Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2026 – 03:42 am BST

PDB ID	:	1O7T / pdb_00001o7t
Title	:	Metal nanoclusters bound to the Ferric Binding Protein from Neisseria gonorrhoeae.
Authors	:	Alexeev, D.; Zu, H.; Guo, M.; Zhong, W.; Hunter, D.J.B.; Yang, W.; Campopiano, D.J.; Sadler, P.J.
Deposited on	:	2002-11-12
Resolution	:	1.65 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

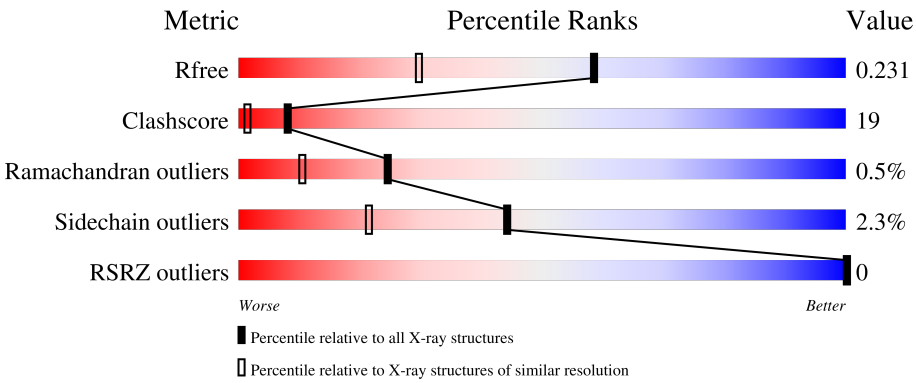
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	74% 23% •
1	B	309	73% 25% •
1	C	309	72% 27% •
1	D	309	64% 34% •

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Mol	Chain	Length	Quality of chain
1	E	309	69% 28% •
1	F	309	69% 29% •
1	G	309	65% 33% •
1	H	309	58% 37% 5%
1	I	309	64% 32% •

2 Entry composition (i)

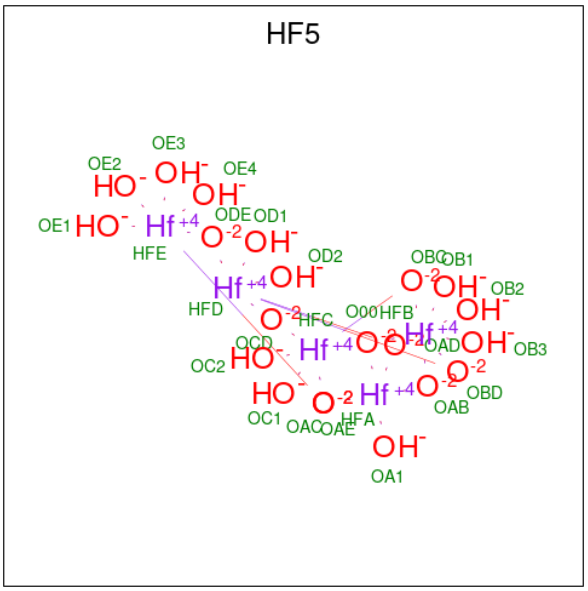
There are 5 unique types of molecules in this entry. The entry contains 23605 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 IRON BINDING PROTEIN.

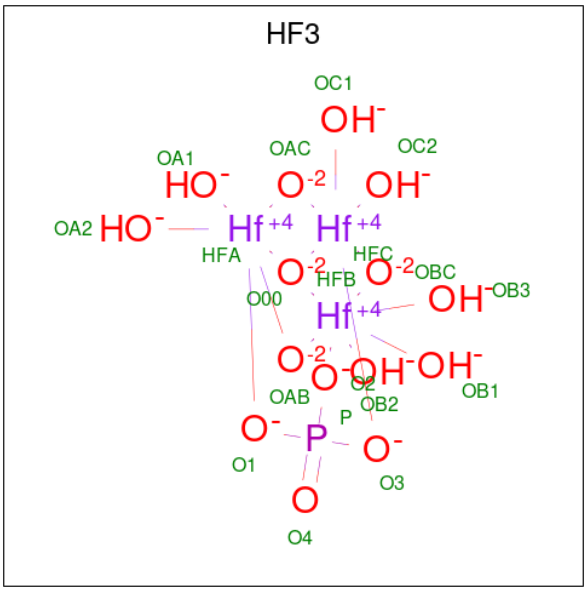
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2377	1507	423	446	1	0	0	0
1	B	309	2377	1507	423	446	1	0	0	0
1	C	309	2377	1507	423	446	1	0	0	0
1	D	309	2377	1507	423	446	1	0	0	0
1	E	309	2377	1507	423	446	1	0	0	0
1	F	309	2377	1507	423	446	1	0	0	0
1	G	309	2377	1507	423	446	1	0	0	0
1	H	309	2377	1507	423	446	1	0	0	0
1	I	309	2377	1507	423	446	1	0	0	0

- Molecule 2 is HF OXO CLUSTER HF5 (CCD ID: HF5) (formula: $H_{12}Hf_5O_{21}$).



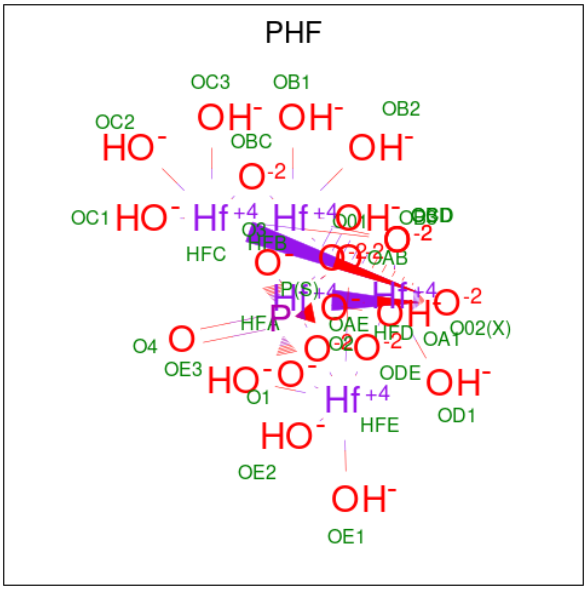
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Hf	O	0	0
			26	5	21		
2	B	1	Total	Hf	O	0	0
			26	5	21		
2	C	1	Total	Hf	O	0	0
			26	5	21		
2	E	1	Total	Hf	O	0	0
			26	5	21		
2	F	1	Total	Hf	O	0	0
			26	5	21		

- Molecule 3 is SMALLEST HF-OXO-PHOSPHATE CLUSTER HF3 (CCD ID: HF3) (formula: $H_7Hf_3O_{15}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Hf	O	P		
3	D	1	19	3	15	1	0	0

- Molecule 4 is HF-OXO-PHOSPHATE CLUSTER PHF (CCD ID: PHF) (formula: $H_{11}Hf_5O_{23}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Hf	O	P		
4	G	1	29	5	23	1	0	0
4	H	1	29	5	23	1	0	0
4	I	1	29	5	23	1	0	0

- Molecule 5 is water.

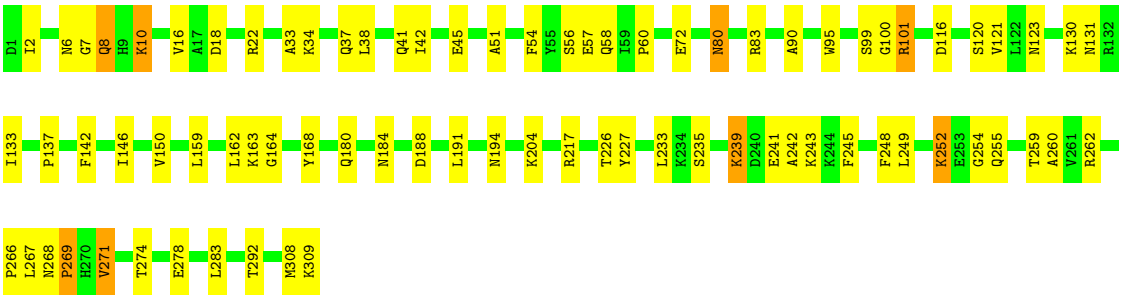
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	256	256	256	0	0
			Total	O		
5	B	220	220	220	0	0
			Total	O		
5	C	223	223	223	0	0
			Total	O		
5	D	210	210	210	0	0
			Total	O		
5	E	243	243	243	0	0
			Total	O		
5	F	227	227	227	0	0
			Total	O		
5	G	212	212	212	0	0
			Total	O		
5	H	188	188	188	0	0
			Total	O		
5	I	197	197	197	0	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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

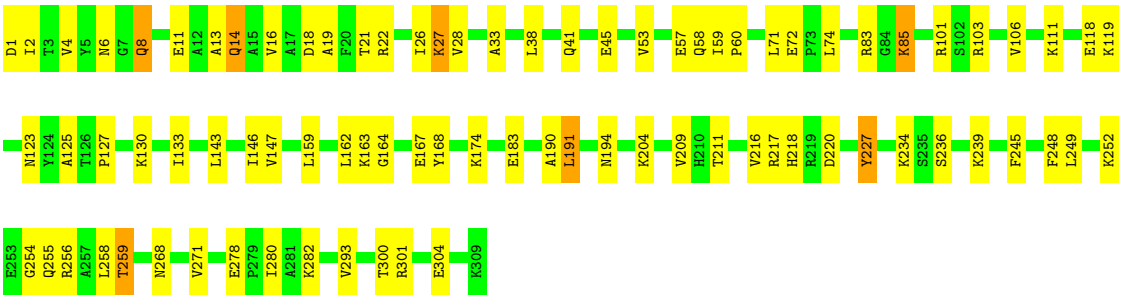
- Molecule 1: IRON BINDING PROTEIN

Chain A:



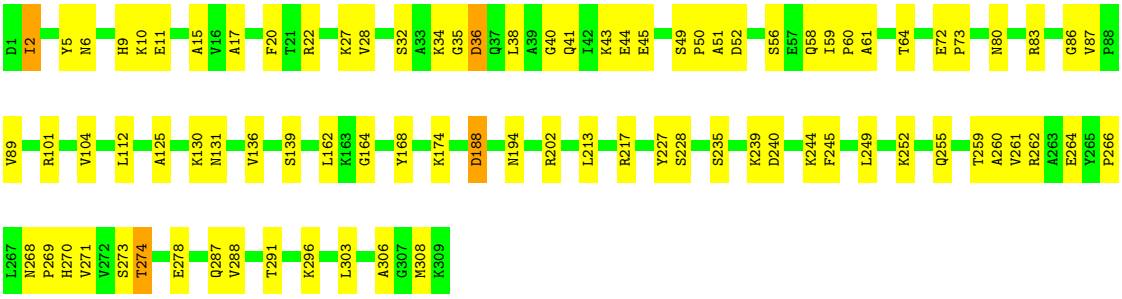
- Molecule 1: IRON BINDING PROTEIN

Chain B:



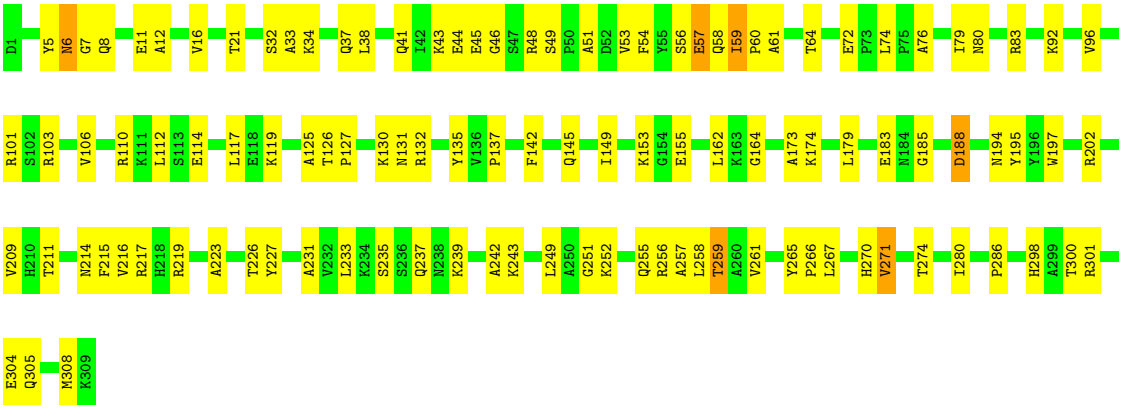
- Molecule 1: IRON BINDING PROTEIN

Chain C:



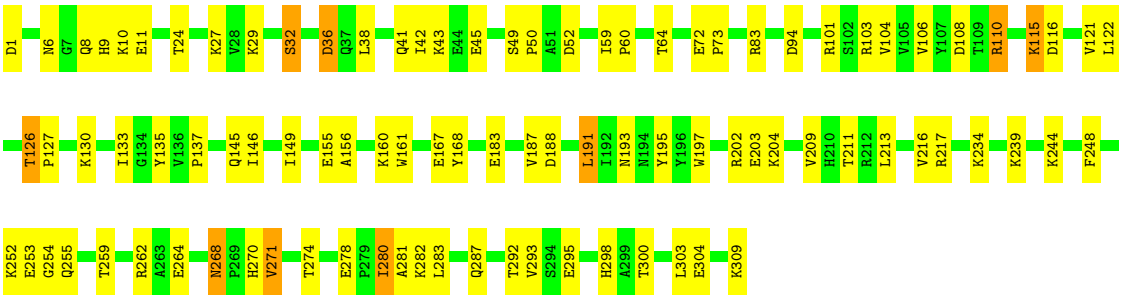
• Molecule 1: IRON BINDING PROTEIN

Chain D: 64% 34% •



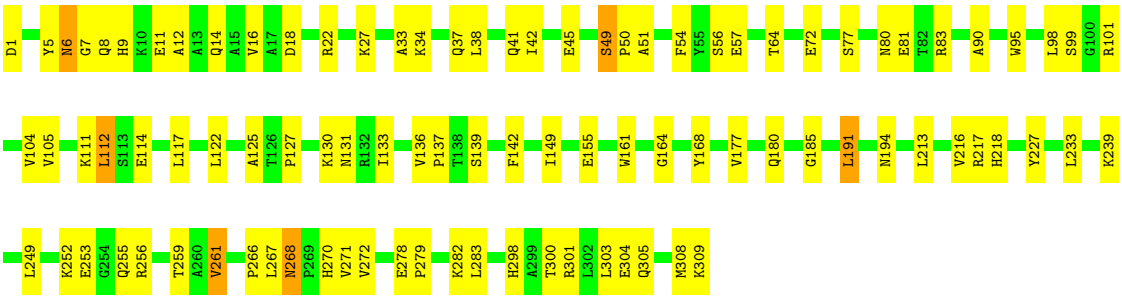
• Molecule 1: IRON BINDING PROTEIN

Chain E: 69% 28% •



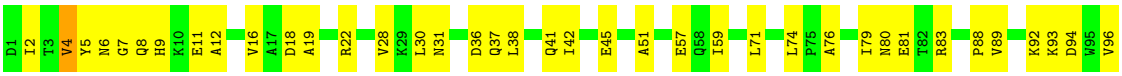
• Molecule 1: IRON BINDING PROTEIN

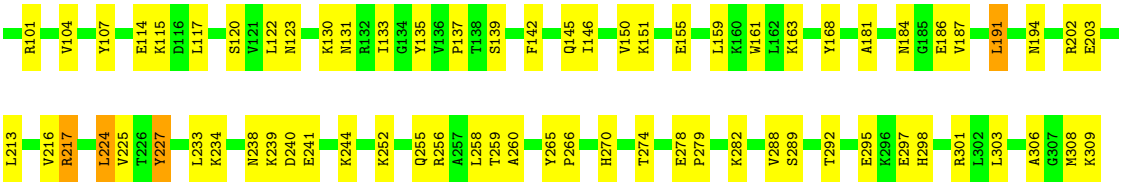
Chain F: 69% 29% •



• Molecule 1: IRON BINDING PROTEIN

Chain G: 65% 33% •



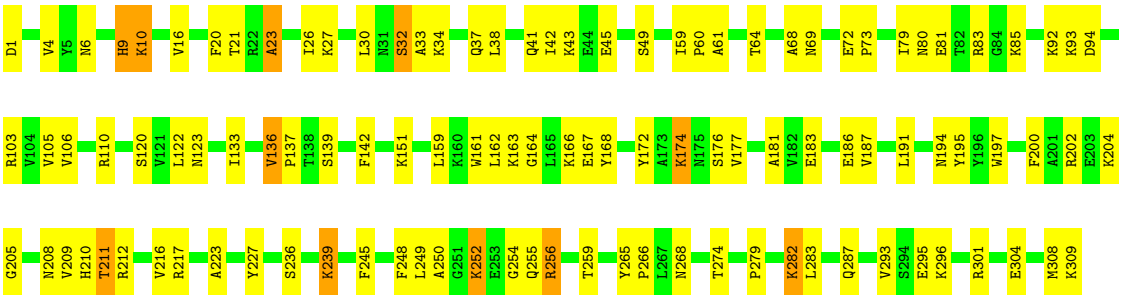


- Molecule 1: IRON BINDING PROTEIN

Chain H:

