



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:23 PM BST

PDB ID : 2BCC
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

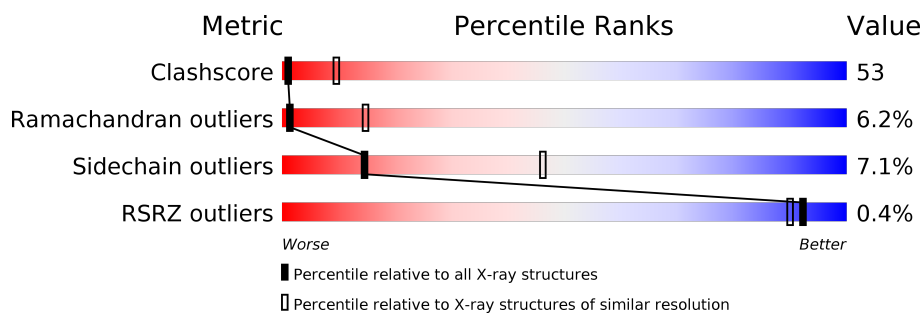
1 Overall quality at a glance

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	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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 $\leq 5\%$. 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	<div> <div>39%</div> <div>53%</div> <div>7%</div> <div>.</div> </div>
2	B	422	<div> <div>35%</div> <div>51%</div> <div>10%</div> <div>.</div> </div>
3	C	380	<div> <div>30%</div> <div>57%</div> <div>11%</div> <div>.</div> </div>
4	D	241	<div> <div>42%</div> <div>54%</div> <div>.</div> </div>
5	E	196	<div> <div>2%</div> <div>34%</div> <div>56%</div> <div>9%</div> <div>.</div> </div>
6	F	109	<div> <div>50%</div> <div>33%</div> <div>8%</div> <div>8%</div> </div>
7	G	81	<div> <div>31%</div> <div>54%</div> <div>9%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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
12	U10	C	383	-	-	-	X
13	PEE	C	384	X	-	-	-
13	PEE	E	198	X	-	-	-

2 Entry composition

There are 16 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
1	A	442	Total	C	N	O	S	0	0	0
			3423	2147	601	657	18			

- 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			

- 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			

- 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			

- 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			

- 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			

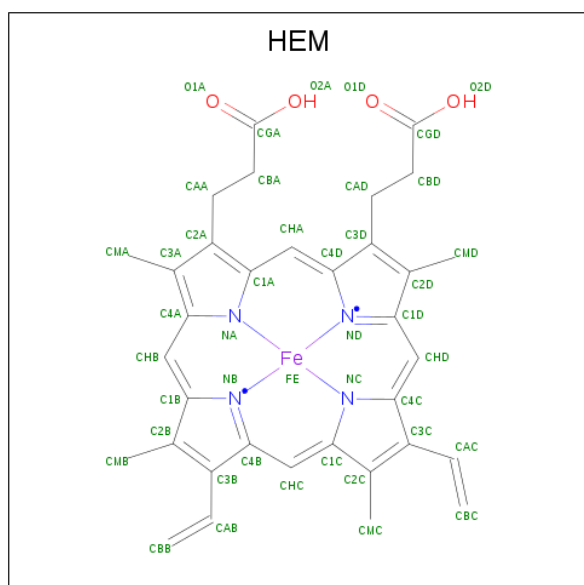
- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

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.

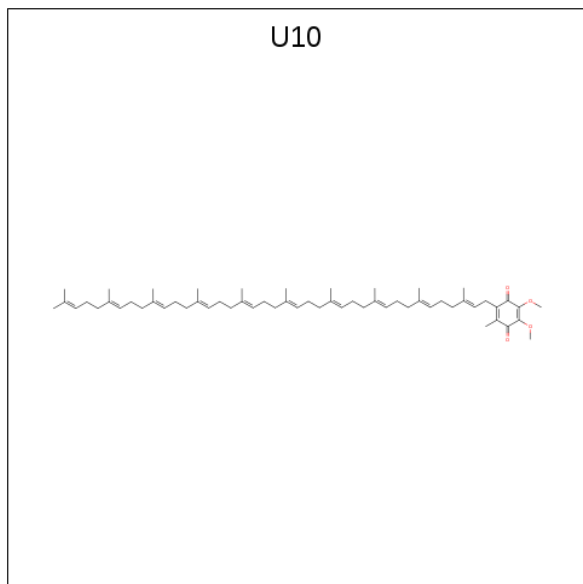
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			459	299	78	82			

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



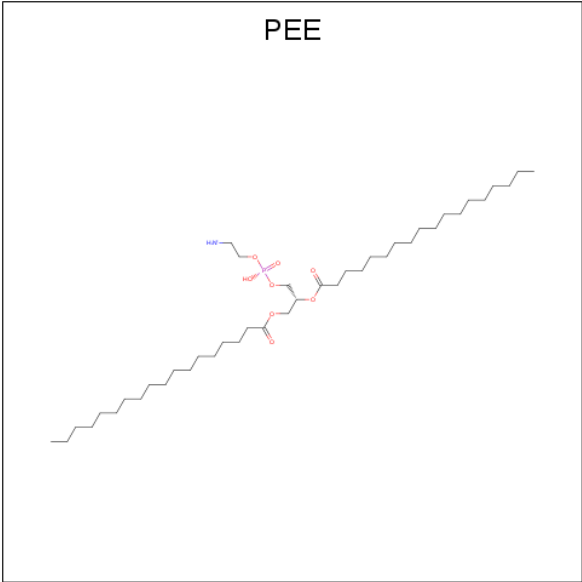
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



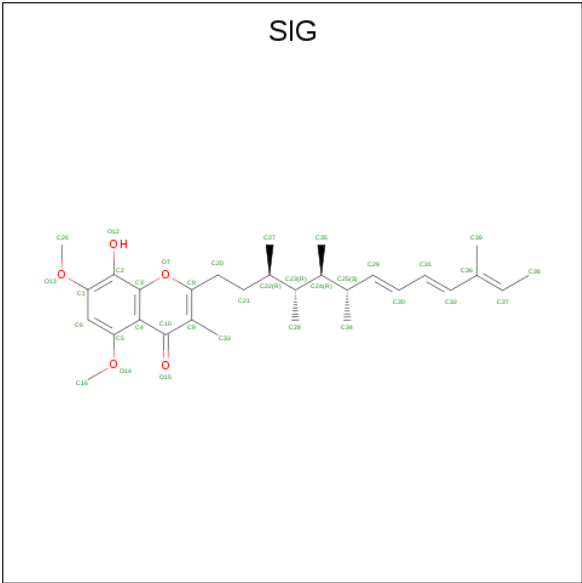
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			29	25	4		

- Molecule 13 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



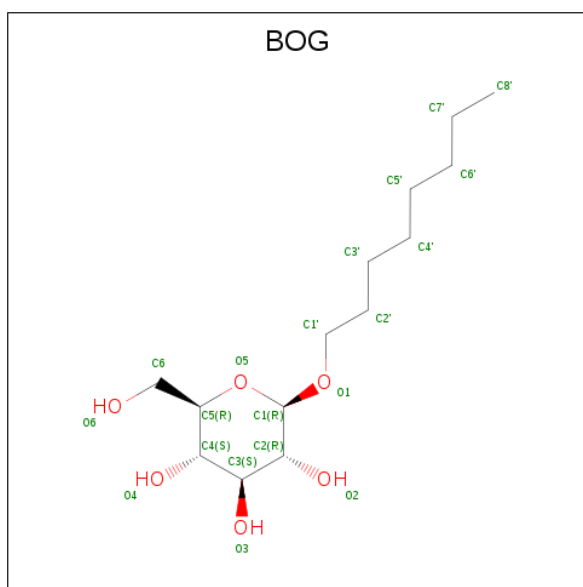
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is STIGMATELLIN (three-letter code: SIG) (formula: C₃₀H₄₂O₅).



