Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 07:56 PM EDT

PDB ID	:	7TAY
Title	:	Bos Taurus Mitochondrial BC1 in complex with Pyramoxadone
Authors	:	Xia, D.; Zhou, F.; Esser, L.
Deposited on	:	2021-12-21
Resolution	:	2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

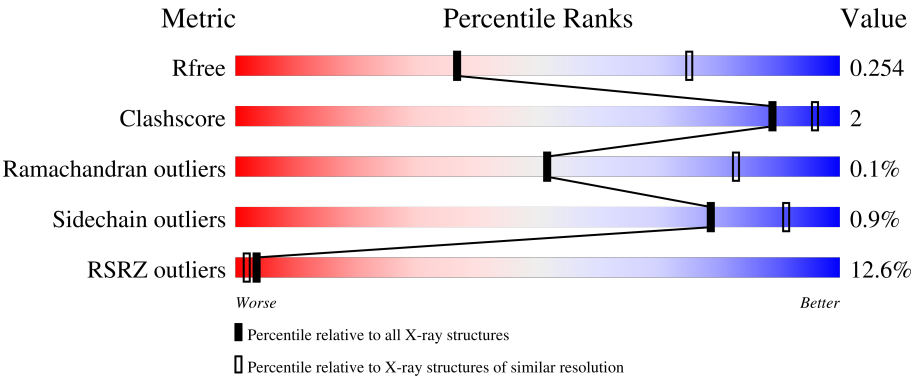
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	4% 96%
2	B	439	2% 94%
3	C	379	4% 92% 8%
4	D	241	17% 95% 5%
5	E	196	35% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	110	12% 93% 5%
7	G	80	9% 85% 9% 6%
8	H	78	36% 79% 6% 14%
9	I	78	18% 38% 5% 56%
10	J	63	38% 79% 17%
11	K	56	38% 75% 11% 12%

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	CDL	C	1006	-	-	-	X
13	CDL	D	1002	-	-	-	X
21	PX4	J	101	-	-	-	X

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 33549 atoms, of which 16706 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	446	6799	2161	3341	609	668	20	0	0	0

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	425	6328	1998	3147	564	612	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	377	6042	2009	3046	470	499	18	0	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	241	3778	1225	1859	330	349	15	0	0	0

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	196	3015	957	1497	263	290	8	0	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	105	1816	576	905	166	167	2	0	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0	0
			1261	410	633	118	99	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	67	Total	C	H	N	O	S	0	0	0
			1075	332	527	99	112	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	I	34	Total	C	H	N	O	S	0	0	0
			509	149	265	51	43	1			

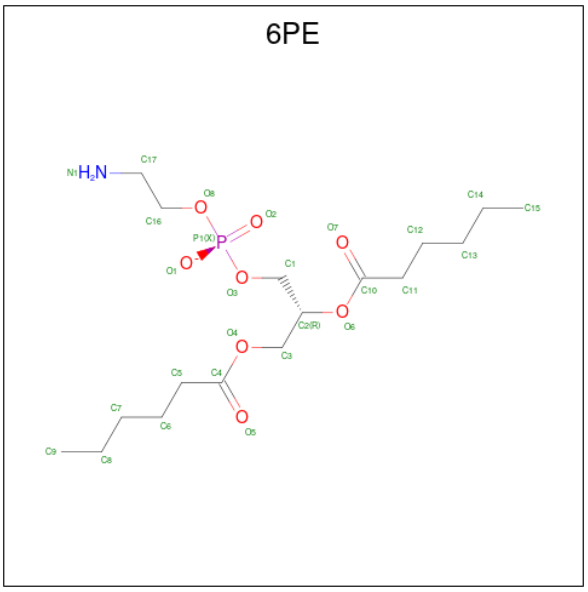
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	61	Total	C	H	N	O	0	0	0
			1004	329	502	87	86			

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

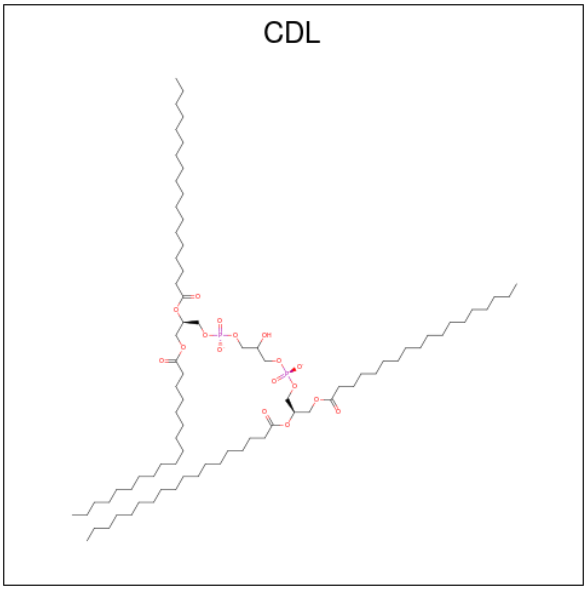
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	H	N	O	0	0	0
			801	267	400	72	62			

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: $C_{17}H_{33}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	A	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		
12	K	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



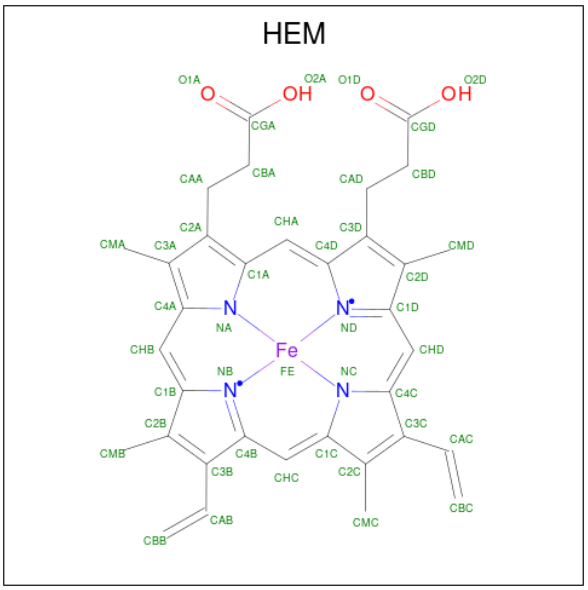
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	O	P	0	0
			124	41	64	17	2		
13	C	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

Continued on next page...

Continued from previous page...

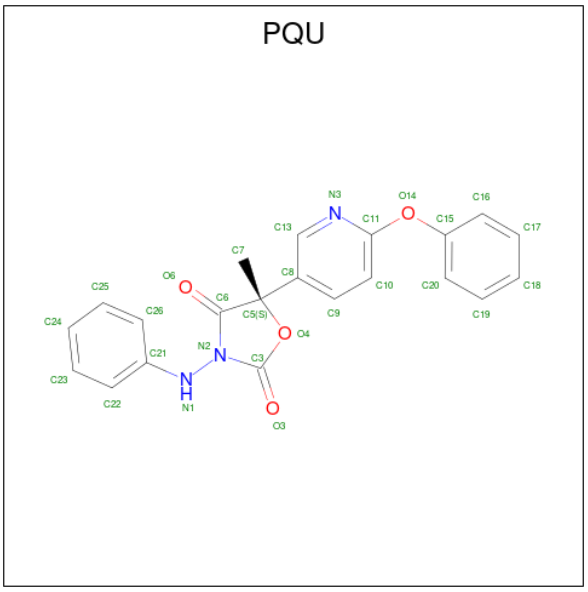
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



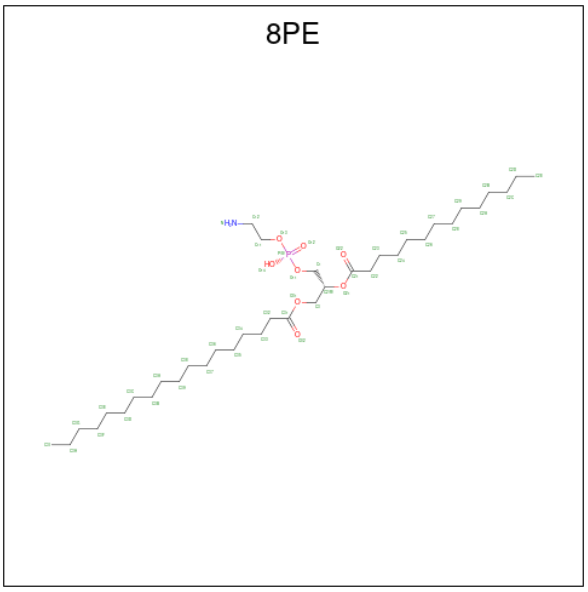
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
14	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 15 is (5S)-3-anilino-5-methyl-5-(6-phenoxypyridin-3-yl)-1,3-oxazolidine-2,4-dione (three-letter code: PQU) (formula: $C_{21}H_{17}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



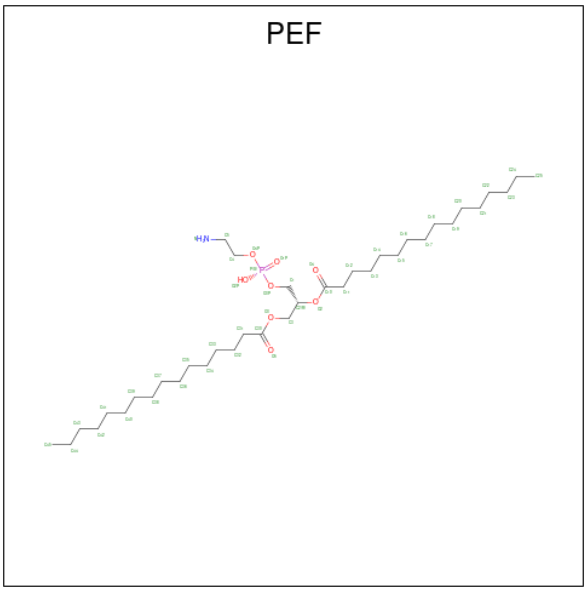
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	H	N	O	0	0
			45	21	17	3	4		

- Molecule 16 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	C	1	Total	C	H	N	O	P	0	0
			120	37	73	1	8	1		

- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).