- Molecule 1: IRON BINDING PROTEIN

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	148.13Å 148.13Å 115.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.65 30.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.65) 99.9 (30.00-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.55Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.164 , 0.262 0.165 , 0.231	Depositor DCC
R_{free} test set	27813 reflections (6.84%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.090 for -h,-k,l 0.089 for h,-h-k,-l 0.427 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	23605	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: HF3, HF5, PHF

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	0.48	0/2422	1.02	13/3279 (0.4%)
1	B	0.46	0/2422	0.95	5/3279 (0.2%)
1	C	0.46	0/2422	0.98	7/3279 (0.2%)
1	D	0.47	0/2422	0.93	5/3279 (0.2%)
1	E	0.48	0/2422	0.95	9/3279 (0.3%)
1	F	0.47	0/2422	0.99	7/3279 (0.2%)
1	G	0.45	0/2422	0.95	5/3279 (0.2%)
1	H	0.44	0/2422	1.00	13/3279 (0.4%)
1	I	0.45	0/2422	0.95	9/3279 (0.3%)
All	All	0.46	0/21798	0.97	73/29511 (0.2%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	GLN	OE1-CD-NE2	-9.42	113.18	122.60
1	B	194	ASN	N-CA-C	8.40	120.52	111.36
1	A	194	ASN	N-CA-C	8.31	119.97	111.07
1	G	194	ASN	N-CA-C	8.02	120.74	111.11
1	F	194	ASN	N-CA-C	7.95	119.58	111.07
1	C	194	ASN	N-CA-C	7.94	120.63	111.11
1	H	70	LEU	N-CA-C	-7.90	103.71	112.72
1	C	239	LYS	N-CA-C	7.28	119.30	111.36
1	D	227	TYR	N-CA-C	7.18	121.36	109.95
1	H	188	ASP	N-CA-C	6.95	118.51	111.07
1	B	227	TYR	N-CA-C	6.80	120.95	110.42
1	E	32	SER	N-CA-C	6.77	119.72	108.96
1	F	6	ASN	N-CA-C	6.70	119.64	108.73
1	F	261	VAL	N-CA-C	6.65	117.28	111.90
1	D	271	VAL	N-CA-C	6.55	117.73	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	6	ASN	N-CA-C	6.48	119.27	108.96
1	A	8	GLN	CG-CD-NE2	6.47	126.10	116.40
1	H	194	ASN	N-CA-C	6.38	119.92	111.75
1	H	155	GLU	N-CA-C	6.36	117.87	111.07
1	E	217	ARG	CB-CA-C	-6.32	108.27	115.79
1	H	247	ALA	N-CA-C	-6.31	104.69	112.38
1	A	6	ASN	N-CA-C	6.29	119.13	107.99
1	G	6	ASN	N-CA-C	6.27	118.94	108.73
1	A	239	LYS	N-CA-C	6.27	118.91	111.33
1	C	188	ASP	N-CA-C	6.12	117.95	111.28
1	I	136	VAL	CA-C-N	6.08	125.97	119.28
1	I	136	VAL	C-N-CA	6.08	125.97	119.28
1	H	227	TYR	N-CA-C	5.96	119.66	110.42
1	H	72	GLU	CA-C-N	5.94	127.26	119.84
1	H	72	GLU	C-N-CA	5.94	127.26	119.84
1	I	239	LYS	N-CA-C	5.90	117.79	111.36
1	F	49	SER	CA-C-N	5.87	126.38	120.04
1	F	49	SER	C-N-CA	5.87	126.38	120.04
1	I	211	THR	N-CA-C	5.86	119.19	110.52
1	A	269	PRO	N-CA-C	5.86	121.23	114.03
1	A	227	TYR	N-CA-C	5.83	119.45	110.42
1	C	52	ASP	N-CA-C	-5.82	106.72	113.88
1	I	227	TYR	N-CA-C	5.79	119.15	109.95
1	G	4	VAL	N-CA-C	5.78	116.17	107.80
1	F	227	TYR	N-CA-C	5.77	119.09	110.14
1	A	242	ALA	N-CA-C	-5.74	104.48	112.45
1	E	188	ASP	N-CA-C	5.64	117.88	111.11
1	C	10	LYS	N-CA-C	5.64	117.88	111.11
1	H	6	ASN	N-CA-C	5.60	117.86	108.73
1	A	260	ALA	N-CA-C	-5.51	106.39	113.23
1	H	218	HIS	N-CA-C	5.48	118.75	111.30
1	B	252	LYS	N-CA-C	5.44	117.64	111.11
1	E	271	VAL	N-CA-C	5.41	116.77	108.71
1	E	52	ASP	N-CA-C	-5.40	105.75	112.93
1	I	256	ARG	N-CA-C	-5.39	105.31	111.14
1	I	32	SER	N-CA-C	5.38	118.39	109.46
1	H	79	ILE	N-CA-C	5.37	115.58	110.42
1	A	10	LYS	N-CA-C	5.31	117.07	111.28
1	A	188	ASP	N-CA-C	5.20	117.34	111.11
1	D	242	ALA	N-CA-C	-5.18	105.75	111.71
1	H	107	TYR	N-CA-C	5.17	117.25	109.23
1	E	126	THR	CA-C-N	5.16	125.45	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	126	THR	C-N-CA	5.16	125.45	119.47
1	F	112	LEU	N-CA-C	5.16	116.91	109.07
1	G	217	ARG	CB-CA-C	-5.13	109.11	115.89
1	G	227	TYR	N-CA-C	5.11	118.08	109.95
1	D	188	ASP	N-CA-C	5.11	117.24	111.11
1	C	87	VAL	CA-C-N	5.10	125.39	119.93
1	C	87	VAL	C-N-CA	5.10	125.39	119.93
1	E	116	ASP	N-CA-C	-5.10	106.65	112.92
1	A	274	THR	N-CA-C	-5.08	106.78	113.17
1	H	238	ASN	N-CA-C	-5.08	104.38	110.88
1	B	280	ILE	N-CA-C	5.07	116.40	110.62
1	D	6	ASN	N-CA-C	5.07	116.99	108.73
1	I	274	THR	N-CA-C	-5.05	107.12	113.28
1	A	271	VAL	N-CA-C	5.02	115.81	108.53
1	B	217	ARG	CB-CA-C	-5.01	109.28	115.89
1	I	252	LYS	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

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	2377	0	2422	59	0
1	B	2377	0	2422	74	0
1	C	2377	0	2422	84	0
1	D	2377	0	2422	109	0
1	E	2377	0	2422	79	0
1	F	2377	0	2422	82	0
1	G	2377	0	2422	103	0
1	H	2377	0	2422	141	0
1	I	2377	0	2422	102	0
2	A	26	0	0	3	0
2	B	26	0	0	1	0
2	C	26	0	0	2	0
2	E	26	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	26	0	0	0	0
3	D	19	0	0	2	0
4	G	29	0	0	2	0
4	H	29	0	0	2	0
4	I	29	0	0	3	0
5	A	256	0	0	8	0
5	B	220	0	0	12	0
5	C	223	0	0	7	0
5	D	210	0	0	12	0
5	E	243	0	0	10	0
5	F	227	0	0	5	0
5	G	212	0	0	13	0
5	H	188	0	0	19	0
5	I	197	0	0	7	0
All	All	23605	0	21798	846	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 19.

