wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2026 – 08:05 AM EDT

PDB ID	:	2BCC / pdb_00002bcc
Title	:	STIGMATELLIN-BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors	:	Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.; Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on	:	1998-09-18
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

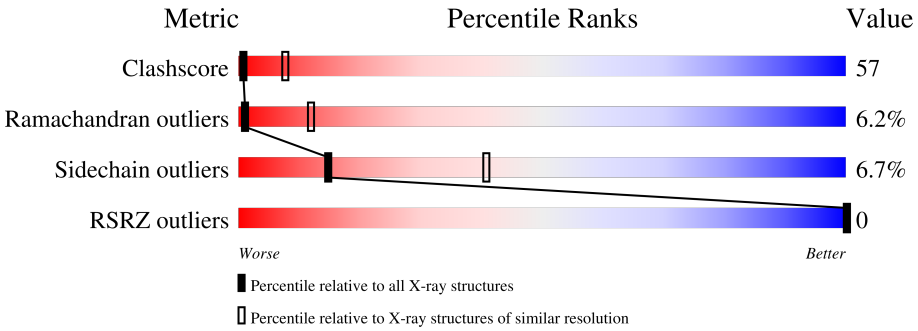
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.50 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.



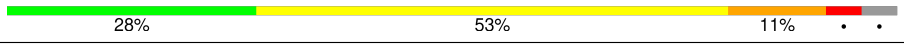
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	446	33% 56% 10%
2	B	422	32% 52% 11%
3	C	380	25% 56% 17%
4	D	241	34% 54% 11%
5	E	196	31% 54% 14%
6	F	109	43% 39% 10% 8%

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Mol	Chain	Length	Quality of chain
7	G	81	
8	H	78	
9	I	33	
10	J	62	

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
13	PEE	C	384	X	-	-	-
13	PEE	E	198	X	-	-	-
16	HEC	D	243	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 15754 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3423	2147	601	657	18	0	0	0

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	406	2994	1878	518	591	7	0	0	0

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3002	2013	473	504	12	0	0	0

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1899	1214	326	345	14	0	0	0

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1512	953	266	285	8	0	0	0

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	100	875	557	153	162	3	0	0	0

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	78	Total	C	N	O	S	0	0	0
			626	411	114	100	1			

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			490	301	88	96	5			

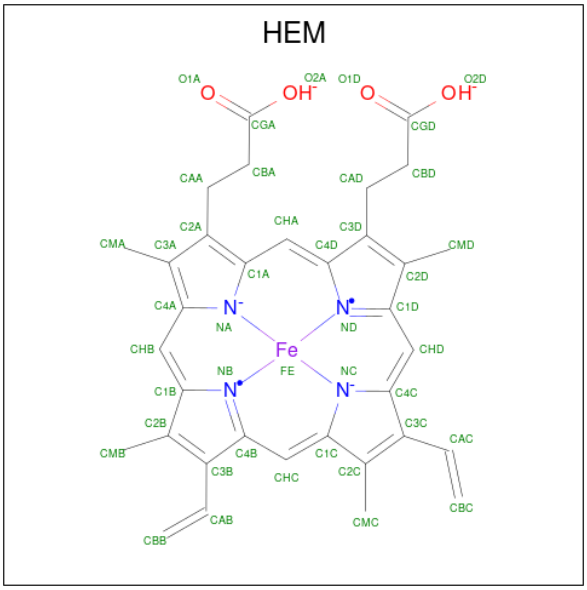
- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	0	0	0
			159	92	33	34			

- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

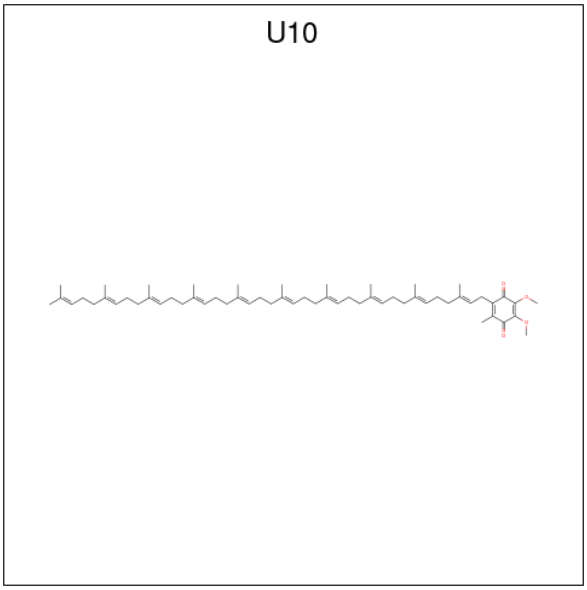
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			459	299	78	82			

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



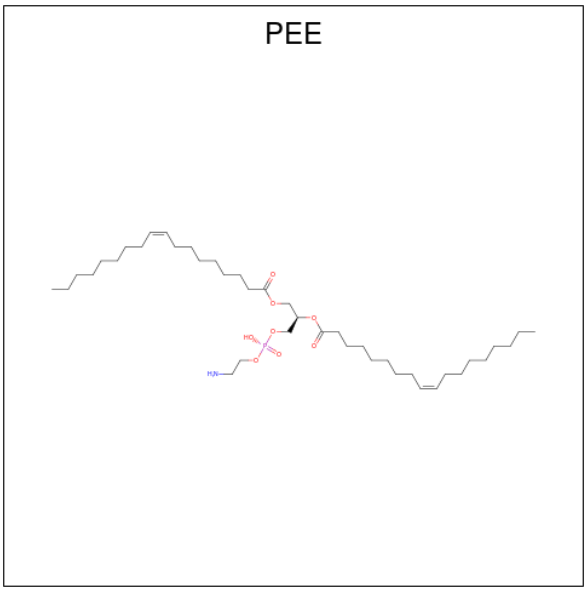
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



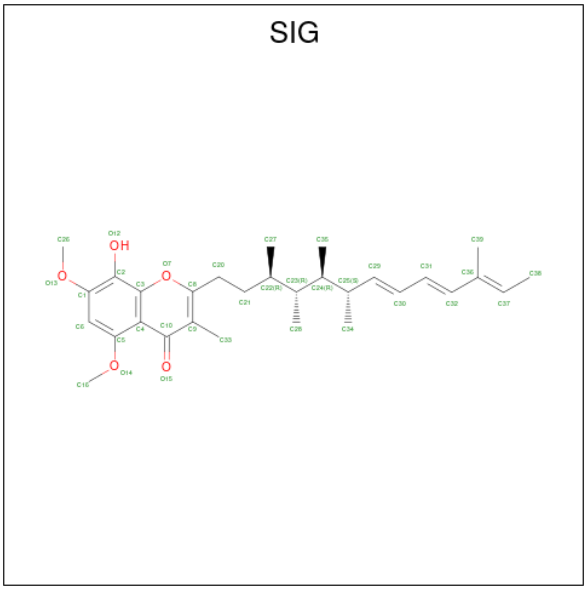
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			29	25	4		

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



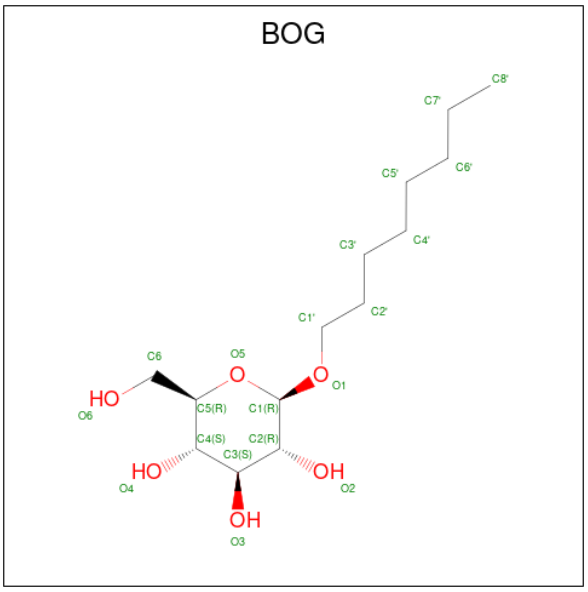
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is STIGMATELLIN (CCD ID: SIG) (formula: $C_{30}H_{42}O_5$).



