Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 02:22 pm BST

PDB ID	:	6G0L / pdb_00006g0l
EMDB ID	:	EMD-4336
Title	:	Structure of two molecules of the chromatin remodelling enzyme Chd1 bound to a nucleosome
Authors	:	Sundaramoorthy, R.; Owen-hughes, T.; Norman, D.G.; Hughes, A.
Deposited on	:	2018-03-19
Resolution	:	10.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

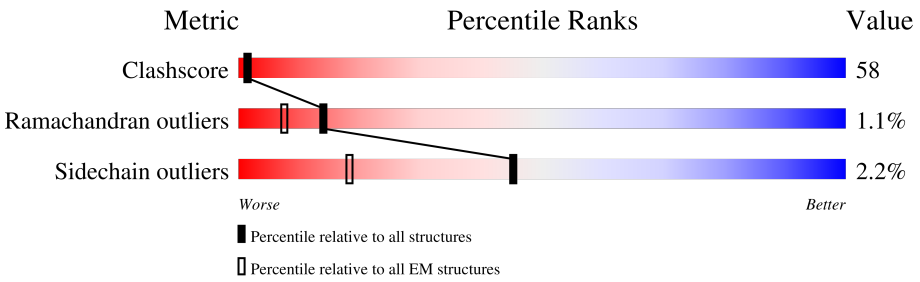
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

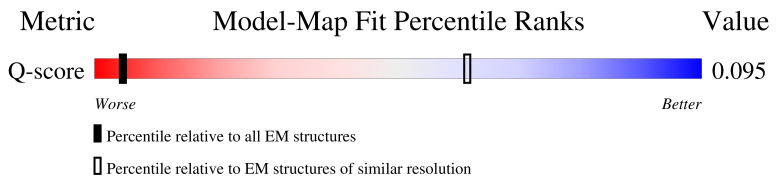
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	147 (9.50 - 10.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	136	7%; 17%, 40%, 12%, •, 29%
1	E	136	•; 19%, 35%, 17%, •, 29%
2	B	103	•; 15%, 47%, 17%, •, 19%
2	F	103	14%; 26%, 45%, 16%, •, 11%

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Mol	Chain	Length	Quality of chain
3	C	130	7% 23% 32% 21% 21%
4	D	126	11% 26% 37% 10% 25%
4	H	126	21% 42% 11% 26%
5	G	130	18% 19% 45% 15% 19%
6	I	176	9% 22% 78%
7	J	177	14% 16% 83%
8	M	1468	8% 47% 11% 42%
8	W	1468	25% 21% 31% 7% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ADP	W	1502	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 27526 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	97	800	504	155	138	3	0	0
1	E	97	799	502	155	139	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	83	662	418	129	114	1	0	0
2	F	92	686	430	134	121	1	0	0

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	103	795	501	155	139	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	106	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	95	745	469	134	140	2	0	0
4	H	93	726	457	130	137	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP A0A1L8G0X3
H	29	THR	SER	conflict	UNP A0A1L8G0X3

- Molecule 5 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	105	809	510	158	141	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 6 is a DNA chain called DNA (176-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	176	3590	1704	657	1053	176	0	0

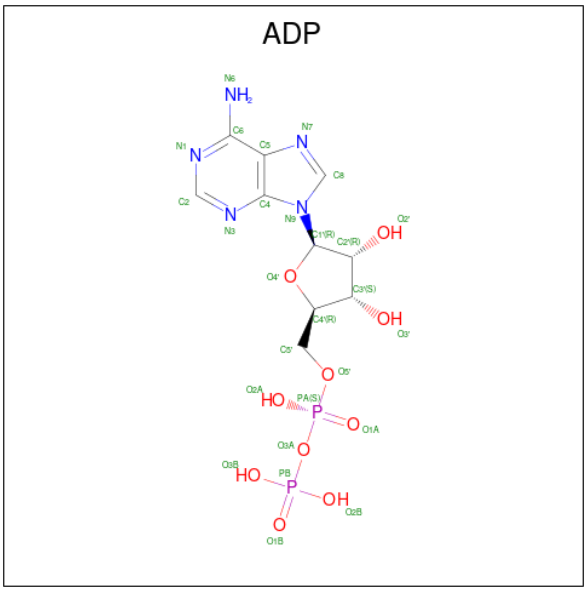
- Molecule 7 is a DNA chain called DNA (177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	177	3646	1727	676	1066	177	0	0

- Molecule 8 is a protein called Chromo domain-containing protein 1.

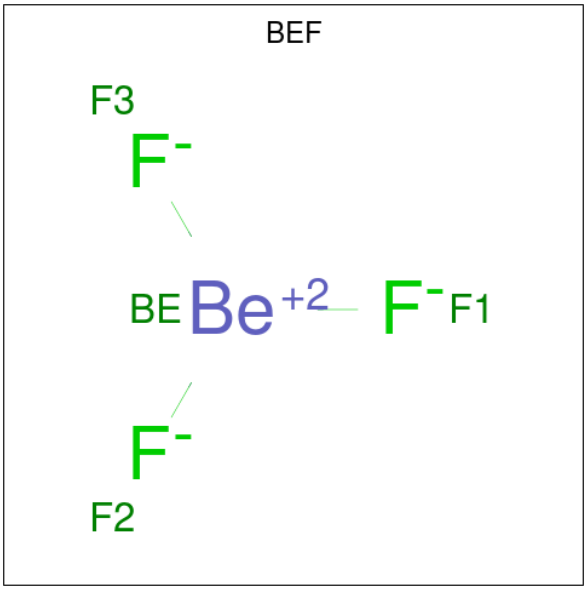
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	855	7017	4461	1221	1308	27	0	0
			Total	C	N	O	S		
8	W	878	7189	4568	1260	1334	27	2	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	M	1	27	10	5	10	2	0
			Total	C	N	O	P	
9	W	1	27	10	5	10	2	0

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



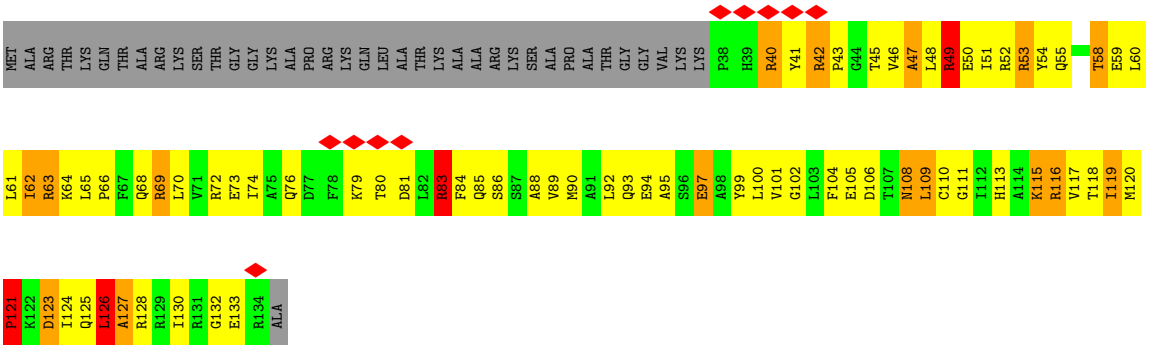
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
10	M	1	4	1	3	0
			Total	Be	F	
10	W	1	4	1	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

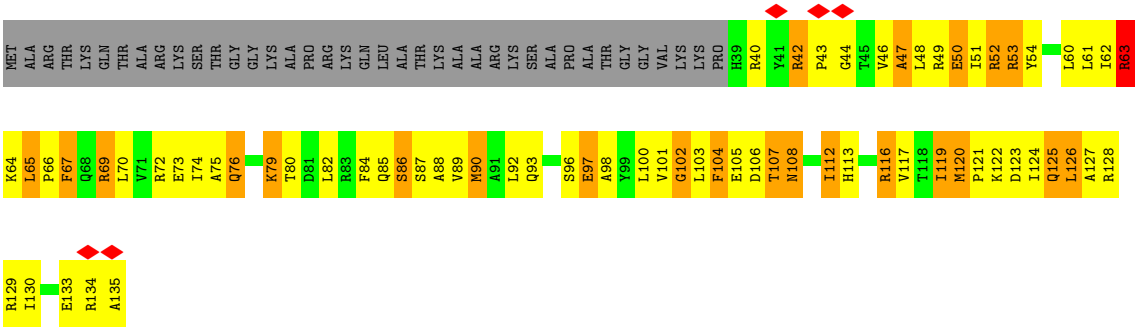
- Molecule 1: Histone H3

Chain A:



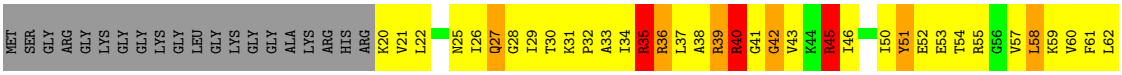
- Molecule 1: Histone H3

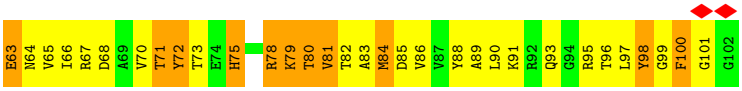
Chain E:



- Molecule 2: Histone H4

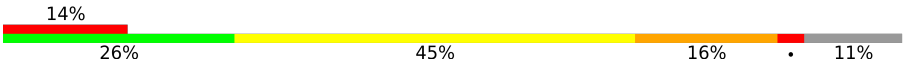
Chain B:

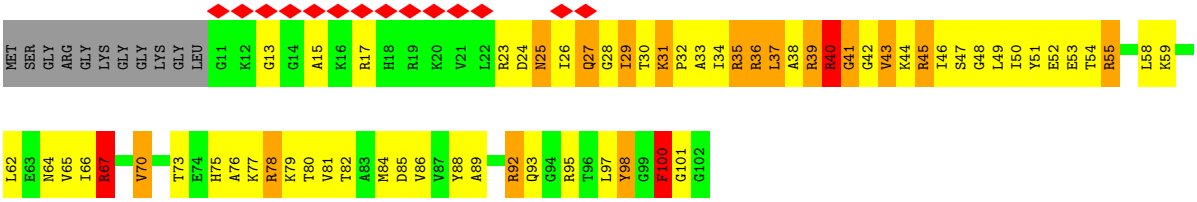




• Molecule 2: Histone H4

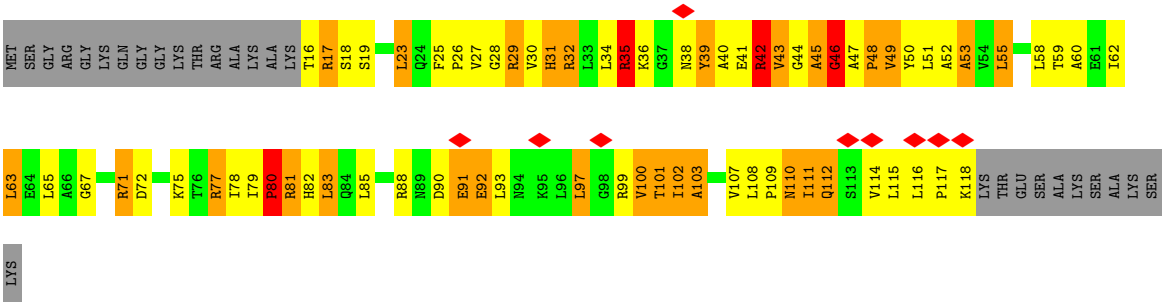
Chain F:





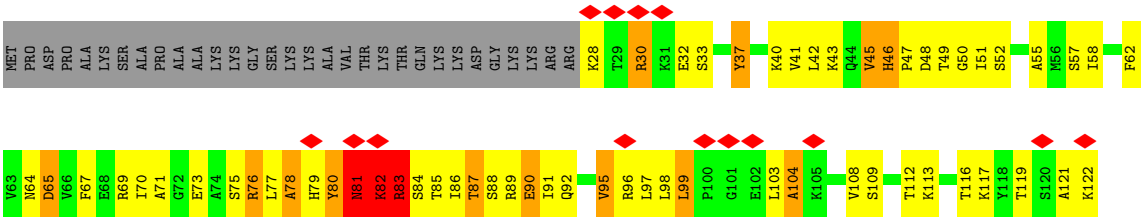
• Molecule 3: Histone H2A type 1

Chain C:



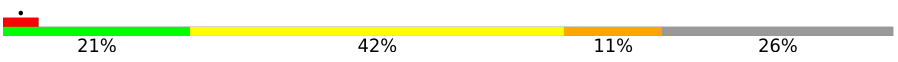
• Molecule 4: Histone H4

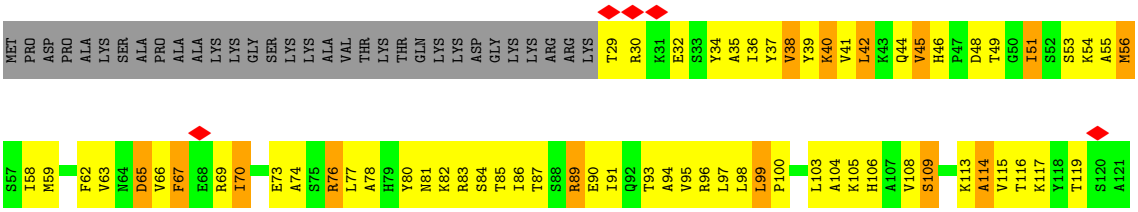
Chain D:



• Molecule 4: Histone H4

Chain H:

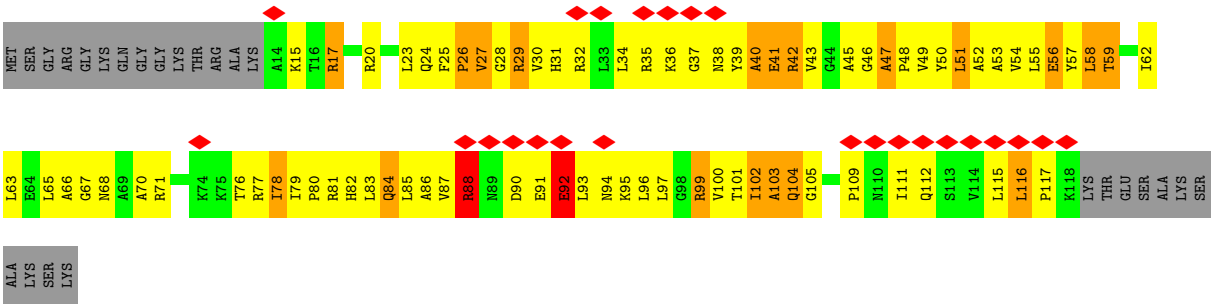




LYS

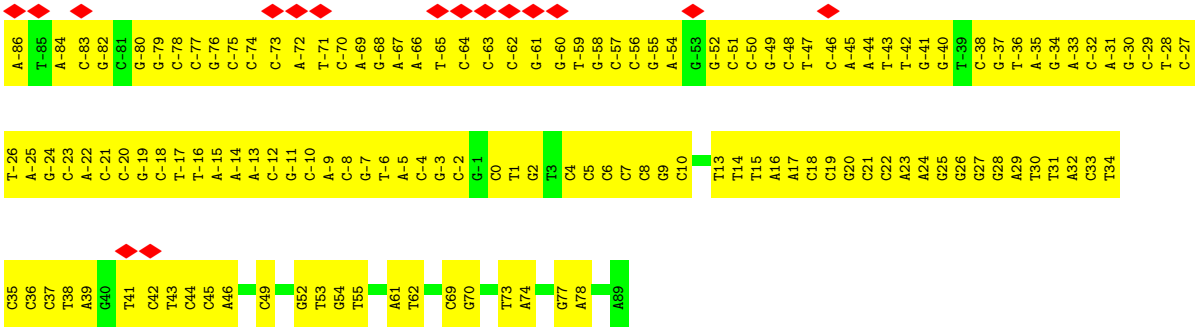
• Molecule 5: Histone H2A type 1

Chain G:



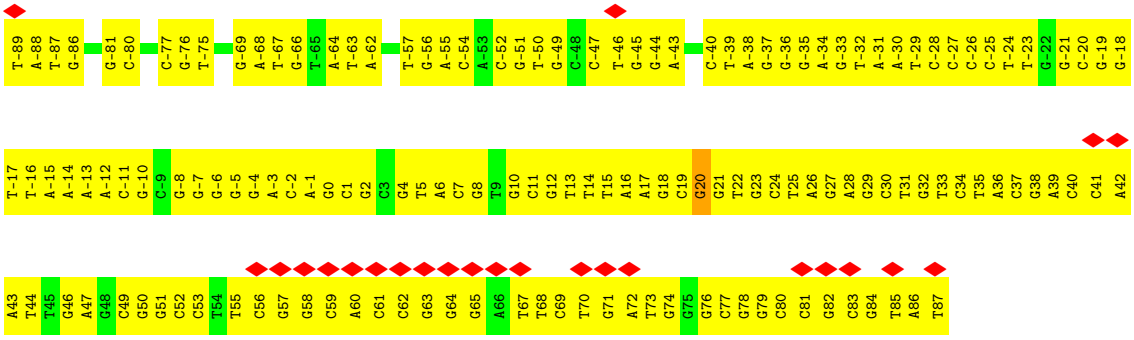
• Molecule 6: DNA (176-MER)

Chain I:



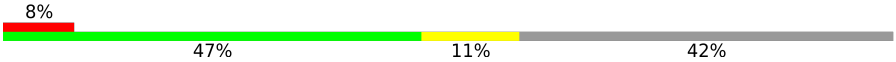
• Molecule 7: DNA (177-MER)

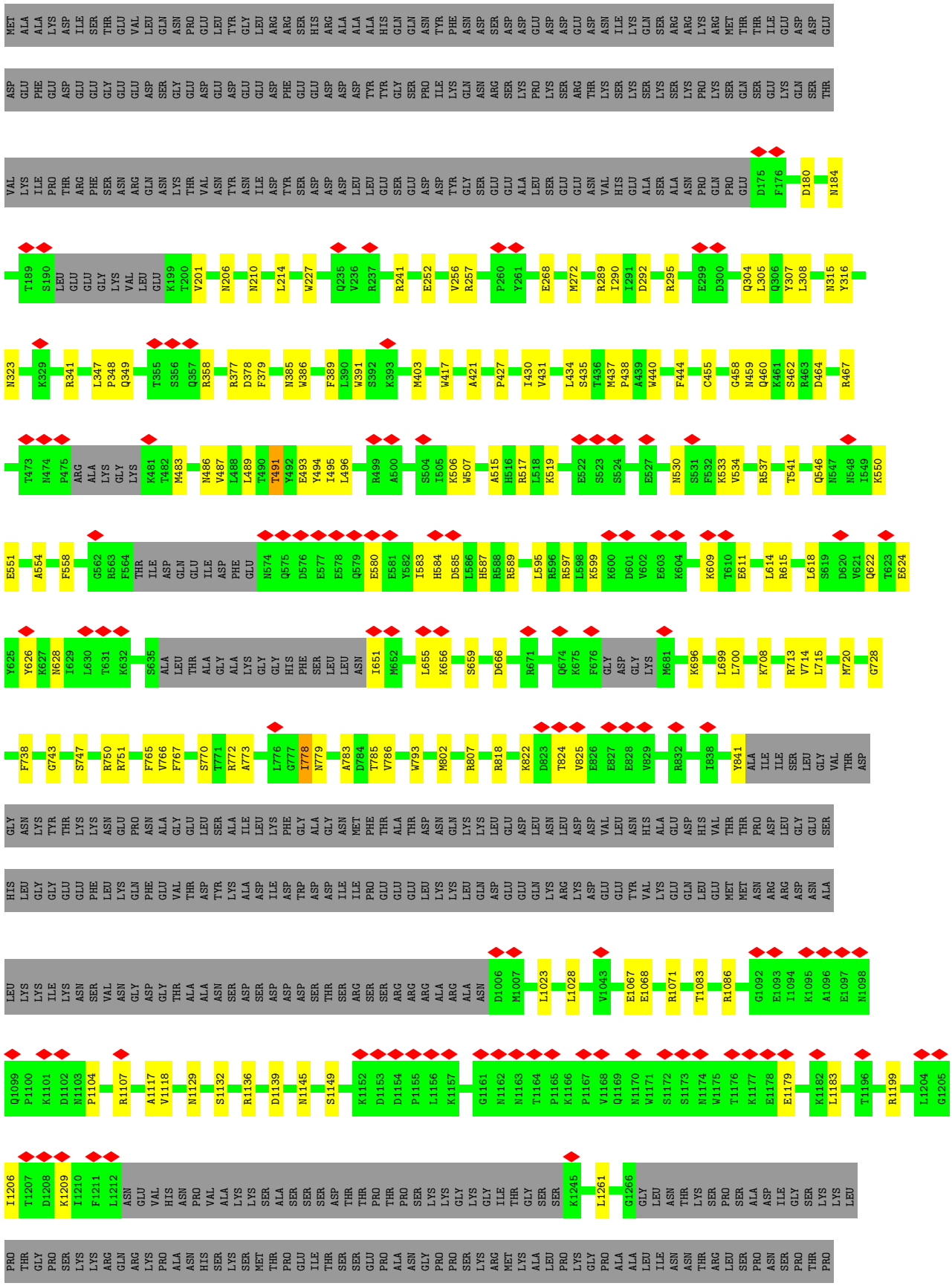
Chain J:



• Molecule 8: Chromo domain-containing protein 1

Chain M:

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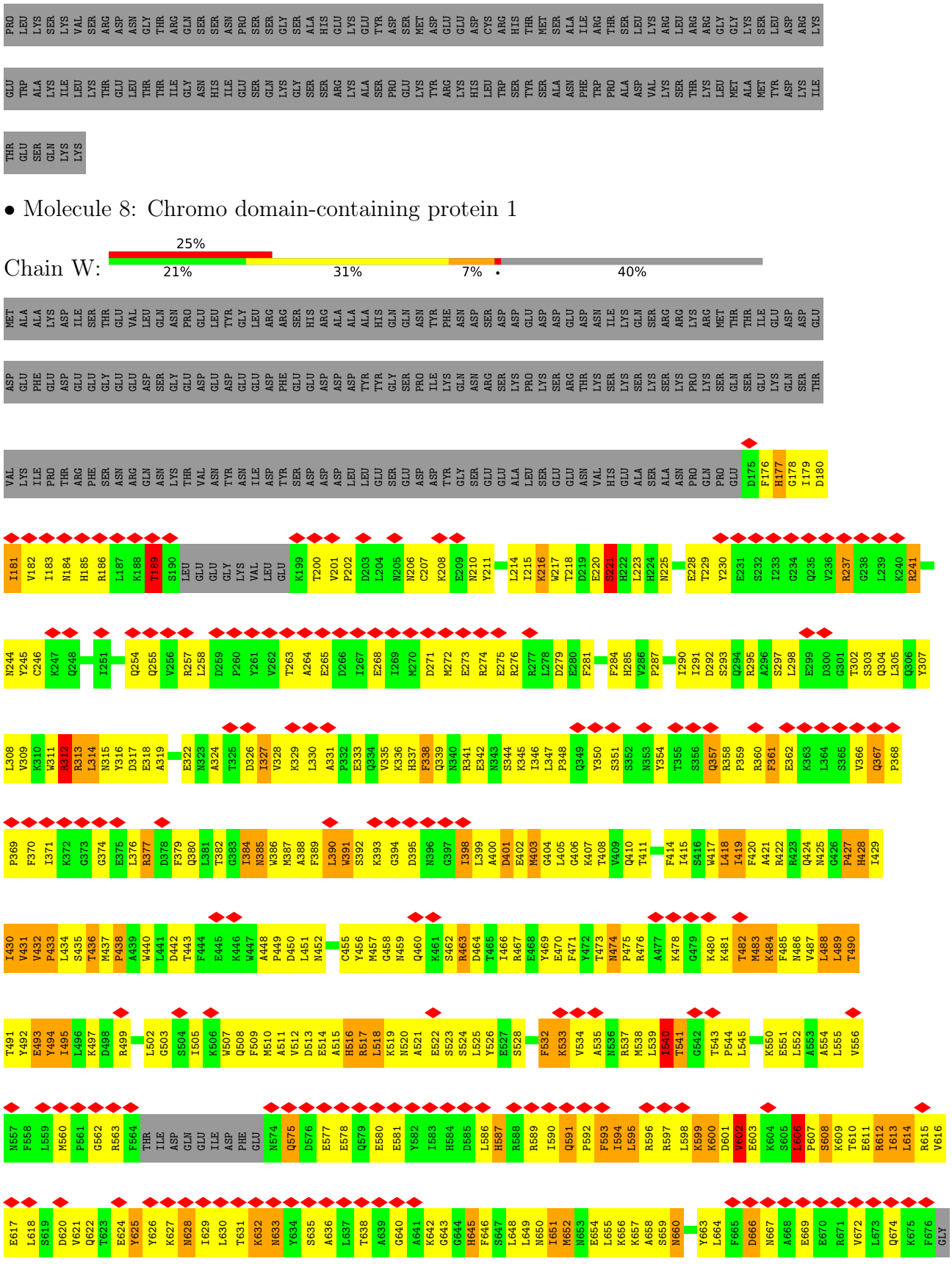
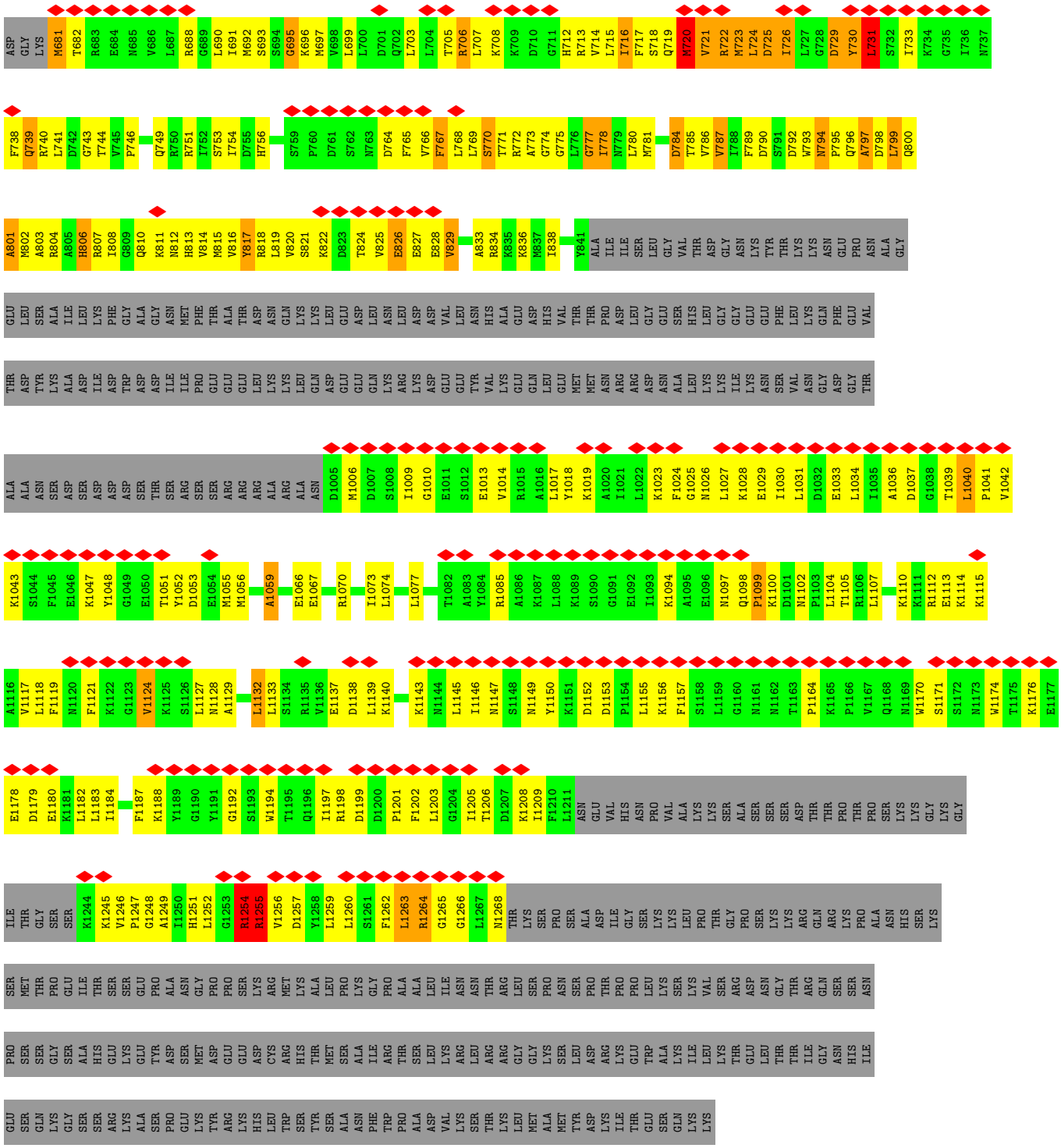
ASP GLU PHE GLU ASP GLU GLU GLY GLU GLU ASP SER GLY GLU ASP GLU GLU ASP GLU ASP PHE GLU GLU ASP ASP ASP TYR TYR GLY SER PRO ILE LYS GLN ASN ARG SER LYS PRO LYS SER ARG THR LYS SER LYS SER LYS SER LYS PRO LYS SER GLN SER GLU LYS GLN SER THR
VAL LYS ILE PRO THR ARG PHE SER ASN ARG GLN ASN LYS THR VAL ASN TYR ASN ILE ASP TYR SER ASP ASP ASP LEU LEU GLU SER GLU GLU ASP ASP TYR GLY SER GLU GLU ALA LEU SER GLU GLU ASN VAL HIS GLU ALA SER ALA ASN PRO GLN PRO GLU D175 F176 D180 N184
T189 S190 LEU GLU GLU GLY LYS VAL LEU GLU K199 T200 V201 N206 N210 L214 W227 Q235 V236 R237 R241 E252 V256 R257 P260 Y261 E268 M272 R289 I290 I291 D292 R295 E299 D300 Q304 L305 Q306 Y307 L308 N315 Y316
N323 K329 R341 L347 P348 Q349 T355 S356 Q357 R358 R377 D378 F379 N385 W386 F389 L390 W391 S392 K393 M403 W417 A421 P427 I430 V431 L434 S435 T436 M437 P438 A439 W440 F444 C455 G458 N459 Q460 K461 S462 R463 D464 R467
T473 N474 P475 ARG ALA LYS GLY LYS K481 T482 M483 N486 V487 L488 L489 T490 T491 Y492 E493 Y494 I495 L496 R499 A500 S504 I505 K506 W507 A515 H516 R517 L518 K519 E522 S523 S524 E527 N530 S531 F532 K533 V534 R537 T541 Q546 N547 N548 I549 K550
E551 A554 F558 G562 R563 F564 THR ILE ASP GLN GLU ILE ASP PHE GLU N574 Q575 D576 E577 E578 E579 E580 E581 Y582 I583 H584 D585 L586 H587 R588 R589 L595 R596 R597 L598 K599 K600 D601 V602 E603 K604 K609 T610 E611 L614 R615 L618 S619 D620 V621 Q622 T623 E624
Y625 Y626 K627 N628 I629 L630 T631 K632 S635 ALA LEU THR ALA GLY ALA LYS GLY GLY HIS PHE SER LEU LEU ASN I651 M652 L655 K656 S659 D666 R671 Q674 K675 F676 GLY ASP GLY LYS M681 K696 L699 L700 K708 R713 V714 L715 M720 G728
F738 G743 S747 R750 R751 F765 V766 F767 S770 T771 R772 A773 L776 G777 I778 N779 A783 D784 T785 V786 W793 M802 R807 R818 K822 D823 T824 V825 E826 E827 E828 V829 R832 I838 Y841 ALA ILE ILE SER LEU GLY VAL THR ASP
GLY ASN LYS TYR THR LYS LYS ASN GLU PRO ASN ALA GLY GLU LEU SER ALA ILE LEU LYS PHE GLY ALA ALA GLY ASN MET PHE THR ALA ALA THR ASP ASN GLN LYS LYS LEU GLU ASP LEU ASN LEU LEU ASP ASP VAL LEU ASN HIS ALA GLU ASP HIS VAL THR THR PRO ASP LEU GLY GLU SER
HIS LEU GLY GLY GLU GLU PHE LEU LYS GLN PHE GLU VAL THR ASP TYR LYS ALA ASP ILE ASP TRP ASP ASP ILE ILE PRO GLU GLU GLU LEU LYS LYS LEU GLN ASP GLU GLU GLN LYS ARG LYS ASP GLU TYR VAL LYS GLU GLN LEU GLU MET MET ASN ARG ARG ASP ASN ALA
LEU LYS LYS ILE LYS ASN SER VAL ASN GLY ASP GLY THR ALA ALA ASN SER ASP SER ASP ASP SER THR SER ARG SER SER ARG ARG ARG ALA ARG ALA ASN D1006 M1007 L1023 L1028 V1043 E1067 E1068 R1071 T1083 R1086 G1092 E1093 I1094 K1095 A1096 E1097 N1098
Q1099 P1100 K1101 D1102 N1103 P1104 R1107 A1117 V1118 N1129 S1132 R1136 D1139 N1145 S1149 K1152 D1153 D1154 P1155 L1156 K1157 G1161 N1162 N1163 T1164 P1165 K1166 P1167 V1168 Q1169 N1170 W1171 S1172 S1173 N1174 W1175 T1176 K1177 E1178 E1179 K1182 L1183 T1196 R1199 L1204 G1205
I1206 T1207 D1208 K1209 I1210 F1211 L1212 ASN GLU VAL HIS ASN PRO VAL ALA ALA LYS LYS SER ALA SER SER SER SER ASP THR THR PRO THR PRO ALA PRO ASN SER LYS LYS GLY LYS GLY ILE THR GLY SER SER K1245 L1261 G1266 GLY LEU ASN THR LYS SER PRO SER ALA ASP ILE GLY SER LYS LYS LEU
PRO THR GLY PRO SER LYS LYS ARG GLN ARG LYS PRO ALA ASN HIS SER LYS SER MET THR PRO GLU ILE THR SER SER GLU PRO ALA ASN GLY PRO PRO SER LYS ARG MET LYS ALA LEU PRO LYS GLY PRO ALA ALA LEU ILE ASN ASN THR ARG LEU SER PRO ASN SER PRO THR PRO



• Molecule 8: Chromo domain-containing protein 1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F738 Q739 R740 L741 D742 G743 T744 V745 P746 Q749 R750 R751 T752 S753 I754 D755 H756 S759 P760 D761 S762 N763 D764 F765 V766 F767 L768 L769 S770 T771 R772 A773 G774 G775 L776 G777 I778 N779 L780 M781 D784 T785 V786 V787 I788 F789 D790 S791 D792 W793 N794 P795 Q796 A797 D798 L799 Q800
A801 M802 A803 R804 A805 H806 R807 I808 G809 Q810 K811 N812 H813 V814 M815 V816 Y817 R818 L819 V820 S821 K822 D823 T824 V825 E826 E827 E828 V829 A833 R834 K835 K836 M837 I838 Y841 ALA ILE ILE SER LEU GLY VAL THR ASP GLY ASN LYS TYR THR LYS LYS ASN GLU PRO ASN ALA GLY
GLU LEU SER ALA ILE LEU LYS PHE GLY ALA GLY ASN MET PHE THR ALA THR ASP ASN GLN LYS LYS LEU GLU ASP LEU ASN LEU ASP ASP VAL LEU ASN HIS ALA GLU ASP HIS VAL THR THR PRO ASP LEU GLY GLU SER HIS LEU GLY GLY GLU GLU PHE LEU LYS GLN PHE GLU VAL
THR ASP TYR LYS ALA ASP ILE ASP TRP ASP ASP ILE ILE PRO GLU GLU GLU LEU LYS LYS LEU GLN ASP GLU GLU GLN LYS ARG LYS ASP GLU TYR VAL LYS GLU GLN LEU GLU MET MET ASN ARG ARG ASP ASN ALA LEU LYS LYS ILE LYS ASN SER VAL ASN GLY ASP GLY THR
ALA ALA ASN SER ASP SER ASP ASP ASP SER THR SER ARG SER SER ARG ARG ARG ALA ARG ALA ASN D1005 M1006 D1007 S1008 I1009 G1010 E1011 S1012 E1013 V1014 R1015 A1016 L1017 Y1018 K1019 A1020 I1021 L1022 K1023 F1024 G1025 N1026 L1027 K1028 E1029 I1030 L1031 D1032 E1033 L1034 I1035 A1036 D1037 G1038 T1039 L1040 P1041 V1042
K1043 S1044 F1045 E1046 K1047 Y1048 G1049 E1050 T1051 Y1052 D1053 E1054 M1055 M1056 A1059 E1066 E1067 R1070 I1073 L1074 L1077 T1082 A1083 Y1084 R1085 A1086 K1087 L1088 K1089 S1090 G1091 E1092 I1093 K1094 A1095 E1096 N1097 Q1098 P1099 K1100 D1101 N1102 P1103 L1104 T1105 R1106 L1107 K1110 K1111 R1112 E1113 K1114 K1115
A1116 V1117 L1118 F1119 N1120 F1121 K1122 G1123 V1124 K1125 S1126 L1127 N1128 A1129 L1132 L1133 S1134 R1135 V1136 E1137 D1138 L1139 K1140 K1143 N1144 L1145 I1146 N1147 S1148 N1149 Y1150 K1151 D1152 D1153 P1154 L1155 K1156 F1157 S1158 L1159 G1160 N1161 N1162 T1163 P1164 K1165 P1166 V1167 Q1168 N1169 W1170 S1171 S1172 N1173 W1174 T1175 K1176 E1177
E1178 D1179 E1180 K1181 L1182 L1183 I1184 F1187 K1188 Y1189 G1190 Y1191 G1192 S1193 W1194 T1195 Q1196 I1197 R1198 D1199 D1200 P1201 F1202 L1203 G1204 I1205 T1206 D1207 K1208 I1209 F1210 L1211 ASN GLU VAL HIS ASN PRO VAL ALA LYS LYS SER ALA SER SER SER SER LYS LYS LYS GLY LYS GLY
ILE THR GLY SER SER K1244 K1245 V1246 P1247 G1248 A1249 I1250 H1251 L1252 G1253 R1254 R1255 V1256 D1257 Y1258 L1259 L1260 S1261 F1262 L1263 R1264 G1265 G1266 L1267 N1268 THR LYS SER PRO SER ALA ASP ILE GLY SER LYS LYS LEU PRO THR GLY PRO SER LYS LYS ARG GLN ARG LYS PRO ALA ASN HIS SER LYS
SER MET THR PRO GLU ILE THR SER SER GLU PRO ALA ASN GLY PRO PRO SER LYS ARG MET LYS ALA LEU PRO LYS GLY PRO ALA ALA LEU ILE ASN ASN THR ARG LEU SER PRO ASN SER PRO THR PRO LEU LYS SER LYS VAL SER ARG ASP ASN GLY THR ARG GLN ARG SER SER ASN
PRO SER SER GLY SER ALA HIS GLU LYS GLU TYR ASP SER MET ASP GLU GLU ASP CYS ARG HIS THR MET SER ALA ILE ARG THR SER LEU LYS ARG LEU ARG ARG GLY GLY LYS SER LEU ASP ARG LYS GLU TRP ALA LYS ILE LEU LYS THR GLU GLU LEU THR THR ILE GLY ASN HIS ILE
GLU SER GLN LYS GLY SER SER ARG LYS ALA SER PRO GLU LYS TYR ARG LYS HIS LEU TRP SER TYR SER ALA ASN PHE TRP PRO ALA ASP VAL LYS SER THR LYS LEU MET ALA MET TYR ASP LYS ILE THR GLU SER GLN LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.56	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	98591	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	369.19998, 369.19998, 369.19998	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.42, 1.42, 1.42	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BEF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.62	14/812 (1.7%)	1.76	11/1088 (1.0%)
1	E	1.45	8/810 (1.0%)	1.83	19/1084 (1.8%)
2	B	1.58	9/669 (1.3%)	2.01	17/894 (1.9%)
2	F	1.67	13/693 (1.9%)	1.96	21/929 (2.3%)
3	C	1.83	21/805 (2.6%)	2.00	31/1088 (2.8%)
4	D	1.62	18/756 (2.4%)	1.79	10/1015 (1.0%)
4	H	1.51	9/737 (1.2%)	1.84	20/993 (2.0%)
5	G	1.73	18/819 (2.2%)	1.90	21/1106 (1.9%)
6	I	0.26	0/4023	0.46	0/6199
7	J	0.26	0/4091	0.47	1/6315 (0.0%)
8	M	0.09	0/7152	0.23	0/9632
8	W	1.43	94/7334 (1.3%)	1.54	64/9875 (0.6%)
All	All	1.05	204/28701 (0.7%)	1.18	215/40218 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	E	0	6
2	B	0	5
2	F	0	7
3	C	0	7
4	D	0	3
4	H	0	4
5	G	0	4
8	W	0	19
All	All	0	62