All (846) 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)
1:F:259:THR:HG21	1:F:266:PRO:HG3	1.29	1.12
1:D:202:ARG:HH22	1:D:274:THR:HG22	1.08	1.08
1:H:288:VAL:HG12	1:H:289:SER:H	1.17	1.05
1:A:259:THR:HG21	1:A:266:PRO:HG3	1.37	1.03
1:C:202:ARG:HH22	1:C:274:THR:HG23	1.21	1.03
1:D:101:ARG:HH12	1:D:226:THR:HB	1.18	1.03
1:H:106:VAL:HG22	1:H:211:THR:HG21	1.38	1.01
1:H:1:ASP:N	1:H:26:ILE:HG23	1.74	1.01
1:E:197:TRP:HE1	1:E:211:THR:HG23	1.22	1.00
1:I:255:GLN:NE2	1:I:268:ASN:HB2	1.76	1.00
1:H:80:ASN:HD21	1:H:83:ARG:HH11	1.10	0.99
1:H:1:ASP:H1	1:H:26:ILE:HG23	1.28	0.99
1:C:162:LEU:HD22	1:C:308:MET:HE1	1.44	0.98
1:G:83:ARG:HE	1:G:83:ARG:HA	1.27	0.95
1:D:80:ASN:HA	1:D:83:ARG:HG2	1.48	0.95
1:G:83:ARG:HH22	1:G:89:VAL:HG22	1.30	0.94
1:I:259:THR:HG21	1:I:266:PRO:HG3	1.48	0.92
1:H:259:THR:HG23	1:H:273:SER:HA	1.49	0.92
1:H:5:TYR:HB3	1:H:38:LEU:HD13	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:THR:CG2	1:C:273:SER:HA	2.02	0.90
1:H:27:LYS:HG2	1:H:28:VAL:H	1.35	0.90
1:E:202:ARG:NH2	1:E:274:THR:HG22	1.87	0.89
1:A:146:ILE:HD11	1:A:162:LEU:HD21	1.54	0.88
1:C:86:GLY:HA2	1:C:287:GLN:HE21	1.39	0.88
1:D:202:ARG:NH2	1:D:274:THR:HG22	1.89	0.88
1:H:33:ALA:HB3	1:H:38:LEU:HD21	1.56	0.87
1:H:71:LEU:HG	1:H:94:ASP:HB2	1.56	0.87
1:E:115:LYS:HE2	1:E:115:LYS:HA	1.57	0.86
1:C:259:THR:HG21	1:C:273:SER:HA	1.57	0.86
1:E:202:ARG:HH22	1:E:274:THR:HG22	1.37	0.86
1:A:80:ASN:ND2	1:A:83:ARG:HD3	1.89	0.85
1:A:34:LYS:HA	1:A:34:LYS:HE2	1.59	0.85
1:F:34:LYS:HG3	1:F:37:GLN:H	1.41	0.85
1:D:101:ARG:NH1	1:D:226:THR:HB	1.92	0.85
1:D:41:GLN:HE21	1:D:45:GLU:CD	1.84	0.85
1:E:197:TRP:NE1	1:E:211:THR:HG23	1.92	0.84
1:A:130:LYS:HE3	1:A:131:ASN:HD21	1.41	0.84
1:G:79:ILE:HG12	1:G:96:VAL:HG22	1.57	0.84
1:G:241:GLU:HA	1:G:244:LYS:HD2	1.61	0.83
1:G:83:ARG:HA	1:G:83:ARG:NE	1.94	0.82
1:D:34:LYS:HB3	1:D:37:GLN:HG2	1.62	0.81
1:G:83:ARG:NH2	1:G:89:VAL:HG22	1.96	0.81
1:G:303:LEU:HD22	1:G:309:LYS:HB2	1.61	0.81
1:H:293:VAL:HG23	5:H:2177:HOH:O	1.79	0.81
1:D:197:TRP:HE1	1:D:211:THR:HG23	1.46	0.80
1:A:130:LYS:HE3	1:A:131:ASN:ND2	1.96	0.80
1:G:259:THR:HG21	1:G:266:PRO:HG3	1.64	0.79
1:F:11:GLU:HG2	1:F:261:VAL:HG11	1.63	0.79
1:B:58:GLN:HE21	1:B:60:PRO:HG2	1.48	0.78
1:H:252:LYS:HE2	1:H:270:HIS:HB3	1.64	0.78
1:I:255:GLN:HE22	1:I:268:ASN:HB2	1.48	0.78
1:C:2:ILE:HD11	1:C:28:VAL:HG22	1.65	0.78
1:E:10:LYS:HG2	5:E:2012:HOH:O	1.84	0.78
1:G:4:VAL:HB	1:G:30:LEU:HD23	1.66	0.78
1:F:137:PRO:HB3	1:F:308:MET:HE3	1.65	0.77
1:I:72:GLU:OE1	1:I:73:PRO:HD2	1.83	0.77
1:I:174:LYS:HG3	1:I:177:VAL:HG23	1.67	0.77
1:A:80:ASN:HD21	1:A:83:ARG:HD3	1.46	0.77
1:H:71:LEU:HD11	1:H:231:ALA:HB1	1.65	0.77
1:F:133:ILE:HD11	1:F:191:LEU:HD13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ARG:NH1	4:G:1310:PHF:OC1	2.17	0.76
1:H:10:LYS:HE2	1:H:32:SER:HB2	1.66	0.76
1:H:79:ILE:HD13	1:H:93:LYS:HD2	1.67	0.76
1:A:7:GLY:HA2	1:A:33:ALA:O	1.85	0.76
1:G:80:ASN:HA	1:G:83:ARG:HG2	1.67	0.76
1:H:27:LYS:HG2	1:H:28:VAL:N	2.00	0.76
1:C:41:GLN:O	1:C:45:GLU:HG3	1.85	0.75
1:B:282:LYS:HA	1:B:282:LYS:HE2	1.68	0.75
1:H:4:VAL:HG22	1:H:53:VAL:HB	1.66	0.75
1:H:211:THR:HB	5:H:2112:HOH:O	1.86	0.75
1:D:135:TYR:HE2	1:D:308:MET:HE3	1.50	0.74
1:H:259:THR:CG2	1:H:273:SER:HA	2.16	0.74
1:I:166:LYS:HD3	1:I:308:MET:HG2	1.67	0.74
2:C:1310:HF5:OB3	2:C:1310:HF5:OBC	2.04	0.74
1:B:33:ALA:HB3	1:B:38:LEU:HD21	1.71	0.73
1:H:38:LEU:O	1:H:42:ILE:HG13	1.88	0.73
1:I:259:THR:CG2	1:I:266:PRO:HG3	2.19	0.73
1:D:101:ARG:HH11	1:D:101:ARG:HB2	1.51	0.73
1:H:240:ASP:O	1:H:244:LYS:HD3	1.89	0.72
1:C:86:GLY:HA2	1:C:287:GLN:NE2	2.03	0.72
1:F:259:THR:CG2	1:F:266:PRO:HG3	2.16	0.72
1:H:106:VAL:HG22	1:H:211:THR:CG2	2.17	0.72
1:G:202:ARG:HH22	1:G:274:THR:HG22	1.53	0.72
1:D:58:GLN:HE21	1:D:61:ALA:H	1.35	0.72
1:I:61:ALA:O	1:I:64:THR:HG22	1.89	0.72
1:C:202:ARG:NH2	1:C:274:THR:HG23	1.99	0.72
1:H:107:TYR:O	1:H:211:THR:HG23	1.90	0.72
1:A:204:LYS:HE2	5:A:2169:HOH:O	1.89	0.72
1:D:301:ARG:HA	1:D:301:ARG:HH11	1.54	0.71
1:I:34:LYS:HB2	1:I:37:GLN:HG3	1.71	0.71
1:E:204:LYS:HE3	5:E:2170:HOH:O	1.90	0.71
1:F:34:LYS:HG2	1:F:37:GLN:HB2	1.72	0.71
1:G:224:LEU:HD13	1:G:225:VAL:N	2.04	0.71
1:H:99:SER:HA	1:H:267:LEU:HG	1.73	0.71
1:E:262:ARG:HG2	1:E:264:GLU:HG3	1.71	0.71
1:H:1:ASP:H2	1:H:26:ILE:HG23	1.57	0.70
1:D:101:ARG:HH12	1:D:226:THR:CB	1.99	0.70
1:E:72:GLU:HG3	1:E:239:LYS:HE3	1.73	0.70
1:G:202:ARG:NH2	1:G:274:THR:HG22	2.06	0.70
1:A:146:ILE:CD1	1:A:162:LEU:HD21	2.22	0.70
1:D:130:LYS:HE3	1:D:131:ASN:ND2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:LYS:O	1:I:256:ARG:HG2	1.91	0.70
1:I:79:ILE:HG22	1:I:83:ARG:NH1	2.07	0.69
1:E:255:GLN:O	1:E:259:THR:HG22	1.92	0.69
1:H:59:ILE:N	1:H:60:PRO:HD2	2.08	0.69
1:C:27:LYS:NZ	1:C:27:LYS:HB3	2.08	0.68
1:D:79:ILE:HG12	1:D:96:VAL:HG22	1.75	0.68
1:D:135:TYR:CE2	1:D:308:MET:HE3	2.28	0.68
1:B:14:GLN:HE21	1:B:14:GLN:HA	1.58	0.67
1:D:197:TRP:NE1	1:D:211:THR:HG23	2.08	0.67
1:C:130:LYS:HA	1:C:168:TYR:HB3	1.77	0.67
1:H:288:VAL:HG12	1:H:289:SER:N	1.98	0.67
1:I:259:THR:HG21	1:I:266:PRO:CG	2.22	0.67
1:H:41:GLN:O	1:H:45:GLU:HB2	1.94	0.67
1:E:130:LYS:HD3	1:E:168:TYR:HD2	1.60	0.67
2:E:1310:HF5:OB3	2:E:1310:HF5:OBC	2.13	0.66
1:C:252:LYS:HE2	1:C:270:HIS:HB2	1.75	0.66
1:I:79:ILE:HD12	1:I:93:LYS:HE2	1.78	0.66
1:F:16:VAL:HG11	1:F:249:LEU:CD2	2.26	0.66
1:G:79:ILE:HG12	1:G:96:VAL:CG2	2.26	0.66
1:I:93:LYS:HE3	5:I:2058:HOH:O	1.96	0.66
1:H:234:LYS:C	1:H:234:LYS:HD2	2.21	0.65
1:A:239:LYS:O	1:A:243:LYS:HG3	1.96	0.65
4:I:1310:PHF:O02	4:I:1310:PHF:OBC	2.14	0.65
1:D:80:ASN:HA	1:D:83:ARG:CG	2.26	0.65
1:C:59:ILE:HD11	1:C:227:TYR:HB2	1.78	0.65
1:I:10:LYS:HE2	1:I:32:SER:HB2	1.79	0.65
1:C:2:ILE:CD1	1:C:28:VAL:HG22	2.27	0.64
1:G:292:THR:OG1	1:G:295:GLU:HG3	1.96	0.64
1:F:14:GLN:HE21	1:F:18:ASP:CG	2.06	0.64
1:G:41:GLN:O	1:G:45:GLU:HG3	1.98	0.64
1:G:59:ILE:HD11	1:G:88:PRO:HG2	1.80	0.64
1:I:159:LEU:O	1:I:163:LYS:HG2	1.97	0.64
1:A:57:GLU:HB2	1:A:101:ARG:HH22	1.63	0.64
1:D:45:GLU:O	1:D:48:ARG:HB3	1.97	0.64
1:D:257:ALA:HB1	5:D:2017:HOH:O	1.96	0.64
1:G:139:SER:HB3	1:G:142:PHE:HB2	1.80	0.64
1:G:259:THR:CG2	1:G:266:PRO:HG3	2.28	0.64
1:E:280:ILE:HD12	1:E:283:LEU:HD12	1.79	0.63
1:C:252:LYS:HE2	1:C:270:HIS:CB	2.27	0.63
1:B:59:ILE:HD11	1:B:227:TYR:HB2	1.81	0.63
1:C:43:LYS:HE3	1:C:64:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:LYS:HD2	1:H:244:LYS:N	2.14	0.63
1:F:255:GLN:HB2	1:F:271:VAL:HG21	1.81	0.63
1:H:33:ALA:HB3	1:H:38:LEU:CD2	2.28	0.63
1:H:255:GLN:CB	1:H:271:VAL:HG21	2.28	0.63
1:F:301:ARG:HH21	1:F:304:GLU:CD	2.07	0.62
1:D:106:VAL:HG22	1:D:211:THR:OG1	1.99	0.62
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.64	0.62
1:H:101:ARG:NH1	4:H:1310:PHF:OC1	2.31	0.62
1:D:265:TYR:HB3	1:D:280:ILE:HG23	1.80	0.62
1:H:38:LEU:HD12	1:H:54:PHE:HE1	1.63	0.62
1:B:58:GLN:HG2	1:B:60:PRO:HD2	1.81	0.62
1:C:202:ARG:HH22	1:C:274:THR:CG2	2.06	0.62
1:E:45:GLU:HB2	1:E:49:SER:HB2	1.82	0.62
1:F:268:ASN:HD22	1:F:270:HIS:H	1.47	0.62
1:H:12:ALA:HB1	1:H:258:LEU:CD1	2.30	0.62
1:A:41:GLN:O	1:A:45:GLU:HG3	2.00	0.62
1:E:202:ARG:HH22	1:E:274:THR:CG2	2.10	0.62
1:B:33:ALA:HB3	1:B:38:LEU:CD2	2.29	0.62
1:F:34:LYS:CG	1:F:37:GLN:HB2	2.29	0.62
1:I:105:VAL:HG22	1:I:191:LEU:HD13	1.81	0.62
1:A:130:LYS:HA	1:A:168:TYR:HB3	1.80	0.62
1:C:255:GLN:NE2	1:C:268:ASN:H	1.97	0.62
1:D:45:GLU:HB2	1:D:49:SER:HB2	1.82	0.62
1:E:72:GLU:HG2	1:E:234:LYS:HA	1.81	0.62
1:I:34:LYS:O	1:I:38:LEU:HG	1.99	0.62
2:A:1310:HF5:OAB	2:A:1310:HF5:OA1	2.18	0.61
1:D:125:ALA:HB1	1:D:164:GLY:HA3	1.81	0.61
1:E:268:ASN:C	1:E:268:ASN:HD22	2.08	0.61
1:A:248:PHE:O	1:A:254:GLY:HA3	2.00	0.61
1:D:12:ALA:HB1	1:D:258:LEU:CD1	2.31	0.61
1:H:292:THR:OG1	1:H:295:GLU:HG3	2.00	0.61
1:A:245:PHE:O	1:A:249:LEU:HG	2.01	0.61
1:D:33:ALA:HB3	1:D:38:LEU:HD21	1.81	0.61
1:F:217:ARG:HD3	1:F:282:LYS:O	2.01	0.61
1:H:70:LEU:HD13	5:H:2018:HOH:O	2.01	0.61
1:H:16:VAL:HG11	1:H:249:LEU:CD2	2.29	0.61
1:H:240:ASP:HB2	1:H:244:LYS:NZ	2.15	0.61
1:F:125:ALA:HB1	1:F:164:GLY:HA3	1.83	0.61
1:E:304:GLU:HG2	1:E:309:LYS:HD3	1.82	0.60
1:G:59:ILE:CD1	1:G:88:PRO:HG2	2.31	0.60
1:G:135:TYR:HE2	1:G:308:MET:HE3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:VAL:HG22	1:H:242:ALA:HB1	1.82	0.60
1:G:36:ASP:OD2	1:G:37:GLN:HG3	2.01	0.60
1:B:58:GLN:HG2	1:B:60:PRO:HG2	1.83	0.60
1:G:83:ARG:HE	1:G:83:ARG:CA	2.08	0.60
1:G:8:GLN:HG3	1:G:9:HIS:N	2.16	0.60
1:G:151:LYS:HE2	1:G:289:SER:OG	2.01	0.60
1:H:59:ILE:H	1:H:60:PRO:HD2	1.66	0.60
1:H:78:THR:HG23	1:H:247:ALA:HA	1.84	0.60
4:I:1310:PHF:OBC	4:I:1310:PHF:OB3	2.20	0.60
1:B:18:ASP:O	1:B:21:THR:HG22	2.01	0.60
1:D:256:ARG:HA	1:D:259:THR:HG22	1.83	0.60
1:B:83:ARG:HD3	5:B:2063:HOH:O	2.02	0.60
1:F:9:HIS:CE1	1:F:11:GLU:HB3	2.37	0.60
1:H:8:GLN:HG2	5:H:2030:HOH:O	2.01	0.59
1:B:103:ARG:HD3	5:B:2086:HOH:O	2.01	0.59
1:E:293:VAL:HG23	5:E:2230:HOH:O	2.01	0.59
1:G:159:LEU:HD11	1:G:163:LYS:HE2	1.84	0.59
1:E:9:HIS:CE1	1:E:11:GLU:HB3	2.37	0.59
1:I:174:LYS:HD2	1:I:176:SER:HB3	1.84	0.59
1:B:125:ALA:HB1	1:B:164:GLY:HA3	1.85	0.59
1:C:255:GLN:HE21	1:C:268:ASN:CB	2.15	0.59
1:H:211:THR:HG22	1:H:212:ARG:N	2.16	0.59
1:B:72:GLU:HG2	1:B:234:LYS:HA	1.85	0.59
1:B:111:LYS:HD3	5:B:2139:HOH:O	2.03	0.59
1:D:101:ARG:NH1	1:D:101:ARG:HB2	2.16	0.59
1:B:74:LEU:HB2	5:B:2055:HOH:O	2.01	0.59
1:G:255:GLN:O	1:G:259:THR:HG23	2.03	0.59
1:I:120:SER:HB3	1:I:123:ASN:ND2	2.18	0.59
1:G:133:ILE:HD11	1:G:191:LEU:HD13	1.85	0.58
1:G:137:PRO:HB3	1:G:308:MET:CE	2.33	0.58
1:I:252:LYS:HE3	1:I:256:ARG:HH21	1.67	0.58
1:B:1:ASP:N	1:B:26:ILE:HG23	2.18	0.58
1:H:252:LYS:HE2	1:H:270:HIS:CB	2.31	0.58
1:I:162:LEU:HD22	1:I:308:MET:HE1	1.83	0.58
1:I:209:VAL:HG12	1:I:211:THR:H	1.68	0.58
1:E:203:GLU:OE1	1:E:204:LYS:HE2	2.03	0.58
1:D:54:PHE:CZ	1:D:56:SER:HB3	2.38	0.58
1:D:209:VAL:CG1	1:D:211:THR:HG22	2.33	0.58
1:E:130:LYS:HA	1:E:168:TYR:HB3	1.83	0.58
1:D:7:GLY:HA2	1:D:33:ALA:O	2.03	0.58
1:C:59:ILE:N	1:C:60:PRO:HD2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:PHE:O	1:C:249:LEU:HG	2.04	0.58
1:H:80:ASN:ND2	1:H:83:ARG:HH11	1.93	0.58
1:I:191:LEU:HD12	5:I:2080:HOH:O	2.03	0.58
3:D:1310:HF3:OAC	3:D:1310:HF3:OC2	2.20	0.58
1:H:240:ASP:HA	1:H:243:LYS:HG3	1.86	0.58
1:I:166:LYS:HD3	1:I:308:MET:CG	2.33	0.58
1:F:34:LYS:HE2	1:F:37:GLN:HB2	1.86	0.58
1:B:85:LYS:HA	1:B:85:LYS:HE3	1.85	0.58
1:B:106:VAL:HG12	1:B:190:ALA:O	2.04	0.58
1:B:183:GLU:OE1	1:B:209:VAL:HG13	2.04	0.58
1:B:159:LEU:O	1:B:163:LYS:HG3	2.04	0.57
1:F:217:ARG:HG2	1:F:283:LEU:O	2.04	0.57
1:C:5:TYR:CE1	1:C:51:ALA:HB2	2.40	0.57
1:C:130:LYS:HE3	1:C:131:ASN:ND2	2.20	0.57
1:B:258:LEU:HD13	1:B:258:LEU:C	2.30	0.57
1:D:142:PHE:CE2	1:D:308:MET:HE1	2.40	0.57
1:E:8:GLN:HG3	1:E:9:HIS:N	2.20	0.57
1:B:59:ILE:N	1:B:60:PRO:HD2	2.20	0.57
1:E:115:LYS:HA	1:E:115:LYS:CE	2.32	0.57
1:G:81:GLU:OE1	1:G:252:LYS:NZ	2.37	0.57
1:D:112:LEU:HD21	1:D:132:ARG:HH21	1.70	0.57
1:E:187:VAL:HB	5:E:2130:HOH:O	2.05	0.56
1:H:72:GLU:OE1	1:H:234:LYS:HA	2.04	0.56
1:I:34:LYS:HB2	1:I:37:GLN:CG	2.34	0.56
1:G:120:SER:HB3	1:G:123:ASN:ND2	2.20	0.56
1:A:278:GLU:HG2	5:A:2210:HOH:O	2.04	0.56
1:E:108:ASP:CG	1:E:110:ARG:HH11	2.13	0.56
1:A:133:ILE:HD11	1:A:191:LEU:HD13	1.87	0.56
1:C:9:HIS:CD2	1:C:11:GLU:HG2	2.41	0.56
1:D:12:ALA:HB1	1:D:258:LEU:HD12	1.88	0.56
1:F:41:GLN:O	1:F:45:GLU:HG3	2.05	0.56
1:H:80:ASN:HD21	1:H:83:ARG:NH1	1.93	0.56
1:H:16:VAL:HG11	1:H:249:LEU:HD22	1.87	0.56
1:C:101:ARG:HD2	5:C:2083:HOH:O	2.06	0.56
1:G:74:LEU:HD12	1:G:96:VAL:HG23	1.87	0.56
1:I:4:VAL:HB	1:I:30:LEU:HD23	1.87	0.56
1:G:202:ARG:HH22	1:G:274:THR:CG2	2.16	0.55
1:H:255:GLN:HB2	1:H:271:VAL:HG21	1.87	0.55
1:D:58:GLN:HE21	1:D:61:ALA:N	2.02	0.55
1:C:27:LYS:HB3	1:C:27:LYS:HZ3	1.71	0.55
1:B:1:ASP:HA	1:B:27:LYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:HA	1:B:259:THR:HG22	1.88	0.55
1:I:282:LYS:HB3	1:I:282:LYS:HZ2	1.71	0.55
1:A:252:LYS:HE3	1:H:237:GLN:HB3	1.89	0.55
1:B:4:VAL:HG22	1:B:53:VAL:HB	1.88	0.55
1:B:14:GLN:HA	1:B:14:GLN:NE2	2.21	0.55
1:I:69:ASN:ND2	1:I:92:LYS:HZ2	2.04	0.55
1:I:183:GLU:HG3	1:I:200:PHE:HE1	1.71	0.55
1:D:265:TYR:CB	1:D:280:ILE:HG23	2.36	0.55
1:E:252:LYS:HG2	1:E:270:HIS:HB2	1.88	0.55
1:F:38:LEU:O	1:F:42:ILE:HG13	2.07	0.55
1:I:69:ASN:HD21	1:I:92:LYS:NZ	2.05	0.55
1:C:40:GLY:O	1:C:44:GLU:HG3	2.07	0.55
1:H:8:GLN:HG3	1:H:9:HIS:N	2.20	0.55
1:A:57:GLU:HB2	1:A:101:ARG:NH2	2.21	0.55
1:G:137:PRO:HB3	1:G:308:MET:HE3	1.88	0.55
1:D:255:GLN:HE22	1:D:267:LEU:H	1.53	0.54
1:B:27:LYS:NZ	1:B:27:LYS:HB3	2.22	0.54
1:F:303:LEU:HD22	1:F:308:MET:HE2	1.89	0.54
1:I:174:LYS:CG	1:I:177:VAL:HG23	2.36	0.54
1:B:19:ALA:HA	1:B:22:ARG:NH2	2.21	0.54
1:C:240:ASP:O	1:C:244:LYS:HG3	2.07	0.54
1:F:185:GLY:HA2	5:F:2112:HOH:O	2.08	0.54
1:G:31:ASN:HB2	5:G:2026:HOH:O	2.06	0.54
1:I:106:VAL:CG2	1:I:211:THR:HG21	2.38	0.54
1:A:80:ASN:HB3	5:H:2023:HOH:O	2.06	0.54
1:D:6:ASN:HB3	1:D:32:SER:HA	1.89	0.54
1:F:300:THR:O	1:F:304:GLU:HG3	2.07	0.54
1:B:58:GLN:HG2	1:B:60:PRO:CG	2.37	0.54
1:D:114:GLU:OE1	1:D:117:LEU:HD22	2.07	0.54
1:H:3:THR:HG23	1:H:29:LYS:HG3	1.89	0.54
1:I:69:ASN:ND2	1:I:92:LYS:NZ	2.55	0.54
1:I:79:ILE:HG22	1:I:83:ARG:HH12	1.72	0.54
1:B:58:GLN:HG2	1:B:60:PRO:CD	2.38	0.54
1:E:216:VAL:HG13	5:E:2174:HOH:O	2.08	0.54
1:C:80:ASN:HA	1:C:83:ARG:NH2	2.22	0.54
1:E:108:ASP:OD2	1:E:110:ARG:CD	2.55	0.54
1:G:139:SER:HB3	1:G:142:PHE:CB	2.38	0.54
1:H:42:ILE:HG22	5:H:2018:HOH:O	2.07	0.54
1:C:72:GLU:OE2	1:C:73:PRO:HD2	2.08	0.54
1:C:80:ASN:OD1	1:C:83:ARG:NH2	2.41	0.54
1:B:119:LYS:HE3	5:B:2101:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLU:N	1:D:57:GLU:OE1	2.41	0.54
1:D:219:ARG:NH1	5:D:2145:HOH:O	2.40	0.54
1:E:133:ILE:HD11	1:E:191:LEU:HD13	1.90	0.54
1:E:300:THR:HG22	1:E:304:GLU:OE2	2.08	0.54
1:H:17:ALA:O	1:H:20:PHE:HB3	2.08	0.54
1:H:133:ILE:HD11	1:H:191:LEU:CD1	2.39	0.54
1:I:174:LYS:HG3	1:I:177:VAL:CG2	2.36	0.54
1:B:255:GLN:HB2	1:B:271:VAL:HG21	1.91	0.53
1:F:64:THR:HG23	5:F:2058:HOH:O	2.08	0.53
1:G:297:GLU:O	1:G:301:ARG:HG3	2.09	0.53
1:I:85:LYS:HE2	5:I:2079:HOH:O	2.07	0.53
1:E:108:ASP:OD2	1:E:110:ARG:HD2	2.08	0.53
1:H:288:VAL:CG1	1:H:289:SER:H	2.01	0.53
1:A:120:SER:HB3	1:A:123:ASN:ND2	2.24	0.53
1:C:268:ASN:HD22	1:C:269:PRO:HD2	1.72	0.53
1:G:163:LYS:HD3	1:G:306:ALA:HA	1.89	0.53
1:H:29:LYS:HD2	1:H:30:LEU:N	2.23	0.53
1:C:255:GLN:HE21	1:C:268:ASN:H	1.54	0.53
1:H:11:GLU:HG2	1:H:261:VAL:HG11	1.89	0.53
1:H:38:LEU:HD12	1:H:54:PHE:CE1	2.43	0.53
1:A:259:THR:CG2	1:A:266:PRO:HG3	2.25	0.53
1:E:155:GLU:OE2	1:E:298:HIS:HE1	1.91	0.53
1:D:130:LYS:HE3	1:D:131:ASN:HD21	1.73	0.53
1:F:101:ARG:HG3	1:F:101:ARG:HH11	1.74	0.53
1:C:259:THR:O	1:C:274:THR:HG22	2.08	0.53
1:B:204:LYS:HG2	5:B:2145:HOH:O	2.08	0.53
1:B:255:GLN:NE2	1:B:268:ASN:H	2.07	0.53
1:C:112:LEU:HD11	1:C:188:ASP:HB3	1.91	0.53
1:D:59:ILE:H	1:D:60:PRO:CD	2.21	0.53
1:A:269:PRO:HG3	1:H:48:ARG:HD2	1.92	0.52
1:D:112:LEU:HD21	1:D:132:ARG:NH2	2.24	0.52
1:E:248:PHE:O	1:E:254:GLY:HA3	2.09	0.52
1:G:122:LEU:HA	1:G:161:TRP:CD1	2.44	0.52
1:D:51:ALA:O	1:D:233:LEU:HD22	2.09	0.52
1:G:240:ASP:O	1:G:244:LYS:HG3	2.10	0.52
1:I:245:PHE:O	1:I:248:PHE:HB3	2.09	0.52
1:C:217:ARG:HH11	1:C:217:ARG:HG2	1.74	0.52
1:G:184:ASN:N	1:G:184:ASN:HD22	2.05	0.52
1:D:72:GLU:OE1	1:D:239:LYS:HD3	2.10	0.52
1:I:133:ILE:HD11	1:I:191:LEU:HD22	1.91	0.52
1:E:94:ASP:OD1	1:E:94:ASP:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:GLU:HG2	1:E:282:LYS:HB2	1.89	0.52
1:B:14:GLN:HE21	1:B:14:GLN:CA	2.20	0.52
1:I:20:PHE:CZ	1:I:26:ILE:HD12	2.44	0.52
1:I:133:ILE:HD11	1:I:191:LEU:CD2	2.40	0.52
1:A:241:GLU:HG2	5:A:2195:HOH:O	2.10	0.52
1:C:89:VAL:HG22	5:C:2019:HOH:O	2.08	0.52
1:D:173:ALA:O	1:D:174:LYS:HD3	2.10	0.52
1:E:252:LYS:HG3	5:E:2198:HOH:O	2.09	0.52
1:F:127:PRO:HG3	1:F:168:TYR:CZ	2.45	0.52
1:G:301:ARG:HG2	5:G:2205:HOH:O	2.08	0.52
1:A:101:ARG:NH1	1:A:262:ARG:HH21	2.08	0.52
1:B:255:GLN:CB	1:B:271:VAL:HG21	2.40	0.52
1:G:240:ASP:OD1	1:G:244:LYS:HE3	2.10	0.52
1:H:240:ASP:HA	1:H:243:LYS:CG	2.40	0.52
1:A:34:LYS:HD2	2:A:1310:HF5:OD1	2.10	0.51
1:D:5:TYR:OH	1:D:41:GLN:NE2	2.43	0.51
1:D:216:VAL:HG23	5:D:2139:HOH:O	2.09	0.51
1:E:59:ILE:HB	1:E:60:PRO:HD3	1.92	0.51
1:I:255:GLN:NE2	1:I:268:ASN:CB	2.62	0.51
1:C:80:ASN:CB	1:C:83:ARG:HH22	2.23	0.51
1:D:43:LYS:HE3	1:D:64:THR:HG22	1.92	0.51
1:E:203:GLU:CD	1:E:204:LYS:HE2	2.35	0.51
1:H:235:SER:HB2	5:H:2024:HOH:O	2.10	0.51
1:G:9:HIS:CE1	1:G:11:GLU:HB3	2.46	0.51
1:H:71:LEU:CG	1:H:94:ASP:HB2	2.36	0.51
1:I:248:PHE:O	1:I:254:GLY:HA3	2.10	0.51
1:A:235:SER:HB3	5:A:2052:HOH:O	2.11	0.51
1:C:6:ASN:HB3	1:C:32:SER:HA	1.93	0.51
1:I:122:LEU:HA	1:I:161:TRP:CD1	2.46	0.51
1:G:142:PHE:O	1:G:145:GLN:HB3	2.11	0.51
1:I:38:LEU:O	1:I:42:ILE:HG13	2.09	0.51
1:F:33:ALA:HB3	1:F:38:LEU:HG	1.92	0.51
1:F:104:VAL:HG21	1:F:213:LEU:HD22	1.91	0.51
1:I:1:ASP:HA	1:I:27:LYS:O	2.11	0.51
1:G:93:LYS:HG3	5:G:2082:HOH:O	2.10	0.51
1:D:239:LYS:O	1:D:243:LYS:HG3	2.10	0.51
1:G:71:LEU:O	1:G:234:LYS:HE3	2.10	0.51
1:D:6:ASN:O	1:D:38:LEU:HD11	2.12	0.51
1:D:252:LYS:HE3	1:D:270:HIS:CB	2.41	0.51
1:I:45:GLU:HB2	1:I:49:SER:HB2	1.92	0.51
1:I:204:LYS:O	1:I:208:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:301:ARG:HH11	1:I:304:GLU:CD	2.18	0.51
1:A:233:LEU:N	1:A:233:LEU:HD12	2.26	0.50
1:C:260:ALA:HA	1:C:274:THR:HG21	1.92	0.50
1:F:5:TYR:CE1	1:F:51:ALA:HB2	2.46	0.50
1:G:224:LEU:HD13	1:G:224:LEU:C	2.36	0.50
1:A:72:GLU:OE1	1:A:239:LYS:HE2	2.11	0.50
1:D:48:ARG:O	1:D:48:ARG:HG3	2.10	0.50
1:F:177:VAL:HA	1:F:180:GLN:CD	2.37	0.50
1:H:241:GLU:HB2	5:H:2054:HOH:O	2.11	0.50
1:E:135:TYR:CD2	1:E:137:PRO:HD3	2.47	0.50
1:I:110:ARG:HD3	1:I:210:HIS:ND1	2.26	0.50
1:E:156:ALA:O	1:E:160:LYS:HG3	2.10	0.50
1:F:301:ARG:O	1:F:305:GLN:HG3	2.11	0.50
1:A:101:ARG:HH11	1:A:262:ARG:HH21	1.60	0.50
1:D:251:GLY:O	1:D:255:GLN:HG3	2.11	0.50
1:F:177:VAL:HA	1:F:180:GLN:OE1	2.11	0.50
1:B:72:GLU:OE2	1:B:234:LYS:HG2	2.11	0.50
1:C:15:ALA:CB	1:C:261:VAL:HG21	2.42	0.50
1:C:262:ARG:HG3	1:C:264:GLU:HG3	1.94	0.50
1:H:272:VAL:HA	5:H:2163:HOH:O	2.11	0.50
1:B:1:ASP:H2	1:B:26:ILE:HG23	1.74	0.50
1:E:255:GLN:HB2	1:E:271:VAL:HG21	1.94	0.50
1:H:41:GLN:HG3	1:H:42:ILE:N	2.25	0.50
1:H:238:ASN:HB3	1:H:241:GLU:HB3	1.94	0.50
1:C:255:GLN:HE21	1:C:268:ASN:HB3	1.77	0.49
1:C:291:THR:HG22	1:C:296:LYS:HG3	1.94	0.49
1:H:234:LYS:NZ	1:H:235:SER:HB3	2.27	0.49
1:I:137:PRO:HA	1:I:142:PHE:CD2	2.47	0.49
1:C:268:ASN:HD22	1:C:269:PRO:CD	2.25	0.49
1:D:256:ARG:HG2	1:D:271:VAL:HG13	1.94	0.49
1:E:146:ILE:HD11	1:E:303:LEU:HD21	1.93	0.49
1:F:54:PHE:CE2	1:F:56:SER:HB2	2.46	0.49
1:H:127:PRO:HG3	1:H:168:TYR:CZ	2.47	0.49
1:I:33:ALA:HB3	1:I:38:LEU:HD21	1.94	0.49