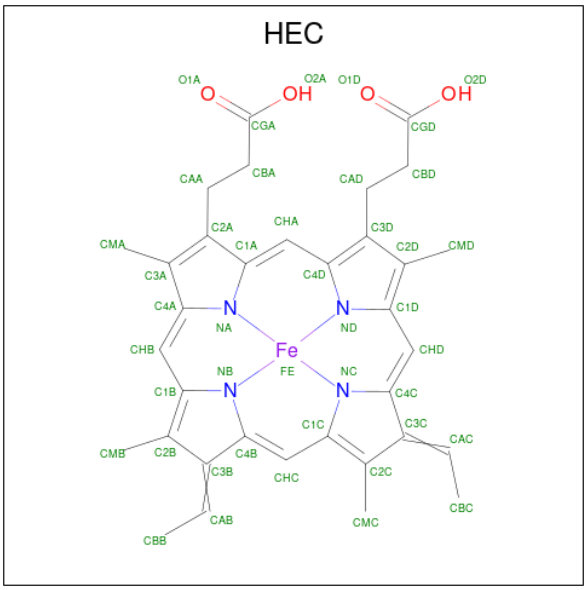


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
17	C	1	Total	C	H	N	O	P	0	0
			119	37	72	1	8	1		

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

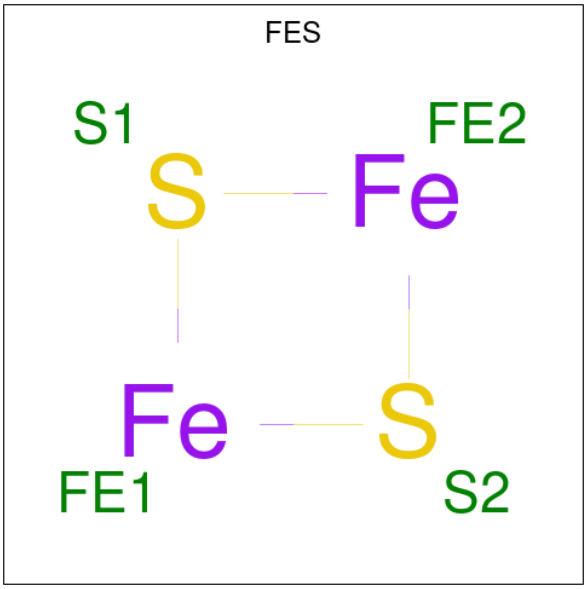
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	1	Total	Cl	0	0
			1	1		

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



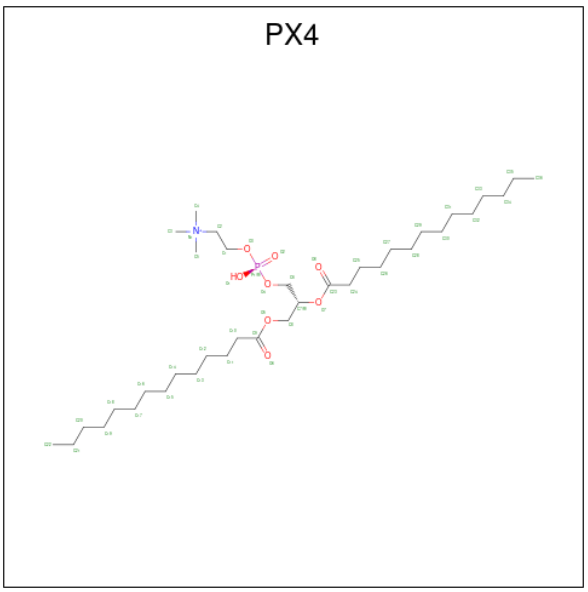
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	D	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
21	J	1	Total	C	H	N	O	P	0	0
			118	36	72	1	8	1		

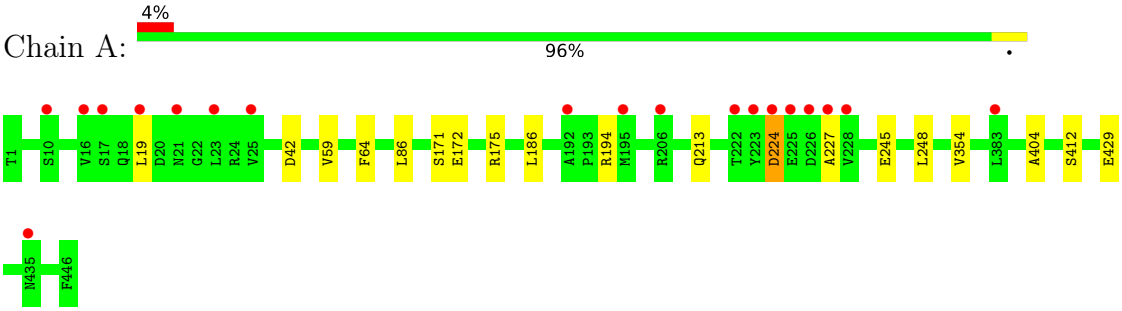
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	C	1	Total	O	0	0
			1	1		

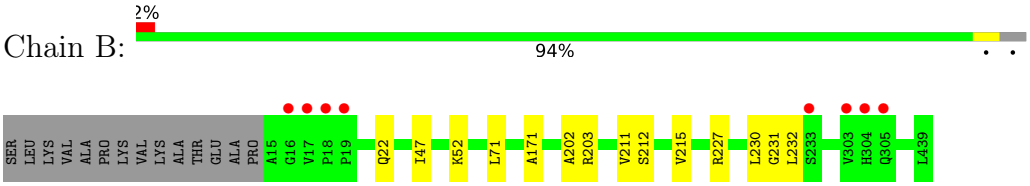
3 Residue-property plots (i)

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.

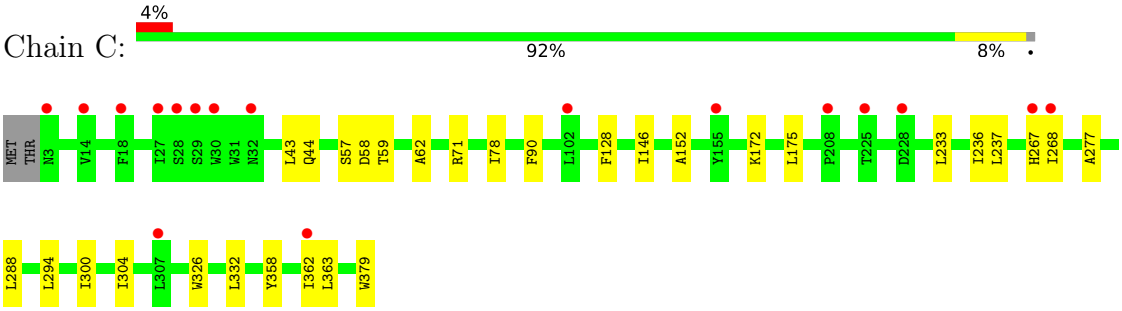
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



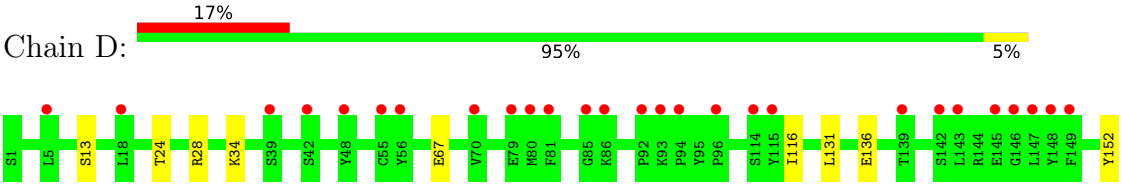
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

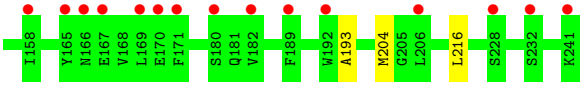


• Molecule 3: Cytochrome b



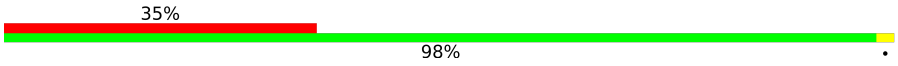
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

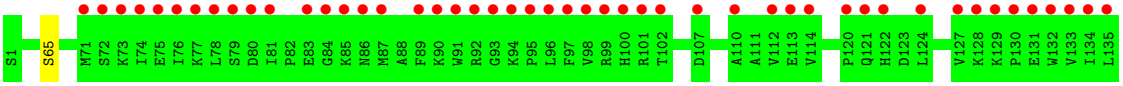


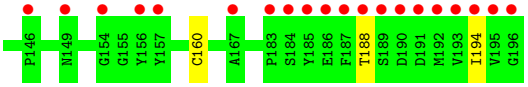


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:

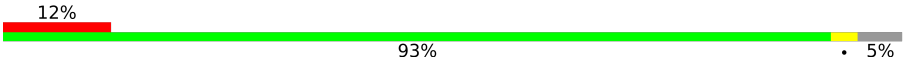


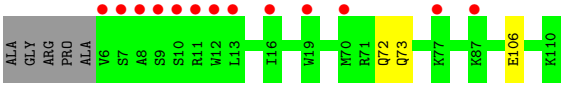




• Molecule 6: Cytochrome b-c1 complex subunit 7

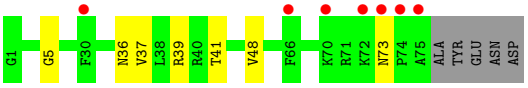
Chain F:





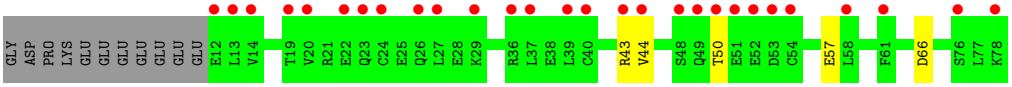
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:



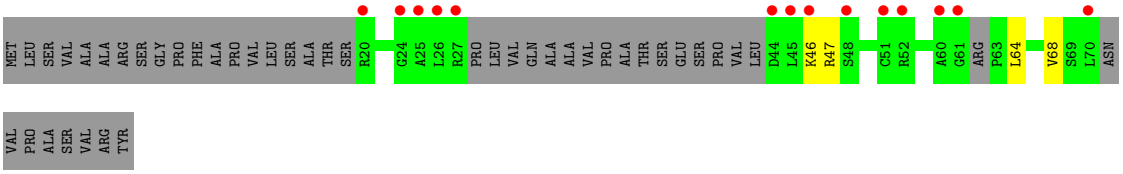
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



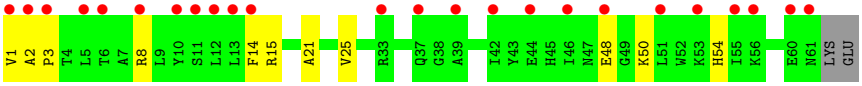
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:

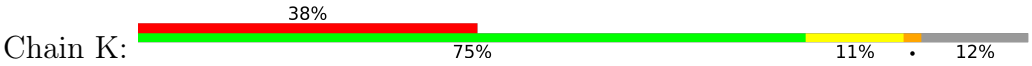


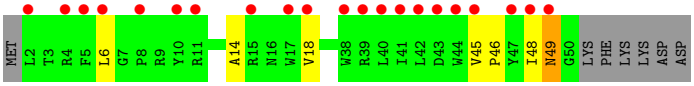
• Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:



• Molecule 11: Cytochrome b-c1 complex subunit 10





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.39Å 153.39Å 590.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.58 – 2.95 41.58 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.58-2.95) 93.2 (41.58-2.93)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.20_4444	Depositor
R, R_{free}	0.227 , 0.258 0.226 , 0.254	Depositor DCC
R_{free} test set	1994 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33549	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: CDL, 6PE, PQU, FES, HEM, 8PE, CL, HEC, PX4, PEF

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	0.32	0/3531	0.58	0/4792
2	B	0.38	0/3241	0.61	0/4398
3	C	0.32	0/3093	0.55	0/4232
4	D	0.31	0/1978	0.59	0/2684
5	E	0.28	0/1552	0.52	0/2100
6	F	0.35	0/930	0.59	0/1246
7	G	0.34	0/649	0.62	0/878
8	H	0.30	0/553	0.64	0/741
9	I	0.37	0/242	0.82	0/319
10	J	0.32	0/515	0.62	0/696
11	K	0.30	0/416	0.64	0/573
All	All	0.33	0/16700	0.59	0/22659

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3458	3341	3356	12	0
2	B	3181	3147	3160	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2996	3046	3058	18	0
4	D	1919	1859	1868	10	0
5	E	1518	1497	1503	2	0
6	F	911	905	906	2	0
7	G	628	633	636	5	0
8	H	548	527	530	3	0
9	I	244	265	265	1	0
10	J	502	502	505	9	0
11	K	401	400	400	4	0
12	A	27	33	33	0	0
12	K	27	33	33	0	0
13	A	60	64	64	0	0
13	C	60	64	64	0	0
13	D	60	64	64	0	0
14	C	86	60	60	2	0
15	C	28	17	0	1	0
16	C	47	73	73	0	0
17	C	47	72	73	1	0
18	C	1	0	0	0	0
19	D	43	32	30	4	0
20	E	4	0	0	0	0
21	J	46	72	72	3	0
22	C	1	0	0	0	0
All	All	16843	16706	16753	64	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 2.