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	102	ILE	C-O	12.01	1.36	1.24
4	D	87	THR	C-O	-11.77	1.10	1.23
3	C	92	GLU	C-O	11.53	1.35	1.23
1	A	121	PRO	C-O	-10.44	1.10	1.24
5	G	51	LEU	C-O	-9.94	1.12	1.24
5	G	112	GLN	C-O	-9.81	1.11	1.23
3	C	111	ILE	C-O	-9.47	1.13	1.24
3	C	109	PRO	C-O	-9.44	1.13	1.23
3	C	55	LEU	C-O	-9.38	1.13	1.24
8	W	216	LYS	C-O	9.34	1.35	1.24
8	W	784	ASP	N-CA	9.26	1.57	1.46
8	W	767	PHE	C-O	-9.23	1.13	1.23
4	D	57	SER	C-O	9.17	1.35	1.24
2	F	85	ASP	N-CA	-9.07	1.35	1.46
1	A	111	GLY	C-O	-8.93	1.13	1.23
1	E	98	ALA	N-CA	-8.86	1.35	1.46
8	W	430	ILE	C-O	-8.82	1.14	1.24
1	A	127	ALA	C-O	-8.81	1.13	1.24
8	W	729	ASP	CG-OD2	8.80	1.42	1.25
8	W	550	LYS	N-CA	8.78	1.56	1.46
8	W	797	ALA	N-CA	8.74	1.57	1.46
2	F	13	GLY	N-CA	8.74	1.57	1.45
2	B	35	ARG	C-O	8.63	1.34	1.24
8	W	730	TYR	N-CA	8.53	1.56	1.46
2	F	37	LEU	C-O	-8.24	1.13	1.24
5	G	40	ALA	C-O	-8.17	1.15	1.23
1	A	106	ASP	C-O	8.16	1.33	1.24
8	W	431	VAL	C-O	-8.13	1.15	1.24
5	G	84	GLN	C-O	8.09	1.33	1.24
1	A	118	THR	C-O	8.03	1.33	1.24
5	G	42	ARG	N-CA	7.93	1.55	1.46
4	D	95	VAL	C-O	7.82	1.33	1.24
4	D	64	ASN	C-O	-7.74	1.14	1.24
2	B	36	ARG	C-O	7.74	1.33	1.24
2	B	101	GLY	C-O	-7.70	1.14	1.23
1	A	127	ALA	N-CA	-7.70	1.36	1.46
8	W	338	PHE	N-CA	7.62	1.55	1.46
8	W	625	TYR	N-CA	-7.61	1.37	1.46
4	D	83	ARG	C-O	-7.54	1.14	1.23
4	D	65	ASP	CG-OD2	-7.50	1.11	1.25
8	W	533	LYS	C-O	-7.49	1.14	1.24
4	H	53	SER	C-O	-7.47	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	45	ARG	N-CA	7.46	1.56	1.46
8	W	342	GLU	C-O	-7.46	1.15	1.24
8	W	820	VAL	C-O	-7.43	1.16	1.23
8	W	494	TYR	N-CA	-7.43	1.37	1.46
8	W	436	THR	N-CA	7.42	1.55	1.46
2	F	41	GLY	C-O	-7.34	1.15	1.24
8	W	499	ARG	C-O	-7.34	1.15	1.24
2	B	78	ARG	C-O	7.28	1.32	1.23
8	W	401	ASP	N-CA	7.25	1.55	1.45
3	C	110	ASN	N-CA	-7.25	1.36	1.46
8	W	770	SER	N-CA	7.23	1.54	1.45
8	W	716	ILE	C-O	-7.21	1.16	1.24
3	C	36	LYS	C-O	-7.21	1.14	1.24
4	D	76	ARG	C-O	-7.20	1.15	1.24
2	F	43	VAL	C-O	-7.17	1.15	1.24
8	W	599	LYS	C-O	-7.16	1.15	1.24
3	C	29	ARG	CD-NE	7.09	1.56	1.46
8	W	488	LEU	C-O	-7.06	1.15	1.23
4	D	95	VAL	N-CA	-7.01	1.38	1.46
3	C	23	LEU	C-O	-6.99	1.14	1.23
1	E	102	GLY	N-CA	-6.96	1.37	1.45
3	C	35	ARG	C-O	-6.95	1.15	1.24
5	G	66	ALA	N-CA	-6.94	1.37	1.46
8	W	792	ASP	N-CA	6.94	1.55	1.46
3	C	53	ALA	C-O	6.91	1.32	1.24
8	W	489	LEU	C-O	-6.91	1.16	1.24
5	G	41	GLU	C-O	-6.88	1.16	1.24
8	W	361	PHE	N-CA	6.83	1.53	1.45
2	B	40	ARG	C-O	-6.78	1.16	1.24
2	F	40	ARG	NE-CZ	6.76	1.40	1.33
1	A	47	ALA	C-O	-6.74	1.15	1.24
8	W	652	MET	N-CA	6.69	1.54	1.45
8	W	632	LYS	N-CA	6.65	1.54	1.46
5	G	88	ARG	N-CA	6.65	1.54	1.46
8	W	767	PHE	N-CA	-6.62	1.37	1.46
8	W	357	GLN	C-O	6.62	1.31	1.23
8	W	753	SER	C-O	6.61	1.32	1.24
4	D	45	VAL	C-O	-6.60	1.16	1.24
4	D	78	ALA	C-O	-6.59	1.16	1.24
8	W	327	ILE	C-O	-6.50	1.16	1.24
1	A	108	ASN	C-O	6.44	1.31	1.24
5	G	105	GLY	C-O	6.44	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	73	GLU	CD-OE2	6.42	1.37	1.25
3	C	58	LEU	C-O	6.42	1.31	1.24
8	W	452	ASN	N-CA	6.41	1.54	1.45
5	G	116	LEU	N-CA	-6.41	1.36	1.45
8	W	651	ILE	N-CA	6.36	1.54	1.46
8	W	1254[A]	ARG	C-O	6.33	1.31	1.24
8	W	1254[B]	ARG	C-O	6.33	1.31	1.24
5	G	23	LEU	C-O	-6.33	1.16	1.23
8	W	669	GLU	N-CA	6.29	1.54	1.46
5	G	49	VAL	C-O	-6.29	1.17	1.24
5	G	86	ALA	C-O	-6.27	1.16	1.24
4	H	114	ALA	N-CA	-6.26	1.38	1.46
8	W	490	THR	N-CA	-6.26	1.38	1.46
8	W	433	PRO	C-O	6.23	1.30	1.23
2	B	57	VAL	N-CA	-6.23	1.39	1.46
8	W	725	ASP	N-CA	6.22	1.53	1.46
8	W	424	GLN	C-O	-6.18	1.16	1.24
1	A	94	GLU	C-O	6.17	1.31	1.24
5	G	27	VAL	N-CA	-6.16	1.39	1.46
8	W	724	LEU	N-CA	-6.13	1.38	1.46
8	W	669	GLU	CD-OE2	-6.12	1.13	1.25
8	W	494	TYR	C-O	-6.12	1.16	1.24
3	C	83	LEU	C-O	-6.12	1.17	1.24
5	G	37	GLY	C-O	-6.10	1.20	1.24
8	W	790	ASP	C-O	-6.06	1.16	1.23
8	W	756	HIS	C-O	-6.05	1.16	1.24
1	E	97	GLU	C-O	-6.04	1.17	1.24
4	H	67	PHE	C-O	-6.02	1.17	1.24
4	D	46	HIS	CE1-NE2	6.01	1.38	1.32
1	A	126	LEU	C-O	-5.99	1.17	1.24
1	E	112	ILE	C-O	5.96	1.30	1.24
8	W	817	TYR	N-CA	-5.94	1.38	1.46
8	W	594	ILE	N-CA	-5.92	1.39	1.46
8	W	731	LEU	C-O	5.90	1.31	1.24
8	W	826	GLU	CD-OE2	-5.86	1.14	1.25
4	H	70	ILE	C-O	-5.85	1.17	1.24
4	H	56	MET	CG-SD	-5.81	1.66	1.80
1	E	97	GLU	N-CA	-5.81	1.39	1.46
2	F	29	ILE	C-O	5.80	1.30	1.24
4	H	40	LYS	C-O	5.80	1.30	1.24
5	G	56	GLU	N-CA	-5.80	1.39	1.46
3	C	49	VAL	C-O	5.79	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	596	ARG	N-CA	5.78	1.53	1.46
4	D	82	LYS	N-CA	5.77	1.53	1.46
8	W	493	GLU	CD-OE2	5.76	1.36	1.25
8	W	591	GLN	N-CA	5.74	1.53	1.46
8	W	394	GLY	N-CA	5.73	1.53	1.45
2	F	25	ASN	N-CA	-5.73	1.38	1.46
1	A	49	ARG	NE-CZ	5.71	1.39	1.33
4	D	117	LYS	C-O	5.71	1.30	1.24
8	W	532	PHE	N-CA	5.69	1.53	1.46
8	W	464	ASP	C-O	5.68	1.30	1.24
8	W	257	ARG	N-CA	5.67	1.53	1.46
8	W	801	ALA	C-O	-5.67	1.17	1.24
8	W	729	ASP	C-O	-5.66	1.17	1.24
2	B	51	TYR	C-O	-5.66	1.17	1.24
1	A	123	ASP	N-CA	-5.63	1.39	1.46
8	W	720	MET	N-CA	-5.62	1.39	1.46
3	C	46	GLY	C-O	5.59	1.31	1.23
8	W	610	THR	N-CA	5.58	1.53	1.46
2	F	70	VAL	N-CA	-5.56	1.39	1.46
8	W	743	GLY	C-O	-5.53	1.16	1.23
8	W	730	TYR	C-O	-5.52	1.17	1.24
3	C	45	ALA	C-O	5.51	1.31	1.24
4	D	65	ASP	C-O	-5.51	1.17	1.24
8	W	1249	ALA	C-O	-5.50	1.17	1.24
8	W	398	ILE	C-O	-5.48	1.18	1.24
8	W	562	GLY	N-CA	5.47	1.53	1.45
3	C	31	HIS	CE1-NE2	5.45	1.38	1.32
8	W	516	HIS	N-CA	-5.44	1.38	1.46
8	W	339	GLN	C-O	5.43	1.30	1.24
3	C	72	ASP	C-O	5.42	1.30	1.24
8	W	411	THR	N-CA	5.40	1.53	1.46
4	H	116	THR	C-O	5.39	1.30	1.24
8	W	428	HIS	CE1-NE2	5.38	1.38	1.32
5	G	103	ALA	C-O	-5.37	1.17	1.24
1	E	86	SER	C-O	5.37	1.30	1.24
1	A	97	GLU	N-CA	-5.37	1.40	1.46
8	W	652	MET	C-O	-5.35	1.17	1.24
3	C	100	VAL	C-O	-5.32	1.18	1.24
2	B	79	LYS	CA-C	-5.31	1.47	1.52
8	W	719	GLN	C-O	-5.29	1.17	1.24
8	W	418	LEU	N-CA	-5.29	1.39	1.46
1	E	67	PHE	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	104	PHE	N-CA	-5.27	1.40	1.46
8	W	384	ILE	N-CA	-5.27	1.40	1.46
2	F	98	TYR	N-CA	-5.27	1.39	1.45
8	W	554	ALA	N-CA	5.25	1.52	1.46
8	W	419	ILE	N-CA	5.25	1.51	1.45
2	F	78	ARG	C-O	5.23	1.30	1.24
8	W	729	ASP	N-CA	-5.22	1.40	1.46
8	W	787	VAL	C-O	-5.22	1.18	1.24
8	W	403	MET	N-CA	5.22	1.53	1.46
3	C	112	GLN	C-O	-5.20	1.17	1.23
3	C	107	VAL	C-O	-5.20	1.16	1.23
4	D	104	ALA	C-O	-5.20	1.18	1.24
8	W	1053	ASP	C-O	5.19	1.30	1.24
8	W	438	PRO	C-O	5.18	1.30	1.24
4	H	39	TYR	C-O	5.18	1.30	1.24
2	F	35	ARG	C-O	5.17	1.30	1.24
8	W	499	ARG	N-CA	5.16	1.52	1.46
8	W	337	HIS	N-CA	-5.16	1.40	1.46
4	H	105	LYS	C-O	-5.16	1.18	1.24
8	W	726	ILE	N-CA	-5.16	1.40	1.46
8	W	312	ARG	N-CA	5.15	1.52	1.46
8	W	463	ARG	N-CA	-5.15	1.39	1.46
8	W	777	GLY	C-O	-5.13	1.16	1.23
8	W	382	THR	C-O	5.12	1.30	1.24
4	D	33	SER	C-O	-5.12	1.17	1.23
8	W	614	LEU	C-O	-5.11	1.18	1.23
2	F	27	GLN	N-CA	5.11	1.52	1.46
1	A	53	ARG	C-O	5.09	1.30	1.24
5	G	27	VAL	C-O	-5.09	1.18	1.24
8	W	314	LEU	N-CA	-5.09	1.39	1.46
8	W	1248	GLY	C-O	-5.07	1.19	1.23
8	W	1265	GLY	N-CA	5.06	1.52	1.45
4	D	90	GLU	CD-OE2	-5.05	1.15	1.25
8	W	593	PHE	C-O	-5.04	1.16	1.23
8	W	1266	GLY	N-CA	5.03	1.52	1.45
8	W	221	SER	N-CA	5.00	1.52	1.46

