wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 09:28 PM EDT

PDB ID	:	1BCC
Title	:	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	:	1998-03-23
Resolution	:	3.16 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:

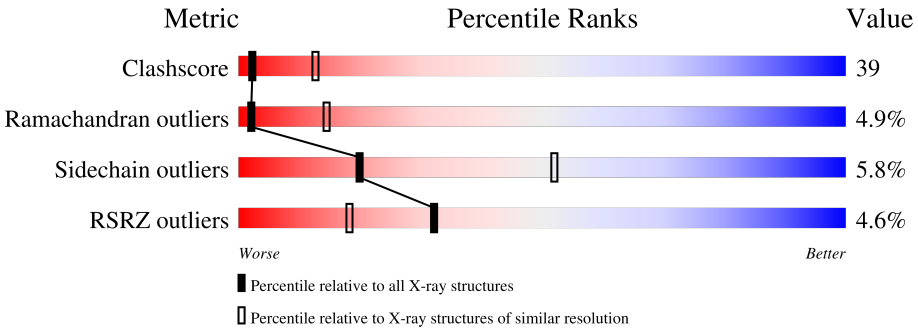
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.16 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	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	2% 42% 50% 7%
2	B	422	4% 40% 47% 9%
3	C	380	2% 45% 48% 6%
4	D	241	3% 44% 50% 6%
5	E	196	23% 38% 58%
6	F	109	2% 56% 32% 8%

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Mol	Chain	Length	Quality of chain
7	G	81	2% 47% 40% 10%
8	H	78	% 51% 32% 15%
9	I	33	64% 36%
10	J	62	3% 56% 37% 5%

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	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 15719 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
1	A	442	Total	C	N	O	S	0	0	0
			3423	2147	601	657	18			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	THR	conflict	UNP P13272
A	23	VAL	LEU	conflict	UNP P13272
A	59	LEU	VAL	conflict	UNP P13272
A	72	GLN	GLY	conflict	UNP P13272
A	91	SER	THR	conflict	UNP P13272
A	106	VAL	LEU	conflict	UNP P13272
A	135	VAL	LEU	conflict	UNP P13272
A	136	ARG	GLN	conflict	UNP P13272
A	147	GLU	ASP	conflict	UNP P13272
A	162	GLY	PRO	conflict	UNP P13272
A	174	ILE	VAL	conflict	UNP P13272
A	188	THR	ARG	conflict	UNP P13272
A	191	THR	LYS	conflict	UNP P13272
A	203	VAL	LEU	conflict	UNP P13272
A	206	GLN	ARG	conflict	UNP P13272
A	210	GLU	ASP	conflict	UNP P13272
A	217	GLY	SER	conflict	UNP P13272
A	219	VAL	LEU	conflict	UNP P13272
A	220	PRO	SER	conflict	UNP P13272
A	221	PHE	GLY	conflict	UNP P13272
A	225	ASP	GLU	conflict	UNP P13272
A	233	LYS	PRO	conflict	UNP P13272
A	242	ARG	CYS	conflict	UNP P13272
A	267	LEU	ASN	conflict	UNP P13272
A	282	ARG	CYS	conflict	UNP P13272
A	288	LEU	ALA	conflict	UNP P13272
A	290	SER	LEU	conflict	UNP P13272

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	VAL	ALA	conflict	UNP P13272
A	311	SER	ASN	conflict	UNP P13272
A	315	SER	ALA	conflict	UNP P13272
A	316	GLU	ASP	conflict	UNP P13272
A	320	PHE	LEU	conflict	UNP P13272
A	322	PHE	ALA	conflict	UNP P13272
A	323	TYR	HIS	conflict	UNP P13272
A	328	ARG	HIS	conflict	UNP P13272
A	349	ILE	ALA	conflict	UNP P13272
A	350	SER	THR	conflict	UNP P13272
A	360	PHE	LEU	conflict	UNP P13272
A	382	GLU	SER	conflict	UNP P13272
A	393	GLU	ALA	conflict	UNP P13272
A	397	GLU	SER	conflict	UNP P13272
A	399	LEU	ILE	conflict	UNP P13272
A	406	MET	VAL	conflict	UNP P13272
A	415	ILE	PHE	conflict	UNP P13272
A	425	PRO	PHE	conflict	UNP P13272

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

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

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ILE	PHE	conflict	UNP P23004
B	28	LYS	ARG	conflict	UNP P23004
B	42	SER	ALA	conflict	UNP P23004
B	44	GLY	ALA	conflict	UNP P23004
B	46	THR	ARG	conflict	UNP P23004
B	49	VAL	LEU	conflict	UNP P23004
B	61	SER	ASN	conflict	UNP P23004
B	99	GLU	THR	conflict	UNP P23004
B	117	GLU	ASP	conflict	UNP P23004
B	134	PRO	ARG	conflict	UNP P23004
B	139	ASP	ALA	conflict	UNP P23004
B	145	LYS	ARG	conflict	UNP P23004
B	152	PHE	LEU	conflict	UNP P23004
B	157	THR	ALA	conflict	UNP P23004

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Chain	Residue	Modelled	Actual	Comment	Reference
B	174	ASP	ASN	conflict	UNP P23004
B	188	SER	PRO	conflict	UNP P23004
B	194	PHE	TYR	conflict	UNP P23004
B	207	VAL	ILE	conflict	UNP P23004
B	218	ASN	GLN	conflict	UNP P23004
B	223	LEU	PHE	conflict	UNP P23004
B	240	ARG	HIS	conflict	UNP P23004
B	257	ILE	LEU	conflict	UNP P23004
B	266	GLY	SER	conflict	UNP P23004
B	282	ASN	GLY	conflict	UNP P23004
B	321	LEU	SER	conflict	UNP P23004
B	332	TYR	SER	conflict	UNP P23004
B	335	GLN	ASP	conflict	UNP P23004
B	352	VAL	LEU	conflict	UNP P23004
B	355	GLU	PRO	conflict	UNP P23004
B	356	ASN	ASP	conflict	UNP P23004
B	367	LYS	GLY	conflict	UNP P23004
B	380	GLU	ASP	conflict	UNP P23004
B	393	ASN	THR	conflict	UNP P23004
B	412	LYS	ASN	conflict	UNP P23004
B	420	ARG	GLY	conflict	UNP P23004
B	421	GLN	ARG	conflict	UNP P23004
B	436	VAL	ILE	conflict	UNP P23004

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

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PRO	LEU	conflict	UNP P00125
D	143	VAL	LEU	conflict	UNP P00125
D	167	ASP	GLU	conflict	UNP P00125

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	VAL	LEU	conflict	UNP P00125
D	221	TYR	ALA	conflict	UNP P00125

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

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ASN	ASP	conflict	UNP P13272
E	17	PRO	GLU	conflict	UNP P13272
E	18	ASP	VAL	conflict	UNP P13272
E	19	ASP	LEU	conflict	UNP P13272
E	20	TYR	ASP	conflict	UNP P13272
E	26	ARG	LYS	conflict	UNP P13272
E	29	ASP	SER	conflict	UNP P13272
E	30	PRO	GLU	conflict	UNP P13272
E	31	SER	ALA	conflict	UNP P13272
E	42	VAL	THR	conflict	UNP P13272
E	45	LEU	VAL	conflict	UNP P13272
E	56	THR	SER	conflict	UNP P13272

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

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	TYR	LEU	conflict	UNP P00129
F	38	TYR	HIS	conflict	UNP P00129
F	59	MET	VAL	conflict	UNP P00129
F	69	ASN	SER	conflict	UNP P00129
F	87	VAL	LYS	conflict	UNP P00129
F	88	PRO	SER	conflict	UNP P00129
F	108	ASP	ALA	conflict	UNP P00129

- 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			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	LEU	VAL	conflict	UNP P13271
G	25	PRO	ALA	conflict	UNP P13271
G	34	VAL	ILE	conflict	UNP P13271
G	38	TRP	LEU	conflict	UNP P13271
G	41	LEU	THR	conflict	UNP P13271
G	53	LEU	VAL	conflict	UNP P13271
G	58	LEU	VAL	conflict	UNP P13271
G	78	VAL	GLU	conflict	UNP P13271

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	59	PHE	LEU	conflict	UNP P00126

- 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			

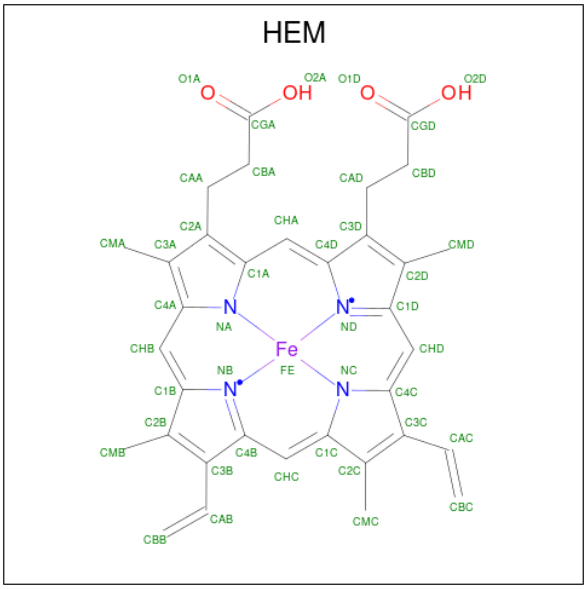
- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