All (64) 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)
19:D:1001:HEC:HBC3	19:D:1001:HEC:HMC1	1.67	0.75
11:K:45:VAL:O	11:K:49:ASN:ND2	2.26	0.69
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.25	0.65
4:D:131:LEU:HD11	19:D:1001:HEC:HMB2	1.79	0.64
1:A:171:SER:OG	1:A:175:ARG:NH1	2.31	0.63
3:C:59:THR:OG1	3:C:172:LYS:NZ	2.29	0.63
8:H:43:ARG:NH2	8:H:57:GLU:OE2	2.31	0.63
2:B:47:ILE:HD11	2:B:211:VAL:HG21	1.80	0.62
1:A:42:ASP:O	1:A:194:ARG:NH2	2.34	0.59
4:D:13:SER:O	10:J:50:LYS:NZ	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:332:LEU:HD21	3:C:358:TYR:CE1	2.38	0.59
10:J:48:GLU:O	10:J:54:HIS:ND1	2.36	0.58
6:F:72:GLN:O	7:G:39:ARG:NH2	2.36	0.58
10:J:25:VAL:HG22	21:J:101:PX4:H34	1.89	0.54
2:B:202:ALA:O	2:B:232:LEU:HD21	2.08	0.54
3:C:57:SER:O	3:C:175:LEU:HD12	2.08	0.53
3:C:152:ALA:O	3:C:288:LEU:HD13	2.08	0.53
3:C:237:LEU:HD22	4:D:216:LEU:HD11	1.89	0.53
14:C:1001:HEM:HMC1	14:C:1001:HEM:HBC2	1.89	0.53
19:D:1001:HEC:HBB3	19:D:1001:HEC:HMB1	1.90	0.53
3:C:71:ARG:NH2	4:D:193:ALA:O	2.41	0.52
10:J:1:VAL:HG13	10:J:8:ARG:NH2	2.25	0.52
1:A:172:GLU:N	1:A:172:GLU:OE1	2.43	0.51
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.42	0.50
8:H:44:VAL:HG13	8:H:50:THR:HG21	1.93	0.50
1:A:59:VAL:HG11	1:A:186:LEU:HD21	1.94	0.48
3:C:304:ILE:HD11	3:C:362:ILE:HG23	1.95	0.48
1:A:224:ASP:HB2	1:A:227:ALA:HB3	1.94	0.48
4:D:152:TYR:OH	8:H:66:ASP:OD2	2.23	0.48
10:J:14:PHE:O	21:J:101:PX4:H8	2.13	0.48
7:G:37:VAL:O	7:G:41:THR:HG23	2.14	0.47
1:A:19:LEU:HD22	1:A:213:GLN:HG2	1.97	0.47
10:J:2:ALA:HB3	10:J:3:PRO:HD3	1.96	0.47
1:A:224:ASP:CB	1:A:227:ALA:HB3	2.44	0.47
5:E:188:THR:HG21	5:E:194:ILE:HD12	1.96	0.47
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.95	0.47
1:A:429:GLU:OE1	7:G:5:GLY:N	2.45	0.46
3:C:233:LEU:HD23	4:D:216:LEU:HD23	1.98	0.46
4:D:116:ILE:HG12	19:D:1001:HEC:HMA3	1.97	0.46
3:C:59:THR:HG1	3:C:172:LYS:HZ3	1.60	0.46
6:F:73:GLN:NE2	7:G:36:ASN:OD1	2.49	0.46
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.98	0.45
11:K:45:VAL:HG11	11:K:48:ILE:HD12	1.98	0.45
2:B:212:SER:OG	2:B:215:VAL:HG23	2.17	0.45
3:C:268:ILE:HD12	5:E:160:CYS:SG	2.56	0.45
14:C:1002:HEM:HBC2	14:C:1002:HEM:HMC2	1.99	0.44
4:D:24:THR:HG22	4:D:28:ARG:NH1	2.32	0.44
11:K:14:ALA:O	11:K:18:VAL:HG23	2.16	0.44
1:A:245:GLU:HG3	1:A:248:LEU:HG	1.99	0.44
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.99	0.44
10:J:21:ALA:O	10:J:25:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.33	0.44
1:A:412:SER:O	10:J:15:ARG:NH2	2.51	0.43
3:C:78:ILE:HD12	4:D:204:MET:CE	2.48	0.43
11:K:45:VAL:HG11	11:K:48:ILE:CD1	2.49	0.43
10:J:1:VAL:HG12	10:J:1:VAL:O	2.19	0.43
17:C:1005:PEF:H122	17:C:1005:PEF:H311	2.01	0.42
1:A:64:PHE:CD1	1:A:86:LEU:HD21	2.54	0.42
2:B:52:LYS:O	2:B:203:ARG:NH2	2.50	0.42
3:C:146:ILE:HD11	15:C:1003:PQU:C26	2.50	0.42
2:B:203:ARG:NH1	2:B:231:GLY:O	2.54	0.41
3:C:58:ASP:O	3:C:62:ALA:N	2.54	0.41
3:C:43:LEU:HD23	3:C:44:GLN:OE1	2.20	0.41
3:C:236:ILE:HD11	21:J:101:PX4:H71	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	438 (99%)	6 (1%)	0	100	100
2	B	423/439 (96%)	419 (99%)	3 (1%)	1 (0%)	47	79
3	C	375/379 (99%)	369 (98%)	6 (2%)	0	100	100
4	D	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
6	F	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
7	G	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
8	H	65/78 (83%)	65 (100%)	0	0	100	100
9	I	28/78 (36%)	24 (86%)	4 (14%)	0	100	100
10	J	59/63 (94%)	58 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	47/56 (84%)	44 (94%)	1 (2%)	2 (4%)	2 12
All	All	2050/2166 (95%)	2012 (98%)	35 (2%)	3 (0%)	51 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	49	ASN
11	K	46	PRO
2	B	171	ALA

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	370/370 (100%)	369 (100%)	1 (0%)	92 97
2	B	332/343 (97%)	329 (99%)	3 (1%)	78 91
3	C	325/327 (99%)	321 (99%)	4 (1%)	71 88
4	D	206/206 (100%)	205 (100%)	1 (0%)	88 95
5	E	168/168 (100%)	167 (99%)	1 (1%)	86 94
6	F	96/98 (98%)	95 (99%)	1 (1%)	76 90
7	G	66/70 (94%)	65 (98%)	1 (2%)	65 85
8	H	64/74 (86%)	64 (100%)	0	100 100
9	I	25/60 (42%)	22 (88%)	3 (12%)	5 19
10	J	51/53 (96%)	51 (100%)	0	100 100
11	K	39/46 (85%)	38 (97%)	1 (3%)	46 75
All	All	1742/1815 (96%)	1726 (99%)	16 (1%)	78 91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	22	GLN
2	B	227	ARG
2	B	230	LEU
3	C	90	PHE
3	C	128	PHE
3	C	267	HIS
3	C	379	TRP
4	D	136	GLU
5	E	65	SER
6	F	106	GLU
7	G	73	ASN
9	I	46	LYS
9	I	47	ARG
9	I	64	LEU
11	K	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	104	ASN
2	B	158	HIS
2	B	162	ASN
2	B	276	GLN
2	B	342	ASN
3	C	267	HIS
6	F	73	GLN
7	G	36	ASN
11	K	12	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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	CDL	D	1002	-	59,59,99	0.49	0	65,71,111	0.70	2 (3%)
15	PQU	C	1003	-	29,31,31	0.77	0	33,44,44	1.37	3 (9%)
19	HEC	D	1001	4	32,50,50	2.12	4 (12%)	24,82,82	1.42	2 (8%)
14	HEM	C	1002	3	41,50,50	1.47	6 (14%)	45,82,82	1.35	8 (17%)
13	CDL	A	502	-	59,59,99	0.38	0	65,71,111	0.64	1 (1%)
16	8PE	C	1004	-	46,46,46	0.94	2 (4%)	49,51,51	0.89	1 (2%)
14	HEM	C	1001	3	41,50,50	1.51	6 (14%)	45,82,82	1.46	6 (13%)
17	PEF	C	1005	-	46,46,46	0.91	3 (6%)	49,51,51	0.96	3 (6%)
12	6PE	A	501	-	26,26,26	0.87	0	29,31,31	0.96	2 (6%)
12	6PE	K	101	-	26,26,26	1.00	2 (7%)	29,31,31	0.89	1 (3%)
21	PX4	J	101	-	45,45,45	1.28	4 (8%)	51,53,53	0.98	2 (3%)
13	CDL	C	1006	-	59,59,99	0.39	0	65,71,111	0.66	1 (1%)
20	FES	E	1001	5	0,4,4	-	-	-		

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	CDL	D	1002	-	-	28/70/70/110	-
15	PQU	C	1003	-	-	4/14/33/33	0/4/4/4
19	HEC	D	1001	4	-	3/10/54/54	-
14	HEM	C	1002	3	-	4/12/54/54	-
13	CDL	A	502	-	-	29/70/70/110	-
16	8PE	C	1004	-	-	20/50/50/50	-
14	HEM	C	1001	3	-	3/12/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PEF	C	1005	-	-	19/50/50/50	-
12	6PE	A	501	-	-	14/30/30/30	-
12	6PE	K	101	-	-	15/30/30/30	-
21	PX4	J	101	-	-	18/49/49/49	-
13	CDL	C	1006	-	-	38/70/70/110	-
20	FES	E	1001	5	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	1001	HEC	C3C-C2C	-6.09	1.34	1.40
19	D	1001	HEC	C3D-C2D	5.51	1.54	1.37
19	D	1001	HEC	C2B-C3B	-5.35	1.35	1.40
14	C	1002	HEM	C3C-C2C	-4.21	1.34	1.40
14	C	1001	HEM	C3C-CAC	4.07	1.56	1.47
14	C	1002	HEM	C3C-CAC	3.62	1.55	1.47
14	C	1001	HEM	C3C-C2C	-3.54	1.35	1.40
16	C	1004	8PE	P-O11	3.51	1.73	1.59
17	C	1005	PEF	P-O3P	3.15	1.72	1.59
21	J	101	PX4	O7-C23	3.13	1.43	1.34
21	J	101	PX4	O5-C9	3.11	1.42	1.33
14	C	1002	HEM	CAB-C3B	3.09	1.55	1.47
14	C	1001	HEM	CAB-C3B	2.95	1.55	1.47
16	C	1004	8PE	P-O13	2.73	1.70	1.59
12	K	101	6PE	P1-O3	2.57	1.69	1.59
17	C	1005	PEF	P-O4P	2.48	1.69	1.59
21	J	101	PX4	O7-C7	-2.42	1.40	1.46
14	C	1001	HEM	FE-NB	2.41	2.08	1.96
17	C	1005	PEF	C3-C2	2.28	1.57	1.50
14	C	1002	HEM	CMB-C2B	2.27	1.55	1.50
21	J	101	PX4	P1-O4	2.15	1.68	1.59
14	C	1002	HEM	CMD-C2D	2.10	1.55	1.50
12	K	101	6PE	P1-O8	2.09	1.67	1.59
14	C	1001	HEM	CMB-C2B	2.05	1.55	1.50
19	D	1001	HEC	CAD-C3D	2.02	1.55	1.52
14	C	1001	HEM	CMD-C2D	2.01	1.55	1.50
14	C	1002	HEM	FE-NB	2.00	2.06	1.96