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	39	TYR	N-CA-C	10.11	121.98	110.97
2	B	40	ARG	NE-CZ-NH1	-9.12	112.38	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	17	ARG	CA-C-O	-8.79	111.59	120.82
5	G	104	GLN	CA-C-O	-8.68	111.88	122.03
1	E	119	ILE	N-CA-CB	8.61	122.05	110.26
2	B	75	HIS	CA-CB-CG	-8.52	105.28	113.80
5	G	109	PRO	N-CA-C	-8.36	98.18	110.80
4	D	81	ASN	CB-CA-C	8.19	124.94	110.37
1	E	127	ALA	O-C-N	8.14	130.79	122.08
2	B	27	GLN	CB-CG-CD	-8.09	98.84	112.60
8	W	495	ILE	N-CA-CB	7.87	118.89	110.62
3	C	42	ARG	CB-CA-C	-7.87	100.70	113.37
8	W	442	ASP	CA-CB-CG	7.66	120.26	112.60
2	B	63	GLU	CB-CG-CD	7.55	125.44	112.60
5	G	37	GLY	CA-C-O	7.53	125.89	119.04
5	G	47	ALA	CA-C-O	7.52	126.22	119.08
5	G	92	GLU	CB-CG-CD	7.48	125.31	112.60
3	C	62	ILE	N-CA-C	7.39	117.98	110.82
2	B	98	TYR	CA-C-O	-7.35	112.23	120.32
1	A	49	ARG	CB-CG-CD	7.32	128.14	111.30
1	E	90	MET	N-CA-C	-7.24	102.57	111.33
5	G	17	ARG	O-C-N	7.23	129.51	122.07
4	D	80	TYR	CA-C-N	-7.08	110.38	122.56
4	D	80	TYR	C-N-CA	-7.08	110.38	122.56
1	A	53	ARG	CA-C-O	7.05	128.24	120.63
5	G	29	ARG	CA-C-O	6.93	127.77	120.42
4	H	39	TYR	CA-CB-CG	-6.92	101.45	113.90
4	D	46	HIS	CA-CB-CG	6.89	120.69	113.80
2	B	100	PHE	CA-C-N	-6.86	114.94	121.46
2	B	100	PHE	C-N-CA	-6.86	114.94	121.46
5	G	45	ALA	CA-C-N	-6.85	111.89	122.30
5	G	45	ALA	C-N-CA	-6.85	111.89	122.30
2	F	40	ARG	CB-CG-CD	-6.82	95.62	111.30
2	B	53	GLU	CB-CG-CD	6.81	124.17	112.60
8	W	432	VAL	N-CA-CB	-6.81	105.88	111.67
1	E	107	THR	N-CA-C	-6.75	103.00	111.11
2	B	42	GLY	CA-C-O	6.74	126.54	118.86
8	W	516	HIS	N-CA-C	-6.72	104.30	113.30
1	E	52	ARG	NE-CZ-NH1	-6.64	114.86	121.50
8	W	608	SER	N-CA-C	6.61	119.09	110.43
1	A	115	LYS	CB-CA-C	-6.59	100.26	111.26
2	F	100	PHE	CA-C-O	-6.55	113.29	120.36
2	F	100	PHE	O-C-N	6.50	131.03	123.30
2	F	36	ARG	N-CA-C	-6.50	103.47	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	18	SER	N-CA-C	-6.48	104.13	111.07
8	W	729	ASP	N-CA-CB	-6.43	100.64	110.16
2	F	36	ARG	CA-C-O	6.42	127.56	120.63
4	H	45	VAL	N-CA-C	6.41	117.09	111.90
8	W	756	HIS	CA-CB-CG	6.36	120.16	113.80
8	W	432	VAL	CA-C-N	6.35	126.30	119.76
8	W	432	VAL	C-N-CA	6.35	126.30	119.76
3	C	91	GLU	N-CA-C	6.34	118.19	111.28
8	W	385	ASN	CA-CB-CG	6.32	118.92	112.60
8	W	177	HIS	CA-C-N	6.32	127.01	121.58
8	W	177	HIS	C-N-CA	6.32	127.01	121.58
2	F	52	GLU	CA-C-O	-6.30	114.16	120.90
8	W	271	ASP	CA-CB-CG	6.26	118.86	112.60
4	H	40	LYS	N-CA-C	6.25	118.64	111.02
8	W	575	GLN	CA-C-N	6.24	128.97	120.54
8	W	575	GLN	C-N-CA	6.24	128.97	120.54
1	E	102	GLY	N-CA-C	-6.23	105.10	112.64
3	C	48	PRO	CA-C-O	6.22	129.56	119.86
3	C	42	ARG	N-CA-C	-6.22	99.23	109.80
8	W	695	GLY	CA-C-O	6.22	127.25	120.66
1	E	120	MET	CA-C-O	6.20	127.04	120.66
4	H	65	ASP	CA-C-O	6.19	127.32	120.63
8	W	730	TYR	CB-CA-C	-6.19	100.39	110.79
8	W	279	ASP	CA-CB-CG	6.18	118.78	112.60
3	C	97	LEU	CA-C-N	6.17	126.66	119.94
3	C	97	LEU	C-N-CA	6.17	126.66	119.94
5	G	109	PRO	CB-CA-C	6.12	118.87	111.46
8	W	420	PHE	N-CA-C	-6.12	104.45	112.41
5	G	26	PRO	CB-CA-C	-6.12	106.73	111.87
2	B	36	ARG	CA-C-O	-6.11	114.08	120.55
8	W	292	ASP	CA-CB-CG	6.09	118.69	112.60
2	F	52	GLU	CB-CG-CD	6.05	122.89	112.60
8	W	1202	PHE	CA-CB-CG	6.05	119.85	113.80
2	F	40	ARG	NE-CZ-NH2	6.04	124.63	119.20
4	D	90	GLU	CB-CA-C	6.03	120.35	110.88
3	C	63	LEU	CA-C-O	6.01	127.33	120.90
8	W	390	LEU	N-CA-C	-5.96	105.66	113.17
8	W	612	ARG	CG-CD-NE	5.94	125.07	112.00
1	E	133	GLU	N-CA-C	-5.94	103.58	111.24
2	F	55	ARG	N-CA-C	-5.90	104.93	111.36
8	W	599	LYS	CA-C-O	-5.89	114.81	121.00
2	F	38	ALA	CA-C-O	5.89	126.66	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	433	PRO	N-CA-C	5.87	120.30	111.14
2	F	70	VAL	N-CA-C	-5.87	104.63	110.62
1	E	125	GLN	CA-C-O	-5.85	114.67	120.82
8	W	464	ASP	N-CA-C	5.84	117.73	111.36
2	B	85	ASP	CA-C-O	-5.84	114.36	120.55
8	W	806	HIS	CB-CA-C	-5.83	101.88	111.68
7	J	20	DG	C2'-C3'-O3'	-5.80	102.80	111.50
3	C	42	ARG	CA-C-O	-5.80	114.62	120.77
2	B	58	LEU	N-CA-C	-5.79	104.32	111.33
8	W	418	LEU	N-CA-C	-5.78	106.00	113.16
8	W	1188	LYS	N-CA-C	5.76	118.77	111.69
4	H	99	LEU	CA-C-N	5.75	125.77	119.90
4	H	99	LEU	C-N-CA	5.75	125.77	119.90
2	F	31	LYS	CB-CA-C	-5.75	102.06	112.76
3	C	39	TYR	CB-CA-C	-5.75	102.11	110.96
5	G	46	GLY	O-C-N	-5.74	116.52	121.97
8	W	770	SER	O-C-N	-5.74	116.18	122.84
4	H	76	ARG	NE-CZ-NH1	-5.74	115.76	121.50
3	C	50	TYR	CB-CG-CD1	-5.70	112.25	120.80
4	H	105	LYS	CB-CA-C	5.69	120.52	110.85
3	C	102	ILE	CA-C-O	5.67	126.60	120.43
4	H	81	ASN	N-CA-CB	5.66	119.17	110.79
2	F	49	LEU	CA-C-O	5.66	126.76	120.82
8	W	1265	GLY	CA-C-N	5.65	126.22	120.00
8	W	1265	GLY	C-N-CA	5.65	126.22	120.00
8	W	628	ASN	CA-CB-CG	-5.65	106.95	112.60
1	E	119	ILE	N-CA-C	-5.65	101.53	109.21
1	E	119	ILE	CA-CB-CG1	5.64	119.99	110.40
2	F	55	ARG	CB-CG-CD	5.62	124.23	111.30
8	W	1099	PRO	N-CA-C	5.62	120.15	111.21
8	W	792	ASP	CA-C-N	5.61	130.92	122.68
8	W	792	ASP	C-N-CA	5.61	130.92	122.68
3	C	59	THR	CA-C-O	5.59	126.47	120.55
2	B	40	ARG	NH1-CZ-NH2	5.59	126.56	119.30
8	W	606	LEU	CA-C-N	5.58	125.53	119.78
8	W	606	LEU	C-N-CA	5.58	125.53	119.78
2	B	71	THR	OG1-CB-CG2	-5.58	98.14	109.30
5	G	26	PRO	N-CA-CB	5.57	106.04	102.92
8	W	1137	GLU	N-CA-C	5.56	117.42	111.36
3	C	102	ILE	N-CA-C	5.56	116.29	108.17
8	W	771	THR	CA-CB-OG1	-5.55	101.27	109.60
3	C	103	ALA	CA-C-O	-5.55	115.67	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	67	ARG	O-C-N	5.54	127.86	122.09
8	W	287	PRO	CB-CA-C	5.54	118.56	110.63
5	G	41	GLU	CA-C-O	-5.53	114.69	120.55
1	A	109	LEU	CA-C-O	5.51	126.60	120.82
8	W	337	HIS	CA-C-N	5.51	127.92	120.38
8	W	337	HIS	C-N-CA	5.51	127.92	120.38
8	W	666	ASP	N-CA-CB	-5.50	101.67	110.19
1	E	97	GLU	N-CA-C	-5.48	105.21	111.07
2	B	95	ARG	CB-CG-CD	5.47	123.89	111.30
1	E	126	LEU	O-C-N	5.47	127.78	122.09
1	A	62	ILE	CB-CA-C	-5.46	104.09	111.63
5	G	45	ALA	CA-C-O	5.45	126.38	119.78
4	H	39	TYR	N-CA-C	5.45	116.90	111.07
8	W	432	VAL	CA-CB-CG1	5.44	119.65	110.40
2	F	36	ARG	CG-CD-NE	-5.44	100.04	112.00
3	C	32	ARG	CB-CA-C	-5.43	101.62	110.85
8	W	595	LEU	CA-C-O	-5.43	113.58	120.20
4	D	99	LEU	CD1-CG-CD2	5.41	122.71	110.80
8	W	1031	LEU	CA-C-O	-5.40	115.12	120.90
8	W	1059	ALA	N-CA-C	5.39	116.84	111.07
4	H	76	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	F	35	ARG	N-CA-C	-5.38	105.42	111.28
1	A	83	ARG	NE-CZ-NH1	-5.37	116.13	121.50
4	H	115	VAL	N-CA-C	-5.37	105.15	110.62
4	H	38	VAL	CA-C-O	5.36	126.52	120.95
4	H	65	ASP	CA-CB-CG	5.36	117.95	112.60
8	W	771	THR	CA-C-O	-5.34	115.19	120.80
4	H	119	THR	CA-CB-OG1	-5.34	101.60	109.60
8	W	587	HIS	CA-CB-CG	5.33	119.13	113.80
3	C	102	ILE	CA-C-N	5.32	131.18	121.97
3	C	102	ILE	C-N-CA	5.32	131.18	121.97
3	C	46	GLY	CA-C-N	5.32	126.37	119.78
3	C	46	GLY	C-N-CA	5.32	126.37	119.78
8	W	493	GLU	CB-CG-CD	-5.32	103.56	112.60
3	C	101	THR	CA-C-N	-5.31	115.05	122.75
3	C	101	THR	C-N-CA	-5.31	115.05	122.75
1	E	50	GLU	N-CA-C	-5.30	105.50	111.28
4	H	40	LYS	CB-CA-C	-5.30	102.49	110.92
4	H	74	ALA	CA-C-O	5.29	126.38	120.82
1	E	53	ARG	CA-C-O	5.29	126.02	120.42
2	F	55	ARG	CG-CD-NE	-5.28	100.38	112.00
4	H	109	SER	CA-C-O	-5.27	115.29	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	23	LEU	CA-C-O	5.27	127.02	121.33
1	E	79	LYS	CA-C-O	5.26	126.86	121.23
8	W	492	TYR	CA-C-O	-5.26	114.85	120.42
3	C	50	TYR	CB-CG-CD2	5.26	128.69	120.80
8	W	1206	THR	N-CA-C	5.25	117.01	111.28
8	W	189	THR	N-CA-C	5.25	117.46	108.90
2	B	101	GLY	CA-C-O	-5.24	116.76	121.47
1	A	102	GLY	CA-C-O	5.21	125.91	120.80
8	W	1255	ARG	N-CA-C	5.20	116.64	111.07
5	G	58	LEU	CA-C-O	5.20	126.06	120.55
8	W	273	GLU	O-C-N	5.19	127.62	122.12
8	W	596	ARG	N-CA-CB	5.19	118.75	110.65
2	B	93	GLN	OE1-CD-NE2	5.18	127.78	122.60
4	D	50	GLY	CA-C-O	5.18	127.73	121.77
8	W	367	GLN	CA-C-O	5.18	123.45	119.46
8	W	482	THR	CA-CB-OG1	-5.17	101.84	109.60
1	E	108	ASN	CB-CA-C	-5.17	102.53	110.81
8	W	724	LEU	CA-C-O	-5.17	114.94	120.42
3	C	62	ILE	CA-C-N	5.16	127.51	120.54
3	C	62	ILE	C-N-CA	5.16	127.51	120.54
5	G	102	ILE	N-CA-C	5.16	115.33	108.11
5	G	105	GLY	CA-C-O	5.14	126.34	121.05
1	E	126	LEU	CB-CA-C	-5.13	102.61	110.81
8	W	1040	LEU	N-CA-C	5.12	118.44	109.48
1	A	53	ARG	N-CA-C	-5.12	105.14	111.33
2	F	35	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	58	THR	CA-C-N	5.11	128.11	120.90
1	A	58	THR	C-N-CA	5.11	128.11	120.90
3	C	43	VAL	N-CA-CB	-5.11	103.08	111.45
3	C	72	ASP	CA-CB-CG	5.10	117.70	112.60
2	F	93	GLN	CA-C-O	5.09	125.30	119.35
4	H	48	ASP	CA-C-O	-5.09	116.38	122.13
4	D	64	ASN	N-CA-C	-5.08	105.82	111.36
2	F	58	LEU	CD1-CG-CD2	-5.07	99.64	110.80
4	H	42	LEU	CB-CA-C	-5.07	102.87	110.92
1	A	49	ARG	NE-CZ-NH2	5.05	123.75	119.20
4	D	50	GLY	O-C-N	-5.04	118.90	123.29
4	D	113	LYS	N-CA-C	-5.04	105.70	111.14
8	W	790	ASP	CA-C-O	-5.03	115.22	121.06
8	W	432	VAL	O-C-N	-5.03	117.10	121.57
8	W	829	VAL	N-CA-C	-5.02	105.50	110.62
1	E	105	GLU	CB-CG-CD	5.01	121.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	59	THR	CA-C-O	5.01	126.26	120.90
3	C	80	PRO	CA-C-N	5.00	126.98	120.28
3	C	80	PRO	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	63	ARG	Sidechain
1	A	69	ARG	Sidechain
1	A	83	ARG	Sidechain
2	B	35	ARG	Sidechain
2	B	39	ARG	Sidechain
2	B	40	ARG	Sidechain
2	B	45	ARG	Sidechain
2	B	72	TYR	Sidechain
3	C	101	THR	Peptide
3	C	29	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	42	ARG	Sidechain
3	C	71	ARG	Sidechain
3	C	77	ARG	Sidechain
3	C	81	ARG	Sidechain
4	D	30	ARG	Sidechain
4	D	81	ASN	Mainchain
4	D	83	ARG	Peptide
1	E	116	ARG	Sidechain
1	E	40	ARG	Sidechain
1	E	63	ARG	Sidechain
1	E	69	ARG	Sidechain
1	E	72	ARG	Sidechain
1	E	97	GLU	Mainchain
2	F	100	PHE	Peptide
2	F	39	ARG	Sidechain
2	F	40	ARG	Sidechain
2	F	45	ARG	Sidechain
2	F	67	ARG	Sidechain
2	F	92	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	F	95	ARG	Sidechain
5	G	71	ARG	Sidechain
5	G	77	ARG	Sidechain
5	G	88	ARG	Sidechain
5	G	99	ARG	Sidechain
4	H	34	TYR	Sidechain
4	H	76	ARG	Sidechain
4	H	89	ARG	Sidechain
4	H	96	ARG	Sidechain
8	W	1085	ARG	Sidechain
8	W	1112	ARG	Sidechain
8	W	1254[A]	ARG	Sidechain
8	W	1254[B]	ARG	Sidechain
8	W	1264	ARG	Sidechain
8	W	189	THR	Peptide
8	W	237	ARG	Sidechain
8	W	241	ARG	Sidechain
8	W	274	ARG	Sidechain
8	W	276	ARG	Sidechain
8	W	312	ARG	Sidechain
8	W	313	ARG	Sidechain
8	W	377	ARG	Sidechain
8	W	517	ARG	Sidechain
8	W	563	ARG	Sidechain
8	W	706	ARG	Sidechain
8	W	720	MET	Mainchain
8	W	722	ARG	Sidechain
8	W	797	ALA	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	800	0	837	197	0
1	E	799	0	834	163	0
2	B	662	0	709	169	0
2	F	686	0	693	190	0
3	C	795	0	844	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	745	0	773	131	0
4	H	726	0	746	114	0
5	G	809	0	864	180	0
6	I	3590	0	1969	644	0
7	J	3646	0	1989	702	0
8	M	7017	0	7011	173	0
8	W	7189	0	7206	956	0
9	M	27	0	12	1	0
9	W	27	0	12	12	0
10	M	4	0	0	1	0
10	W	4	0	0	0	0
All	All	27526	0	24499	2995	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (2995) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:26:DA:H2"	7:J:27:DG:C8	1.33	1.59
6:I:30:DT:C6	6:I:31:DT:H72	1.40	1.52
1:A:63:ARG:CZ	7:J:17:DA:H5'	1.40	1.50
6:I:22:DC:P	8:W:520:ASN:HB3	1.52	1.50
6:I:-84:DA:H2	7:J:86:DA:C2	1.30	1.48
7:J:-17:DT:H5'	8:W:493:GLU:CB	1.43	1.47
6:I:23:DA:OP1	8:W:519:LYS:CE	1.66	1.43
8:W:345:LYS:HB3	8:W:1036:ALA:CB	1.48	1.42
1:E:61:LEU:CD1	2:F:37:LEU:HA	1.50	1.41
6:I:-84:DA:C2	7:J:86:DA:C2	2.08	1.41
6:I:-80:DG:H1	7:J:82:DG:N2	1.17	1.40
1:A:117:VAL:HB	6:I:-3:DG:P	1.62	1.40
6:I:-80:DG:N1	7:J:82:DG:N2	1.68	1.37
1:E:61:LEU:HD13	2:F:37:LEU:CA	1.54	1.37
1:A:63:ARG:CZ	7:J:17:DA:C5'	2.04	1.36
5:G:15:LYS:NZ	6:I:46:DA:H4'	1.07	1.36
6:I:-84:DA:C2	7:J:86:DA:H2	1.43	1.36
3:C:77:ARG:HB2	6:I:-55:DG:OP1	1.21	1.35
1:A:85:GLN:CG	6:I:-24:DG:OP1	1.72	1.35
8:W:481:LYS:HG3	8:W:483:MET:CE	1.55	1.34
6:I:-86:DA:N1	7:J:87:DT:N3	1.73	1.34
2:B:78:ARG:CB	7:J:28:DA:OP1	1.76	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HD22	3:C:39:TYR:CE2	1.63	1.33
1:E:61:LEU:HD12	2:F:37:LEU:CD1	1.57	1.33
3:C:40:ALA:HB2	4:D:86:ILE:CD1	1.56	1.32
6:I:-3:DG:C5	6:I:-2:DC:N3	1.91	1.32
7:J:26:DA:C2'	7:J:27:DG:C8	2.13	1.32
5:G:91:GLU:O	5:G:95:LYS:HG3	1.29	1.32
5:G:43:VAL:N	6:I:39:DA:OP1	1.62	1.31
8:W:518:LEU:HD12	8:W:518:LEU:O	1.30	1.31
4:H:66:VAL:O	4:H:70:ILE:HD13	1.13	1.30
7:J:-11:DC:N4	7:J:-10:DG:O6	1.61	1.30
3:C:17:ARG:HD2	6:I:-43:DT:OP1	1.15	1.30
6:I:34:DT:H2"	6:I:35:DC:C6	1.65	1.29
4:H:36:ILE:HD11	6:I:49:DC:OP2	1.25	1.29
1:A:117:VAL:HB	6:I:-3:DG:OP1	1.31	1.29
7:J:19:DC:H2"	7:J:20:DG:C8	1.67	1.28
1:E:63:ARG:NE	7:J:-13:DA:H5'	1.48	1.27
3:C:34:LEU:CD2	3:C:39:TYR:HE2	1.46	1.27
6:I:-76:DG:N1	7:J:76:DG:N2	1.82	1.27
8:W:607:PRO:HB2	8:W:813:HIS:N	1.48	1.27
6:I:-6:DT:H2"	6:I:-5:DA:C8	1.70	1.26
1:A:83:ARG:O	1:A:84:PHE:HD1	1.15	1.26
6:I:-19:DG:O5'	8:M:743:GLY:HA3	1.17	1.26
7:J:26:DA:N7	7:J:27:DG:O6	1.68	1.26
8:W:390:LEU:CD1	8:W:393:LYS:HD2	1.65	1.25
1:A:85:GLN:HA	6:I:-24:DG:O5'	1.31	1.25
6:I:-23:DC:H2"	6:I:-22:DA:C5'	1.66	1.25
8:W:481:LYS:CG	8:W:483:MET:HE3	1.63	1.25
2:F:17:ARG:CB	8:W:722:ARG:NH2	2.01	1.24
6:I:-28:DT:H2"	6:I:-27:DC:C5	1.73	1.24
7:J:-37:DG:H2"	7:J:-36:DG:N7	1.52	1.24
8:W:345:LYS:CB	8:W:1036:ALA:CB	2.17	1.23
1:E:61:LEU:CD1	2:F:37:LEU:HD12	1.66	1.23
1:A:85:GLN:HA	6:I:-24:DG:P	1.78	1.23
6:I:22:DC:P	8:W:520:ASN:CB	2.27	1.23
5:G:15:LYS:NZ	6:I:46:DA:C4'	2.00	1.22
2:F:45:ARG:HA	6:I:8:DC:OP1	1.39	1.22
2:F:46:ILE:H	6:I:8:DC:P	1.61	1.22
6:I:22:DC:OP2	8:W:520:ASN:CB	1.88	1.22
7:J:13:DT:OP1	8:M:241:ARG:HG2	1.06	1.22
6:I:-18:DC:C5'	8:M:434:LEU:HD21	1.68	1.22
8:W:414:PHE:CE2	8:W:538:MET:HE1	1.74	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-17:DT:C5'	8:W:493:GLU:HB3	1.71	1.21
6:I:-77:DC:O2	7:J:78:DG:N2	1.73	1.21
7:J:21:DG:C4'	8:M:517:ARG:HH21	1.51	1.21
7:J:-11:DC:C4	7:J:-10:DG:C6	2.29	1.21
7:J:32:DG:C2'	7:J:33:DT:H71	1.69	1.20
1:A:63:ARG:NH2	7:J:17:DA:H5'	1.56	1.20
8:W:607:PRO:HG3	8:W:811:LYS:C	1.64	1.20
1:A:84:PHE:CE1	2:B:81:VAL:HB	1.77	1.19
5:G:43:VAL:H	6:I:39:DA:P	1.64	1.19
8:W:607:PRO:CB	8:W:813:HIS:H	1.52	1.19
7:J:21:DG:H4'	8:M:517:ARG:NH2	1.57	1.19
7:J:26:DA:C5	7:J:27:DG:C6	2.29	1.19
6:I:-77:DC:C2	7:J:78:DG:N2	2.11	1.19
5:G:91:GLU:O	5:G:95:LYS:CG	1.90	1.19
1:E:63:ARG:HE	7:J:-13:DA:C5'	1.54	1.18
6:I:-3:DG:C4	6:I:-2:DC:N3	2.09	1.18
8:W:345:LYS:CB	8:W:1036:ALA:HB3	1.72	1.18
8:W:414:PHE:CD2	8:W:538:MET:HE1	1.76	1.18
1:E:116:ARG:NH2	7:J:-2:DC:OP2	1.74	1.18
7:J:-38:DA:C5	7:J:-37:DG:C6	2.31	1.18
3:C:17:ARG:CD	6:I:-43:DT:OP1	1.90	1.18
6:I:20:DG:H3'	8:W:524:SER:OG	1.40	1.18
8:W:777:GLY:O	8:W:778:ILE:HG22	1.36	1.18
4:H:66:VAL:O	4:H:70:ILE:CD1	1.92	1.17
6:I:-19:DG:H3'	8:M:743:GLY:CA	1.72	1.17
7:J:-35:DG:H2"	7:J:-34:DA:C8	1.78	1.17
7:J:-46:DT:H1'	7:J:-45:DG:C5	1.79	1.17
6:I:23:DA:OP1	8:W:519:LYS:HE2	1.20	1.16
8:W:650:ASN:HA	8:W:654:GLU:HB3	1.27	1.16
6:I:-86:DA:N1	7:J:87:DT:C4	2.14	1.15
7:J:24:DC:OP1	8:M:793:TRP:CD1	1.98	1.15
3:C:97:LEU:HD11	4:D:62:PHE:CE2	1.80	1.15
6:I:-38:DC:C4	6:I:-37:DG:O6	2.00	1.15
6:I:21:DC:OP2	8:W:524:SER:OG	1.63	1.15
8:W:398:ILE:HG23	8:W:539:LEU:HD11	1.26	1.15
6:I:-35:DA:C8	6:I:-34:DG:N7	2.13	1.15
7:J:13:DT:OP1	8:M:241:ARG:CG	1.94	1.14
4:H:36:ILE:HD11	6:I:49:DC:P	1.86	1.14
7:J:-46:DT:C1'	7:J:-45:DG:C5	2.26	1.14
8:W:1150:TYR:HD1	8:W:1156:LYS:HE2	1.04	1.14
1:A:83:ARG:O	1:A:84:PHE:CD1	2.01	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-35:DA:N7	6:I:-34:DG:C6	2.15	1.14
6:I:-38:DC:C4	6:I:-37:DG:C6	2.35	1.14
6:I:5:DC:H2"	6:I:6:DC:C5	1.81	1.14
7:J:-17:DT:H5'	8:W:493:GLU:CG	1.73	1.13
6:I:-18:DC:O3'	8:M:493:GLU:OE2	1.65	1.13
2:B:26:ILE:HD13	2:B:59:LYS:HD3	1.30	1.13
6:I:22:DC:OP2	8:W:520:ASN:HB3	0.95	1.13
8:W:518:LEU:CD1	8:W:555:LEU:HD12	1.78	1.13
7:J:-17:DT:C7	7:J:-16:DT:O4	1.96	1.13
6:I:42:DC:H2"	6:I:43:DT:O5'	1.42	1.12
8:W:523:SER:HB2	8:W:526:TYR:HB2	1.12	1.12
5:G:51:LEU:CD2	4:H:91:ILE:HG21	1.79	1.11
6:I:-77:DC:OP2	8:W:1254[A]:ARG:NH2	1.82	1.11
6:I:-18:DC:H5"	8:M:434:LEU:HD21	1.22	1.11
7:J:-21:DG:H2"	7:J:-20:DC:O5'	1.38	1.11
2:B:45:ARG:HD3	7:J:8:DG:H5'	1.25	1.11
6:I:20:DG:C3'	8:W:524:SER:OG	1.98	1.11
6:I:21:DC:P	8:W:524:SER:OG	2.09	1.10
7:J:-25:DC:C2'	7:J:-24:DT:H72	1.81	1.10
7:J:20:DG:H5"	8:M:496:LEU:HD23	1.33	1.10
1:E:116:ARG:HB3	7:J:-3:DA:OP1	1.47	1.10
6:I:23:DA:OP1	8:W:519:LYS:HE3	1.48	1.10
6:I:-3:DG:C2'	6:I:-2:DC:C5	2.34	1.10
7:J:6:DA:H2"	7:J:7:DC:C5	1.87	1.10
2:F:30:THR:HB	7:J:-13:DA:H3'	1.24	1.10
2:F:30:THR:HG21	7:J:-13:DA:C5'	1.81	1.10
6:I:-18:DC:C4'	8:M:434:LEU:HD21	1.81	1.10
7:J:-17:DT:C5	7:J:-16:DT:C4	2.39	1.10
8:W:295:ARG:HD2	8:W:1198:ARG:NH2	1.66	1.10
6:I:-30:DG:C8	6:I:-29:DC:C5	2.40	1.09
7:J:21:DG:H4'	8:M:517:ARG:HH21	0.93	1.09
8:W:408:THR:HG23	8:W:440:TRP:CZ3	1.87	1.09
8:W:615:ARG:HB3	8:W:822:LYS:HD3	1.11	1.09
7:J:-19:DG:OP1	8:W:772:ARG:HB2	1.49	1.09
2:F:45:ARG:CA	6:I:8:DC:OP1	2.00	1.09
6:I:30:DT:C6	6:I:31:DT:C7	2.34	1.09
1:A:63:ARG:HE	7:J:17:DA:H4'	1.10	1.09
3:C:40:ALA:CB	4:D:86:ILE:CD1	2.30	1.09
4:D:62:PHE:HA	2:F:98:TYR:CE1	1.86	1.09
7:J:-25:DC:H2'	7:J:-24:DT:H72	1.32	1.09
3:C:34:LEU:CD2	3:C:39:TYR:CE2	2.28	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:CG2	7:J:-13:DA:H4'	1.81	1.09
6:I:43:DT:H2"	6:I:44:DC:O5'	1.44	1.09
8:W:390:LEU:HD12	8:W:393:LYS:HD2	1.20	1.08
3:C:30:VAL:HG13	4:D:67:PHE:HE1	1.15	1.08
8:W:419:ILE:HG21	8:W:451:LEU:HD11	1.35	1.08
8:W:1150:TYR:CD1	8:W:1156:LYS:HE2	1.87	1.08
1:A:120:MET:HB3	1:A:121:PRO:HD2	1.29	1.08
8:W:481:LYS:CD	8:W:483:MET:HE1	1.84	1.08
6:I:-62:DC:O2	7:J:63:DG:N2	1.86	1.08
7:J:26:DA:N7	7:J:27:DG:C6	2.20	1.08
6:I:-68:DG:N2	7:J:69:DC:N3	2.02	1.07
8:W:345:LYS:HE2	8:W:1037:ASP:HB2	1.22	1.07
1:A:73:GLU:HG2	2:B:22:LEU:O	1.54	1.07
6:I:-3:DG:H2'	6:I:-2:DC:C5	1.90	1.07
7:J:24:DC:C2'	7:J:25:DT:H71	1.84	1.07
7:J:72:DA:C8	7:J:73:DT:H72	1.89	1.07
6:I:34:DT:H2"	6:I:35:DC:C5	1.90	1.07
3:C:79:ILE:HG23	3:C:80:PRO:HD2	1.31	1.07
2:F:15:ALA:HA	8:W:729:ASP:HB3	1.15	1.07
1:A:63:ARG:NE	7:J:17:DA:C5'	2.17	1.06
6:I:-80:DG:N2	7:J:82:DG:H21	1.52	1.06
6:I:-23:DC:N4	6:I:-22:DA:H62	1.52	1.06
6:I:-3:DG:H2"	6:I:-2:DC:C6	1.89	1.06
7:J:-25:DC:C2'	7:J:-24:DT:C7	2.34	1.06
7:J:-46:DT:C2'	7:J:-45:DG:C6	2.28	1.06
1:A:85:GLN:HG2	6:I:-24:DG:P	1.95	1.06
7:J:-11:DC:N4	7:J:-10:DG:C6	2.23	1.06
7:J:34:DC:H2'	7:J:35:DT:C7	1.85	1.06
7:J:34:DC:H2'	7:J:35:DT:H71	1.07	1.05
7:J:-37:DG:H2"	7:J:-36:DG:C8	1.90	1.05
7:J:42:DA:H2"	7:J:43:DA:O5'	1.48	1.05
6:I:-86:DA:N6	7:J:87:DT:O4	1.89	1.05
6:I:-23:DC:N4	6:I:-22:DA:N6	2.04	1.05
6:I:-3:DG:C4	6:I:-2:DC:C4	2.33	1.05
3:C:77:ARG:CB	6:I:-55:DG:OP1	2.04	1.05
8:M:778:ILE:HG22	8:M:779:ASN:H	1.17	1.05
8:W:345:LYS:HB3	8:W:1036:ALA:HB1	1.11	1.05
6:I:20:DG:O3'	8:W:524:SER:HB2	1.50	1.05
8:W:1055:MET:HE3	8:W:1121:PHE:CE2	1.92	1.05
3:C:40:ALA:CB	4:D:86:ILE:HD12	1.87	1.04
6:I:-86:DA:C2	7:J:87:DT:N3	2.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:20:DG:O3'	8:W:524:SER:CB	2.04	1.04
6:I:-35:DA:C5	6:I:-34:DG:C6	2.44	1.04
8:W:481:LYS:CG	8:W:483:MET:CE	2.28	1.04
1:A:73:GLU:CG	2:B:22:LEU:O	2.05	1.04
7:J:32:DG:H2"	7:J:33:DT:H71	1.05	1.04
6:I:-23:DC:C2'	6:I:-22:DA:H5'	1.87	1.04
6:I:-19:DG:H2'	8:M:743:GLY:O	1.58	1.04
1:A:63:ARG:NE	7:J:17:DA:H4'	1.72	1.04
6:I:-76:DG:H1	7:J:76:DG:N2	1.49	1.04
6:I:-19:DG:O5'	8:M:743:GLY:CA	2.05	1.04
3:C:32:ARG:HH21	6:I:-43:DT:H72	1.24	1.03
1:A:63:ARG:HE	7:J:17:DA:C4'	1.71	1.03
3:C:34:LEU:HD22	3:C:39:TYR:HE2	0.88	1.03
3:C:112:GLN:HB2	3:C:115:LEU:HD12	1.37	1.03
2:F:30:THR:HB	7:J:-13:DA:C3'	1.88	1.03
7:J:4:DG:H2'	7:J:5:DT:H71	1.40	1.03
6:I:-19:DG:H3'	8:M:743:GLY:HA2	1.41	1.03
1:E:66:PRO:HB2	2:F:29:ILE:HG12	1.35	1.03
6:I:-80:DG:C2	7:J:82:DG:N2	2.25	1.03
6:I:-16:DT:OP2	8:M:459:ASN:HB3	1.58	1.03
1:E:60:LEU:HD13	1:E:93:GLN:CD	1.84	1.02
7:J:-25:DC:H2"	7:J:-24:DT:C7	1.89	1.02
1:A:65:LEU:HD22	7:J:17:DA:OP2	1.60	1.02
1:E:60:LEU:HD13	1:E:93:GLN:NE2	1.73	1.02
7:J:-17:DT:C5	7:J:-16:DT:O4	2.12	1.02
7:J:-17:DT:H71	7:J:-16:DT:O4	1.57	1.02
8:W:1138:ASP:HB3	8:W:1260:LEU:HD23	1.37	1.02
2:B:78:ARG:HB3	7:J:28:DA:P	1.99	1.02
8:W:643:GLY:HA2	8:W:646:PHE:CZ	1.93	1.02
8:W:599:LYS:O	8:W:601:ASP:N	1.91	1.02
7:J:-46:DT:C1'	7:J:-45:DG:C6	2.42	1.02
8:W:518:LEU:CD1	8:W:555:LEU:CD1	2.37	1.02
8:W:645:HIS:CE1	8:W:649:LEU:HD11	1.93	1.02
7:J:-33:DG:H2"	7:J:-32:DT:O5'	1.56	1.01
7:J:-32:DT:H2"	7:J:-31:DA:C8	1.95	1.01
1:A:117:VAL:CB	6:I:-3:DG:OP1	2.09	1.01
6:I:-12:DC:N4	6:I:-11:DG:O6	1.94	1.01
8:W:345:LYS:HB3	8:W:1036:ALA:HB3	1.33	1.01
8:W:607:PRO:HG3	8:W:812:ASN:N	1.73	1.01
8:W:523:SER:CB	8:W:526:TYR:HB2	1.91	1.01
7:J:32:DG:H2"	7:J:33:DT:C7	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:ILE:N	6:I:8:DC:OP1	1.94	1.00
4:D:84:SER:OG	6:I:-35:DA:H3'	1.60	1.00
6:I:-35:DA:N7	6:I:-34:DG:C5	2.29	1.00
7:J:20:DG:H4'	8:M:496:LEU:HD22	1.42	1.00
8:W:295:ARG:HD2	8:W:1198:ARG:HH22	1.22	1.00
1:A:100:LEU:HD23	2:B:37:LEU:HD13	1.43	1.00
7:J:24:DC:H2"	7:J:25:DT:H71	1.41	1.00
7:J:33:DT:H2"	7:J:34:DC:H5	1.26	1.00
1:E:63:ARG:HE	7:J:-13:DA:H5'	0.83	1.00
8:W:474:ASN:HB2	8:W:475:PRO:HD2	1.39	0.99
2:F:46:ILE:O	6:I:7:DC:H3'	1.62	0.99
4:H:62:PHE:O	4:H:66:VAL:HG23	1.62	0.99
4:D:85:THR:N	6:I:-34:DG:OP1	1.95	0.99
6:I:-28:DT:H2"	6:I:-27:DC:C6	1.97	0.99
3:C:40:ALA:HB2	4:D:86:ILE:HD12	1.41	0.99
6:I:-37:DG:H2"	6:I:-36:DT:C5	1.96	0.99
3:C:32:ARG:HD2	6:I:-44:DA:P	2.02	0.99
6:I:-79:DG:N2	7:J:80:DC:O2	1.96	0.99
2:B:78:ARG:HB3	7:J:28:DA:OP1	0.81	0.99
3:C:97:LEU:HD11	4:D:62:PHE:HE2	1.28	0.99
2:F:17:ARG:CB	8:W:722:ARG:HH21	1.69	0.99
7:J:33:DT:H2"	7:J:34:DC:C5	1.98	0.99
2:F:30:THR:HG21	7:J:-13:DA:H4'	1.45	0.99
2:F:17:ARG:HA	8:W:722:ARG:HH22	1.28	0.98
2:F:30:THR:CG2	7:J:-13:DA:C4'	2.40	0.98
1:A:85:GLN:CA	6:I:-24:DG:P	2.50	0.98
6:I:-6:DT:C5	6:I:-5:DA:N6	2.30	0.98
8:W:345:LYS:HE2	8:W:1037:ASP:CB	1.92	0.98
8:W:518:LEU:HD11	8:W:555:LEU:CD1	1.93	0.98
7:J:24:DC:H2"	7:J:25:DT:C5	1.97	0.98
5:G:67:GLY:HA2	5:G:78:ILE:HD11	1.43	0.98
7:J:-11:DC:C4	7:J:-10:DG:C5	2.51	0.98
6:I:-84:DA:N1	7:J:86:DA:N1	2.10	0.98
6:I:-49:DG:H1	7:J:49:DC:H42	1.05	0.98
6:I:-18:DC:H5"	8:M:434:LEU:CD2	1.92	0.98
7:J:-19:DG:OP1	8:W:772:ARG:CB	2.12	0.98
1:A:63:ARG:NH2	7:J:17:DA:C4'	2.27	0.98
2:F:30:THR:CB	7:J:-13:DA:H5"	1.95	0.97
6:I:-70:DC:O2	7:J:71:DG:N2	1.95	0.97
6:I:-19:DG:C2'	8:M:743:GLY:O	2.12	0.97
6:I:21:DC:P	8:W:524:SER:HG	1.87	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:611:GLU:HG2	8:W:816:VAL:HG12	1.46	0.97
2:F:45:ARG:C	6:I:8:DC:OP1	2.07	0.97
7:J:34:DC:C6	7:J:34:DC:H5'	2.00	0.97
6:I:-18:DC:H4'	8:M:434:LEU:HD21	1.47	0.97
8:W:523:SER:HB2	8:W:526:TYR:CB	1.94	0.97
6:I:15:DT:H2"	6:I:16:DA:C8	2.00	0.97
6:I:-3:DG:C2'	6:I:-2:DC:C6	2.48	0.97
7:J:24:DC:H2"	7:J:25:DT:C6	1.98	0.97
7:J:24:DC:H2"	7:J:25:DT:C7	1.95	0.97
6:I:-77:DC:OP2	8:W:1254[B]:ARG:NH1	1.97	0.96
7:J:-11:DC:C5	7:J:-10:DG:N7	2.33	0.96
8:W:650:ASN:HA	8:W:654:GLU:CB	1.95	0.96
1:E:65:LEU:H	1:E:66:PRO:HD2	1.29	0.96
8:W:345:LYS:CE	8:W:1037:ASP:HB2	1.94	0.96
2:B:98:TYR:CE1	4:H:62:PHE:HA	1.99	0.96
1:A:100:LEU:CD2	2:B:37:LEU:HD13	1.94	0.96
2:F:47:SER:HA	6:I:7:DC:O5'	1.65	0.96
6:I:-35:DA:C8	6:I:-34:DG:C5	2.52	0.96
8:W:770:SER:HB2	8:W:773:ALA:HB3	1.45	0.96
2:F:30:THR:HG21	7:J:-13:DA:C4'	1.95	0.96
6:I:-23:DC:H2"	6:I:-22:DA:H5'	0.98	0.96
1:A:59:GLU:OE2	1:A:60:LEU:O	1.84	0.96
8:W:367:GLN:CD	8:W:371:ILE:HD11	1.91	0.96
7:J:6:DA:H2"	7:J:7:DC:C6	1.99	0.96
7:J:78:DG:C6	7:J:79:DG:C6	2.53	0.96
4:H:51:ILE:HD13	4:H:56:MET:HE3	1.48	0.95
8:W:609:LYS:HA	8:W:814:VAL:HB	1.47	0.95
7:J:60:DA:H2"	7:J:61:DC:C5	2.02	0.95
8:W:502:LEU:O	8:W:507:TRP:HZ3	1.50	0.95
7:J:24:DC:C2'	7:J:25:DT:C7	2.44	0.95
8:W:770:SER:CB	8:W:773:ALA:HB3	1.96	0.95
8:W:390:LEU:HD13	8:W:393:LYS:HD2	1.49	0.95
5:G:84:GLN:NE2	5:G:102:ILE:CG1	2.30	0.95
8:W:518:LEU:O	8:W:518:LEU:CD1	2.13	0.95
5:G:41:GLU:O	6:I:39:DA:H5"	1.66	0.95
3:C:63:LEU:HD12	4:D:41:VAL:HG12	1.47	0.95
2:B:45:ARG:CD	7:J:8:DG:H5'	1.97	0.94
3:C:32:ARG:HH21	6:I:-43:DT:C7	1.79	0.94
2:F:32:PRO:O	2:F:36:ARG:HG2	1.67	0.94
8:W:650:ASN:CA	8:W:654:GLU:HB3	1.97	0.94
5:G:97:LEU:O	5:G:100:VAL:HG22	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-6:DT:H2"	6:I:-5:DA:N7	1.82	0.94
5:G:91:GLU:O	5:G:95:LYS:CD	2.14	0.94
4:H:36:ILE:CD1	6:I:49:DC:OP2	2.15	0.94
6:I:30:DT:C5	6:I:31:DT:H72	2.02	0.94
7:J:20:DG:H4'	7:J:21:DG:OP1	1.64	0.94
1:A:85:GLN:HG2	6:I:-24:DG:OP1	0.77	0.94
7:J:-33:DG:C2'	7:J:-32:DT:O5'	2.15	0.94
3:C:30:VAL:HG13	4:D:67:PHE:CE1	2.02	0.94
8:W:656:LYS:HE2	8:W:826:GLU:HA	1.48	0.94
1:E:65:LEU:HD13	6:I:17:DA:H2'	1.49	0.94
2:F:15:ALA:CA	8:W:729:ASP:HB3	1.98	0.94
7:J:20:DG:N2	7:J:21:DG:C6	2.36	0.94
8:W:229:THR:HG22	8:W:230:TYR:H	1.32	0.94
5:G:15:LYS:HZ1	6:I:46:DA:H4'	1.20	0.94
7:J:-17:DT:H5'	8:W:493:GLU:HB3	0.94	0.94
7:J:19:DC:C5	7:J:20:DG:O6	2.21	0.94
8:W:607:PRO:HD2	8:W:810:GLN:O	1.68	0.94
2:B:98:TYR:HE1	4:H:62:PHE:HA	1.28	0.93
8:W:1246:VAL:HG13	8:W:1247:PRO:HA	1.51	0.93
2:F:15:ALA:HA	8:W:729:ASP:CB	1.99	0.93
7:J:26:DA:C2'	7:J:27:DG:N7	2.30	0.93
7:J:26:DA:C8	7:J:27:DG:C5	2.56	0.93
1:A:63:ARG:NH2	7:J:17:DA:C5'	2.21	0.93
2:B:45:ARG:HD3	7:J:8:DG:C5'	1.97	0.93
4:H:55:ALA:HA	4:H:58:ILE:HD12	1.50	0.93
3:C:65:LEU:CD2	3:C:90:ASP:OD2	2.16	0.93
8:W:481:LYS:CD	8:W:483:MET:CE	2.45	0.93
5:G:51:LEU:HD21	4:H:91:ILE:HG21	1.46	0.93
8:W:390:LEU:HD12	8:W:393:LYS:CD	1.97	0.93
3:C:40:ALA:HB2	4:D:86:ILE:HD11	1.48	0.93
6:I:-16:DT:OP2	8:M:459:ASN:CB	2.15	0.93
3:C:43:VAL:HG12	7:J:38:DG:H3'	1.51	0.93
1:E:65:LEU:HB3	6:I:17:DA:O5'	1.68	0.93
6:I:23:DA:C5	6:I:24:DA:N6	2.37	0.93
7:J:5:DT:H2"	7:J:6:DA:C8	2.04	0.93
8:W:414:PHE:CE2	8:W:538:MET:CE	2.52	0.93
6:I:34:DT:C2'	6:I:35:DC:C5	2.51	0.93
7:J:-25:DC:H2"	7:J:-24:DT:C6	2.03	0.92
6:I:-37:DG:H2"	6:I:-36:DT:C7	1.99	0.92
8:W:656:LYS:HE3	8:W:829:VAL:CG2	2.00	0.92
2:B:84:MET:HE1	2:B:88:TYR:OH	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-79:DG:N2	7:J:80:DC:C2	2.37	0.92
8:W:813:HIS:O	8:W:814:VAL:HG23	1.68	0.92
1:A:63:ARG:HH21	7:J:17:DA:C4'	1.80	0.92
5:G:15:LYS:HZ3	6:I:46:DA:H4'	1.21	0.92
8:W:470:GLU:HG2	8:W:485:PHE:CE2	2.04	0.92
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.50	0.92
8:W:347:LEU:HD22	8:W:483:MET:O	1.68	0.92
2:B:25:ASN:OD1	2:B:26:ILE:N	2.03	0.92
6:I:34:DT:H2"	6:I:35:DC:H6	1.28	0.92
7:J:-38:DA:C5	7:J:-37:DG:O6	2.22	0.92
7:J:14:DT:H2"	7:J:15:DT:C7	1.99	0.92
8:W:607:PRO:HG3	8:W:811:LYS:CA	1.98	0.92
8:W:794:ASN:OD1	8:W:795:PRO:HD2	1.68	0.92
6:I:-73:DC:C4	6:I:-72:DA:N6	2.38	0.92
7:J:-16:DT:OP2	8:W:497:LYS:CD	2.17	0.92
8:W:474:ASN:CB	8:W:475:PRO:CD	2.48	0.92
8:W:607:PRO:HB2	8:W:813:HIS:H	0.77	0.92
8:W:1026:ASN:HA	8:W:1052:TYR:OH	1.70	0.92
5:G:51:LEU:HD23	4:H:91:ILE:HG21	1.47	0.92
8:W:611:GLU:HG2	8:W:816:VAL:CG1	1.99	0.92
6:I:19:DC:H42	7:J:-19:DG:H22	1.02	0.92
8:W:433:PRO:HD3	8:W:513:ASP:HB3	1.49	0.92
1:A:116:ARG:NH1	1:A:120:MET:HG2	1.84	0.91
7:J:26:DA:C8	7:J:27:DG:C6	2.59	0.91
8:W:607:PRO:CD	8:W:811:LYS:HA	1.98	0.91
1:E:63:ARG:CZ	7:J:-13:DA:H5'	2.00	0.91
2:F:17:ARG:CA	8:W:722:ARG:NH2	2.32	0.91
6:I:23:DA:C6	6:I:24:DA:N6	2.38	0.91
1:A:41:TYR:HB3	1:A:45:THR:HG21	1.53	0.91
1:E:65:LEU:HB2	6:I:17:DA:H3'	1.49	0.91
2:F:46:ILE:N	6:I:8:DC:P	2.41	0.91
8:W:398:ILE:HG12	8:W:539:LEU:HD21	1.52	0.91
8:W:379:PHE:HE1	8:W:597:ARG:HD2	1.31	0.91
3:C:79:ILE:HG12	4:D:52:SER:HB3	1.49	0.91
4:D:62:PHE:HA	2:F:98:TYR:HE1	1.31	0.91
1:E:42:ARG:H	1:E:43:PRO:CD	1.82	0.91
2:F:46:ILE:O	6:I:7:DC:H5'	1.70	0.91
8:W:1073:ILE:HG21	8:W:1110:LYS:HE2	1.53	0.91
7:J:-17:DT:C5'	8:W:493:GLU:CB	2.37	0.91
7:J:-46:DT:H1'	7:J:-45:DG:C4	2.06	0.91
8:W:654:GLU:OE2	8:W:664:LEU:HD23	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:21:DG:H2"	7:J:22:DT:O5'	1.68	0.90
2:F:17:ARG:HA	8:W:722:ARG:NH2	1.87	0.90
1:E:61:LEU:HD12	2:F:37:LEU:HD12	0.91	0.90
6:I:-23:DC:C5	6:I:-22:DA:N7	2.40	0.90
7:J:-35:DG:H2"	7:J:-34:DA:H8	1.31	0.90
7:J:-33:DG:H2"	7:J:-32:DT:C5'	2.01	0.90
8:W:646:PHE:HA	8:W:649:LEU:HD12	1.53	0.90
1:A:88:ALA:HA	2:B:83:ALA:HB2	1.53	0.90
4:H:87:THR:HG22	4:H:90:GLU:HG2	1.52	0.90
6:I:-22:DA:C5	6:I:-21:DC:C4	2.60	0.90
8:W:419:ILE:HG21	8:W:451:LEU:CD1	2.00	0.90
5:G:47:ALA:HB3	5:G:48:PRO:HD3	1.54	0.90
2:B:58:LEU:CD2	2:B:62:LEU:HD11	2.01	0.90
5:G:91:GLU:HB3	5:G:95:LYS:HE3	1.52	0.90
5:G:83:LEU:HD13	4:H:59:MET:SD	2.12	0.89
6:I:-30:DG:N7	6:I:-29:DC:C4	2.40	0.89
5:G:26:PRO:O	5:G:30:VAL:HG22	1.72	0.89
6:I:-28:DT:C2'	6:I:-27:DC:C5	2.54	0.89
7:J:-37:DG:C2'	7:J:-36:DG:N7	2.36	0.89
7:J:-17:DT:H2"	7:J:-16:DT:O5'	1.71	0.89
1:A:117:VAL:CB	6:I:-3:DG:P	2.57	0.89
7:J:-38:DA:N7	7:J:-37:DG:O6	2.05	0.89
8:W:629:ILE:HG21	8:W:650:ASN:ND2	1.87	0.89
8:W:638:THR:HB	8:W:667:ASN:ND2	1.87	0.89
1:E:65:LEU:CD1	6:I:17:DA:H2'	2.02	0.89
5:G:84:GLN:NE2	5:G:102:ILE:HG13	1.88	0.89
6:I:-12:DC:C4	6:I:-11:DG:O6	2.25	0.89
7:J:26:DA:C8	7:J:27:DG:N7	2.41	0.89
1:A:83:ARG:C	1:A:84:PHE:CD1	2.51	0.89
4:D:28:LYS:NZ	7:J:51:DG:H5"	1.88	0.89
6:I:-84:DA:C2	7:J:86:DA:N1	2.41	0.89
8:W:315:ASN:OD1	8:W:316:TYR:N	2.04	0.89
1:E:116:ARG:CZ	7:J:-2:DC:OP2	2.21	0.89
1:E:63:ARG:NE	2:F:30:THR:HG21	1.87	0.89
7:J:-35:DG:C5	7:J:-34:DA:C6	2.61	0.89
8:M:778:ILE:HG22	8:M:779:ASN:N	1.84	0.89
6:I:-68:DG:N2	7:J:69:DC:C2	2.40	0.88
7:J:-46:DT:H2"	7:J:-45:DG:O6	1.72	0.88
1:A:63:ARG:NE	7:J:17:DA:C4'	2.35	0.88
1:A:88:ALA:HA	2:B:83:ALA:CB	2.02	0.88
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:HG22	7:J:-13:DA:H4'	1.55	0.88
7:J:-35:DG:C2'	7:J:-34:DA:C8	2.56	0.88
8:W:691:ILE:HD12	8:W:697:MET:HB3	1.52	0.88
3:C:81:ARG:O	3:C:85:LEU:HG	1.73	0.88
4:D:30:ARG:NH2	6:I:-45:DA:OP1	2.07	0.88
8:W:436:THR:O	8:W:440:TRP:CD1	2.27	0.88
7:J:-46:DT:H2"	7:J:-45:DG:C6	1.62	0.88
8:W:777:GLY:O	8:W:778:ILE:CG2	2.21	0.88
1:A:84:PHE:CD1	2:B:81:VAL:HB	2.07	0.88
6:I:24:DA:H2"	6:I:25:DG:C8	2.09	0.88
7:J:34:DC:H2"	7:J:35:DT:O5'	1.73	0.88
7:J:69:DC:H2"	7:J:70:DT:H71	1.53	0.88
1:A:48:LEU:HA	1:A:51:ILE:HD12	1.54	0.88
7:J:67:DT:H2"	7:J:68:DT:C7	2.04	0.88
1:A:85:GLN:CB	6:I:-24:DG:P	2.62	0.88
8:W:471:PHE:HE1	8:W:481:LYS:HE2	1.38	0.88
8:W:376:LEU:HD13	8:W:380:GLN:HB3	1.54	0.88
1:A:73:GLU:HG3	2:B:25:ASN:HD22	1.38	0.87
6:I:-19:DG:C5'	8:M:743:GLY:HA3	2.02	0.87
7:J:39:DA:H2"	7:J:40:DC:H5'	1.56	0.87
8:W:617:GLU:OE1	8:W:618:LEU:O	1.92	0.87
2:F:66:ILE:O	2:F:70:VAL:HG23	1.73	0.87
8:M:206:ASN:O	8:M:210:ASN:HB2	1.74	0.87
8:W:615:ARG:CB	8:W:822:LYS:HD3	2.00	0.87
1:A:120:MET:HB3	1:A:121:PRO:CD	2.04	0.87
7:J:14:DT:H2'	7:J:15:DT:H72	1.56	0.87
1:E:84:PHE:N	7:J:-23:DT:OP1	2.08	0.87
6:I:5:DC:C2'	6:I:6:DC:C5	2.58	0.87
8:W:348:PRO:HG2	8:W:483:MET:HB3	1.56	0.87
7:J:20:DG:C4'	8:M:496:LEU:HD22	2.03	0.87
1:E:116:ARG:CB	7:J:-3:DA:OP1	2.22	0.87
6:I:-66:DA:H2"	6:I:-65:DT:H71	1.55	0.87
6:I:-38:DC:N3	6:I:-37:DG:C6	2.43	0.87
6:I:-19:DG:C3'	8:M:743:GLY:CA	2.52	0.87
7:J:-18:DG:O4'	8:W:493:GLU:OE2	1.91	0.87
7:J:19:DC:C2'	7:J:20:DG:C8	2.56	0.87
2:B:45:ARG:CD	7:J:8:DG:C5'	2.52	0.87
7:J:51:DG:H2"	7:J:52:DC:OP2	1.73	0.87
8:M:778:ILE:CG2	8:M:779:ASN:H	1.87	0.87
8:W:474:ASN:CB	8:W:475:PRO:HD2	2.03	0.87
8:W:767:PHE:CE2	8:W:769:LEU:HD11	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:NE	7:J:17:DA:H5"	1.88	0.87
5:G:103:ALA:C	5:G:104:GLN:OE1	2.18	0.87
7:J:-17:DT:C5'	8:W:493:GLU:CG	2.52	0.87
8:W:182:VAL:HG11	8:W:245:TYR:CE2	2.10	0.86
4:D:28:LYS:NZ	7:J:51:DG:C5'	2.38	0.86
6:I:-12:DC:C4	6:I:-11:DG:C6	2.63	0.86
7:J:14:DT:C2'	7:J:15:DT:H72	2.05	0.86
8:W:1119:PHE:CE2	8:W:1129:ALA:HB2	2.10	0.86
6:I:-82:DG:C2	7:J:84:DG:N2	2.43	0.86
6:I:-77:DC:P	8:W:1254[A]:ARG:HH21	1.98	0.86
6:I:15:DT:H2"	6:I:16:DA:H8	1.37	0.86
7:J:14:DT:H2"	7:J:15:DT:C6	2.10	0.86
8:W:1164:PRO:HD2	8:W:1176:LYS:HE3	1.57	0.86
6:I:-80:DG:H22	7:J:82:DG:H21	1.23	0.86
8:W:295:ARG:CD	8:W:1198:ARG:NH2	2.38	0.86
8:W:786:VAL:CG2	8:W:816:VAL:HG22	2.06	0.86
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.11	0.86
7:J:69:DC:H2"	7:J:70:DT:C7	2.05	0.86
7:J:-16:DT:OP2	8:W:497:LYS:CG	2.23	0.86
7:J:14:DT:C2'	7:J:15:DT:C7	2.52	0.86
4:D:84:SER:OG	6:I:-35:DA:C3'	2.23	0.85
5:G:28:GLY:HA3	7:J:-43:DA:P	2.15	0.85
7:J:32:DG:C2'	7:J:33:DT:C7	2.51	0.85
2:F:30:THR:CG2	7:J:-13:DA:C5'	2.54	0.85
7:J:20:DG:H5"	8:M:496:LEU:CD2	2.06	0.85
2:B:26:ILE:CD1	2:B:59:LYS:HD3	2.06	0.85
6:I:-4:DC:N3	7:J:4:DG:N2	2.24	0.85
7:J:-28:DC:C5	7:J:-27:DC:N4	2.44	0.85
1:A:63:ARG:CZ	7:J:17:DA:C4'	2.55	0.85
6:I:-58:DG:C2	7:J:58:DG:N1	2.45	0.85
7:J:23:DG:C8	7:J:24:DC:H5	1.95	0.85
6:I:21:DC:C4	6:I:22:DC:N4	2.44	0.85
5:G:15:LYS:HZ2	6:I:46:DA:H4'	1.02	0.85
7:J:58:DG:H2"	7:J:59:DC:C5	2.12	0.84
8:W:720:MET:SD	8:W:721:VAL:N	2.49	0.84
1:A:89:VAL:HG12	1:A:90:MET:CE	2.07	0.84
7:J:34:DC:C2'	7:J:35:DT:C6	2.60	0.84
2:F:44:LYS:O	6:I:8:DC:H5"	1.77	0.84
6:I:34:DT:C2'	6:I:35:DC:C6	2.57	0.84
7:J:-25:DC:H2"	7:J:-24:DT:C5	2.12	0.84
7:J:4:DG:C2'	7:J:5:DT:C6	2.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:307:TYR:HD2	8:W:327:ILE:HD13	1.41	0.84
8:W:551:GLU:O	8:W:555:LEU:HD13	1.77	0.84
8:W:681:MET:SD	8:W:682:THR:N	2.50	0.84
8:W:182:VAL:HG11	8:W:245:TYR:CD2	2.13	0.84
8:W:436:THR:O	8:W:440:TRP:HD1	1.59	0.84
8:W:1059:ALA:HB2	8:W:1132:LEU:HD21	1.58	0.84
1:A:85:GLN:CA	6:I:-24:DG:OP2	2.25	0.84
6:I:-18:DC:H5"	8:M:434:LEU:HD11	1.57	0.84
6:I:-13:DA:N6	7:J:12:DG:O6	2.10	0.84
8:W:793:TRP:O	8:W:794:ASN:HB2	1.75	0.84
3:C:39:TYR:CZ	4:D:71:ALA:HB1	2.12	0.84
2:F:32:PRO:HG2	7:J:-13:DA:H2'	1.59	0.84
6:I:-19:DG:H2"	6:I:-18:DC:C5	2.13	0.84
7:J:-16:DT:OP2	8:W:497:LYS:HD3	1.78	0.84
7:J:-11:DC:C6	7:J:-10:DG:N7	2.45	0.84
7:J:37:DC:C2	7:J:38:DG:N7	2.46	0.84
7:J:51:DG:C5	7:J:52:DC:C4	2.65	0.84
1:A:85:GLN:CA	6:I:-24:DG:O5'	2.23	0.84
6:I:-30:DG:C5	6:I:-29:DC:C4	2.66	0.84
7:J:19:DC:H2"	7:J:20:DG:N7	1.92	0.84
8:W:457:MET:HG3	8:W:457:MET:O	1.77	0.84
8:W:1132:LEU:HD12	8:W:1133:LEU:N	1.93	0.84
8:W:524:SER:O	8:W:528:SER:HB2	1.77	0.84
2:B:58:LEU:HD23	2:B:62:LEU:CD1	2.07	0.84
4:D:28:LYS:HZ2	7:J:51:DG:H5"	1.42	0.84
7:J:19:DC:C2'	7:J:20:DG:N7	2.41	0.84
1:E:63:ARG:NE	7:J:-13:DA:C5'	2.27	0.83
8:W:207:CYS:HA	8:W:211:TYR:CD2	2.13	0.83
1:E:117:VAL:CG2	7:J:-4:DG:H5"	2.08	0.83
8:W:609:LYS:HD2	8:W:814:VAL:HG11	1.60	0.83
6:I:-66:DA:H2"	6:I:-65:DT:C7	2.08	0.83
6:I:-19:DG:H3'	8:M:743:GLY:HA3	1.59	0.83
6:I:20:DG:O3'	8:W:524:SER:OG	1.92	0.83
7:J:30:DC:H2"	7:J:31:DT:O5'	1.78	0.83
8:W:723:MET:HE3	8:W:789:PHE:CE2	2.14	0.83
2:B:58:LEU:HD23	2:B:62:LEU:HD11	1.57	0.83
6:I:-19:DG:C3'	8:M:743:GLY:HA3	2.09	0.83
8:W:502:LEU:O	8:W:507:TRP:CZ3	2.32	0.83
1:A:43:PRO:HB2	6:I:-5:DA:H5"	1.59	0.83
8:W:481:LYS:HD2	8:W:483:MET:HE1	1.58	0.83
4:H:113:LYS:O	4:H:117:LYS:HG3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:806:HIS:ND1	8:W:814:VAL:HG21	1.93	0.83
3:C:31:HIS:HB2	3:C:48:PRO:HB3	1.61	0.83
7:J:13:DT:P	8:M:241:ARG:HG2	2.18	0.83
7:J:21:DG:C4'	8:M:517:ARG:NH2	2.25	0.83
2:F:30:THR:HG21	7:J:-13:DA:H5"	1.59	0.82
7:J:24:DC:H2'	7:J:25:DT:H71	1.61	0.82
8:W:387:MET:HE3	8:W:538:MET:HE2	1.61	0.82
3:C:45:ALA:N	7:J:38:DG:OP1	2.12	0.82
1:A:88:ALA:CA	2:B:83:ALA:HB2	2.09	0.82
4:D:28:LYS:NZ	7:J:51:DG:O5'	2.12	0.82
6:I:-20:DC:H2"	6:I:-19:DG:C8	2.14	0.82
8:W:591:GLN:HG3	8:W:592:PRO:HD3	1.60	0.82
5:G:42:ARG:HB3	6:I:38:DT:H4'	1.61	0.82
6:I:27:DG:H2"	6:I:28:DG:C8	2.15	0.82
1:A:116:ARG:HH11	1:A:120:MET:HG2	1.42	0.82
6:I:-52:DG:H2"	6:I:-51:DC:O5'	1.79	0.82
7:J:67:DT:H2"	7:J:68:DT:C5	2.14	0.82
2:F:88:TYR:OH	4:H:80:TYR:CE1	2.32	0.82
6:I:-57:DC:H2"	6:I:-56:DC:C5	2.14	0.82
8:W:1143:LYS:HD3	8:W:1187:PHE:CE1	2.14	0.82
7:J:-32:DT:H2"	7:J:-31:DA:H8	1.43	0.82
8:W:1150:TYR:CE2	8:W:1157:PHE:HA	2.15	0.82
2:F:48:GLY:HA2	2:F:51:TYR:HE2	1.44	0.82
3:C:26:PRO:HG3	4:D:37:TYR:CE2	2.15	0.82
1:E:134:ARG:NH1	1:E:135:ALA:HB3	1.95	0.82
6:I:-23:DC:C4	6:I:-22:DA:N7	2.48	0.81
6:I:4:DC:H2"	6:I:5:DC:O5'	1.78	0.81
7:J:17:DA:H2"	7:J:18:DG:C8	2.15	0.81
7:J:24:DC:H2'	7:J:25:DT:C7	2.09	0.81
8:W:345:LYS:CB	8:W:1036:ALA:HB1	1.99	0.81
8:W:345:LYS:HB2	8:W:1036:ALA:CB	2.09	0.81
2:F:30:THR:CG2	7:J:-13:DA:H5"	2.09	0.81
7:J:20:DG:C4'	8:M:496:LEU:CD2	2.58	0.81
8:W:348:PRO:HB3	8:W:425:ASN:O	1.80	0.81
8:W:602:VAL:HG13	8:W:808:ILE:HG23	1.61	0.81
8:W:807:ARG:HH22	9:W:1502:ADP:PB	2.03	0.81
1:A:73:GLU:HG3	2:B:22:LEU:O	1.80	0.81
1:A:83:ARG:C	1:A:84:PHE:HD1	1.87	0.81
1:A:83:ARG:HH22	7:J:26:DA:H4'	1.45	0.81
1:A:95:ALA:HB2	2:B:97:LEU:HD11	1.62	0.81
2:F:17:ARG:CA	8:W:722:ARG:HH22	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-86:DA:C6	7:J:87:DT:O4	2.33	0.81
6:I:-19:DG:H2"	6:I:-18:DC:H5	1.43	0.81
7:J:-38:DA:C6	7:J:-37:DG:C6	2.68	0.81
8:W:612:ARG:N	8:W:816:VAL:O	2.13	0.81
2:B:20:LYS:HE2	8:M:666:ASP:OD2	1.78	0.81
2:F:75:HIS:ND1	4:H:93:THR:HG21	1.95	0.81
1:A:85:GLN:CG	6:I:-24:DG:P	2.62	0.81
8:W:1025:GLY:HA3	8:W:1139:LEU:HD21	1.60	0.81
6:I:5:DC:H2"	6:I:6:DC:H5	1.46	0.81
6:I:30:DT:C2	6:I:31:DT:C6	2.68	0.81
2:F:80:THR:OG1	6:I:28:DG:H5"	1.81	0.81
4:H:36:ILE:CD1	6:I:49:DC:P	2.69	0.81
6:I:-18:DC:C4'	8:M:434:LEU:CD2	2.58	0.81
6:I:19:DC:N4	7:J:-19:DG:H22	1.77	0.81
1:E:61:LEU:CD1	2:F:37:LEU:CD1	2.40	0.81
6:I:-12:DC:H2'	6:I:-11:DG:C8	2.16	0.81
8:W:807:ARG:NH2	9:W:1502:ADP:O3B	2.13	0.81
1:A:132:GLY:O	3:C:99:ARG:NH1	2.14	0.81
7:J:4:DG:H2'	7:J:5:DT:C7	2.10	0.80
1:E:103:LEU:O	1:E:107:THR:HG23	1.80	0.80
5:G:51:LEU:HD21	4:H:91:ILE:HG12	1.63	0.80
6:I:-3:DG:C4	6:I:-2:DC:C2	2.68	0.80
5:G:25:PHE:CD2	5:G:52:ALA:O	2.34	0.80
7:J:23:DG:C8	7:J:24:DC:C5	2.70	0.80
7:J:34:DC:H5'	7:J:34:DC:H6	1.45	0.80
8:W:655:LEU:CD2	8:W:825:VAL:HB	2.11	0.80
1:A:76:GLN:OE1	2:B:21:VAL:HA	1.81	0.80
8:W:476:ARG:NH1	8:W:480:LYS:O	2.13	0.80
6:I:-18:DC:H4'	8:M:434:LEU:CD2	2.12	0.80
7:J:-16:DT:OP2	8:W:497:LYS:HG2	1.80	0.80
8:W:348:PRO:CG	8:W:483:MET:HB3	2.10	0.80
8:W:387:MET:CE	8:W:538:MET:HE2	2.12	0.80
1:A:70:LEU:HD13	2:B:25:ASN:CG	2.07	0.80
3:C:100:VAL:HG21	2:F:98:TYR:HE2	1.46	0.80
8:W:1246:VAL:CG1	8:W:1247:PRO:HA	2.11	0.80
6:I:-38:DC:C5	6:I:-37:DG:O6	2.34	0.80
6:I:-38:DC:N4	6:I:-37:DG:O6	2.15	0.80
8:W:345:LYS:HB2	8:W:1036:ALA:HB3	1.64	0.80
1:E:42:ARG:H	1:E:43:PRO:HD2	1.45	0.80
8:W:315:ASN:HD21	8:W:458:GLY:HA2	1.47	0.80
8:W:794:ASN:OD1	8:W:795:PRO:CD	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:1119:PHE:HE2	8:W:1129:ALA:HB2	1.46	0.80
3:C:25:PHE:CG	3:C:26:PRO:HD2	2.16	0.80
6:I:-35:DA:C5	6:I:-34:DG:C5	2.69	0.80
6:I:-3:DG:H2'	6:I:-2:DC:H5	1.41	0.80
7:J:4:DG:H2"	7:J:5:DT:C6	2.17	0.80
8:W:713:ARG:HA	8:W:765:PHE:HB2	1.64	0.80
2:B:90:LEU:CD1	2:B:97:LEU:HD11	2.12	0.79
7:J:26:DA:N9	7:J:27:DG:C5	2.51	0.79
8:W:429:ILE:HG23	8:W:510:MET:SD	2.22	0.79
8:W:663:TYR:OH	8:W:672:VAL:HG11	1.81	0.79
8:W:429:ILE:HB	8:W:507:TRP:CD1	2.18	0.79
8:W:1039:THR:HG22	8:W:1040:LEU:HD12	1.62	0.79
1:A:43:PRO:HG2	6:I:-5:DA:H5'	1.62	0.79
8:W:254:GLN:HA	8:W:258:LEU:HB2	1.64	0.79
8:W:433:PRO:CD	8:W:513:ASP:HB3	2.13	0.79
8:W:607:PRO:HB2	8:W:813:HIS:CA	2.11	0.79
3:C:79:ILE:HG23	3:C:80:PRO:CD	2.11	0.79
7:J:-8:DG:H2"	7:J:-7:DG:C8	2.18	0.79
3:C:110:ASN:O	3:C:111:ILE:HD13	1.82	0.79
5:G:51:LEU:HD21	4:H:91:ILE:CG2	2.13	0.79
5:G:50:TYR:O	5:G:54:VAL:HG23	1.83	0.79
4:H:51:ILE:HD13	4:H:56:MET:CE	2.13	0.79
6:I:-76:DG:C2	7:J:76:DG:N2	2.50	0.79
2:B:45:ARG:HB3	7:J:8:DG:OP1	1.83	0.79
1:E:122:LYS:O	1:E:125:GLN:N	2.14	0.79
6:I:-35:DA:N7	6:I:-34:DG:O6	2.15	0.79
8:W:390:LEU:CD1	8:W:393:LYS:CD	2.53	0.79
8:W:615:ARG:HB3	8:W:822:LYS:CD	2.05	0.79
3:C:32:ARG:CD	6:I:-44:DA:P	2.71	0.79
6:I:-38:DC:H2"	6:I:-37:DG:OP2	1.81	0.79
8:W:177:HIS:CE1	8:W:217:TRP:CE2	2.71	0.79
7:J:19:DC:C5	7:J:20:DG:C6	2.71	0.79
8:W:606:LEU:C	8:W:606:LEU:HD12	2.08	0.79
8:W:518:LEU:HD13	8:W:555:LEU:HD12	1.66	0.78
3:C:32:ARG:CD	6:I:-44:DA:OP2	2.31	0.78
8:W:398:ILE:HG23	8:W:539:LEU:CD1	2.10	0.78
8:W:645:HIS:CE1	8:W:649:LEU:CD1	2.66	0.78
3:C:44:GLY:HA3	4:D:87:THR:HA	1.64	0.78
6:I:-78:DC:N4	7:J:78:DG:H1	1.80	0.78
7:J:20:DG:H3'	8:M:496:LEU:CD2	2.13	0.78
8:W:624:GLU:OE1	8:W:625:TYR:CD1	2.36	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ARG:HD3	6:I:-44:DA:OP2	1.84	0.78
1:E:84:PHE:O	7:J:-23:DT:OP1	2.00	0.78
2:F:47:SER:O	2:F:50:ILE:HG22	1.84	0.78
5:G:15:LYS:HZ1	6:I:46:DA:C4'	1.81	0.78
7:J:5:DT:H2"	7:J:6:DA:N7	1.98	0.78
8:M:268:GLU:O	8:M:272:MET:HB2	1.84	0.78
8:W:419:ILE:CG2	8:W:451:LEU:HD11	2.11	0.78
8:W:813:HIS:O	8:W:814:VAL:CG2	2.31	0.78
1:E:74:ILE:HG21	2:F:59:LYS:HE3	1.65	0.78
7:J:26:DA:H2"	7:J:27:DG:H8	0.95	0.78
8:W:324:ALA:O	8:W:327:ILE:HG22	1.83	0.78
3:C:44:GLY:N	4:D:86:ILE:O	2.18	0.77
3:C:79:ILE:CG2	3:C:80:PRO:HD2	2.13	0.77
2:F:82:THR:HG22	2:F:84:MET:H	1.47	0.77
1:A:117:VAL:CA	6:I:-3:DG:OP1	2.32	0.77
6:I:-86:DA:N1	7:J:87:DT:O4	2.17	0.77
8:W:391:TRP:CE3	8:W:391:TRP:O	2.38	0.77
8:W:656:LYS:CE	8:W:826:GLU:HA	2.13	0.77
3:C:32:ARG:NH2	6:I:-43:DT:H72	2.00	0.77
1:E:66:PRO:HB2	2:F:29:ILE:CG1	2.15	0.77
1:E:48:LEU:HA	1:E:51:ILE:HD12	1.65	0.77
2:F:75:HIS:HE2	4:H:90:GLU:CD	1.92	0.77
4:H:97:LEU:HD12	4:H:98:LEU:N	1.99	0.77
5:G:31:HIS:CD2	5:G:43:VAL:HG11	2.19	0.77
7:J:20:DG:C5'	8:M:496:LEU:HD23	2.12	0.77
5:G:80:PRO:HG3	4:H:55:ALA:HB2	1.65	0.77
6:I:-80:DG:N2	7:J:82:DG:N2	2.31	0.77
2:B:90:LEU:HD12	2:B:97:LEU:HD11	1.67	0.77
4:D:121:ALA:O	4:D:122:LYS:HB2	1.83	0.77
7:J:67:DT:H2"	7:J:68:DT:H71	1.66	0.77
4:D:28:LYS:HZ2	7:J:51:DG:C5'	1.96	0.77
2:F:32:PRO:HD2	7:J:-13:DA:H3'	1.66	0.77
7:J:-17:DT:C4	7:J:-16:DT:C4	2.73	0.77
7:J:24:DC:OP1	8:M:793:TRP:NE1	2.18	0.77
4:D:84:SER:C	6:I:-34:DG:OP1	2.28	0.77
6:I:7:DC:H42	7:J:-7:DG:H1	1.33	0.77
8:W:379:PHE:HE1	8:W:597:ARG:CD	1.97	0.77
6:I:-49:DG:H1	7:J:49:DC:N4	1.79	0.76
6:I:30:DT:N1	6:I:31:DT:H72	2.00	0.76
8:W:408:THR:HG23	8:W:440:TRP:CE3	2.19	0.76
6:I:32:DA:H1'	6:I:33:DC:H5'	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LEU:HD12	4:D:41:VAL:CG1	2.15	0.76
6:I:-79:DG:C2	7:J:79:DG:N2	2.53	0.76
1:A:65:LEU:CD2	7:J:17:DA:OP2	2.32	0.76
1:A:85:GLN:HB3	6:I:-24:DG:OP2	1.86	0.76
2:F:34:ILE:HD11	2:F:55:ARG:HH11	1.48	0.76
6:I:-12:DC:H42	7:J:11:DC:N4	1.82	0.76
8:W:350:TYR:HE1	8:W:1042:VAL:CG1	1.98	0.76
8:W:474:ASN:HB3	8:W:475:PRO:CD	2.14	0.76
6:I:-68:DG:N2	7:J:69:DC:O2	2.17	0.76
8:W:434:LEU:HD12	8:W:435:SER:N	1.99	0.76
3:C:39:TYR:O	4:D:75:SER:OG	2.01	0.76
8:W:433:PRO:HG2	8:W:514:GLU:OE1	1.85	0.76
3:C:65:LEU:HD23	3:C:90:ASP:OD2	1.85	0.76
1:E:75:ALA:HB1	1:E:82:LEU:CD2	2.15	0.76
7:J:-33:DG:C5	7:J:-32:DT:C4	2.72	0.76
8:W:200:THR:O	8:W:258:LEU:HD13	1.86	0.76
8:W:654:GLU:O	8:W:658:ALA:N	2.19	0.76
8:W:715:LEU:HD21	8:W:780:LEU:HD22	1.67	0.76
8:W:723:MET:HE3	8:W:789:PHE:HE2	1.49	0.76
8:W:508:GLN:HB2	8:W:535:ALA:HB3	1.68	0.76
8:W:607:PRO:C	8:W:813:HIS:HA	2.09	0.76
8:W:654:GLU:O	8:W:657:LYS:N	2.18	0.76
2:B:45:ARG:NE	7:J:8:DG:C5'	2.49	0.76
5:G:84:GLN:NE2	5:G:102:ILE:HG12	2.00	0.76
7:J:78:DG:C6	7:J:79:DG:O6	2.39	0.76
2:B:26:ILE:HD13	2:B:59:LYS:CD	2.14	0.75
8:W:608:SER:N	8:W:813:HIS:HA	2.00	0.75
1:E:89:VAL:HA	1:E:92:LEU:HD12	1.68	0.75
1:A:63:ARG:HE	7:J:17:DA:C5'	1.90	0.75
2:F:45:ARG:HA	6:I:8:DC:P	2.26	0.75
1:A:84:PHE:CE1	2:B:81:VAL:CB	2.66	0.75
1:A:119:ILE:HD11	2:B:46:ILE:HG12	1.68	0.75
6:I:-68:DG:H2"	6:I:-67:DA:C8	2.21	0.75
6:I:-3:DG:C6	6:I:-2:DC:N3	2.53	0.75
7:J:-46:DT:H1'	7:J:-45:DG:C6	2.15	0.75
1:A:89:VAL:HG12	1:A:90:MET:HE2	1.67	0.75
3:C:46:GLY:C	4:D:88:SER:HB3	2.11	0.75
4:D:79:HIS:NE2	5:G:38:ASN:ND2	2.35	0.75
7:J:26:DA:C1'	7:J:27:DG:C8	2.70	0.75
8:W:518:LEU:HD11	8:W:555:LEU:HD12	1.53	0.75
3:C:32:ARG:NH2	6:I:-43:DT:C7	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LEU:HD13	4:D:42:LEU:N	2.02	0.75
5:G:25:PHE:CE1	5:G:56:GLU:HA	2.22	0.75
6:I:-28:DT:C6	6:I:-27:DC:N4	2.55	0.75
8:W:1119:PHE:HE2	8:W:1129:ALA:CB	1.99	0.75
7:J:79:DG:H2"	7:J:80:DC:OP2	1.87	0.75
8:W:376:LEU:HD13	8:W:380:GLN:CB	2.17	0.75
8:W:432:VAL:HG11	8:W:440:TRP:CD1	2.21	0.75
8:W:586:LEU:HG	8:W:590:ILE:HD12	1.69	0.75
3:C:39:TYR:CE2	4:D:71:ALA:HB1	2.21	0.74
6:I:-18:DC:H5"	8:M:434:LEU:CD1	2.16	0.74
8:W:474:ASN:HB2	8:W:475:PRO:CD	2.12	0.74
6:I:30:DT:C2	6:I:31:DT:C5	2.74	0.74
8:W:540:ILE:HD12	8:W:540:ILE:O	1.86	0.74
8:W:617:GLU:CD	8:W:618:LEU:N	2.45	0.74
8:W:638:THR:HB	8:W:667:ASN:HD22	1.51	0.74
8:W:666:ASP:OD1	8:W:667:ASN:N	2.18	0.74
1:A:85:GLN:CB	6:I:-24:DG:OP2	2.35	0.74
3:C:110:ASN:C	3:C:111:ILE:HD13	2.12	0.74
7:J:60:DA:H2"	7:J:61:DC:C6	2.21	0.74
8:W:345:LYS:HE2	8:W:1037:ASP:CA	2.16	0.74
3:C:63:LEU:CD1	4:D:41:VAL:HG12	2.17	0.74
6:I:45:DC:C4	7:J:-46:DT:C4	2.74	0.74
7:J:24:DC:C2'	7:J:25:DT:C5	2.68	0.74
7:J:69:DC:H2"	7:J:70:DT:C5	2.23	0.74
8:W:177:HIS:NE2	8:W:217:TRP:CG	2.55	0.74
8:W:180:ASP:HB2	8:W:218:THR:HA	1.68	0.74
8:W:620:ASP:OD1	8:W:621:VAL:N	2.16	0.74
5:G:83:LEU:CD1	4:H:59:MET:SD	2.76	0.74
6:I:23:DA:H2"	6:I:24:DA:OP2	1.87	0.74
7:J:20:DG:C3'	8:M:496:LEU:CD2	2.64	0.74
8:W:466:ILE:O	8:W:470:GLU:HB2	1.87	0.74
2:B:97:LEU:HD23	5:G:101:THR:CG2	2.18	0.74
1:E:65:LEU:H	1:E:66:PRO:CD	2.01	0.74
6:I:23:DA:H2"	6:I:24:DA:C8	2.23	0.74
6:I:-29:DC:H2"	6:I:-28:DT:O5'	1.88	0.74
7:J:4:DG:H2'	7:J:5:DT:C6	2.21	0.74
8:W:690:LEU:O	8:W:697:MET:SD	2.46	0.74
1:A:73:GLU:OE1	1:A:74:ILE:HD12	1.88	0.74
6:I:-30:DG:N7	6:I:-29:DC:C5	2.56	0.74
6:I:7:DC:H2"	6:I:8:DC:C6	2.22	0.74
8:W:602:VAL:CG1	8:W:808:ILE:HG23	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ALA:CB	4:D:91:ILE:HD11	2.19	0.73
2:F:29:ILE:HG22	2:F:30:THR:N	2.01	0.73
2:B:82:THR:HG22	2:B:84:MET:H	1.52	0.73
2:F:15:ALA:CB	8:W:690:LEU:CD1	2.66	0.73
5:G:88:ARG:O	5:G:94:ASN:ND2	2.21	0.73
6:I:-32:DC:H2"	6:I:-31:DA:C8	2.23	0.73
6:I:-31:DA:H2"	6:I:-30:DG:OP2	1.88	0.73
7:J:-38:DA:H2"	7:J:-37:DG:O5'	1.88	0.73
7:J:14:DT:H2"	7:J:15:DT:C5	2.23	0.73
8:W:624:GLU:OE1	8:W:625:TYR:CE1	2.41	0.73
1:A:117:VAL:HG11	6:I:-4:DC:H5"	1.68	0.73
3:C:28:GLY:O	6:I:-44:DA:H5"	1.87	0.73
3:C:30:VAL:CG1	4:D:67:PHE:HE1	1.96	0.73
2:F:46:ILE:O	6:I:7:DC:C3'	2.35	0.73
8:W:385:ASN:O	8:W:389:PHE:HB2	1.87	0.73
8:W:591:GLN:CG	8:W:592:PRO:HD3	2.17	0.73
3:C:25:PHE:CD1	3:C:26:PRO:HD2	2.24	0.73
3:C:43:VAL:HG12	7:J:38:DG:C3'	2.18	0.73
6:I:5:DC:H1'	6:I:6:DC:C6	2.23	0.73
7:J:-21:DG:C2'	7:J:-20:DC:O5'	2.29	0.73
7:J:4:DG:H2"	7:J:5:DT:H6	1.52	0.73
7:J:38:DG:C2	7:J:39:DA:C4	2.77	0.73
6:I:23:DA:H2"	6:I:24:DA:H8	1.52	0.73
8:W:178:GLY:O	8:W:218:THR:OG1	2.05	0.73
8:W:613:ILE:O	8:W:614:LEU:HD12	1.87	0.73
3:C:34:LEU:HD23	3:C:39:TYR:CE2	2.19	0.73
2:F:80:THR:OG1	6:I:28:DG:C5'	2.35	0.73
1:E:65:LEU:CB	6:I:17:DA:H3'	2.18	0.73
1:E:84:PHE:O	7:J:-23:DT:P	2.47	0.73
6:I:-82:DG:N2	7:J:84:DG:C2	2.56	0.73
8:W:298:LEU:HD11	8:W:304:GLN:HG2	1.70	0.73
8:W:481:LYS:HD3	8:W:483:MET:HE1	1.68	0.73
2:B:79:LYS:O	2:B:81:VAL:N	2.22	0.73
8:W:607:PRO:HD3	8:W:811:LYS:HA	1.68	0.73
8:W:807:ARG:NH2	9:W:1502:ADP:PB	2.62	0.73