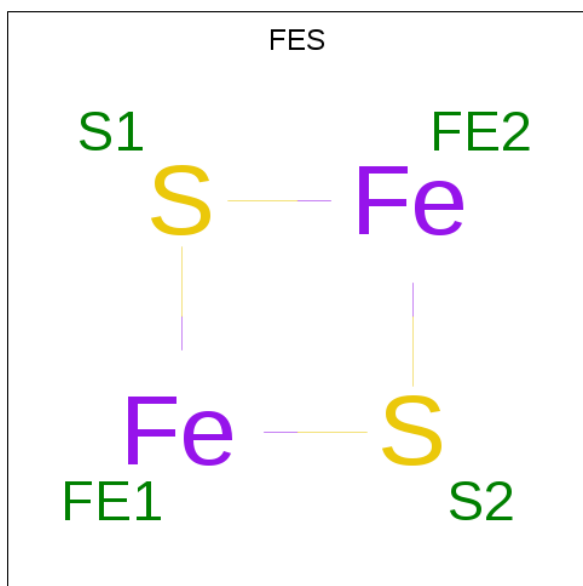
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			35	30	5		

- Molecule 15 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

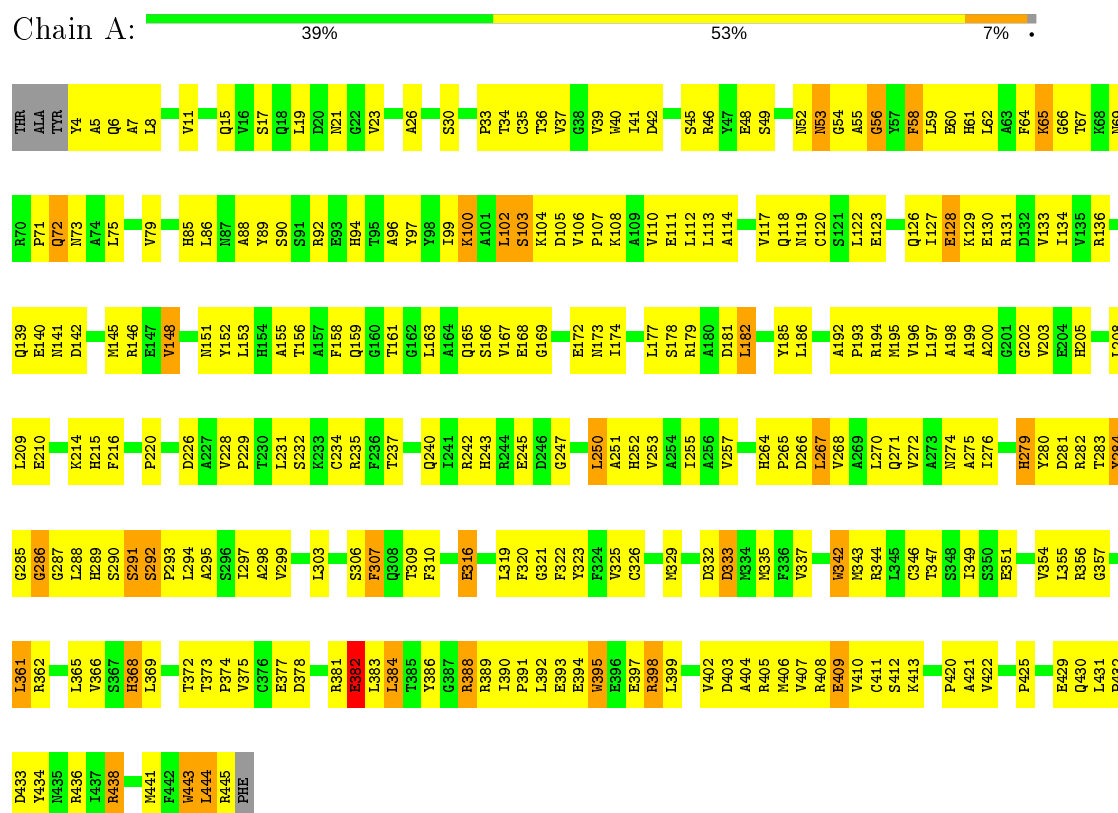


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		

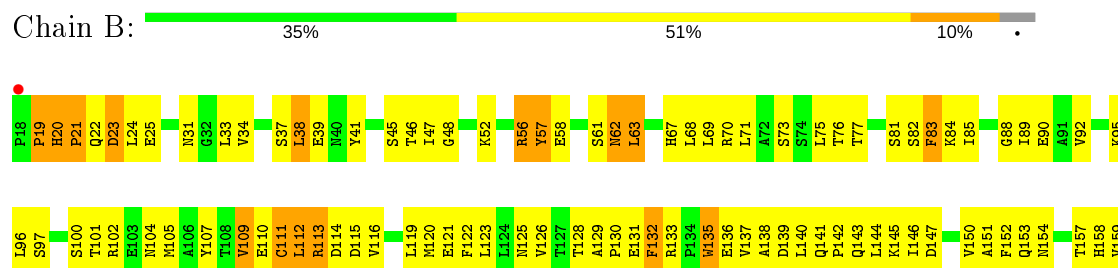
3 Residue-property plots

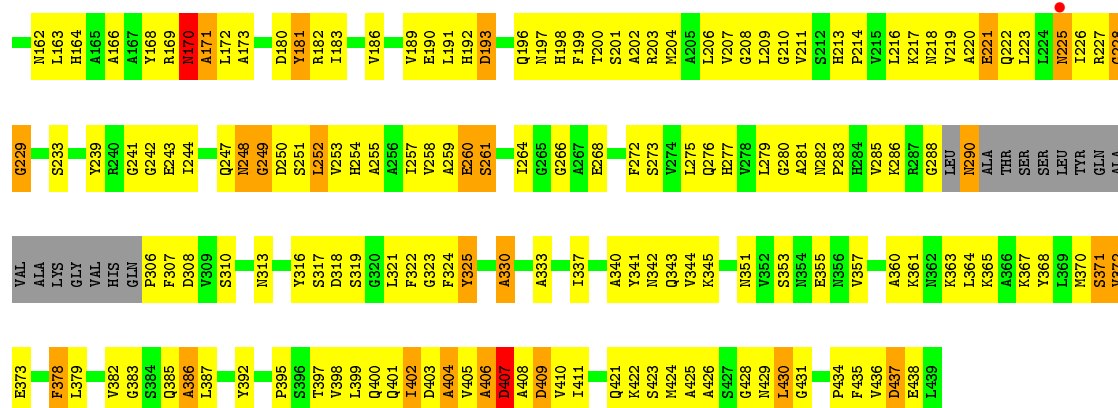
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



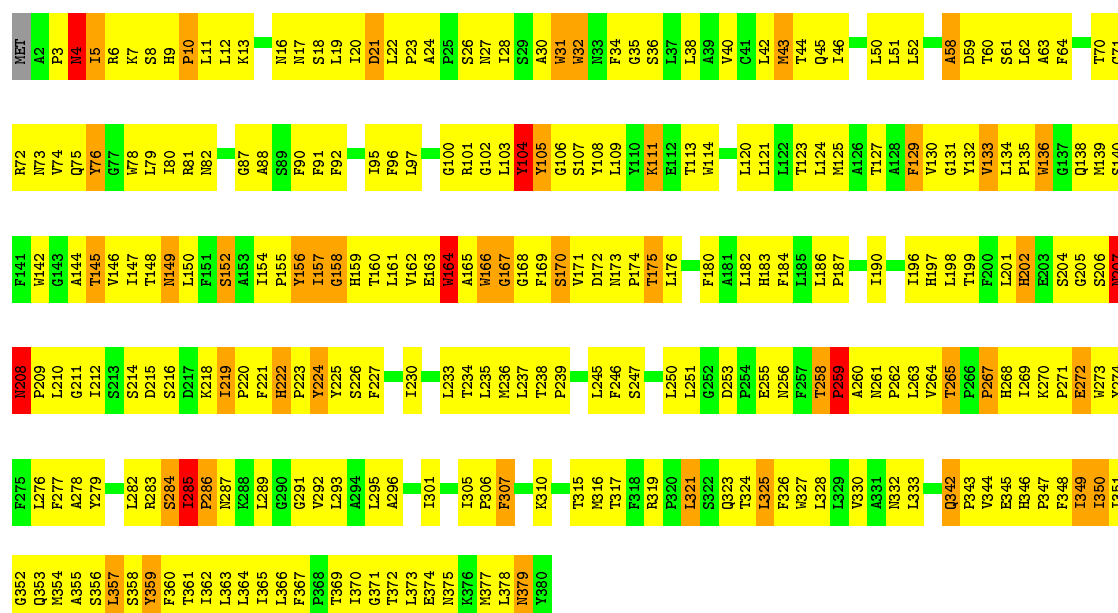
• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE





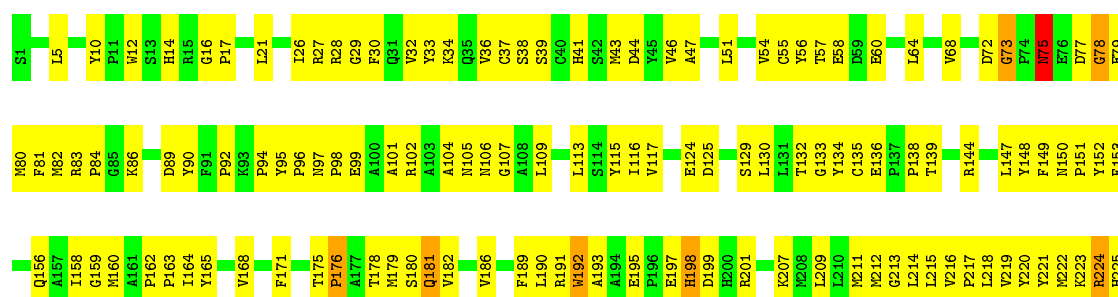
• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain C: 30% 57% 11%



• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain D: 42% 54%

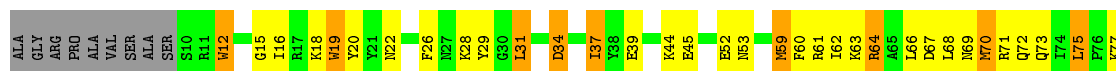




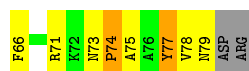
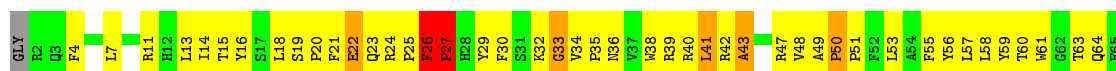
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

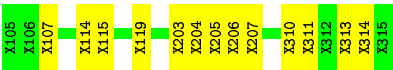


• Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE





● Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



4 Data and refinement statistics

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 87.05 – 3.02	Depositor EDS
% Data completeness (in resolution range)	85.6 (12.00-3.50) 62.8 (87.05-3.02)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.01Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.284 , 0.317 0.286 , (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)	0.27 , 21.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.229 for k,h,-l	Xtriage
F_o, F_c correlation	0.82	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, SIG, FES, HEM, PEE, BOG

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	0.45	0/3495	0.78	1/4742 (0.0%)
2	B	0.43	0/3046	0.73	0/4132
3	C	0.52	0/3104	0.85	5/4252 (0.1%)
4	D	0.50	0/1960	0.81	1/2665 (0.0%)
5	E	0.46	0/1548	0.78	1/2095 (0.0%)
6	F	0.49	0/896	0.76	0/1206
7	G	0.53	0/648	1.17	3/882 (0.3%)
8	H	0.44	0/495	0.69	0/669
10	J	0.52	0/470	0.80	1/635 (0.2%)
All	All	0.48	0/15662	0.81	12/21278 (0.1%)

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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	26	PHE	C-N-CD	-18.95	78.91	120.60
7	G	26	PHE	C-N-CA	13.72	179.63	122.00
7	G	27	PRO	CA-N-CD	-7.67	100.76	111.50
10	J	61	ASN	N-CA-C	6.56	128.72	111.00
3	C	267	PRO	N-CA-C	-6.18	96.03	112.10

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

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	359	0
2	B	2994	0	2906	345	0
3	C	3002	0	3036	423	0
4	D	1899	0	1822	216	0
5	E	1512	0	1483	177	0
6	F	875	0	839	70	0
7	G	626	0	591	83	0
8	H	490	0	445	57	0
9	I	159	0	46	20	0
10	J	459	0	424	53	0
11	C	86	0	60	19	0
11	D	43	0	30	2	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	E	4	0	0	1	0
All	All	15754	0	15211	1654	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 53.

The worst 5 of 1654 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.36	1.05
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.19	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	3	23
2	B	404/422 (96%)	295 (73%)	78 (19%)	31 (8%)	1	10
3	C	377/380 (99%)	278 (74%)	68 (18%)	31 (8%)	1	9
4	D	239/241 (99%)	194 (81%)	34 (14%)	11 (5%)	2	21
5	E	194/196 (99%)	151 (78%)	28 (14%)	15 (8%)	1	10
6	F	98/109 (90%)	84 (86%)	12 (12%)	2 (2%)	7	39
7	G	76/81 (94%)	52 (68%)	18 (24%)	6 (8%)	1	10
8	H	64/78 (82%)	56 (88%)	7 (11%)	1 (2%)	9	43
10	J	57/62 (92%)	32 (56%)	20 (35%)	5 (9%)	1	8
All	All	1949/2015 (97%)	1479 (76%)	350 (18%)	120 (6%)	1	15

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 ⓘ

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%)	333 (93%)	26 (7%)	14	45
2	B	307/336 (91%)	286 (93%)	21 (7%)	16	48
3	C	326/329 (99%)	298 (91%)	28 (9%)	10	38
4	D	201/207 (97%)	193 (96%)	8 (4%)	31	64
5	E	165/169 (98%)	153 (93%)	12 (7%)	14	45
6	F	90/98 (92%)	80 (89%)	10 (11%)	6	28
7	G	60/72 (83%)	53 (88%)	7 (12%)	5	26
8	H	51/74 (69%)	51 (100%)	0	100	100
10	J	41/52 (79%)	40 (98%)	1 (2%)	49	76
All	All	1600/1713 (93%)	1487 (93%)	113 (7%)	14	46

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	104	TYR
3	C	208	ASN
6	F	107	TRP
3	C	129	PHE
3	C	152	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	429	ASN
3	C	86	ASN
7	G	64	GLN
3	C	16	ASN
3	C	138	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	E	198	-	48,48,50	2.32	7 (14%)	51,53,55	4.31	18 (35%)
15	BOG	D	242	-	20,20,20	1.16	2 (10%)	25,25,25	0.84	1 (4%)
11	HEM	D	243	4	27,50,50	1.90	6 (22%)	17,82,82	2.95	5 (29%)
16	FES	E	197	5	0,4,4	0.00	-	-	-	-
13	PEE	C	384	-	48,48,50	2.41	9 (18%)	51,53,55	4.28	17 (33%)
14	SIG	C	385	-	32,36,36	3.35	11 (34%)	40,50,50	2.36	12 (30%)
12	U10	C	383	-	29,29,63	3.10	5 (17%)	35,38,79	1.99	8 (22%)
11	HEM	C	382	3	27,50,50	2.12	8 (29%)	17,82,82	2.34	4 (23%)
11	HEM	C	381	3	27,50,50	2.08	8 (29%)	17,82,82	2.68	9 (52%)

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
12	U10	C	383	-	-	7/23/47/87	0/1/1/1
15	BOG	D	242	-	-	5/11/31/31	0/1/1/1
11	HEM	D	243	4	-	2/6/54/54	-
16	FES	E	197	5	-	-	0/1/1/1
13	PEE	C	384	-	1/1/4/4	23/52/52/54	-
14	SIG	C	385	-	-	15/29/30/30	0/2/2/2
13	PEE	E	198	-	1/1/4/4	29/52/52/54	-
11	HEM	C	382	3	-	3/6/54/54	-
11	HEM	C	381	3	-	0/6/54/54	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	385	SIG	C24-C23	-14.79	1.47	1.56
12	C	383	U10	C13-C14	12.23	1.62	1.33
13	E	198	PEE	O5-C30	11.72	1.57	1.22
13	C	384	PEE	O5-C30	11.24	1.55	1.22
12	C	383	U10	C6-C1	7.27	1.48	1.35

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	384	PEE	O4-C10-C11	-18.62	51.07	123.73
13	E	198	PEE	O4-C10-C11	-18.59	51.22	123.73
13	E	198	PEE	O3-C30-C31	12.63	151.56	111.91
13	C	384	PEE	O3-C30-C31	12.57	151.35	111.91
13	C	384	PEE	O3-C30-O5	-11.28	95.11	123.59

All (2) chirality outliers are listed below:

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

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	E	198	PEE	O4-C10-O2-C2
13	E	198	PEE	C31-C30-O3-C3
13	E	198	PEE	O5-C30-O3-C3
11	D	243	HEM	C1A-C2A-CAA-CBA