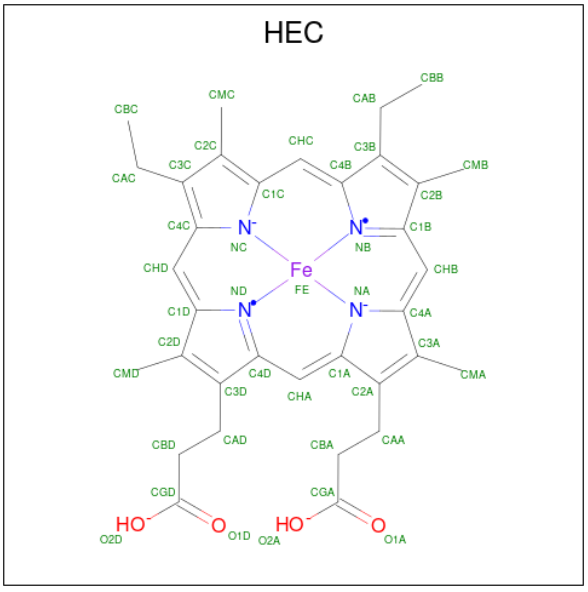
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O		0	0
			35	30	5			

- Molecule 15 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



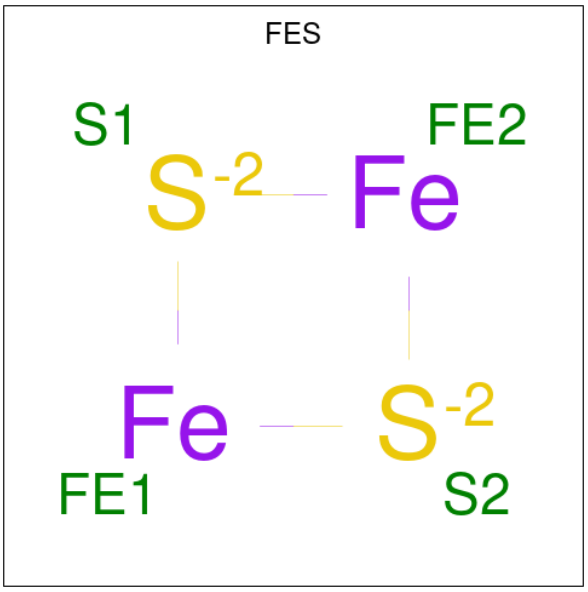
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C O 20 14 6	0	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
17	E	1	4	2	2	0	0

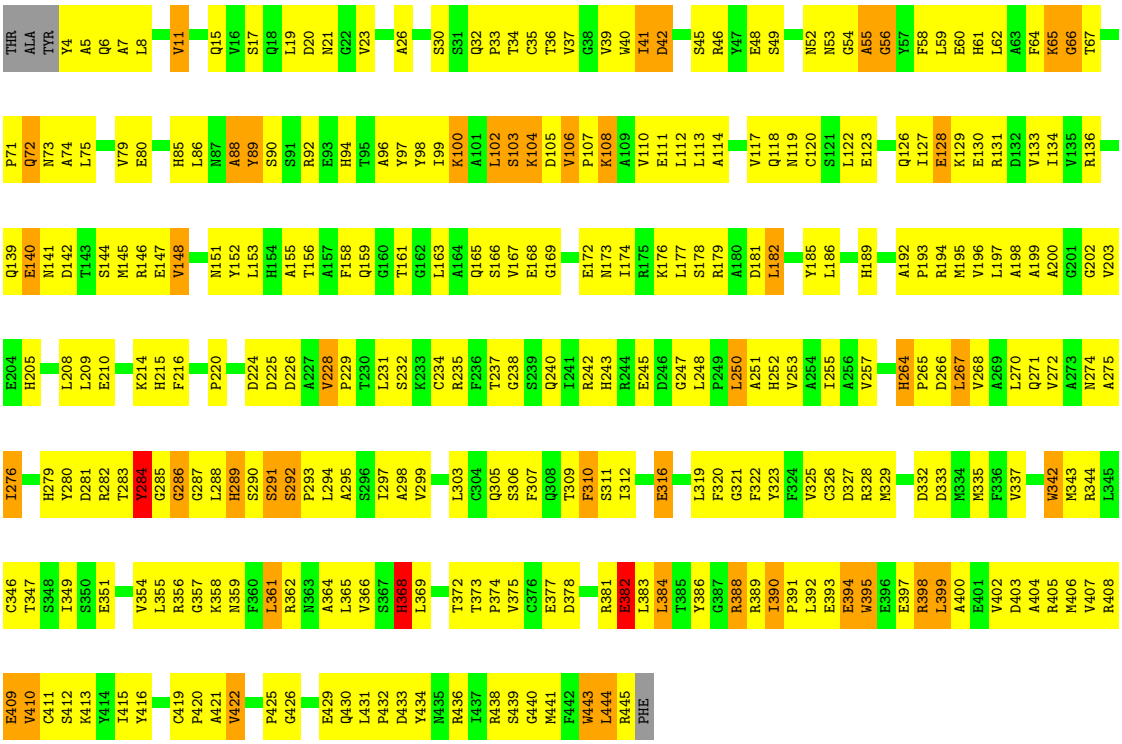
3 Residue-property plots (i)

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: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

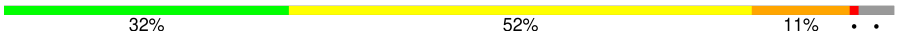
Chain A:



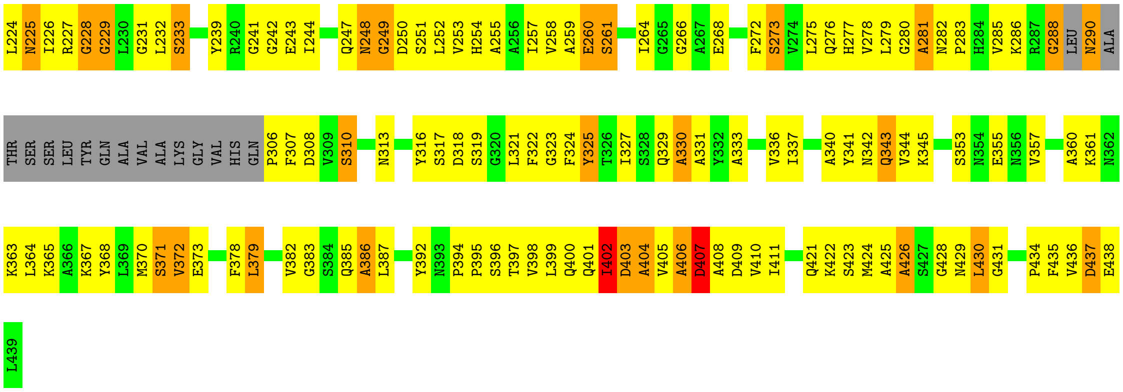


• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain B:

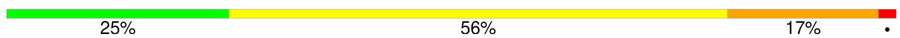


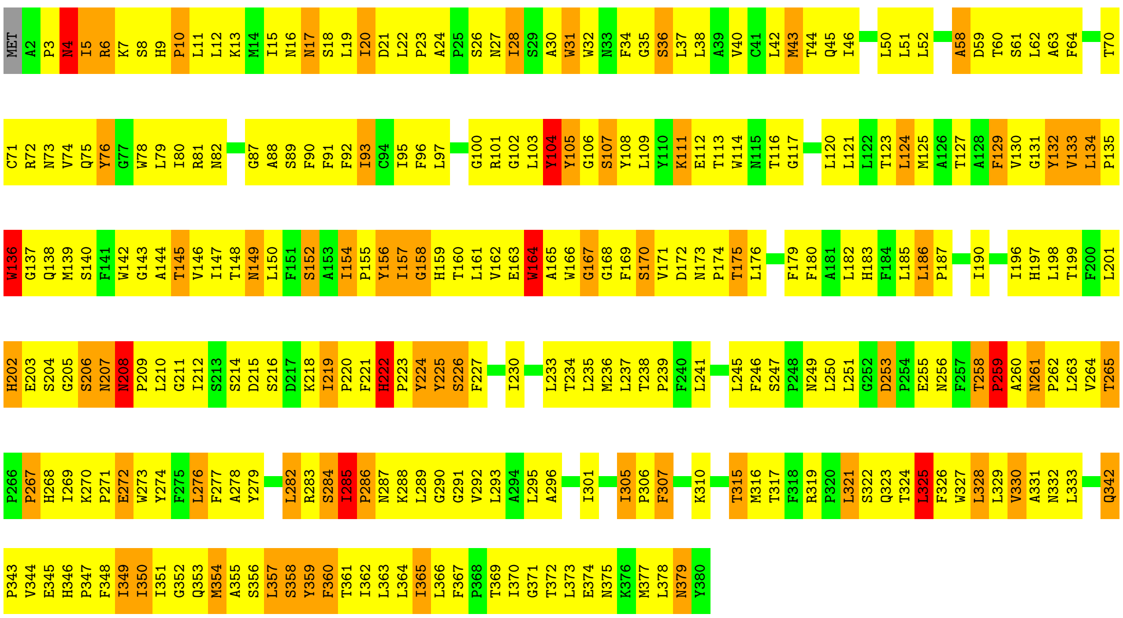




• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain C:

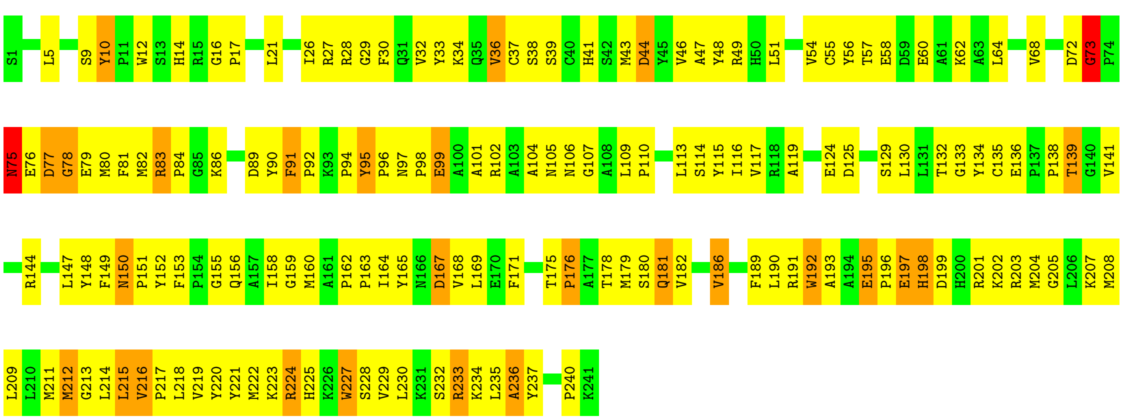




• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

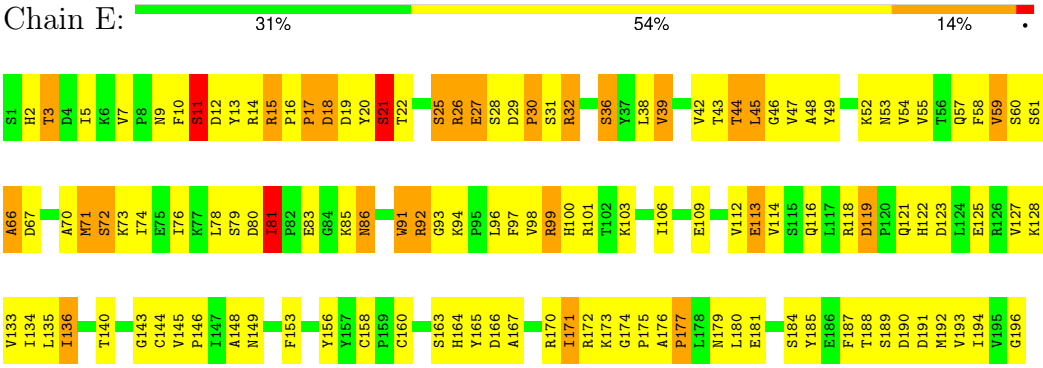
Chain D:





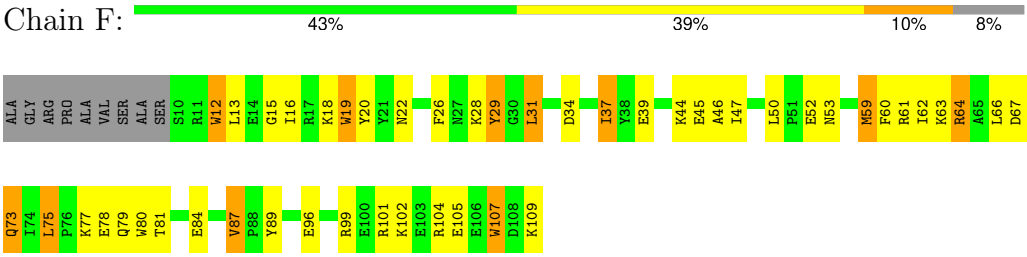
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain E:



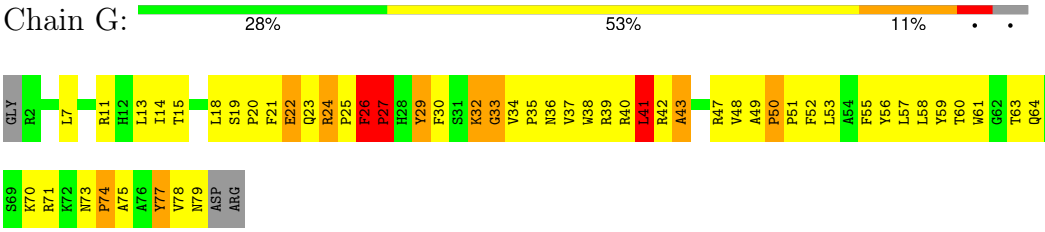
• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain F:



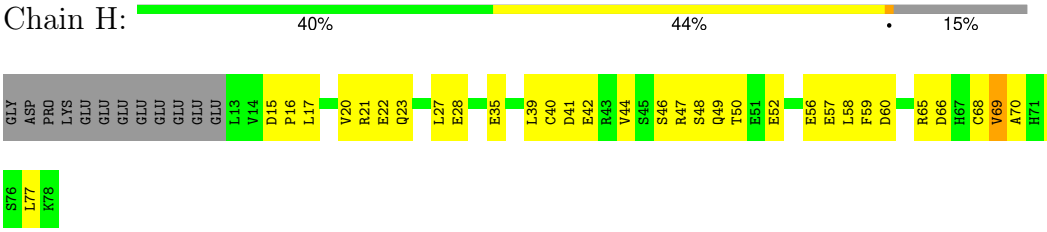
• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain G:



• Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain H:



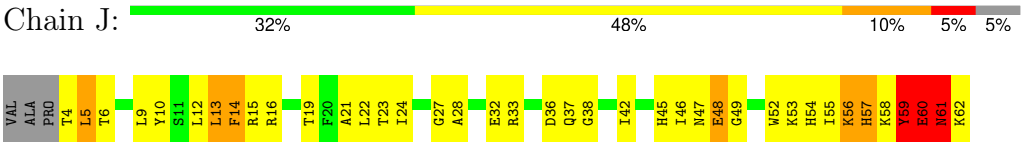
• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I:



• Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain J:


32%
48%
10%
5%
5%
VAL
ALA
PRO
T4
L5
T6
L9
Y10
S11
L12
L13
F14
R15
R16
T19
F20
A21
L22
T23
I24
G27
A28
E32
R33
D36
Q37
G38
T42
H45
I46
N47
E48
G49
W52
K53
H54
I55
K56
H57
K58
Y59
E60
N61
K62

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.50 12.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (12.00-3.50) 70.6 (12.00-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.01Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.284 , 0.317 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 101.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.29$, $< L^2 > = 0.12$	Xtriage
Estimated twinning fraction	0.229 for k,h,-l	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	15754	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIG, HEM, HEC, FES, BOG, U10, PEE

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	0.57	0/3495	1.22	44/4742 (0.9%)
2	B	0.55	1/3046 (0.0%)	1.11	19/4132 (0.5%)
3	C	0.67	0/3104	1.26	44/4252 (1.0%)
4	D	0.66	0/1960	1.33	30/2665 (1.1%)
5	E	0.57	0/1548	1.23	18/2095 (0.9%)
6	F	0.64	0/896	1.14	6/1206 (0.5%)
7	G	0.66	0/648	2.63	9/882 (1.0%)
8	H	0.55	0/495	0.96	1/669 (0.1%)
10	J	0.70	1/470 (0.2%)	1.20	6/635 (0.9%)
All	All	0.61	2/15662 (0.0%)	1.30	177/21278 (0.8%)

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
3	C	0	1
10	J	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	288	GLY	CA-C	7.52	1.57	1.52
10	J	60	GLU	CA-C	5.09	1.59	1.52

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	26	PHE	CA-C-N	47.84	179.63	119.84
7	G	26	PHE	C-N-CA	47.84	179.63	119.84
7	G	26	PHE	C-N-CD	-11.24	78.91	125.00
3	C	265	THR	N-CA-C	-11.04	96.16	110.07
7	G	41	LEU	N-CA-C	-10.88	97.74	111.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	76	TYR	Sidechain
10	J	59	TYR	Sidechain

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	3423	0	3286	381	0
2	B	2994	0	2906	359	0
3	C	3002	0	3036	463	0
4	D	1899	0	1822	227	0
5	E	1512	0	1483	183	0
6	F	875	0	839	76	0
7	G	626	0	591	91	0
8	H	490	0	445	62	0
9	I	159	0	46	20	0
10	J	459	0	424	57	0
11	C	86	0	60	19	0
12	C	29	0	33	9	0
13	C	49	0	70	7	0
13	E	49	0	70	4	0
14	C	35	0	42	12	0
15	D	20	0	28	1	0
16	D	43	0	30	5	0
17	E	4	0	0	1	0
All	All	15754	0	15211	1768	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 57.

The worst 5 of 1768 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)
3:C:166:TRP:HB2	3:C:175:THR:HB	1.22	1.17
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.22	1.17
2:B:280:GLY:H	2:B:283:PRO:HD2	1.06	1.16
4:D:132:THR:HA	4:D:179:MET:HE2	1.32	1.08
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.36	1.05

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	440/446 (99%)	337 (77%)	85 (19%)	18 (4%)	2 19
2	B	404/422 (96%)	295 (73%)	78 (19%)	31 (8%)	1 8
3	C	377/380 (99%)	278 (74%)	68 (18%)	31 (8%)	0 8
4	D	239/241 (99%)	194 (81%)	34 (14%)	11 (5%)	2 17
5	E	194/196 (99%)	151 (78%)	28 (14%)	15 (8%)	1 8
6	F	98/109 (90%)	84 (86%)	12 (12%)	2 (2%)	6 32
7	G	76/81 (94%)	52 (68%)	18 (24%)	6 (8%)	1 8
8	H	64/78 (82%)	56 (88%)	7 (11%)	1 (2%)	7 36
10	J	57/62 (92%)	32 (56%)	20 (35%)	5 (9%)	0 7
All	All	1949/2015 (97%)	1479 (76%)	350 (18%)	120 (6%)	1 12

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	284	TYR
2	B	19	PRO
2	B	20	HIS
2	B	23	ASP

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	359/376 (96%)	336 (94%)	23 (6%)	16	42
2	B	307/336 (91%)	291 (95%)	16 (5%)	21	47
3	C	326/329 (99%)	298 (91%)	28 (9%)	10	33
4	D	201/207 (97%)	189 (94%)	12 (6%)	17	44
5	E	165/169 (98%)	153 (93%)	12 (7%)	13	38
6	F	90/98 (92%)	81 (90%)	9 (10%)	7	28
7	G	60/72 (83%)	55 (92%)	5 (8%)	10	34
8	H	51/74 (69%)	51 (100%)	0	100	100
10	J	41/52 (79%)	39 (95%)	2 (5%)	22	48
All	All	1600/1713 (93%)	1493 (93%)	107 (7%)	15	41