1:A:73:GLU:HG3	2:B:25:ASN:ND2	2.03	0.73
7:J:61:DC:H2"	7:J:62:DC:H5"	1.71	0.73
4:D:91:ILE:O	4:D:95:VAL:HG23	1.88	0.73
2:F:48:GLY:HA2	2:F:51:TYR:CE2	2.23	0.73
8:W:348:PRO:HG2	8:W:483:MET:CB	2.18	0.73
8:W:656:LYS:HE3	8:W:829:VAL:HG23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:1039:THR:HG22	8:W:1040:LEU:CD1	2.19	0.73
6:I:-23:DC:H42	6:I:-22:DA:N6	1.87	0.72
6:I:-4:DC:N4	7:J:4:DG:H1	1.86	0.72
7:J:50:DG:H2"	7:J:51:DG:OP2	1.88	0.72
8:W:354:TYR:CE2	8:W:359:PRO:HG3	2.23	0.72
8:W:1146:ILE:HG13	8:W:1150:TYR:HB2	1.71	0.72
1:A:58:THR:HB	5:G:104:GLN:HB3	1.71	0.72
4:D:46:HIS:HB3	4:D:49:THR:OG1	1.89	0.72
1:A:95:ALA:CB	2:B:90:LEU:HD11	2.18	0.72
1:A:124:ILE:HD12	2:B:50:ILE:HG21	1.72	0.72
8:W:795:PRO:HG3	8:W:836:LYS:HB2	1.72	0.72
8:W:1119:PHE:HE2	8:W:1129:ALA:CA	2.02	0.72
1:A:100:LEU:HD23	2:B:37:LEU:CD1	2.19	0.72
4:D:83:ARG:HE	6:I:-34:DG:H2"	1.54	0.72
8:M:417:TRP:O	8:M:421:ALA:HB3	1.88	0.72
2:B:66:ILE:O	2:B:70:VAL:HG23	1.90	0.72
7:J:-30:DA:C8	7:J:-29:DT:C7	2.72	0.72
1:A:41:TYR:HB3	1:A:45:THR:CG2	2.19	0.72
1:A:42:ARG:O	1:A:45:THR:HG22	1.89	0.72
2:B:63:GLU:O	2:B:66:ILE:HG13	1.90	0.72
4:H:51:ILE:CD1	4:H:56:MET:HE3	2.19	0.72
8:W:608:SER:O	8:W:814:VAL:N	2.23	0.72
5:G:96:LEU:HD12	4:H:100:PRO:HD3	1.70	0.72
5:G:97:LEU:HB3	5:G:100:VAL:CG2	2.20	0.72
2:F:47:SER:HA	6:I:7:DC:P	2.29	0.72
7:J:26:DA:C5	7:J:27:DG:O6	2.36	0.72
7:J:42:DA:C2'	7:J:43:DA:O5'	2.33	0.72
6:I:5:DC:H1'	6:I:6:DC:C5	2.25	0.72
7:J:26:DA:C8	7:J:27:DG:O6	2.43	0.72
3:C:79:ILE:HG12	4:D:52:SER:CB	2.20	0.71
5:G:24:GLN:O	4:H:37:TYR:CD2	2.43	0.71
7:J:-21:DG:C5	7:J:-20:DC:C4	2.77	0.71
6:I:-79:DG:N2	7:J:79:DG:N2	2.38	0.71
7:J:26:DA:C4	7:J:27:DG:C5	2.77	0.71
8:W:470:GLU:HG2	8:W:485:PHE:HE2	1.50	0.71
8:W:518:LEU:CD1	8:W:555:LEU:HD11	2.20	0.71
3:C:65:LEU:HD22	3:C:90:ASP:OD2	1.90	0.71
1:E:117:VAL:HG22	7:J:-4:DG:H5"	1.72	0.71
6:I:-25:DA:H1'	6:I:-24:DG:C8	2.25	0.71
7:J:15:DT:O2	7:J:16:DA:C5	2.43	0.71
8:W:781:MET:HE1	9:W:1502:ADP:H4'	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:HIS:O	3:C:35:ARG:HG3	1.89	0.71
2:F:84:MET:CE	2:F:101:GLY:O	2.39	0.71
5:G:84:GLN:HE21	5:G:102:ILE:CG1	2.01	0.71
5:G:91:GLU:O	5:G:95:LYS:HD2	1.91	0.71
8:W:616:VAL:CG1	8:W:695:GLY:HA3	2.21	0.71
3:C:80:PRO:HD3	4:D:55:ALA:HB2	1.71	0.71
5:G:43:VAL:N	6:I:39:DA:P	2.47	0.71
6:I:-82:DG:N2	7:J:84:DG:N2	2.37	0.71
1:A:116:ARG:HD3	6:I:-3:DG:H3'	1.71	0.71
1:A:117:VAL:N	6:I:-3:DG:OP1	2.24	0.71
4:D:89:ARG:O	4:D:92:GLN:HB3	1.91	0.71
1:E:62:ILE:HD13	2:F:33:ALA:O	1.89	0.71
2:F:35:ARG:HH21	2:F:39:ARG:HH22	1.37	0.71
6:I:-17:DT:P	8:M:493:GLU:OE2	2.49	0.71
7:J:-26:DC:H2"	7:J:-25:DC:C6	2.26	0.71
7:J:78:DG:C5	7:J:79:DG:C6	2.79	0.71
8:W:607:PRO:CG	8:W:811:LYS:C	2.55	0.71
2:B:36:ARG:NH2	6:I:-13:DA:OP2	2.24	0.71
5:G:25:PHE:CZ	5:G:56:GLU:HA	2.25	0.71
6:I:45:DC:H4'	6:I:46:DA:O4'	1.90	0.71
7:J:-11:DC:H2"	7:J:-10:DG:O4'	1.90	0.71
2:F:17:ARG:CB	8:W:722:ARG:HH22	2.02	0.71
2:F:88:TYR:HH	4:H:80:TYR:HE1	1.31	0.71
5:G:26:PRO:HD3	4:H:37:TYR:CD2	2.25	0.71
5:G:34:LEU:HD23	4:H:67:PHE:HZ	1.54	0.71
7:J:20:DG:C5'	8:M:496:LEU:CD2	2.69	0.71
1:E:61:LEU:HD12	2:F:37:LEU:HD13	1.67	0.71
1:A:95:ALA:CB	2:B:90:LEU:CD1	2.69	0.70
3:C:42:ARG:HB3	7:J:38:DG:H4'	1.72	0.70
8:W:429:ILE:CG2	8:W:510:MET:SD	2.78	0.70
7:J:-38:DA:C8	7:J:-37:DG:N7	2.59	0.70
7:J:19:DC:C6	7:J:20:DG:C6	2.79	0.70
8:W:229:THR:HG22	8:W:230:TYR:N	2.06	0.70
8:W:470:GLU:HG2	8:W:485:PHE:CZ	2.26	0.70
8:W:545:LEU:HD13	8:W:552:LEU:HD13	1.73	0.70
6:I:45:DC:H5"	6:I:46:DA:P	2.31	0.70
7:J:-11:DC:C5	7:J:-10:DG:C5	2.78	0.70
7:J:15:DT:H2"	7:J:16:DA:C8	2.26	0.70
7:J:26:DA:C4	7:J:27:DG:C6	2.79	0.70
8:W:740:ARG:HB2	8:W:768:LEU:HD11	1.74	0.70
5:G:47:ALA:N	5:G:48:PRO:CD	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-6:DT:C2'	6:I:-5:DA:N7	2.54	0.70
6:I:0:DC:H2'	6:I:1:DT:H72	1.72	0.70
8:W:616:VAL:HG22	8:W:699:LEU:HD12	1.74	0.70
6:I:-35:DA:C6	6:I:-34:DG:C6	2.80	0.70
7:J:-46:DT:C2'	7:J:-45:DG:O6	2.34	0.70
7:J:34:DC:H2'	7:J:35:DT:C5	2.27	0.70
8:W:388:ALA:N	8:W:414:PHE:HE1	1.89	0.70
8:W:627:LYS:O	8:W:630:LEU:HG	1.91	0.70
8:W:768:LEU:HD12	8:W:768:LEU:O	1.91	0.70
8:W:179:ILE:HD13	8:W:217:TRP:CZ3	2.26	0.70
3:C:45:ALA:HB2	7:J:38:DG:OP1	1.90	0.70
6:I:-22:DA:C5	6:I:-21:DC:N4	2.59	0.70
7:J:84:DG:H2"	7:J:85:DT:C5	2.27	0.70
1:E:46:VAL:HG12	1:E:50:GLU:HG3	1.74	0.70
6:I:45:DC:N4	7:J:-46:DT:C4	2.59	0.70
7:J:-25:DC:C2	7:J:-24:DT:C4	2.80	0.70
7:J:-11:DC:C6	7:J:-10:DG:C8	2.80	0.70
5:G:97:LEU:HD22	5:G:100:VAL:HG11	1.74	0.70
6:I:-28:DT:C6	6:I:-27:DC:C4	2.80	0.70
7:J:-7:DG:H2"	7:J:-6:DG:N7	2.06	0.70
2:F:46:ILE:O	6:I:7:DC:C5'	2.39	0.69
5:G:25:PHE:HB3	5:G:52:ALA:HB1	1.74	0.69
5:G:65:LEU:HD12	5:G:68:ASN:HB2	1.72	0.69
8:W:660:ASN:CB	8:W:696:LYS:HZ2	2.04	0.69
6:I:-30:DG:H2"	6:I:-29:DC:OP2	1.92	0.69
6:I:30:DT:H2'	6:I:31:DT:H73	1.74	0.69
7:J:30:DC:C4	7:J:31:DT:C4	2.79	0.69
8:M:256:VAL:HG12	8:M:257:ARG:HG3	1.74	0.69
8:W:474:ASN:HB3	8:W:475:PRO:HD3	1.74	0.69
2:F:88:TYR:OH	4:H:80:TYR:HE1	1.73	0.69
6:I:-86:DA:C2	7:J:87:DT:C2	2.79	0.69
6:I:24:DA:H2"	6:I:25:DG:N7	2.06	0.69
7:J:-11:DC:C4	7:J:-10:DG:O6	2.30	0.69
8:W:357:GLN:HG3	8:W:358:ARG:H	1.58	0.69
1:A:83:ARG:HH12	7:J:26:DA:C4'	2.04	0.69
8:W:398:ILE:CG2	8:W:539:LEU:HD11	2.13	0.69
8:W:602:VAL:HG12	8:W:808:ILE:HD12	1.73	0.69
2:B:96:THR:O	5:G:101:THR:HG22	1.93	0.69
3:C:41:GLU:OE1	6:I:-35:DA:H5"	1.91	0.69
6:I:-58:DG:H2"	6:I:-57:DC:C5	2.28	0.69
8:W:602:VAL:CG1	8:W:808:ILE:HD12	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:HA	6:I:-24:DG:OP2	1.90	0.69
2:F:48:GLY:O	2:F:51:TYR:CE2	2.46	0.69
8:W:328:VAL:HG21	8:W:1201:PRO:HB2	1.74	0.69
8:W:380:GLN:O	8:W:384:ILE:HG13	1.93	0.69
8:W:656:LYS:HA	8:W:825:VAL:HG13	1.74	0.69
1:A:113:HIS:HB2	1:E:126:LEU:HD21	1.75	0.69
7:J:38:DG:N2	7:J:39:DA:N3	2.40	0.69
4:D:109:SER:O	4:D:112:THR:HG22	1.92	0.69
4:H:30:ARG:HG2	4:H:32:GLU:OE2	1.92	0.69
6:I:-37:DG:H4'	6:I:-36:DT:OP1	1.92	0.69
8:W:184:ASN:OD1	8:W:185:HIS:N	2.25	0.69
8:W:431:VAL:O	8:W:431:VAL:HG13	1.92	0.69
8:W:1014:VAL:HG12	8:W:1124:VAL:CG2	2.23	0.69
1:A:83:ARG:NH2	7:J:26:DA:H4'	2.07	0.69
4:D:84:SER:OG	6:I:-34:DG:P	2.51	0.69
5:G:24:GLN:CD	4:H:41:VAL:HG12	2.18	0.69
5:G:34:LEU:HD23	4:H:67:PHE:CZ	2.28	0.69
5:G:51:LEU:CD2	4:H:91:ILE:CG2	2.65	0.69
8:W:215:ILE:HD12	8:W:228:GLU:HB2	1.74	0.69
8:W:616:VAL:CG2	8:W:699:LEU:HD12	2.22	0.69
2:B:98:TYR:HE1	4:H:62:PHE:CA	2.04	0.69
4:D:51:ILE:O	4:D:51:ILE:HD12	1.93	0.68
4:D:77:LEU:HD12	4:D:78:ALA:N	2.08	0.68
6:I:-84:DA:H2"	6:I:-83:DC:C5	2.28	0.68
6:I:-74:DC:H1'	6:I:-73:DC:H5'	1.74	0.68
6:I:9:DG:C5	6:I:10:DC:C4	2.81	0.68
8:M:385:ASN:O	8:M:389:PHE:HB2	1.92	0.68
8:W:656:LYS:HE2	8:W:826:GLU:CA	2.23	0.68
7:J:34:DC:C2'	7:J:35:DT:O5'	2.41	0.68
8:W:482:THR:O	8:W:483:MET:HB2	1.91	0.68
7:J:-17:DT:C6	7:J:-16:DT:C4	2.81	0.68
8:W:532:PHE:O	8:W:533:LYS:C	2.33	0.68
8:W:181:ILE:HG22	8:W:182:VAL:N	2.08	0.68
8:W:263:THR:HG22	8:W:264:ALA:H	1.59	0.68
8:W:473:THR:OG1	8:W:476:ARG:NH2	2.26	0.68
8:W:1192:GLY:HA2	8:W:1194:TRP:CH2	2.28	0.68
1:A:104:PHE:CD2	2:B:38:ALA:HA	2.28	0.68
2:F:84:MET:HE1	2:F:101:GLY:O	1.94	0.68
6:I:43:DT:C2'	6:I:44:DC:O5'	2.31	0.68
8:W:575:GLN:HB2	8:W:578:GLU:HB2	1.74	0.68
4:H:38:VAL:O	4:H:42:LEU:HG	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:114:ALA:HA	4:H:117:LYS:HD2	1.74	0.68
1:A:47:ALA:O	1:A:51:ILE:HG13	1.92	0.68
3:C:116:LEU:CD1	3:C:118:LYS:HB2	2.24	0.68
2:F:30:THR:OG1	2:F:33:ALA:HB2	1.94	0.68
8:W:1143:LYS:HA	8:W:1187:PHE:HE1	1.57	0.68
8:W:189:THR:OG1	8:W:210:ASN:OD1	2.11	0.68
8:W:655:LEU:HD23	8:W:825:VAL:HB	1.75	0.68
2:B:90:LEU:HD12	2:B:97:LEU:CD1	2.23	0.68
3:C:46:GLY:HA3	4:D:88:SER:CB	2.24	0.68
3:C:77:ARG:HB2	6:I:-55:DG:P	2.33	0.68
1:E:65:LEU:CB	6:I:17:DA:O5'	2.36	0.68
6:I:-43:DT:C4	6:I:-42:DT:O4	2.46	0.68
7:J:-33:DG:H2"	7:J:-32:DT:H5'	1.76	0.68
8:W:347:LEU:HB3	8:W:348:PRO:HD2	1.76	0.68
7:J:17:DA:H2"	7:J:18:DG:H8	1.58	0.67
7:J:33:DT:C2'	7:J:34:DC:H5	2.06	0.67
8:W:377:ARG:NE	8:W:602:VAL:HG23	2.09	0.67
8:W:430:ILE:CG1	8:W:511:ALA:HB3	2.23	0.67
8:W:491:THR:HB	8:W:494:TYR:CD2	2.29	0.67
8:W:607:PRO:CG	8:W:811:LYS:CA	2.72	0.67
8:W:616:VAL:HG22	8:W:699:LEU:CD1	2.24	0.67
8:W:650:ASN:O	8:W:655:LEU:N	2.27	0.67
2:B:68:ASP:OD1	2:B:72:TYR:HE1	1.77	0.67
6:I:-86:DA:H2	7:J:87:DT:C2	2.12	0.67
6:I:-35:DA:C6	6:I:-34:DG:N1	2.61	0.67
7:J:34:DC:C2	7:J:35:DT:C4	2.81	0.67
8:M:1132:SER:O	8:M:1136:ARG:HB2	1.93	0.67
2:F:30:THR:CB	7:J:-13:DA:C5'	2.72	0.67
4:H:95:VAL:HG13	4:H:99:LEU:HD13	1.76	0.67
7:J:-17:DT:C4	7:J:-16:DT:N3	2.62	0.67
7:J:23:DG:C4	7:J:24:DC:C5	2.82	0.67
7:J:51:DG:N7	7:J:52:DC:N4	2.42	0.67
8:W:1039:THR:C	8:W:1040:LEU:HD12	2.20	0.67
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.18	0.67
3:C:34:LEU:HD11	3:C:51:LEU:HD23	1.76	0.67
1:E:42:ARG:N	1:E:43:PRO:CD	2.56	0.67
1:E:63:ARG:HD3	6:I:17:DA:H5"	1.76	0.67
7:J:-25:DC:H2"	7:J:-24:DT:H73	1.73	0.67
8:W:185:HIS:O	8:W:186:ARG:NH1	2.27	0.67
8:W:608:SER:O	8:W:813:HIS:C	2.36	0.67
7:J:-38:DA:N7	7:J:-37:DG:C6	2.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:358:ARG:HD3	8:W:392:SER:O	1.94	0.67
8:W:1205:ILE:HD12	8:W:1208:LYS:HD2	1.77	0.67
2:F:32:PRO:HD3	7:J:-12:DA:OP2	1.95	0.67
7:J:32:DG:H2'	7:J:33:DT:H71	1.70	0.67
8:W:350:TYR:HE1	8:W:1042:VAL:HG13	1.58	0.67
8:W:430:ILE:HG13	8:W:511:ALA:HB3	1.76	0.67
4:D:32:GLU:HG2	7:J:49:DC:H5"	1.75	0.67
4:D:45:VAL:O	4:D:46:HIS:ND1	2.27	0.67
2:F:75:HIS:ND1	4:H:93:THR:CG2	2.58	0.67
6:I:-72:DA:H2"	6:I:-71:DT:H71	1.76	0.67
8:W:284:PHE:O	8:W:311:TRP:CD1	2.47	0.67
8:W:541:THR:HG23	8:W:543:THR:H	1.60	0.67
8:W:654:GLU:O	8:W:655:LEU:C	2.38	0.67
5:G:67:GLY:CA	5:G:78:ILE:HD11	2.23	0.67
4:H:54:LYS:O	4:H:58:ILE:HG13	1.94	0.67
7:J:-11:DC:N3	7:J:-10:DG:C6	2.61	0.67
8:W:419:ILE:CD1	8:W:451:LEU:HD13	2.24	0.67
8:W:660:ASN:OD1	8:W:821:SER:HB2	1.95	0.67
6:I:-28:DT:C2'	6:I:-27:DC:C6	2.78	0.67
7:J:-25:DC:H2'	7:J:-24:DT:C7	2.06	0.67
8:W:307:TYR:CD2	8:W:327:ILE:HD13	2.27	0.67
8:W:738:PHE:O	8:W:739:GLN:OE1	2.13	0.67
2:B:62:LEU:O	2:B:66:ILE:HG23	1.95	0.67
1:E:134:ARG:HH12	1:E:135:ALA:HB3	1.58	0.67
5:G:59:THR:O	5:G:63:LEU:HB2	1.95	0.67
7:J:4:DG:H2'	7:J:5:DT:C5	2.29	0.67
2:F:15:ALA:HB3	8:W:690:LEU:HD11	1.77	0.66
4:D:78:ALA:O	4:D:83:ARG:O	2.13	0.66
7:J:-37:DG:C2'	7:J:-36:DG:C8	2.74	0.66
8:W:415:ILE:HA	8:W:418:LEU:CD2	2.25	0.66
3:C:39:TYR:CZ	4:D:71:ALA:CB	2.78	0.66
2:F:29:ILE:CG2	2:F:30:THR:N	2.57	0.66
6:I:22:DC:H5"	8:W:519:LYS:HB3	1.77	0.66
6:I:23:DA:C2'	6:I:24:DA:C8	2.78	0.66
7:J:-3:DA:H2"	7:J:-2:DC:C6	2.30	0.66
8:W:177:HIS:CE1	8:W:217:TRP:CD2	2.84	0.66
8:W:655:LEU:HD21	8:W:825:VAL:HB	1.76	0.66
8:W:1180:GLU:O	8:W:1183:LEU:HG	1.96	0.66
1:A:100:LEU:CD2	2:B:37:LEU:CD1	2.70	0.66
2:B:45:ARG:CD	7:J:8:DG:H5"	2.23	0.66
3:C:46:GLY:CA	4:D:88:SER:HB3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:GLY:HA2	3:C:78:ILE:HD11	1.77	0.66
5:G:97:LEU:HB3	5:G:100:VAL:HG21	1.77	0.66
6:I:-73:DC:O2	7:J:74:DG:N2	2.28	0.66
8:W:345:LYS:HE2	8:W:1037:ASP:N	2.11	0.66
8:W:656:LYS:CD	8:W:826:GLU:HA	2.24	0.66
3:C:40:ALA:HB3	4:D:86:ILE:HD12	1.74	0.66
5:G:24:GLN:NE2	4:H:44:GLN:OE1	2.29	0.66
8:W:180:ASP:O	8:W:181:ILE:HG13	1.95	0.66
1:E:48:LEU:HB3	1:E:52:ARG:HH12	1.61	0.66
6:I:-3:DG:C1'	6:I:-2:DC:C5	2.79	0.66
1:E:117:VAL:HG21	7:J:-4:DG:H5"	1.78	0.66
5:G:42:ARG:HB3	6:I:38:DT:C4'	2.25	0.66
7:J:34:DC:H2"	7:J:35:DT:C6	2.30	0.66
7:J:34:DC:H2"	7:J:35:DT:H6	1.61	0.66
8:W:177:HIS:HE2	8:W:217:TRP:CG	2.13	0.66
8:W:419:ILE:HD12	8:W:451:LEU:HD13	1.78	0.66
8:W:614:LEU:HB2	8:W:819:LEU:HA	1.77	0.66
8:W:1170:TRP:HE3	8:W:1174:TRP:NE1	1.94	0.66
1:A:60:LEU:HD13	1:A:93:GLN:HG2	1.77	0.65
6:I:5:DC:C1'	6:I:6:DC:C5	2.79	0.65
7:J:-32:DT:C2'	7:J:-31:DA:C8	2.77	0.65
1:E:69:ARG:HB3	2:F:24:ASP:CB	2.26	0.65
5:G:57:TYR:HH	4:H:106:HIS:HD1	1.45	0.65
6:I:-57:DC:H2"	6:I:-56:DC:C6	2.31	0.65
8:W:525:LEU:HA	8:W:528:SER:HB3	1.77	0.65
7:J:-38:DA:H2"	7:J:-37:DG:C8	2.31	0.65
7:J:-38:DA:C4	7:J:-37:DG:C6	2.85	0.65
7:J:-37:DG:C4	7:J:-36:DG:C6	2.85	0.65
7:J:-25:DC:C2'	7:J:-24:DT:C5	2.77	0.65
8:W:655:LEU:HD23	8:W:825:VAL:CB	2.26	0.65
8:W:660:ASN:CG	8:W:696:LYS:NZ	2.54	0.65
8:W:1171:SER:HB3	8:W:1245:LYS:HE3	1.77	0.65
7:J:14:DT:H2"	7:J:15:DT:H73	1.78	0.65
8:W:315:ASN:ND2	8:W:458:GLY:HA2	2.11	0.65
8:W:471:PHE:CE1	8:W:481:LYS:HE2	2.24	0.65
8:W:611:GLU:CG	8:W:816:VAL:CG1	2.74	0.65
3:C:41:GLU:HB3	4:D:84:SER:O	1.96	0.65
4:D:65:ASP:OD2	2:F:98:TYR:OH	2.12	0.65
4:D:76:ARG:NH2	4:D:80:TYR:OH	2.30	0.65
4:D:116:THR:O	4:D:119:THR:HG22	1.97	0.65
8:W:599:LYS:C	8:W:601:ASP:N	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:606:LEU:HD12	8:W:607:PRO:O	1.96	0.65
8:W:1183:LEU:HD12	8:W:1184:ILE:N	2.11	0.65
4:D:70:ILE:HD13	4:D:98:LEU:CD1	2.27	0.65
4:D:121:ALA:O	4:D:122:LYS:CB	2.44	0.65
6:I:9:DG:N7	6:I:10:DC:N4	2.45	0.65
6:I:37:DC:H42	7:J:-38:DA:N6	1.95	0.65
8:W:223:LEU:HD11	8:W:285:HIS:HA	1.79	0.65
8:W:795:PRO:HG3	8:W:836:LYS:CB	2.26	0.65
3:C:97:LEU:HB3	3:C:100:VAL:CG2	2.27	0.65
5:G:42:ARG:C	6:I:39:DA:OP1	2.38	0.65
7:J:78:DG:C2'	7:J:79:DG:C8	2.79	0.65
8:W:214:LEU:HD21	8:W:225:ASN:HB2	1.77	0.65
8:W:656:LYS:HA	8:W:825:VAL:CG1	2.26	0.65
8:W:1013:GLU:HG2	8:W:1041:PRO:HG2	1.79	0.65
2:B:98:TYR:OH	4:H:65:ASP:HB3	1.97	0.65
2:F:30:THR:HB	7:J:-13:DA:H5"	1.78	0.65
6:I:-73:DC:N3	6:I:-72:DA:N6	2.45	0.65
7:J:-39:DT:H2"	7:J:-38:DA:OP2	1.97	0.65
8:W:290:ILE:O	8:W:341:ARG:NH2	2.29	0.65
8:W:813:HIS:C	8:W:814:VAL:HG23	2.22	0.65
1:A:86:SER:N	6:I:-24:DG:OP2	2.30	0.65
8:W:362:GLU:N	8:W:362:GLU:OE1	2.30	0.65
8:W:508:GLN:OE1	8:W:508:GLN:N	2.30	0.65
8:W:795:PRO:HD3	8:W:836:LYS:HD2	1.79	0.65
2:B:31:LYS:HB3	2:B:32:PRO:HD3	1.79	0.64
7:J:-35:DG:C6	7:J:-34:DA:C6	2.85	0.64
7:J:15:DT:N3	7:J:16:DA:N6	2.44	0.64
7:J:26:DA:N9	7:J:27:DG:N7	2.45	0.64
8:W:391:TRP:HD1	8:W:414:PHE:CZ	2.14	0.64
8:W:437:MET:HE1	8:W:457:MET:SD	2.36	0.64
7:J:-35:DG:C4	7:J:-34:DA:C5	2.86	0.64
1:A:76:GLN:HG3	1:A:80:THR:HG22	1.78	0.64
8:W:654:GLU:OE2	8:W:658:ALA:HB2	1.97	0.64
1:A:88:ALA:HB2	2:B:83:ALA:N	2.13	0.64
8:W:607:PRO:CD	8:W:810:GLN:O	2.45	0.64
8:W:696:LYS:HG2	8:W:819:LEU:HD23	1.80	0.64
8:W:1025:GLY:CA	8:W:1139:LEU:HD21	2.27	0.64
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.07	0.64
8:W:1099:PRO:HG2	8:W:1102:ASN:HB3	1.78	0.64
1:A:63:ARG:NH2	7:J:17:DA:O4'	2.25	0.64
3:C:112:GLN:HE22	1:E:108:ASN:CG	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ALA:O	2:F:77:LYS:CG	2.45	0.64
7:J:-38:DA:C4	7:J:-37:DG:C5	2.86	0.64
8:W:603:GLU:HG2	8:W:603:GLU:O	1.98	0.64
8:W:1143:LYS:HD3	8:W:1187:PHE:CD1	2.32	0.64
1:A:70:LEU:CD1	2:B:25:ASN:CG	2.70	0.64
2:B:68:ASP:OD2	2:B:89:ALA:HA	1.97	0.64
7:J:-17:DT:C4	7:J:-16:DT:O4	2.51	0.64
7:J:14:DT:H2"	7:J:15:DT:H6	1.62	0.64
8:W:720:MET:SD	8:W:720:MET:C	2.79	0.64
8:W:807:ARG:NH2	9:W:1502:ADP:O1B	2.30	0.64
2:B:84:MET:CE	2:B:88:TYR:OH	2.43	0.64
3:C:45:ALA:HB2	7:J:38:DG:P	2.38	0.64
8:W:437:MET:CG	8:W:438:PRO:HD3	2.28	0.64
8:W:650:ASN:HA	8:W:654:GLU:CG	2.26	0.64
2:F:30:THR:CB	7:J:-13:DA:C3'	2.71	0.64
6:I:-80:DG:C8	6:I:-79:DG:C6	2.86	0.64
6:I:-23:DC:H2"	6:I:-22:DA:O5'	1.98	0.64
8:W:317:ASP:OD1	8:W:318:GLU:N	2.31	0.64
1:A:133:GLU:HA	3:C:99:ARG:HH22	1.63	0.63
3:C:97:LEU:CD1	4:D:62:PHE:HE2	2.07	0.63
1:E:47:ALA:N	6:I:9:DG:OP1	2.31	0.63
6:I:-30:DG:N7	6:I:-29:DC:N4	2.46	0.63
7:J:-38:DA:C2'	7:J:-37:DG:C8	2.81	0.63
7:J:19:DC:H2'	7:J:20:DG:N7	2.11	0.63
8:W:371:ILE:HG13	8:W:371:ILE:O	1.98	0.63
8:W:387:MET:CB	8:W:414:PHE:CE1	2.80	0.63
8:W:656:LYS:HD2	8:W:826:GLU:HA	1.80	0.63
3:C:34:LEU:CD2	3:C:39:TYR:CZ	2.82	0.63
5:G:42:ARG:HG2	6:I:39:DA:H5'	1.80	0.63
6:I:-52:DG:C2'	6:I:-51:DC:O5'	2.46	0.63
6:I:-35:DA:C8	6:I:-34:DG:C8	2.85	0.63
6:I:23:DA:C5	6:I:24:DA:C6	2.87	0.63
3:C:112:GLN:NE2	1:E:108:ASN:CG	2.56	0.63
7:J:6:DA:H8	7:J:6:DA:OP2	1.80	0.63
8:W:293:SER:HB3	8:W:307:TYR:CD1	2.33	0.63
8:W:510:MET:O	8:W:538:MET:HB3	1.98	0.63
1:A:84:PHE:O	6:I:-24:DG:H3'	1.98	0.63
2:B:26:ILE:CD1	2:B:59:LYS:CD	2.76	0.63
7:J:21:DG:OP1	8:M:496:LEU:HD22	1.98	0.63
8:W:643:GLY:HA2	8:W:646:PHE:CE2	2.33	0.63
8:W:1104:LEU:HD12	8:W:1105:THR:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:O	1:A:50:GLU:HG3	1.98	0.63
3:C:100:VAL:HG21	2:F:98:TYR:CE2	2.33	0.63
6:I:-59:DT:C2	6:I:-58:DG:C2	2.86	0.63
7:J:-17:DT:H2'	7:J:-16:DT:C6	2.34	0.63
8:W:387:MET:C	8:W:414:PHE:CE1	2.76	0.63
8:W:612:ARG:O	8:W:817:TYR:HA	1.97	0.63
7:J:23:DG:H2"	7:J:24:DC:O5'	1.99	0.63
8:M:1068:GLU:HG2	8:M:1071:ARG:HH22	1.64	0.63
1:A:63:ARG:NH1	7:J:17:DA:H5'	2.05	0.63
2:B:98:TYR:OH	4:H:65:ASP:CG	2.42	0.63
6:I:-80:DG:H22	7:J:82:DG:N2	1.95	0.63
6:I:30:DT:H2'	6:I:31:DT:C7	2.29	0.63
8:W:402:GLU:CD	8:W:403:MET:N	2.56	0.63
6:I:-12:DC:N3	6:I:-11:DG:C6	2.67	0.63
8:W:674:GLN:OE1	8:W:674:GLN:N	2.32	0.63
2:B:98:TYR:OH	4:H:65:ASP:CB	2.47	0.62
3:C:47:ALA:HB1	4:D:91:ILE:HD11	1.81	0.62
5:G:26:PRO:HB3	4:H:37:TYR:CZ	2.35	0.62
6:I:-17:DT:H5'	8:M:493:GLU:CD	2.24	0.62
8:W:607:PRO:CG	8:W:811:LYS:HA	2.27	0.62
8:W:1098:GLN:OE1	8:W:1104:LEU:HD21	1.99	0.62
1:A:63:ARG:CZ	7:J:17:DA:H5"	2.17	0.62
3:C:63:LEU:HD22	4:D:42:LEU:HB2	1.81	0.62
3:C:112:GLN:HE22	1:E:108:ASN:ND2	1.97	0.62
1:E:61:LEU:HD13	2:F:37:LEU:HA	0.70	0.62
5:G:15:LYS:HZ2	6:I:46:DA:C4'	1.91	0.62
6:I:-23:DC:C4	6:I:-22:DA:C5	2.88	0.62
7:J:78:DG:C5	7:J:79:DG:C5	2.87	0.62
8:W:481:LYS:HG3	8:W:483:MET:HE3	0.71	0.62
8:W:599:LYS:O	8:W:600:LYS:C	2.43	0.62
8:W:660:ASN:CB	8:W:696:LYS:NZ	2.61	0.62
8:W:1070:ARG:NH2	8:W:1113:GLU:HG2	2.14	0.62
1:A:63:ARG:CZ	7:J:17:DA:H4'	2.22	0.62
2:F:44:LYS:O	6:I:8:DC:C5'	2.47	0.62
5:G:42:ARG:CG	6:I:39:DA:H5'	2.29	0.62
6:I:24:DA:C2'	6:I:25:DG:C8	2.82	0.62
6:I:30:DT:C4	6:I:31:DT:C4	2.87	0.62
7:J:20:DG:H3'	8:M:496:LEU:HD21	1.81	0.62
8:W:348:PRO:HG2	8:W:483:MET:CG	2.29	0.62
2:B:59:LYS:O	2:B:63:GLU:HG3	1.99	0.62
1:A:52:ARG:HD2	5:G:111:ILE:HD11	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:ARG:O	3:C:85:LEU:CG	2.47	0.62
2:F:30:THR:OG1	7:J:-13:DA:H5"	1.98	0.62
8:W:556:VAL:HG22	8:W:593:PHE:HE2	1.63	0.62
8:W:730:TYR:CD2	8:W:731:LEU:HD12	2.34	0.62
2:B:52:GLU:OE1	2:B:52:GLU:N	2.30	0.62
6:I:-6:DT:C6	6:I:-5:DA:N6	2.68	0.62
8:W:207:CYS:HG	8:W:246:CYS:HG	1.36	0.62
5:G:116:LEU:HD12	5:G:117:PRO:HD3	1.80	0.62
7:J:-30:DA:C8	7:J:-29:DT:H73	2.34	0.62
8:M:435:SER:O	8:M:751:ARG:NH2	2.33	0.62
1:E:48:LEU:HB3	1:E:52:ARG:NH1	2.15	0.62
6:I:5:DC:H2"	6:I:6:DC:C6	2.32	0.62
7:J:13:DT:OP2	8:M:241:ARG:NE	2.32	0.62
7:J:24:DC:OP1	8:M:793:TRP:HD1	1.78	0.62
7:J:43:DA:H2"	7:J:44:DT:OP2	1.99	0.62
8:M:580:GLU:O	8:M:584:HIS:HB2	2.00	0.62
8:W:488:LEU:CD2	8:W:490:THR:HG22	2.30	0.62
1:A:83:ARG:HB2	2:B:80:THR:OG1	1.98	0.62
3:C:40:ALA:CB	4:D:86:ILE:HD13	2.25	0.62
4:D:46:HIS:CB	4:D:49:THR:OG1	2.47	0.62
6:I:23:DA:C4	6:I:24:DA:C5	2.88	0.62
7:J:-38:DA:C6	7:J:-37:DG:N1	2.68	0.62
7:J:-11:DC:N3	7:J:-10:DG:C5	2.68	0.62
8:W:181:ILE:CG2	8:W:182:VAL:N	2.63	0.62
8:W:241:ARG:O	8:W:244:ASN:OD1	2.18	0.62
8:W:414:PHE:O	8:W:418:LEU:HD23	2.00	0.62
8:W:1023:LYS:HZ2	8:W:1024:PHE:HE1	1.48	0.62
1:A:64:LYS:HB3	7:J:18:DG:OP2	1.99	0.62
4:D:97:LEU:C	4:D:97:LEU:HD12	2.25	0.62
1:E:63:ARG:HD2	2:F:30:THR:HG23	1.82	0.62
8:W:781:MET:O	8:W:810:GLN:NE2	2.32	0.62
1:A:117:VAL:HG11	6:I:-4:DC:C3'	2.30	0.61
5:G:28:GLY:C	7:J:-44:DG:H5"	2.25	0.61
6:I:-73:DC:N4	6:I:-72:DA:N6	2.48	0.61
7:J:-15:DA:OP2	7:J:-15:DA:H8	1.83	0.61
7:J:25:DT:OP2	7:J:25:DT:H6	1.83	0.61
8:W:1174:TRP:HE1	8:W:1247:PRO:HD3	1.63	0.61
1:A:100:LEU:HD22	2:B:37:LEU:HD13	1.79	0.61
6:I:-8:DC:N3	6:I:-7:DG:C6	2.69	0.61
6:I:-7:DG:H2"	6:I:-6:DT:C5	2.34	0.61
7:J:50:DG:C6	7:J:51:DG:C6	2.87	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:611:GLU:HA	8:W:816:VAL:HB	1.83	0.61
8:W:660:ASN:HB2	8:W:696:LYS:HZ2	1.64	0.61
8:W:1043:LYS:HD2	8:W:1048:TYR:CE1	2.34	0.61
1:A:132:GLY:O	3:C:99:ARG:CZ	2.48	0.61
3:C:83:LEU:HD21	4:D:55:ALA:HB1	1.82	0.61
1:E:79:LYS:HD2	1:E:80:THR:H	1.65	0.61
6:I:-18:DC:H5"	8:M:434:LEU:CG	2.29	0.61
8:W:629:ILE:CG2	8:W:650:ASN:ND2	2.63	0.61
8:W:1164:PRO:CD	8:W:1176:LYS:HE3	2.29	0.61
3:C:43:VAL:HG12	7:J:39:DA:P	2.40	0.61
8:W:784:ASP:OD1	8:W:785:THR:N	2.32	0.61
3:C:71:ARG:HH12	4:D:49:THR:HG23	1.65	0.61
7:J:4:DG:C2'	7:J:5:DT:H6	2.06	0.61
7:J:51:DG:C8	7:J:52:DC:C5	2.89	0.61
8:M:440:TRP:O	8:M:444:PHE:HB2	2.01	0.61
2:B:68:ASP:OD1	2:B:72:TYR:CE1	2.53	0.61
2:B:73:THR:OG1	2:B:81:VAL:HG22	2.01	0.61
4:D:83:ARG:HE	6:I:-34:DG:C2'	2.13	0.61
2:F:97:LEU:HD22	2:F:100:PHE:CD2	2.35	0.61
5:G:24:GLN:O	4:H:37:TYR:HD2	1.82	0.61
6:I:-78:DC:C2	7:J:79:DG:N2	2.69	0.61
6:I:-16:DT:P	8:M:459:ASN:HB2	2.40	0.61
6:I:15:DT:C2'	6:I:16:DA:C8	2.80	0.61
8:W:390:LEU:HD11	8:W:395:ASP:HB2	1.83	0.61
8:W:391:TRP:O	8:W:391:TRP:HE3	1.82	0.61
8:W:723:MET:HA	8:W:726:ILE:HD12	1.82	0.61
2:B:50:ILE:O	2:B:54:THR:HG23	2.00	0.61
6:I:-4:DC:N4	7:J:4:DG:N1	2.48	0.61
8:W:414:PHE:HE2	8:W:509:PHE:CZ	2.19	0.61
8:W:1170:TRP:HE3	8:W:1174:TRP:CD1	2.18	0.61
7:J:46:DG:H4'	7:J:47:DA:OP1	2.00	0.61
8:W:1192:GLY:HA2	8:W:1194:TRP:CZ3	2.36	0.61
1:A:62:ILE:HG22	1:A:63:ARG:N	2.15	0.61
3:C:34:LEU:HD23	3:C:39:TYR:OH	2.01	0.61
7:J:69:DC:C2'	7:J:70:DT:H71	2.29	0.61
8:W:1264:ARG:HH11	8:W:1264:ARG:HG3	1.65	0.61
1:A:47:ALA:HB1	2:B:39:ARG:NH2	2.15	0.61
6:I:-22:DA:C6	6:I:-21:DC:N4	2.69	0.61
7:J:51:DG:N7	7:J:52:DC:C4	2.69	0.61
8:W:834:ARG:O	8:W:838:ILE:HG13	2.01	0.61
1:E:121:PRO:O	2:F:53:GLU:OE1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:30:DT:C5	6:I:31:DT:C7	2.77	0.60
7:J:-35:DG:C5	7:J:-34:DA:N6	2.68	0.60
8:W:379:PHE:CE1	8:W:597:ARG:NE	2.69	0.60
1:A:65:LEU:HD13	7:J:17:DA:OP2	2.01	0.60
2:B:45:ARG:O	2:B:46:ILE:HG13	2.01	0.60
7:J:26:DA:C5	7:J:27:DG:N1	2.68	0.60
8:W:313:ARG:NH2	8:W:751:ARG:NH2	2.48	0.60
8:W:1059:ALA:CB	8:W:1132:LEU:HD11	2.31	0.60
1:E:62:ILE:HA	2:F:33:ALA:HB1	1.83	0.60
7:J:15:DT:C2	7:J:16:DA:C5	2.88	0.60
7:J:51:DG:H1'	7:J:52:DC:H5'	1.83	0.60
8:W:295:ARG:CD	8:W:1198:ARG:HH22	2.01	0.60
8:W:664:LEU:HG	8:W:664:LEU:O	2.01	0.60
1:A:51:ILE:O	1:A:55:GLN:HG3	2.01	0.60
2:F:33:ALA:HA	2:F:36:ARG:HG3	1.84	0.60
7:J:23:DG:N9	7:J:24:DC:C5	2.68	0.60
8:W:419:ILE:HD12	8:W:451:LEU:CD1	2.31	0.60
8:W:609:LYS:HD3	8:W:806:HIS:CG	2.36	0.60
8:W:696:LYS:HE2	8:W:819:LEU:HB3	1.83	0.60
4:H:55:ALA:O	4:H:59:MET:HG2	2.01	0.60
4:H:73:GLU:O	4:H:77:LEU:HD13	2.02	0.60
6:I:36:DC:H2"	6:I:37:DC:C6	2.37	0.60
8:W:586:LEU:C	8:W:586:LEU:HD23	2.26	0.60
8:W:795:PRO:O	8:W:796:GLN:HB2	2.02	0.60
2:B:58:LEU:CD2	2:B:62:LEU:CD1	2.73	0.60
3:C:44:GLY:HA3	4:D:87:THR:CA	2.29	0.60
3:C:112:GLN:NE2	1:E:108:ASN:ND2	2.49	0.60
2:F:82:THR:HG22	2:F:84:MET:N	2.16	0.60
7:J:69:DC:C2'	7:J:70:DT:C7	2.78	0.60
8:W:696:LYS:CG	8:W:819:LEU:HD23	2.31	0.60
7:J:86:DA:H2"	7:J:87:DT:H71	1.83	0.60
8:W:379:PHE:CE1	8:W:597:ARG:CD	2.83	0.60
8:W:642:LYS:C	8:W:646:PHE:CE2	2.79	0.60
8:W:1026:ASN:OD1	8:W:1028:LYS:HG2	2.01	0.60
3:C:45:ALA:CA	7:J:38:DG:OP1	2.50	0.60
2:F:50:ILE:O	2:F:54:THR:HG23	2.02	0.60
4:H:98:LEU:HG	4:H:99:LEU:HD12	1.82	0.60
6:I:-58:DG:N1	7:J:58:DG:C6	2.70	0.60
6:I:-38:DC:N4	7:J:37:DC:H42	2.00	0.60
8:W:210:ASN:O	8:W:211:TYR:CD1	2.55	0.60
8:W:368:PRO:O	8:W:370:PHE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:540:ILE:O	8:W:540:ILE:CG1	2.46	0.60
2:B:45:ARG:CB	7:J:8:DG:OP1	2.50	0.60
3:C:63:LEU:HD13	4:D:42:LEU:CA	2.31	0.60
6:I:-12:DC:N4	7:J:11:DC:N4	2.50	0.60
6:I:38:DT:H2'	6:I:39:DA:C8	2.36	0.60
6:I:0:DC:H2"	6:I:1:DT:C6	2.37	0.60
7:J:-30:DA:C8	7:J:-29:DT:H71	2.36	0.60
7:J:78:DG:H2"	7:J:79:DG:O5'	2.01	0.60
6:I:-22:DA:C6	6:I:-21:DC:C4	2.90	0.59
6:I:-3:DG:N9	6:I:-2:DC:C5	2.40	0.59
7:J:-11:DC:H2"	7:J:-10:DG:C5'	2.32	0.59
7:J:6:DA:C2'	7:J:7:DC:C5	2.74	0.59
7:J:38:DG:C2	7:J:39:DA:C5	2.89	0.59
8:W:386:TRP:HA	8:W:389:PHE:HB3	1.85	0.59
3:C:46:GLY:HA3	4:D:88:SER:OG	2.02	0.59
2:F:30:THR:HB	7:J:-13:DA:C4'	2.31	0.59
3:C:23:LEU:HD13	3:C:53:ALA:HA	1.82	0.59
3:C:63:LEU:CD1	4:D:41:VAL:CG1	2.79	0.59
4:H:78:ALA:O	4:H:83:ARG:N	2.35	0.59
6:I:-38:DC:C2	6:I:-37:DG:C5	2.90	0.59
7:J:38:DG:N2	7:J:39:DA:C2	2.70	0.59
8:W:255:GLN:CG	8:W:255:GLN:O	2.50	0.59
8:W:330:LEU:HD12	8:W:331:ALA:N	2.17	0.59
8:W:390:LEU:HD12	8:W:393:LYS:HB2	1.84	0.59
8:W:645:HIS:HE1	8:W:649:LEU:HD11	1.63	0.59
8:W:660:ASN:HB3	8:W:696:LYS:CE	2.32	0.59
6:I:-4:DC:H2"	6:I:-3:DG:C8	2.37	0.59
6:I:-3:DG:H2"	6:I:-2:DC:H6	1.62	0.59
6:I:5:DC:O3'	6:I:6:DC:C6	2.56	0.59
7:J:-28:DC:C6	7:J:-27:DC:N4	2.70	0.59
8:M:751:ARG:NH2	8:M:778:ILE:HD11	2.17	0.59
8:W:208:LYS:HG2	8:W:230:TYR:CD2	2.38	0.59
8:W:357:GLN:HG3	8:W:358:ARG:N	2.18	0.59
8:W:616:VAL:HG11	8:W:695:GLY:HA3	1.82	0.59
5:G:115:LEU:C	5:G:115:LEU:HD12	2.26	0.59
6:I:24:DA:H1'	6:I:25:DG:C8	2.38	0.59
1:A:108:ASN:ND2	2:B:42:GLY:O	2.36	0.59
1:E:76:GLN:NE2	1:E:80:THR:HA	2.17	0.59
8:W:368:PRO:C	8:W:370:PHE:H	2.10	0.59
6:I:-14:DA:C2	6:I:-13:DA:C4	2.90	0.59
7:J:20:DG:N2	7:J:21:DG:C5	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:660:ASN:CG	8:W:696:LYS:HZ1	2.10	0.59
3:C:45:ALA:CB	7:J:38:DG:OP1	2.50	0.59
4:D:84:SER:N	6:I:-34:DG:OP1	2.36	0.59
5:G:42:ARG:HA	6:I:39:DA:P	2.42	0.59
8:W:649:LEU:O	8:W:654:GLU:CB	2.51	0.59
2:F:84:MET:SD	2:F:101:GLY:HA3	2.42	0.59
5:G:55:LEU:O	5:G:59:THR:HG23	2.03	0.59
8:W:380:GLN:HG3	9:W:1502:ADP:N6	2.18	0.59
1:E:74:ILE:HG21	2:F:59:LYS:CE	2.33	0.59
4:H:86:ILE:HG22	4:H:91:ILE:HD11	1.83	0.59
7:J:23:DG:C5	7:J:24:DC:C5	2.91	0.59
8:W:348:PRO:CD	8:W:483:MET:HB3	2.33	0.59
8:W:350:TYR:CE1	8:W:1042:VAL:CG1	2.82	0.59
8:W:367:GLN:CG	8:W:371:ILE:HD11	2.33	0.59
8:W:626:TYR:CE1	8:W:824:THR:HG22	2.38	0.59
8:W:767:PHE:CD2	8:W:769:LEU:HD11	2.37	0.59
2:F:29:ILE:HD13	2:F:55:ARG:NH2	2.17	0.58
4:H:63:VAL:O	4:H:67:PHE:N	2.34	0.58
6:I:-78:DC:H1'	6:I:-77:DC:H5'	1.84	0.58
8:W:388:ALA:HA	8:W:391:TRP:HB2	1.85	0.58
2:B:45:ARG:NE	7:J:8:DG:H5"	2.16	0.58
6:I:-28:DT:C5	6:I:-27:DC:N4	2.71	0.58
7:J:78:DG:C2'	7:J:79:DG:H8	2.16	0.58
4:D:49:THR:O	6:I:-54:DA:OP1	2.22	0.58
1:E:50:GLU:HB3	1:E:54:TYR:CE2	2.38	0.58
1:E:66:PRO:HA	2:F:23:ARG:O	2.03	0.58
6:I:-49:DG:N2	7:J:50:DG:C2	2.72	0.58
6:I:36:DC:OP2	6:I:36:DC:H6	1.86	0.58
7:J:78:DG:C4	7:J:79:DG:C5	2.91	0.58
8:W:361:PHE:CE1	8:W:362:GLU:O	2.56	0.58
8:W:1246:VAL:CG1	8:W:1247:PRO:CA	2.81	0.58
1:A:116:ARG:NH1	1:A:120:MET:CG	2.64	0.58
3:C:79:ILE:CG2	3:C:80:PRO:CD	2.79	0.58
1:E:66:PRO:HG2	1:E:67:PHE:H	1.68	0.58
5:G:35:ARG:HG3	5:G:43:VAL:HG21	1.86	0.58
5:G:55:LEU:HA	5:G:58:LEU:HD12	1.85	0.58
7:J:-28:DC:C6	7:J:-27:DC:C4	2.91	0.58
7:J:17:DA:C2'	7:J:18:DG:C8	2.86	0.58
8:M:434:LEU:HD23	8:M:491:THR:HG21	1.85	0.58
8:M:1023:LEU:O	8:M:1136:ARG:NH1	2.36	0.58
6:I:-78:DC:N4	7:J:78:DG:N1	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-45:DA:H2"	6:I:-44:DA:C8	2.39	0.58
6:I:23:DA:N9	6:I:24:DA:N7	2.52	0.58
7:J:-38:DA:C6	7:J:-37:DG:O6	2.56	0.58
8:W:207:CYS:HA	8:W:211:TYR:HD2	1.62	0.58
8:W:400:ALA:H	8:W:595:LEU:HB2	1.69	0.58
8:W:509:PHE:HZ	8:W:538:MET:CE	2.16	0.58
8:W:540:ILE:O	8:W:540:ILE:CD1	2.51	0.58
3:C:43:VAL:CG1	7:J:38:DG:H3'	2.29	0.58
6:I:-73:DC:C2	6:I:-72:DA:N7	2.72	0.58
6:I:-19:DG:H3'	8:M:743:GLY:C	2.28	0.58
6:I:45:DC:H3'	6:I:46:DA:OP2	2.02	0.58
8:W:177:HIS:HE2	8:W:217:TRP:CD1	2.21	0.58
8:W:655:LEU:O	8:W:659:SER:HB3	2.03	0.58
6:I:24:DA:C4	6:I:25:DG:C6	2.92	0.58
8:W:305:LEU:HD21	8:W:307:TYR:OH	2.03	0.58
8:W:402:GLU:HB3	8:W:405:LEU:HG	1.86	0.58
8:W:654:GLU:OE2	8:W:664:LEU:CD2	2.48	0.58
2:F:15:ALA:HB3	8:W:690:LEU:CD1	2.32	0.58
4:H:97:LEU:HD12	4:H:97:LEU:C	2.29	0.58
7:J:33:DT:C2'	7:J:34:DC:C5	2.82	0.58
7:J:80:DC:O3'	7:J:81:DC:O4'	2.21	0.58
8:W:244:ASN:OD1	8:W:245:TYR:N	2.37	0.58
8:W:707:LEU:HD23	8:W:712:HIS:HB2	1.86	0.58
1:A:73:GLU:OE1	1:A:74:ILE:CD1	2.51	0.58
2:B:73:THR:CB	2:B:81:VAL:HG22	2.34	0.58
5:G:78:ILE:O	5:G:78:ILE:HG22	2.03	0.58
4:H:84:SER:HB2	7:J:-35:DG:H4'	1.84	0.58
6:I:9:DG:C5	6:I:10:DC:N4	2.72	0.58
8:W:206:ASN:O	8:W:210:ASN:N	2.36	0.58
8:W:518:LEU:HD12	8:W:555:LEU:CD1	2.31	0.58
8:W:593:PHE:O	8:W:594:ILE:HD13	2.04	0.58
6:I:-17:DT:OP1	8:M:494:TYR:OH	2.17	0.58
6:I:20:DG:C3'	8:W:524:SER:CB	2.77	0.58
8:W:628:ASN:OD1	8:W:633:ASN:ND2	2.36	0.58
4:D:84:SER:OG	6:I:-35:DA:O3'	2.21	0.57
6:I:-11:DG:H2"	6:I:-10:DC:C6	2.38	0.57
2:B:58:LEU:HD21	2:B:62:LEU:HD11	1.85	0.57
5:G:80:PRO:HG3	4:H:55:ALA:CB	2.35	0.57
7:J:26:DA:H2'	7:J:27:DG:N7	2.17	0.57
7:J:34:DC:C2'	7:J:35:DT:C5	2.87	0.57
8:W:345:LYS:CG	8:W:1036:ALA:HB3	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:607:PRO:CG	8:W:812:ASN:N	2.58	0.57
1:E:116:ARG:CA	7:J:-3:DA:OP1	2.51	0.57
5:G:97:LEU:HD11	4:H:62:PHE:HE2	1.68	0.57
7:J:51:DG:C5	7:J:52:DC:N3	2.72	0.57
8:W:221:SER:HB3	8:W:311:TRP:CZ2	2.39	0.57
8:W:589:ARG:O	8:W:593:PHE:HE1	1.86	0.57
8:W:681:MET:HE3	8:W:682:THR:O	2.04	0.57
5:G:47:ALA:HB3	5:G:48:PRO:CD	2.31	0.57
6:I:5:DC:C2'	6:I:6:DC:C6	2.88	0.57
7:J:-40:DC:C6	7:J:-39:DT:H72	2.40	0.57
7:J:-25:DC:C2'	7:J:-24:DT:C6	2.84	0.57
7:J:37:DC:C2	7:J:38:DG:C5	2.92	0.57
7:J:37:DC:O2	7:J:38:DG:C5	2.58	0.57
8:M:1067:GLU:HG2	8:M:1118:VAL:HG22	1.85	0.57
8:W:348:PRO:HD2	8:W:483:MET:HB3	1.86	0.57
8:W:593:PHE:O	8:W:594:ILE:HG12	2.03	0.57
8:W:723:MET:O	8:W:723:MET:SD	2.62	0.57
1:E:46:VAL:O	1:E:49:ARG:N	2.37	0.57
6:I:-41:DG:C6	6:I:-40:DG:C6	2.92	0.57
7:J:-46:DT:N1	7:J:-45:DG:C6	2.72	0.57
7:J:-35:DG:N7	7:J:-34:DA:N6	2.53	0.57
7:J:-25:DC:H2"	7:J:-24:DT:H6	1.60	0.57
8:W:361:PHE:CD1	8:W:362:GLU:N	2.72	0.57
1:A:65:LEU:HB3	1:A:66:PRO:CD	2.31	0.57
2:B:78:ARG:HD2	7:J:28:DA:O5'	2.05	0.57
4:H:84:SER:O	4:H:85:THR:HG23	2.04	0.57
4:H:87:THR:HG23	4:H:89:ARG:H	1.69	0.57
8:W:347:LEU:HD13	8:W:483:MET:O	2.04	0.57
8:W:463:ARG:O	8:W:467:ARG:HG3	2.05	0.57
8:W:483:MET:HE2	8:W:483:MET:HA	1.86	0.57
8:W:681:MET:SD	8:W:682:THR:HG22	2.45	0.57
1:A:101:VAL:HG13	2:B:41:GLY:N	2.19	0.57
3:C:65:LEU:CD2	3:C:90:ASP:CG	2.75	0.57
5:G:42:ARG:CB	6:I:38:DT:H4'	2.32	0.57
8:W:180:ASP:C	8:W:181:ILE:HG13	2.30	0.57
8:W:730:TYR:HD2	8:W:731:LEU:HD12	1.69	0.57
8:W:770:SER:HB2	8:W:773:ALA:CB	2.27	0.57
8:W:1119:PHE:CD2	8:W:1129:ALA:HB2	2.39	0.57
3:C:31:HIS:NE2	3:C:35:ARG:HD2	2.19	0.57
3:C:34:LEU:HD23	3:C:39:TYR:CZ	2.39	0.57
2:F:30:THR:HB	7:J:-13:DA:C5'	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:22:DC:P	8:W:520:ASN:HB2	2.37	0.57
7:J:67:DT:C2'	7:J:68:DT:C7	2.80	0.57
8:W:387:MET:HB2	8:W:414:PHE:CE1	2.40	0.57
1:A:65:LEU:HD22	7:J:17:DA:P	2.44	0.57
1:A:99:TYR:HD1	1:A:100:LEU:HD12	1.69	0.57
2:F:39:ARG:O	2:F:42:GLY:N	2.38	0.57
2:F:86:VAL:O	2:F:89:ALA:HB3	2.05	0.57
5:G:32:ARG:NE	7:J:-45:DG:H3'	2.20	0.57
6:I:-52:DG:C2'	6:I:-51:DC:C6	2.88	0.57
6:I:-23:DC:C2'	6:I:-22:DA:C5'	2.61	0.57
6:I:-16:DT:P	8:M:459:ASN:CB	2.93	0.57
6:I:27:DG:H2"	6:I:28:DG:N7	2.19	0.57
7:J:-35:DG:C6	7:J:-34:DA:N1	2.73	0.57
8:M:622:GLN:O	8:M:626:TYR:HB2	2.05	0.57
8:W:183:ILE:HG23	8:W:281:PHE:CD2	2.40	0.57
8:W:460:GLN:O	8:W:463:ARG:HB3	2.05	0.57
6:I:-43:DT:C2	6:I:-42:DT:C4	2.93	0.57
6:I:36:DC:H2"	6:I:37:DC:H6	1.70	0.57
7:J:32:DG:H2"	7:J:33:DT:C5	2.40	0.57
8:W:181:ILE:CG2	8:W:182:VAL:H	2.18	0.57
8:W:741:LEU:HD22	8:W:769:LEU:HG	1.87	0.57
8:W:827:GLU:HG3	8:W:828:GLU:CD	2.30	0.57
1:A:76:GLN:CG	1:A:80:THR:HG22	2.36	0.56
1:E:63:ARG:HD2	2:F:30:THR:CG2	2.35	0.56
2:F:75:HIS:CE1	4:H:90:GLU:HA	2.40	0.56
6:I:-22:DA:C4	6:I:-21:DC:C5	2.92	0.56
6:I:-6:DT:C4	6:I:-5:DA:N6	2.73	0.56
7:J:34:DC:H2'	7:J:35:DT:C6	2.38	0.56
8:M:583:ILE:O	8:M:587:HIS:HB2	2.04	0.56
8:W:387:MET:C	8:W:414:PHE:HE1	2.12	0.56
2:F:47:SER:HA	6:I:7:DC:C5'	2.35	0.56
6:I:-12:DC:H42	7:J:11:DC:H42	1.53	0.56
1:E:66:PRO:CB	2:F:29:ILE:HG12	2.23	0.56
5:G:53:ALA:O	5:G:56:GLU:HB3	2.05	0.56
4:H:87:THR:O	4:H:91:ILE:HD12	2.04	0.56
6:I:-67:DA:C2	7:J:68:DT:O2	2.59	0.56
6:I:-64:DC:H2"	6:I:-63:DC:C5	2.40	0.56
6:I:-49:DG:H1'	6:I:-48:DC:C2	2.40	0.56
6:I:-22:DA:C4	6:I:-21:DC:C4	2.93	0.56
6:I:-20:DC:H2"	6:I:-19:DG:H8	1.66	0.56
6:I:4:DC:C2'	6:I:5:DC:O5'	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:38:DT:C2'	6:I:39:DA:C8	2.88	0.56
8:W:470:GLU:HA	8:W:485:PHE:HE2	1.69	0.56
8:W:603:GLU:HA	8:W:606:LEU:HD23	1.86	0.56
8:W:650:ASN:C	8:W:654:GLU:HB3	2.30	0.56
8:W:744:THR:HG22	8:W:744:THR:O	2.04	0.56
8:W:1059:ALA:CB	8:W:1132:LEU:HD21	2.32	0.56
2:B:97:LEU:HD23	5:G:101:THR:HG21	1.87	0.56
4:D:70:ILE:CD1	4:D:98:LEU:CD1	2.84	0.56
4:D:119:THR:O	4:D:121:ALA:O	2.23	0.56
5:G:25:PHE:CZ	5:G:56:GLU:CA	2.89	0.56
5:G:31:HIS:HD2	5:G:43:VAL:HG11	1.68	0.56
5:G:84:GLN:HE22	5:G:102:ILE:HG12	1.68	0.56
6:I:-23:DC:C6	6:I:-22:DA:N7	2.73	0.56
3:C:79:ILE:CG1	4:D:52:SER:HB3	2.29	0.56
6:I:19:DC:H42	7:J:-19:DG:N2	1.87	0.56
8:M:546:GLN:NE2	8:M:841:TYR:O	2.38	0.56
8:M:583:ILE:O	8:M:587:HIS:CB	2.53	0.56
8:W:618:LEU:HG	8:W:622:GLN:CD	2.31	0.56
8:W:1014:VAL:HG12	8:W:1124:VAL:HG22	1.87	0.56
6:I:-49:DG:N2	7:J:50:DG:N2	2.54	0.56
6:I:34:DT:C2'	6:I:35:DC:H5	2.14	0.56
7:J:26:DA:C1'	7:J:27:DG:N7	2.69	0.56
8:W:471:PHE:HE1	8:W:481:LYS:CE	2.14	0.56
8:W:505:ILE:O	8:W:507:TRP:CE3	2.59	0.56
8:W:586:LEU:HG	8:W:590:ILE:CD1	2.36	0.56
8:W:601:ASP:C	8:W:603:GLU:H	2.14	0.56
8:W:648:LEU:HA	8:W:651:ILE:HD12	1.86	0.56
8:W:754:ILE:HG12	8:W:778:ILE:HD11	1.87	0.56
1:A:88:ALA:CB	2:B:83:ALA:CA	2.84	0.56
2:B:98:TYR:CE1	4:H:62:PHE:CA	2.83	0.56
5:G:87:VAL:O	5:G:94:ASN:HB3	2.05	0.56
5:G:90:ASP:HB2	5:G:93:LEU:HB2	1.86	0.56
8:M:417:TRP:O	8:M:421:ALA:CB	2.52	0.56
8:W:263:THR:HG22	8:W:264:ALA:N	2.21	0.56
8:W:656:LYS:HE3	8:W:829:VAL:HG21	1.85	0.56
8:W:691:ILE:HD11	8:W:697:MET:O	2.05	0.56
8:W:781:MET:CE	9:W:1502:ADP:H4'	2.35	0.56
3:C:46:GLY:CA	4:D:88:SER:CB	2.84	0.56
3:C:97:LEU:CD1	4:D:62:PHE:CE2	2.72	0.56
4:D:81:ASN:O	4:D:82:LYS:HB2	2.06	0.56
4:H:62:PHE:O	4:H:66:VAL:CG2	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:290:ILE:O	8:M:341:ARG:NH2	2.38	0.56
8:W:611:GLU:HA	8:W:816:VAL:O	2.06	0.56
8:W:643:GLY:N	8:W:646:PHE:CE2	2.74	0.56
4:H:46:HIS:O	4:H:49:THR:HB	2.05	0.56
6:I:-38:DC:C5	6:I:-37:DG:C6	2.92	0.56
6:I:-38:DC:H42	7:J:37:DC:H42	1.54	0.56
6:I:-37:DG:H2"	6:I:-36:DT:H71	1.86	0.56
7:J:21:DG:C2'	7:J:22:DT:O5'	2.49	0.56
7:J:58:DG:H2"	7:J:59:DC:H5	1.70	0.56
7:J:80:DC:O5'	7:J:80:DC:H6	1.89	0.56
8:W:590:ILE:O	8:W:594:ILE:HG12	2.05	0.56
1:E:65:LEU:HD12	6:I:17:DA:H2'	1.84	0.56
6:I:30:DT:N1	6:I:31:DT:C5	2.74	0.56
8:W:305:LEU:HD21	8:W:307:TYR:CZ	2.41	0.56
8:W:1009:ILE:HA	8:W:1043:LYS:HE2	1.87	0.56
1:E:122:LYS:O	1:E:123:ASP:C	2.49	0.55
5:G:42:ARG:HA	6:I:39:DA:C5'	2.37	0.55
6:I:23:DA:P	8:W:519:LYS:CE	2.91	0.55
8:W:183:ILE:HB	8:W:214:LEU:HD22	1.87	0.55
8:W:347:LEU:CD2	8:W:483:MET:O	2.48	0.55
8:W:717:PHE:CE1	8:W:769:LEU:CB	2.88	0.55
1:A:63:ARG:NH2	7:J:17:DA:H4'	2.18	0.55
1:A:117:VAL:CG1	6:I:-4:DC:O3'	2.54	0.55
2:B:91:LYS:HD2	4:D:76:ARG:HH22	1.71	0.55
7:J:-18:DG:H2"	7:J:-17:DT:OP2	2.05	0.55
8:W:183:ILE:HD11	8:W:216:LYS:CE	2.36	0.55
8:W:414:PHE:CE2	8:W:509:PHE:CZ	2.94	0.55
8:W:427:PRO:HA	8:W:486:ASN:HA	1.87	0.55
8:W:766:VAL:O	8:W:766:VAL:HG13	2.07	0.55
8:W:291:ILE:HB	8:W:308:LEU:HD23	1.88	0.55
8:W:311:TRP:HZ3	8:W:319:ALA:HA	1.71	0.55
8:W:379:PHE:CE1	8:W:597:ARG:HD2	2.24	0.55
8:W:591:GLN:HG3	8:W:592:PRO:CD	2.33	0.55
8:W:1139:LEU:HD12	8:W:1140:LYS:N	2.21	0.55
5:G:97:LEU:HB3	5:G:100:VAL:HG22	1.87	0.55
6:I:-67:DA:H2	7:J:68:DT:O2	1.89	0.55
6:I:27:DG:C2	6:I:28:DG:C2	2.95	0.55
7:J:-6:DG:H2"	7:J:-5:DG:C8	2.41	0.55
7:J:26:DA:C6	7:J:27:DG:N1	2.74	0.55
8:W:179:ILE:HD12	8:W:215:ILE:HG21	1.87	0.55
1:A:83:ARG:HH12	7:J:26:DA:H4'	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:25:PHE:HA	4:H:37:TYR:CD2	2.40	0.55
5:G:31:HIS:CD2	5:G:31:HIS:C	2.84	0.55
6:I:-72:DA:C2'	6:I:-71:DT:H71	2.36	0.55
6:I:-9:DA:C8	6:I:-8:DC:C5	2.94	0.55
7:J:20:DG:C4'	7:J:21:DG:OP1	2.46	0.55
7:J:30:DC:C4	7:J:31:DT:O4	2.60	0.55
7:J:68:DT:H2"	7:J:69:DC:C5	2.42	0.55
8:W:417:TRP:O	8:W:421:ALA:HB3	2.06	0.55
8:W:433:PRO:HD3	8:W:513:ASP:CB	2.32	0.55
8:W:607:PRO:CG	8:W:813:HIS:H	2.15	0.55
5:G:91:GLU:HB3	5:G:95:LYS:CE	2.29	0.55
7:J:-19:DG:OP1	8:W:772:ARG:HB3	2.01	0.55
7:J:-17:DT:H2"	7:J:-16:DT:C5'	2.37	0.55
8:M:347:LEU:HD22	8:M:349:GLN:HE22	1.72	0.55
3:C:25:PHE:CD2	3:C:26:PRO:HD2	2.41	0.55
5:G:97:LEU:O	5:G:100:VAL:N	2.36	0.55
8:W:182:VAL:CG1	8:W:245:TYR:CE2	2.87	0.55
8:W:417:TRP:O	8:W:417:TRP:CD1	2.60	0.55
8:W:429:ILE:HB	8:W:507:TRP:NE1	2.22	0.55
8:W:1157:PHE:CE2	8:W:1183:LEU:HD21	2.41	0.55
5:G:39:TYR:O	5:G:40:ALA:HB2	2.06	0.55
6:I:-19:DG:C2'	8:M:743:GLY:C	2.79	0.55
8:M:720:MET:N	8:M:720:MET:SD	2.80	0.55
8:W:359:PRO:HG2	8:W:422:ARG:HD2	1.89	0.55
8:W:434:LEU:HD12	8:W:434:LEU:C	2.32	0.55
8:W:1170:TRP:HB2	8:W:1174:TRP:HD1	1.72	0.55
4:D:62:PHE:CA	2:F:98:TYR:CE1	2.76	0.55
8:M:483:MET:N	8:M:483:MET:SD	2.80	0.55
8:W:295:ARG:HG2	8:W:303:SER:OG	2.07	0.55
8:W:786:VAL:HG22	8:W:816:VAL:HG22	1.85	0.55
2:B:78:ARG:CB	7:J:28:DA:P	2.77	0.55
1:E:50:GLU:HG2	1:E:53:ARG:HH21	1.72	0.55
1:E:76:GLN:HE22	1:E:80:THR:HA	1.71	0.55
6:I:26:DG:H2"	6:I:27:DG:C8	2.41	0.55
8:W:437:MET:HG2	8:W:438:PRO:HD3	1.87	0.55
2:B:39:ARG:HH11	2:B:39:ARG:CG	2.16	0.54
2:F:84:MET:SD	2:F:101:GLY:O	2.64	0.54
4:H:97:LEU:HD12	4:H:98:LEU:CA	2.37	0.54
6:I:-35:DA:N6	6:I:-34:DG:N1	2.55	0.54
2:F:97:LEU:HD22	2:F:100:PHE:HD2	1.73	0.54
6:I:-61:DG:H2"	6:I:-60:DG:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:464:ASP:OD1	8:M:467:ARG:NH2	2.34	0.54
8:W:376:LEU:HD22	9:W:1502:ADP:N6	2.22	0.54
8:W:593:PHE:O	8:W:594:ILE:CG1	2.56	0.54
1:E:89:VAL:HG13	1:E:90:MET:N	2.21	0.54
8:M:696:LYS:O	8:M:700:LEU:HB2	2.06	0.54
8:W:518:LEU:HD12	8:W:555:LEU:HD11	1.88	0.54
8:W:707:LEU:HD23	8:W:712:HIS:CB	2.38	0.54
8:W:717:PHE:CE1	8:W:769:LEU:HB3	2.43	0.54
8:W:767:PHE:CD2	8:W:769:LEU:CD1	2.91	0.54
4:D:84:SER:H	6:I:-34:DG:P	2.29	0.54
6:I:30:DT:N1	6:I:31:DT:C7	2.66	0.54
7:J:-45:DG:N2	7:J:-44:DG:C2	2.75	0.54
7:J:-38:DA:C8	7:J:-37:DG:C5	2.95	0.54
7:J:23:DG:C5	7:J:24:DC:C4	2.96	0.54
7:J:37:DC:O2	7:J:38:DG:C8	2.60	0.54
8:W:544:PRO:HG2	8:W:796:GLN:OE1	2.07	0.54
8:W:614:LEU:N	8:W:818:ARG:O	2.41	0.54
8:W:1029:GLU:HG2	8:W:1030:ILE:HG23	1.88	0.54
3:C:39:TYR:C	4:D:75:SER:HG	2.14	0.54
3:C:97:LEU:HD21	4:D:62:PHE:CE2	2.43	0.54
1:E:119:ILE:HG23	2:F:43:VAL:HG21	1.88	0.54
6:I:-19:DG:C2'	6:I:-18:DC:C5	2.88	0.54
6:I:32:DA:H2"	6:I:33:DC:O5'	2.07	0.54
7:J:34:DC:C1'	7:J:35:DT:C6	2.90	0.54
8:M:599:LYS:HD3	8:M:609:LYS:HE2	1.89	0.54
8:W:1247:PRO:HB2	8:W:1251:HIS:HB2	1.89	0.54
2:B:27:GLN:O	2:B:28:GLY:C	2.50	0.54
7:J:52:DC:H2"	7:J:53:DC:C5	2.42	0.54
8:W:625:TYR:OH	8:W:667:ASN:O	2.20	0.54
8:W:794:ASN:OD1	8:W:795:PRO:N	2.40	0.54
1:E:120:MET:C	2:F:50:ILE:HD12	2.32	0.54
5:G:29:ARG:HA	7:J:-44:DG:OP1	2.07	0.54
6:I:-23:DC:H41	6:I:-22:DA:H62	1.47	0.54
6:I:-22:DA:C8	6:I:-21:DC:C5	2.95	0.54
6:I:23:DA:C1'	6:I:24:DA:C8	2.91	0.54
8:M:348:PRO:HB3	8:M:427:PRO:HD3	1.89	0.54
8:W:476:ARG:HD2	8:W:480:LYS:HB2	1.88	0.54
8:W:660:ASN:HB3	8:W:696:LYS:HE3	1.90	0.54
8:W:768:LEU:HD12	8:W:768:LEU:C	2.32	0.54
8:W:1055:MET:HA	8:W:1121:PHE:CE1	2.43	0.54
3:C:44:GLY:H	4:D:86:ILE:C	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:29:ARG:N	7:J:-44:DG:H5"	2.23	0.54
4:H:84:SER:HB2	7:J:-35:DG:C3'	2.38	0.54
6:I:-38:DC:H2"	6:I:-37:DG:C8	2.43	0.54
6:I:17:DA:H1'	6:I:18:DC:H5'	1.90	0.54
8:W:482:THR:O	8:W:483:MET:CB	2.56	0.54
3:C:77:ARG:HG3	4:D:51:ILE:N	2.23	0.54
4:D:84:SER:CA	6:I:-34:DG:OP1	2.56	0.54
1:E:119:ILE:HG13	2:F:50:ILE:HD13	1.88	0.54
5:G:34:LEU:HD21	4:H:67:PHE:HE1	1.73	0.54
8:W:476:ARG:HG2	8:W:480:LYS:C	2.33	0.54
1:A:95:ALA:HB2	2:B:90:LEU:CD1	2.37	0.54
2:B:32:PRO:HA	2:B:35:ARG:NH1	2.23	0.54
3:C:41:GLU:CD	6:I:-35:DA:H5"	2.32	0.54
1:E:42:ARG:H	1:E:43:PRO:HD3	1.70	0.54
2:F:30:THR:CG2	7:J:-13:DA:C3'	2.86	0.54
5:G:104:GLN:OE1	5:G:104:GLN:N	2.41	0.54
7:J:37:DC:O2	7:J:38:DG:N7	2.41	0.54
8:W:503:GLY:HA2	8:W:532:PHE:CD1	2.43	0.54
8:W:518:LEU:HD11	8:W:555:LEU:HD11	1.82	0.54
8:W:793:TRP:O	8:W:794:ASN:CB	2.48	0.54
3:C:32:ARG:HD2	6:I:-44:DA:O5'	2.08	0.53
5:G:116:LEU:HD12	5:G:117:PRO:CD	2.38	0.53
4:H:93:THR:CG2	4:H:94:ALA:N	2.71	0.53
6:I:-49:DG:H2"	6:I:-48:DC:C5	2.43	0.53
6:I:-23:DC:C6	6:I:-22:DA:C8	2.95	0.53
7:J:51:DG:C2'	7:J:52:DC:OP2	2.52	0.53
8:W:328:VAL:CG2	8:W:1201:PRO:HB2	2.38	0.53
8:W:643:GLY:CA	8:W:646:PHE:CZ	2.80	0.53
8:W:1114:LYS:O	8:W:1115:LYS:HG2	2.07	0.53
8:W:1132:LEU:HD12	8:W:1132:LEU:C	2.31	0.53
1:A:88:ALA:CB	2:B:83:ALA:N	2.70	0.53
1:A:113:HIS:CB	1:E:126:LEU:HD21	2.37	0.53
1:A:116:ARG:NH2	1:E:113:HIS:HE1	2.07	0.53
4:D:103:LEU:HD23	4:D:103:LEU:C	2.34	0.53
2:F:78:ARG:NH2	6:I:28:DG:H3'	2.23	0.53
6:I:30:DT:H2"	6:I:31:DT:O5'	2.07	0.53
8:M:458:GLY:HA3	8:M:462:SER:HB2	1.90	0.53
8:W:295:ARG:CD	8:W:1198:ARG:HH21	2.18	0.53
1:A:45:THR:HG23	1:A:46:VAL:HG23	1.89	0.53
1:E:63:ARG:HD3	6:I:17:DA:C5'	2.38	0.53
1:E:85:GLN:NE2	2:F:82:THR:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:96:LEU:HD12	4:H:100:PRO:CD	2.38	0.53
7:J:14:DT:H2'	7:J:15:DT:C7	2.26	0.53
8:W:220:GLU:OE1	8:W:220:GLU:HA	2.08	0.53
1:A:63:ARG:HH21	7:J:17:DA:H4'	1.72	0.53
3:C:25:PHE:HD2	3:C:52:ALA:HB1	1.72	0.53
5:G:102:ILE:O	5:G:103:ALA:C	2.50	0.53
8:W:615:ARG:HD2	8:W:822:LYS:HG2	1.89	0.53
2:B:78:ARG:CA	7:J:28:DA:OP1	2.53	0.53
1:E:117:VAL:N	7:J:-3:DA:OP1	2.41	0.53
2:F:30:THR:CB	7:J:-13:DA:C4'	2.86	0.53
2:F:75:HIS:HE1	4:H:90:GLU:HA	1.73	0.53
6:I:-78:DC:N4	7:J:78:DG:C6	2.70	0.53
7:J:10:DG:H2"	7:J:11:DC:H5'	1.90	0.53
7:J:15:DT:C2	7:J:16:DA:N7	2.77	0.53
8:W:377:ARG:HE	8:W:602:VAL:CG2	2.20	0.53
8:W:486:ASN:OD1	8:W:487:VAL:N	2.41	0.53
3:C:65:LEU:HD23	3:C:90:ASP:CG	2.32	0.53
5:G:42:ARG:HB3	6:I:38:DT:O3'	2.08	0.53
4:H:70:ILE:HD12	4:H:70:ILE:H	1.73	0.53
6:I:-19:DG:P	8:M:743:GLY:H	2.31	0.53
8:W:183:ILE:HA	8:W:281:PHE:CE2	2.44	0.53
8:W:418:LEU:HD11	8:W:428:HIS:CE1	2.44	0.53
2:F:73:THR:OG1	2:F:81:VAL:HG22	2.08	0.53
5:G:34:LEU:HD21	4:H:67:PHE:CE1	2.44	0.53
6:I:-17:DT:OP1	8:M:494:TYR:CZ	2.62	0.53
6:I:23:DA:C6	6:I:24:DA:C6	2.96	0.53
7:J:24:DC:C2	7:J:25:DT:C4	2.97	0.53
8:W:650:ASN:HA	8:W:654:GLU:HG2	1.91	0.53
8:W:715:LEU:HD21	8:W:780:LEU:CD2	2.38	0.53
1:A:100:LEU:HD22	2:B:37:LEU:CD1	2.36	0.53
1:E:70:LEU:HD13	2:F:24:ASP:O	2.09	0.53
2:F:64:ASN:O	2:F:67:ARG:HB3	2.09	0.53
5:G:81:ARG:HG2	5:G:85:LEU:HD13	1.90	0.53
6:I:-86:DA:H2	7:J:87:DT:O2	1.90	0.53
6:I:30:DT:C6	6:I:31:DT:C5	2.97	0.53
7:J:-33:DG:C6	7:J:-32:DT:C4	2.95	0.53
8:M:515:ALA:H	8:M:541:THR:HB	1.73	0.53
8:W:176:PHE:CD2	8:W:237:ARG:HD2	2.44	0.53
2:B:30:THR:HB	6:I:-12:DC:P	2.49	0.53
2:F:33:ALA:HA	2:F:36:ARG:CG	2.39	0.53
6:I:-6:DT:C7	6:I:-5:DA:N6	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:78:DG:O6	7:J:79:DG:O6	2.27	0.53
8:M:358:ARG:NH1	8:M:391:TRP:O	2.42	0.53
8:M:714:VAL:HA	8:M:785:THR:HB	1.91	0.53
8:W:786:VAL:HG23	8:W:786:VAL:O	2.08	0.53
1:A:65:LEU:HD21	1:A:69:ARG:NE	2.24	0.52
3:C:51:LEU:HD11	4:D:70:ILE:HG21	1.91	0.52
1:E:62:ILE:HG23	2:F:33:ALA:HB1	1.90	0.52
2:F:76:ALA:O	2:F:77:LYS:HG3	2.10	0.52
6:I:-78:DC:N3	7:J:79:DG:N2	2.56	0.52
6:I:-52:DG:H2"	6:I:-51:DC:C6	2.44	0.52
6:I:-48:DC:H1'	6:I:-47:DT:H5'	1.91	0.52
6:I:-16:DT:H1'	6:I:-15:DA:C8	2.44	0.52
8:W:415:ILE:HA	8:W:418:LEU:HD21	1.91	0.52
8:W:626:TYR:CE1	8:W:655:LEU:HD11	2.44	0.52
8:W:794:ASN:CG	8:W:795:PRO:HD2	2.33	0.52
6:I:-57:DC:C2	7:J:58:DG:N2	2.77	0.52
6:I:-4:DC:C2	7:J:4:DG:N2	2.66	0.52
8:W:611:GLU:HG2	8:W:816:VAL:CB	2.39	0.52
8:W:718:SER:HB3	8:W:724:LEU:HD21	1.90	0.52
1:A:70:LEU:HD13	2:B:25:ASN:OD1	2.09	0.52
2:B:78:ARG:CG	7:J:28:DA:P	2.98	0.52
5:G:24:GLN:HB3	4:H:40:LYS:HE3	1.90	0.52
6:I:-58:DG:H22	7:J:59:DC:H42	1.55	0.52
6:I:-16:DT:OP2	8:M:459:ASN:HB2	2.04	0.52
6:I:45:DC:C4	7:J:-46:DT:O4	2.62	0.52
7:J:-3:DA:N7	7:J:-2:DC:N4	2.57	0.52
7:J:-3:DA:C5	7:J:-2:DC:C4	2.98	0.52
8:W:1025:GLY:HA3	8:W:1139:LEU:CD2	2.34	0.52
8:W:1102:ASN:O	8:W:1105:THR:HG22	2.09	0.52
3:C:97:LEU:HB3	3:C:100:VAL:HG22	1.91	0.52
1:E:121:PRO:HB2	2:F:53:GLU:OE2	2.09	0.52
4:H:73:GLU:OE2	4:H:97:LEU:HD21	2.09	0.52
7:J:38:DG:H2"	7:J:39:DA:OP2	2.09	0.52
8:W:284:PHE:CE1	8:W:314:LEU:HD22	2.44	0.52
2:B:45:ARG:NE	7:J:8:DG:H5'	2.19	0.52
2:F:64:ASN:OD1	2:F:65:VAL:N	2.43	0.52
5:G:31:HIS:CD2	5:G:31:HIS:O	2.62	0.52
5:G:84:GLN:OE1	5:G:88:ARG:HG2	2.09	0.52
6:I:-69:DA:H2"	6:I:-68:DG:C8	2.44	0.52
8:W:284:PHE:HE1	8:W:314:LEU:HD13	1.74	0.52
8:W:359:PRO:O	8:W:360:ARG:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:593:PHE:O	8:W:594:ILE:CD1	2.58	0.52
8:W:643:GLY:CA	8:W:646:PHE:CE2	2.92	0.52
1:E:62:ILE:HD11	2:F:37:LEU:HD22	1.92	0.52
6:I:-43:DT:C6	6:I:-42:DT:H73	2.44	0.52
7:J:-33:DG:C6	7:J:-32:DT:O4	2.63	0.52
8:W:380:GLN:OE1	8:W:410:GLN:HG3	2.10	0.52
8:W:387:MET:HB2	8:W:414:PHE:CD1	2.44	0.52
8:W:1013:GLU:CG	8:W:1041:PRO:HG2	2.39	0.52
8:W:1099:PRO:O	8:W:1100:LYS:C	2.52	0.52
1:E:100:LEU:HD13	2:F:37:LEU:CD2	2.40	0.52
5:G:76:THR:O	4:H:49:THR:HA	2.09	0.52
5:G:83:LEU:O	5:G:87:VAL:HG23	2.10	0.52
4:H:51:ILE:CD1	4:H:56:MET:CE	2.83	0.52
6:I:-78:DC:N3	7:J:79:DG:C2	2.78	0.52
8:W:606:LEU:CD1	8:W:607:PRO:O	2.57	0.52
8:W:767:PHE:HE2	8:W:769:LEU:HD11	1.69	0.52
8:W:800:GLN:O	8:W:803:ALA:N	2.41	0.52
3:C:28:GLY:O	6:I:-44:DA:H3'	2.09	0.52
6:I:-59:DT:C6	6:I:-58:DG:C6	2.98	0.52
8:W:295:ARG:HH11	8:W:303:SER:CB	2.23	0.52
8:W:431:VAL:O	8:W:512:VAL:HA	2.09	0.52
2:B:65:VAL:HG23	2:B:66:ILE:N	2.24	0.52
3:C:23:LEU:CD1	3:C:53:ALA:HB2	2.39	0.52
2:F:76:ALA:O	2:F:77:LYS:HG2	2.09	0.52
6:I:30:DT:C2'	6:I:31:DT:H73	2.40	0.52
8:W:510:MET:HB3	8:W:537:ARG:HA	1.92	0.52
8:W:622:GLN:NE2	8:W:659:SER:O	2.43	0.52
8:W:655:LEU:CD2	8:W:825:VAL:CB	2.85	0.52
8:W:1143:LYS:HA	8:W:1187:PHE:CE1	2.42	0.52
1:A:40:ARG:HG3	7:J:10:DG:H5'	1.92	0.52
1:A:104:PHE:HD2	2:B:38:ALA:HA	1.75	0.52
3:C:39:TYR:OH	4:D:71:ALA:CB	2.57	0.52
3:C:97:LEU:HD21	4:D:62:PHE:HE2	1.74	0.52
6:I:-61:DG:C2	7:J:62:DC:O2	2.63	0.52
6:I:-30:DG:O6	7:J:29:DG:O6	2.28	0.52
7:J:-44:DG:C6	7:J:-43:DA:C6	2.98	0.52
7:J:78:DG:H2'	7:J:79:DG:C8	2.45	0.52
8:W:200:THR:HG22	8:W:201:VAL:HG23	1.92	0.52
8:W:433:PRO:HG2	8:W:514:GLU:CD	2.34	0.52
8:W:1009:ILE:HG13	8:W:1013:GLU:HB2	1.90	0.52
8:W:1171:SER:CB	8:W:1245:LYS:HE3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:PRO:O	3:C:118:LYS:C	2.53	0.51
2:F:47:SER:CB	6:I:7:DC:OP1	2.58	0.51
6:I:-64:DC:H2"	6:I:-63:DC:C6	2.45	0.51
7:J:17:DA:C6	7:J:18:DG:C6	2.99	0.51
8:W:208:LYS:HG2	8:W:230:TYR:HD2	1.73	0.51
8:W:1119:PHE:CE2	8:W:1129:ALA:CB	2.82	0.51
8:M:1206:ILE:HG22	8:M:1209:LYS:HD2	1.93	0.51
8:W:350:TYR:CE1	8:W:1042:VAL:HG11	2.45	0.51
5:G:91:GLU:CB	5:G:95:LYS:HE3	2.31	0.51
6:I:-47:DT:H2"	6:I:-46:DC:C4	2.45	0.51
6:I:-38:DC:N3	6:I:-37:DG:N1	2.57	0.51
7:J:-29:DT:H2"	7:J:-28:DC:O5'	2.09	0.51
7:J:34:DC:C6	7:J:34:DC:C5'	2.85	0.51
8:M:751:ARG:CZ	8:M:778:ILE:HD11	2.40	0.51
8:W:415:ILE:O	8:W:419:ILE:HG13	2.10	0.51
8:W:729:ASP:O	8:W:733:ILE:HG12	2.10	0.51
8:W:1070:ARG:HH21	8:W:1113:GLU:HG2	1.76	0.51