1:G:71:LEU:O	1:G:234:LYS:HG3	2.12	0.49
1:E:110:ARG:NH2	1:E:183:GLU:O	2.43	0.49
1:D:117:LEU:N	1:D:117:LEU:HD12	2.27	0.49
1:H:107:TYR:C	1:H:211:THR:HG23	2.37	0.49
1:H:245:PHE:O	1:H:248:PHE:HB3	2.12	0.49
1:D:162:LEU:HD22	1:D:308:MET:SD	2.52	0.49
1:F:252:LYS:HD3	5:F:2181:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ILE:HD12	5:G:2072:HOH:O	2.13	0.49
2:C:1310:HF5:OC2	2:C:1310:HF5:OAC	2.30	0.49
1:D:60:PRO:HG2	5:D:2197:HOH:O	2.12	0.49
2:E:1310:HF5:OAC	2:E:1310:HF5:OAE	2.30	0.49
1:G:181:ALA:HA	1:G:186:GLU:OE2	2.12	0.49
1:B:16:VAL:HG21	1:B:249:LEU:HD23	1.94	0.49
1:E:38:LEU:O	1:E:42:ILE:HG13	2.13	0.49
1:E:41:GLN:O	1:E:45:GLU:HG3	2.12	0.49
1:G:252:LYS:HD2	1:G:252:LYS:N	2.28	0.49
1:I:80:ASN:OD1	1:I:83:ARG:HD2	2.13	0.49
1:I:174:LYS:HD3	1:I:176:SER:H	1.78	0.49
1:I:216:VAL:HG13	5:I:2128:HOH:O	2.13	0.49
1:B:106:VAL:CG2	1:B:211:THR:HG21	2.43	0.49
1:H:64:THR:HG23	5:H:2036:HOH:O	2.13	0.49
1:D:194:ASN:HB2	5:D:2125:HOH:O	2.11	0.48
1:G:233:LEU:HD12	1:G:233:LEU:N	2.27	0.48
1:H:256:ARG:HG2	1:H:271:VAL:HG13	1.95	0.48
1:F:99:SER:HA	1:F:267:LEU:HG	1.96	0.48
1:I:106:VAL:HG23	1:I:211:THR:CG2	2.43	0.48
1:I:197:TRP:NE1	1:I:211:THR:HG22	2.28	0.48
1:I:211:THR:CG2	1:I:212:ARG:N	2.74	0.48
1:E:104:VAL:HG21	1:E:213:LEU:HD22	1.96	0.48
5:A:2158:HOH:O	1:F:22:ARG:HG2	2.13	0.48
1:B:301:ARG:NE	5:B:2208:HOH:O	2.46	0.48
1:D:32:SER:HB3	5:D:2005:HOH:O	2.13	0.48
1:H:70:LEU:HD22	5:H:2144:HOH:O	2.12	0.48
1:I:20:PHE:HZ	1:I:26:ILE:HD12	1.79	0.48
1:A:146:ILE:O	1:A:150:VAL:HG23	2.14	0.48
1:A:180:GLN:HG2	5:A:2157:HOH:O	2.13	0.48
1:G:59:ILE:HD11	1:G:227:TYR:HB2	1.95	0.48
1:H:297:GLU:O	1:H:301:ARG:HG2	2.13	0.48
1:D:12:ALA:O	1:D:16:VAL:HG23	2.14	0.48
1:H:33:ALA:O	1:H:38:LEU:HG	2.14	0.48
1:H:71:LEU:CD1	1:H:231:ALA:HB1	2.41	0.48
1:H:211:THR:CG2	1:H:212:ARG:N	2.76	0.48
1:I:20:PHE:CE2	1:I:26:ILE:HB	2.47	0.48
1:F:130:LYS:HE3	1:F:131:ASN:ND2	2.28	0.48
1:G:22:ARG:HD3	5:G:2003:HOH:O	2.13	0.48
1:H:33:ALA:O	1:H:34:LYS:C	2.57	0.48
1:H:240:ASP:HB2	1:H:244:LYS:HZ2	1.78	0.48
1:I:9:HIS:O	1:I:10:LYS:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:293:VAL:HG23	5:I:2181:HOH:O	2.13	0.48
1:E:59:ILE:N	1:E:60:PRO:CD	2.77	0.48
1:I:106:VAL:CG2	1:I:211:THR:CG2	2.92	0.48
1:I:164:GLY:O	1:I:168:TYR:HD1	1.97	0.48
1:C:5:TYR:CD1	1:C:51:ALA:HB2	2.49	0.48
1:C:5:TYR:HB3	1:C:38:LEU:HD13	1.96	0.48
1:F:72:GLU:OE1	1:F:239:LYS:HE2	2.13	0.48
1:A:255:GLN:HB2	1:A:271:VAL:HG21	1.96	0.48
1:F:101:ARG:HG3	1:F:101:ARG:NH1	2.29	0.48
1:F:122:LEU:HA	1:F:161:TRP:CD1	2.49	0.48
1:H:83:ARG:HG2	1:H:84:GLY:N	2.29	0.48
1:D:74:LEU:CD1	1:D:96:VAL:HG23	2.44	0.47
1:B:71:LEU:O	1:B:234:LYS:HE3	2.14	0.47
1:B:106:VAL:CG2	1:B:211:THR:CG2	2.92	0.47
1:G:83:ARG:HG3	5:G:2068:HOH:O	2.14	0.47
1:G:151:LYS:HD2	1:G:288:VAL:HG12	1.96	0.47
1:B:130:LYS:HA	1:B:168:TYR:HB3	1.96	0.47
1:C:262:ARG:CG	1:C:264:GLU:HG3	2.45	0.47
1:D:41:GLN:NE2	1:D:45:GLU:OE2	2.47	0.47
1:E:292:THR:OG1	1:E:295:GLU:HG3	2.12	0.47
1:F:114:GLU:HA	1:F:117:LEU:HG	1.95	0.47
1:F:130:LYS:HE3	1:F:131:ASN:HD21	1.80	0.47
1:B:216:VAL:O	1:B:218:HIS:CE1	2.68	0.47
1:C:278:GLU:HG2	5:C:2189:HOH:O	2.13	0.47
1:D:256:ARG:O	1:D:259:THR:HG22	2.14	0.47
1:E:83:ARG:HG2	1:E:83:ARG:NH1	2.28	0.47
1:F:7:GLY:HA2	1:F:33:ALA:O	2.14	0.47
1:E:145:GLN:O	1:E:149:ILE:HG13	2.14	0.47
1:E:209:VAL:HG13	1:E:211:THR:HG22	1.96	0.47
1:G:19:ALA:O	1:G:22:ARG:HB3	2.15	0.47
1:G:151:LYS:HZ1	1:G:295:GLU:CD	2.22	0.47
1:H:4:VAL:HG21	1:H:245:PHE:CE2	2.49	0.47
1:H:9:HIS:HD2	5:H:2155:HOH:O	1.96	0.47
1:I:43:LYS:HE2	1:I:68:ALA:HB2	1.96	0.47
1:G:5:TYR:CE1	1:G:51:ALA:HB2	2.50	0.47
1:G:36:ASP:OD2	1:G:37:GLN:N	2.46	0.47
1:A:159:LEU:HG	1:A:163:LYS:HE3	1.97	0.47
1:C:2:ILE:HD13	1:C:2:ILE:H	1.80	0.47
1:C:303:LEU:HD23	1:C:308:MET:HE3	1.97	0.47
1:D:155:GLU:OE2	1:D:298:HIS:HE1	1.97	0.47
1:F:33:ALA:HB3	1:F:38:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:GLU:HG2	5:F:2190:HOH:O	2.14	0.47
1:G:151:LYS:HD2	1:G:288:VAL:CG1	2.45	0.47
1:H:103:ARG:O	1:H:104:VAL:HG13	2.14	0.47
1:H:240:ASP:HA	1:H:243:LYS:CD	2.44	0.47
1:H:240:ASP:HA	1:H:243:LYS:HD2	1.96	0.47
1:I:265:TYR:CE2	1:I:283:LEU:HD11	2.50	0.47
1:A:58:GLN:HB2	1:A:60:PRO:HD2	1.97	0.47
1:G:76:ALA:HB2	5:G:2061:HOH:O	2.15	0.47
1:H:6:ASN:HB3	1:H:32:SER:OG	2.15	0.47
1:H:94:ASP:OD2	1:H:94:ASP:N	2.41	0.47
1:B:133:ILE:HD11	1:B:191:LEU:HD13	1.96	0.47
1:E:1:ASP:CG	1:E:27:LYS:HB2	2.40	0.47
1:G:83:ARG:HH12	1:G:89:VAL:CG1	2.28	0.47
1:I:183:GLU:HG3	1:I:200:PHE:CE1	2.50	0.47
1:I:304:GLU:HG2	1:I:309:LYS:HB3	1.96	0.47
1:E:133:ILE:HD11	1:E:191:LEU:CD1	2.45	0.47
1:F:11:GLU:HG2	1:F:261:VAL:CG1	2.40	0.47
1:I:194:ASN:CG	1:I:195:TYR:H	2.23	0.47
1:I:296:LYS:HE2	5:I:2179:HOH:O	2.15	0.47
1:A:18:ASP:O	1:A:22:ARG:HG3	2.15	0.46
1:D:126:THR:HB	1:D:127:PRO:CD	2.45	0.46
1:D:197:TRP:CD1	1:D:211:THR:HG23	2.50	0.46
1:A:162:LEU:O	1:A:308:MET:HE3	2.14	0.46
1:D:137:PRO:HB3	1:D:308:MET:HE2	1.97	0.46
1:E:43:LYS:HE3	1:E:64:THR:HG22	1.96	0.46
1:G:146:ILE:O	1:G:150:VAL:HG23	2.15	0.46
1:I:304:GLU:HG2	1:I:309:LYS:HD3	1.97	0.46
1:D:59:ILE:N	1:D:60:PRO:CD	2.79	0.46
1:F:259:THR:HG21	1:F:266:PRO:CG	2.21	0.46
1:E:253:GLU:HG2	5:E:2199:HOH:O	2.16	0.46
1:H:253:GLU:HB2	5:H:2057:HOH:O	2.14	0.46
1:B:11:GLU:HA	1:B:11:GLU:OE2	2.15	0.46
1:E:304:GLU:CG	1:E:309:LYS:HD3	2.44	0.46
1:G:184:ASN:N	1:G:184:ASN:ND2	2.63	0.46
1:G:203:GLU:HB2	5:G:2138:HOH:O	2.15	0.46
1:G:303:LEU:CD2	1:G:309:LYS:HB2	2.41	0.46
1:I:194:ASN:CG	1:I:195:TYR:N	2.73	0.46
1:B:41:GLN:O	1:B:45:GLU:HG3	2.15	0.46
1:E:122:LEU:HA	1:E:161:TRP:CD1	2.51	0.46
1:G:130:LYS:HE3	1:G:131:ASN:ND2	2.31	0.46
1:I:6:ASN:O	1:I:38:LEU:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PHE:O	1:B:254:GLY:HA3	2.16	0.46
1:E:106:VAL:HG22	1:E:211:THR:OG1	2.16	0.46
1:F:233:LEU:N	1:F:233:LEU:HD12	2.30	0.46
1:F:301:ARG:HA	1:F:301:ARG:NE	2.30	0.46
1:G:51:ALA:O	1:G:233:LEU:HD22	2.16	0.46
1:I:105:VAL:HG22	1:I:191:LEU:CD1	2.44	0.46
1:A:164:GLY:O	1:A:168:TYR:HD1	1.99	0.46
2:A:1310:HF5:OB3	2:A:1310:HF5:OBC	2.33	0.46
1:B:57:GLU:HB2	1:B:101:ARG:NH2	2.31	0.46
1:B:293:VAL:HG23	5:B:2200:HOH:O	2.16	0.46
1:C:125:ALA:HB1	1:C:164:GLY:HA3	1.98	0.46
1:H:151:LYS:HD2	1:H:288:VAL:CG1	2.46	0.46
1:H:255:GLN:HG3	1:H:268:ASN:CB	2.46	0.46
1:I:92:LYS:HB2	1:I:94:ASP:OD1	2.16	0.46
1:A:2:ILE:HG23	1:A:241:GLU:OE2	2.15	0.45
1:B:19:ALA:HA	1:B:22:ARG:CZ	2.46	0.45
1:C:9:HIS:NE2	1:C:11:GLU:HG2	2.31	0.45
1:D:5:TYR:CE1	1:D:51:ALA:HB2	2.51	0.45
1:E:29:LYS:HG3	5:E:2027:HOH:O	2.16	0.45
1:H:8:GLN:HB2	5:H:2141:HOH:O	2.16	0.45
1:I:69:ASN:HD21	1:I:92:LYS:HZ3	1.62	0.45
1:B:245:PHE:O	1:B:248:PHE:HB3	2.15	0.45
1:H:259:THR:OG1	1:H:266:PRO:HG3	2.16	0.45
1:I:181:ALA:O	1:I:186:GLU:HB2	2.17	0.45
1:D:145:GLN:O	1:D:149:ILE:HG13	2.17	0.45
1:H:114:GLU:OE2	1:H:214:ASN:ND2	2.49	0.45
1:I:34:LYS:HB2	1:I:37:GLN:CD	2.41	0.45
1:C:130:LYS:HE3	1:C:131:ASN:HD21	1.80	0.45
1:F:8:GLN:HG3	1:F:9:HIS:H	1.82	0.45
1:G:216:VAL:HG13	1:G:217:ARG:N	2.31	0.45
1:H:155:GLU:OE2	1:H:298:HIS:HE1	2.00	0.45
1:I:81:GLU:HB3	1:I:250:ALA:O	2.17	0.45
1:A:133:ILE:HD11	1:A:191:LEU:CD1	2.46	0.45
1:F:34:LYS:CE	1:F:37:GLN:HB2	2.46	0.45
1:G:101:ARG:HD2	5:G:2047:HOH:O	2.16	0.45
1:H:72:GLU:CD	1:H:234:LYS:HA	2.42	0.45
1:B:72:GLU:CG	1:B:234:LYS:HA	2.46	0.45
1:B:255:GLN:HG3	1:B:268:ASN:CB	2.46	0.45
1:B:255:GLN:HG3	1:B:268:ASN:HB2	1.99	0.45
1:F:33:ALA:HB3	1:F:38:LEU:HD21	1.98	0.45
1:F:268:ASN:ND2	1:F:270:HIS:H	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:261:VAL:HG12	1:H:261:VAL:O	2.17	0.45
1:I:174:LYS:CD	1:I:176:SER:HB3	2.45	0.45
1:D:137:PRO:HB3	1:D:308:MET:CE	2.46	0.45
1:D:219:ARG:HD2	1:D:219:ARG:N	2.31	0.45
1:D:300:THR:O	1:D:304:GLU:HG3	2.17	0.45
1:H:137:PRO:HA	1:H:142:PHE:CD2	2.52	0.45
1:H:234:LYS:HD2	1:H:235:SER:N	2.31	0.45
1:H:255:GLN:HE22	1:H:267:LEU:H	1.65	0.45
1:I:216:VAL:HG23	1:I:223:ALA:HB2	1.98	0.45
1:B:216:VAL:HG11	1:B:220:ASP:CB	2.47	0.45
1:B:300:THR:O	1:B:304:GLU:HG3	2.17	0.45
1:B:106:VAL:HG23	1:B:211:THR:CG2	2.48	0.44
1:A:54:PHE:CE2	1:A:56:SER:HB3	2.52	0.44
1:C:35:GLY:HA3	1:C:58:GLN:HE21	1.83	0.44
1:D:194:ASN:CG	1:D:195:TYR:N	2.75	0.44
1:E:278:GLU:HG2	1:E:282:LYS:CB	2.47	0.44
1:E:280:ILE:HG23	1:E:281:ALA:N	2.33	0.44
1:F:155:GLU:OE2	1:F:298:HIS:HE1	2.00	0.44
1:H:75:PRO:C	1:H:77:SER:N	2.75	0.44
1:I:279:PRO:HB2	1:I:282:LYS:HG2	2.00	0.44
1:C:303:LEU:HD23	1:C:308:MET:CE	2.47	0.44
1:D:21:THR:HG22	1:D:21:THR:O	2.17	0.44
1:D:119:LYS:HA	1:D:119:LYS:HD3	1.79	0.44
1:E:72:GLU:OE1	1:E:73:PRO:HD2	2.17	0.44
1:G:265:TYR:HA	1:G:266:PRO:HD3	1.86	0.44
1:H:59:ILE:N	1:H:60:PRO:CD	2.75	0.44
1:H:259:THR:CG2	1:H:259:THR:O	2.65	0.44
1:D:301:ARG:HA	1:D:301:ARG:NH1	2.28	0.44
1:I:43:LYS:HE2	1:I:68:ALA:CB	2.47	0.44
1:E:259:THR:HG23	5:E:2210:HOH:O	2.18	0.44
1:G:133:ILE:O	1:G:133:ILE:HG23	2.18	0.44
1:I:21:THR:C	1:I:23:ALA:H	2.24	0.44
1:I:304:GLU:OE2	1:I:309:LYS:HD3	2.17	0.44
1:A:51:ALA:HB3	1:A:233:LEU:HD22	1.98	0.44
1:D:110:ARG:NH2	1:D:183:GLU:O	2.49	0.44
1:D:112:LEU:HD11	1:D:188:ASP:HB3	1.99	0.44
3:D:1310:HF3:OBC	3:D:1310:HF3:OB3	2.35	0.44
1:A:16:VAL:HG11	1:A:249:LEU:CD2	2.47	0.44
1:A:252:LYS:NZ	1:A:252:LYS:CB	2.81	0.44
1:C:255:GLN:CB	1:C:271:VAL:HG21	2.48	0.44
1:D:255:GLN:O	1:D:259:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ARG:HD2	5:D:2204:HOH:O	2.17	0.44
1:E:108:ASP:OD2	1:E:110:ARG:HD3	2.17	0.44
1:E:193:ASN:HB3	1:E:195:TYR:CE1	2.53	0.44
1:E:203:GLU:OE2	1:E:204:LYS:HE2	2.18	0.44
1:F:16:VAL:HG11	1:F:249:LEU:HD21	1.99	0.44
1:F:142:PHE:HE2	1:F:308:MET:HE1	1.82	0.44
1:F:255:GLN:CB	1:F:271:VAL:HG21	2.48	0.44
1:F:256:ARG:HH12	1:F:272:VAL:H	1.66	0.44
1:C:306:ALA:HB3	1:C:308:MET:HE2	2.00	0.44
1:E:72:GLU:HG3	1:E:239:LYS:CE	2.44	0.44
1:E:72:GLU:HG2	1:E:234:LYS:HG2	2.00	0.44
1:F:105:VAL:HG22	1:F:191:LEU:HD12	2.00	0.44
1:D:34:LYS:O	1:D:38:LEU:HG	2.18	0.44
1:D:44:GLU:HG3	5:D:2033:HOH:O	2.17	0.44
1:D:235:SER:O	1:D:237:GLN:NE2	2.49	0.44
1:F:142:PHE:CE2	1:F:308:MET:HE1	2.52	0.44
1:H:82:THR:HG23	1:H:250:ALA:HB1	1.99	0.44
1:C:259:THR:OG1	1:C:266:PRO:HG3	2.18	0.43
1:G:36:ASP:HB3	5:G:2201:HOH:O	2.18	0.43
1:G:133:ILE:HD11	1:G:191:LEU:CD1	2.46	0.43
1:H:19:ALA:HB2	5:H:2007:HOH:O	2.18	0.43
1:C:101:ARG:NH2	1:C:228:SER:HB3	2.33	0.43
1:F:12:ALA:O	1:F:16:VAL:HG23	2.18	0.43
1:B:111:LYS:HE2	1:B:111:LYS:HB3	1.85	0.43
1:D:6:ASN:ND2	1:D:8:GLN:O	2.52	0.43
1:F:90:ALA:HB2	1:F:95:TRP:CE2	2.53	0.43
1:B:216:VAL:O	1:B:218:HIS:ND1	2.51	0.43
1:E:197:TRP:CD1	1:E:211:THR:HG23	2.53	0.43
1:G:114:GLU:HA	1:G:117:LEU:HD23	2.00	0.43
1:H:244:LYS:N	1:H:244:LYS:CD	2.81	0.43
1:H:255:GLN:HG3	1:H:268:ASN:HB3	1.99	0.43
1:D:114:GLU:OE1	1:D:114:GLU:HA	2.18	0.43
1:E:268:ASN:HD22	1:E:270:HIS:H	1.64	0.43
1:G:92:LYS:HB2	1:G:94:ASP:OD1	2.18	0.43
1:H:70:LEU:O	1:H:234:LYS:HG3	2.19	0.43
1:I:83:ARG:HG3	1:I:83:ARG:HH11	1.83	0.43
1:C:260:ALA:HA	1:C:274:THR:CG2	2.48	0.43
1:F:49:SER:HA	1:F:50:PRO:HD3	1.76	0.43
1:G:71:LEU:C	1:G:234:LYS:HG3	2.44	0.43
1:H:66:SER:C	1:H:68:ALA:H	2.27	0.43
1:I:59:ILE:N	1:I:60:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB3	1:A:38:LEU:HD21	2.01	0.43
1:D:53:VAL:HG13	1:D:231:ALA:O	2.18	0.43
1:F:8:GLN:HG3	1:F:9:HIS:N	2.33	0.43
1:G:38:LEU:O	1:G:42:ILE:HG13	2.18	0.43
1:G:252:LYS:O	1:G:256:ARG:HG3	2.18	0.43
1:H:262:ARG:HD3	5:H:2155:HOH:O	2.18	0.43
1:B:11:GLU:HG3	5:B:2005:HOH:O	2.18	0.43
1:C:43:LYS:NZ	1:C:64:THR:HG23	2.33	0.43
1:E:126:THR:HB	1:E:127:PRO:HD2	2.01	0.43
1:E:268:ASN:ND2	1:E:270:HIS:H	2.16	0.43
1:F:34:LYS:HE3	1:F:37:GLN:N	2.33	0.43
1:G:239:LYS:HB2	1:G:239:LYS:HE3	1.86	0.43
1:G:266:PRO:HD2	5:G:2176:HOH:O	2.19	0.43
1:H:300:THR:CG2	1:H:309:LYS:NZ	2.82	0.43
1:C:101:ARG:HH21	1:C:228:SER:HB3	1.84	0.43
1:D:114:GLU:HA	1:D:117:LEU:HD13	2.00	0.43
1:F:253:GLU:HG2	5:F:2182:HOH:O	2.17	0.43
1:F:304:GLU:OE2	1:F:309:LYS:NZ	2.46	0.43
1:G:252:LYS:HE3	1:G:270:HIS:CD2	2.54	0.43
1:H:5:TYR:CE1	1:H:51:ALA:HB2	2.54	0.43
1:H:12:ALA:HB1	1:H:258:LEU:HD11	1.99	0.43
1:H:240:ASP:HB2	1:H:244:LYS:HZ3	1.84	0.43
1:A:90:ALA:HB2	1:A:95:TRP:CD2	2.54	0.43
1:B:236:SER:HB3	1:B:239:LYS:HG2	2.00	0.43
1:D:223:ALA:HB3	1:D:286:PRO:HD3	2.01	0.43
1:G:7:GLY:HA3	1:G:57:GLU:OE2	2.19	0.43
1:G:130:LYS:HA	1:G:168:TYR:HB3	1.99	0.43
1:H:246:VAL:C	1:H:248:PHE:N	2.73	0.43
1:I:136:VAL:HG13	1:I:172:TYR:O	2.18	0.43
1:I:282:LYS:HB3	1:I:282:LYS:NZ	2.34	0.43
1:B:174:LYS:HB3	5:B:2215:HOH:O	2.18	0.42
1:C:58:GLN:O	1:C:58:GLN:HG3	2.18	0.42
1:D:185:GLY:HA2	5:D:2081:HOH:O	2.17	0.42
1:F:111:LYS:C	1:F:112:LEU:HG	2.43	0.42
1:G:2:ILE:HG13	1:G:28:VAL:HG13	2.00	0.42
1:G:18:ASP:O	1:G:22:ARG:HB2	2.19	0.42
1:G:83:ARG:HH12	1:G:89:VAL:CG2	2.31	0.42
1:G:104:VAL:HG21	1:G:213:LEU:HD22	2.00	0.42
1:G:155:GLU:OE1	1:G:298:HIS:HE1	2.02	0.42
1:H:53:VAL:CG2	1:H:242:ALA:HB1	2.48	0.42
2:B:1310:HF5:OC2	5:B:2217:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ALA:O	1:C:64:THR:HB	2.19	0.42
1:C:104:VAL:HG21	1:C:213:LEU:HD22	2.00	0.42
1:H:1:ASP:H1	1:H:26:ILE:CG2	2.14	0.42
1:A:100:GLY:HA2	1:A:226:THR:O	2.20	0.42
1:B:278:GLU:HG2	5:B:2186:HOH:O	2.19	0.42
1:C:174:LYS:HE2	5:C:2137:HOH:O	2.18	0.42
2:E:1310:HF5:OAC	2:E:1310:HF5:OC2	2.37	0.42
1:F:33:ALA:HB3	1:F:38:LEU:CG	2.49	0.42
1:F:57:GLU:HB2	1:F:101:ARG:HH21	1.84	0.42
1:F:279:PRO:HD2	1:F:282:LYS:HG3	2.01	0.42
1:A:255:GLN:CB	1:A:271:VAL:HG21	2.50	0.42
1:B:143:LEU:O	1:B:147:VAL:HG23	2.19	0.42
1:F:1:ASP:CG	1:F:27:LYS:HB2	2.44	0.42
1:A:255:GLN:HG3	1:A:268:ASN:HB2	2.01	0.42
1:B:6:ASN:OD1	1:B:13:ALA:HB2	2.20	0.42
1:C:235:SER:HB3	5:C:2035:HOH:O	2.19	0.42
1:D:16:VAL:HG11	1:D:249:LEU:CD2	2.50	0.42
1:D:267:LEU:HD23	1:D:280:ILE:CD1	2.49	0.42
1:F:6:ASN:OD1	1:F:8:GLN:HB3	2.19	0.42
1:H:238:ASN:O	1:H:239:LYS:C	2.62	0.42
4:H:1310:PHF:OBC	4:H:1310:PHF:OB3	2.37	0.42
1:H:82:THR:HA	1:H:267:LEU:O	2.20	0.42
1:H:233:LEU:N	1:H:233:LEU:HD12	2.35	0.42
1:H:279:PRO:O	1:H:282:LYS:N	2.46	0.42
1:I:41:GLN:O	1:I:45:GLU:HG3	2.19	0.42
1:B:2:ILE:CG1	1:B:28:VAL:HG22	2.50	0.42
1:C:34:LYS:HE3	1:C:34:LYS:HB3	1.82	0.42
1:C:56:SER:O	1:C:228:SER:HB2	2.19	0.42
1:D:92:LYS:HE2	5:D:2049:HOH:O	2.20	0.42
1:D:126:THR:HB	1:D:127:PRO:HD2	2.00	0.42
1:F:104:VAL:CG2	1:F:213:LEU:HD22	2.50	0.42
1:F:136:VAL:HA	1:F:137:PRO:HD2	1.91	0.42
4:G:1310:PHF:OBD	4:G:1310:PHF:OB1	2.37	0.42
1:I:197:TRP:CD1	1:I:211:THR:HG22	2.55	0.42
1:D:215:PHE:HA	5:D:2074:HOH:O	2.20	0.42
1:G:303:LEU:HD23	1:G:308:MET:HB2	2.00	0.42
1:H:36:ASP:OD2	1:H:36:ASP:N	2.46	0.42
1:H:151:LYS:HE2	1:H:295:GLU:OE2	2.18	0.42
1:I:200:PHE:CE2	1:I:204:LYS:HG3	2.55	0.42
1:A:121:VAL:HB	5:A:2122:HOH:O	2.20	0.42
1:A:308:MET:O	1:A:309:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:VAL:O	1:C:139:SER:HB3	2.20	0.42
1:D:34:LYS:HE3	1:D:37:GLN:N	2.35	0.42
1:E:36:ASP:OD2	1:E:36:ASP:N	2.53	0.42
1:H:49:SER:HA	1:H:50:PRO:HD3	1.86	0.42
1:A:99:SER:HA	1:A:267:LEU:HG	2.01	0.42
1:A:292:THR:HG22	5:A:2112:HOH:O	2.20	0.42
1:C:268:ASN:HD22	1:C:268:ASN:C	2.27	0.42
1:D:34:LYS:HE3	1:D:37:GLN:H	1.85	0.42
1:D:301:ARG:O	1:D:305:GLN:HB2	2.19	0.42
1:E:49:SER:HA	1:E:50:PRO:HD3	1.79	0.42
1:F:217:ARG:HB3	1:F:218:HIS:H	1.71	0.42
1:H:112:LEU:HD22	1:H:116:ASP:HB2	2.01	0.42
1:D:11:GLU:HG2	1:D:261:VAL:HG11	2.02	0.41
1:D:46:GLY:C	1:D:48:ARG:H	2.27	0.41
1:D:153:LYS:HE3	5:D:2107:HOH:O	2.19	0.41
1:E:10:LYS:NZ	1:E:32:SER:HB2	2.34	0.41
1:A:180:GLN:O	1:A:184:ASN:ND2	2.53	0.41
1:D:265:TYR:HA	1:D:266:PRO:HD3	1.95	0.41
1:E:101:ARG:HD2	1:E:264:GLU:OE2	2.20	0.41
1:F:122:LEU:HD21	1:F:149:ILE:HD13	2.01	0.41
1:G:224:LEU:C	1:G:224:LEU:CD1	2.93	0.41
1:H:45:GLU:HG2	1:H:49:SER:CA	2.51	0.41
1:A:54:PHE:CZ	1:A:56:SER:HB3	2.55	0.41
1:D:74:LEU:HD12	1:D:96:VAL:HG23	2.01	0.41
1:G:11:GLU:HB2	5:G:2009:HOH:O	2.20	0.41
1:G:59:ILE:HG12	5:G:2161:HOH:O	2.20	0.41
1:C:22:ARG:HB2	5:C:2012:HOH:O	2.20	0.41
1:D:106:VAL:HG21	1:D:179:LEU:CD1	2.50	0.41
1:E:1:ASP:HB3	5:E:2027:HOH:O	2.19	0.41
1:F:304:GLU:HG2	1:F:309:LYS:O	2.20	0.41
1:G:12:ALA:O	1:G:16:VAL:HG23	2.19	0.41
1:A:42:ILE:HD13	1:A:233:LEU:HD21	2.01	0.41
1:C:80:ASN:HB3	1:C:83:ARG:HH22	1.86	0.41
1:C:306:ALA:CB	1:C:308:MET:HE2	2.50	0.41
1:E:24:THR:HG21	1:E:244:LYS:HE2	2.01	0.41
1:G:278:GLU:OE1	1:G:282:LYS:HB3	2.20	0.41
1:I:16:VAL:HG11	1:I:249:LEU:HD23	2.02	0.41
1:I:136:VAL:O	1:I:139:SER:HB2	2.19	0.41
1:B:159:LEU:HD11	1:B:163:LYS:HE3	2.03	0.41
1:C:17:ALA:O	1:C:20:PHE:HB3	2.20	0.41
1:F:256:ARG:NH1	1:F:272:VAL:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:LEU:C	1:G:260:ALA:H	2.29	0.41
1:H:12:ALA:HB2	5:H:2155:HOH:O	2.21	0.41
1:B:127:PRO:HG3	1:B:168:TYR:CZ	2.55	0.41
1:C:36:ASP:N	1:C:58:GLN:NE2	2.69	0.41
1:C:59:ILE:N	1:C:60:PRO:CD	2.84	0.41
1:H:91:ALA:C	1:H:93:LYS:H	2.29	0.41
1:H:215:PHE:O	1:H:217:ARG:HG3	2.20	0.41
1:A:217:ARG:HA	1:A:283:LEU:O	2.20	0.41
1:C:266:PRO:HD2	5:C:2196:HOH:O	2.20	0.41
1:D:76:ALA:O	1:D:80:ASN:ND2	2.54	0.41
1:H:8:GLN:OE1	1:H:101:ARG:NH2	2.54	0.41
1:H:21:THR:HA	1:H:26:ILE:O	2.19	0.41
1:H:45:GLU:HG2	1:H:49:SER:HA	2.01	0.41
1:H:272:VAL:HG13	5:H:2163:HOH:O	2.20	0.41
1:I:136:VAL:CG1	1:I:139:SER:OG	2.69	0.41
4:I:1310:PHF:OE3	4:I:1310:PHF:OAE	2.39	0.41
1:B:146:ILE:HD13	1:B:162:LEU:HD11	2.02	0.41
1:I:79:ILE:CD1	1:I:93:LYS:HE2	2.47	0.41
1:I:83:ARG:NH1	1:I:83:ARG:HG3	2.36	0.41
1:I:103:ARG:HD3	5:I:2077:HOH:O	2.21	0.41
1:I:236:SER:HB3	1:I:239:LYS:HG3	2.03	0.41
1:B:58:GLN:NE2	1:B:60:PRO:HG2	2.27	0.41
1:G:5:TYR:CD1	1:G:51:ALA:HB2	2.56	0.41
1:H:71:LEU:HD21	1:H:94:ASP:O	2.21	0.41
1:I:265:TYR:CD1	1:I:265:TYR:N	2.88	0.41
1:C:291:THR:HG22	1:C:296:LYS:HE3	2.02	0.40
1:F:77:SER:O	1:F:81:GLU:HG2	2.22	0.40
1:F:80:ASN:OD1	1:F:83:ARG:HD3	2.21	0.40
1:G:278:GLU:O	1:G:279:PRO:C	2.64	0.40
1:I:151:LYS:NZ	1:I:295:GLU:OE1	2.55	0.40
1:I:216:VAL:HG23	1:I:217:ARG:N	2.36	0.40
1:A:137:PRO:HA	1:A:142:PHE:CD2	2.57	0.40
1:B:118:GLU:HB3	1:B:123:ASN:HB2	2.02	0.40
1:C:45:GLU:OE1	1:C:49:SER:HB2	2.22	0.40
1:C:268:ASN:HD22	1:C:269:PRO:N	2.20	0.40
1:F:98:LEU:C	1:F:267:LEU:HG	2.46	0.40
1:G:238:ASN:HD22	1:G:238:ASN:HA	1.69	0.40
1:H:34:LYS:HB3	1:H:36:ASP:OD2	2.21	0.40
1:H:78:THR:CG2	1:H:247:ALA:HA	2.50	0.40
1:H:184:ASN:HB3	5:H:2114:HOH:O	2.21	0.40
1:D:183:GLU:OE1	1:D:211:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:VAL:CG2	1:H:211:THR:HG21	2.28	0.40
1:H:8:GLN:CG	1:H:9:HIS:N	2.85	0.40
1:B:209:VAL:HG12	1:B:211:THR:H	1.86	0.40
1:C:49:SER:HA	1:C:50:PRO:HD3	1.90	0.40
1:C:259:THR:HG23	1:C:273:SER:HA	1.97	0.40
1:D:106:VAL:CG2	1:D:211:THR:OG1	2.68	0.40
1:G:107:TYR:OH	1:G:114:GLU:HG2	2.20	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 X-ray entries followed by that with respect to entries of similar resolution.