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	272	GLU
4	D	136	GLU
6	F	107	TRP
3	C	285	ILE
3	C	350	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	421	GLN
3	C	138	GLN
8	H	75	ASN
5	E	86	ASN
2	B	429	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)

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	$\#\|Z\| > 2$
13	PEE	C	384	-	48,48,50	2.67	11 (22%)	51,53,55	4.31	17 (33%)
15	BOG	D	242	-	20,20,20	1.14	2 (10%)	25,25,25	0.85	1 (4%)
17	FES	E	197	5	0,4,4	-	-	-		
14	SIG	C	385	-	35,36,36	3.22	14 (40%)	42,50,50	1.76	10 (23%)
11	HEM	C	382	3	50,50,50	1.61	10 (20%)	67,82,82	2.28	26 (38%)
16	HEC	D	243	4	50,50,50	1.14	2 (4%)	68,82,82	1.96	19 (27%)
11	HEM	C	381	3	50,50,50	1.48	6 (12%)	67,82,82	2.08	21 (31%)
12	U10	C	383	-	29,29,63	3.16	5 (17%)	36,38,79	2.00	11 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	PEE	E	198	-	48,48,50	2.57	9 (18%)	51,53,55	4.34	18 (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
13	PEE	C	384	-	1/1/4/8	22/52/52/54	-
15	BOG	D	242	-	-	5/11/31/31	0/1/1/1
17	FES	E	197	5	-	-	0/1/1/1
14	SIG	C	385	-	-	16/30/30/30	0/2/2/2
11	HEM	C	382	3	-	11/14/54/54	-
16	HEC	D	243	4	1/1/3/7	10/14/54/54	-
11	HEM	C	381	3	-	6/14/54/54	-
12	U10	C	383	-	-	6/23/47/87	0/1/1/1
13	PEE	E	198	-	1/1/4/8	26/52/52/54	-

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	385	SIG	C24-C23	-13.33	1.47	1.55
12	C	383	U10	C13-C14	12.71	1.62	1.33
13	E	198	PEE	O5-C30	11.67	1.57	1.22
13	C	384	PEE	O5-C30	11.20	1.55	1.22
12	C	383	U10	C6-C1	7.41	1.48	1.35

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	384	PEE	O4-C10-C11	-18.59	51.07	123.78
13	E	198	PEE	O4-C10-C11	-18.55	51.22	123.78
13	E	198	PEE	O3-C30-C31	13.03	151.56	111.83
13	C	384	PEE	O3-C30-C31	12.96	151.35	111.83
13	C	384	PEE	O3-C30-O5	-11.40	95.11	123.63

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	384	PEE	C2

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Mol	Chain	Res	Type	Atom
13	E	198	PEE	C2
16	D	243	HEC	NA

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	HEM	C2B-C3B-CAB-CBB
11	C	381	HEM	C4B-C3B-CAB-CBB
11	C	382	HEM	C1A-C2A-CAA-CBA
11	C	382	HEM	C2C-C3C-CAC-CBC
11	C	382	HEM	C4C-C3C-CAC-CBC

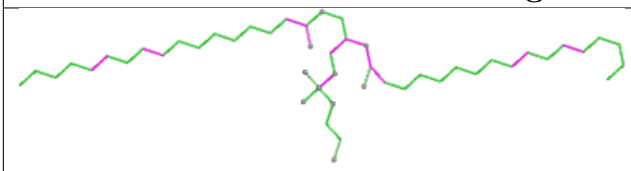
There are no ring outliers.

9 monomers are involved in 58 short contacts:

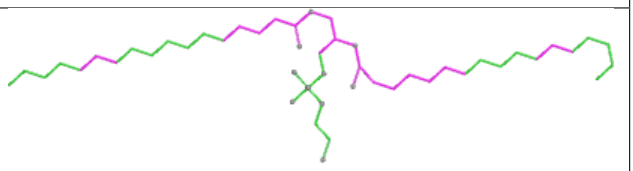
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	384	PEE	7	0
15	D	242	BOG	1	0
17	E	197	FES	1	0
14	C	385	SIG	12	0
11	C	382	HEM	12	0
16	D	243	HEC	5	0
11	C	381	HEM	7	0
12	C	383	U10	9	0
13	E	198	PEE	4	0

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.

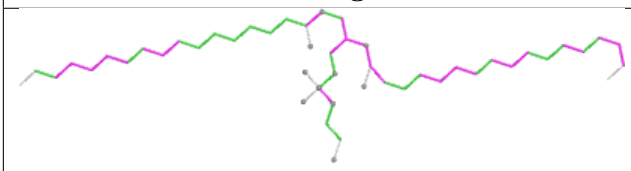
Ligand PEE C 384



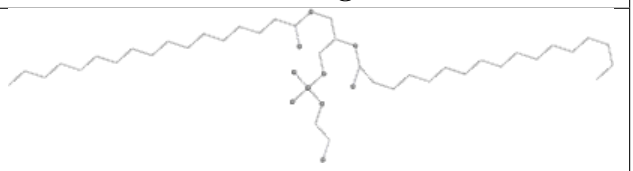
Bond lengths



Bond angles

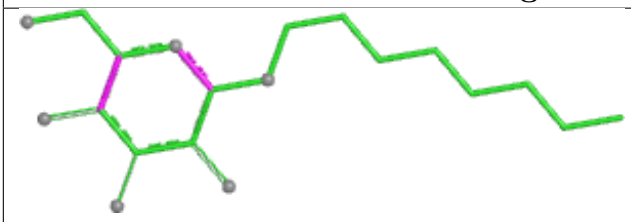


Torsions

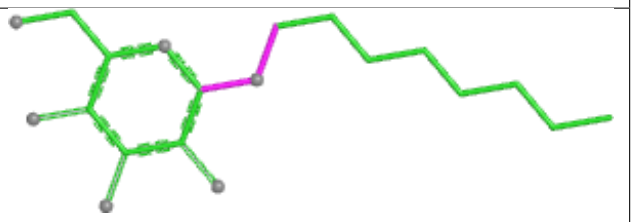


Rings

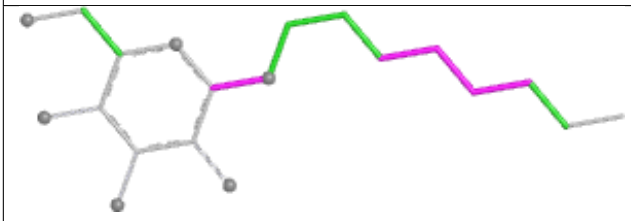
Ligand BOG D 242



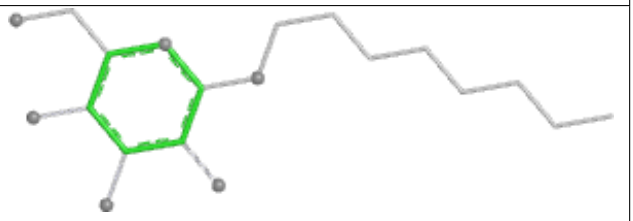
Bond lengths



Bond angles

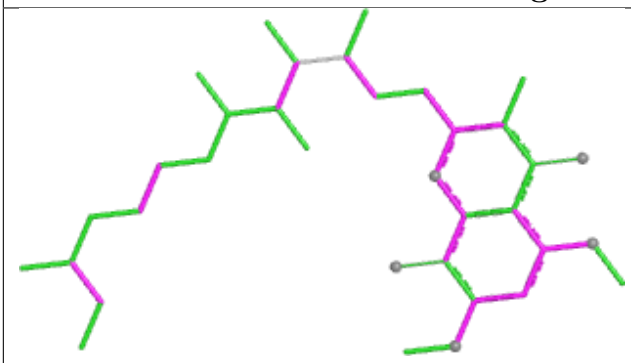


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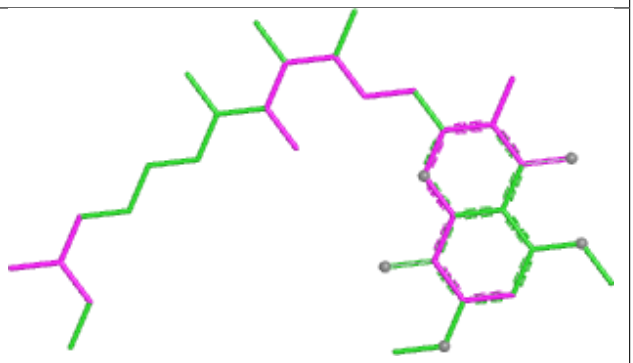