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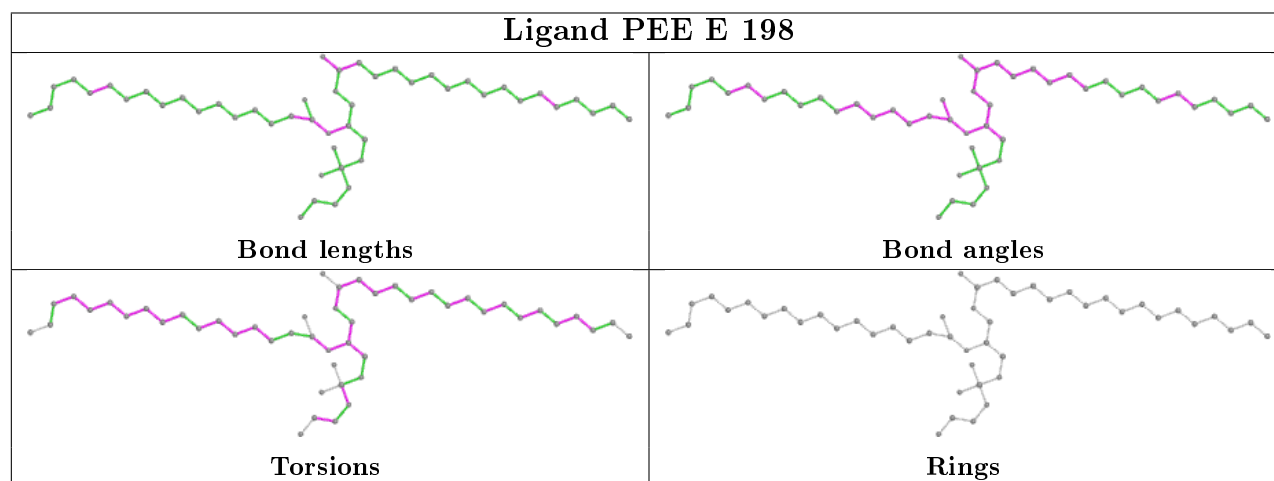
Mol	Chain	Res	Type	Atoms
11	D	243	HEM	C3A-C2A-CAA-CBA

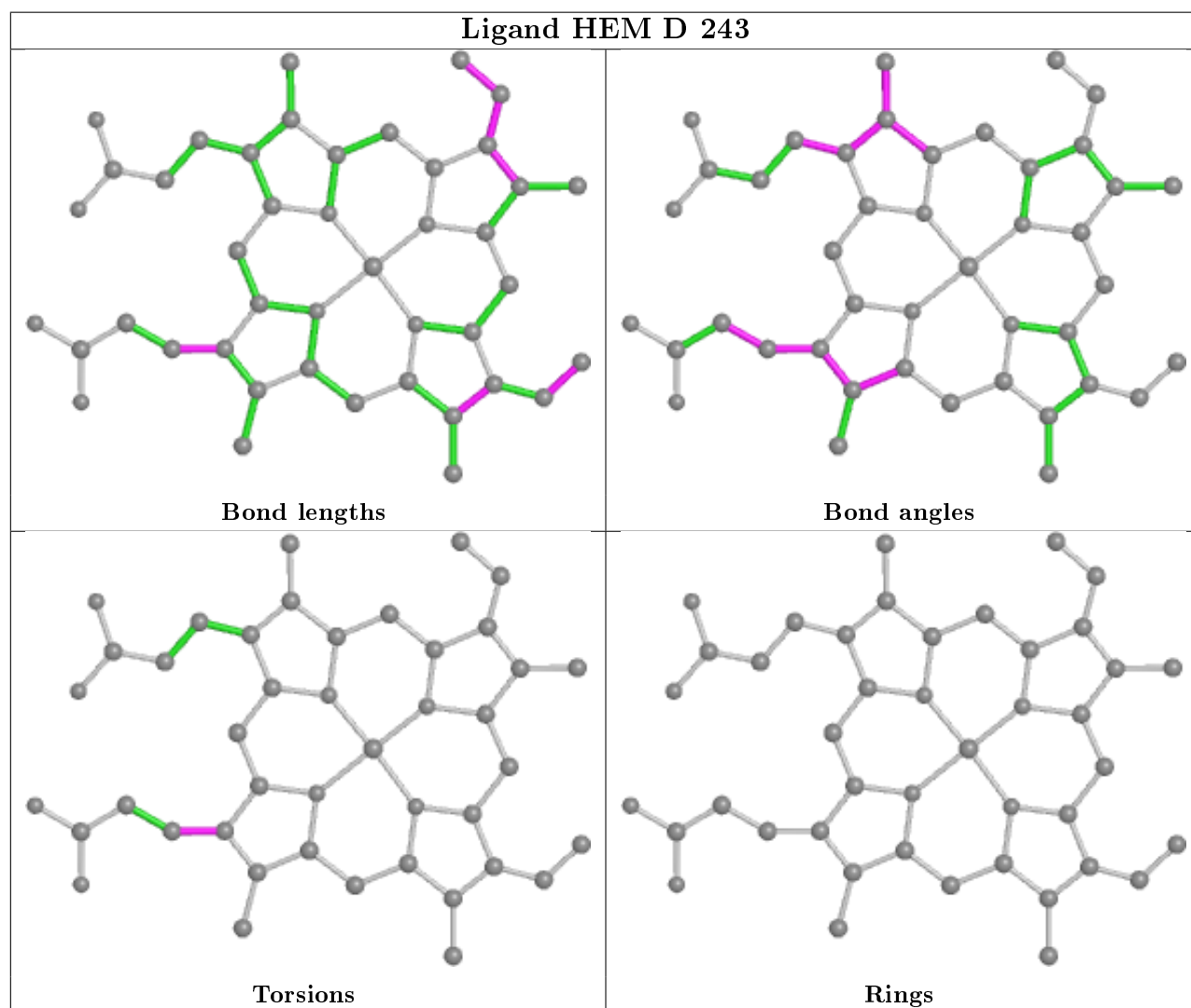
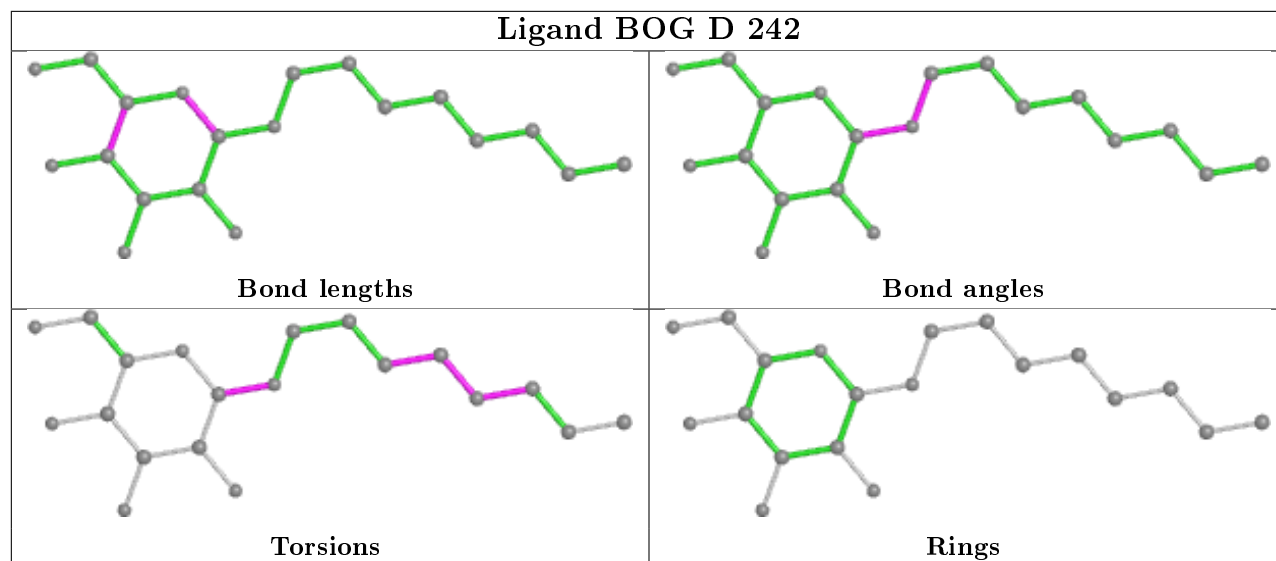
There are no ring outliers.