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	1003	PQU	C15-O14-C11	4.09	128.62	118.83
15	C	1003	PQU	C21-N1-N2	4.06	124.05	116.23
21	J	101	PX4	O7-C23-C24	3.67	119.42	111.50
19	D	1001	HEC	CMC-C2C-C1C	-3.33	123.34	128.46
14	C	1001	HEM	C4C-CHD-C1D	3.16	126.73	122.56
14	C	1001	HEM	CBA-CAA-C2A	-3.06	107.40	112.62
14	C	1002	HEM	C4B-CHC-C1C	3.03	126.56	122.56
14	C	1001	HEM	C4B-CHC-C1C	3.02	126.55	122.56
15	C	1003	PQU	C13-N3-C11	2.88	119.17	116.63
14	C	1001	HEM	C4D-ND-C1D	2.84	108.01	105.07
17	C	1005	PEF	O2P-P-O1P	2.78	125.97	112.24
14	C	1001	HEM	C1B-NB-C4B	2.75	107.92	105.07
16	C	1004	8PE	O14-P-O12	2.72	125.66	112.24
14	C	1002	HEM	C4D-ND-C1D	2.67	107.83	105.07
12	K	101	6PE	P1-O8-C16	-2.64	108.57	121.59
14	C	1002	HEM	C4C-CHD-C1D	2.63	126.03	122.56
13	D	1002	CDL	CB2-C1-CA2	-2.63	105.05	112.79
14	C	1002	HEM	CBD-CAD-C3D	-2.58	105.45	112.63
17	C	1005	PEF	P-O4P-C4	-2.53	109.13	121.59
13	C	1006	CDL	CB2-C1-CA2	-2.52	105.39	112.79
12	A	501	6PE	P1-O8-C16	-2.52	109.21	121.59
21	J	101	PX4	O5-C9-C10	2.49	119.72	111.91
14	C	1002	HEM	O2A-CGA-CBA	2.46	121.93	114.03
14	C	1002	HEM	CMC-C2C-C3C	2.42	129.22	124.68
14	C	1001	HEM	C3D-C4D-ND	-2.27	107.64	110.17
13	A	502	CDL	CB2-C1-CA2	-2.26	106.14	112.79
13	D	1002	CDL	OA6-CA4-CA3	-2.26	100.23	108.40
14	C	1002	HEM	C1B-NB-C4B	2.25	107.40	105.07
19	D	1001	HEC	CMB-C2B-C1B	-2.20	125.09	128.46
12	A	501	6PE	P1-O3-C1	-2.17	108.98	121.68
17	C	1005	PEF	O2-C10-C11	2.13	116.10	111.50
14	C	1002	HEM	O1A-CGA-CBA	-2.06	116.45	123.08

There are no chirality outliers.

All (195) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	501	6PE	C1-O3-P1-O2
12	A	501	6PE	C1-O3-P1-O8
12	A	501	6PE	O7-C10-O6-C2
12	A	501	6PE	C11-C10-O6-C2
12	A	501	6PE	O8-C16-C17-N1
12	K	101	6PE	C16-O8-P1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	K	101	6PE	O8-C16-C17-N1
13	A	502	CDL	CB2-C1-CA2-OA2
13	A	502	CDL	CA2-OA2-PA1-OA3
13	A	502	CDL	CA3-OA5-PA1-OA3
13	A	502	CDL	CA3-OA5-PA1-OA4
13	C	1006	CDL	CA3-OA5-PA1-OA4
13	D	1002	CDL	CA3-OA5-PA1-OA2
13	D	1002	CDL	CB3-OB5-PB2-OB3
13	D	1002	CDL	OB7-CB5-OB6-CB4
16	C	1004	8PE	C1-O11-P-O14
17	C	1005	PEF	O4P-C4-C5-N
17	C	1005	PEF	C11-C10-O2-C2
21	J	101	PX4	C1-O3-P1-O2
21	J	101	PX4	O3-C1-C2-N1
21	J	101	PX4	O4-C6-C7-O7
13	D	1002	CDL	C31-CA7-OA8-CA6
13	D	1002	CDL	OA9-CA7-OA8-CA6
13	D	1002	CDL	OB9-CB7-OB8-CB6
16	C	1004	8PE	O32-C31-O31-C3
17	C	1005	PEF	O4-C10-O2-C2
13	D	1002	CDL	C51-CB5-OB6-CB4
13	A	502	CDL	C31-CA7-OA8-CA6
13	D	1002	CDL	C71-CB7-OB8-CB6
16	C	1004	8PE	C32-C31-O31-C3
13	D	1002	CDL	O1-C1-CB2-OB2
13	C	1006	CDL	C71-CB7-OB8-CB6
13	D	1002	CDL	C11-CA5-OA6-CA4
21	J	101	PX4	C10-C9-O5-C8
13	A	502	CDL	OA9-CA7-OA8-CA6
13	C	1006	CDL	OB9-CB7-OB8-CB6
21	J	101	PX4	O6-C9-O5-C8
13	D	1002	CDL	OA7-CA5-OA6-CA4
17	C	1005	PEF	C31-C30-O3-C3
13	C	1006	CDL	OA5-CA3-CA4-OA6
13	A	502	CDL	CB5-C51-C52-C53
13	A	502	CDL	CB7-C71-C72-C73
17	C	1005	PEF	O5-C30-O3-C3
12	A	501	6PE	C10-C11-C12-C13
13	C	1006	CDL	CA7-C31-C32-C33
13	D	1002	CDL	CA5-C11-C12-C13
13	A	502	CDL	O1-C1-CA2-OA2
21	J	101	PX4	C24-C23-O7-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	K	101	6PE	C16-O8-P1-O3
13	A	502	CDL	CA2-OA2-PA1-OA5
13	A	502	CDL	CA3-OA5-PA1-OA2
13	A	502	CDL	CB3-OB5-PB2-OB2
13	C	1006	CDL	CA3-OA5-PA1-OA2
16	C	1004	8PE	C1-O11-P-O13
21	J	101	PX4	O8-C23-O7-C7
13	C	1006	CDL	C11-CA5-OA6-CA4
13	C	1006	CDL	OA7-CA5-OA6-CA4
13	C	1006	CDL	CB5-C51-C52-C53
13	D	1002	CDL	C11-C12-C13-C14
13	D	1002	CDL	C33-C34-C35-C36
13	D	1002	CDL	OB5-CB3-CB4-OB6
21	J	101	PX4	C28-C29-C30-C31
21	J	101	PX4	C18-C19-C20-C21
17	C	1005	PEF	C10-C11-C12-C13
21	J	101	PX4	C24-C25-C26-C27
13	D	1002	CDL	C72-C73-C74-C75
16	C	1004	8PE	O13-C11-C12-N
17	C	1005	PEF	C17-C18-C19-C20
12	K	101	6PE	C11-C10-O6-C2
13	A	502	CDL	C51-CB5-OB6-CB4
21	J	101	PX4	C9-C10-C11-C12
13	C	1006	CDL	O1-C1-CA2-OA2
13	D	1002	CDL	C51-C52-C53-C54
13	A	502	CDL	OB7-CB5-OB6-CB4
12	A	501	6PE	C5-C4-O4-C3
12	A	501	6PE	O5-C4-O4-C3
12	K	101	6PE	O7-C10-O6-C2
12	K	101	6PE	C5-C4-O4-C3
13	D	1002	CDL	CA7-C31-C32-C33
16	C	1004	8PE	C22-C21-O21-C2
21	J	101	PX4	C11-C12-C13-C14
16	C	1004	8PE	O22-C21-O21-C2
13	C	1006	CDL	CB2-OB2-PB2-OB5
21	J	101	PX4	O4-C6-C7-C8
13	C	1006	CDL	C72-C73-C74-C75
13	D	1002	CDL	C31-C32-C33-C34
16	C	1004	8PE	C3B-C3C-C3D-C3E
12	A	501	6PE	C1-C2-C3-O4
13	A	502	CDL	C73-C74-C75-C76
13	C	1006	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	1005	PEF	C33-C34-C35-C36
15	C	1003	PQU	C10-C11-O14-C15
13	C	1006	CDL	C34-C35-C36-C37
13	A	502	CDL	C71-C72-C73-C74
13	D	1002	CDL	CA6-CA4-OA6-CA5
13	D	1002	CDL	CB6-CB4-OB6-CB5
17	C	1005	PEF	C3-C2-O2-C10
12	K	101	6PE	O5-C4-O4-C3
12	A	501	6PE	O6-C2-C3-O4
17	C	1005	PEF	C35-C36-C37-C38
13	C	1006	CDL	C14-C15-C16-C17
13	D	1002	CDL	OB5-CB3-CB4-CB6
13	A	502	CDL	C54-C55-C56-C57
21	J	101	PX4	C27-C28-C29-C30
17	C	1005	PEF	C21-C22-C23-C24
14	C	1001	HEM	C3D-CAD-CBD-CGD
13	A	502	CDL	CA3-CA4-CA6-OA8
16	C	1004	8PE	C1-C2-C3-O31
12	K	101	6PE	C5-C6-C7-C8
13	A	502	CDL	C74-C75-C76-C77
21	J	101	PX4	C16-C17-C18-C19
16	C	1004	8PE	C11-O13-P-O11
13	C	1006	CDL	C32-C33-C34-C35
12	K	101	6PE	O6-C2-C3-O4
16	C	1004	8PE	C25-C26-C27-C28
12	A	501	6PE	C2-C1-O3-P1
13	C	1006	CDL	OB7-CB5-OB6-CB4
13	D	1002	CDL	C12-C13-C14-C15
12	K	101	6PE	C1-C2-C3-O4
17	C	1005	PEF	C1-C2-C3-O3
13	C	1006	CDL	C51-CB5-OB6-CB4
13	A	502	CDL	OB5-CB3-CB4-OB6
13	C	1006	CDL	OB6-CB4-CB6-OB8
16	C	1004	8PE	O21-C2-C3-O31
21	J	101	PX4	C30-C31-C32-C33
13	A	502	CDL	C14-C15-C16-C17
12	K	101	6PE	C16-O8-P1-O2
13	A	502	CDL	CA2-OA2-PA1-OA4
13	A	502	CDL	CB3-OB5-PB2-OB3
13	A	502	CDL	CB3-OB5-PB2-OB4
13	C	1006	CDL	CA3-OA5-PA1-OA3
16	C	1004	8PE	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	1006	CDL	OA5-CA3-CA4-CA6
17	C	1005	PEF	C15-C16-C17-C18
12	K	101	6PE	C4-C5-C6-C7
13	A	502	CDL	C13-C14-C15-C16
13	A	502	CDL	C34-C35-C36-C37
13	D	1002	CDL	C13-C14-C15-C16
16	C	1004	8PE	C24-C25-C26-C27
17	C	1005	PEF	C18-C19-C20-C21
15	C	1003	PQU	N3-C11-O14-C15
16	C	1004	8PE	C3D-C3E-C3F-C3G
17	C	1005	PEF	C20-C21-C22-C23
13	D	1002	CDL	CB3-OB5-PB2-OB2
13	D	1002	CDL	C74-C75-C76-C77
12	K	101	6PE	C2-C1-O3-P1
12	A	501	6PE	C4-C5-C6-C7
13	A	502	CDL	C51-C52-C53-C54
16	C	1004	8PE	C38-C39-C3A-C3B
17	C	1005	PEF	C38-C39-C40-C41
13	C	1006	CDL	C31-CA7-OA8-CA6
14	C	1002	HEM	CAA-CBA-CGA-O1A
13	C	1006	CDL	CA2-OA2-PA1-OA5
13	A	502	CDL	C32-C33-C34-C35
13	C	1006	CDL	C12-C13-C14-C15
13	A	502	CDL	OA6-CA4-CA6-OA8
13	C	1006	CDL	C73-C74-C75-C76
14	C	1002	HEM	CAA-CBA-CGA-O2A
13	C	1006	CDL	C74-C75-C76-C77
21	J	101	PX4	C26-C27-C28-C29
13	C	1006	CDL	OA9-CA7-OA8-CA6
13	D	1002	CDL	C73-C74-C75-C76
17	C	1005	PEF	C11-C12-C13-C14
14	C	1001	HEM	CAD-CBD-CGD-O1D
16	C	1004	8PE	C34-C35-C36-C37
14	C	1001	HEM	CAD-CBD-CGD-O2D
19	D	1001	HEC	CAA-CBA-CGA-O2A
16	C	1004	8PE	C23-C24-C25-C26
13	C	1006	CDL	C52-C51-CB5-OB6
12	A	501	6PE	C5-C6-C7-C8
12	K	101	6PE	O4-C4-C5-C6
16	C	1004	8PE	C28-C29-C2A-C2B
19	D	1001	HEC	CAA-CBA-CGA-O1A
19	D	1001	HEC	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	1006	CDL	C72-C71-CB7-OB8
13	C	1006	CDL	C32-C31-CA7-OA8
13	C	1006	CDL	C52-C51-CB5-OB7
12	K	101	6PE	O5-C4-C5-C6
13	C	1006	CDL	CA5-C11-C12-C13
17	C	1005	PEF	C37-C38-C39-C40
13	C	1006	CDL	C33-C34-C35-C36
13	C	1006	CDL	CA2-OA2-PA1-OA3
13	C	1006	CDL	CB2-OB2-PB2-OB3
13	D	1002	CDL	CA2-OA2-PA1-OA3
16	C	1004	8PE	C11-O13-P-O12
13	C	1006	CDL	C12-C11-CA5-OA6
15	C	1003	PQU	C6-C5-C8-C13
15	C	1003	PQU	C6-C5-C8-C9
12	A	501	6PE	O6-C10-C11-C12
17	C	1005	PEF	C31-C32-C33-C34
14	C	1002	HEM	CAD-CBD-CGD-O1D
14	C	1002	HEM	CAD-CBD-CGD-O2D
13	C	1006	CDL	C32-C31-CA7-OA9
13	C	1006	CDL	C72-C71-CB7-OB9
21	J	101	PX4	C13-C14-C15-C16

There are no ring outliers.