Rings

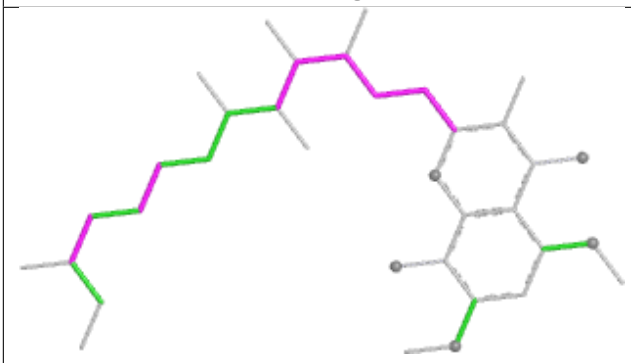
Ligand SIG C 385



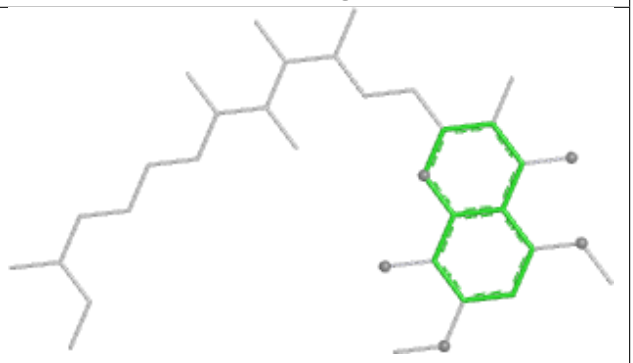
Bond lengths



Bond angles

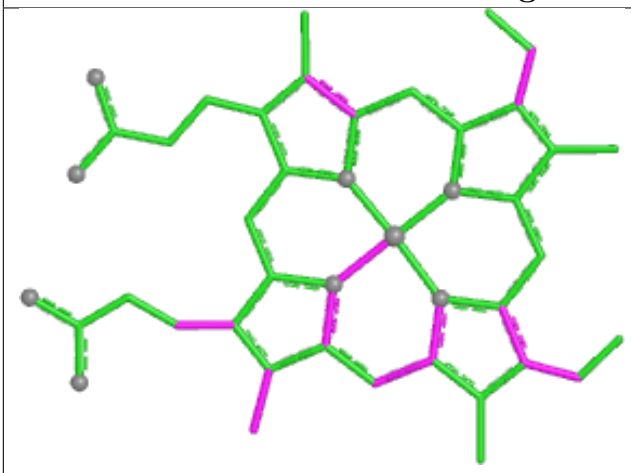


Torsions

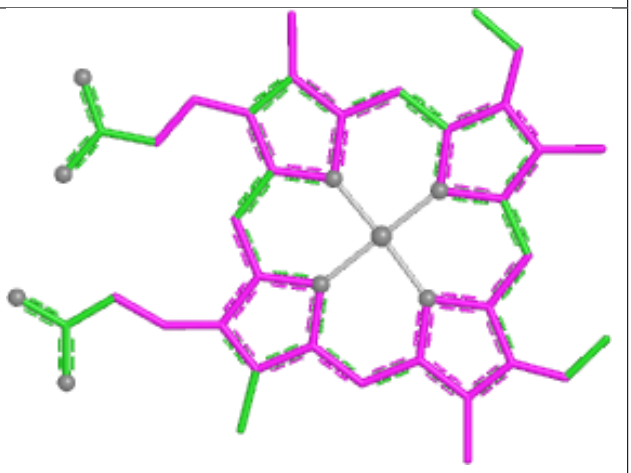


Rings

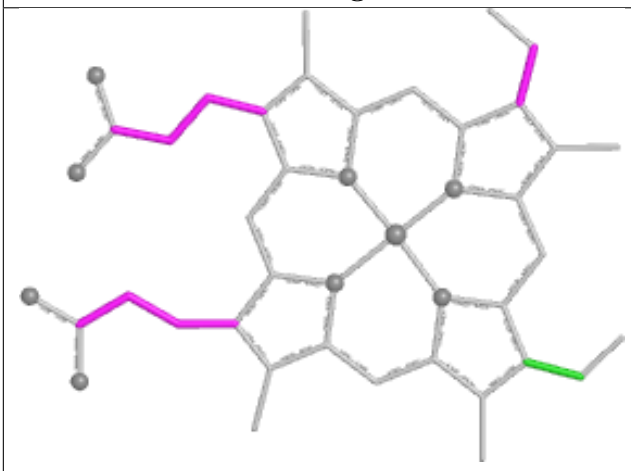
Ligand HEM C 382



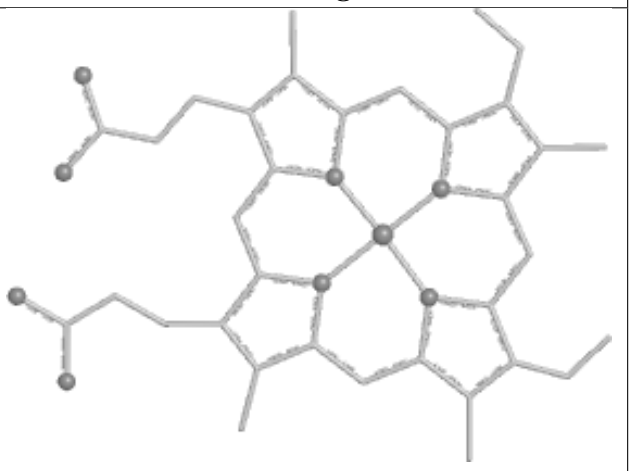
Bond lengths



Bond angles

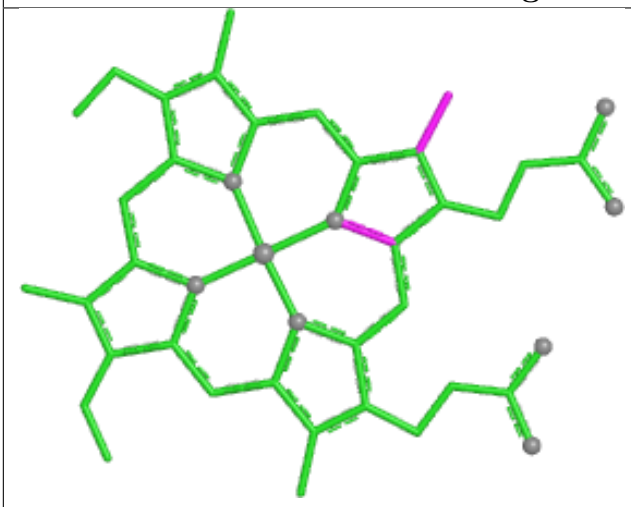


Torsions

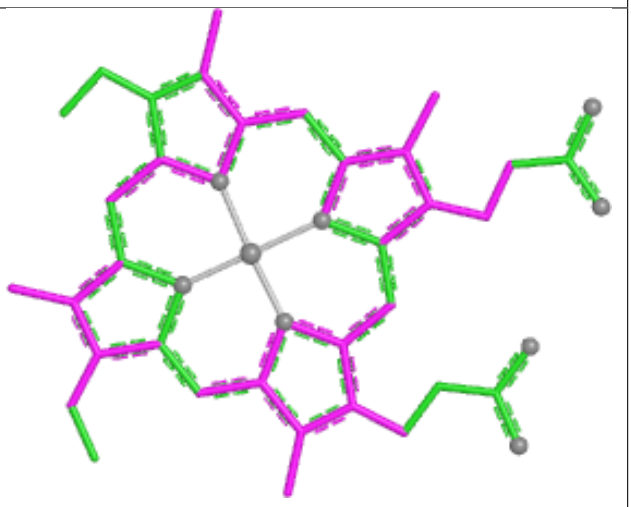


Rings

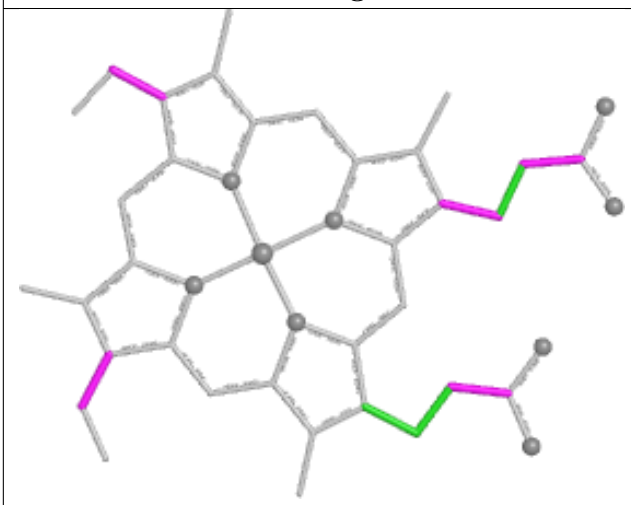
Ligand HEC D 243



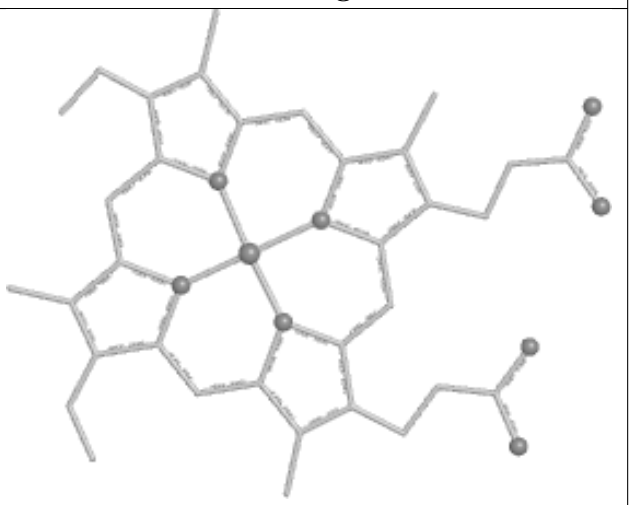
Bond lengths



Bond angles

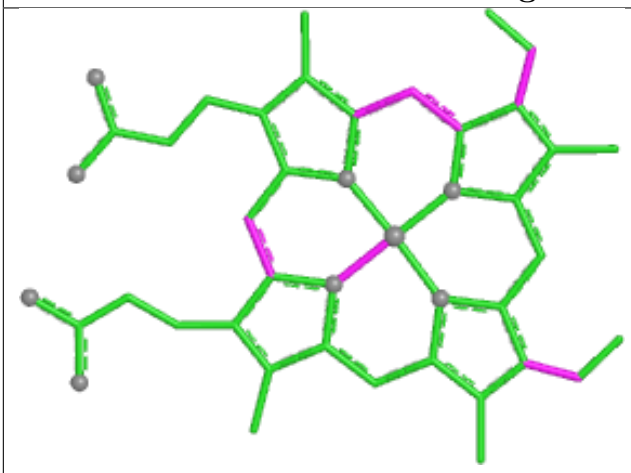


Torsions

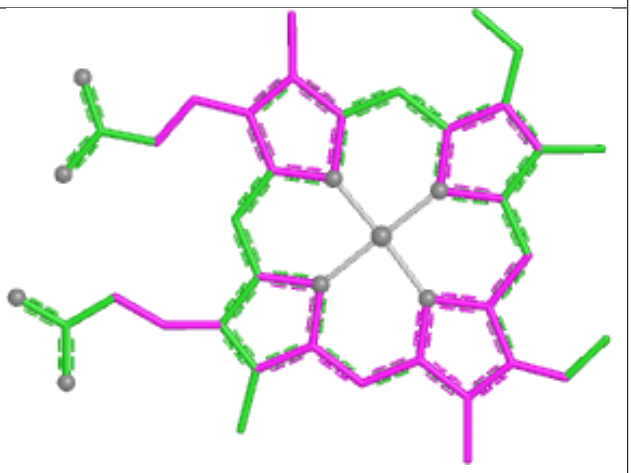


Rings

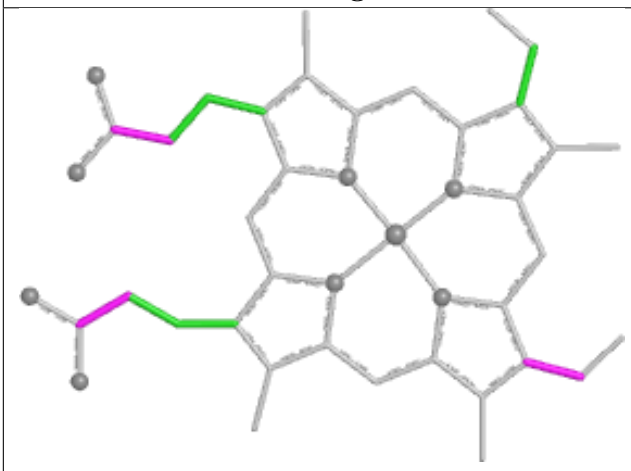
Ligand HEM C 381



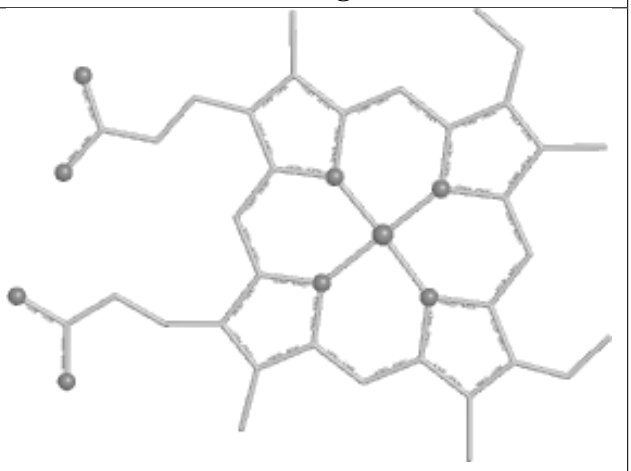
Bond lengths



Bond angles

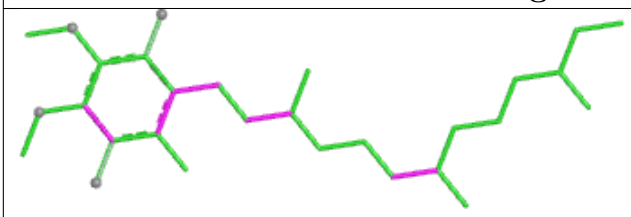


Torsions

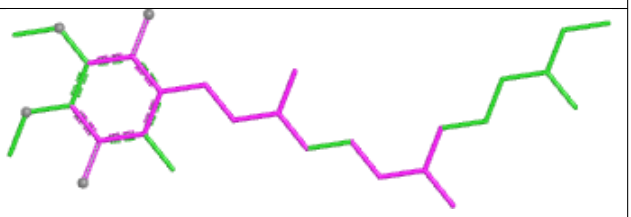


Rings