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

There is a discrepancy between the modelled and reference sequences:

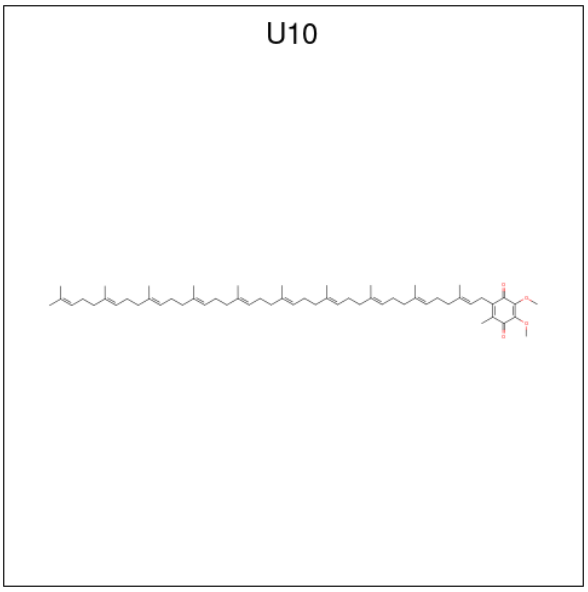
Chain	Residue	Modelled	Actual	Comment	Reference
J	30	LEU	PHE	conflict	UNP P00130

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



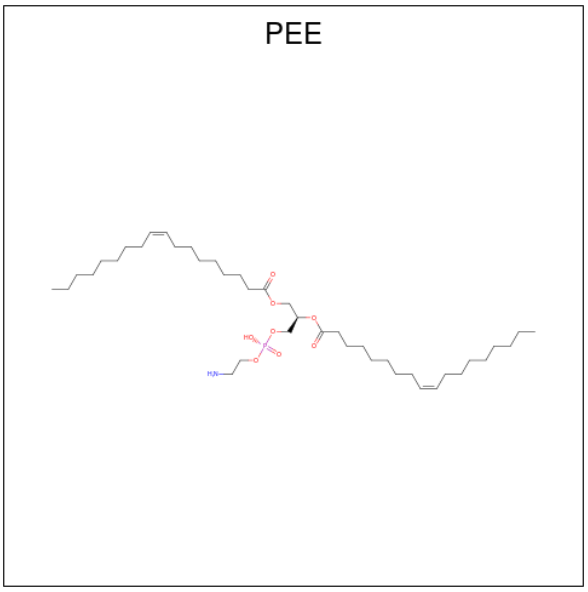
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



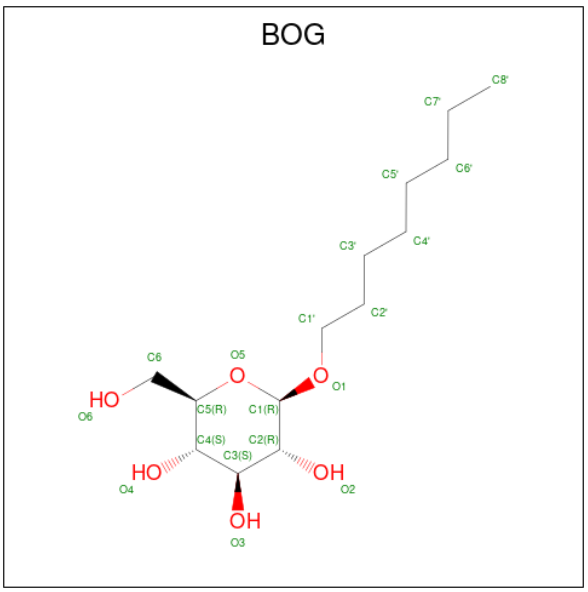
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			29	25	4		

- Molecule 13 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



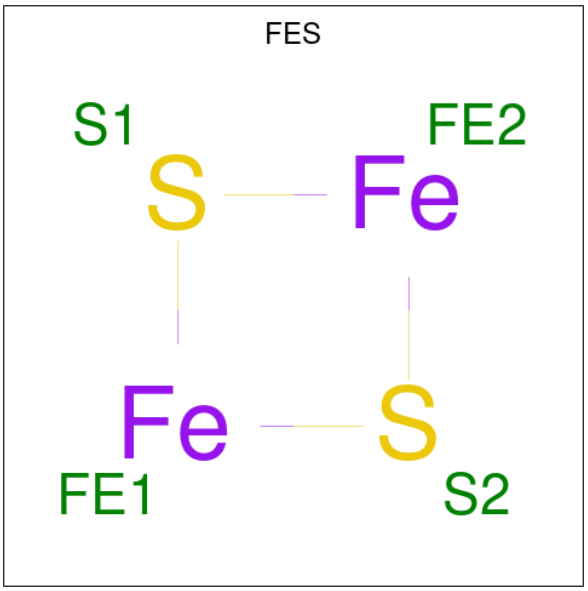
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



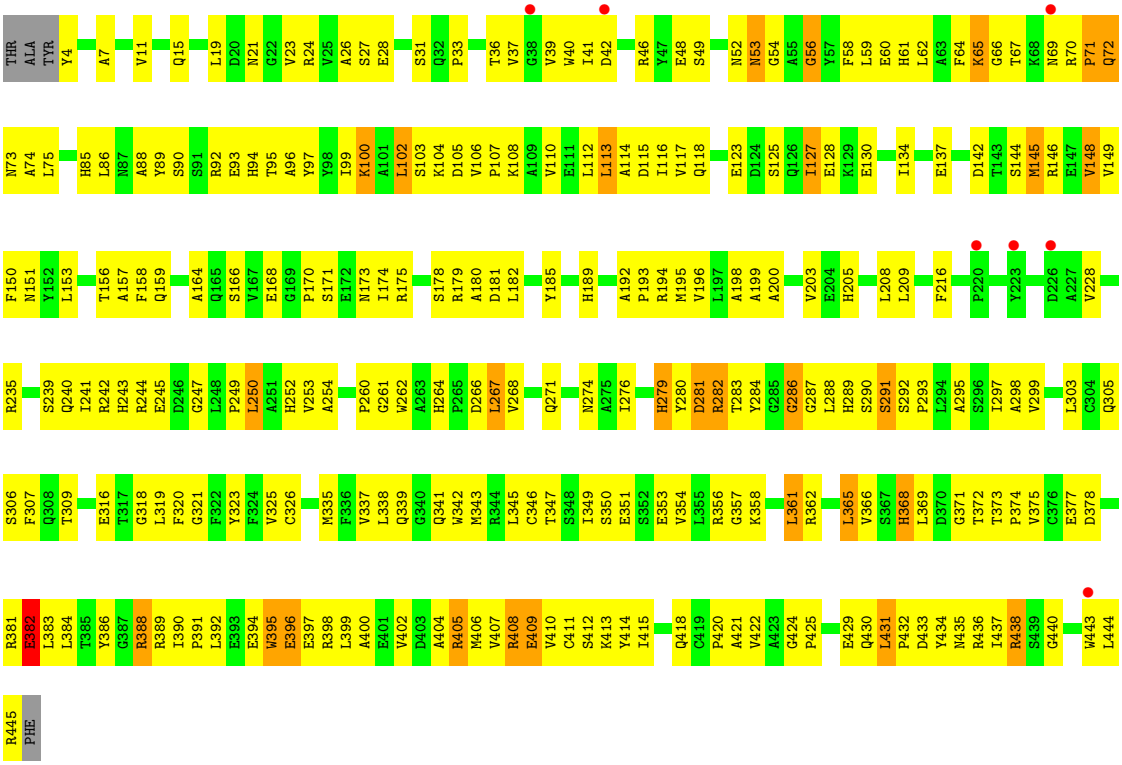
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total Fe S 4 2 2	0	0

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.