2:B:75:HIS:HE1	4:D:89:ARG:HD3	1.75	0.51
5:G:35:ARG:CG	5:G:43:VAL:HG21	2.40	0.51
6:I:0:DC:H2'	6:I:1:DT:C7	2.38	0.51
6:I:24:DA:C2	6:I:25:DG:C2	2.98	0.51
7:J:-38:DA:C5	7:J:-37:DG:C5	2.93	0.51
8:M:507:TRP:HB2	8:M:534:VAL:HG12	1.91	0.51
8:W:1118:LEU:C	8:W:1118:LEU:HD12	2.36	0.51
8:W:1198:ARG:HB2	8:W:1209:ILE:HD13	1.92	0.51
1:E:124:ILE:HD12	2:F:53:GLU:OE1	2.10	0.51
5:G:47:ALA:N	5:G:48:PRO:HD2	2.25	0.51
6:I:-28:DT:H4'	6:I:-27:DC:OP1	2.11	0.51
7:J:21:DG:O4'	8:M:517:ARG:NH2	2.43	0.51
8:W:177:HIS:HE1	8:W:217:TRP:CE2	2.28	0.51
1:A:83:ARG:O	2:B:80:THR:HA	2.11	0.51
1:A:42:ARG:O	1:A:45:THR:CG2	2.59	0.51
5:G:54:VAL:O	5:G:58:LEU:HG	2.10	0.51
6:I:-12:DC:N4	6:I:-11:DG:C6	2.73	0.51
6:I:21:DC:C4	6:I:22:DC:C4	2.99	0.51
8:M:289:ARG:HE	8:M:290:ILE:H	1.58	0.51
8:W:350:TYR:CE1	8:W:1042:VAL:HG13	2.43	0.51
8:W:720:MET:SD	8:W:721:VAL:CG1	2.99	0.51
3:C:108:LEU:HD12	3:C:110:ASN:HB2	1.92	0.51
2:F:79:LYS:N	6:I:28:DG:OP1	2.42	0.51
5:G:32:ARG:HA	5:G:35:ARG:HE	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:84:SER:HB2	7:J:-35:DG:O3'	2.11	0.51
8:M:1145:ASN:O	8:M:1149:SER:CB	2.59	0.51
8:W:268:GLU:O	8:W:272:MET:HB2	2.10	0.51
8:W:462:SER:O	8:W:463:ARG:C	2.54	0.51
8:W:778:ILE:O	8:W:804:ARG:HD2	2.11	0.51
8:W:799:LEU:O	8:W:802:MET:HG2	2.10	0.51
8:W:1055:MET:HE3	8:W:1121:PHE:CD2	2.43	0.51
1:A:115:LYS:HG2	1:A:115:LYS:O	2.11	0.51
1:E:122:LYS:C	1:E:124:ILE:N	2.68	0.51
2:F:31:LYS:N	7:J:-12:DA:OP2	2.44	0.51
6:I:-8:DC:C2	6:I:-7:DG:C5	2.99	0.51
7:J:38:DG:N3	7:J:39:DA:C4	2.79	0.51
8:W:663:TYR:OH	8:W:672:VAL:CG1	2.53	0.51
8:W:1017:LEU:HD12	8:W:1027:LEU:HD21	1.93	0.51
8:W:1119:PHE:HE2	8:W:1129:ALA:HA	1.76	0.51
2:B:34:ILE:HD11	2:B:55:ARG:HE	1.76	0.51
5:G:42:ARG:CB	6:I:38:DT:O3'	2.59	0.51
6:I:-38:DC:C2	6:I:-37:DG:C6	2.99	0.51
8:M:696:LYS:O	8:M:700:LEU:CB	2.59	0.51
8:W:207:CYS:HA	8:W:211:TYR:HB2	1.93	0.51
2:B:62:LEU:O	2:B:65:VAL:CG2	2.59	0.50
3:C:40:ALA:HB3	4:D:86:ILE:CD1	2.29	0.50
3:C:43:VAL:O	7:J:38:DG:H5"	2.10	0.50
3:C:63:LEU:HB3	4:D:42:LEU:CD1	2.41	0.50
4:H:70:ILE:HD12	4:H:70:ILE:N	2.26	0.50
7:J:-21:DG:C5	7:J:-20:DC:N4	2.79	0.50
7:J:69:DC:H2"	7:J:70:DT:C6	2.46	0.50
8:W:515:ALA:H	8:W:541:THR:HB	1.75	0.50
8:W:764:ASP:OD1	8:W:764:ASP:O	2.29	0.50
8:W:795:PRO:CD	8:W:836:LYS:HD2	2.40	0.50
8:W:1170:TRP:CZ3	8:W:1247:PRO:HG3	2.46	0.50
1:A:83:ARG:NH1	7:J:26:DA:H4'	2.26	0.50
1:A:116:ARG:HH21	1:E:113:HIS:HE1	1.59	0.50
3:C:27:VAL:HG13	3:C:49:VAL:HA	1.92	0.50
6:I:-58:DG:C2	7:J:58:DG:C2	2.99	0.50
8:M:316:TYR:HH	8:M:455:CYS:HG	1.53	0.50
8:W:390:LEU:HD12	8:W:393:LYS:CB	2.41	0.50
8:W:408:THR:HG22	8:W:443:THR:HG21	1.92	0.50
8:W:602:VAL:HG13	8:W:602:VAL:O	2.11	0.50
8:W:1152:ASP:OD1	8:W:1153:ASP:N	2.44	0.50
3:C:39:TYR:OH	4:D:71:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-19:DG:H2"	8:M:743:GLY:O	2.04	0.50
6:I:0:DC:H2"	6:I:1:DT:H6	1.74	0.50
7:J:-30:DA:N7	7:J:-29:DT:H73	2.27	0.50
7:J:15:DT:H2"	7:J:16:DA:H8	1.74	0.50
7:J:22:DT:H2"	7:J:23:DG:OP2	2.11	0.50
7:J:78:DG:C4	7:J:79:DG:N7	2.79	0.50
8:W:1102:ASN:OD1	8:W:1104:LEU:HG	2.12	0.50
6:I:-18:DC:C5'	8:M:434:LEU:HD11	2.36	0.50
7:J:37:DC:H2"	7:J:38:DG:OP2	2.12	0.50
7:J:38:DG:N2	7:J:39:DA:C4	2.79	0.50
7:J:51:DG:C5	7:J:52:DC:N4	2.79	0.50
8:W:229:THR:CG2	8:W:230:TYR:H	2.14	0.50
8:W:387:MET:O	8:W:391:TRP:HB2	2.11	0.50
4:D:87:THR:HG23	4:D:89:ARG:H	1.75	0.50
7:J:-14:DA:H2"	7:J:-13:DA:C8	2.47	0.50
7:J:1:DC:H2"	7:J:2:DG:C8	2.46	0.50
8:M:1145:ASN:O	8:M:1149:SER:OG	2.27	0.50
8:W:429:ILE:HG23	8:W:429:ILE:O	2.11	0.50
1:E:63:ARG:NH2	7:J:-13:DA:H5'	2.25	0.50
8:W:183:ILE:HB	8:W:214:LEU:CD2	2.41	0.50
8:W:458:GLY:HA3	8:W:462:SER:CB	2.41	0.50
8:W:488:LEU:HD23	8:W:489:LEU:N	2.26	0.50
8:W:626:TYR:HD2	8:W:627:LYS:HZ2	1.57	0.50
8:W:751:ARG:O	8:W:754:ILE:HG22	2.12	0.50
4:D:48:ASP:OD1	6:I:-54:DA:H4'	2.11	0.50
2:F:75:HIS:NE2	4:H:90:GLU:OE1	2.42	0.50
5:G:26:PRO:HD3	4:H:37:TYR:CG	2.47	0.50
4:H:51:ILE:HD13	4:H:56:MET:HB2	1.92	0.50
6:I:-58:DG:N1	7:J:58:DG:N1	2.60	0.50
6:I:-17:DT:H5'	8:M:493:GLU:OE2	2.10	0.50
6:I:21:DC:H2'	6:I:22:DC:C6	2.46	0.50
6:I:5:DC:O2	6:I:6:DC:N3	2.45	0.50
7:J:-69:DG:H2"	7:J:-68:DA:H8	1.77	0.50
8:M:184:ASN:H	8:M:214:LEU:HB3	1.77	0.50
8:M:437:MET:HG3	8:M:489:LEU:HD22	1.92	0.50
8:W:390:LEU:HD13	8:W:393:LYS:CD	2.32	0.50
8:W:595:LEU:HD13	8:W:597:ARG:HH22	1.76	0.50
8:W:599:LYS:C	8:W:601:ASP:H	2.20	0.50
3:C:42:ARG:HD3	7:J:38:DG:C4'	2.42	0.50
1:E:50:GLU:HB3	1:E:54:TYR:HE2	1.76	0.50
4:H:87:THR:CG2	4:H:90:GLU:HG2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-18:DC:C5'	8:M:434:LEU:CD2	2.58	0.50
7:J:19:DC:C6	7:J:20:DG:O6	2.61	0.50
8:M:786:VAL:HG11	8:M:802:MET:HG2	1.94	0.50
8:M:1139:ASP:HB3	8:M:1261:LEU:HD13	1.94	0.50
8:W:431:VAL:O	8:W:431:VAL:CG1	2.58	0.50
8:W:455:CYS:SG	8:W:456:TYR:N	2.84	0.50
1:A:92:LEU:N	2:B:86:VAL:HG11	2.26	0.49
1:E:69:ARG:CB	2:F:24:ASP:CB	2.90	0.49
5:G:25:PHE:CE2	5:G:55:LEU:HB2	2.47	0.49
4:H:35:ALA:HB1	4:H:56:MET:SD	2.52	0.49
6:I:7:DC:H2"	6:I:8:DC:C5	2.46	0.49
8:W:387:MET:HB3	8:W:414:PHE:CE1	2.46	0.49
8:W:398:ILE:HG12	8:W:539:LEU:CD2	2.35	0.49
8:W:415:ILE:HA	8:W:418:LEU:HD23	1.94	0.49
1:A:85:GLN:C	6:I:-24:DG:OP2	2.55	0.49
7:J:-64:DA:H2'	7:J:-63:DT:H71	1.93	0.49
8:M:530:ASN:HA	8:M:537:ARG:HH22	1.77	0.49
8:W:705:THR:O	8:W:708:LYS:HB3	2.12	0.49
8:W:746:PRO:HB2	8:W:749:GLN:HG2	1.94	0.49
2:B:62:LEU:O	2:B:65:VAL:HG22	2.11	0.49
4:D:55:ALA:HA	4:D:58:ILE:HD12	1.94	0.49
2:F:29:ILE:CG2	2:F:30:THR:H	2.24	0.49
6:I:-30:DG:N9	6:I:-29:DC:C6	2.80	0.49
6:I:5:DC:O3'	6:I:6:DC:H6	1.94	0.49
6:I:45:DC:H3'	6:I:46:DA:P	2.53	0.49
7:J:67:DT:H2"	7:J:68:DT:C6	2.48	0.49
8:W:488:LEU:CD2	8:W:490:THR:CG2	2.90	0.49
1:A:73:GLU:CG	2:B:25:ASN:HD22	2.18	0.49
3:C:116:LEU:C	3:C:116:LEU:HD12	2.37	0.49
5:G:34:LEU:CD2	4:H:67:PHE:CZ	2.95	0.49
4:H:84:SER:HB2	7:J:-35:DG:C4'	2.41	0.49
6:I:-4:DC:N3	7:J:4:DG:C2	2.80	0.49
6:I:34:DT:H2'	6:I:35:DC:H5	1.76	0.49
8:W:293:SER:HB3	8:W:307:TYR:HD1	1.75	0.49
8:W:516:HIS:HB3	8:W:543:THR:HB	1.93	0.49
8:W:1034:LEU:O	8:W:1037:ASP:O	2.30	0.49
6:I:-12:DC:N4	7:J:11:DC:H42	2.11	0.49
7:J:-11:DC:H2"	7:J:-10:DG:O5'	2.13	0.49
7:J:79:DG:C2'	7:J:80:DC:OP2	2.60	0.49
8:W:437:MET:CE	8:W:457:MET:SD	3.01	0.49
8:W:611:GLU:OE2	8:W:818:ARG:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:717:PHE:CE1	8:W:769:LEU:HB2	2.48	0.49
4:H:51:ILE:HD13	4:H:56:MET:SD	2.52	0.49
6:I:-58:DG:H2"	6:I:-57:DC:C6	2.47	0.49
7:J:34:DC:H6	7:J:34:DC:C5'	2.20	0.49
8:W:387:MET:HE2	8:W:538:MET:HE2	1.92	0.49
8:W:545:LEU:HD13	8:W:552:LEU:CD1	2.42	0.49
8:W:1114:LYS:O	8:W:1115:LYS:HD3	2.13	0.49
8:W:1124:VAL:HB	8:W:1127:LEU:HD11	1.94	0.49
3:C:32:ARG:NH2	6:I:-43:DT:H71	2.25	0.49
6:I:-40:DG:H1	7:J:40:DC:N4	2.11	0.49
6:I:24:DA:C2'	6:I:25:DG:N7	2.76	0.49
7:J:32:DG:H2"	7:J:33:DT:C6	2.48	0.49
8:M:550:LYS:O	8:M:554:ALA:HB2	2.13	0.49
8:W:177:HIS:NE2	8:W:217:TRP:CD2	2.80	0.49
8:W:1170:TRP:CE3	8:W:1174:TRP:CD1	2.99	0.49
8:W:1247:PRO:HB2	8:W:1251:HIS:CB	2.42	0.49
2:B:78:ARG:HG2	7:J:28:DA:P	2.53	0.49
1:E:116:ARG:HA	7:J:-3:DA:OP2	2.12	0.49
2:F:78:ARG:HH22	6:I:28:DG:H3'	1.78	0.49
6:I:-73:DC:C2	6:I:-72:DA:C5	3.01	0.49
6:I:-17:DT:C5'	8:M:493:GLU:OE2	2.61	0.49
8:W:649:LEU:O	8:W:654:GLU:HB2	2.13	0.49
8:W:1056:MET:HE2	8:W:1133:LEU:HD23	1.95	0.49
8:W:1205:ILE:HD12	8:W:1208:LYS:HB2	1.95	0.49
3:C:34:LEU:CD2	3:C:39:TYR:OH	2.61	0.49
1:E:120:MET:HE3	1:E:121:PRO:HD2	1.93	0.49
4:H:51:ILE:CG1	4:H:56:MET:HE3	2.43	0.49
6:I:5:DC:C1'	6:I:6:DC:C6	2.94	0.49
8:M:1104:PRO:HA	8:M:1107:ARG:HG2	1.93	0.49
1:A:104:PHE:CD2	2:B:38:ALA:CA	2.96	0.49
3:C:42:ARG:HD3	7:J:38:DG:H4'	1.95	0.49
3:C:63:LEU:HB3	4:D:42:LEU:HD12	1.94	0.49
4:D:70:ILE:HD13	4:D:98:LEU:HD12	1.95	0.49
2:F:30:THR:HG21	7:J:-13:DA:H5'	1.87	0.49
2:F:34:ILE:O	2:F:37:LEU:HB3	2.12	0.49
2:F:39:ARG:C	2:F:41:GLY:N	2.68	0.49
6:I:-83:DC:H2"	6:I:-82:DG:C8	2.48	0.49
6:I:41:DT:C2	6:I:42:DC:C5	3.01	0.49
7:J:38:DG:N3	7:J:39:DA:C5	2.81	0.49
7:J:50:DG:H1'	7:J:51:DG:H5'	1.95	0.49
8:W:417:TRP:O	8:W:417:TRP:CG	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:HB2	6:I:-5:DA:C5'	2.37	0.48
1:A:45:THR:O	1:A:49:ARG:HG3	2.12	0.48
1:A:65:LEU:CD1	7:J:17:DA:OP2	2.61	0.48
3:C:102:ILE:HD11	4:D:58:ILE:CG2	2.42	0.48
4:H:45:VAL:HG12	4:H:46:HIS:ND1	2.28	0.48
6:I:-79:DG:N1	7:J:79:DG:N1	2.61	0.48
6:I:-68:DG:H2"	6:I:-67:DA:N7	2.28	0.48
7:J:24:DC:O2	7:J:25:DT:C2	2.66	0.48
7:J:30:DC:C5	7:J:31:DT:C4	3.01	0.48
7:J:39:DA:C2'	7:J:40:DC:H5'	2.36	0.48
8:M:430:ILE:HD13	8:M:487:VAL:HG13	1.95	0.48
8:W:419:ILE:HD13	8:W:451:LEU:HD13	1.94	0.48
8:W:517:ARG:O	8:W:519:LYS:N	2.44	0.48
8:W:611:GLU:CB	8:W:816:VAL:HB	2.42	0.48
8:W:1094:LYS:HE2	8:W:1097:ASN:HB3	1.95	0.48
3:C:23:LEU:HD11	3:C:53:ALA:HB2	1.94	0.48
3:C:40:ALA:HB2	4:D:86:ILE:HD13	1.73	0.48
3:C:97:LEU:HD11	4:D:62:PHE:CD2	2.40	0.48
6:I:-67:DA:C2	6:I:-66:DA:C2	3.01	0.48
6:I:21:DC:C5	6:I:22:DC:N4	2.81	0.48
7:J:33:DT:C2	7:J:34:DC:N4	2.81	0.48
8:M:292:ASP:H	8:M:308:LEU:HB3	1.78	0.48
8:W:312:ARG:HD3	8:W:313:ARG:N	2.28	0.48
8:W:556:VAL:HG22	8:W:593:PHE:CE2	2.47	0.48
1:E:106:ASP:O	1:E:107:THR:C	2.56	0.48
5:G:24:GLN:CD	4:H:41:VAL:CG1	2.87	0.48
6:I:7:DC:H2"	6:I:8:DC:H6	1.72	0.48
8:M:180:ASP:O	8:M:241:ARG:NH1	2.40	0.48
8:W:295:ARG:HD2	8:W:1198:ARG:HH21	1.66	0.48
8:W:525:LEU:HA	8:W:528:SER:CB	2.43	0.48
8:W:586:LEU:HD23	8:W:587:HIS:N	2.28	0.48
8:W:1077:LEU:HD23	8:W:1107:LEU:HA	1.94	0.48
1:A:125:GLN:HG2	1:A:128:ARG:HH12	1.78	0.48
3:C:63:LEU:HD22	4:D:42:LEU:HD13	1.95	0.48
1:E:61:LEU:HD22	2:F:36:ARG:C	2.38	0.48
2:F:15:ALA:CB	8:W:690:LEU:HD12	2.41	0.48
6:I:-18:DC:C3'	8:M:434:LEU:CD2	2.91	0.48
6:I:-8:DC:C2	6:I:-7:DG:C6	3.02	0.48
6:I:-6:DT:C6	6:I:-5:DA:C6	3.01	0.48
6:I:24:DA:C2	6:I:25:DG:N1	2.82	0.48
7:J:-68:DA:H2'	7:J:-67:DT:H71	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-25:DC:C6	7:J:-24:DT:H72	2.48	0.48
1:A:69:ARG:HB3	2:B:22:LEU:HD23	1.94	0.48
5:G:17:ARG:HD3	5:G:27:VAL:HG11	1.95	0.48
6:I:-75:DC:H2'	6:I:-74:DC:C6	2.49	0.48
6:I:-62:DC:H2"	6:I:-61:DG:H5"	1.96	0.48
6:I:21:DC:N4	6:I:22:DC:N4	2.61	0.48
7:J:58:DG:C2'	7:J:59:DC:C5	2.91	0.48
8:W:221:SER:HB3	8:W:311:TRP:CH2	2.48	0.48
8:W:370:PHE:CE1	8:W:417:TRP:HZ3	2.30	0.48
8:W:520:ASN:ND2	8:W:522:GLU:HB3	2.29	0.48
8:W:814:VAL:HG12	8:W:815:MET:N	2.29	0.48
8:W:1047:LYS:O	8:W:1051:THR:HG23	2.14	0.48
8:W:1174:TRP:NE1	8:W:1247:PRO:HD3	2.29	0.48
1:A:88:ALA:CB	2:B:83:ALA:HA	2.43	0.48
2:F:32:PRO:CD	7:J:-12:DA:OP2	2.60	0.48
2:F:88:TYR:O	2:F:92:ARG:HG2	2.14	0.48
5:G:26:PRO:HB2	5:G:29:ARG:HB3	1.95	0.48
5:G:65:LEU:HA	5:G:68:ASN:OD1	2.14	0.48
5:G:88:ARG:C	5:G:94:ASN:HD22	2.22	0.48
6:I:-78:DC:N3	7:J:78:DG:N2	2.61	0.48
6:I:45:DC:N3	7:J:-46:DT:N3	2.62	0.48
7:J:15:DT:H3	7:J:16:DA:N6	2.11	0.48
7:J:21:DG:H4'	8:M:517:ARG:CZ	2.36	0.48
8:W:309:VAL:HG13	8:W:311:TRP:CH2	2.49	0.48
8:W:376:LEU:HD22	9:W:1502:ADP:HN62	1.78	0.48
8:W:399:LEU:HG	8:W:595:LEU:HD12	1.95	0.48
8:W:681:MET:HE1	8:W:682:THR:HG22	1.95	0.48
8:W:1145:LEU:HD21	8:W:1149:ASN:HD21	1.77	0.48
2:B:55:ARG:O	2:B:59:LYS:HG3	2.14	0.48
5:G:26:PRO:HB3	4:H:37:TYR:OH	2.13	0.48
5:G:103:ALA:HB1	5:G:104:GLN:OE1	2.13	0.48
6:I:5:DC:H1'	6:I:6:DC:C4	2.48	0.48
7:J:-8:DG:C5	7:J:-7:DG:C6	3.02	0.48
7:J:17:DA:C5	7:J:18:DG:C6	3.02	0.48
8:W:517:ARG:HA	8:W:517:ARG:HD2	1.51	0.48
8:W:723:MET:SD	8:W:723:MET:C	2.97	0.48
1:A:117:VAL:HG11	6:I:-4:DC:C5'	2.39	0.48
1:E:116:ARG:HD3	7:J:-3:DA:H3'	1.96	0.48
2:F:46:ILE:O	6:I:7:DC:C4'	2.61	0.48
6:I:-73:DC:H2"	6:I:-72:DA:OP2	2.12	0.48
6:I:-18:DC:C3'	8:M:434:LEU:HD22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-3:DG:N3	6:I:-2:DC:C2	2.81	0.48
7:J:20:DG:H3'	8:M:496:LEU:HD23	1.94	0.48
4:D:97:LEU:HD12	4:D:97:LEU:O	2.14	0.48
1:E:48:LEU:CB	1:E:52:ARG:HH12	2.27	0.48
6:I:-56:DC:H2"	6:I:-55:DG:C8	2.49	0.48
6:I:-12:DC:C2'	6:I:-11:DG:C8	2.94	0.48
6:I:-11:DG:H2"	6:I:-10:DC:H6	1.79	0.48
7:J:-26:DC:H2"	7:J:-25:DC:C5	2.49	0.48
7:J:43:DA:C8	7:J:44:DT:C7	2.97	0.48
7:J:51:DG:C8	7:J:52:DC:C4	3.01	0.48
7:J:55:DT:H2"	7:J:56:DC:C5	2.49	0.48
8:W:298:LEU:HB2	8:W:302:THR:HG22	1.96	0.48
8:W:315:ASN:HD21	8:W:458:GLY:CA	2.22	0.48
8:W:521:ALA:HA	8:W:526:TYR:CE2	2.49	0.48
8:W:614:LEU:CB	8:W:819:LEU:HA	2.44	0.48
1:A:70:LEU:HD13	2:B:25:ASN:CB	2.44	0.48
3:C:30:VAL:O	3:C:34:LEU:HG	2.14	0.48
6:I:-19:DG:C4'	8:M:743:GLY:HA3	2.43	0.48
6:I:30:DT:N3	6:I:31:DT:C4	2.81	0.48
7:J:-25:DC:C2'	7:J:-24:DT:H73	2.33	0.48
7:J:-17:DT:C2'	7:J:-16:DT:O5'	2.54	0.48
8:W:315:ASN:OD1	8:W:316:TYR:HD1	1.97	0.48
8:W:611:GLU:CG	8:W:816:VAL:HG12	2.32	0.48
1:E:46:VAL:O	1:E:49:ARG:HB3	2.14	0.47
1:E:63:ARG:HE	2:F:30:THR:HG21	1.76	0.47
2:F:34:ILE:HD11	2:F:55:ARG:HD2	1.96	0.47
5:G:17:ARG:NH1	7:J:-43:DA:OP2	2.46	0.47
5:G:42:ARG:HA	6:I:39:DA:OP1	2.14	0.47
6:I:-75:DC:H3'	6:I:-75:DC:H6	1.78	0.47
7:J:-33:DG:H2'	7:J:-32:DT:C6	2.49	0.47
7:J:67:DT:C2'	7:J:68:DT:H71	2.42	0.47
8:W:333:GLU:OE1	8:W:336:LYS:HE3	2.13	0.47
8:W:663:TYR:CE2	8:W:693:SER:HB3	2.48	0.47
2:B:32:PRO:HG2	6:I:-13:DA:H3'	1.95	0.47
3:C:114:VAL:O	3:C:114:VAL:HG12	2.13	0.47
2:F:80:THR:HG23	6:I:27:DG:H4'	1.95	0.47
6:I:-30:DG:C5	6:I:-29:DC:C5	2.99	0.47
6:I:-6:DT:C2'	6:I:-5:DA:C8	2.66	0.47
6:I:24:DA:C4	6:I:25:DG:C5	3.02	0.47
8:W:326:ASP:HA	8:W:329:LYS:CB	2.44	0.47
8:W:399:LEU:HA	8:W:595:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:488:LEU:HD22	8:W:490:THR:CG2	2.44	0.47
8:W:611:GLU:CA	8:W:816:VAL:HB	2.43	0.47
8:W:681:MET:CE	8:W:682:THR:HG22	2.44	0.47
8:W:754:ILE:HG12	8:W:778:ILE:CD1	2.44	0.47
8:W:1145:LEU:HD23	8:W:1145:LEU:C	2.39	0.47
2:B:27:GLN:O	2:B:29:ILE:N	2.47	0.47
1:E:61:LEU:HD22	2:F:36:ARG:HB2	1.97	0.47
1:E:74:ILE:HG13	1:E:75:ALA:N	2.29	0.47
1:E:104:PHE:HA	1:E:107:THR:OG1	2.14	0.47
6:I:-37:DG:C2'	6:I:-36:DT:C5	2.85	0.47
6:I:-22:DA:C5	6:I:-21:DC:C5	3.03	0.47
8:W:636:ALA:HA	8:W:640:GLY:HA2	1.95	0.47
8:W:1059:ALA:HB1	8:W:1132:LEU:HD11	1.95	0.47
8:W:1157:PHE:CD2	8:W:1183:LEU:HD11	2.49	0.47
1:A:68:GLN:O	1:A:72:ARG:HG2	2.14	0.47
1:A:88:ALA:HA	2:B:83:ALA:CA	2.43	0.47
1:E:47:ALA:CA	6:I:9:DG:OP1	2.63	0.47
6:I:-19:DG:C3'	8:M:743:GLY:C	2.86	0.47
7:J:-20:DC:H4'	8:W:772:ARG:NE	2.29	0.47
7:J:10:DG:H2"	7:J:11:DC:C5'	2.44	0.47
7:J:20:DG:N2	7:J:21:DG:O6	2.44	0.47
7:J:31:DT:H2"	7:J:32:DG:H8	1.79	0.47
8:M:315:ASN:HD21	8:M:458:GLY:HA2	1.78	0.47
8:W:427:PRO:O	8:W:507:TRP:CD1	2.67	0.47
8:W:688:ARG:O	8:W:691:ILE:HG22	2.15	0.47
1:A:99:TYR:CD1	1:A:100:LEU:HD12	2.48	0.47
3:C:31:HIS:HB2	3:C:48:PRO:CB	2.38	0.47
5:G:78:ILE:HD12	4:H:49:THR:CG2	2.44	0.47
7:J:-40:DC:H2"	7:J:-39:DT:OP2	2.14	0.47
7:J:78:DG:H2"	7:J:79:DG:C8	2.49	0.47
8:W:305:LEU:HD21	8:W:307:TYR:CE1	2.50	0.47
8:W:404:GLY:HA2	9:W:1502:ADP:O3B	2.15	0.47
8:W:469:TYR:O	8:W:469:TYR:CG	2.66	0.47
8:W:507:TRP:O	8:W:534:VAL:HA	2.13	0.47
8:W:508:GLN:HB2	8:W:535:ALA:CB	2.42	0.47
8:W:618:LEU:HG	8:W:622:GLN:NE2	2.30	0.47
8:W:663:TYR:OH	8:W:693:SER:HB2	2.15	0.47
8:W:767:PHE:CE2	8:W:769:LEU:CD1	2.92	0.47
8:W:1070:ARG:HG3	8:W:1110:LYS:HE3	1.96	0.47
1:A:61:LEU:HD22	2:B:36:ARG:HD3	1.97	0.47
2:F:51:TYR:O	2:F:54:THR:OG1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:25:PHE:CE1	5:G:56:GLU:CA	2.95	0.47
6:I:-57:DC:C2'	6:I:-56:DC:C5	2.94	0.47
6:I:-33:DA:H2"	6:I:-32:DC:H5'	1.97	0.47
6:I:23:DA:C4	6:I:24:DA:C6	3.03	0.47
7:J:-44:DG:N2	7:J:-43:DA:C2	2.83	0.47
8:M:506:LYS:HG2	8:M:533:LYS:HE2	1.94	0.47
8:W:469:TYR:O	8:W:469:TYR:CD2	2.68	0.47
8:W:723:MET:O	8:W:726:ILE:HB	2.15	0.47
8:W:1073:ILE:CG2	8:W:1110:LYS:HE2	2.36	0.47
8:W:1150:TYR:HD1	8:W:1156:LYS:CE	1.98	0.47
1:A:65:LEU:HD21	1:A:69:ARG:CZ	2.45	0.47
3:C:63:LEU:HD13	4:D:42:LEU:HA	1.96	0.47
3:C:91:GLU:C	3:C:91:GLU:CD	2.82	0.47
4:D:77:LEU:HD11	4:D:90:GLU:HB3	1.96	0.47
2:F:75:HIS:CE1	4:H:93:THR:CG2	2.98	0.47
5:G:29:ARG:HA	7:J:-44:DG:C5'	2.44	0.47
5:G:42:ARG:CG	6:I:38:DT:H4'	2.44	0.47
5:G:47:ALA:O	5:G:51:LEU:HG	2.14	0.47
6:I:23:DA:C8	6:I:24:DA:N7	2.83	0.47
6:I:77:DG:H2"	6:I:78:DA:H5'	1.97	0.47
7:J:-76:DG:C8	7:J:-75:DT:H72	2.49	0.47
7:J:-44:DG:H2"	7:J:-43:DA:H5'	1.95	0.47
7:J:-18:DG:C4'	8:W:493:GLU:OE2	2.62	0.47
7:J:-16:DT:OP2	8:W:497:LYS:CE	2.63	0.47
7:J:78:DG:H2"	7:J:79:DG:H8	1.79	0.47
8:M:486:ASN:OD1	8:M:487:VAL:N	2.46	0.47
8:M:656:LYS:HG2	8:M:825:VAL:HG11	1.97	0.47
8:W:377:ARG:CD	8:W:602:VAL:HG23	2.44	0.47
8:W:488:LEU:HD22	8:W:490:THR:HG22	1.97	0.47
8:W:525:LEU:HD12	8:W:525:LEU:O	2.14	0.47
8:W:606:LEU:HA	8:W:607:PRO:HD2	1.78	0.47
8:W:775:GLY:O	8:W:804:ARG:NH2	2.48	0.47
8:W:793:TRP:CZ3	8:W:829:VAL:HG21	2.50	0.47
8:W:1055:MET:HB2	8:W:1121:PHE:CZ	2.50	0.47
8:W:1067:GLU:C	8:W:1067:GLU:CD	2.83	0.47
8:W:1179:ASP:HA	8:W:1182:LEU:HD12	1.97	0.47
8:W:1197:ILE:O	8:W:1203:LEU:HD12	2.15	0.47
1:A:109:LEU:HD21	1:E:129:ARG:CZ	2.45	0.47
3:C:60:ALA:HA	4:D:41:VAL:CG1	2.45	0.47
1:E:75:ALA:CB	1:E:82:LEU:CD2	2.88	0.47
6:I:-27:DC:H2"	6:I:-26:DT:H72	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1:DT:H2"	6:I:2:DG:C8	2.49	0.47
6:I:54:DG:H2"	6:I:55:DT:C5	2.50	0.47
7:J:-50:DT:O4	7:J:-49:DG:O6	2.31	0.47
7:J:33:DT:C2	7:J:34:DC:C4	3.02	0.47
8:W:214:LEU:CD2	8:W:225:ASN:HB2	2.44	0.47
8:W:410:GLN:O	8:W:414:PHE:HB2	2.15	0.47
8:W:786:VAL:HG23	8:W:816:VAL:HG22	1.94	0.47
1:A:83:ARG:CZ	7:J:26:DA:H4'	2.44	0.47
1:A:119:ILE:HG12	2:B:43:VAL:HG11	1.96	0.47
3:C:97:LEU:HD22	3:C:100:VAL:HG21	1.97	0.47
1:E:64:LYS:O	1:E:64:LYS:HG2	2.14	0.47
1:E:75:ALA:CB	1:E:82:LEU:HD23	2.45	0.47
2:F:30:THR:HG22	7:J:-13:DA:C4'	2.28	0.47
5:G:17:ARG:CD	5:G:27:VAL:HG11	2.45	0.47
6:I:-73:DC:C2	7:J:74:DG:N2	2.82	0.47
6:I:-66:DA:H2"	6:I:-65:DT:C5	2.50	0.47
6:I:-30:DG:H1'	6:I:-29:DC:O5'	2.14	0.47
6:I:30:DT:C2'	6:I:31:DT:C7	2.93	0.47
7:J:13:DT:P	8:M:241:ARG:CG	2.91	0.47
7:J:76:DG:C5	7:J:77:DC:N4	2.83	0.47
8:W:458:GLY:HA3	8:W:462:SER:HB2	1.97	0.47
8:W:602:VAL:HG11	8:W:808:ILE:CG2	2.45	0.47
8:W:626:TYR:OH	8:W:824:THR:HA	2.15	0.47
3:C:116:LEU:HD12	3:C:116:LEU:O	2.15	0.47
5:G:25:PHE:HE2	5:G:55:LEU:HB2	1.80	0.47
6:I:-43:DT:N3	6:I:-42:DT:C4	2.83	0.47
7:J:-18:DG:H4'	8:W:493:GLU:HG2	1.74	0.47
7:J:52:DC:H2"	7:J:53:DC:C6	2.50	0.47
8:W:177:HIS:NE2	8:W:217:TRP:CD1	2.82	0.47
8:W:455:CYS:SG	8:W:489:LEU:HB2	2.55	0.47
2:B:68:ASP:OD1	4:D:97:LEU:HD22	2.14	0.46
5:G:25:PHE:HA	4:H:37:TYR:HD2	1.79	0.46
6:I:-30:DG:N9	6:I:-29:DC:C5	2.80	0.46
8:W:371:ILE:HD12	8:W:374:GLY:O	2.16	0.46
8:W:508:GLN:HA	8:W:535:ALA:H	1.80	0.46
2:B:68:ASP:O	2:B:72:TYR:CD1	2.69	0.46
6:I:-77:DC:OP2	8:W:1254[A]:ARG:NE	2.48	0.46
6:I:-40:DG:H1	7:J:40:DC:H42	1.63	0.46
8:W:390:LEU:HD12	8:W:393:LYS:CG	2.44	0.46
8:W:408:THR:CG2	8:W:443:THR:HG21	2.45	0.46
8:W:523:SER:CB	8:W:526:TYR:CB	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:602:VAL:CG1	8:W:808:ILE:CG2	2.91	0.46
8:W:1245:LYS:HA	8:W:1245:LYS:HD2	1.72	0.46
4:D:43:LYS:HD2	4:D:47:PRO:HA	1.97	0.46
1:E:61:LEU:HD13	2:F:37:LEU:N	2.22	0.46
5:G:101:THR:C	5:G:102:ILE:HD13	2.41	0.46
7:J:-1:DA:H2"	7:J:0:DG:H5'	1.96	0.46
7:J:32:DG:C4	7:J:33:DT:C4	3.03	0.46
8:W:293:SER:HB3	8:W:307:TYR:CE1	2.50	0.46
8:W:380:GLN:HG3	9:W:1502:ADP:HN62	1.80	0.46
8:W:509:PHE:CZ	8:W:538:MET:HE3	2.51	0.46
8:W:696:LYS:HB3	8:W:819:LEU:HD23	1.97	0.46
8:W:720:MET:SD	8:W:721:VAL:HG13	2.56	0.46
1:A:76:GLN:OE1	2:B:21:VAL:HG23	2.15	0.46
1:A:105:GLU:C	1:A:105:GLU:CD	2.84	0.46
1:E:65:LEU:HD13	6:I:17:DA:O5'	2.15	0.46
2:F:35:ARG:NH2	2:F:39:ARG:HH22	2.10	0.46
2:F:75:HIS:O	2:F:75:HIS:CD2	2.69	0.46
6:I:-28:DT:N1	6:I:-27:DC:C4	2.83	0.46
7:J:78:DG:C8	7:J:79:DG:N7	2.83	0.46
8:W:221:SER:CB	8:W:311:TRP:CZ2	2.98	0.46
8:W:284:PHE:CE1	8:W:314:LEU:HD13	2.50	0.46
8:W:681:MET:SD	8:W:681:MET:C	2.95	0.46
8:W:1114:LYS:O	8:W:1115:LYS:CG	2.63	0.46
1:A:125:GLN:HG2	1:A:128:ARG:HH22	1.81	0.46
3:C:17:ARG:NE	6:I:-43:DT:OP1	2.43	0.46
6:I:21:DC:OP1	8:W:525:LEU:N	2.48	0.46
7:J:-57:DT:H4'	7:J:-56:DG:OP1	2.15	0.46
7:J:31:DT:H2"	7:J:32:DG:C8	2.50	0.46
8:M:403:MET:CB	10:M:1502:BEF:F2	2.53	0.46
8:W:330:LEU:HD12	8:W:331:ALA:CB	2.45	0.46
8:W:432:VAL:CG1	8:W:440:TRP:NE1	2.79	0.46
8:W:1070:ARG:O	8:W:1073:ILE:HG22	2.15	0.46
3:C:116:LEU:HD11	3:C:118:LYS:HB2	1.97	0.46
4:D:70:ILE:CD1	4:D:98:LEU:HD12	2.44	0.46
5:G:24:GLN:NE2	4:H:41:VAL:HG12	2.30	0.46
5:G:25:PHE:CE1	5:G:56:GLU:CB	2.99	0.46
6:I:-50:DC:H2"	6:I:-49:DG:C8	2.50	0.46
7:J:-21:DG:OP1	8:W:649:LEU:HD22	2.15	0.46
7:J:23:DG:H5"	8:M:772:ARG:NH2	2.30	0.46
8:W:555:LEU:CD1	8:W:555:LEU:N	2.78	0.46
1:A:97:GLU:O	1:A:101:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PRO:HD3	6:I:-12:DC:OP2	2.16	0.46
2:B:67:ARG:NH2	4:D:96:ARG:O	2.49	0.46
3:C:102:ILE:HD11	4:D:58:ILE:HG23	1.98	0.46
1:E:85:GLN:O	1:E:86:SER:C	2.58	0.46
1:E:121:PRO:HA	2:F:53:GLU:OE1	2.16	0.46
6:I:-35:DA:N6	6:I:-34:DG:C6	2.84	0.46
7:J:-38:DA:H2"	7:J:-37:DG:OP2	2.11	0.46
7:J:-33:DG:C5	7:J:-32:DT:O4	2.69	0.46
7:J:-7:DG:H2"	7:J:-6:DG:C8	2.50	0.46
8:W:183:ILE:HD11	8:W:216:LYS:HE2	1.97	0.46
8:W:361:PHE:CG	8:W:362:GLU:N	2.84	0.46
8:W:417:TRP:O	8:W:421:ALA:CB	2.64	0.46
8:W:419:ILE:CD1	8:W:451:LEU:CD1	2.91	0.46
8:W:1117:VAL:HG12	8:W:1129:ALA:HB3	1.98	0.46
1:A:81:ASP:OD2	8:M:651:ILE:HG23	2.15	0.46
1:A:101:VAL:HG11	2:B:40:ARG:HB3	1.98	0.46
3:C:16:THR:N	3:C:19:SER:HB2	2.30	0.46
1:E:88:ALA:O	1:E:92:LEU:HG	2.16	0.46
5:G:24:GLN:NE2	4:H:44:GLN:CD	2.74	0.46
4:H:104:ALA:O	4:H:108:VAL:HG23	2.16	0.46
6:I:23:DA:C2'	6:I:24:DA:OP2	2.62	0.46
7:J:86:DA:C2'	7:J:87:DT:H71	2.45	0.46
8:W:202:PRO:HA	8:W:206:ASN:HD22	1.81	0.46
1:E:66:PRO:CG	1:E:67:PHE:H	2.29	0.46
1:E:124:ILE:HD11	2:F:50:ILE:HG12	1.98	0.46
6:I:-59:DT:C2	6:I:-58:DG:N1	2.84	0.46
7:J:-44:DG:C6	7:J:-43:DA:N6	2.84	0.46
7:J:51:DG:C4	7:J:52:DC:C4	3.03	0.46
8:W:385:ASN:O	8:W:389:PHE:CB	2.60	0.46
8:W:643:GLY:HA2	8:W:646:PHE:CE1	2.48	0.46
8:W:1164:PRO:HB2	8:W:1259:LEU:HD21	1.98	0.46
8:W:1262:PHE:HD2	8:W:1263:LEU:HD12	1.80	0.46
1:A:95:ALA:CB	2:B:90:LEU:HD13	2.46	0.46
1:E:61:LEU:HD22	2:F:36:ARG:CB	2.46	0.46
1:E:84:PHE:CA	7:J:-23:DT:OP1	2.64	0.46
1:E:128:ARG:NH1	1:E:134:ARG:HB2	2.30	0.46
5:G:28:GLY:HA3	7:J:-43:DA:OP2	2.16	0.46
5:G:42:ARG:HA	6:I:39:DA:H5"	1.97	0.46
5:G:99:ARG:HD3	5:G:99:ARG:HA	1.76	0.46
6:I:-38:DC:C2'	6:I:-37:DG:OP2	2.60	0.46
7:J:-55:DA:H2'	7:J:-54:DC:C4	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:34:DC:C2'	7:J:35:DT:H6	2.16	0.46
8:W:347:LEU:O	8:W:425:ASN:ND2	2.48	0.46
8:W:714:VAL:C	8:W:715:LEU:HD12	2.40	0.46
2:B:50:ILE:O	2:B:50:ILE:HG22	2.14	0.45
3:C:51:LEU:O	3:C:55:LEU:HG	2.16	0.45
3:C:88:ARG:HG3	3:C:108:LEU:HD23	1.98	0.45
3:C:100:VAL:HG23	3:C:100:VAL:O	2.16	0.45
1:E:43:PRO:O	1:E:44:GLY:C	2.58	0.45
6:I:23:DA:H1'	6:I:24:DA:C8	2.51	0.45
6:I:26:DG:N7	6:I:27:DG:C6	2.83	0.45
7:J:19:DC:C4	7:J:20:DG:C6	3.04	0.45
7:J:24:DC:C2'	7:J:25:DT:C6	2.86	0.45
8:W:601:ASP:C	8:W:603:GLU:N	2.74	0.45
8:W:607:PRO:HB2	8:W:813:HIS:HA	1.95	0.45
8:W:770:SER:HB2	8:W:774:GLY:N	2.32	0.45
8:W:1114:LYS:C	8:W:1115:LYS:HG2	2.41	0.45
1:A:43:PRO:HG2	6:I:-5:DA:C5'	2.39	0.45
7:J:-44:DG:N1	7:J:-43:DA:C6	2.85	0.45
7:J:-11:DC:H2'	7:J:-10:DG:C8	2.52	0.45
8:W:1039:THR:O	8:W:1040:LEU:HD12	2.15	0.45
2:B:32:PRO:HA	2:B:35:ARG:HH12	1.80	0.45
1:E:66:PRO:CA	2:F:23:ARG:O	2.64	0.45
2:F:39:ARG:O	2:F:40:ARG:C	2.59	0.45
2:F:62:LEU:O	2:F:66:ILE:HG12	2.16	0.45
6:I:26:DG:C5	6:I:27:DG:C6	3.03	0.45
7:J:64:DG:N2	7:J:65:DG:C2	2.85	0.45
8:M:295:ARG:NH2	8:M:1199:ARG:O	2.50	0.45
8:M:585:ASP:O	8:M:589:ARG:HB2	2.16	0.45
8:W:1018:TYR:OH	8:W:1128:ASN:HB2	2.16	0.45
3:C:79:ILE:CG2	3:C:80:PRO:N	2.79	0.45
4:D:81:ASN:O	4:D:82:LYS:CB	2.65	0.45
6:I:-58:DG:C2	7:J:58:DG:C6	3.04	0.45
6:I:9:DG:N7	6:I:10:DC:C4	2.84	0.45
6:I:24:DA:C1'	6:I:25:DG:C8	2.99	0.45
7:J:-46:DT:O2	7:J:-45:DG:C2	2.69	0.45
8:W:437:MET:HG3	8:W:438:PRO:HD3	1.97	0.45
8:W:512:VAL:CG1	8:W:539:LEU:HA	2.47	0.45
8:W:1043:LYS:HD2	8:W:1048:TYR:CZ	2.50	0.45
8:W:1262:PHE:CD2	8:W:1263:LEU:HD12	2.52	0.45
3:C:44:GLY:CA	4:D:87:THR:HA	2.41	0.45
2:F:66:ILE:HG22	2:F:70:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:47:ALA:O	5:G:48:PRO:C	2.56	0.45
6:I:-58:DG:N1	7:J:58:DG:O6	2.50	0.45
7:J:-87:DT:H2"	7:J:-86:DG:C8	2.51	0.45
7:J:34:DC:H1'	7:J:35:DT:C6	2.51	0.45
7:J:78:DG:H2'	7:J:79:DG:H8	1.81	0.45
8:W:272:MET:O	8:W:275:GLU:HB3	2.17	0.45
8:W:810:GLN:OE1	8:W:812:ASN:HB2	2.16	0.45
8:W:827:GLU:HG3	8:W:828:GLU:OE2	2.16	0.45
8:W:1171:SER:HB3	8:W:1245:LYS:CE	2.45	0.45
3:C:25:PHE:HD2	3:C:52:ALA:CB	2.29	0.45
5:G:42:ARG:CA	6:I:38:DT:O3'	2.65	0.45
8:W:368:PRO:C	8:W:370:PHE:N	2.74	0.45
8:W:443:THR:HG22	8:W:443:THR:O	2.16	0.45
8:W:722:ARG:O	8:W:726:ILE:HG13	2.17	0.45
8:W:1026:ASN:HA	8:W:1052:TYR:CZ	2.50	0.45
8:W:1146:ILE:HG21	8:W:1187:PHE:CE1	2.52	0.45
1:A:92:LEU:HD13	2:B:86:VAL:HG13	1.99	0.45
2:B:28:GLY:O	2:B:30:THR:HG23	2.16	0.45
1:E:62:ILE:CD1	2:F:33:ALA:O	2.62	0.45
1:E:120:MET:N	2:F:50:ILE:HD12	2.32	0.45
5:G:29:ARG:NH2	4:H:32:GLU:HB3	2.31	0.45
6:I:-19:DG:H1'	6:I:-18:DC:C5	2.52	0.45
8:W:326:ASP:HA	8:W:329:LYS:HB2	1.99	0.45
8:W:351:SER:HB2	8:W:425:ASN:H	1.80	0.45
8:W:470:GLU:HA	8:W:485:PHE:CE2	2.49	0.45
8:W:1155:LEU:C	8:W:1157:PHE:H	2.24	0.45
1:E:120:MET:CA	2:F:50:ILE:HD12	2.47	0.45
5:G:36:LYS:O	5:G:36:LYS:HG2	2.16	0.45
8:M:708:LYS:HE2	8:M:708:LYS:HA	1.97	0.45
8:W:312:ARG:O	8:W:313:ARG:C	2.59	0.45
8:W:418:LEU:HD11	8:W:428:HIS:NE2	2.32	0.45
1:A:88:ALA:HA	2:B:83:ALA:HA	1.98	0.45
3:C:43:VAL:HG12	7:J:38:DG:O3'	2.16	0.45
1:E:50:GLU:O	1:E:54:TYR:CD2	2.69	0.45
6:I:-30:DG:C5	6:I:-29:DC:N3	2.85	0.45
7:J:72:DA:N9	7:J:73:DT:H72	2.28	0.45
8:M:431:VAL:HG11	8:M:495:ILE:HD11	1.99	0.45
8:W:696:LYS:CB	8:W:819:LEU:HD23	2.46	0.45
8:W:738:PHE:HB3	8:W:766:VAL:HG13	1.98	0.45
1:E:116:ARG:HA	7:J:-3:DA:P	2.57	0.45
5:G:62:ILE:O	5:G:62:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-73:DC:N1	6:I:-72:DA:N7	2.65	0.45
6:I:-17:DT:H5'	8:M:493:GLU:OE1	2.17	0.45
7:J:-77:DC:H2'	7:J:-76:DG:H8	1.82	0.45
7:J:-35:DG:C5	7:J:-34:DA:C5	3.04	0.45
8:M:379:PHE:O	8:M:597:ARG:NH1	2.38	0.45
8:W:214:LEU:HD21	8:W:225:ASN:CB	2.43	0.45
8:W:265:GLU:O	8:W:268:GLU:HB3	2.17	0.45
8:W:509:PHE:HZ	8:W:538:MET:HE3	1.82	0.45
8:W:580:GLU:HG3	8:W:581:GLU:N	2.32	0.45
2:B:60:VAL:O	2:B:64:ASN:ND2	2.49	0.44
6:I:-28:DT:C6	6:I:-28:DT:OP2	2.70	0.44
6:I:4:DC:H2"	6:I:5:DC:C6	2.52	0.44
7:J:30:DC:H2'	7:J:31:DT:H71	1.98	0.44
7:J:81:DC:OP2	7:J:81:DC:C6	2.70	0.44
8:M:614:LEU:HD21	8:M:699:LEU:HD13	1.98	0.44
8:W:312:ARG:HD3	8:W:313:ARG:H	1.82	0.44
8:W:560:MET:HE2	8:W:560:MET:HB3	1.71	0.44
8:W:617:GLU:CD	8:W:618:LEU:H	2.24	0.44
8:W:1256:VAL:HG13	8:W:1257:ASP:N	2.32	0.44
4:D:40:LYS:O	4:D:43:LYS:HB3	2.17	0.44
2:F:25:ASN:OD1	2:F:26:ILE:N	2.51	0.44
2:F:80:THR:HG1	6:I:28:DG:C5'	2.30	0.44
6:I:0:DC:C2'	6:I:1:DT:C7	2.96	0.44
7:J:-27:DC:H2"	7:J:-26:DC:C5	2.52	0.44
7:J:-11:DC:C2	7:J:-10:DG:C5	3.05	0.44
7:J:51:DG:C6	7:J:52:DC:N3	2.85	0.44
8:W:284:PHE:CD1	8:W:314:LEU:HD22	2.52	0.44
8:W:656:LYS:HE2	8:W:826:GLU:C	2.42	0.44
8:W:674:GLN:H	8:W:674:GLN:CD	2.25	0.44
8:W:716:ILE:HD13	8:W:787:VAL:HB	1.98	0.44
8:W:770:SER:O	8:W:774:GLY:HA3	2.18	0.44
2:B:33:ALA:HA	2:B:36:ARG:HG2	1.99	0.44
3:C:26:PRO:HD3	4:D:37:TYR:CD1	2.53	0.44
3:C:34:LEU:HD22	4:D:71:ALA:HB1	1.97	0.44
3:C:93:LEU:HA	3:C:93:LEU:HD23	1.85	0.44
5:G:80:PRO:CG	4:H:55:ALA:HB2	2.42	0.44
6:I:-59:DT:N3	6:I:-58:DG:N1	2.65	0.44
6:I:27:DG:N2	6:I:28:DG:C2	2.86	0.44
8:M:622:GLN:O	8:M:626:TYR:CB	2.65	0.44
8:W:290:ILE:HB	8:W:338:PHE:CD1	2.52	0.44
8:W:432:VAL:HG11	8:W:440:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:722:ARG:HD2	8:W:722:ARG:HA	1.83	0.44
8:W:1252:LEU:HA	8:W:1255:ARG:HB2	1.98	0.44
5:G:17:ARG:O	5:G:20:ARG:N	2.50	0.44
5:G:24:GLN:HE22	4:H:44:GLN:CD	2.24	0.44
7:J:-5:DG:H1'	7:J:-4:DG:C8	2.53	0.44
7:J:20:DG:N3	7:J:21:DG:N7	2.65	0.44
8:W:470:GLU:CG	8:W:485:PHE:HE2	2.25	0.44
8:W:1164:PRO:CB	8:W:1259:LEU:HD21	2.47	0.44
1:A:62:ILE:CG2	1:A:63:ARG:N	2.80	0.44
1:A:117:VAL:HG11	6:I:-4:DC:C4'	2.48	0.44
6:I:61:DA:H2'	6:I:62:DT:H71	2.00	0.44
7:J:57:DG:H2"	7:J:58:DG:C8	2.52	0.44
8:W:377:ARG:NE	8:W:602:VAL:CG2	2.75	0.44
1:A:76:GLN:HA	1:A:79:LYS:O	2.18	0.44
2:B:20:LYS:O	2:B:22:LEU:HD12	2.18	0.44
2:B:31:LYS:CB	2:B:32:PRO:HD3	2.47	0.44
4:D:83:ARG:HD3	6:I:-34:DG:H3'	1.99	0.44
6:I:-41:DG:O6	6:I:-40:DG:O6	2.36	0.44
6:I:-28:DT:H1'	6:I:-27:DC:C6	2.53	0.44
6:I:13:DT:H2'	6:I:14:DT:H71	1.99	0.44
8:W:417:TRP:CE2	8:W:421:ALA:HB2	2.52	0.44
8:W:418:LEU:HD12	8:W:418:LEU:O	2.18	0.44
8:W:456:TYR:CD1	8:W:466:ILE:HG13	2.52	0.44
8:W:656:LYS:NZ	8:W:829:VAL:HB	2.32	0.44
8:W:706:ARG:HH11	8:W:706:ARG:HG2	1.83	0.44
3:C:108:LEU:CD1	3:C:110:ASN:HB2	2.48	0.44
5:G:24:GLN:O	4:H:37:TYR:CE2	2.70	0.44
5:G:25:PHE:CD1	5:G:56:GLU:HB2	2.53	0.44
7:J:35:DT:O3'	7:J:36:DA:C8	2.71	0.44
1:A:73:GLU:CG	2:B:25:ASN:ND2	2.77	0.44
6:I:21:DC:N4	6:I:22:DC:H42	2.15	0.44
7:J:-47:DC:C6	7:J:-47:DC:H5'	2.52	0.44
7:J:84:DG:H2"	7:J:85:DT:C7	2.48	0.44
8:M:385:ASN:O	8:M:389:PHE:CB	2.62	0.44
8:M:778:ILE:CG2	8:M:779:ASN:N	2.53	0.44
8:W:379:PHE:O	8:W:379:PHE:CG	2.70	0.44
8:W:607:PRO:CB	8:W:813:HIS:N	2.35	0.44
8:W:1017:LEU:CD1	8:W:1027:LEU:HD21	2.48	0.44
8:W:1114:LYS:O	8:W:1115:LYS:CD	2.66	0.44
1:A:124:ILE:HD12	2:B:50:ILE:CG2	2.46	0.44
3:C:25:PHE:CE1	3:C:26:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ILE:HD13	2:F:59:LYS:HE3	2.00	0.44
1:E:122:LYS:O	1:E:124:ILE:N	2.51	0.44
6:I:-30:DG:C4	6:I:-29:DC:C6	3.06	0.44
7:J:0:DG:C2	7:J:1:DC:C2	3.06	0.44
8:M:713:ARG:HB2	8:M:783:ALA:HA	2.00	0.44
8:M:715:LEU:HD22	8:M:767:PHE:HB3	2.00	0.44
8:M:747:SER:HA	8:M:750:ARG:HG2	2.00	0.44
8:W:457:MET:O	8:W:457:MET:CG	2.52	0.44
8:W:502:LEU:HA	8:W:507:TRP:CH2	2.52	0.44
8:W:591:GLN:O	8:W:594:ILE:HB	2.18	0.44
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.82	0.43
1:E:42:ARG:N	1:E:43:PRO:HD2	2.24	0.43
1:E:100:LEU:O	1:E:103:LEU:HB3	2.18	0.43
5:G:26:PRO:O	5:G:30:VAL:CG2	2.56	0.43
7:J:-25:DC:C2	7:J:-24:DT:C5	3.05	0.43
7:J:26:DA:C6	7:J:27:DG:C6	3.00	0.43
8:M:1179:GLU:O	8:M:1183:LEU:HB2	2.18	0.43
9:W:1502:ADP:H8	9:W:1502:ADP:O5'	2.01	0.43
6:I:-19:DG:C1'	6:I:-18:DC:C5	3.01	0.43
6:I:36:DC:OP2	6:I:36:DC:C6	2.70	0.43
7:J:59:DC:C4	7:J:60:DA:N1	2.86	0.43
8:W:436:THR:O	8:W:436:THR:HG22	2.18	0.43
8:W:1010:GLY:O	8:W:1014:VAL:HG23	2.18	0.43
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.34	0.43
3:C:25:PHE:HB3	3:C:52:ALA:HB1	2.01	0.43
4:D:87:THR:HG23	4:D:89:ARG:N	2.33	0.43
1:E:73:GLU:C	1:E:73:GLU:CD	2.86	0.43
1:E:124:ILE:HD11	2:F:50:ILE:CG1	2.48	0.43
2:F:43:VAL:HG12	2:F:45:ARG:H	1.83	0.43
6:I:-25:DA:H4'	6:I:-24:DG:OP1	2.17	0.43
7:J:20:DG:C2	7:J:21:DG:C6	3.03	0.43
1:A:54:TYR:HB3	2:B:40:ARG:HD3	2.00	0.43
2:B:37:LEU:O	2:B:40:ARG:HB2	2.18	0.43
3:C:32:ARG:HD2	6:I:-44:DA:OP1	2.19	0.43
4:D:83:ARG:NE	6:I:-34:DG:H2"	2.28	0.43
1:E:108:ASN:O	1:E:112:ILE:HG13	2.18	0.43
2:F:32:PRO:O	2:F:36:ARG:CG	2.54	0.43
5:G:57:TYR:CE2	4:H:103:LEU:HD12	2.53	0.43
8:M:316:TYR:OH	8:M:455:CYS:SG	2.65	0.43
8:W:505:ILE:HB	8:W:507:TRP:CZ3	2.53	0.43
8:W:577:GLU:OE1	8:W:577:GLU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:630:LEU:C	8:W:630:LEU:HD12	2.44	0.43
8:W:656:LYS:HD3	8:W:825:VAL:HG13	2.00	0.43
8:W:777:GLY:O	8:W:778:ILE:CB	2.66	0.43
8:W:800:GLN:C	8:W:803:ALA:H	2.25	0.43
1:A:99:TYR:CD1	1:A:99:TYR:C	2.96	0.43
2:B:99:GLY:O	2:B:100:PHE:CD1	2.72	0.43
4:D:99:LEU:HD13	4:D:103:LEU:HD22	2.00	0.43
5:G:111:ILE:HG23	5:G:115:LEU:HD11	1.99	0.43
6:I:-80:DG:H2"	6:I:-79:DG:C8	2.54	0.43
6:I:-65:DT:C2	6:I:-64:DC:N3	2.85	0.43
7:J:38:DG:C2	7:J:39:DA:C2	3.07	0.43
8:W:297:SER:HA	8:W:303:SER:HA	2.01	0.43
8:W:333:GLU:OE1	8:W:333:GLU:HA	2.19	0.43
8:W:348:PRO:O	8:W:483:MET:HG3	2.19	0.43
8:W:655:LEU:HG	8:W:825:VAL:CG1	2.48	0.43
8:W:696:LYS:NZ	8:W:789:PHE:O	2.50	0.43
8:W:1138:ASP:HB3	8:W:1260:LEU:CD2	2.27	0.43
8:W:1246:VAL:HG12	8:W:1247:PRO:CA	2.49	0.43
8:W:1259:LEU:HD23	8:W:1259:LEU:HA	1.84	0.43
1:A:85:GLN:HB3	6:I:-24:DG:P	2.52	0.43
1:A:126:LEU:O	1:A:130:ILE:HG23	2.19	0.43
2:B:51:TYR:O	2:B:55:ARG:HG3	2.18	0.43
3:C:81:ARG:O	3:C:85:LEU:CD1	2.67	0.43
6:I:-34:DG:H1'	6:I:-33:DA:C8	2.54	0.43
6:I:38:DT:H2"	6:I:39:DA:C8	2.54	0.43
7:J:41:DC:C2	7:J:42:DA:C8	3.07	0.43
8:W:361:PHE:CD2	8:W:422:ARG:NH2	2.78	0.43
8:W:724:LEU:HD22	8:W:768:LEU:HD13	2.00	0.43
8:W:1198:ARG:HB2	8:W:1209:ILE:CD1	2.48	0.43
1:A:59:GLU:CD	1:A:60:LEU:O	2.58	0.43
1:A:60:LEU:HD13	1:A:93:GLN:CG	2.45	0.43
1:A:88:ALA:HB1	2:B:83:ALA:HA	1.99	0.43
2:B:30:THR:HB	6:I:-12:DC:OP2	2.18	0.43
2:B:61:PHE:O	2:B:65:VAL:HG22	2.19	0.43
3:C:75:LYS:HG3	3:C:77:ARG:O	2.17	0.43
1:E:46:VAL:CG1	1:E:50:GLU:HG3	2.47	0.43
2:F:30:THR:OG1	2:F:33:ALA:CB	2.65	0.43
5:G:29:ARG:HA	7:J:-44:DG:H5"	2.00	0.43
5:G:47:ALA:CB	5:G:48:PRO:CD	2.95	0.43
5:G:97:LEU:HD11	4:H:62:PHE:CE2	2.52	0.43
6:I:-16:DT:P	8:M:459:ASN:HB3	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-38:DA:C2'	7:J:-37:DG:O5'	2.64	0.43
7:J:37:DC:C2	7:J:38:DG:C8	3.06	0.43
7:J:73:DT:OP1	8:W:1019:LYS:NZ	2.52	0.43
8:W:311:TRP:CZ3	8:W:319:ALA:HA	2.53	0.43
8:W:348:PRO:HA	8:W:425:ASN:CB	2.48	0.43
1:E:63:ARG:CD	2:F:30:THR:CG2	2.97	0.43
2:F:48:GLY:CA	2:F:51:TYR:CE2	3.00	0.43
6:I:-19:DG:H1'	6:I:-18:DC:C6	2.53	0.43
7:J:-67:DT:C2	7:J:-66:DG:C8	3.06	0.43
8:W:405:LEU:O	8:W:406:GLY:C	2.62	0.43
8:W:738:PHE:HB3	8:W:766:VAL:CG1	2.49	0.43
8:W:1150:TYR:CD1	8:W:1156:LYS:HG3	2.54	0.43
1:A:120:MET:CB	1:A:121:PRO:CD	2.83	0.43
7:J:-63:DT:H2"	7:J:-62:DA:C8	2.53	0.43
7:J:-38:DA:N9	7:J:-37:DG:C5	2.87	0.43
7:J:-35:DG:C2'	7:J:-34:DA:N7	2.81	0.43
7:J:-13:DA:H1'	7:J:-12:DA:H5'	2.00	0.43
7:J:15:DT:N3	7:J:16:DA:C6	2.87	0.43
8:M:438:PRO:HD2	8:M:751:ARG:HH21	1.84	0.43
8:M:554:ALA:O	8:M:558:PHE:HB2	2.19	0.43
8:M:807:ARG:NH1	9:M:1501:ADP:O5'	2.51	0.43
8:W:207:CYS:SG	8:W:211:TYR:HD2	2.42	0.43
8:W:649:LEU:O	8:W:654:GLU:HB3	2.18	0.43
6:I:-63:DC:O2	7:J:64:DG:N2	2.52	0.43
6:I:7:DC:C2'	6:I:8:DC:C5	3.01	0.43
6:I:43:DT:O4	7:J:-44:DG:O6	2.37	0.43
8:M:1132:SER:O	8:M:1136:ARG:CB	2.63	0.43
8:W:305:LEU:HB2	8:W:1199:ASP:CG	2.43	0.43
8:W:370:PHE:HE1	8:W:417:TRP:HZ3	1.67	0.43
8:W:613:ILE:C	8:W:614:LEU:HD12	2.42	0.43
8:W:828:GLU:OE1	8:W:828:GLU:N	2.41	0.43
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.19	0.42
2:B:73:THR:HG22	2:B:78:ARG:O	2.19	0.42
1:E:61:LEU:O	2:F:36:ARG:HG3	2.19	0.42
1:E:100:LEU:HB2	2:F:37:LEU:HD21	2.00	0.42
8:M:770:SER:HB2	8:M:773:ALA:HB3	2.01	0.42
8:W:180:ASP:HB2	8:W:218:THR:CA	2.44	0.42
8:W:1264:ARG:HH11	8:W:1264:ARG:CG	2.31	0.42
3:C:77:ARG:HD3	6:I:-55:DG:OP2	2.19	0.42
7:J:-21:DG:H2'	7:J:-20:DC:C6	2.54	0.42
7:J:59:DC:C4	7:J:60:DA:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:64:DG:C2	7:J:65:DG:N1	2.87	0.42
8:W:328:VAL:CG1	8:W:335:VAL:HG21	2.49	0.42
8:W:512:VAL:HG13	8:W:539:LEU:HA	2.00	0.42
8:W:1104:LEU:HD12	8:W:1104:LEU:C	2.43	0.42
8:W:1251:HIS:O	8:W:1255:ARG:HG2	2.19	0.42
1:A:95:ALA:HB1	2:B:90:LEU:HD13	2.02	0.42
2:B:90:LEU:CD1	2:B:97:LEU:CD1	2.88	0.42
3:C:100:VAL:CG2	2:F:98:TYR:CE2	3.00	0.42
1:E:65:LEU:N	1:E:66:PRO:HD2	2.12	0.42
5:G:57:TYR:HE2	4:H:103:LEU:HD12	1.84	0.42
5:G:63:LEU:HD23	5:G:63:LEU:HA	1.69	0.42
5:G:104:GLN:N	5:G:104:GLN:CD	2.77	0.42
7:J:-17:DT:C6	7:J:-16:DT:C5	3.07	0.42
7:J:30:DC:C5	7:J:31:DT:O4	2.72	0.42
7:J:64:DG:C2	7:J:65:DG:C2	3.07	0.42
8:W:448:ALA:HA	8:W:449:PRO:HD2	1.83	0.42
8:W:484:LYS:HA	8:W:484:LYS:HD2	1.55	0.42
8:W:609:LYS:HD3	8:W:806:HIS:CD2	2.53	0.42
2:B:30:THR:CG2	6:I:-12:DC:OP1	2.67	0.42
2:B:84:MET:HB3	2:B:84:MET:HE3	1.53	0.42
1:E:63:ARG:HE	7:J:-13:DA:H5”	1.66	0.42
2:F:47:SER:C	2:F:50:ILE:HG22	2.45	0.42
2:F:47:SER:OG	6:I:7:DC:OP1	2.36	0.42
5:G:34:LEU:CD2	4:H:67:PHE:CE1	3.02	0.42
6:I:-22:DA:N9	6:I:-21:DC:C5	2.87	0.42
7:J:24:DC:H2’	7:J:25:DT:H73	1.97	0.42
7:J:43:DA:C2’	7:J:44:DT:OP2	2.66	0.42
8:M:268:GLU:O	8:M:272:MET:CB	2.62	0.42
8:M:290:ILE:HG23	8:M:307:TYR:HB3	2.02	0.42
8:M:1083:THR:HA	8:M:1086:ARG:HE	1.84	0.42
8:W:656:LYS:HE3	8:W:829:VAL:CB	2.47	0.42
8:W:656:LYS:CE	8:W:829:VAL:HB	2.49	0.42
1:A:113:HIS:CG	1:E:126:LEU:HD21	2.53	0.42
1:A:127:ALA:O	1:A:130:ILE:HG13	2.19	0.42
4:D:65:ASP:OD1	4:D:69:ARG:NH2	2.52	0.42
6:I:21:DC:H2”	6:I:22:DC:C5’	2.50	0.42
7:J:20:DG:C5’	8:M:496:LEU:HD22	2.42	0.42
8:W:255:GLN:O	8:W:255:GLN:HG3	2.19	0.42
8:W:345:LYS:HG3	8:W:1033:GLU:O	2.19	0.42
8:W:1119:PHE:CE2	8:W:1129:ALA:HA	2.55	0.42
8:W:1121:PHE:CD2	8:W:1121:PHE:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:1146:ILE:HG23	8:W:1147:ASN:N	2.33	0.42
2:B:68:ASP:O	2:B:71:THR:HG22	2.19	0.42
3:C:102:ILE:HG13	3:C:103:ALA:N	2.33	0.42
1:E:84:PHE:C	7:J:-23:DT:OP1	2.62	0.42
1:E:108:ASN:C	1:E:108:ASN:OD1	2.62	0.42
4:H:109:SER:O	4:H:113:LYS:HG2	2.20	0.42
6:I:-73:DC:N3	6:I:-72:DA:C6	2.87	0.42
6:I:-67:DA:C5	6:I:-66:DA:C6	3.07	0.42
6:I:-35:DA:H1'	6:I:-34:DG:H5'	2.02	0.42
7:J:50:DG:C2'	7:J:51:DG:OP2	2.62	0.42
8:M:519:LYS:HG3	8:M:551:GLU:HG2	2.01	0.42
8:W:399:LEU:HD22	8:W:407:LYS:HD2	2.01	0.42
8:W:414:PHE:CD2	8:W:538:MET:CE	2.71	0.42
8:W:450:ASP:N	8:W:450:ASP:OD1	2.50	0.42
8:W:688:ARG:O	8:W:692:MET:HG2	2.19	0.42
8:W:766:VAL:O	8:W:766:VAL:CG1	2.68	0.42
1:A:72:ARG:HB2	2:B:22:LEU:HD22	2.02	0.42
5:G:31:HIS:HD2	5:G:31:HIS:O	2.03	0.42
6:I:-28:DT:C1'	6:I:-27:DC:C5	3.02	0.42
6:I:45:DC:C3'	6:I:46:DA:P	3.08	0.42
8:W:481:LYS:HD3	8:W:483:MET:CE	2.34	0.42
8:W:754:ILE:HG12	8:W:778:ILE:HG12	2.01	0.42
8:W:1074:LEU:HD21	8:W:1110:LYS:HG3	2.00	0.42
8:W:1145:LEU:CD2	8:W:1149:ASN:HD21	2.32	0.42
8:W:1157:PHE:CE2	8:W:1183:LEU:CD2	3.03	0.42
8:W:1256:VAL:CG2	8:W:1260:LEU:HD13	2.50	0.42
1:A:81:ASP:O	1:A:81:ASP:CG	2.62	0.42
2:B:32:PRO:HB3	2:B:35:ARG:HH22	1.85	0.42
7:J:-89:DT:H2"	7:J:-88:DA:C8	2.55	0.42
7:J:-81:DG:H2"	7:J:-80:DC:C5	2.55	0.42
8:M:1145:ASN:O	8:M:1149:SER:HB2	2.18	0.42
8:W:207:CYS:HA	8:W:211:TYR:CG	2.54	0.42
8:W:207:CYS:CA	8:W:211:TYR:HD2	2.29	0.42
8:W:328:VAL:HG21	8:W:1201:PRO:CB	2.45	0.42
8:W:399:LEU:HB3	8:W:540:ILE:HG22	2.01	0.42
8:W:618:LEU:HD11	8:W:824:THR:HG23	2.02	0.42
8:W:1132:LEU:CD1	8:W:1133:LEU:HG	2.50	0.42
1:A:95:ALA:HB3	2:B:90:LEU:HD11	1.97	0.42
4:H:93:THR:HG23	4:H:94:ALA:N	2.34	0.42
6:I:-37:DG:H2"	6:I:-36:DT:C6	2.51	0.42
6:I:9:DG:C5	6:I:10:DC:N3	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:22:DC:O5'	8:W:520:ASN:HB2	2.20	0.42
6:I:52:DG:H2'	6:I:53:DT:H71	2.01	0.42
7:J:-3:DA:H2"	7:J:-2:DC:H6	1.84	0.42
8:M:377:ARG:HB3	8:M:378:ASP:H	1.59	0.42
1:E:134:ARG:HH11	1:E:135:ALA:HB3	1.80	0.42
6:I:-5:DA:H8	6:I:-5:DA:OP2	2.03	0.42
7:J:78:DG:C5	7:J:79:DG:O6	2.71	0.42
8:W:654:GLU:HG3	8:W:658:ALA:HB3	2.00	0.42
8:W:824:THR:O	8:W:827:GLU:HG2	2.20	0.42
8:W:1155:LEU:C	8:W:1157:PHE:N	2.77	0.42
1:A:117:VAL:HB	6:I:-3:DG:OP2	2.12	0.41
3:C:43:VAL:HB	7:J:39:DA:OP1	2.18	0.41
6:I:-77:DC:N3	7:J:78:DG:C2	2.88	0.41
7:J:-46:DT:C2	7:J:-45:DG:N1	2.88	0.41
7:J:-19:DG:OP1	8:W:772:ARG:HD3	2.20	0.41
7:J:23:DG:C5	7:J:24:DC:N4	2.88	0.41
7:J:34:DC:C2	7:J:35:DT:C5	3.08	0.41
8:M:437:MET:HB3	8:M:438:PRO:HD3	2.02	0.41
8:W:298:LEU:N	8:W:302:THR:O	2.48	0.41
8:W:523:SER:O	8:W:526:TYR:HB3	2.20	0.41
8:W:621:VAL:HG11	8:W:672:VAL:HB	2.02	0.41
2:B:78:ARG:HG2	7:J:28:DA:OP2	2.20	0.41
1:E:63:ARG:CD	2:F:30:THR:HG21	2.47	0.41
2:F:27:GLN:HG3	2:F:28:GLY:N	2.35	0.41
5:G:85:LEU:N	5:G:85:LEU:HD12	2.35	0.41
6:I:28:DG:H2"	6:I:29:DA:H8	1.84	0.41
6:I:69:DC:H2"	6:I:70:DG:C8	2.55	0.41
7:J:-21:DG:N7	7:J:-20:DC:N4	2.67	0.41
7:J:-3:DA:C2'	7:J:-2:DC:C6	3.00	0.41
8:M:252:GLU:O	8:M:256:VAL:HG23	2.20	0.41
8:M:765:PHE:CD2	8:M:766:VAL:HG23	2.55	0.41
8:W:183:ILE:HG23	8:W:281:PHE:HD2	1.83	0.41
8:W:284:PHE:O	8:W:311:TRP:HD1	2.00	0.41
8:W:514:GLU:HA	8:W:541:THR:OG1	2.19	0.41
8:W:545:LEU:HB2	8:W:552:LEU:HD13	2.02	0.41
8:W:626:TYR:O	8:W:630:LEU:HD23	2.21	0.41
8:W:740:ARG:CB	8:W:768:LEU:HD11	2.44	0.41
8:W:1157:PHE:CB	8:W:1184:ILE:HD11	2.50	0.41
1:A:48:LEU:HD12	1:A:48:LEU:N	2.35	0.41
1:E:101:VAL:O	1:E:102:GLY:C	2.61	0.41
5:G:43:VAL:HG23	6:I:39:DA:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:88:ARG:HA	5:G:94:ASN:HB3	2.02	0.41
5:G:92:GLU:HA	5:G:95:LYS:HD2	2.02	0.41
5:G:101:THR:O	5:G:102:ILE:HD13	2.21	0.41
6:I:-30:DG:C6	6:I:-29:DC:N3	2.88	0.41
6:I:-23:DC:C4	6:I:-22:DA:C6	3.08	0.41
7:J:63:DG:H2"	7:J:64:DG:C8	2.55	0.41
8:M:214:LEU:HD13	8:M:227:TRP:CE2	2.55	0.41
8:W:305:LEU:CD2	8:W:307:TYR:OH	2.67	0.41
8:W:589:ARG:O	8:W:593:PHE:CE1	2.71	0.41
8:W:611:GLU:HG2	8:W:816:VAL:HB	2.02	0.41
8:W:720:MET:SD	8:W:721:VAL:HG12	2.61	0.41
8:W:1066:GLU:C	8:W:1066:GLU:CD	2.88	0.41
1:A:40:ARG:CG	7:J:10:DG:H5'	2.50	0.41
4:D:99:LEU:HD23	4:D:99:LEU:HA	1.82	0.41
1:E:60:LEU:CD1	1:E:93:GLN:CD	2.75	0.41
5:G:79:ILE:O	5:G:82:HIS:HB2	2.20	0.41
6:I:-15:DA:H2"	6:I:-14:DA:H8	1.84	0.41
7:J:-21:DG:C8	7:J:-20:DC:C5	3.08	0.41
7:J:23:DG:N7	7:J:24:DC:C5	2.87	0.41
8:W:255:GLN:O	8:W:255:GLN:HG2	2.20	0.41
8:W:656:LYS:HE2	8:W:826:GLU:O	2.21	0.41
8:W:833:ALA:O	8:W:836:LYS:HB2	2.19	0.41
8:W:1043:LYS:HB2	8:W:1048:TYR:CZ	2.56	0.41
2:B:26:ILE:HD12	2:B:26:ILE:HA	1.81	0.41
2:B:80:THR:OG1	7:J:27:DG:H4'	2.20	0.41
3:C:75:LYS:HG2	3:C:82:HIS:HE1	1.85	0.41
3:C:112:GLN:CB	3:C:115:LEU:HD12	2.28	0.41
1:E:63:ARG:CZ	7:J:-13:DA:C5'	2.85	0.41
5:G:42:ARG:HA	6:I:38:DT:O3'	2.20	0.41
5:G:70:ALA:HB2	5:G:78:ILE:HG13	2.02	0.41
6:I:-76:DG:N1	7:J:76:DG:C2	2.69	0.41
6:I:-19:DG:P	8:M:743:GLY:N	2.94	0.41
7:J:-18:DG:C1'	8:W:493:GLU:CD	2.93	0.41
8:M:459:ASN:OD1	8:M:460:GLN:N	2.52	0.41
8:W:179:ILE:CD1	8:W:215:ILE:HG21	2.50	0.41
8:W:391:TRP:HD1	8:W:414:PHE:HZ	1.63	0.41
1:E:87:SER:O	1:E:88:ALA:C	2.64	0.41
5:G:15:LYS:HZ3	6:I:46:DA:C4'	1.98	0.41
5:G:97:LEU:C	5:G:99:ARG:N	2.78	0.41
6:I:37:DC:H42	7:J:-38:DA:H61	1.65	0.41
8:M:1117:ALA:HB1	8:M:1129:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD13	1:A:93:GLN:NE2	2.36	0.41
1:A:83:ARG:HB3	2:B:80:THR:HG23	2.02	0.41
5:G:38:ASN:O	5:G:39:TYR:C	2.62	0.41
6:I:-13:DA:H2"	6:I:-12:DC:O5'	2.20	0.41
6:I:-5:DA:OP2	6:I:-5:DA:H2'	2.20	0.41
7:J:-18:DG:C1'	8:W:493:GLU:OE2	2.67	0.41
7:J:83:DC:H1'	7:J:84:DG:H5'	2.03	0.41
8:W:488:LEU:HD23	8:W:489:LEU:C	2.45	0.41
8:W:589:ARG:O	8:W:592:PRO:HD2	2.21	0.41
8:W:798:ASP:HA	8:W:801:ALA:HB3	2.02	0.41
8:W:1094:LYS:HE2	8:W:1097:ASN:CB	2.50	0.41
1:A:88:ALA:CB	2:B:83:ALA:HB2	2.50	0.41
3:C:112:GLN:CD	1:E:108:ASN:ND2	2.79	0.41
1:E:65:LEU:HB2	6:I:17:DA:C3'	2.36	0.41
2:F:46:ILE:HB	6:I:8:DC:OP2	2.20	0.41
2:F:100:PHE:HD1	2:F:100:PHE:HA	1.61	0.41
6:I:-76:DG:H1'	6:I:-75:DC:H5'	2.03	0.41
6:I:-40:DG:N2	7:J:40:DC:N3	2.68	0.41
6:I:23:DA:P	8:W:519:LYS:HE3	2.54	0.41
6:I:34:DT:H2'	6:I:35:DC:C5	2.44	0.41
7:J:-52:DC:H2"	7:J:-51:DG:C8	2.56	0.41
7:J:69:DC:C2'	7:J:70:DT:C5	3.01	0.41
8:M:615:ARG:HD3	8:M:822:LYS:HD3	2.02	0.41
8:M:728:GLY:HA2	8:M:738:PHE:CZ	2.56	0.41
8:W:379:PHE:O	8:W:379:PHE:CD2	2.73	0.41
8:W:1256:VAL:HG23	8:W:1260:LEU:HD13	2.02	0.41
1:A:95:ALA:HB1	2:B:90:LEU:CD1	2.49	0.41
1:A:110:CYS:SG	1:E:130:ILE:CD1	3.09	0.41
2:B:58:LEU:HD23	2:B:62:LEU:HD12	1.93	0.41
2:B:68:ASP:O	2:B:72:TYR:HD1	2.03	0.41
2:B:97:LEU:HD23	5:G:101:THR:HG23	2.00	0.41
1:E:74:ILE:HG21	2:F:59:LYS:NZ	2.36	0.41
1:E:89:VAL:O	1:E:90:MET:C	2.63	0.41
2:F:33:ALA:C	2:F:36:ARG:HG2	2.45	0.41
2:F:40:ARG:HA	2:F:40:ARG:HD3	1.92	0.41
5:G:93:LEU:HD23	5:G:93:LEU:HA	1.91	0.41
4:H:69:ARG:HB2	4:H:70:ILE:HD12	2.03	0.41
8:M:618:LEU:HD11	8:M:824:THR:HG22	2.02	0.41
8:W:214:LEU:HD11	8:W:225:ASN:OD1	2.20	0.41
8:W:347:LEU:HD22	8:W:484:LYS:HA	2.02	0.41
8:W:347:LEU:HD21	8:W:484:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:437:MET:HG3	8:W:438:PRO:CD	2.51	0.41
8:W:476:ARG:HD2	8:W:480:LYS:CB	2.50	0.41
8:W:505:ILE:O	8:W:507:TRP:CZ3	2.74	0.41
8:W:715:LEU:N	8:W:785:THR:O	2.49	0.41
8:W:1170:TRP:HB2	8:W:1174:TRP:CD1	2.54	0.41
3:C:42:ARG:HD3	7:J:38:DG:O4'	2.21	0.41
4:D:37:TYR:O	4:D:41:VAL:HG23	2.20	0.41
4:D:46:HIS:HB2	4:D:49:THR:CB	2.50	0.41
5:G:29:ARG:CA	7:J:-44:DG:H5"	2.51	0.41
5:G:103:ALA:O	5:G:104:GLN:C	2.64	0.41
6:I:27:DG:C2'	6:I:28:DG:C8	2.95	0.41
6:I:73:DT:H2"	6:I:74:DA:H8	1.86	0.41
7:J:38:DG:C4	7:J:39:DA:C5	3.08	0.41
7:J:84:DG:H2"	7:J:85:DT:C6	2.56	0.41
8:M:611:GLU:OE2	8:M:818:ARG:NH1	2.54	0.41
8:W:646:PHE:HA	8:W:649:LEU:CD1	2.37	0.41
8:W:725:ASP:O	8:W:726:ILE:C	2.64	0.41
8:W:1178:GLU:O	8:W:1182:LEU:HG	2.21	0.41
8:W:1255:ARG:HA	8:W:1255:ARG:HD2	1.51	0.41
1:A:116:ARG:NH2	1:E:113:HIS:CE1	2.88	0.40
1:E:116:ARG:CB	7:J:-3:DA:P	3.08	0.40
2:F:75:HIS:CE1	4:H:93:THR:HG21	2.53	0.40
7:J:24:DC:H2"	7:J:25:DT:OP2	2.21	0.40
8:M:655:LEU:O	8:M:659:SER:OG	2.31	0.40
8:W:348:PRO:HA	8:W:425:ASN:HB2	2.02	0.40
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.64	0.40
4:H:36:ILE:CD1	6:I:49:DC:OP1	2.70	0.40
7:J:-18:DG:C4'	8:W:493:GLU:CD	2.93	0.40
7:J:13:DT:P	8:M:241:ARG:HE	2.44	0.40
8:M:295:ARG:HA	8:M:305:LEU:HA	2.03	0.40
8:W:430:ILE:HG22	8:W:432:VAL:HG23	2.02	0.40
8:W:615:ARG:C	8:W:822:LYS:HE2	2.46	0.40
8:W:1009:ILE:CG1	8:W:1013:GLU:HB2	2.50	0.40
1:A:124:ILE:CD1	2:B:50:ILE:HG21	2.47	0.40
1:E:60:LEU:HD22	1:E:93:GLN:HG2	2.03	0.40
1:E:101:VAL:HG23	2:F:37:LEU:HD11	2.03	0.40
1:E:119:ILE:HD13	1:E:119:ILE:HG21	1.76	0.40
6:I:-59:DT:C5	6:I:-58:DG:O6	2.74	0.40
6:I:-29:DC:H2"	6:I:-28:DT:OP2	2.18	0.40
6:I:23:DA:C4	6:I:24:DA:N7	2.90	0.40
7:J:1:DC:H2"	7:J:2:DG:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:328:VAL:HG13	8:W:335:VAL:HG21	2.04	0.40
8:W:359:PRO:CG	8:W:422:ARG:HD2	2.51	0.40
8:W:525:LEU:HD12	8:W:525:LEU:C	2.45	0.40
8:W:807:ARG:HA	8:W:807:ARG:HD3	1.90	0.40
8:W:1121:PHE:O	8:W:1121:PHE:CG	2.72	0.40
2:B:36:ARG:NH2	6:I:-13:DA:P	2.94	0.40
4:D:104:ALA:O	4:D:108:VAL:HG23	2.21	0.40
2:F:15:ALA:CB	8:W:690:LEU:HD11	2.41	0.40
7:J:-37:DG:C1'	7:J:-36:DG:N7	2.82	0.40
8:M:304:GLN:OE1	8:M:323:ASN:ND2	2.55	0.40
8:W:330:LEU:HD12	8:W:331:ALA:HB2	2.03	0.40
8:W:1157:PHE:HE2	8:W:1183:LEU:HD21	1.85	0.40
3:C:92:GLU:OE1	3:C:92:GLU:N	2.49	0.40
6:I:-49:DG:H2"	6:I:-48:DC:C4	2.57	0.40
7:J:-12:DA:H1'	7:J:-11:DC:H5'	2.04	0.40
8:M:386:TRP:CD1	8:M:595:LEU:HD21	2.57	0.40
8:M:624:GLU:O	8:M:628:ASN:HB2	2.21	0.40
8:W:178:GLY:C	8:W:218:THR:OG1	2.64	0.40
8:W:401:ASP:OD1	8:W:597:ARG:NH2	2.54	0.40
8:W:601:ASP:O	8:W:603:GLU:N	2.55	0.40
8:W:656:LYS:N	8:W:825:VAL:HG11	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	95/136 (70%)	87 (92%)	7 (7%)	1 (1%)	11 46
1	E	95/136 (70%)	86 (90%)	5 (5%)	4 (4%)	2 17
2	B	81/103 (79%)	69 (85%)	10 (12%)	2 (2%)	4 26
2	F	90/103 (87%)	85 (94%)	5 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	101/130 (78%)	83 (82%)	14 (14%)	4 (4%)	2	18
4	D	93/126 (74%)	85 (91%)	7 (8%)	1 (1%)	11	46
4	H	91/126 (72%)	81 (89%)	9 (10%)	1 (1%)	11	46
5	G	103/130 (79%)	93 (90%)	10 (10%)	0	100	100
8	M	839/1468 (57%)	749 (89%)	89 (11%)	1 (0%)	48	83
8	W	868/1468 (59%)	784 (90%)	70 (8%)	14 (2%)	7	38
All	All	2456/3926 (63%)	2202 (90%)	226 (9%)	28 (1%)	14	46