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	307/309 (99%)	298 (97%)	9 (3%)	0	100	100
1	B	307/309 (99%)	298 (97%)	8 (3%)	1 (0%)	36	21
1	C	307/309 (99%)	296 (96%)	11 (4%)	0	100	100
1	D	307/309 (99%)	290 (94%)	15 (5%)	2 (1%)	18	6
1	E	307/309 (99%)	295 (96%)	11 (4%)	1 (0%)	36	21
1	F	307/309 (99%)	293 (95%)	14 (5%)	0	100	100
1	G	307/309 (99%)	294 (96%)	13 (4%)	0	100	100
1	H	307/309 (99%)	281 (92%)	20 (6%)	6 (2%)	6	0
1	I	307/309 (99%)	285 (93%)	18 (6%)	4 (1%)	9	1
All	All	2763/2781 (99%)	2630 (95%)	119 (4%)	14 (0%)	24	10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	239	LYS

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Mol	Chain	Res	Type
1	H	34	LYS
1	H	93	LYS
1	H	280	ILE
1	I	9	HIS
1	I	205	GLY
1	B	8	GLN
1	D	217	ARG
1	H	33	ALA
1	I	10	LYS
1	I	23	ALA
1	E	280	ILE
1	H	77	SER
1	D	59	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 X-ray entries followed by that with respect to entries of similar resolution.