9 monomers are involved in 55 short contacts:

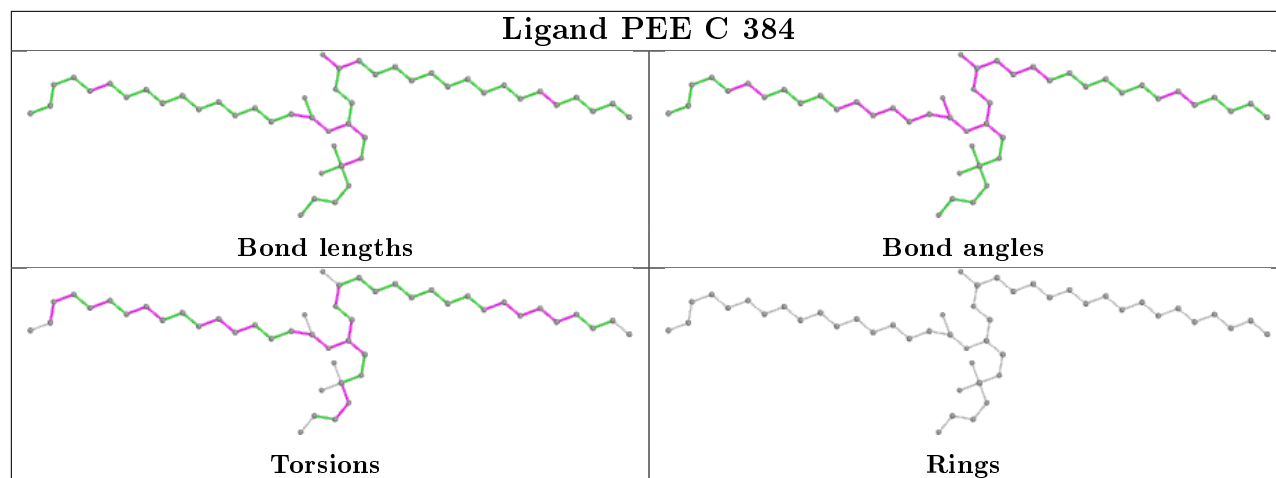
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	198	PEE	4	0
15	D	242	BOG	1	0
11	D	243	HEM	2	0
16	E	197	FES	1	0
13	C	384	PEE	7	0
14	C	385	SIG	12	0
12	C	383	U10	9	0
11	C	382	HEM	12	0
11	C	381	HEM	7	0

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 than 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.