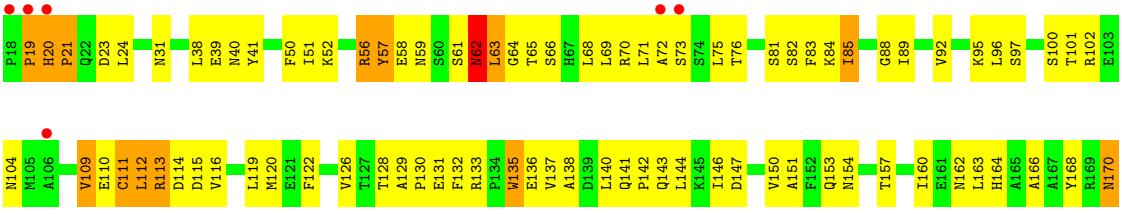
• Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

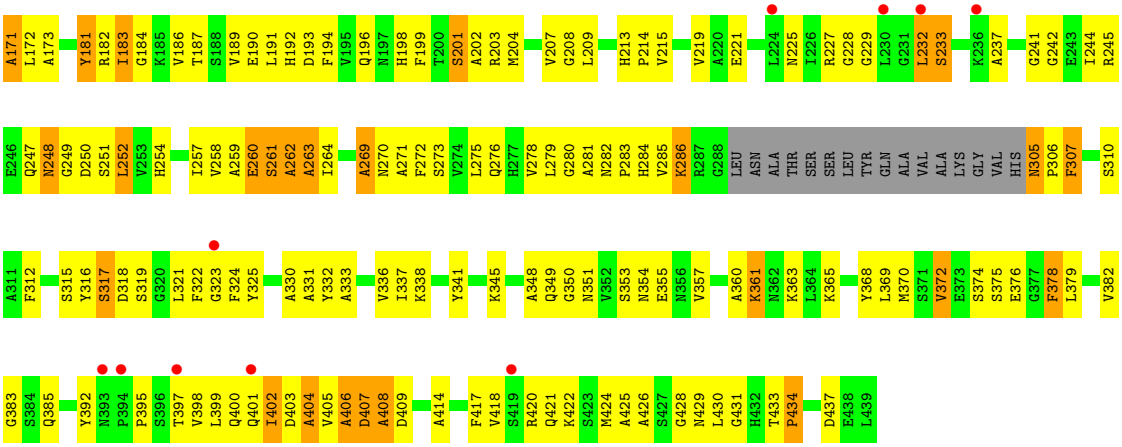
Chain A:



• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

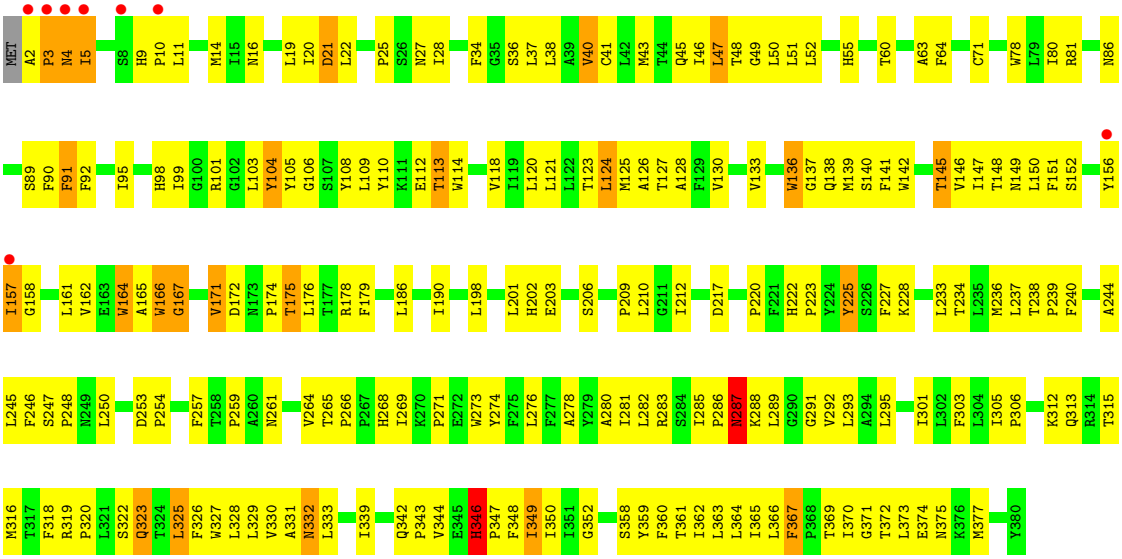
Chain B:





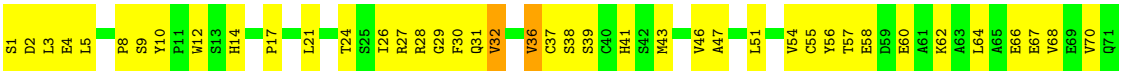
• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

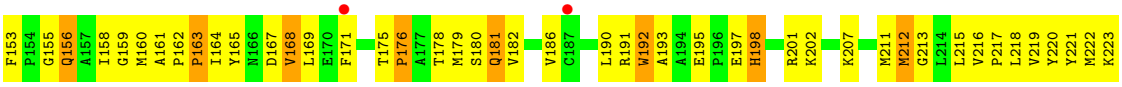
Chain C:

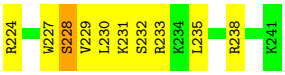


• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

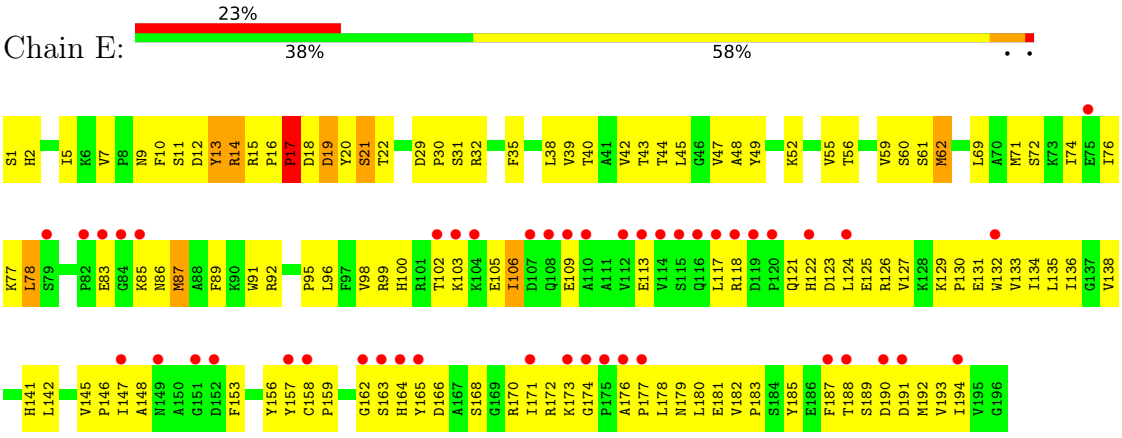
Chain D:



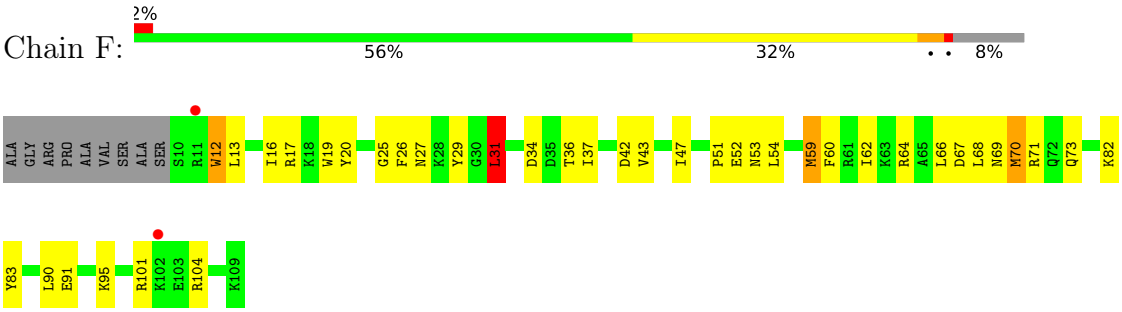




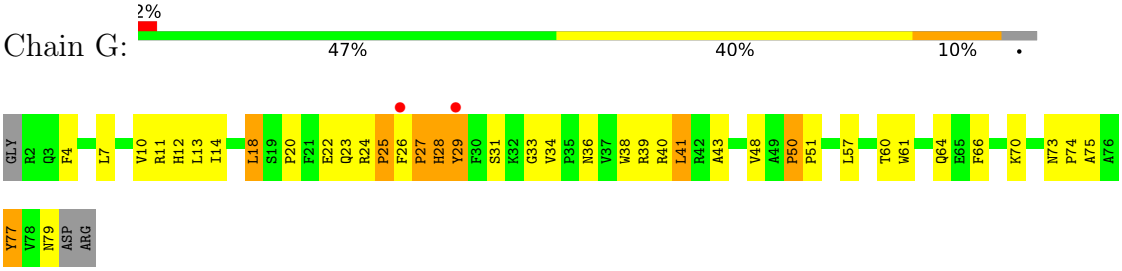
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



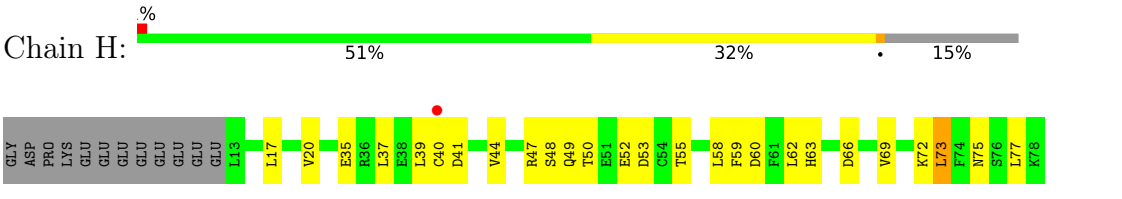
• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



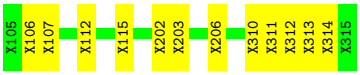
• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