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	82	LYS
1	E	42	ARG
8	M	778	ILE
8	W	474	ASN
8	W	600	LYS
8	W	602	VAL
8	W	778	ILE
8	W	794	ASN
3	C	17	ARG
8	W	221	SER
8	W	518	LEU
2	B	80	THR
1	E	47	ALA
1	E	65	LEU
8	W	459	ASN
8	W	483	MET
1	A	121	PRO
3	C	38	ASN
1	E	63	ARG
4	H	82	LYS
8	W	344	SER
8	W	427	PRO
3	C	46	GLY
3	C	80	PRO
8	W	369	PRO
2	B	81	VAL
8	W	540	ILE
8	W	181	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/111 (77%)	82 (96%)	3 (4%)	32	53
1	E	84/111 (76%)	82 (98%)	2 (2%)	43	64
2	B	68/79 (86%)	67 (98%)	1 (2%)	57	72
2	F	63/79 (80%)	63 (100%)	0	100	100
3	C	82/102 (80%)	82 (100%)	0	100	100
4	D	81/105 (77%)	80 (99%)	1 (1%)	63	75
4	H	79/105 (75%)	77 (98%)	2 (2%)	42	63
5	G	83/101 (82%)	81 (98%)	2 (2%)	43	64
8	M	772/1313 (59%)	769 (100%)	3 (0%)	84	84
8	W	787/1313 (60%)	753 (96%)	34 (4%)	26	47
All	All	2184/3419 (64%)	2136 (98%)	48 (2%)	45	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	119	ILE
1	A	126	LEU
2	B	84	MET
4	D	37	TYR
1	E	76	GLN
1	E	96	SER
5	G	78	ILE
5	G	92	GLU
4	H	29	THR
4	H	51	ILE
8	M	201	VAL
8	M	491	THR
8	M	1028	LEU
8	W	322	GLU
8	W	346	ILE