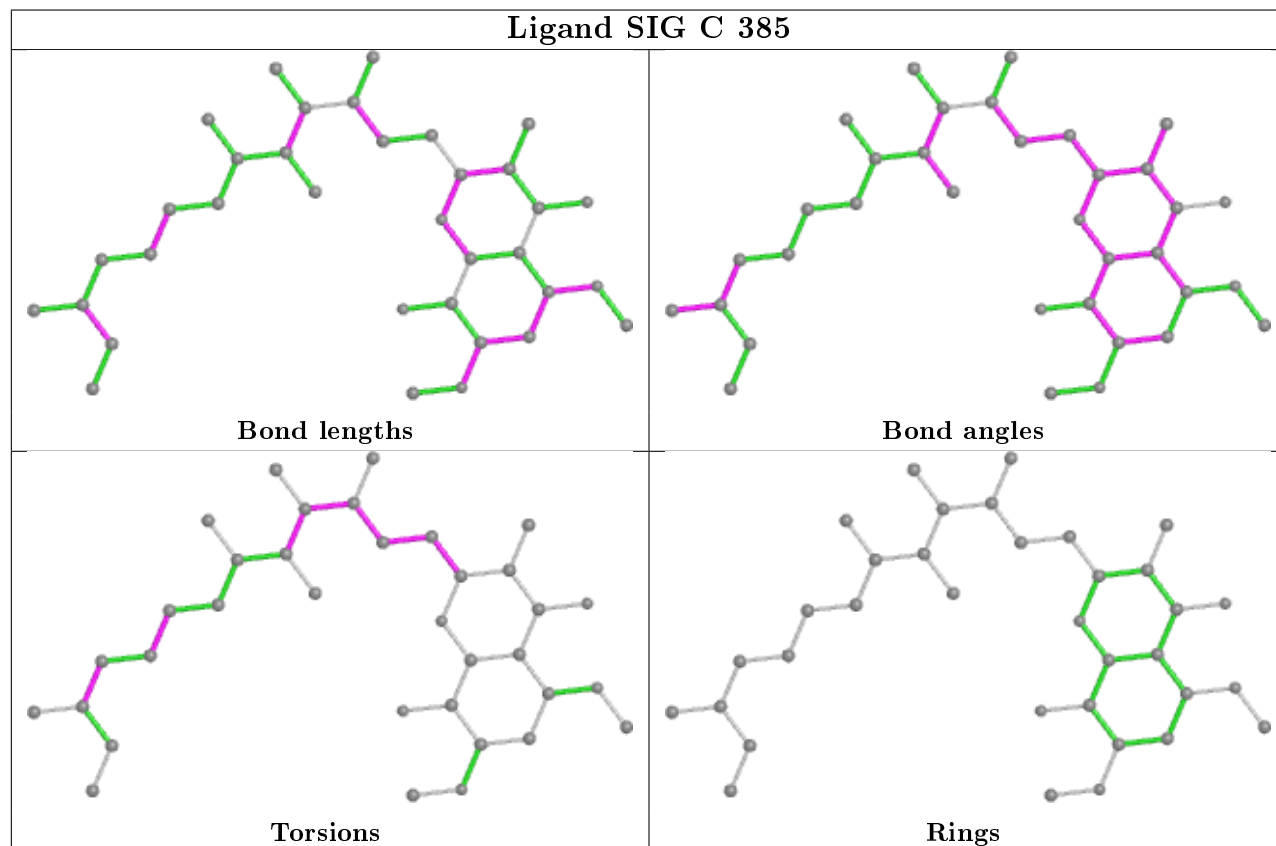




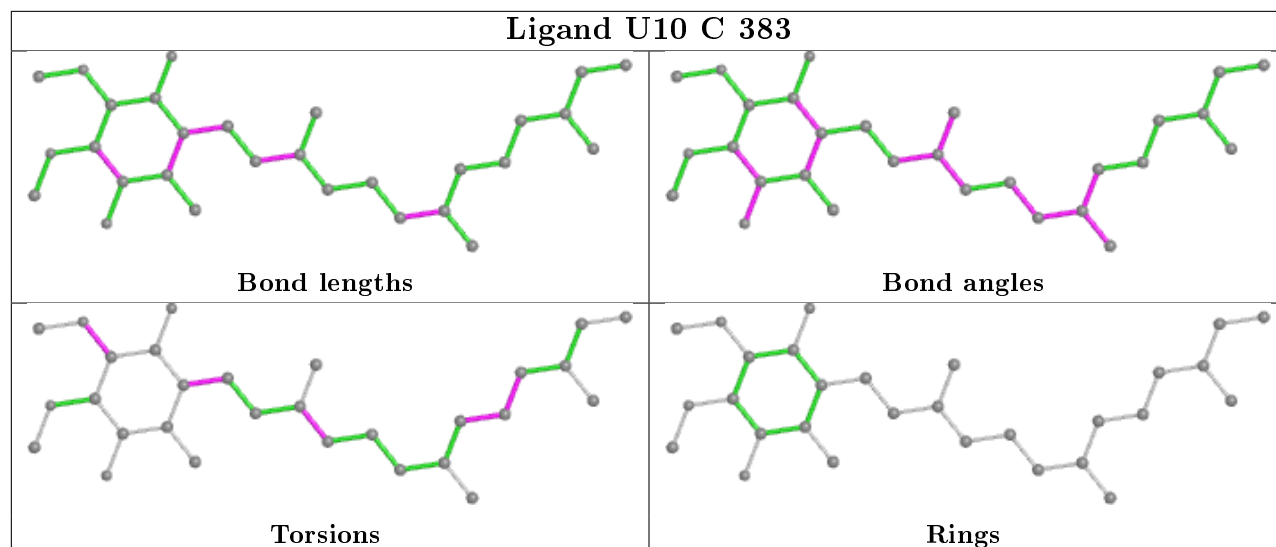
Ligand PEE C 384



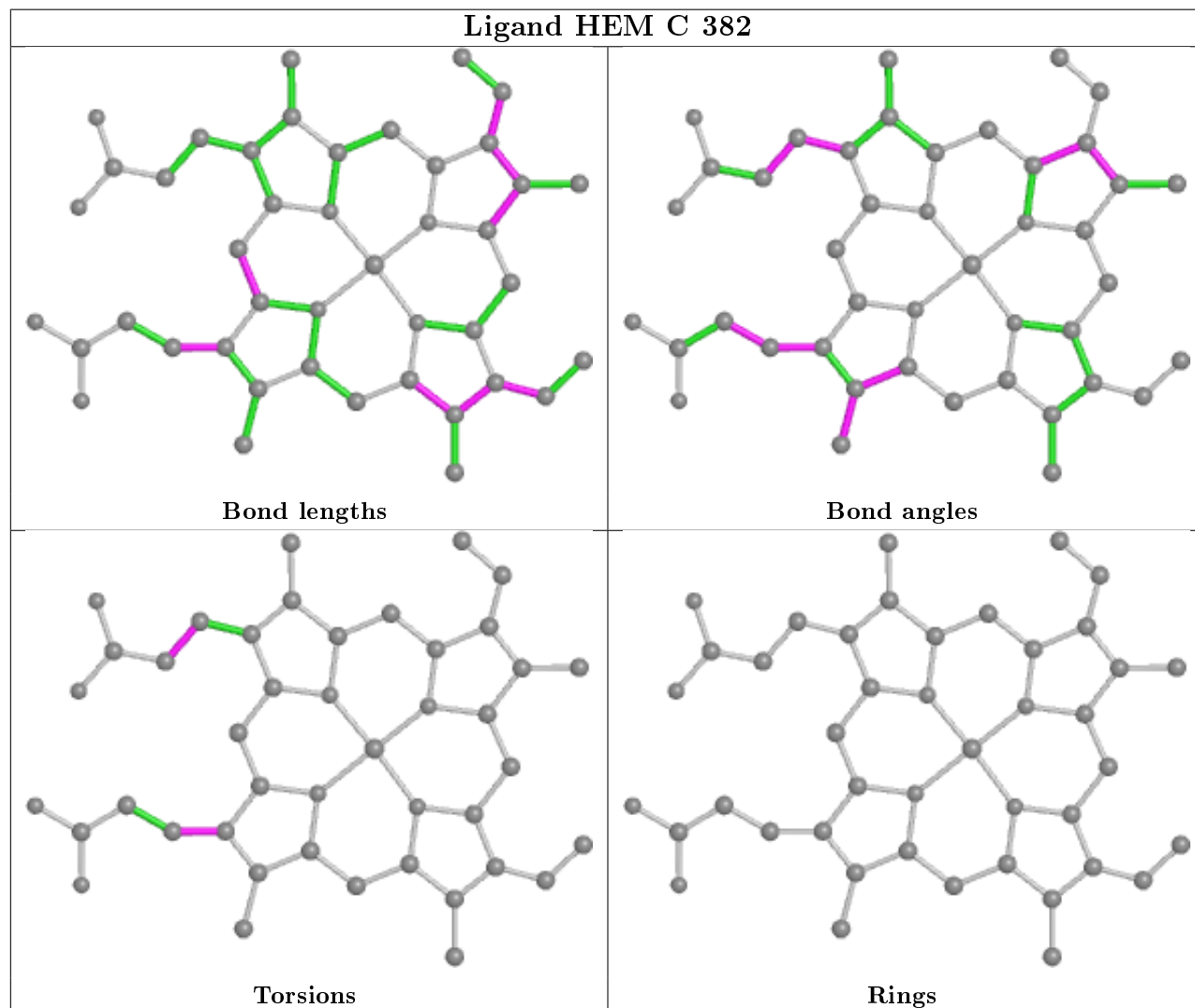
Ligand SIG C 385

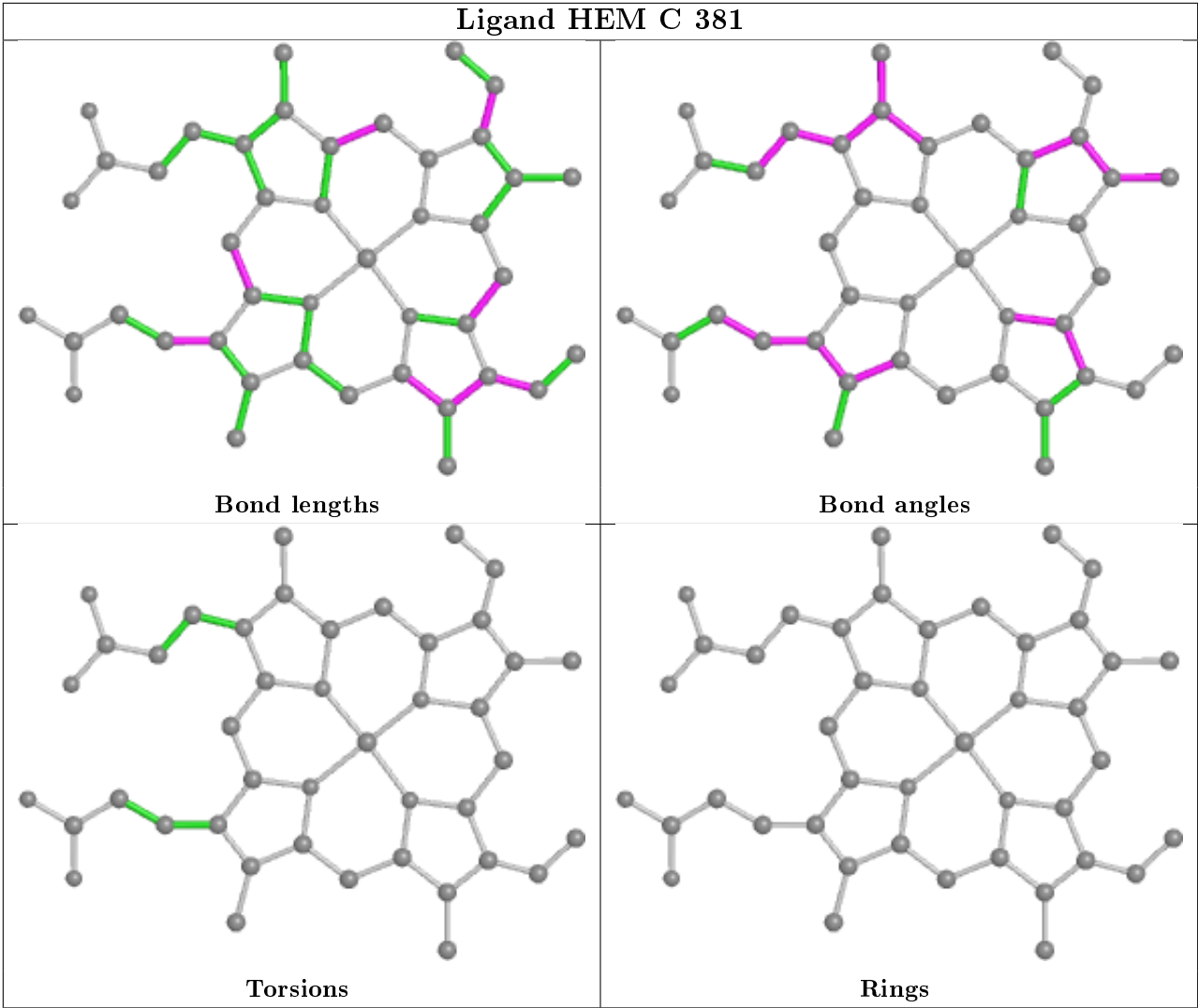


Ligand U10 C 383



Ligand HEM C 382





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	33.76

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

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, 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	442/446 (99%)	-0.60	0 100 100	12, 58, 89, 100	0
2	B	406/422 (96%)	-0.53	2 (0%) 91 88	36, 71, 100, 100	0
3	C	379/380 (99%)	-0.74	0 100 100	4, 32, 71, 91	0
4	D	241/241 (100%)	-0.66	0 100 100	10, 41, 77, 100	0
5	E	196/196 (100%)	-0.25	4 (2%) 65 60	17, 76, 100, 100	0
6	F	100/109 (91%)	-0.68	0 100 100	18, 42, 74, 99	0
7	G	78/81 (96%)	-0.62	0 100 100	26, 54, 89, 100	0
8	H	66/78 (84%)	-0.62	0 100 100	27, 67, 86, 88	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	-0.69	1 (1%) 70 64	37, 53, 86, 100	0
All	All	1967/2048 (96%)	-0.59	7 (0%) 92 90	4, 55, 98, 100	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	PRO	4.1
5	E	185	TYR	3.7
10	J	61	ASN	3.2
2	B	225	ASN	2.6
5	E	191	ASP	2.3