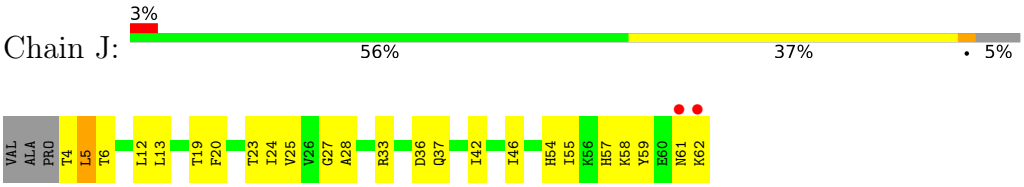
• Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	169.59Å 182.52Å 240.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.16 27.93 – 3.16	Depositor EDS
% Data completeness (in resolution range)	85.5 (12.00-3.16) 90.8 (27.93-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 3.17Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.270 , 0.310 0.288 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	15719	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: U10, PEE, BOG, FES, HEM

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	0.49	0/3495	0.73	1/4742 (0.0%)
2	B	0.45	0/3046	0.70	0/4132
3	C	0.51	0/3104	0.77	1/4252 (0.0%)
4	D	0.49	0/1960	0.75	1/2665 (0.0%)
5	E	0.58	0/1548	0.77	0/2095
6	F	0.50	0/896	0.74	1/1206 (0.1%)
7	G	0.54	0/648	0.75	1/882 (0.1%)
8	H	0.42	0/495	0.64	0/669
10	J	0.46	0/470	0.69	0/635
All	All	0.50	0/15662	0.74	5/21278 (0.0%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	GLY	N-CA-C	-5.71	98.83	113.10
4	D	235	LEU	CA-CB-CG	5.50	127.96	115.30
6	F	31	LEU	CA-CB-CG	5.49	127.92	115.30
7	G	18	LEU	CA-CB-CG	5.43	127.78	115.30
3	C	346	HIS	N-CA-C	5.24	125.15	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	225	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	291	0
2	B	2994	0	2906	278	0
3	C	3002	0	3036	251	0
4	D	1899	0	1822	158	0
5	E	1512	0	1485	159	0
6	F	875	0	839	49	0
7	G	626	0	591	51	0
8	H	490	0	445	35	0
9	I	159	0	42	19	0
10	J	459	0	424	21	0
11	C	86	0	60	12	0
11	D	43	0	30	0	0
12	C	29	0	33	4	0
13	C	49	0	70	2	0
13	E	49	0	70	1	0
14	D	20	0	28	2	0
15	E	4	0	0	1	0
All	All	15719	0	15167	1200	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 39.

The worst 5 of 1200 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)
4:D:158:ILE:HG22	4:D:160:MET:H	1.07	1.15
1:A:282:ARG:NH1	9:I:202:UNK:H	1.47	1.11
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.33	1.10
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.56	1.02
2:B:76:THR:HG22	2:B:82:SER:H	1.23	1.01

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%)	348 (79%)	73 (17%)	19 (4%)	2 17
2	B	404/422 (96%)	291 (72%)	74 (18%)	39 (10%)	0 3
3	C	377/380 (99%)	299 (79%)	64 (17%)	14 (4%)	3 19
4	D	239/241 (99%)	195 (82%)	31 (13%)	13 (5%)	2 12
5	E	194/196 (99%)	167 (86%)	23 (12%)	4 (2%)	7 33
6	F	98/109 (90%)	83 (85%)	15 (15%)	0	100 100
7	G	76/81 (94%)	61 (80%)	10 (13%)	5 (7%)	1 8
8	H	64/78 (82%)	50 (78%)	14 (22%)	0	100 100
10	J	57/62 (92%)	43 (75%)	12 (21%)	2 (4%)	3 21
All	All	1949/2015 (97%)	1537 (79%)	316 (16%)	96 (5%)	2 14

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	65	LYS
1	A	103	SER
1	A	282	ARG
1	A	291	SER

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%)	339 (94%)	20 (6%)	21 53
2	B	307/336 (91%)	286 (93%)	21 (7%)	16 46
3	C	326/329 (99%)	308 (94%)	18 (6%)	21 54
4	D	201/207 (97%)	190 (94%)	11 (6%)	21 54
5	E	165/169 (98%)	156 (94%)	9 (6%)	21 54
6	F	90/98 (92%)	85 (94%)	5 (6%)	21 53
7	G	60/72 (83%)	54 (90%)	6 (10%)	7 28
8	H	51/74 (69%)	49 (96%)	2 (4%)	32 64
10	J	41/52 (79%)	41 (100%)	0	100 100
All	All	1600/1713 (93%)	1508 (94%)	92 (6%)	20 52

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	332	ASN
5	E	17	PRO
4	D	24	THR
4	D	156	GLN
5	E	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	268	HIS
4	D	156	GLN
3	C	287	ASN
3	C	342	GLN
5	E	86	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
15	FES	E	197	5	0,4,4	-	-	-		
13	PEE	C	384	-	48,48,50	2.53	11 (22%)	51,53,55	4.28	18 (35%)
13	PEE	E	198	-	48,48,50	2.47	11 (22%)	51,53,55	4.32	17 (33%)
11	HEM	D	243	4	41,50,50	1.86	10 (24%)	45,82,82	2.23	17 (37%)
12	U10	C	383	-	29,29,63	2.31	9 (31%)	35,38,79	1.77	10 (28%)
11	HEM	C	382	3	41,50,50	1.73	7 (17%)	45,82,82	2.57	16 (35%)
14	BOG	D	242	-	20,20,20	0.75	0	25,25,25	0.93	1 (4%)
11	HEM	C	381	3	41,50,50	1.42	7 (17%)	45,82,82	2.45	16 (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
15	FES	E	197	5	-	-	0/1/1/1
13	PEE	C	384	-	1/1/4/8	23/52/52/54	-
13	PEE	E	198	-	1/1/4/8	28/52/52/54	-
11	HEM	D	243	4	-	6/12/54/54	-
12	U10	C	383	-	-	8/23/47/87	0/1/1/1
11	HEM	C	382	3	-	6/12/54/54	-
14	BOG	D	242	-	-	5/11/31/31	0/1/1/1
11	HEM	C	381	3	-	5/12/54/54	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	198	PEE	O5-C30	11.49	1.56	1.22
13	C	384	PEE	O5-C30	11.21	1.55	1.22
12	C	383	U10	C6-C1	7.48	1.48	1.35
11	D	243	HEM	C3C-C2C	-5.57	1.32	1.40
12	C	383	U10	C7-C6	5.54	1.60	1.51

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	198	PEE	O4-C10-C11	-18.64	51.02	123.73
13	C	384	PEE	O4-C10-C11	-18.62	51.11	123.73
13	E	198	PEE	O3-C30-C31	12.77	151.98	111.91
13	C	384	PEE	O3-C30-C31	12.50	151.15	111.91
13	C	384	PEE	O3-C30-O5	-11.37	94.89	123.59

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	384	PEE	C2
13	E	198	PEE	C2

5 of 81 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
12	C	383	U10	C1-C6-C7-C8
12	C	383	U10	C5-C6-C7-C8
12	C	383	U10	C14-C16-C17-C18

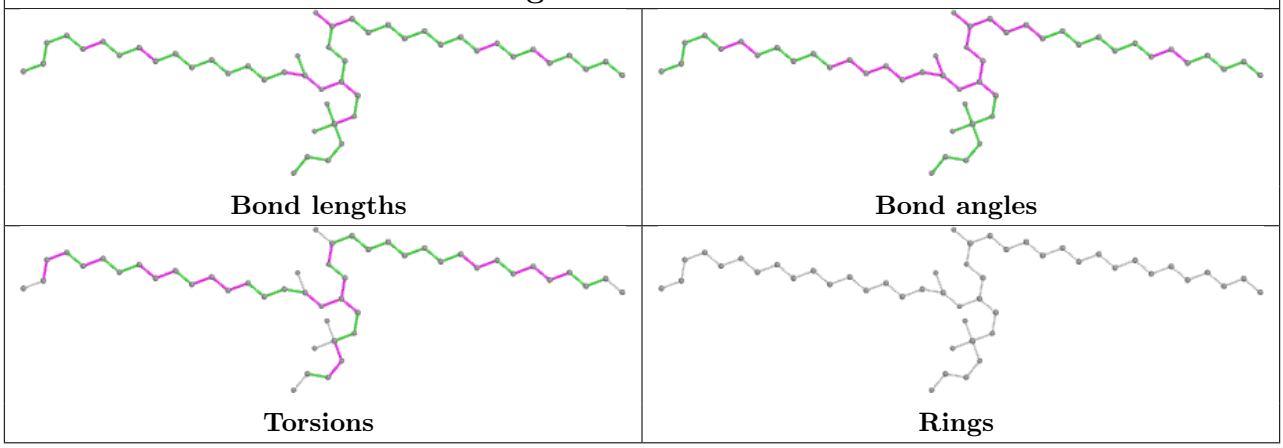
There are no ring outliers.