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	245/245 (100%)	238 (97%)	7 (3%)	37	14
1	B	245/245 (100%)	238 (97%)	7 (3%)	37	14
1	C	245/245 (100%)	241 (98%)	4 (2%)	55	34
1	D	245/245 (100%)	241 (98%)	4 (2%)	55	34
1	E	245/245 (100%)	236 (96%)	9 (4%)	30	8
1	F	245/245 (100%)	241 (98%)	4 (2%)	55	34
1	G	245/245 (100%)	241 (98%)	4 (2%)	55	34
1	H	245/245 (100%)	240 (98%)	5 (2%)	48	26
1	I	245/245 (100%)	239 (98%)	6 (2%)	43	20
All	All	2205/2205 (100%)	2155 (98%)	50 (2%)	44	21

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN

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Mol	Chain	Res	Type
1	A	10	LYS
1	A	37	GLN
1	A	80	ASN
1	A	101	ARG
1	A	116	ASP
1	A	252	LYS
1	B	8	GLN
1	B	14	GLN
1	B	27	LYS
1	B	85	LYS
1	B	167	GLU
1	B	191	LEU
1	B	259	THR
1	C	2	ILE
1	C	36	ASP
1	C	274	THR
1	C	288	VAL
1	D	57	GLU
1	D	103	ARG
1	D	214	ASN
1	D	259	THR
1	E	36	ASP
1	E	103	ARG
1	E	110	ARG
1	E	115	LYS
1	E	121	VAL
1	E	167	GLU
1	E	191	LEU
1	E	268	ASN
1	E	287	GLN
1	F	139	SER
1	F	191	LEU
1	F	216	VAL
1	F	268	ASN
1	G	115	LYS
1	G	187	VAL
1	G	191	LEU
1	G	224	LEU
1	H	69	ASN
1	H	176	SER
1	H	234	LYS
1	H	259	THR