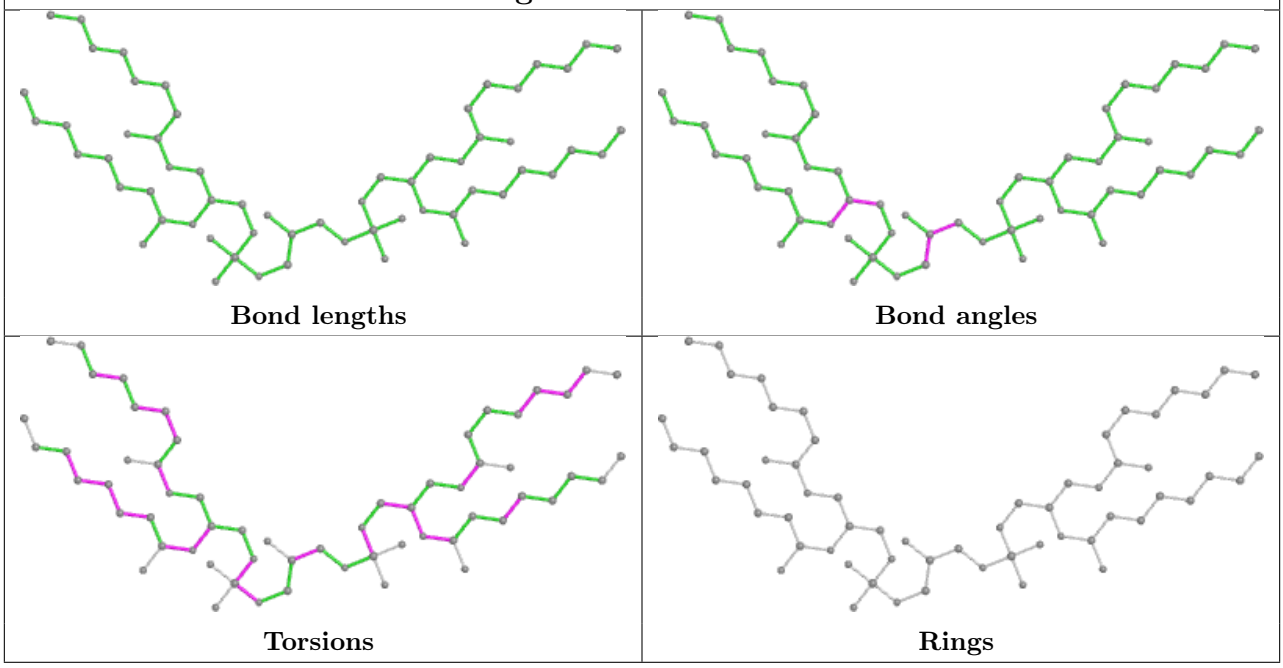
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1003	PQU	1	0
19	D	1001	HEC	4	0
14	C	1002	HEM	1	0
14	C	1001	HEM	1	0
17	C	1005	PEF	1	0
21	J	101	PX4	3	0

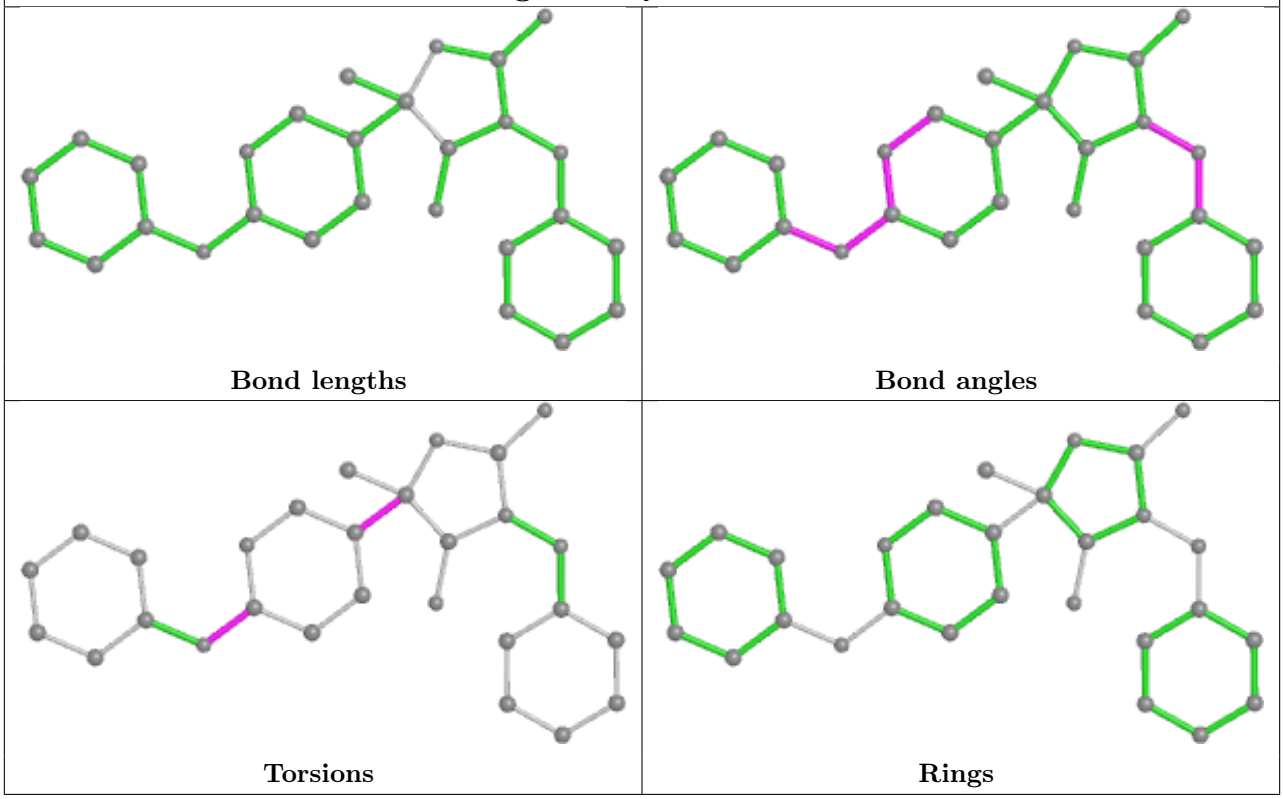
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