7 monomers are involved in 22 short contacts:

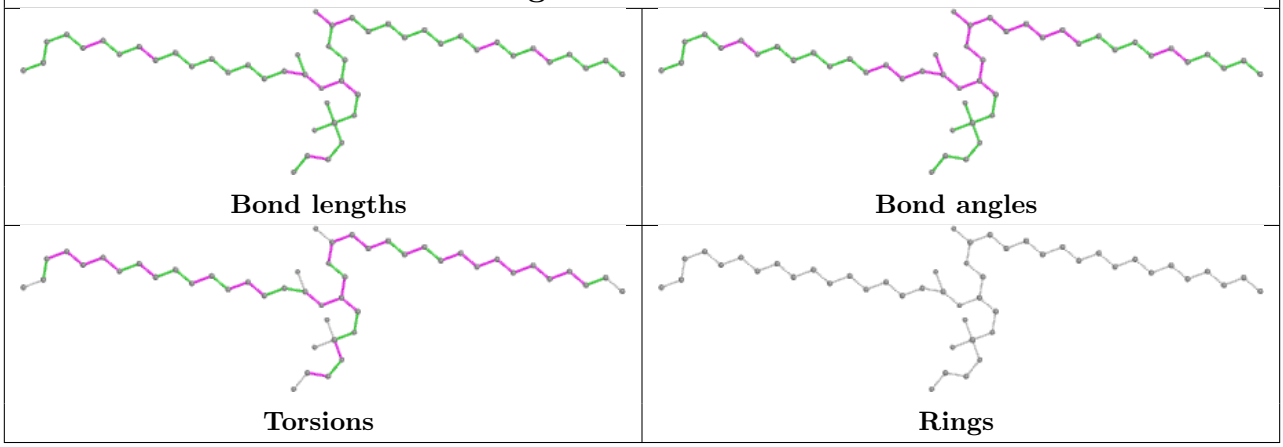
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	197	FES	1	0
13	C	384	PEE	2	0
13	E	198	PEE	1	0
12	C	383	U10	4	0
11	C	382	HEM	7	0
14	D	242	BOG	2	0
11	C	381	HEM	5	0

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.