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Mol	Chain	Res	Type
8	W	366	VAL
8	W	391	TRP
8	W	478	LYS
8	W	484	LYS
8	W	495	ILE
8	W	540	ILE
8	W	541	THR
8	W	598	LEU
8	W	602	VAL
8	W	606	LEU
8	W	613	ILE
8	W	631	THR
8	W	632	LYS
8	W	633	ASN
8	W	635	SER
8	W	645	HIS
8	W	652	MET
8	W	660	ASN
8	W	681	MET
8	W	703	LEU
8	W	720	MET
8	W	721	VAL
8	W	723	MET
8	W	731	LEU
8	W	739	GLN
8	W	799	LEU
8	W	1006	MET
8	W	1124	VAL
8	W	1132	LEU
8	W	1255	ARG
8	W	1263	LEU
8	W	1268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
2	B	75	HIS
3	C	104	GLN
3	C	112	GLN
4	D	60	ASN
1	E	108	ASN

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Mol	Chain	Res	Type
5	G	24	GLN
5	G	31	HIS
5	G	38	ASN
5	G	84	GLN
5	G	112	GLN
8	M	206	ASN
8	M	225	ASN
8	M	349	GLN
8	M	396	ASN
8	M	546	GLN
8	M	548	ASN
8	M	587	HIS
8	M	591	GLN
8	M	622	GLN
8	M	653	ASN
8	M	810	GLN
8	M	813	HIS
8	M	1027	ASN
8	W	304	GLN
8	W	306	GLN
8	W	334	GLN
8	W	343	ASN
8	W	425	ASN
8	W	557	ASN
8	W	645	HIS
8	W	667	ASN
8	W	1147	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	BEF	M	1502	9	0,3,3	-	-	-		
9	ADP	M	1501	10	27,29,29	1.37	4 (14%)	42,45,45	1.99	11 (26%)
10	BEF	W	1501	9	0,3,3	-	-	-		
9	ADP	W	1502	10	27,29,29	1.75	6 (22%)	42,45,45	2.34	15 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	M	1501	10	-	5/16/32/32	0/3/3/3
9	ADP	W	1502	10	-	3/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	1502	ADP	C5-C4	5.39	1.49	1.39
9	M	1501	ADP	C5-C4	4.57	1.47	1.39
9	M	1501	ADP	C5-C6	2.72	1.48	1.41
9	W	1502	ADP	C5-C6	2.65	1.48	1.41
9	W	1502	ADP	C8-N7	2.54	1.36	1.31
9	M	1501	ADP	C8-N7	2.49	1.36	1.31
9	W	1502	ADP	C5-N7	-2.38	1.34	1.39
9	W	1502	ADP	PB-O1B	2.35	1.58	1.50
9	W	1502	ADP	PB-O2B	-2.23	1.46	1.54
9	M	1501	ADP	C5-N7	-2.17	1.34	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	1502	ADP	C5-C4-N3	-6.68	118.04	126.75
9	M	1501	ADP	C5-C4-N3	-6.25	118.59	126.75
9	W	1502	ADP	N3-C4-N9	5.52	136.18	127.08
9	M	1501	ADP	N3-C4-N9	4.84	135.05	127.08
9	W	1502	ADP	C2-N3-C4	4.01	121.22	111.75
9	M	1501	ADP	C2-N3-C4	3.86	120.88	111.75
9	W	1502	ADP	C5-N7-C8	3.78	108.88	103.51
9	W	1502	ADP	C4-C5-N7	-3.74	106.07	110.62
9	W	1502	ADP	C3'-C2'-C1'	3.70	108.45	101.43
9	M	1501	ADP	PA-O3A-PB	-3.63	120.37	132.83
9	W	1502	ADP	N3-C2-N1	-3.44	123.23	128.60
9	W	1502	ADP	PA-O3A-PB	-3.39	121.21	132.83
9	W	1502	ADP	O2B-PB-O1B	3.29	123.57	110.68
9	M	1501	ADP	C4-C5-N7	-3.26	106.64	110.62
9	M	1501	ADP	N3-C2-N1	-3.12	123.73	128.60
9	M	1501	ADP	C5-N7-C8	2.72	107.38	103.51
9	W	1502	ADP	O3B-PB-O3A	-2.70	95.58	104.64
9	W	1502	ADP	C6-C5-N7	2.62	136.91	132.02
9	M	1501	ADP	C4-N9-C8	2.52	108.45	105.73
9	W	1502	ADP	C4-N9-C8	2.52	108.45	105.73
9	M	1501	ADP	C3'-C2'-C1'	2.50	106.17	101.43
9	W	1502	ADP	O5'-PA-O1A	-2.36	99.85	109.07
9	W	1502	ADP	N9-C8-N7	-2.30	110.77	113.91
9	M	1501	ADP	C6-C5-N7	2.15	136.02	132.02
9	W	1502	ADP	C4'-O4'-C1'	2.07	114.03	109.47
9	M	1501	ADP	N9-C8-N7	-2.01	111.17	113.91