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Mol	Chain	Res	Type
1	H	278	GLU
1	I	167	GLU
1	I	174	LYS
1	I	187	VAL
1	I	202	ARG
1	I	282	LYS
1	I	287	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	80	ASN
1	A	123	ASN
1	A	131	ASN
1	A	180	GLN
1	A	255	GLN
1	A	298	HIS
1	B	14	GLN
1	B	58	GLN
1	B	80	ASN
1	B	198	HIS
1	B	208	ASN
1	B	214	ASN
1	B	255	GLN
1	B	298	HIS
1	C	6	ASN
1	C	8	GLN
1	C	31	ASN
1	C	58	GLN
1	C	131	ASN
1	C	180	GLN
1	C	198	HIS
1	C	207	GLN
1	C	208	ASN
1	C	255	GLN
1	C	268	ASN
1	C	287	GLN
1	D	9	HIS
1	D	31	ASN
1	D	37	GLN
1	D	41	GLN

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Mol	Chain	Res	Type
1	D	58	GLN
1	D	131	ASN
1	D	175	ASN
1	D	208	ASN
1	D	218	HIS
1	D	255	GLN
1	D	298	HIS
1	E	180	GLN
1	E	208	ASN
1	E	218	HIS
1	E	255	GLN
1	E	268	ASN
1	E	298	HIS
1	E	305	GLN
1	F	8	GLN
1	F	14	GLN
1	F	131	ASN
1	F	180	GLN
1	F	193	ASN
1	F	198	HIS
1	F	214	ASN
1	F	255	GLN
1	F	268	ASN
1	F	298	HIS
1	G	14	GLN
1	G	123	ASN
1	G	131	ASN
1	G	184	ASN
1	G	193	ASN
1	G	218	HIS
1	G	238	ASN
1	G	255	GLN
1	G	270	HIS
1	G	298	HIS
1	H	41	GLN
1	H	69	ASN
1	H	80	ASN
1	H	198	HIS
1	H	208	ASN
1	H	214	ASN
1	H	238	ASN
1	H	255	GLN

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Mol	Chain	Res	Type
1	H	298	HIS
1	I	9	HIS
1	I	69	ASN
1	I	123	ASN
1	I	131	ASN
1	I	184	ASN
1	I	208	ASN
1	I	238	ASN
1	I	270	HIS
1	I	287	GLN

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)

9 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	$\#\|Z\| > 2$
4	PHF	G	1310	1	6,37,37	3.79	5 (83%)	3,117,117	2.27	1 (33%)
4	PHF	I	1310	1	6,37,37	4.80	4 (66%)	3,117,117	1.47	0
2	HF5	A	1310	1	0,31,31	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HF5	F	1310	1	0,31,31	-	-	-		
2	HF5	C	1310	1	0,31,31	-	-	-		
3	HF3	D	1310	1	4,23,23	3.34	3 (75%)	3,66,66	0.24	0
2	HF5	B	1310	1	0,31,31	-	-	-		
4	PHF	H	1310	1	6,37,37	3.61	4 (66%)	3,117,117	1.55	1 (33%)
2	HF5	E	1310	1	0,31,31	-	-	-		

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1310	PHF	P-O3	8.76	1.73	1.54
4	H	1310	PHF	P-O3	6.66	1.68	1.54
4	G	1310	PHF	P-O2	5.95	1.67	1.54
4	I	1310	PHF	O02-HFC	5.27	2.57	2.27
4	G	1310	PHF	P-O3	-4.91	1.43	1.54
4	H	1310	PHF	O02-HFC	4.87	2.55	2.27
4	I	1310	PHF	P-O2	-4.77	1.43	1.54
3	D	1310	HF3	P-O1	4.52	1.64	1.54
3	D	1310	HF3	P-O2	3.64	1.62	1.54
4	G	1310	PHF	O02-HFA	3.29	2.46	2.27
3	D	1310	HF3	P-O3	3.27	1.61	1.54
4	I	1310	PHF	O02-HFA	3.00	2.44	2.27
4	G	1310	PHF	P-O1	2.97	1.60	1.54
4	G	1310	PHF	P-O4	2.49	1.56	1.48
4	H	1310	PHF	O02-HFA	2.39	2.41	2.27
4	H	1310	PHF	P-O4	2.05	1.55	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1310	PHF	O1-P-O4	3.16	124.76	110.67
4	H	1310	PHF	O1-P-O4	2.25	120.70	110.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1310	PHF	2	0

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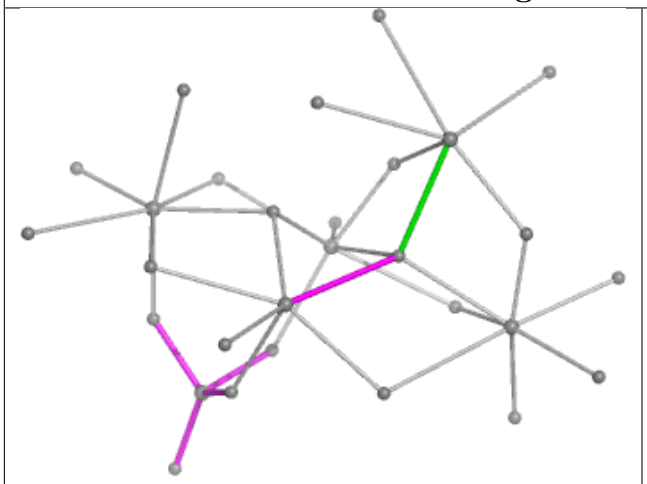
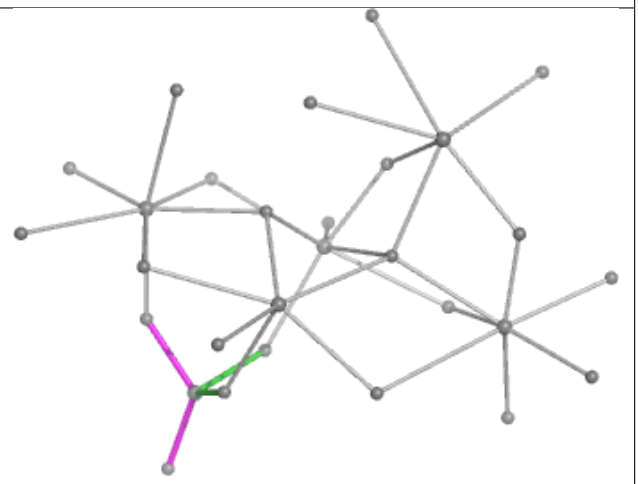
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1310	PHF	3	0
2	A	1310	HF5	3	0
2	C	1310	HF5	2	0
3	D	1310	HF3	2	0
2	B	1310	HF5	1	0
4	H	1310	PHF	2	0
2	E	1310	HF5	3	0