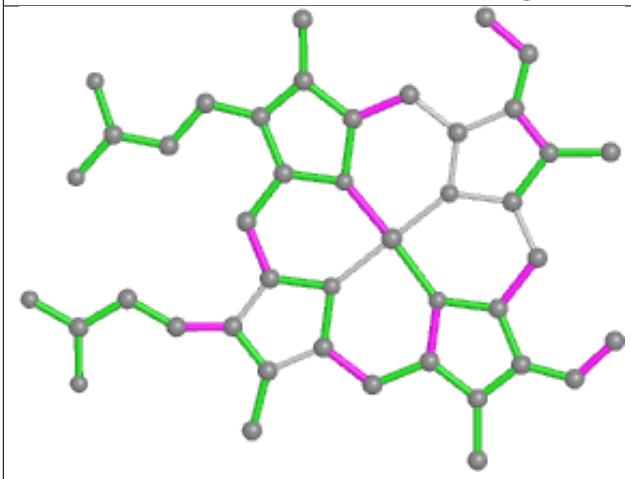
Ligand PEE C 384



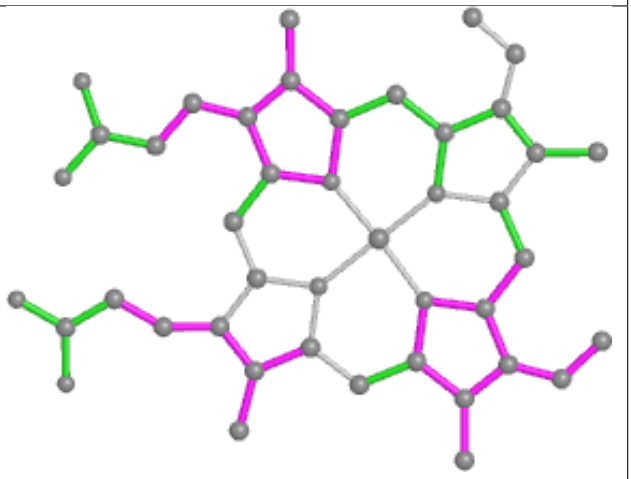
Ligand PEE E 198



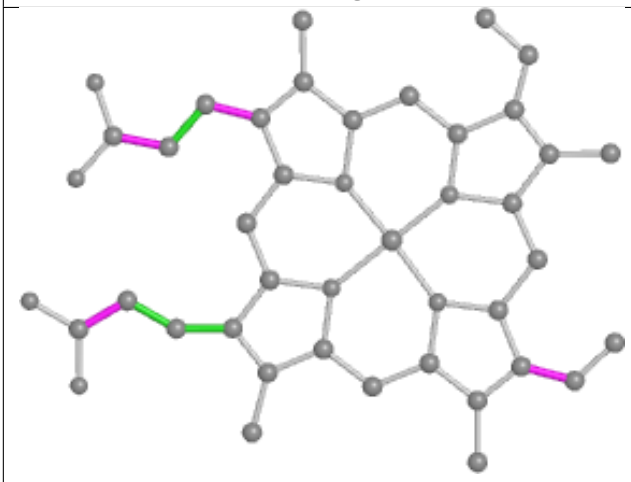
Ligand HEM D 243



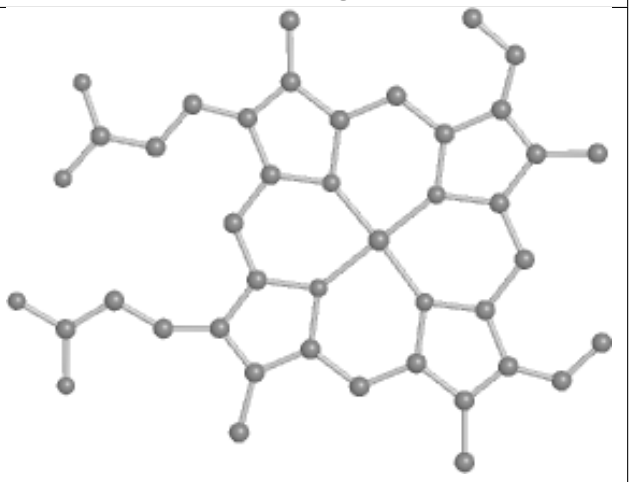
Bond lengths



Bond angles

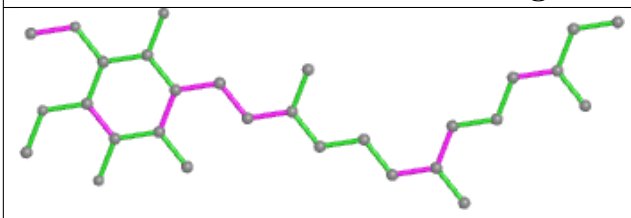


Torsions

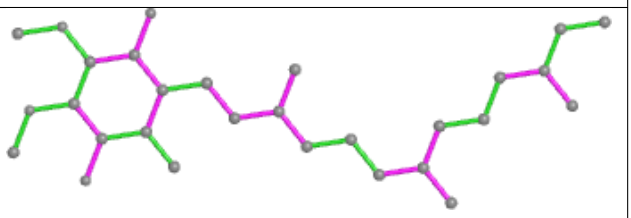


Rings

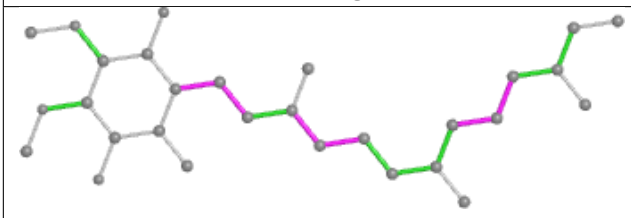
Ligand U10 C 383



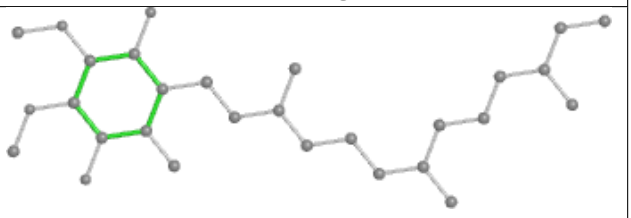
Bond lengths



Bond angles

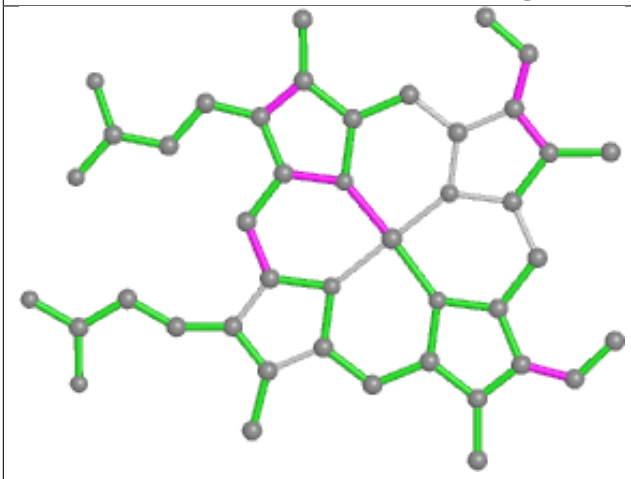


Torsions

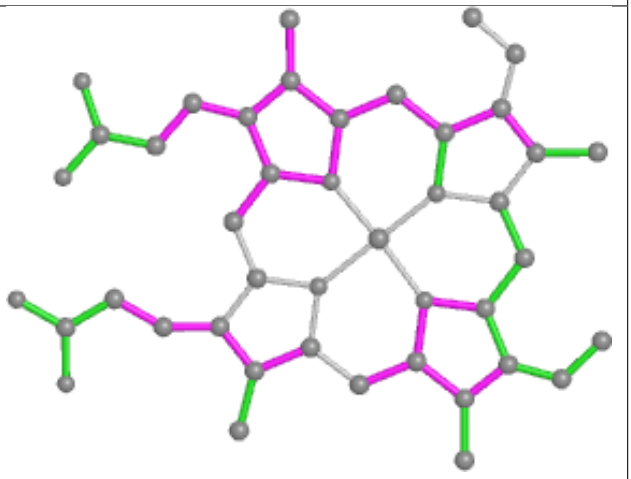


Rings

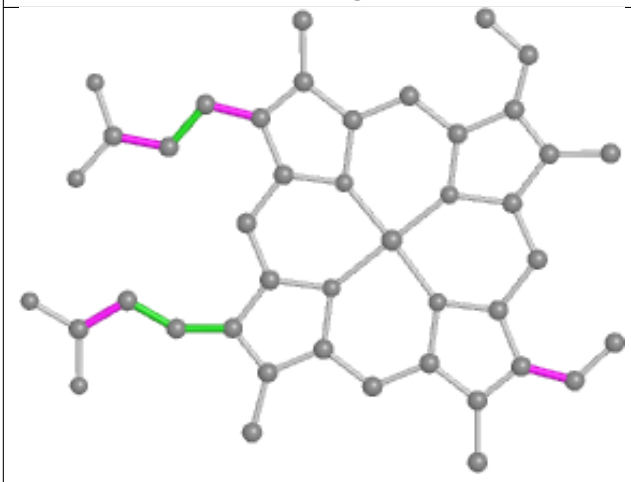
Ligand HEM C 382



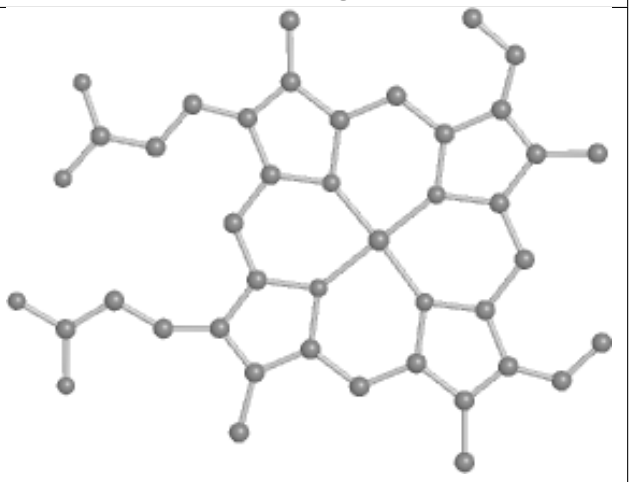
Bond lengths



Bond angles

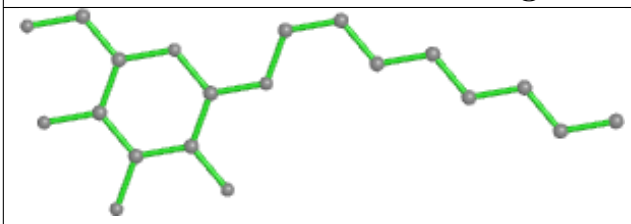


Torsions

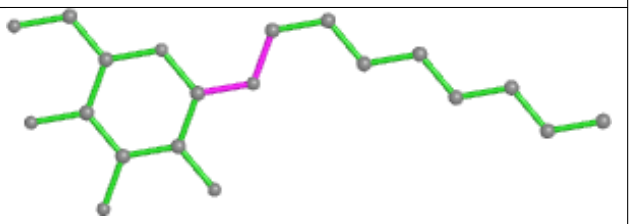


Rings

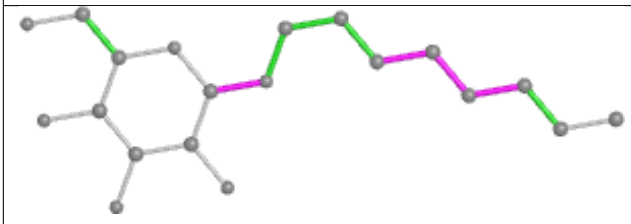
Ligand BOG D 242



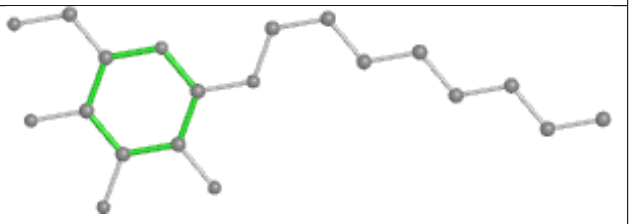
Bond lengths



Bond angles

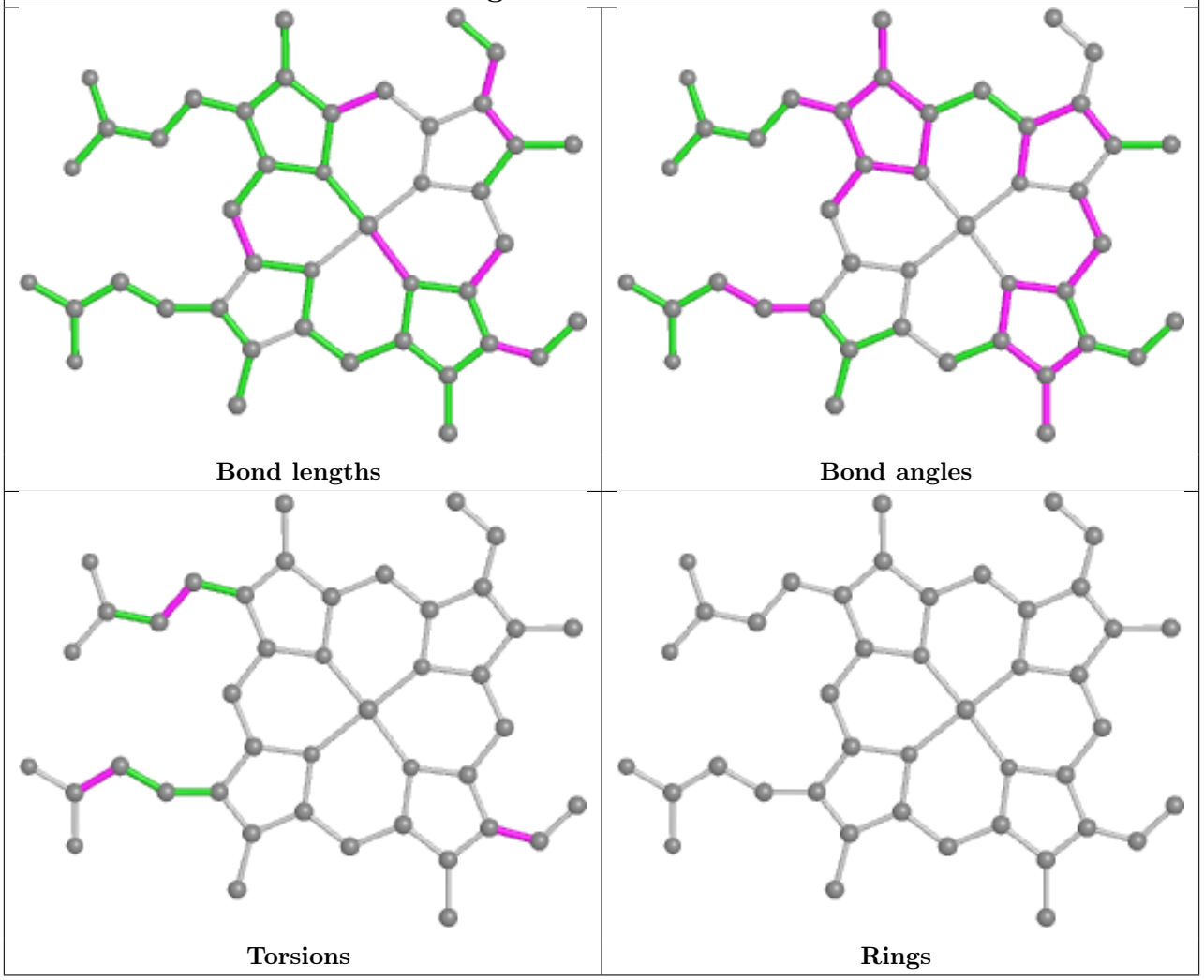


Torsions



Rings

Ligand HEM C 381



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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	33.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	121:UNK	C	202:UNK	N	29.43

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%)	-0.10	7 (1%) 72 59	47, 84, 100, 100	0
2	B	406/422 (96%)	0.09	16 (3%) 39 24	60, 93, 100, 100	0
3	C	379/380 (99%)	-0.24	8 (2%) 63 49	33, 64, 96, 100	0
4	D	241/241 (100%)	-0.03	7 (2%) 51 35	50, 76, 99, 100	0
5	E	196/196 (100%)	0.90	46 (23%) 0 0	54, 100, 100, 100	0
6	F	100/109 (91%)	-0.10	2 (2%) 65 50	50, 73, 98, 100	0
7	G	78/81 (96%)	0.09	2 (2%) 56 40	51, 85, 100, 100	0
8	H	66/78 (84%)	-0.19	1 (1%) 73 61	76, 95, 99, 100	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	-0.05	2 (3%) 45 28	66, 80, 99, 100	0
All	All	1967/2048 (96%)	0.03	91 (4%) 32 18	33, 83, 100, 100	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	114	VAL	6.6
5	E	163	SER	6.3
2	B	18	PRO	5.8
5	E	174	GLY	5.2
10	J	62	LYS	4.6

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 monosaccharides in this entry.