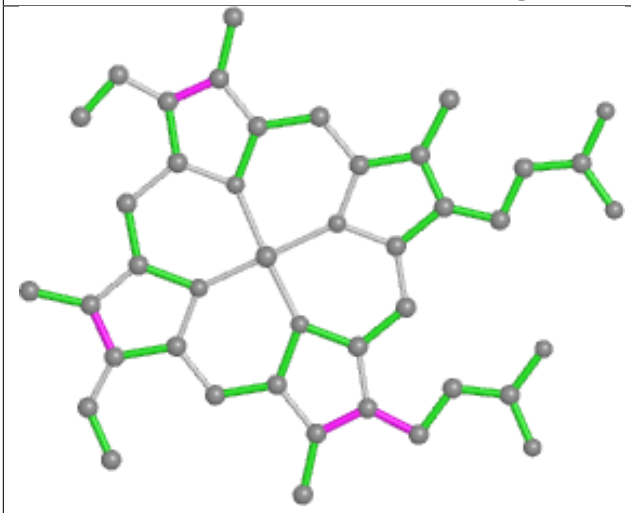
Ligand CDL D 1002



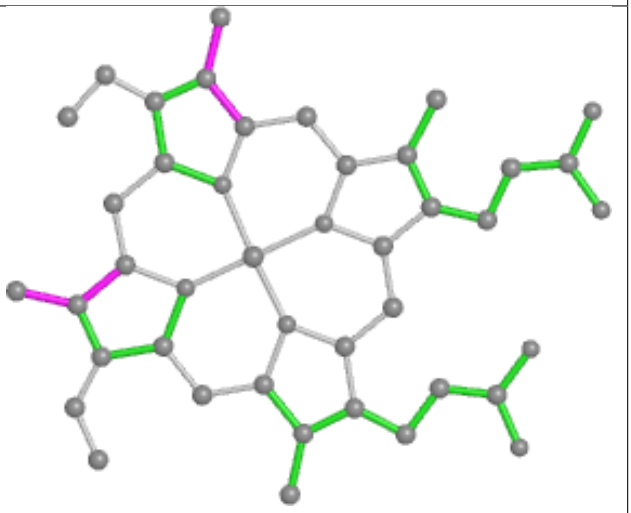
Ligand PQU C 1003



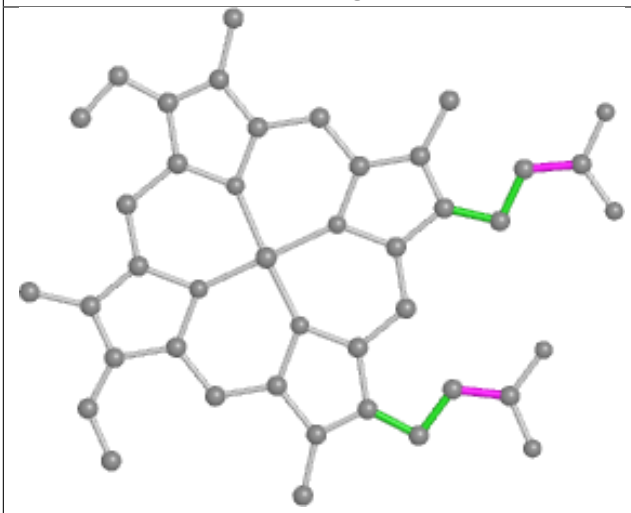
Ligand HEC D 1001



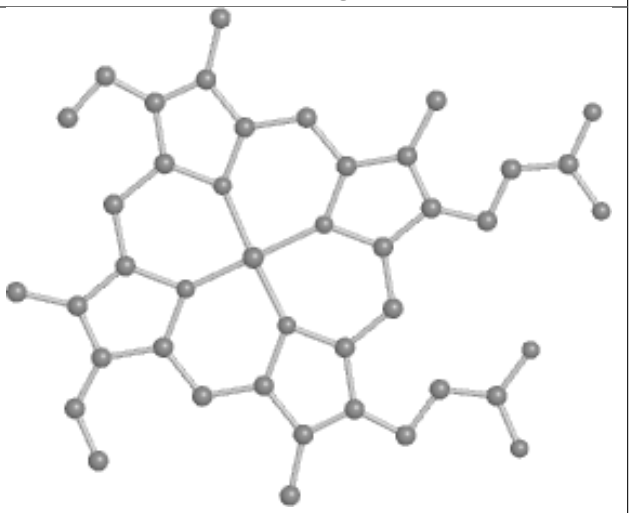
Bond lengths



Bond angles

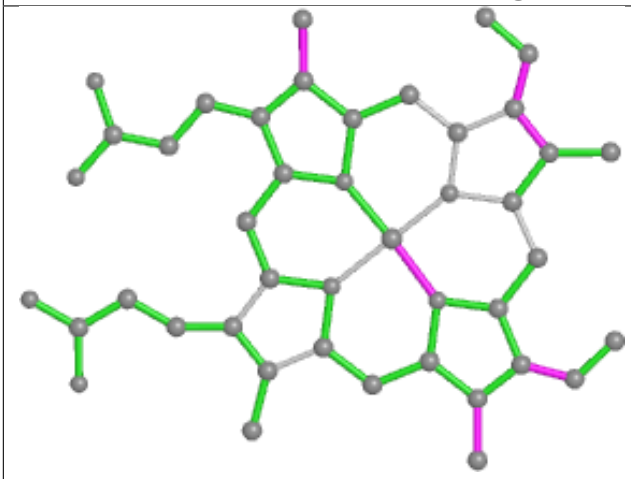


Torsions

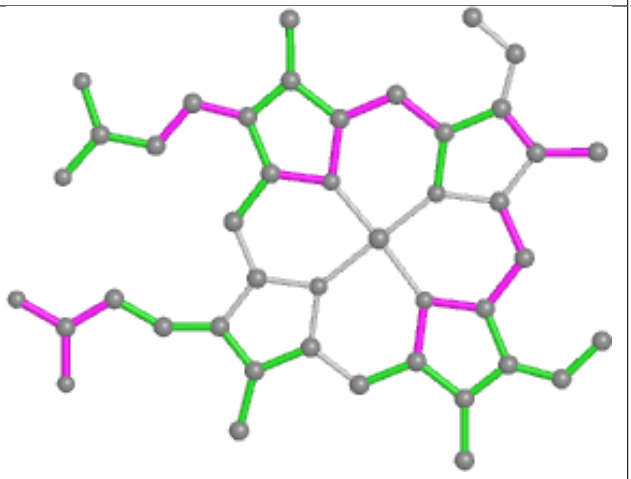


Rings

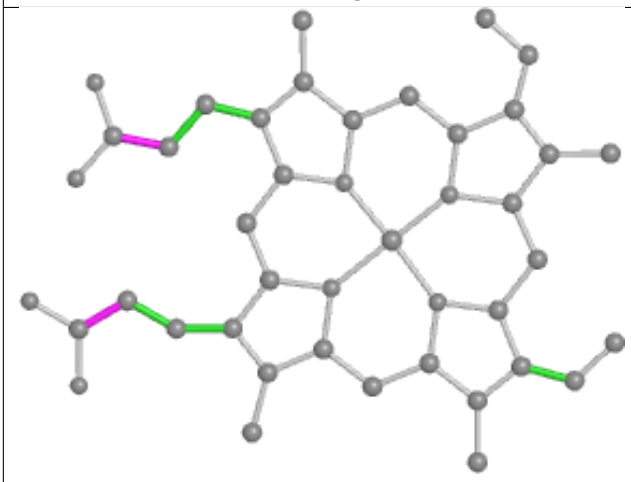
Ligand HEM C 1002



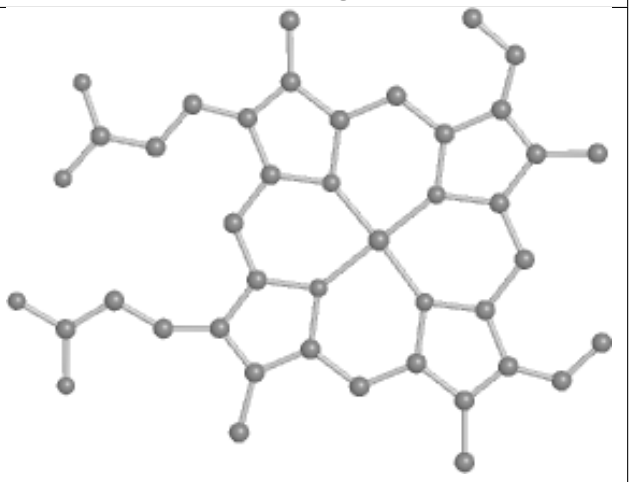
Bond lengths



Bond angles

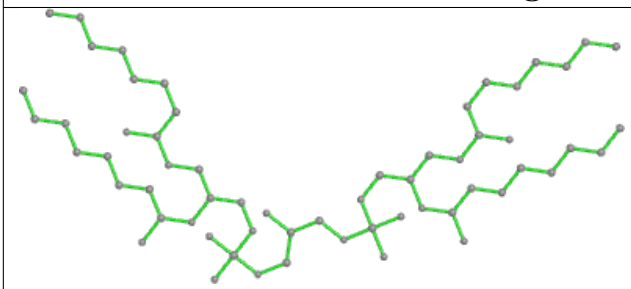


Torsions

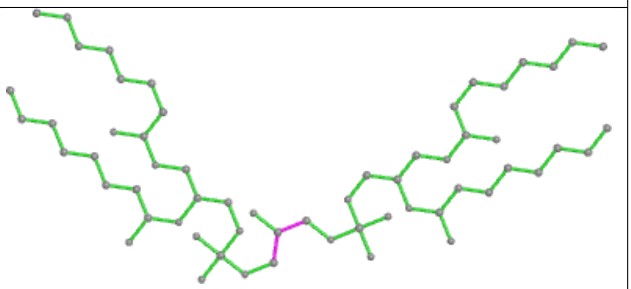


Rings

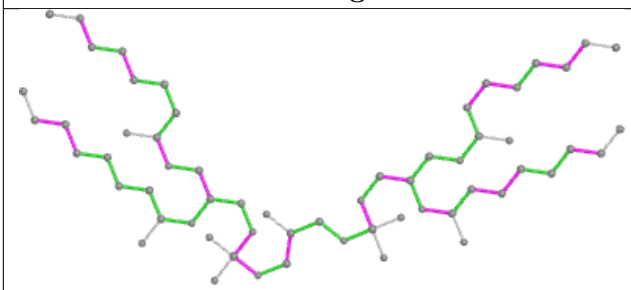
Ligand CDL A 502



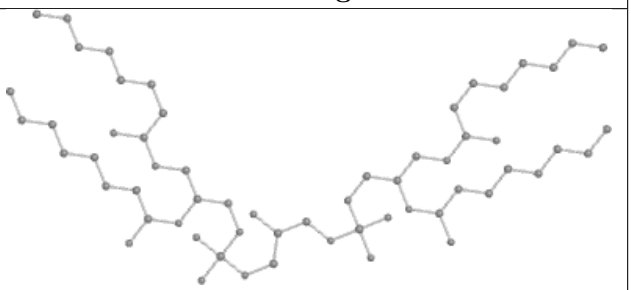
Bond lengths



Bond angles

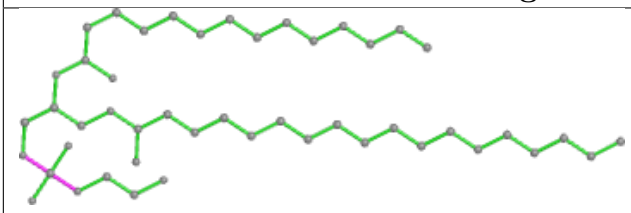


Torsions

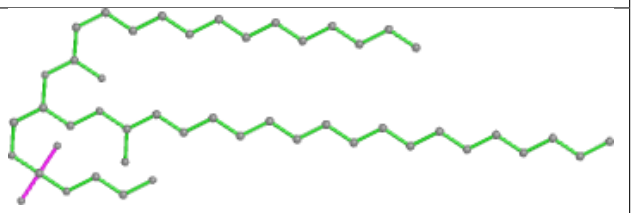


Rings

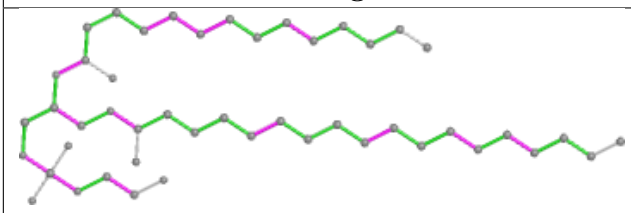
Ligand 8PE C 1004



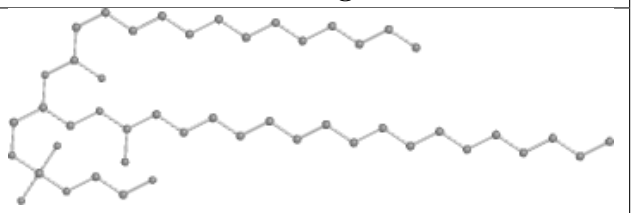
Bond lengths



Bond angles

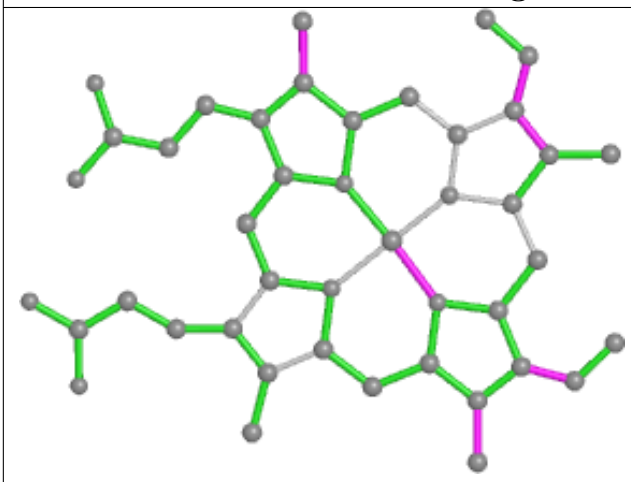


Torsions

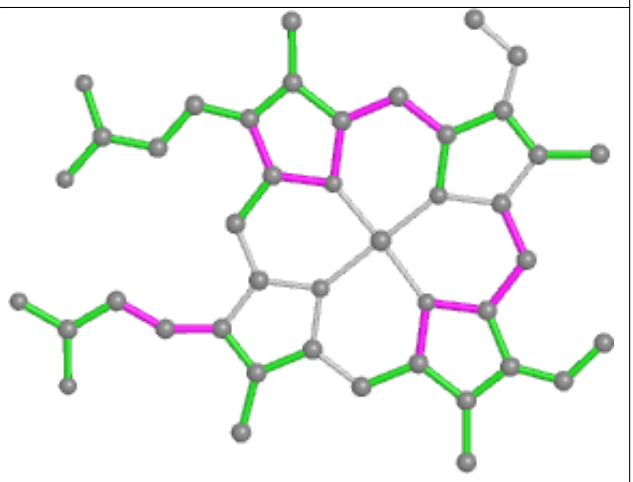


Rings

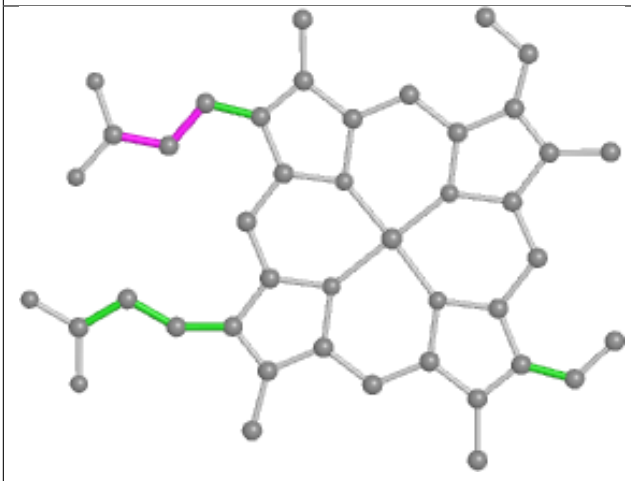
Ligand HEM C 1001



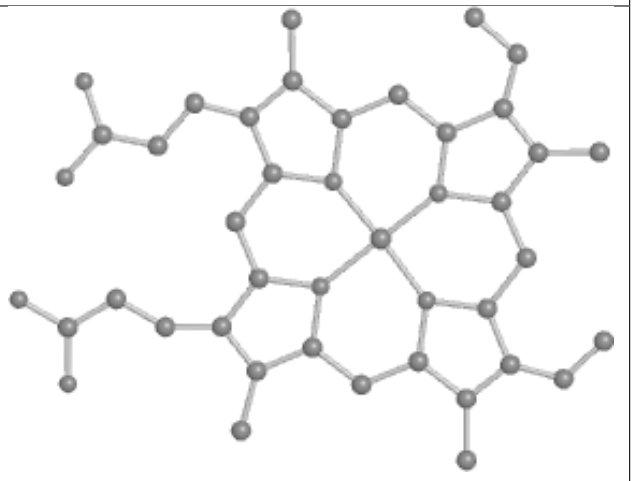
Bond lengths



Bond angles

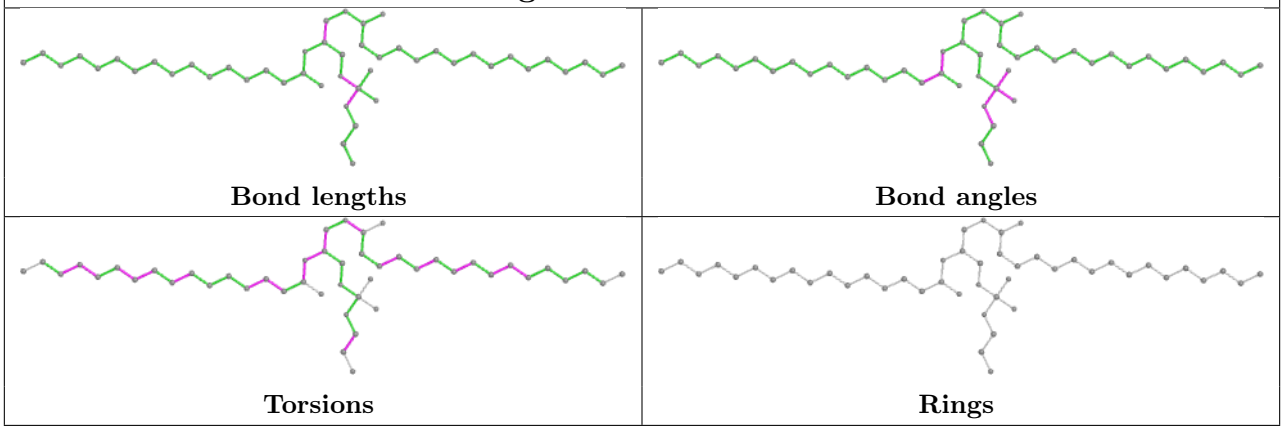


Torsions

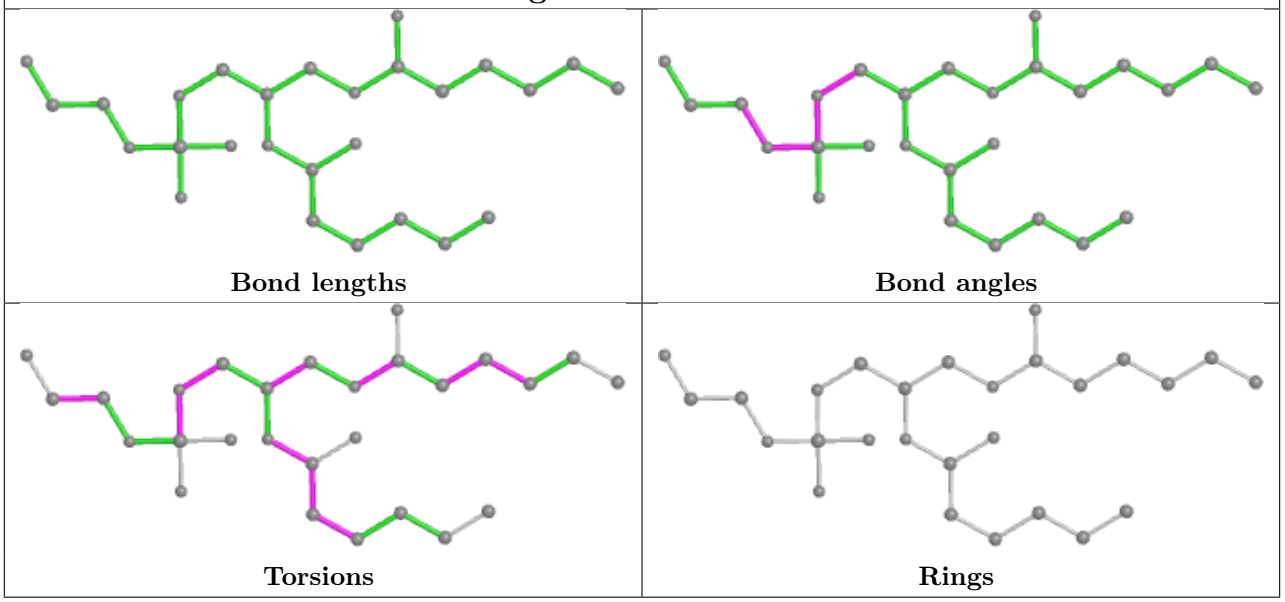


Rings

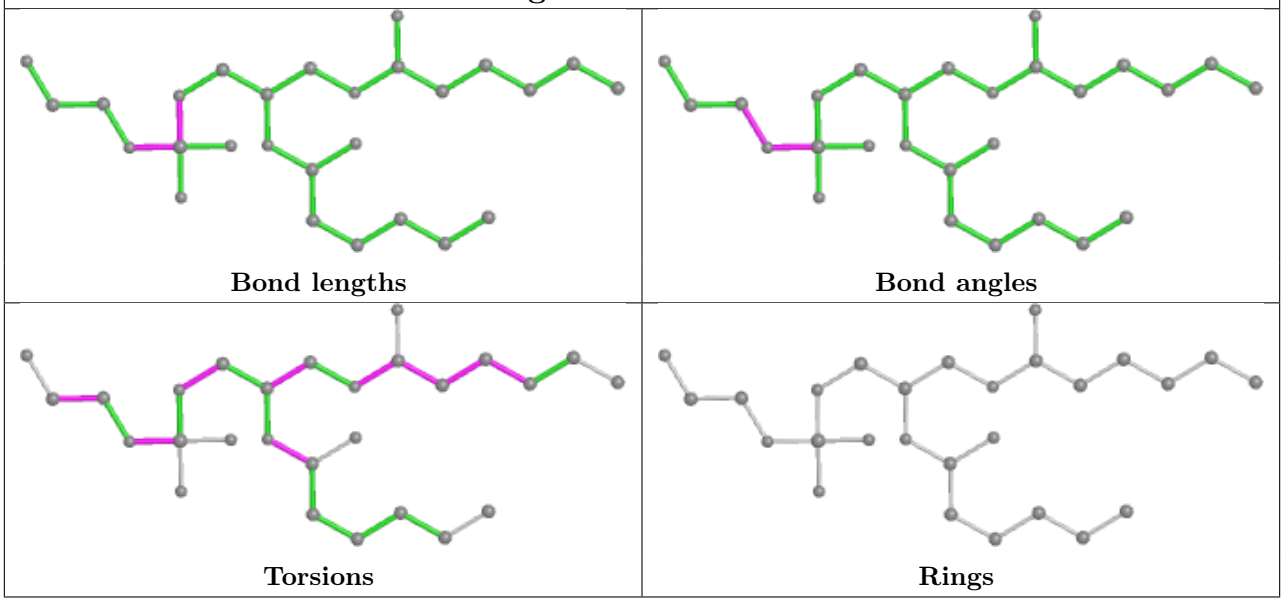
Ligand PEF C 1005



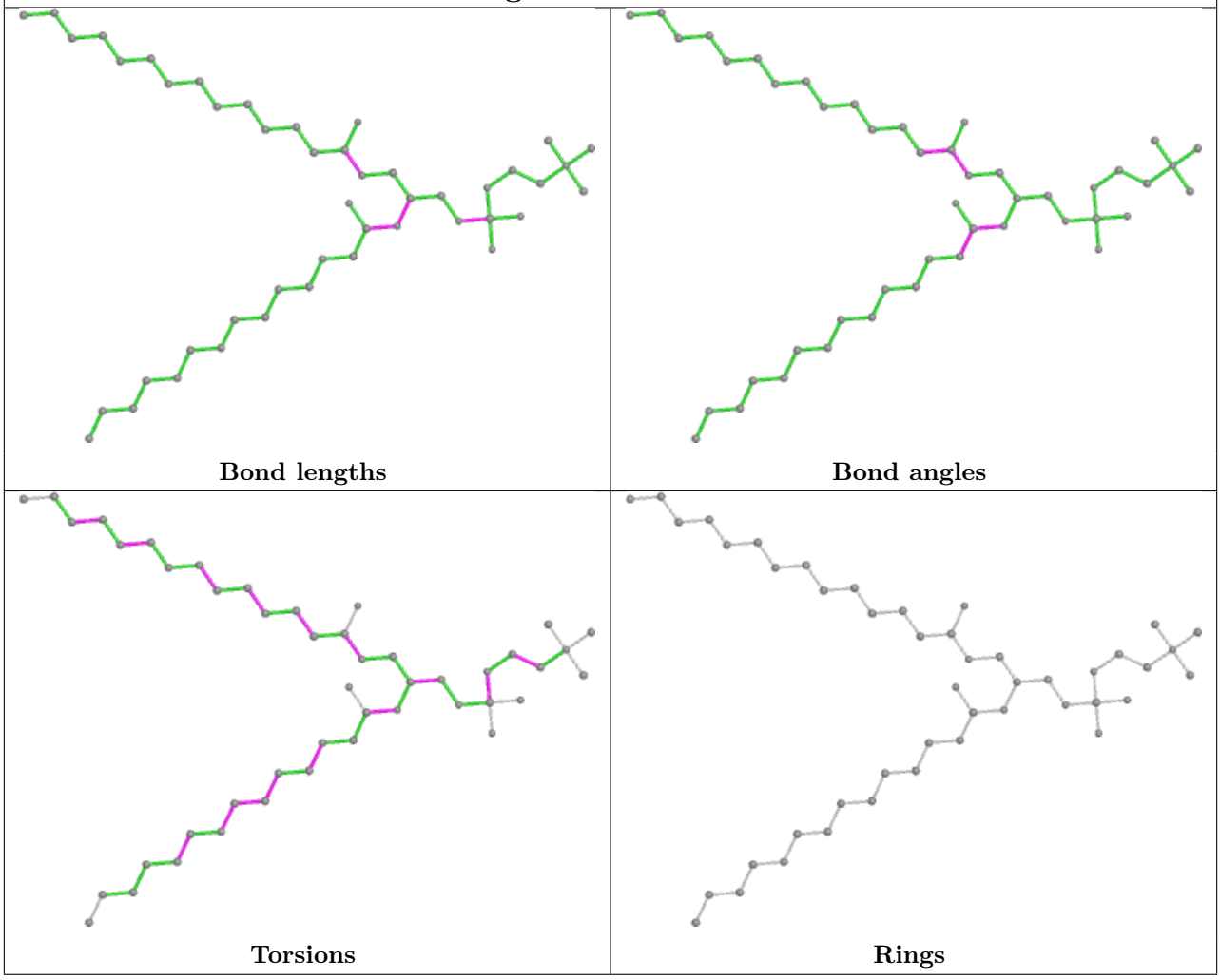
Ligand 6PE A 501



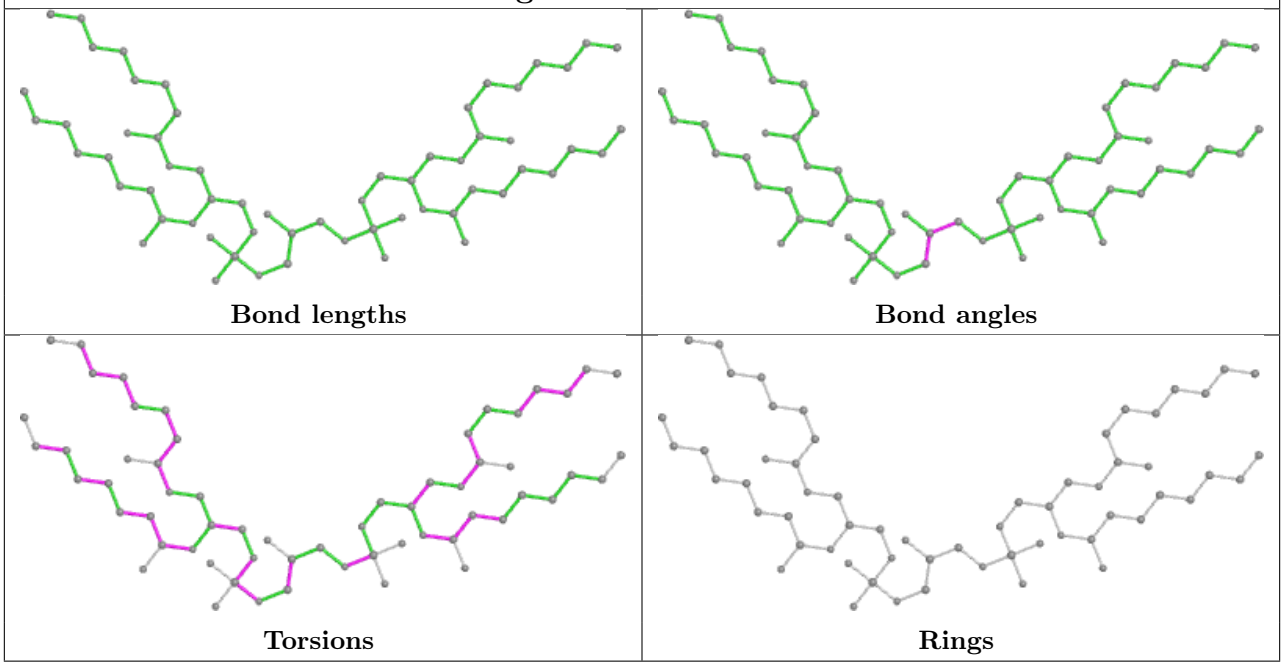
Ligand 6PE K 101



Ligand PX4 J 101



Ligand CDL C 1006



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	446/446 (100%)	0.49	19 (4%) 35 22	55, 79, 117, 208	0
2	B	425/439 (96%)	0.34	8 (1%) 66 49	43, 60, 103, 231	0
3	C	377/379 (99%)	0.57	17 (4%) 33 21	65, 92, 128, 196	0
4	D	241/241 (100%)	1.12	42 (17%) 1 1	65, 138, 167, 198	0
5	E	196/196 (100%)	1.86	68 (34%) 0 0	77, 140, 197, 223	0
6	F	105/110 (95%)	0.75	13 (12%) 4 2	60, 81, 144, 201	0
7	G	75/80 (93%)	0.72	7 (9%) 8 5	63, 112, 138, 197	0
8	H	67/78 (85%)	2.22	28 (41%) 0 0	130, 156, 188, 208	0
9	I	34/78 (43%)	1.69	14 (41%) 0 0	50, 93, 126, 130	0