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 PHF G 1310



Bond lengths

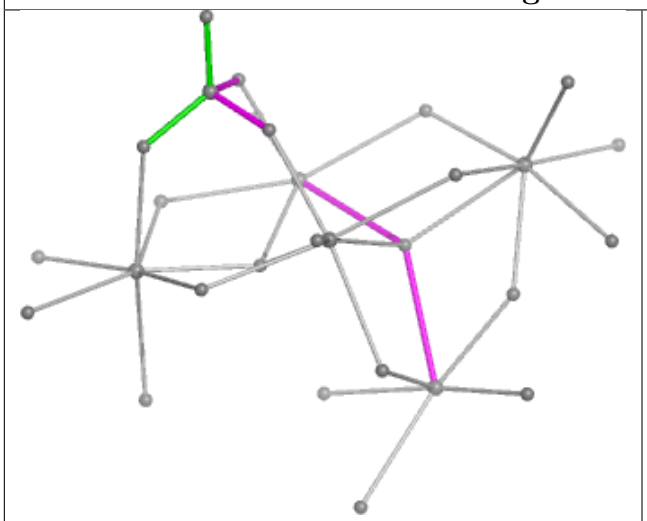


Bond angles

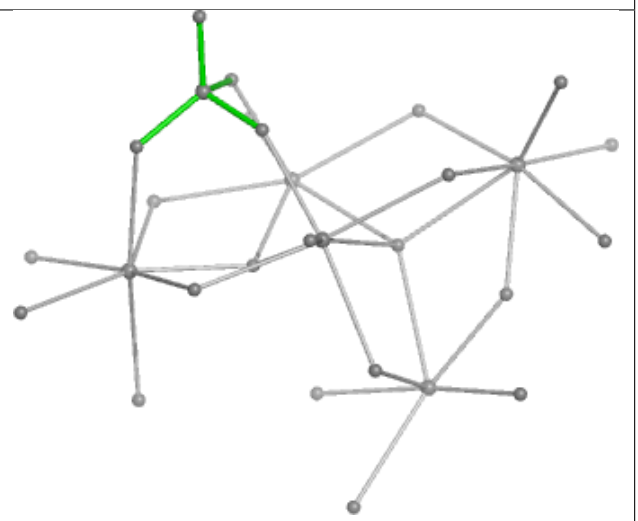
Torsions

Rings

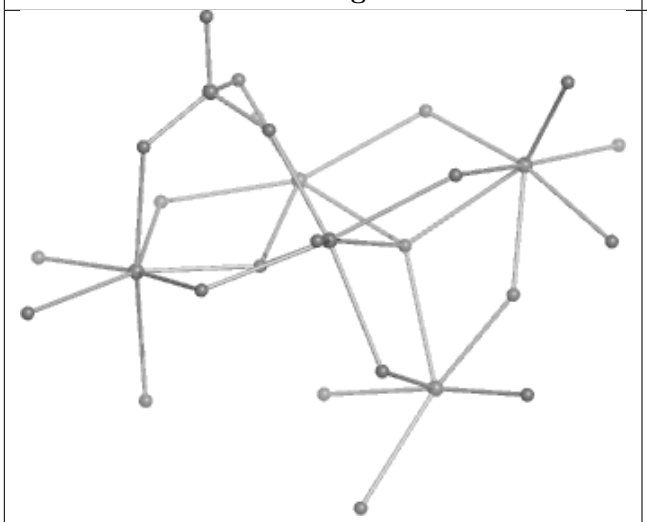
Ligand PHF I 1310



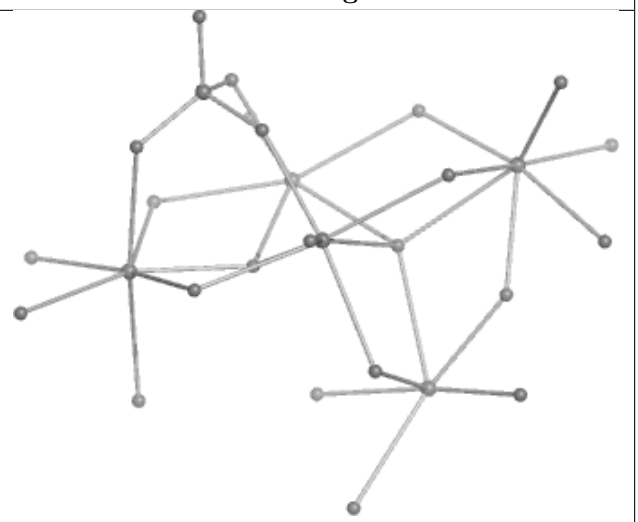
Bond lengths



Bond angles

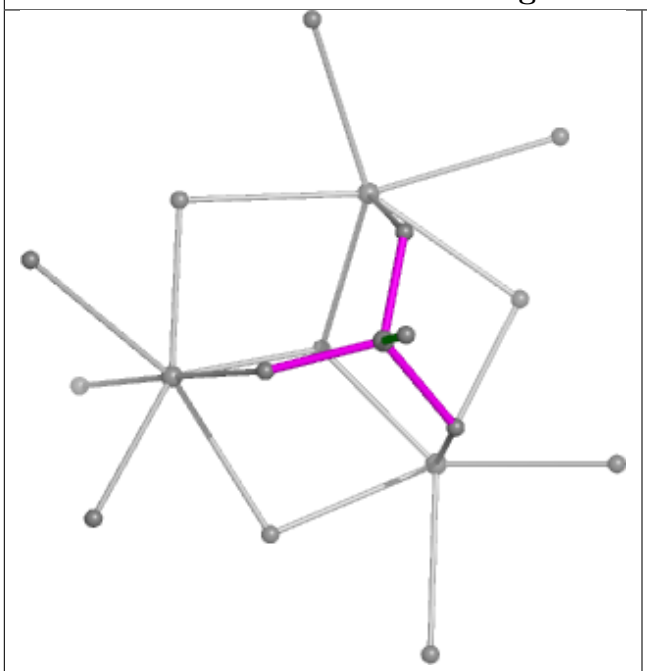


Torsions

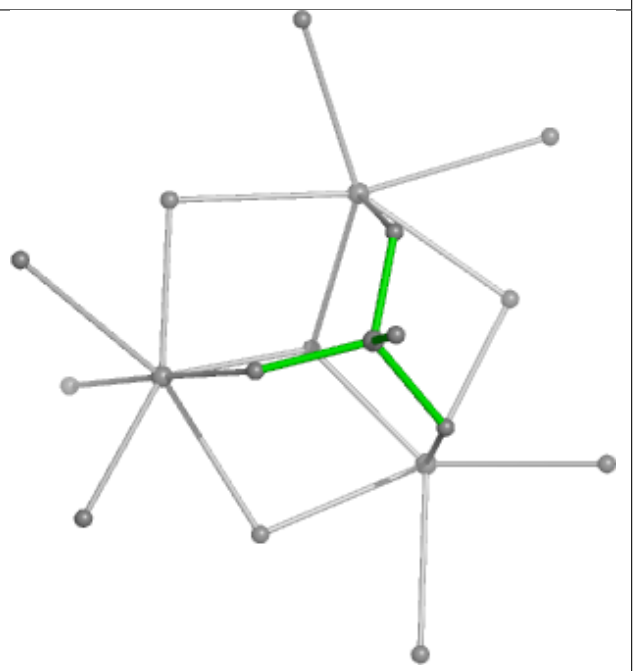


Rings

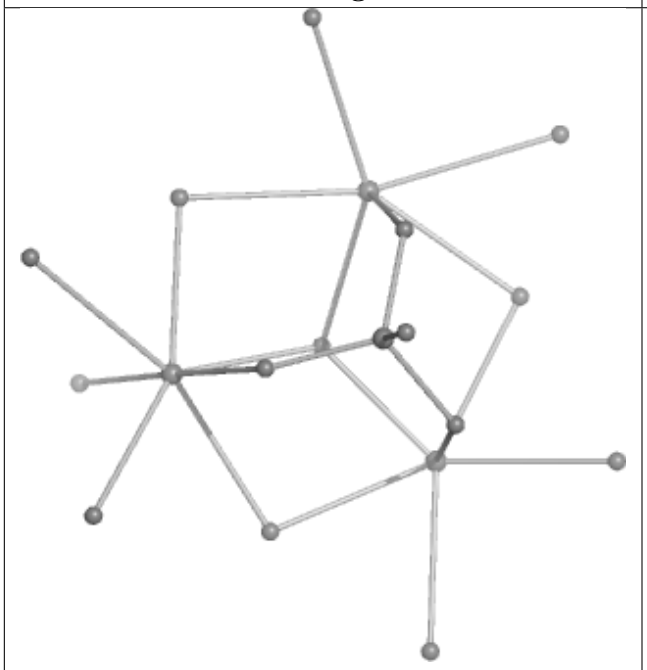
Ligand HF3 D 1310



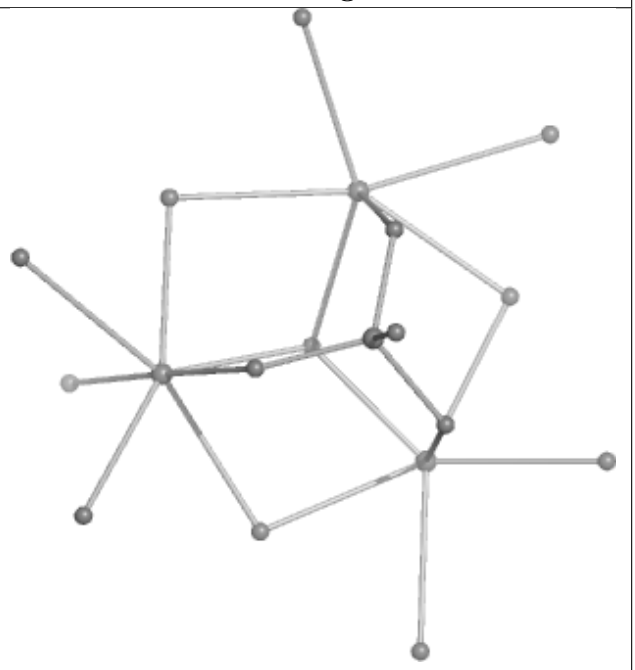
Bond lengths



Bond angles

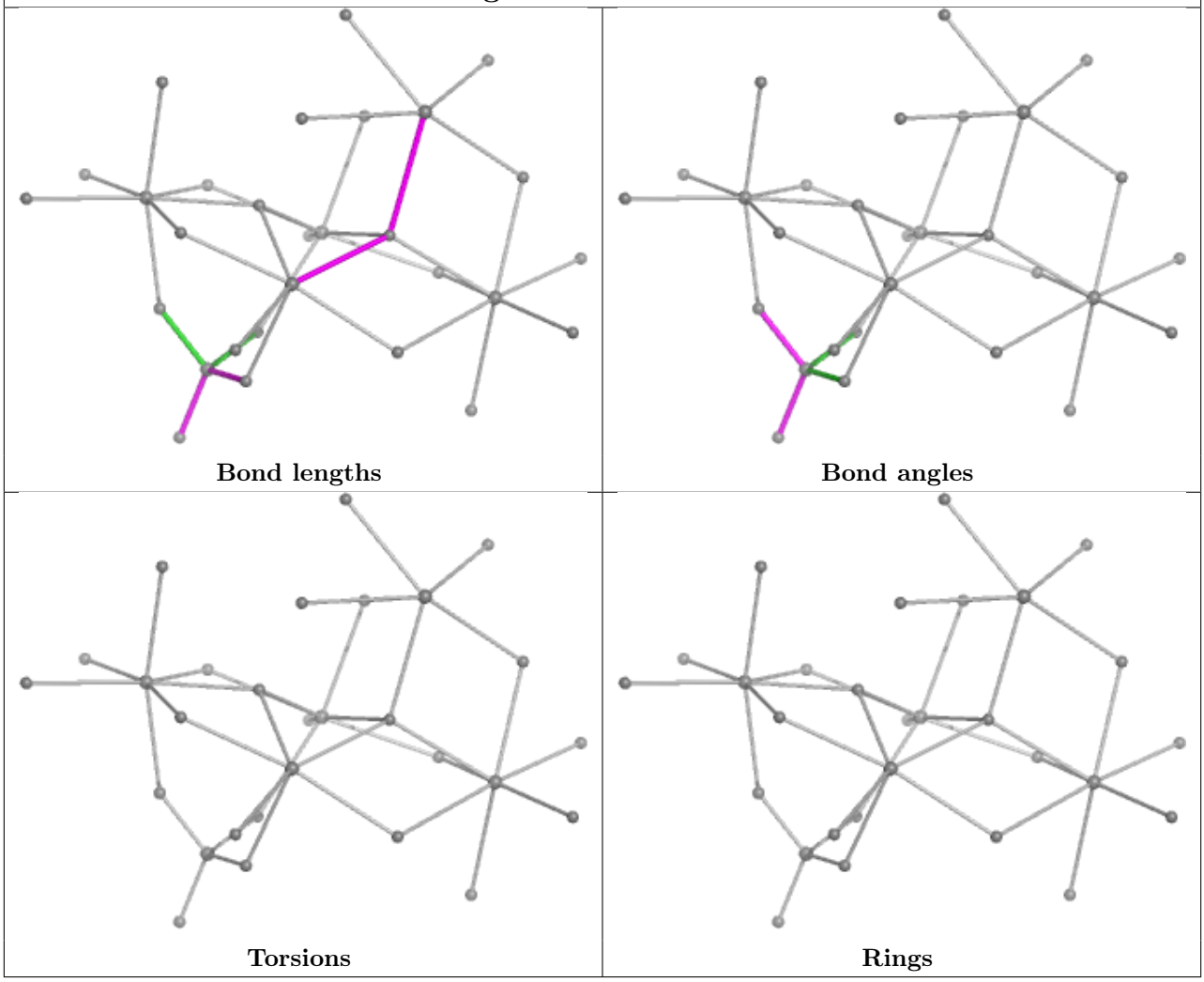


Torsions



Rings

Ligand PHF H 1310



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	309/309 (100%)	-1.32	0	100	100	18, 26, 38, 49	0
1	B	309/309 (100%)	-1.25	0	100	100	16, 29, 45, 61	0
1	C	309/309 (100%)	-1.25	0	100	100	18, 29, 44, 52	0
1	D	309/309 (100%)	-1.25	0	100	100	20, 30, 45, 61	0
1	E	309/309 (100%)	-1.30	0	100	100	18, 27, 38, 47	0
1	F	309/309 (100%)	-1.29	0	100	100	18, 27, 39, 52	0
1	G	309/309 (100%)	-1.25	0	100	100	21, 31, 41, 48	0
1	H	309/309 (100%)	-1.10	0	100	100	20, 34, 59, 65	0
1	I	309/309 (100%)	-1.19	0	100	100	21, 33, 45, 59	0
All	All	2781/2781 (100%)	-1.24	0	100	100	16, 30, 46, 65	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

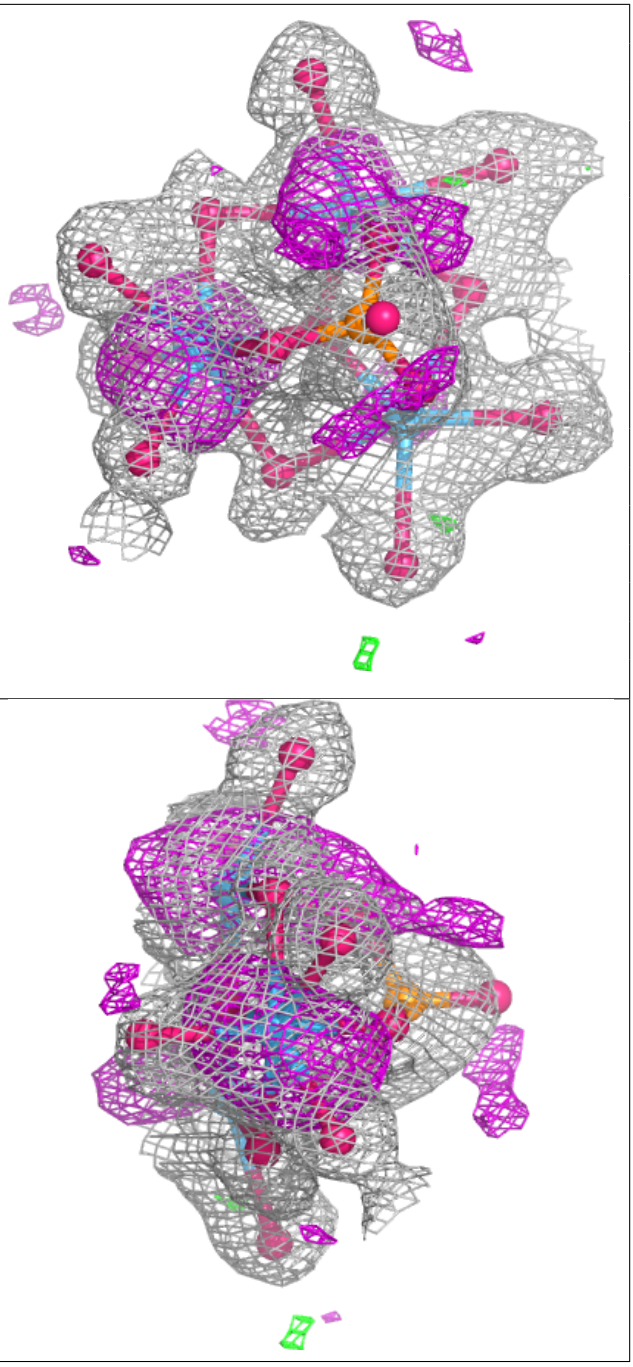
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HF5	A	1310	26/26	1.00	0.05	25,56,99,99	0
2	HF5	B	1310	26/26	1.00	0.05	28,61,99,99	0
2	HF5	C	1310	26/26	1.00	0.05	23,50,99,99	0
2	HF5	E	1310	26/26	1.00	0.04	29,69,99,99	0
2	HF5	F	1310	26/26	1.00	0.04	34,73,99,99	0
3	HF3	D	1310	19/19	1.00	0.03	25,34,66,74	0
4	PHF	G	1310	29/29	1.00	0.04	31,53,90,99	0
4	PHF	H	1310	29/29	1.00	0.05	34,65,83,89	0
4	PHF	I	1310	29/29	1.00	0.05	36,71,99,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

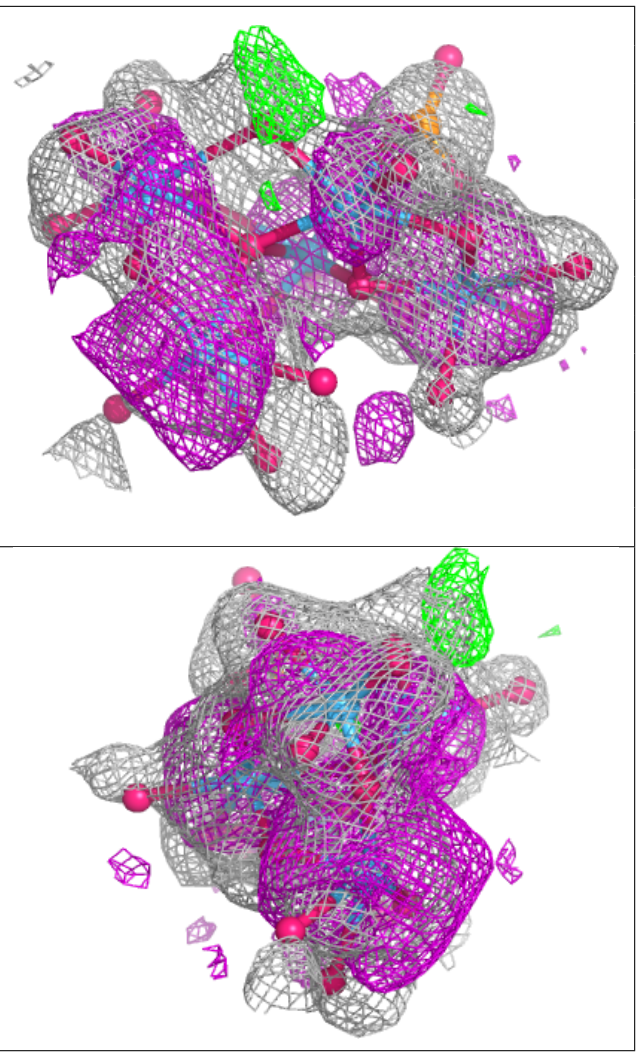
Electron density around HF3 D 1310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



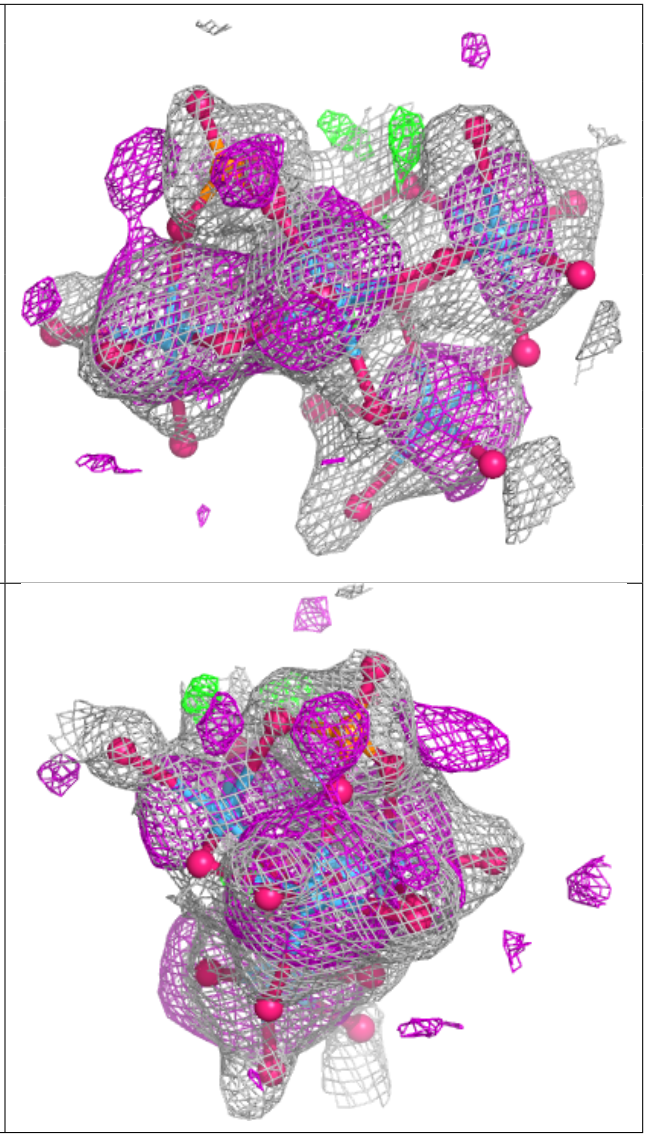
Electron density around PHF G 1310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



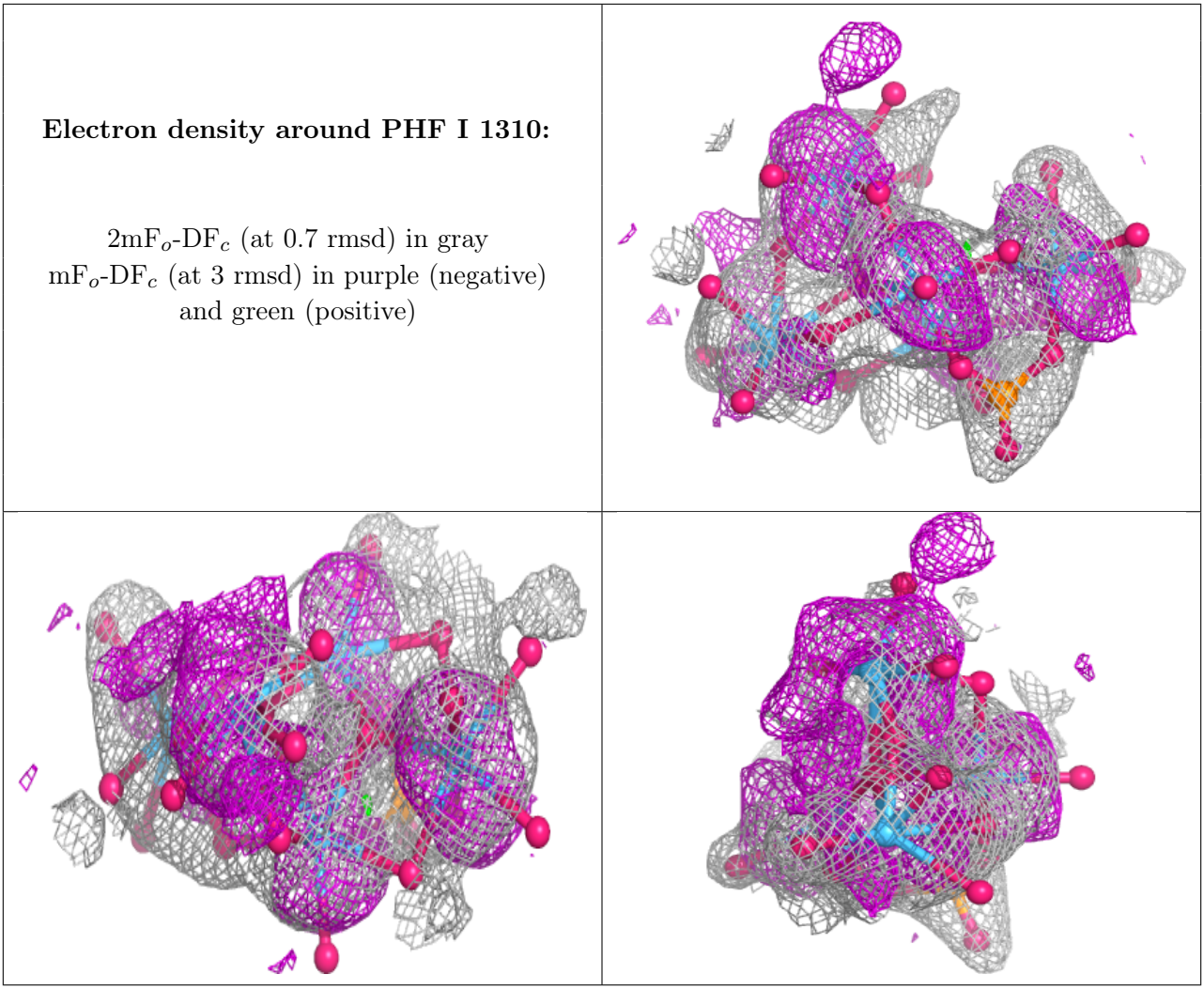
Electron density around PHF H 1310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHF I 1310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.