6.4 Ligands (i)

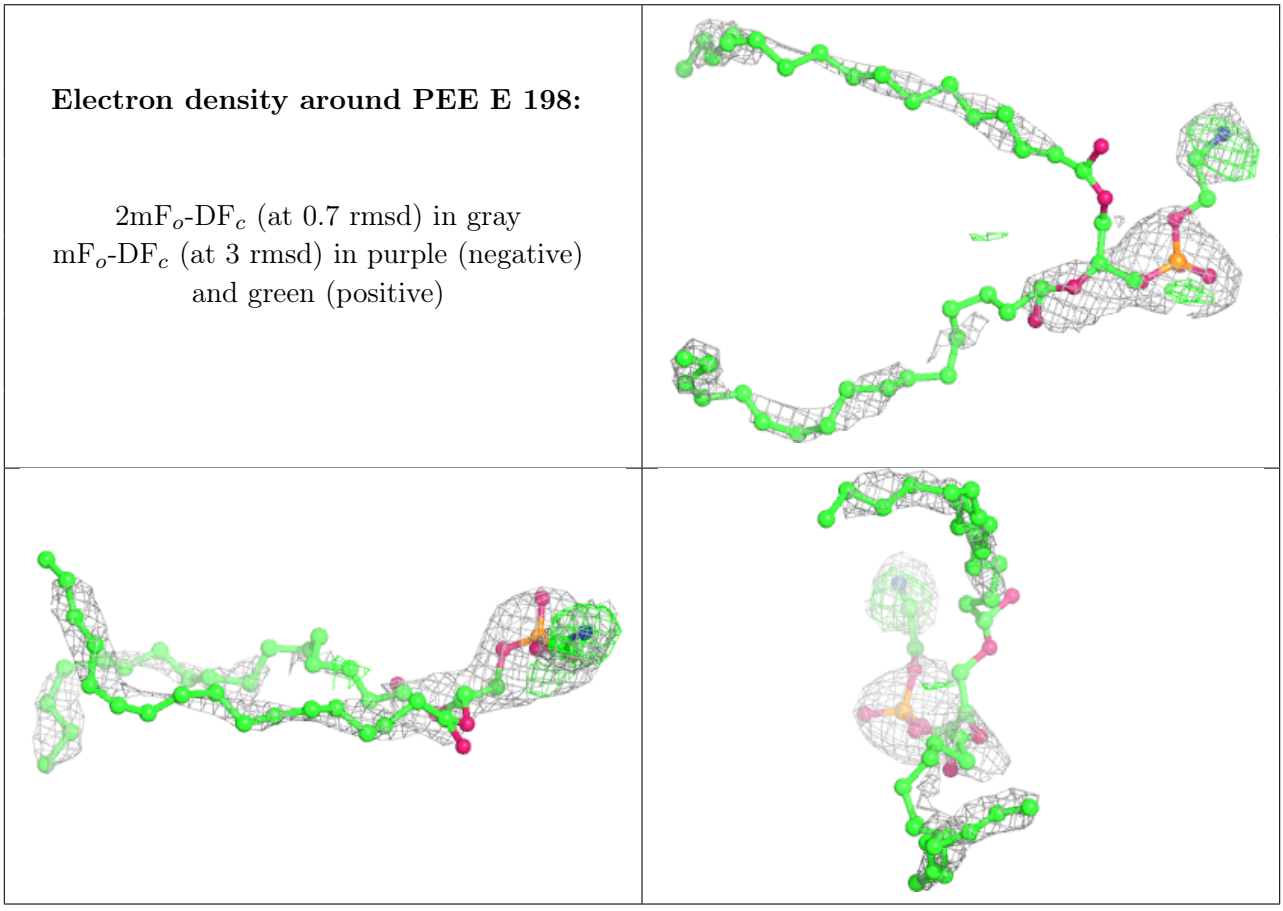
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
13	PEE	E	198	49/51	0.65	0.49	24,45,64,65	49
12	U10	C	383	29/63	0.77	0.39	77,83,100,100	29
13	PEE	C	384	49/51	0.82	0.40	20,39,54,55	49
14	BOG	D	242	20/20	0.90	0.25	37,59,70,72	20
15	FES	E	197	4/4	0.97	0.28	100,100,100,100	0
11	HEM	D	243	43/43	0.98	0.18	46,58,69,74	0
11	HEM	C	381	43/43	0.98	0.23	43,51,59,62	0
11	HEM	C	382	43/43	0.98	0.21	43,46,59,62	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.

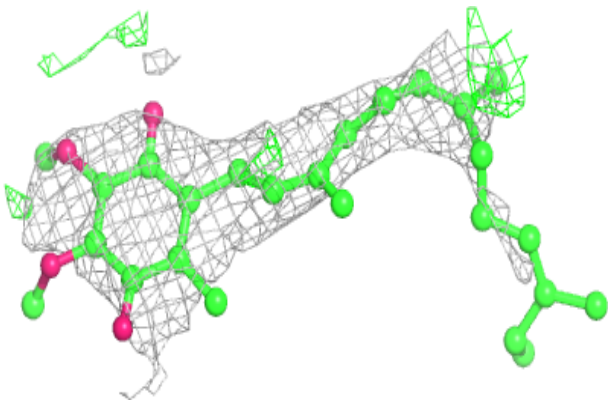
Electron density around PEE E 198:

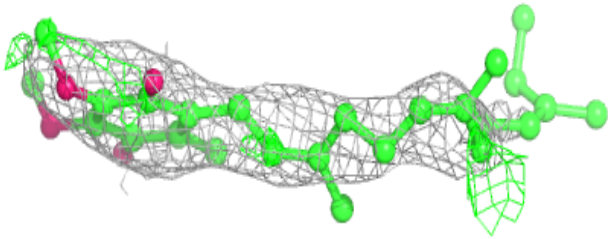
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

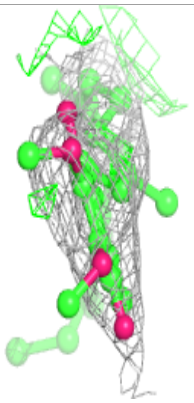


Electron density around U10 C 383:

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

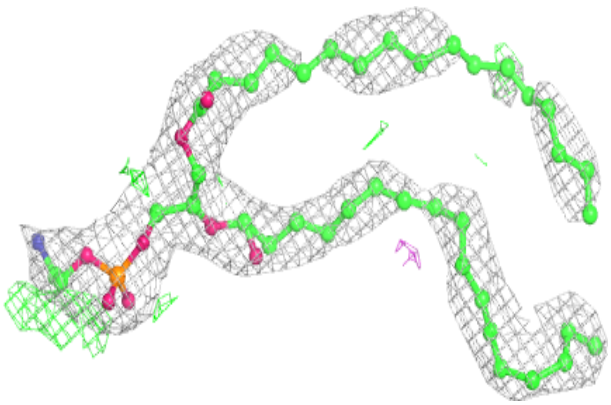


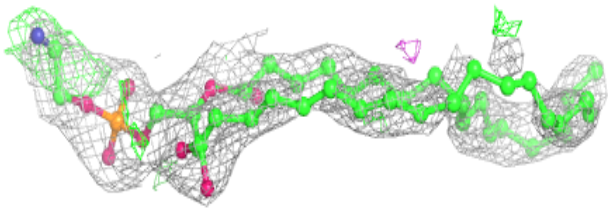


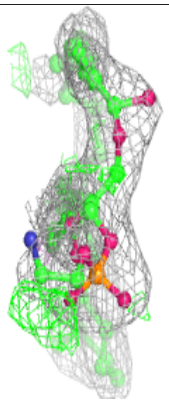


Electron density around PEE C 384:

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

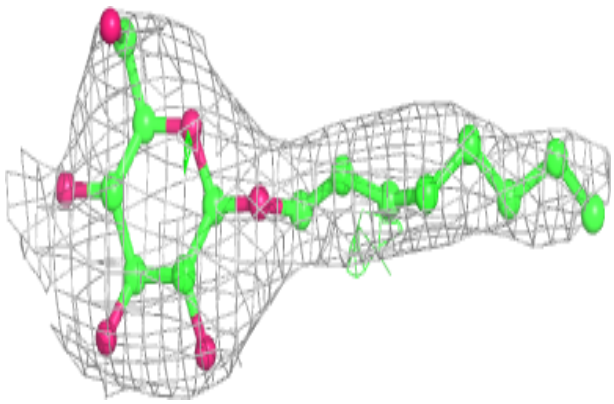


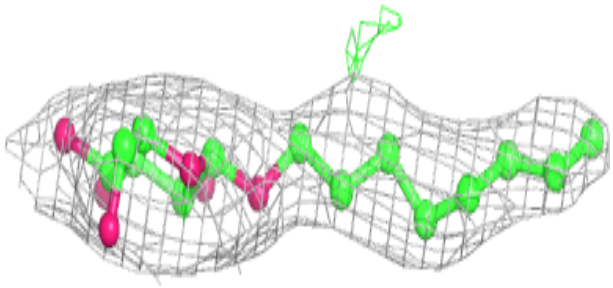


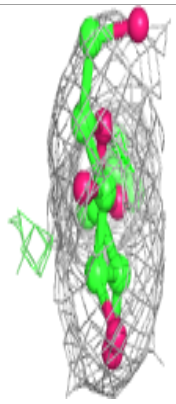


Electron density around BOG D 242:

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

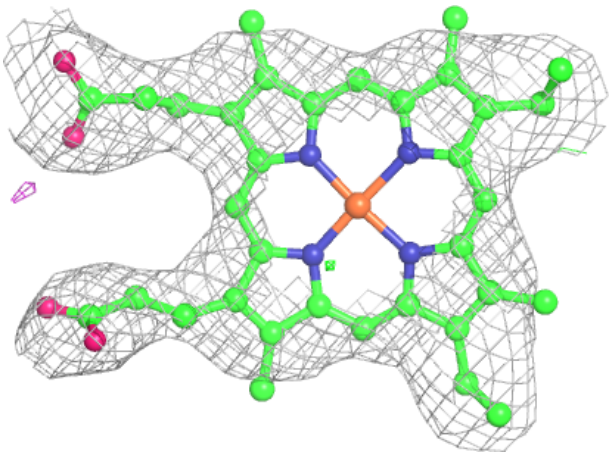


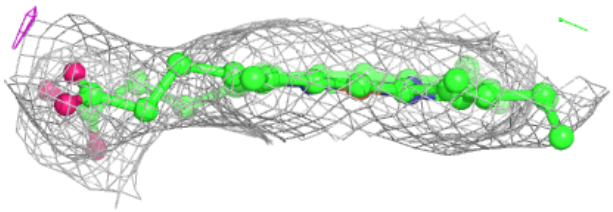


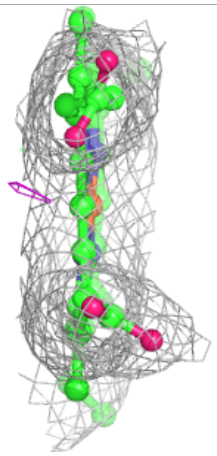


Electron density around HEM D 243:

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

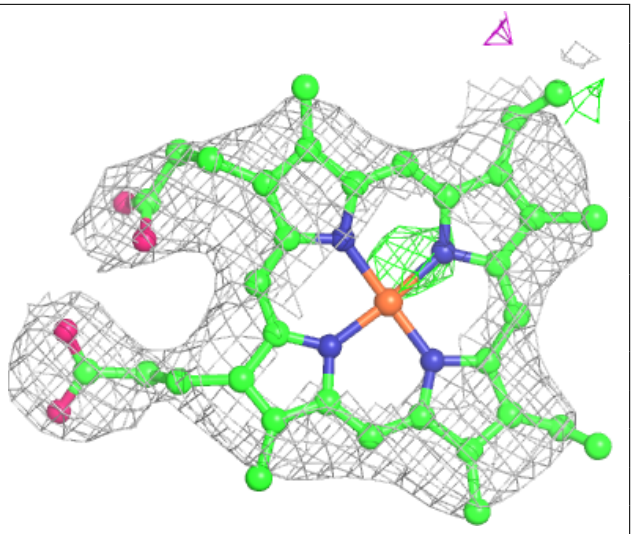


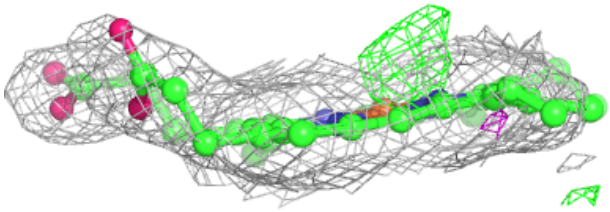


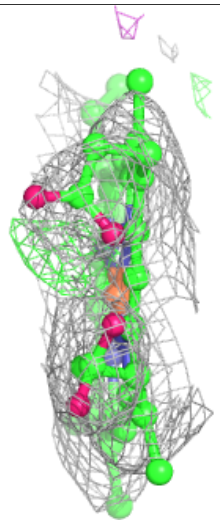


Electron density around HEM C 381:

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

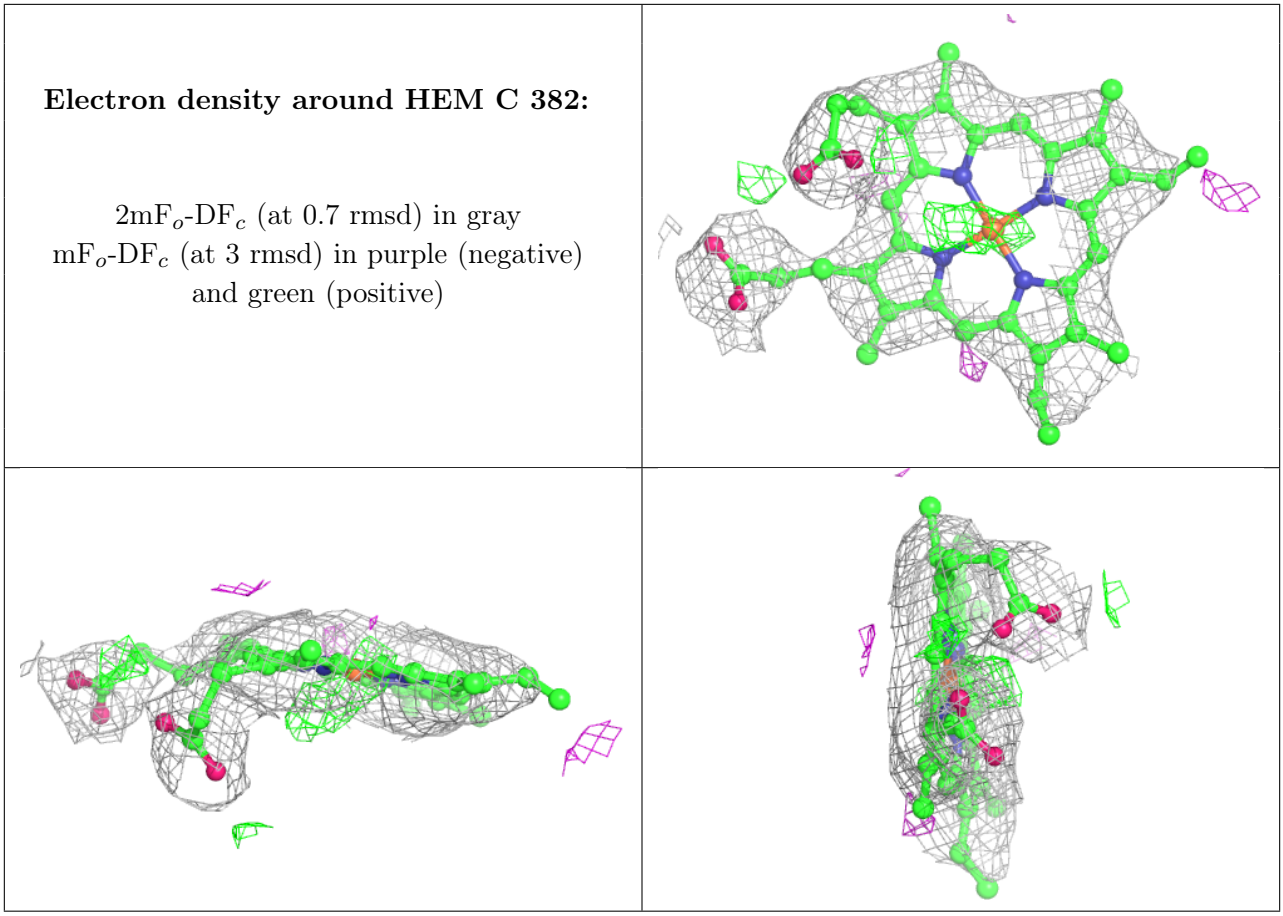






Electron density around HEM C 382:

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



6.5 Other polymers

There are no such residues in this entry.