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 ⓘ

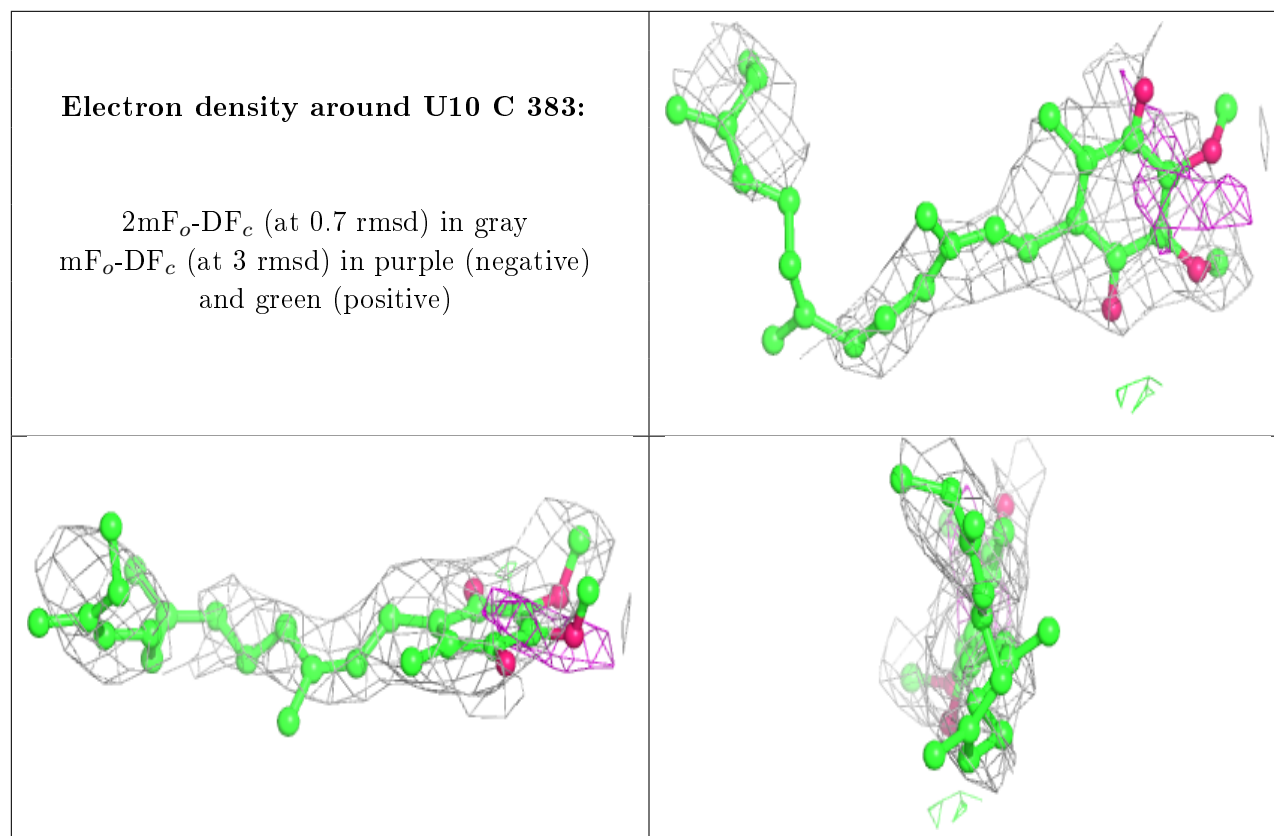
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

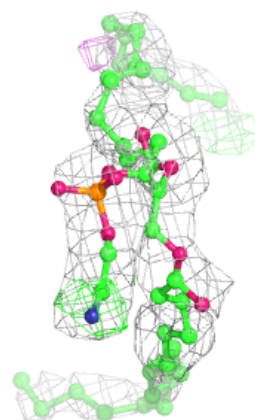
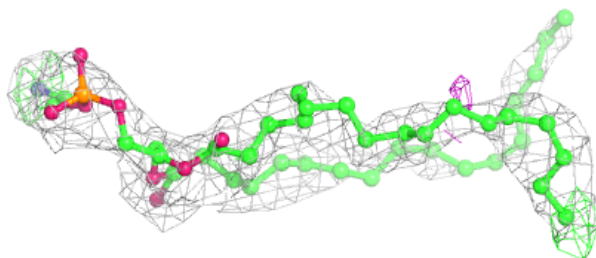
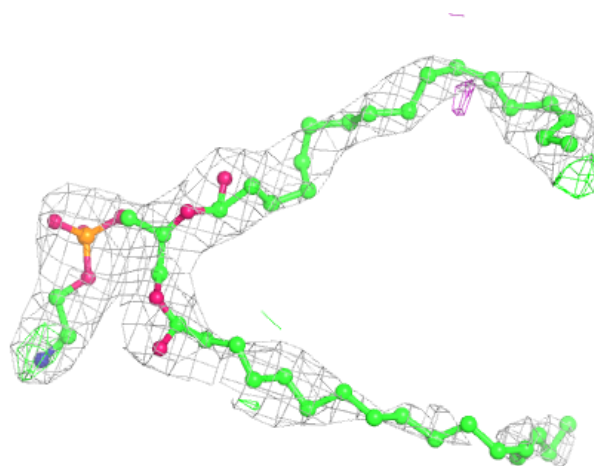
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	U10	C	383	29/63	0.72	0.48	72,88,100,100	0
13	PEE	E	198	49/51	0.81	0.36	43,80,98,100	0
13	PEE	C	384	49/51	0.88	0.42	42,58,76,87	0
15	BOG	D	242	20/20	0.88	0.23	35,68,81,81	0
14	SIG	C	385	35/35	0.95	0.20	2,17,26,29	0
11	HEM	D	243	43/43	0.97	0.16	10,21,32,35	0
11	HEM	C	382	43/43	0.97	0.20	8,20,32,41	0
11	HEM	C	381	43/43	0.97	0.20	6,24,32,43	0
16	FES	E	197	4/4	0.98	0.11	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.



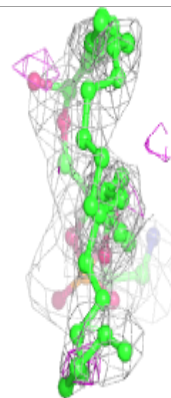
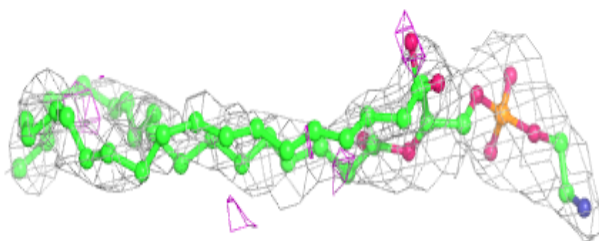
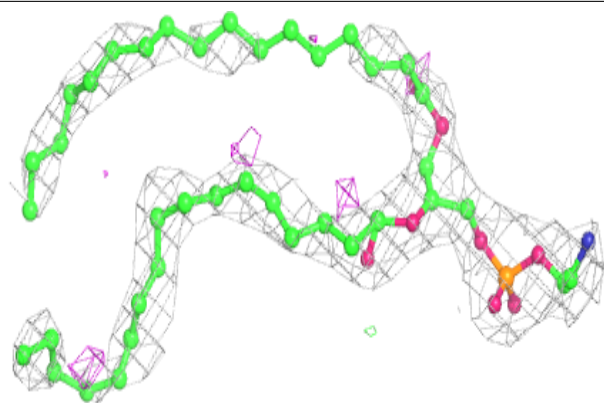
Electron density around PEE E 198:

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

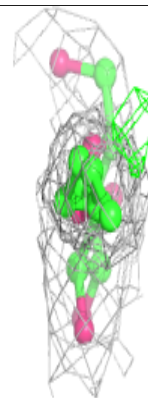
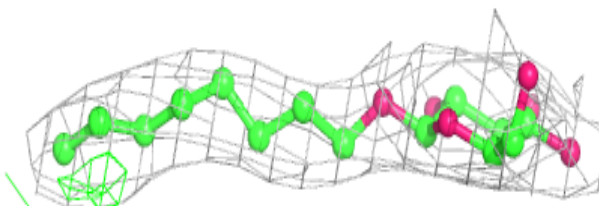
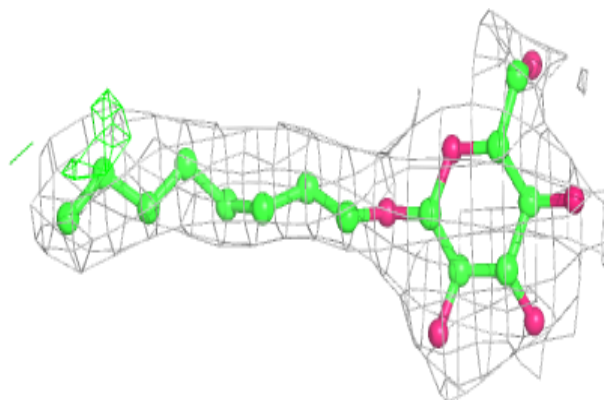


Electron density around PEE C 384:

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

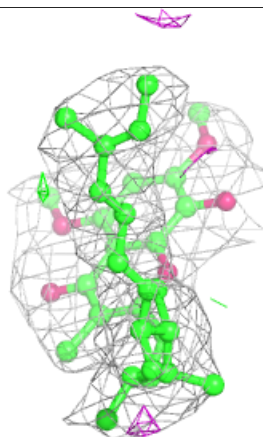
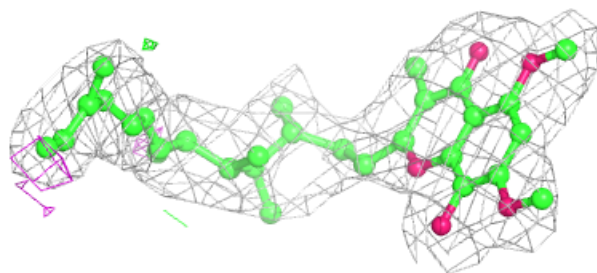
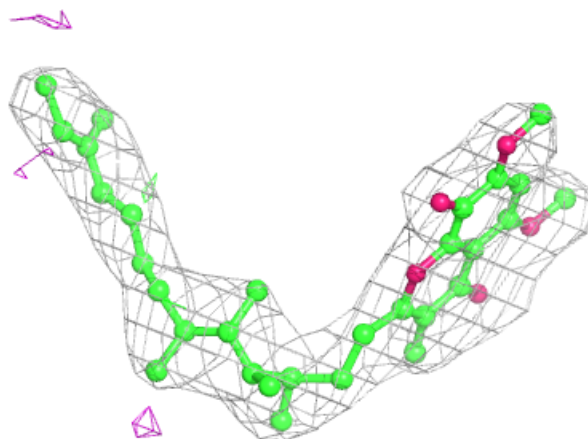
**Electron density around BOG D 242:**