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	1501	ADP	C5'-O5'-PA-O2A
9	M	1501	ADP	C5'-O5'-PA-O3A
9	W	1502	ADP	PA-O3A-PB-O2B
9	M	1501	ADP	PA-O3A-PB-O1B
9	W	1502	ADP	O4'-C4'-C5'-O5'
9	W	1502	ADP	C3'-C4'-C5'-O5'
9	M	1501	ADP	PA-O3A-PB-O2B
9	M	1501	ADP	PA-O3A-PB-O3B

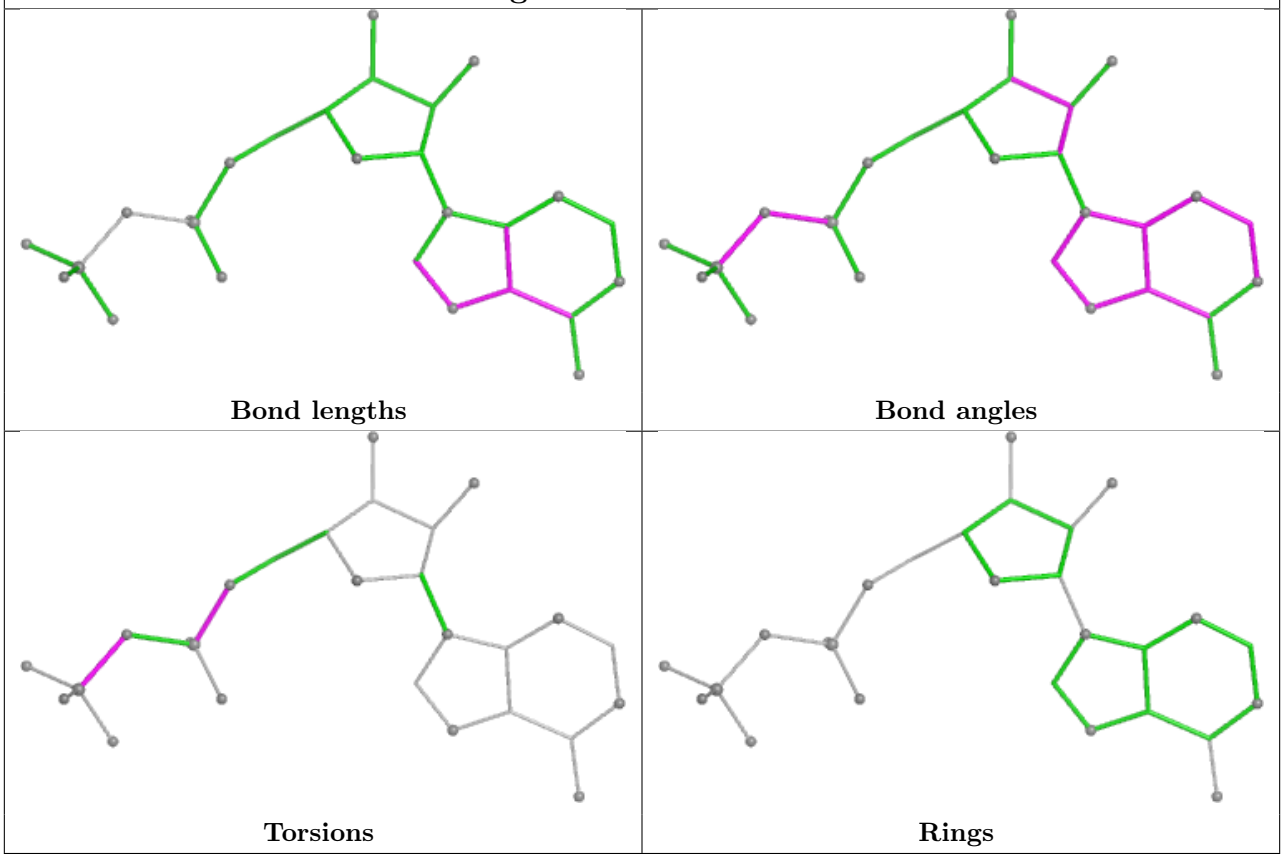
There are no ring outliers.

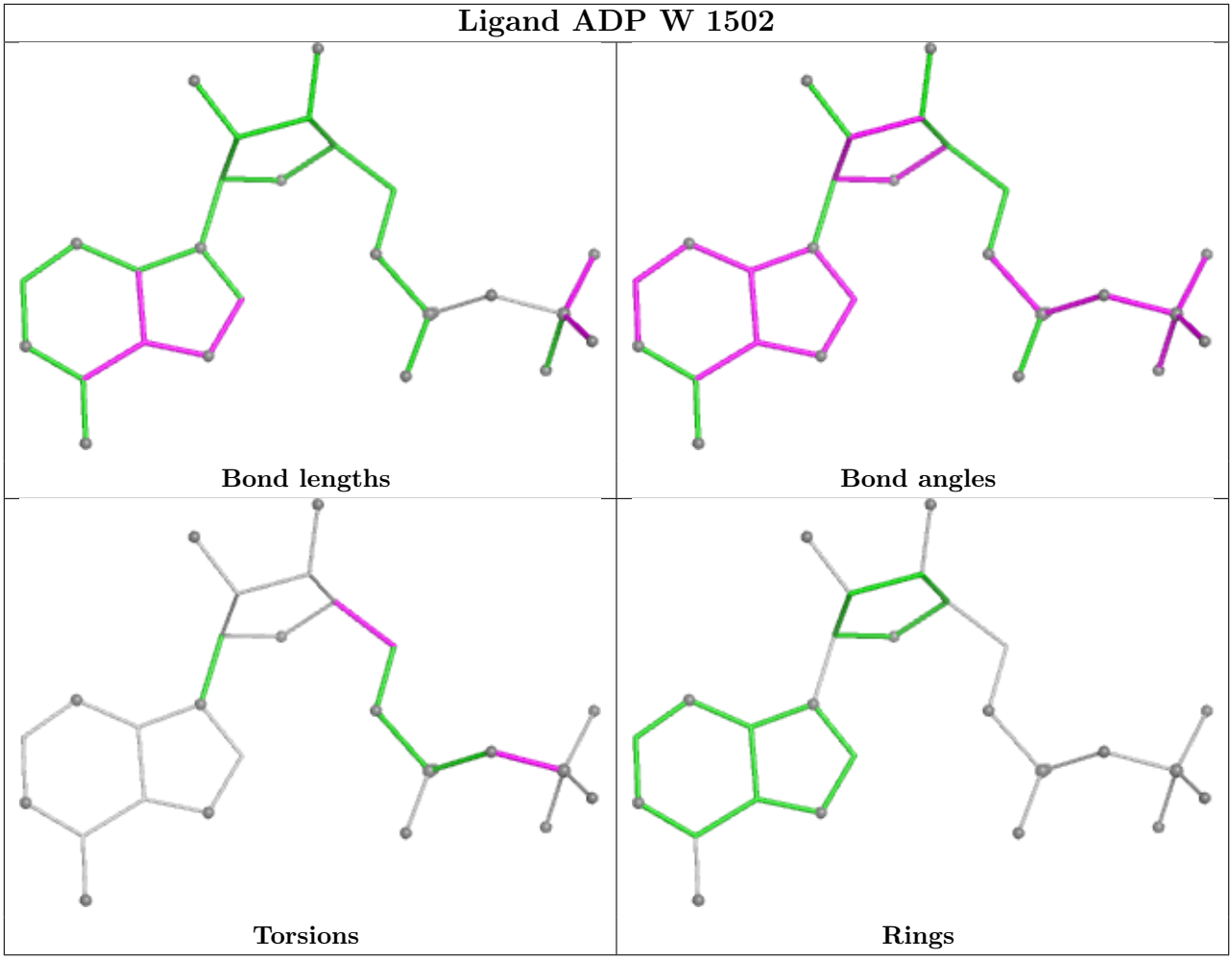
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	1502	BEF	1	0
9	M	1501	ADP	1	0
9	W	1502	ADP	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP M 1501





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	-46:DT	O3'	-45:DG	P	3.92

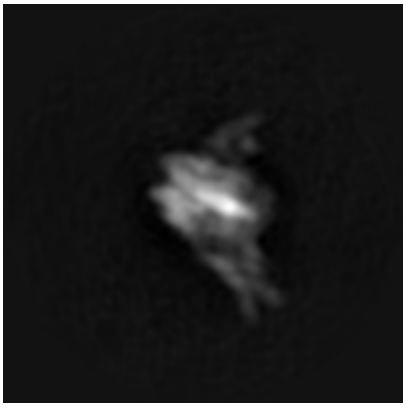
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4336. These allow visual inspection of the internal detail of the map and identification of artifacts.

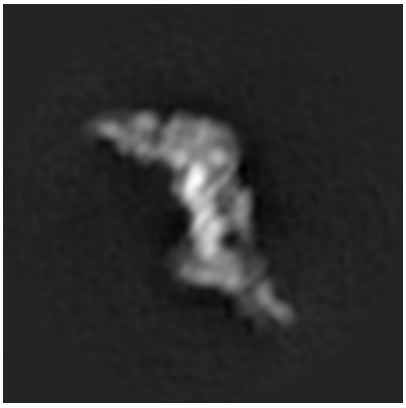
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

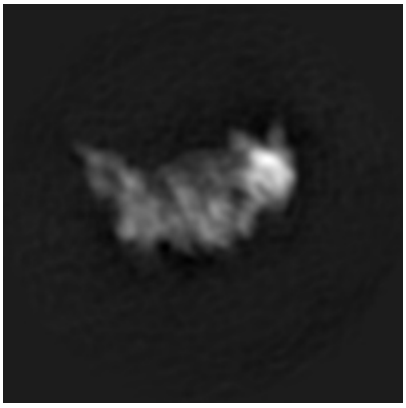
6.1.1 Primary map



X



Y



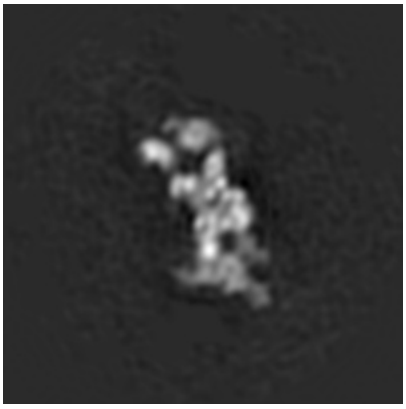
Z

The images above show the map projected in three orthogonal directions.

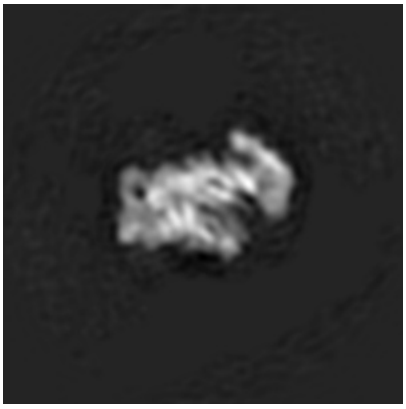
6.2 Central slices (i)

6.2.1 Primary map

X Index: 130



Y Index: 130

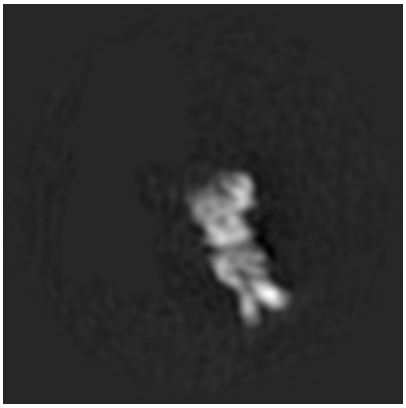


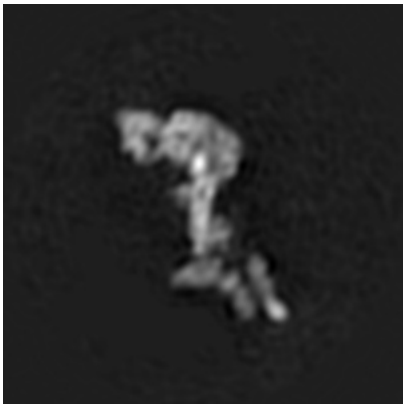
Z Index: 130

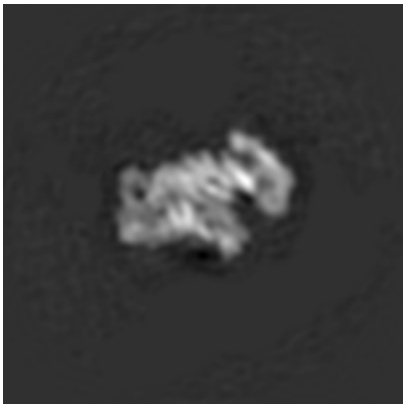
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 177

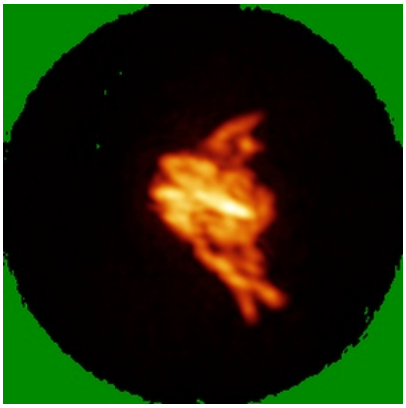

Y Index: 146


Z Index: 128

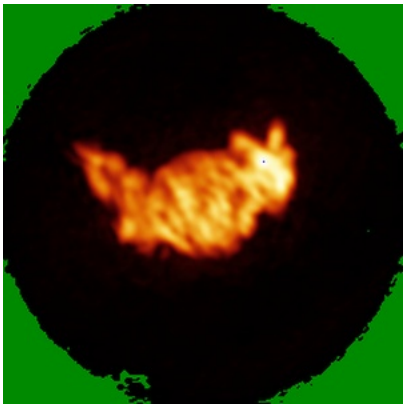
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

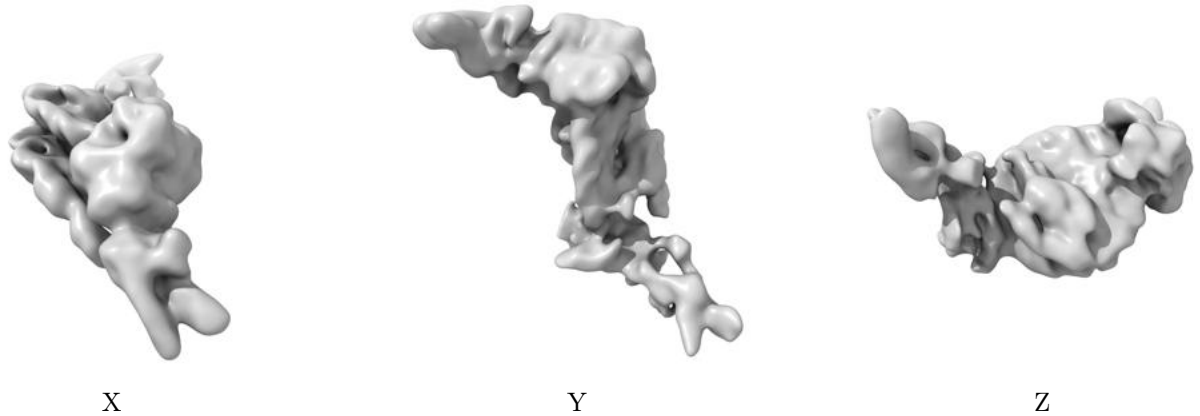
Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

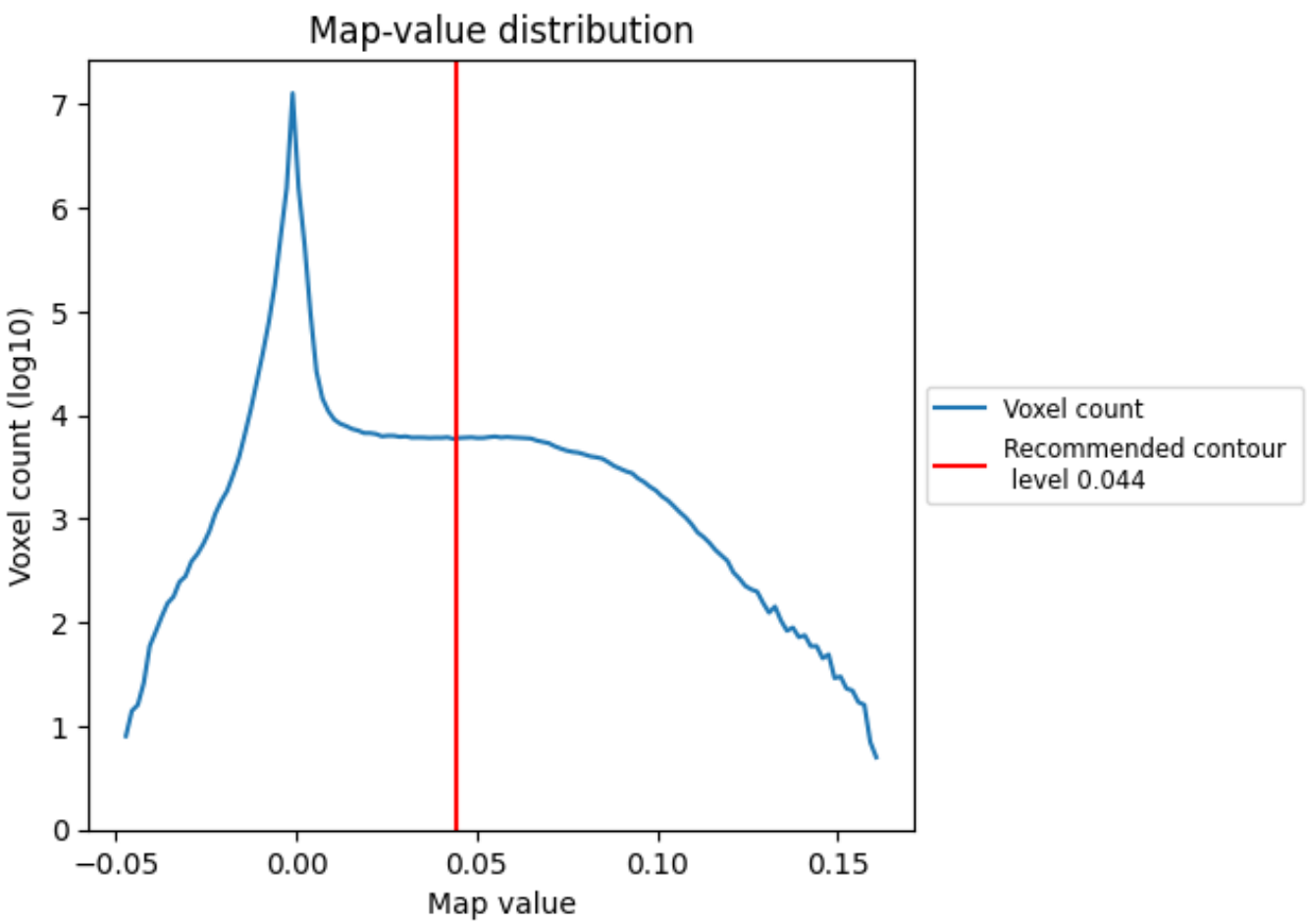
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

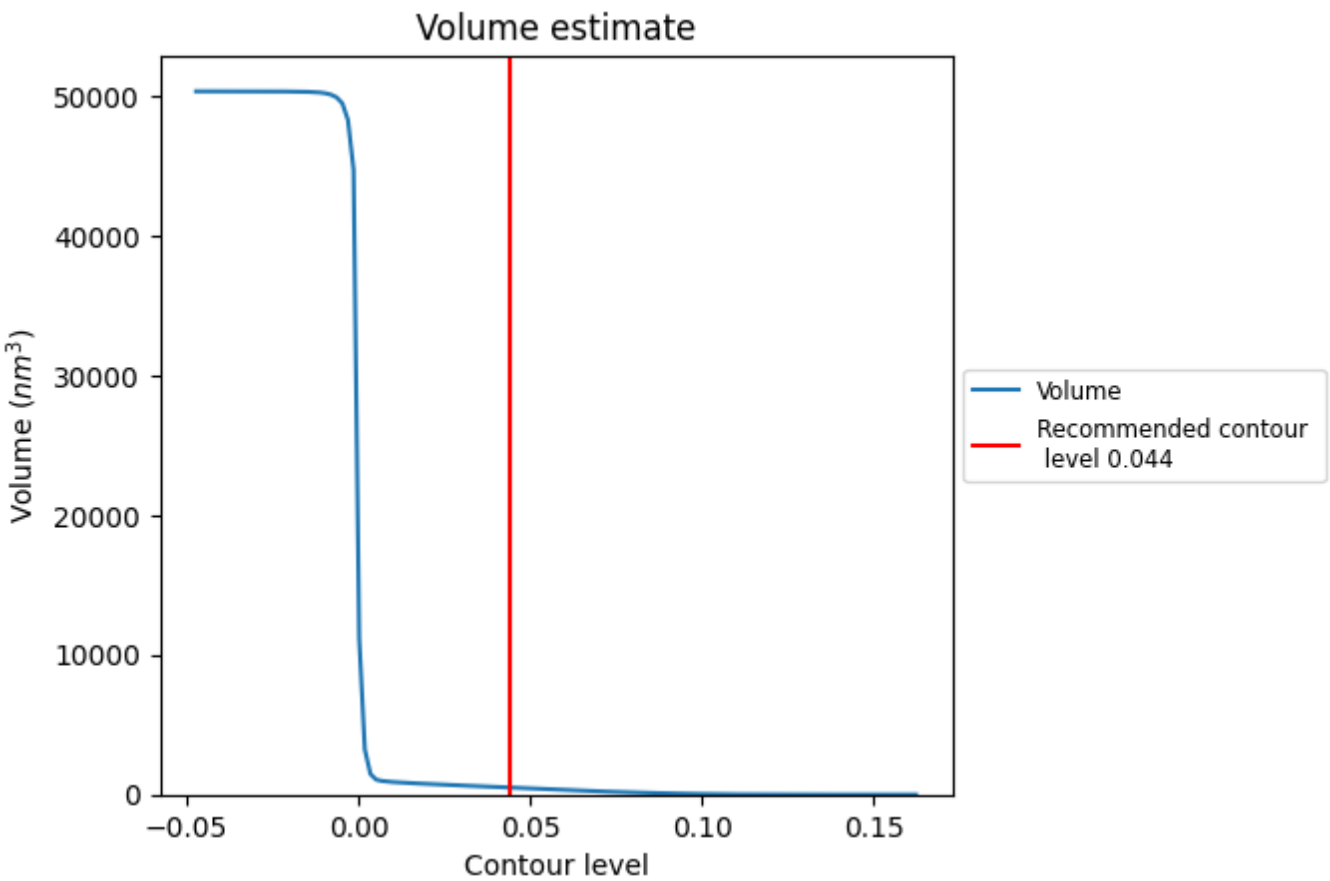
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

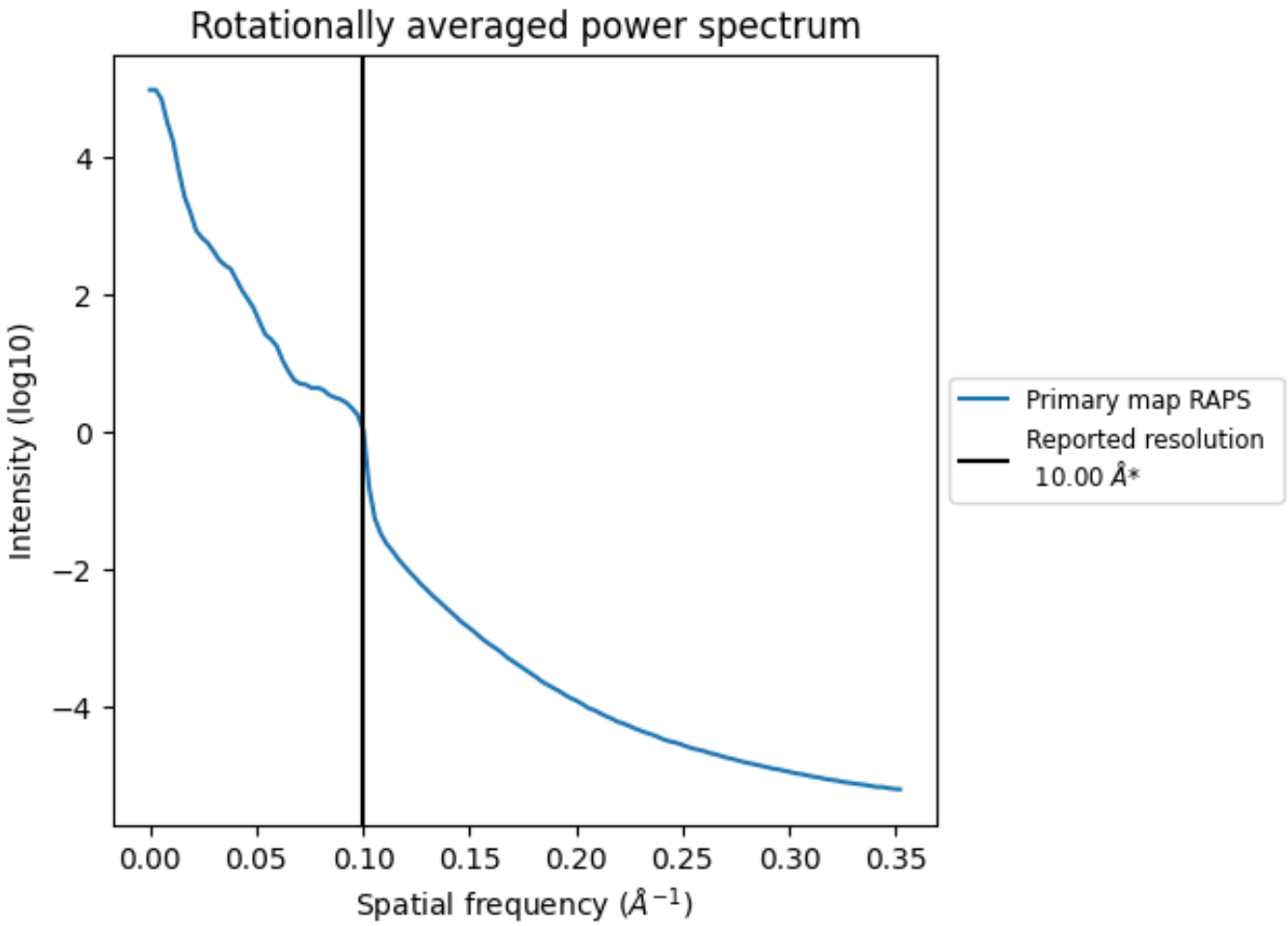
7.2 Volume estimate (i)



The volume at the recommended contour level is 503 nm^3; this corresponds to an approximate mass of 454 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

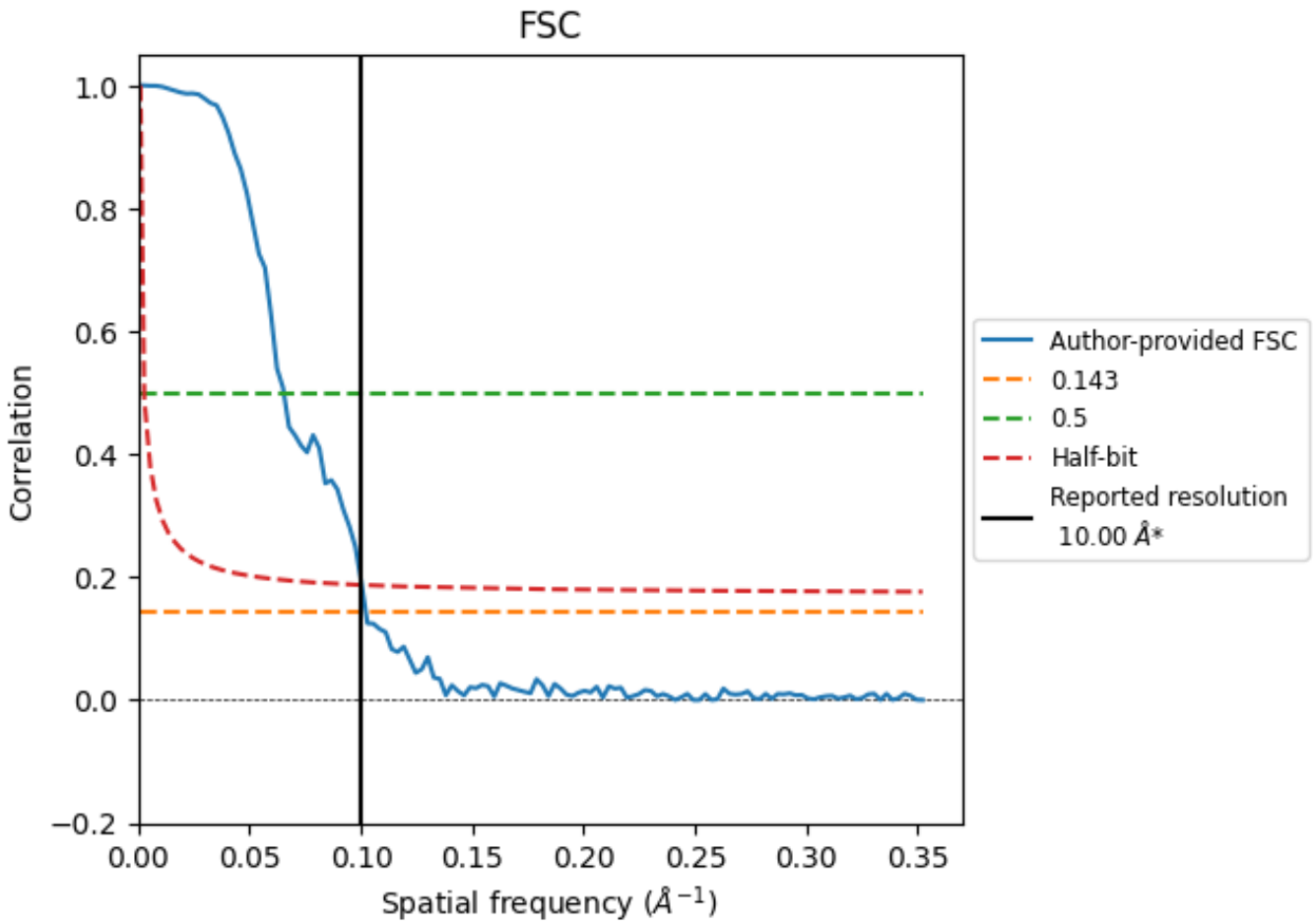


*Reported resolution corresponds to spatial frequency of 0.100 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.100 Å^{-1}

8.2 Resolution estimates (i)

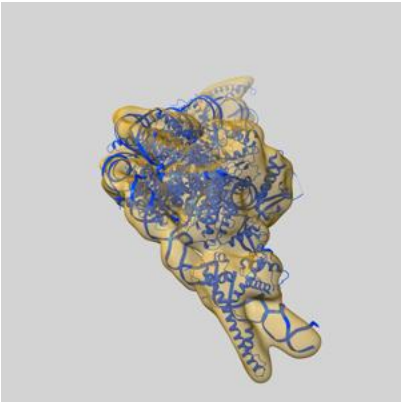
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.78	15.31	9.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

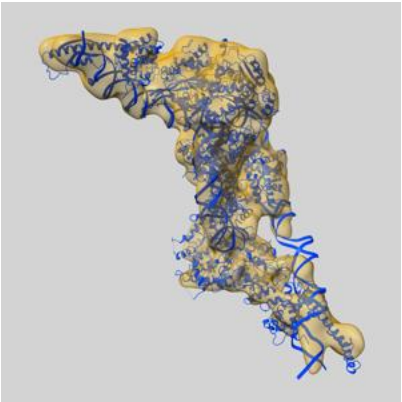
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4336 and PDB model 6G0L. Per-residue inclusion information can be found in section 3 on page 7.

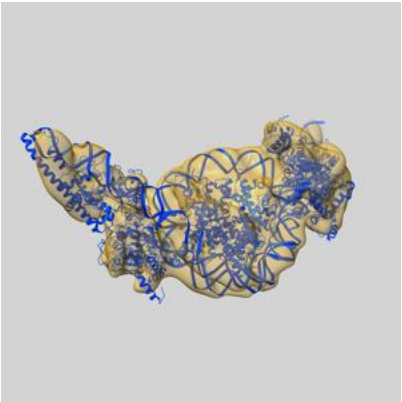
9.1 Map-model overlay (i)



X



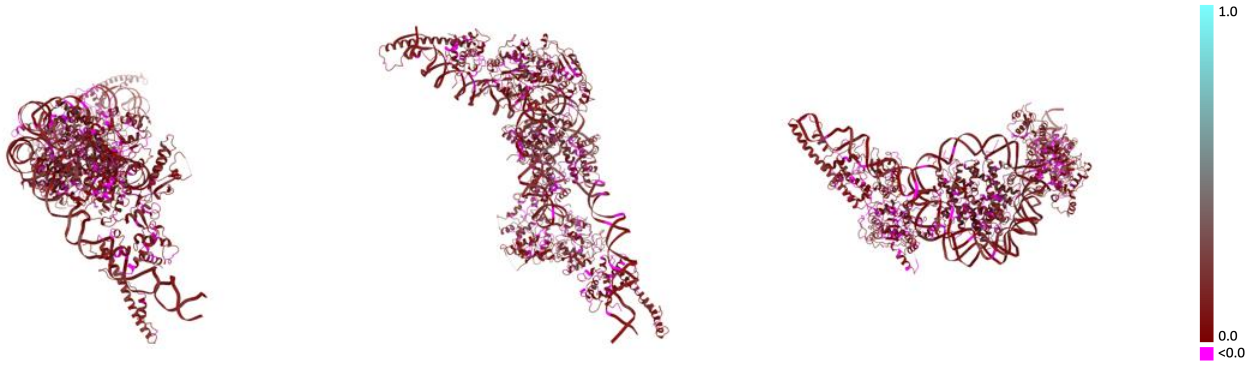
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

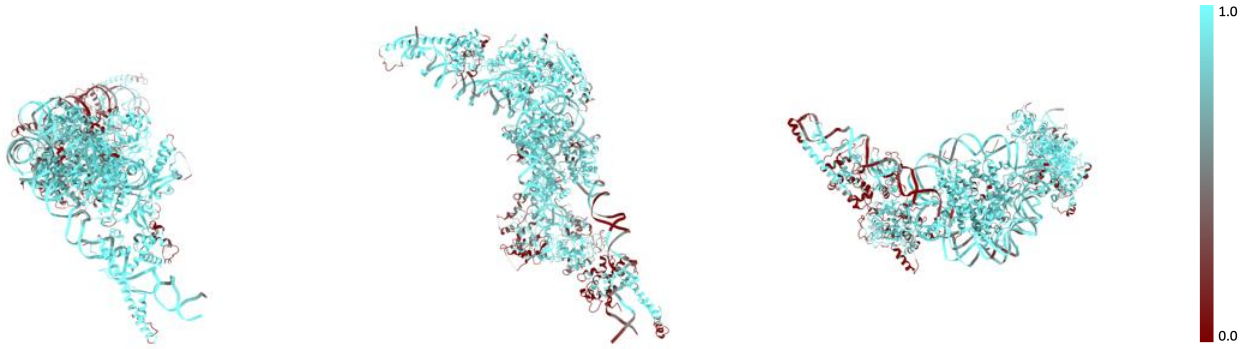
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

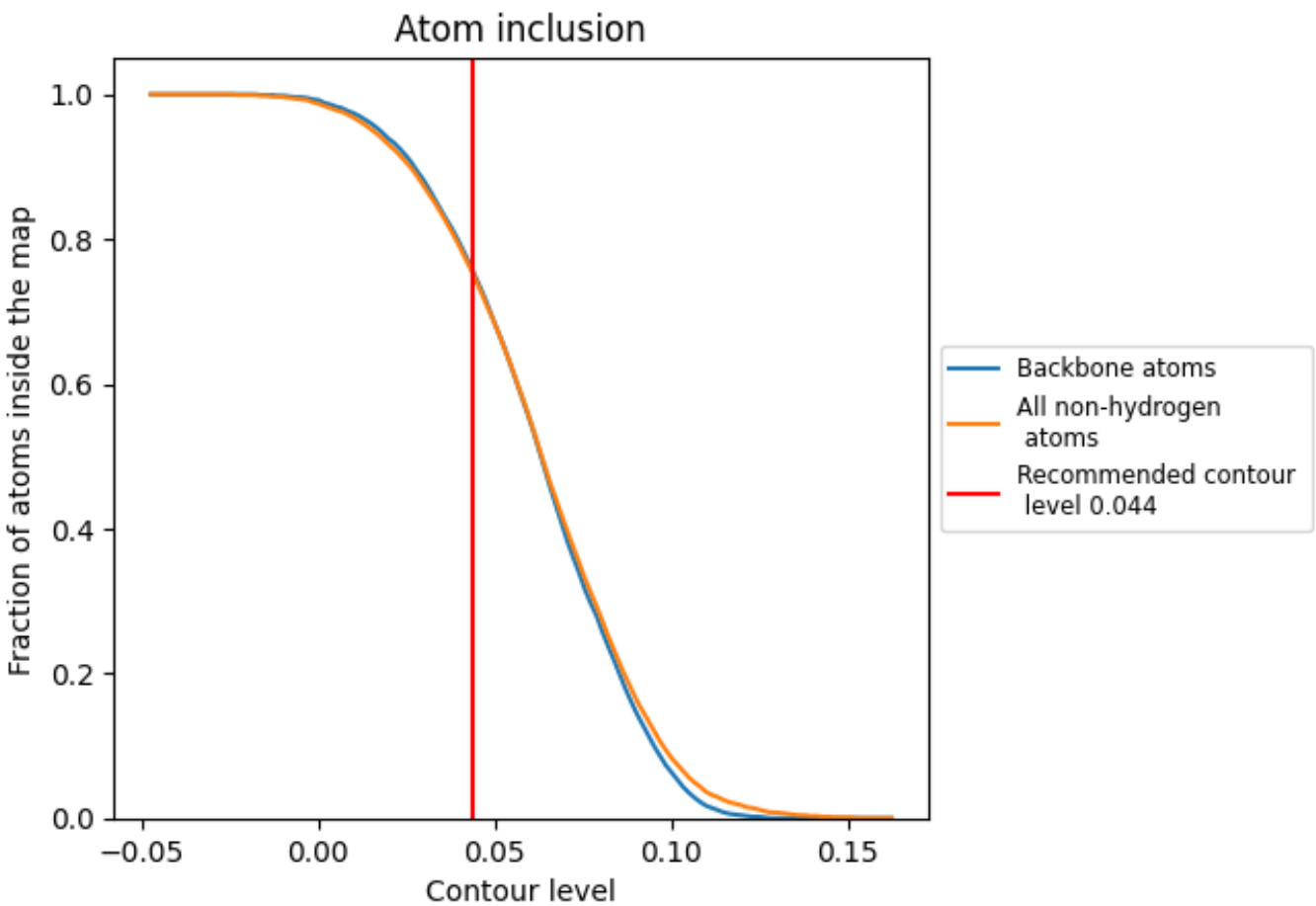
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.044).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.0950
A	0.8440	0.1140
B	0.9500	0.1000
C	0.8830	0.0650
D	0.8120	0.1020
E	0.9270	0.1220
F	0.8510	0.0640
G	0.7410	0.0690
H	0.8980	0.1310
I	0.7910	0.1190
J	0.7580	0.1190
M	0.8330	0.0930
W	0.5540	0.0730