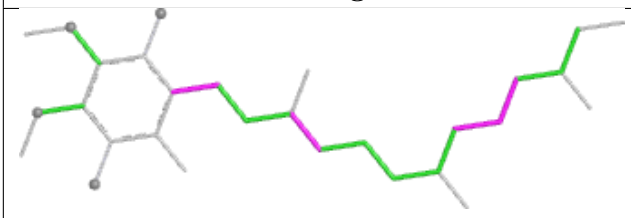
Ligand U10 C 383



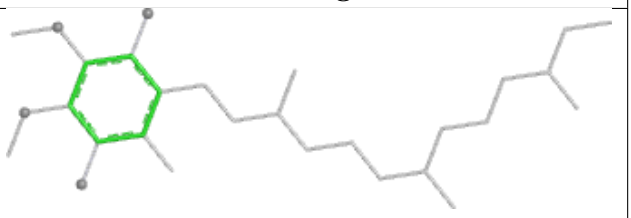
Bond lengths



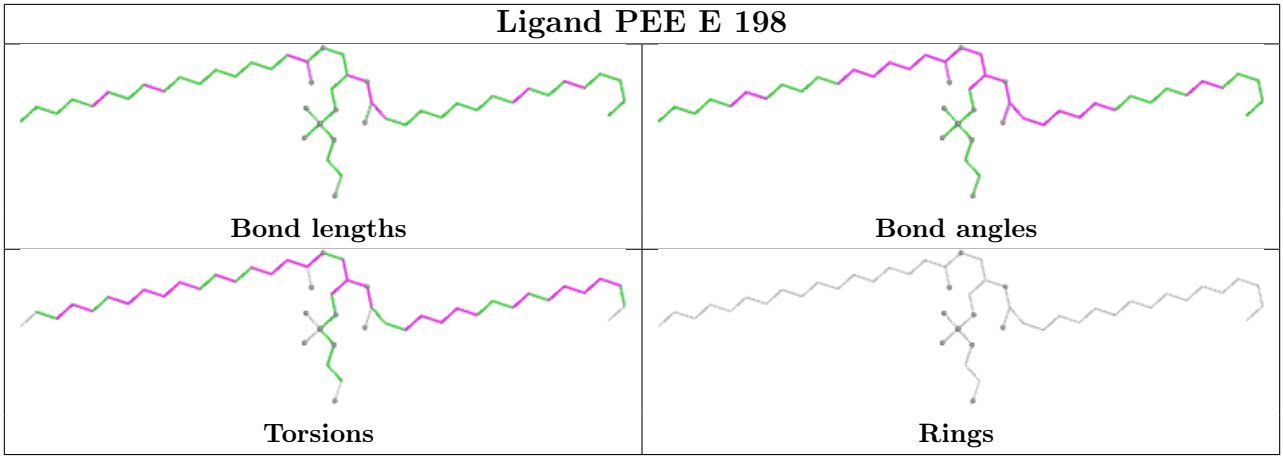
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.76
1	I	121:UNK	C	202:UNK	N	29.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	442/446 (99%)	-0.91	0	100	100	12, 58, 89, 100	0
2	B	406/422 (96%)	-0.78	0	100	100	36, 71, 100, 100	0
3	C	379/380 (99%)	-1.05	0	100	100	4, 32, 71, 91	0
4	D	241/241 (100%)	-0.98	0	100	100	10, 41, 77, 100	0
5	E	196/196 (100%)	-0.74	0	100	100	17, 76, 100, 100	0
6	F	100/109 (91%)	-1.04	0	100	100	18, 42, 74, 99	0
7	G	78/81 (96%)	-0.87	0	100	100	26, 54, 89, 100	0
8	H	66/78 (84%)	-0.88	0	100	100	27, 67, 86, 88	0
9	I	0/33	-	-			-	-
10	J	59/62 (95%)	-0.82	0	100	100	37, 53, 86, 100	0
All	All	1967/2048 (96%)	-0.90	0	100	100	4, 55, 98, 100	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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,