10	J	61/63 (96%)	1.77	24 (39%) 0 0	86, 121, 166, 250	0
11	K	49/56 (87%)	1.63	21 (42%) 0 0	82, 105, 151, 163	0
All	All	2076/2166 (95%)	0.84	261 (12%) 3 2	43, 91, 167, 250	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	187	PHE	12.3
5	E	74	ILE	9.6
10	J	2	ALA	9.4
5	E	76	ILE	9.1
4	D	55	CYS	9.0
10	J	61	ASN	9.0
5	E	195	VAL	8.9
5	E	185	TYR	7.7
5	E	188	THR	7.6
8	H	44	VAL	7.6
5	E	134	ILE	7.6
5	E	190	ASP	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	44	TRP	7.3
8	H	14	VAL	7.3
5	E	133	VAL	7.2
5	E	132	TRP	6.9
6	F	10	SER	6.9
1	A	226	ASP	6.8
5	E	193	VAL	6.8
8	H	13	LEU	6.5
5	E	91	TRP	6.4
7	G	75	ALA	6.3
5	E	96	LEU	6.2
1	A	223	TYR	6.2
5	E	124	LEU	6.2
5	E	192	MET	6.2
4	D	56	TYR	6.1
5	E	92	ARG	6.0
5	E	186	GLU	6.0
5	E	127	VAL	6.0
5	E	72	SER	5.8
5	E	194	ILE	5.8
5	E	90	LYS	5.8
7	G	74	PRO	5.7
2	B	233	SER	5.7
9	I	45	LEU	5.7
10	J	1	VAL	5.5
8	H	12	GLU	5.4
7	G	73	ASN	5.4
5	E	77	LYS	5.3
2	B	17	VAL	5.3
8	H	26	GLN	5.2
8	H	20	VAL	5.2
5	E	83	GLU	5.1
1	A	224	ASP	5.1
11	K	42	LEU	5.0
5	E	89	PHE	5.0
1	A	225	GLU	5.0
6	F	12	TRP	5.0
4	D	143	LEU	5.0
8	H	50	THR	4.9
5	E	86	ASN	4.9
8	H	24	CYS	4.8
5	E	131	GLU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	114	VAL	4.7
4	D	180	SER	4.7
6	F	6	VAL	4.7
8	H	48	SER	4.6
4	D	142	SER	4.6
5	E	99	ARG	4.5
4	D	48	TYR	4.5
5	E	80	ASP	4.5
5	E	101	ARG	4.4
1	A	19	LEU	4.3
2	B	18	PRO	4.3
8	H	76	SER	4.3
4	D	148	TYR	4.3
5	E	75	GLU	4.2
5	E	79	SER	4.2
5	E	78	LEU	4.2
1	A	227	ALA	4.2
10	J	51	LEU	4.2
5	E	191	ASP	4.1
6	F	16	ILE	4.1
5	E	135	LEU	4.1
10	J	44	GLU	4.0
5	E	98	VAL	4.0
9	I	24	GLY	4.0
4	D	79	GLU	3.9
6	F	11	ARG	3.9
10	J	39	ALA	3.9
5	E	128	LYS	3.9
11	K	38	TRP	3.9
11	K	49	ASN	3.9
5	E	184	SER	3.9
4	D	92	PRO	3.8
11	K	43	ASP	3.8
5	E	189	SER	3.7
5	E	121	GLN	3.7
11	K	17	TRP	3.7
5	E	112	VAL	3.7
5	E	81	ILE	3.7
4	D	146	GLY	3.7
11	K	40	LEU	3.7
8	H	22	GLU	3.7
10	J	14	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	3	PRO	3.6
11	K	48	ILE	3.6
11	K	18	VAL	3.6
5	E	100	HIS	3.6
5	E	85	LYS	3.6
10	J	5	LEU	3.6
1	A	23	LEU	3.5
8	H	51	GLU	3.5
3	C	28	SER	3.5
6	F	77	LYS	3.5
5	E	156	TYR	3.5
8	H	49	GLN	3.4
8	H	23	GLN	3.4
5	E	97	PHE	3.4
4	D	149	PHE	3.4