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



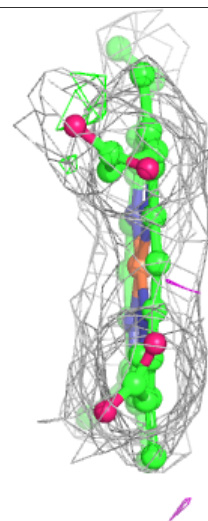
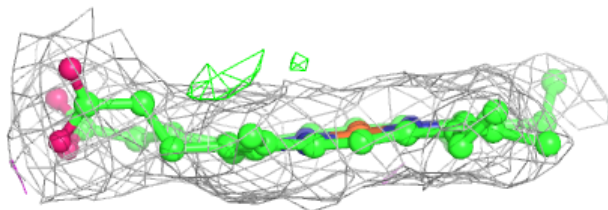
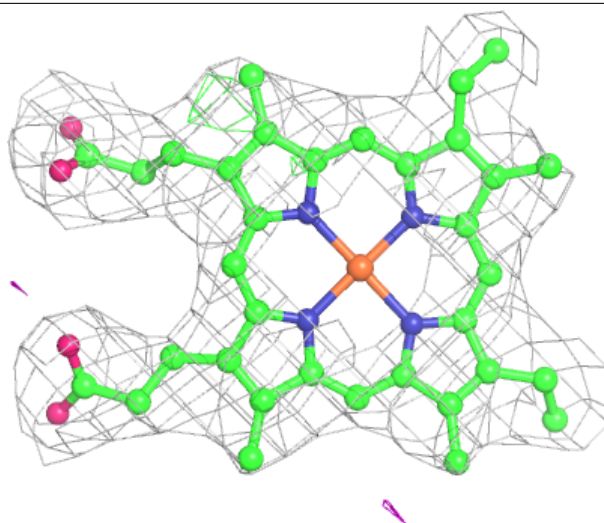
Electron density around SIG C 385:

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



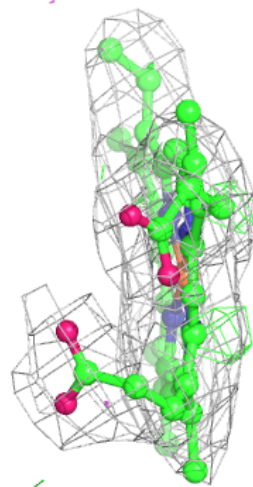
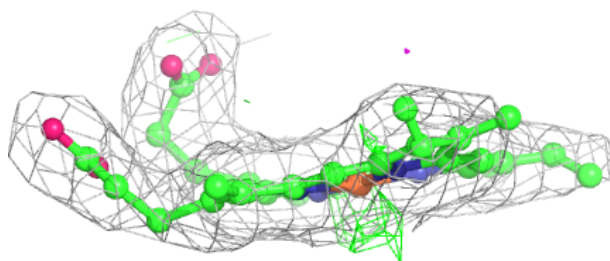
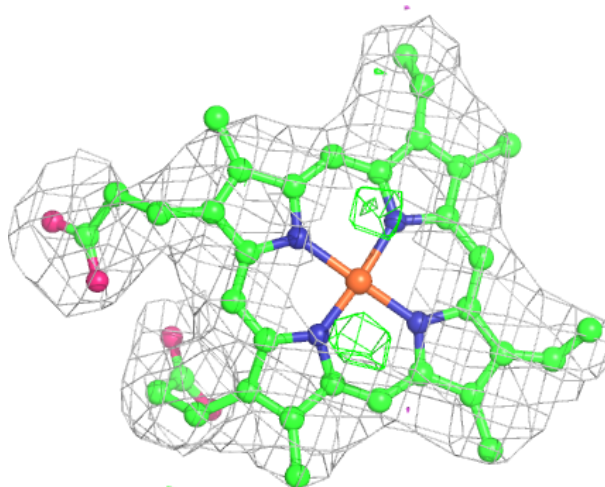
Electron density around HEM D 243:

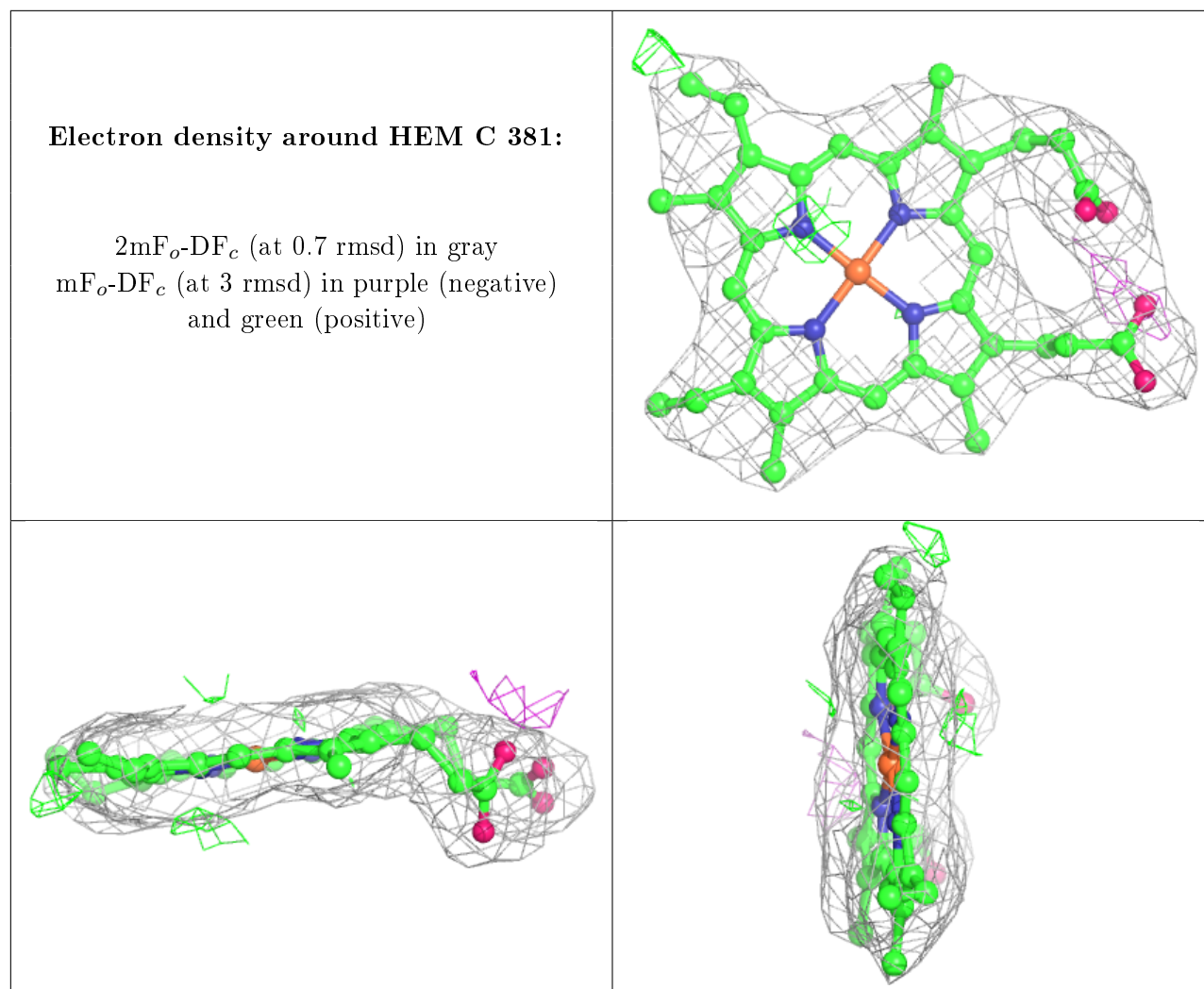
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 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.