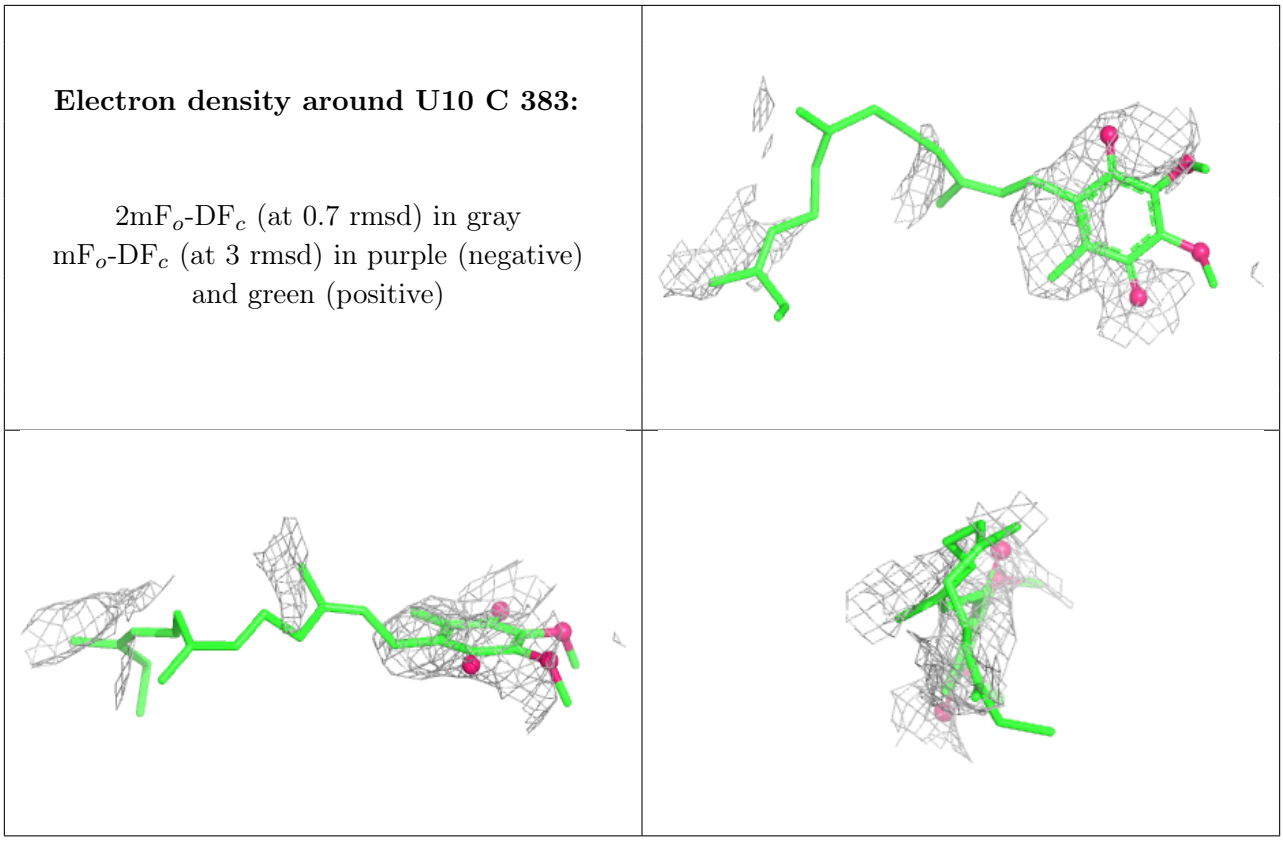
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	U10	C	383	29/63	0.97	0.12	72,88,100,100	0
15	BOG	D	242	20/20	0.97	0.11	35,68,81,81	0
13	PEE	C	384	49/51	0.98	0.08	42,58,76,87	0
11	HEM	C	382	43/43	0.99	0.05	8,20,32,41	0
13	PEE	E	198	49/51	0.99	0.08	43,80,98,100	0
14	SIG	C	385	35/35	0.99	0.05	2,17,26,29	0
11	HEM	C	381	43/43	0.99	0.05	6,24,32,43	0
16	HEC	D	243	43/43	0.99	0.05	10,21,32,35	0
17	FES	E	197	4/4	1.00	0.04	59,60,64,65	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.

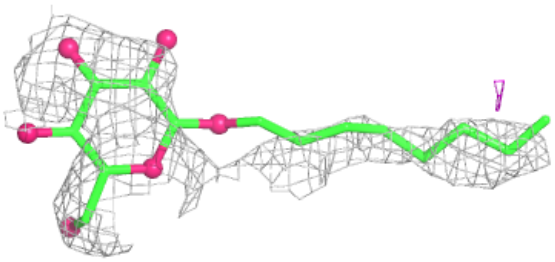
Electron density around U10 C 383:

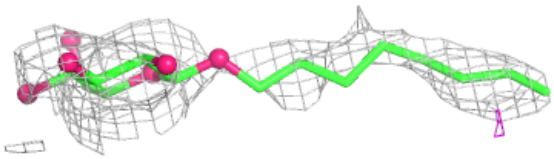
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

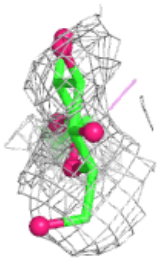


Electron density around BOG D 242:

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

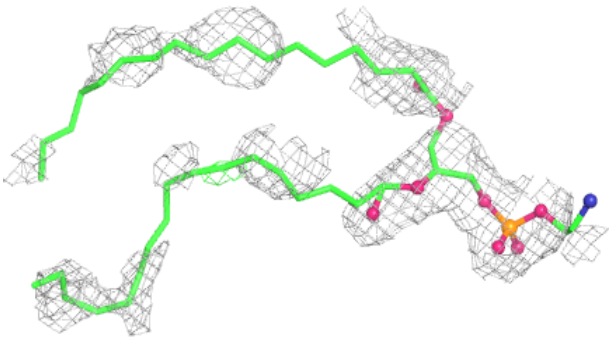


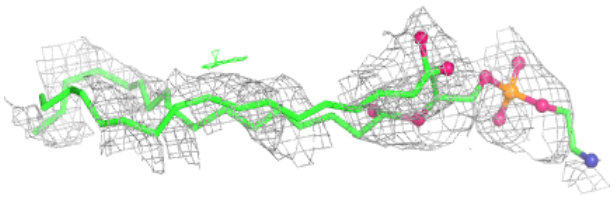




Electron density around PEE C 384:

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

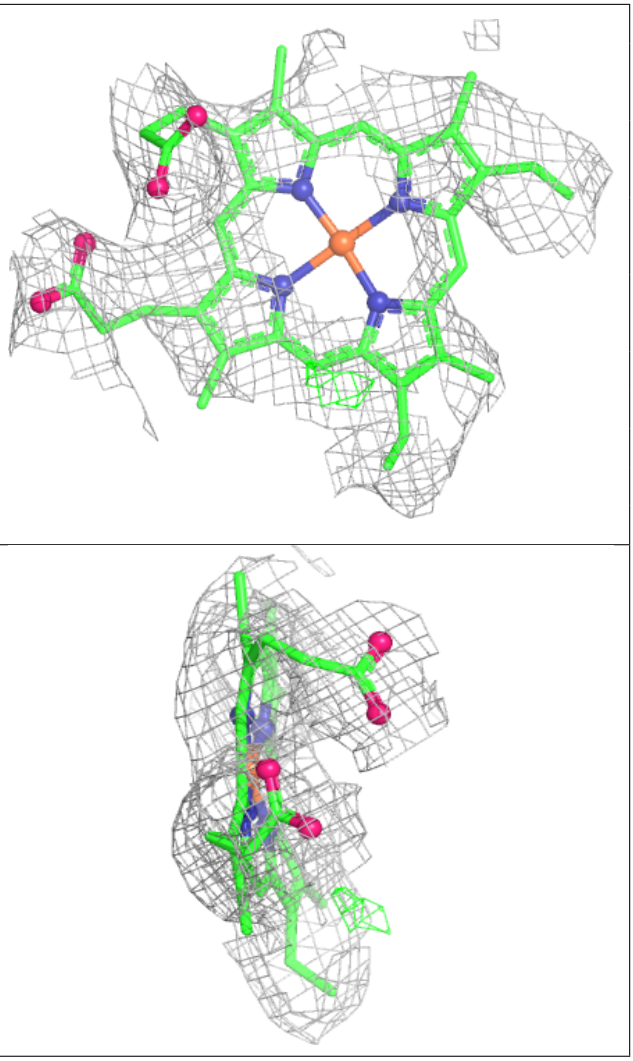






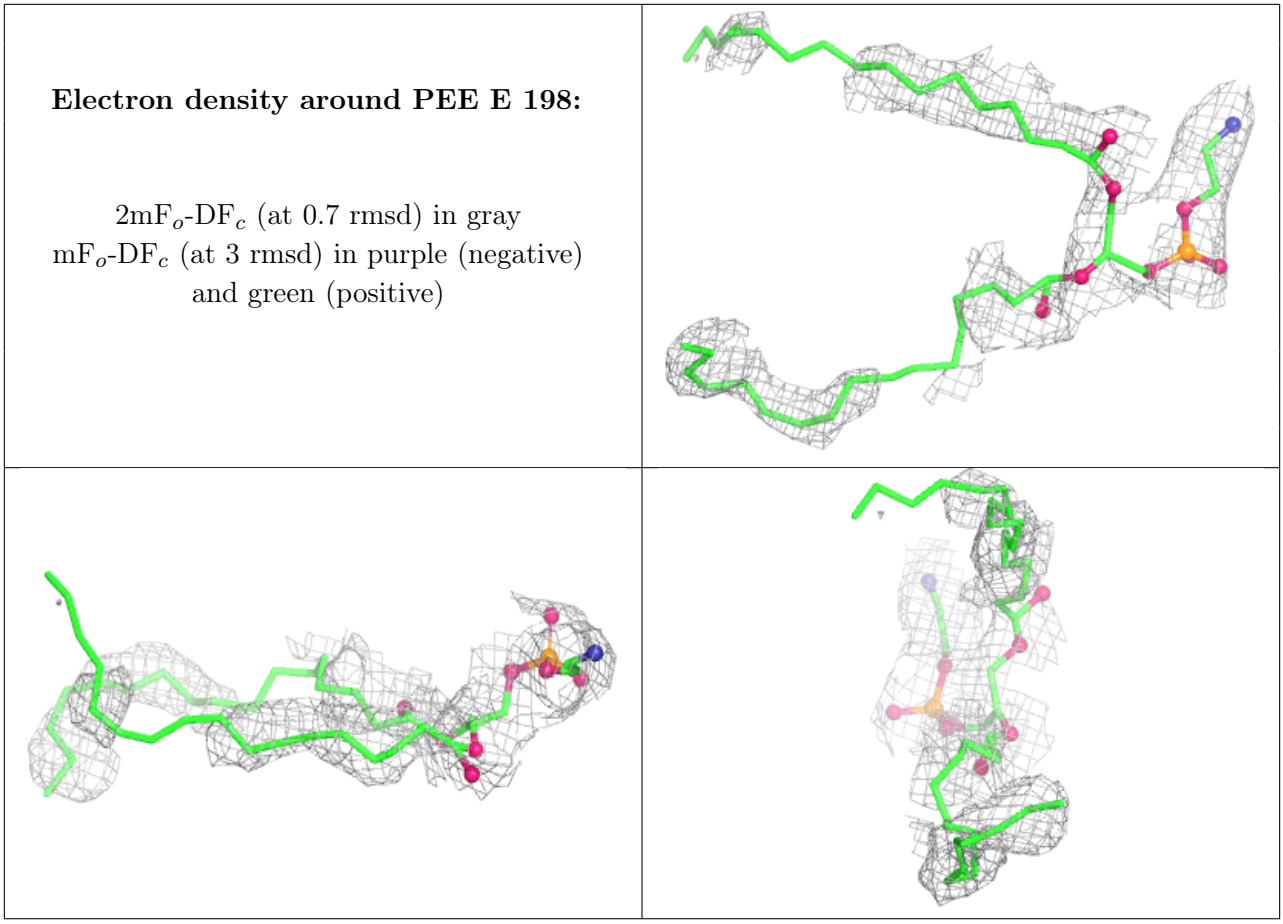
Electron density around HEM C 382:

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



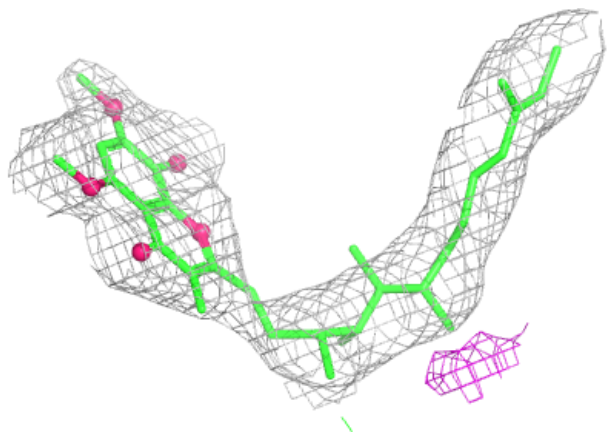
Electron density around PEE E 198:

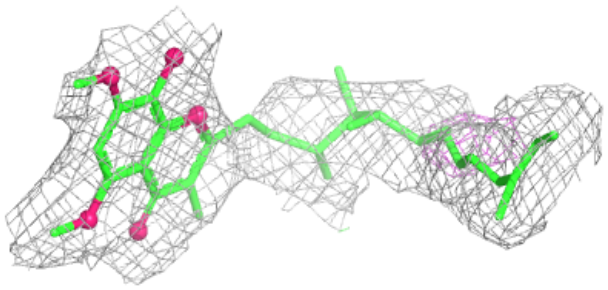
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

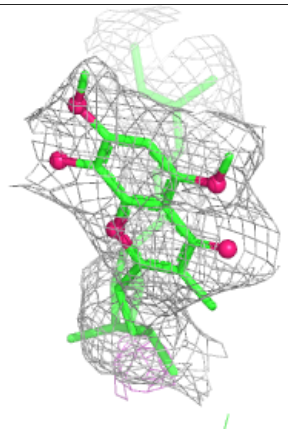


Electron density around SIG C 385:

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

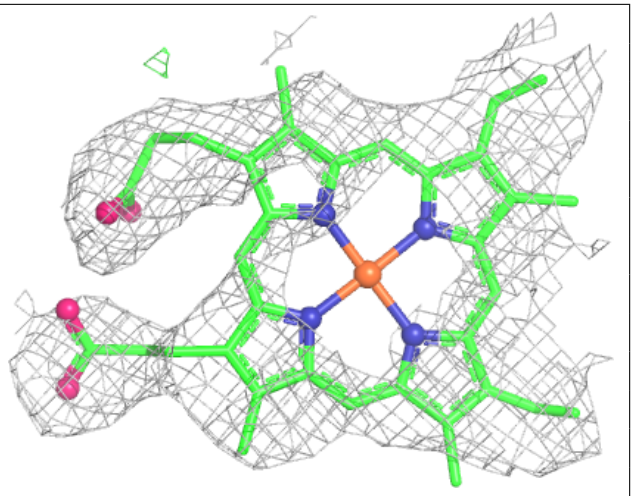


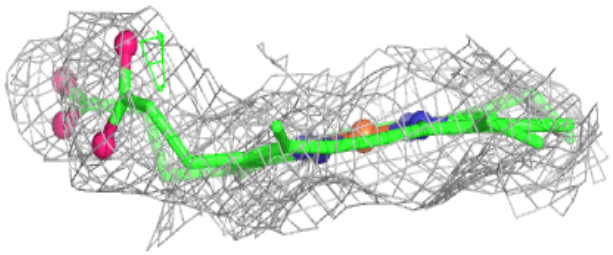


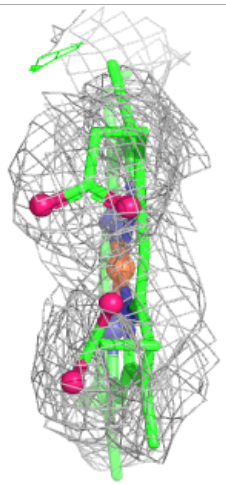


Electron density around HEM C 381:

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

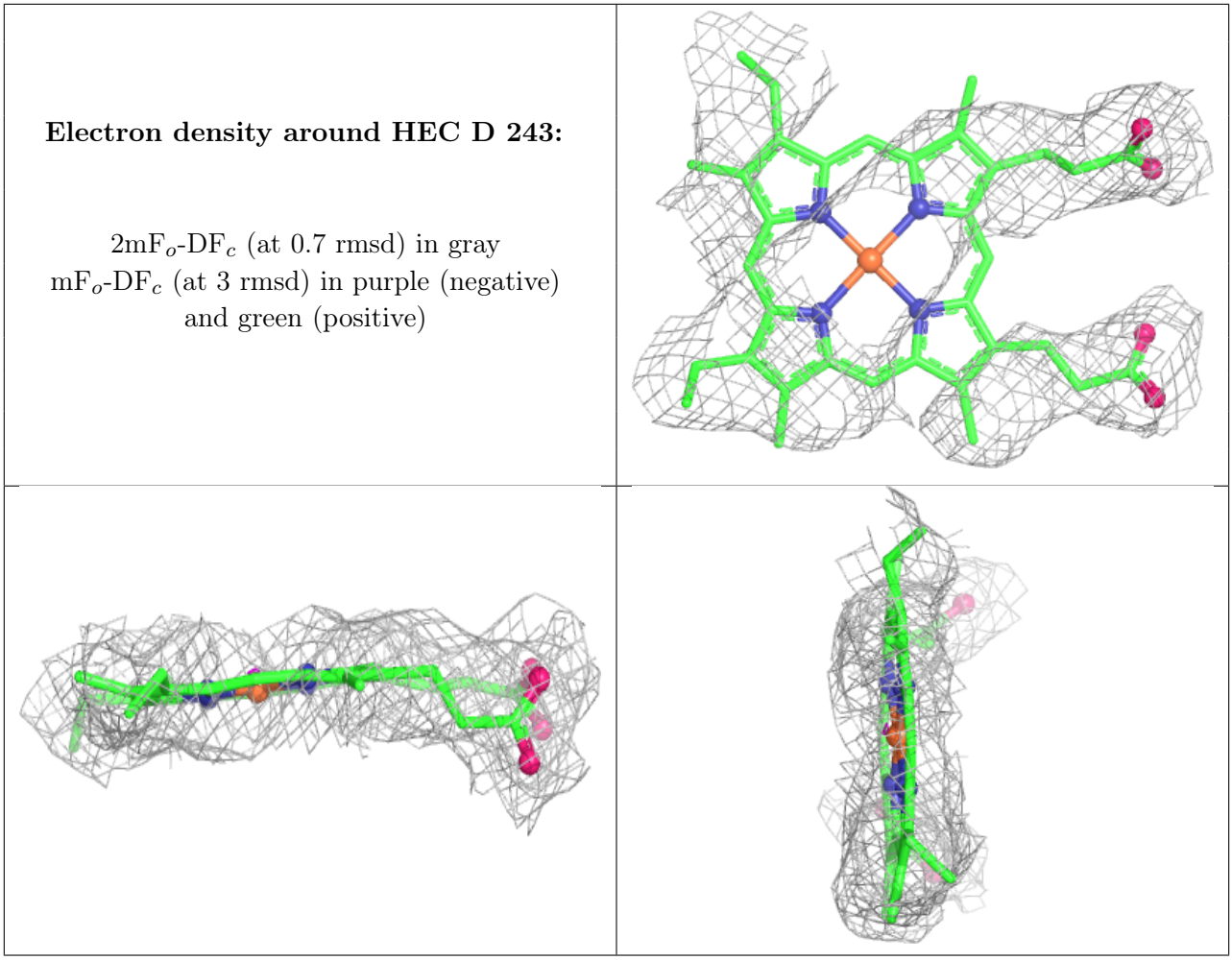






Electron density around HEC D 243:

$2mF_o$-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.