4	D	18	LEU	3.4
10	J	6	THR	3.4
11	K	45	VAL	3.3
10	J	10	TYR	3.3
8	H	19	THR	3.3
4	D	93	LYS	3.3
4	D	166	ASN	3.3
5	E	93	GLY	3.3
11	K	41	ILE	3.3
8	H	27	LEU	3.3
5	E	196	GLY	3.3
4	D	114	SER	3.3
4	D	115	TYR	3.2
8	H	43	ARG	3.2
5	E	87	MET	3.2
3	C	267	HIS	3.2
9	I	27	ARG	3.2
5	E	167	ALA	3.1
11	K	39	ARG	3.1
11	K	47	TYR	3.1
6	F	9	SER	3.1
4	D	158	ILE	3.1
5	E	183	PRO	3.1
1	A	206	ARG	3.1
10	J	48	GLU	3.1
10	J	53	LYS	3.1
10	J	8	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	42	SER	3.0
9	I	48	SER	3.0
7	G	70	LYS	3.0
1	A	383	LEU	3.0
7	G	30	PHE	3.0
4	D	96	PRO	3.0
10	J	42	ILE	3.0
9	I	51	CYS	3.0
3	C	102	LEU	3.0
5	E	94	LYS	3.0
5	E	113	GLU	3.0
8	H	53	ASP	3.0
9	I	20	ARG	3.0
3	C	155	TYR	3.0
8	H	37	LEU	3.0
9	I	44	ASP	3.0
1	A	17	SER	2.9
10	J	56	LYS	2.9
11	K	11	ARG	2.9
5	E	73	LYS	2.9
5	E	129	LYS	2.9
3	C	32	ASN	2.9
10	J	11	SER	2.9
5	E	122	HIS	2.9
8	H	52	GLU	2.9
1	A	195	MET	2.9
10	J	33	ARG	2.9
5	E	84	GLY	2.8
10	J	55	ILE	2.8
4	D	5	LEU	2.8
4	D	169	LEU	2.8
4	D	206	LEU	2.8
2	B	16	GLY	2.8
5	E	154	GLY	2.8
7	G	72	LYS	2.8
11	K	4	ARG	2.7
10	J	12	LEU	2.7
8	H	36	ARG	2.7
3	C	29	SER	2.7
11	K	5	PHE	2.7
11	K	10	TYR	2.7
4	D	167	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	70	LEU	2.6
5	E	130	PRO	2.6
4	D	80	MET	2.6
8	H	39	LEU	2.6
5	E	157	TYR	2.6
8	H	40	CYS	2.6
5	E	71	MET	2.6
4	D	39	SER	2.6
4	D	139	THR	2.5
4	D	86	LYS	2.5
8	H	78	LYS	2.5
9	I	46	LYS	2.5
1	A	228	VAL	2.5
4	D	182	VAL	2.5
6	F	8	ALA	2.5
3	C	307	LEU	2.5
6	F	13	LEU	2.5
4	D	165	TYR	2.5
11	K	6	LEU	2.5
9	I	26	LEU	2.5
8	H	29	LYS	2.5
3	C	30	TRP	2.5
1	A	21	ASN	2.4
3	C	14	VAL	2.4
3	C	225	THR	2.4
5	E	107	ASP	2.4
11	K	15	ARG	2.4
1	A	435	ASN	2.4
10	J	13	LEU	2.4
1	A	10	SER	2.4
5	E	120	PRO	2.4
6	F	87	LYS	2.4
3	C	18	PHE	2.4
9	I	52	ARG	2.4
2	B	304	HIS	2.3
4	D	232	SER	2.3
4	D	94	PRO	2.3
10	J	46	ILE	2.3
10	J	37	GLN	2.3
8	H	54	CYS	2.3
4	D	145	GLU	2.3
9	I	61	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	27	ILE	2.3
4	D	171	PHE	2.3
1	A	25	VAL	2.2
6	F	7	SER	2.2
3	C	208	PRO	2.2
2	B	305	GLN	2.2
3	C	3	ASN	2.2
1	A	16	VAL	2.2
4	D	70	VAL	2.2
4	D	241	LYS	2.2
8	H	61	PHE	2.2
2	B	19	PRO	2.2
5	E	149	ASN	2.2
8	H	58	LEU	2.1
4	D	85	GLY	2.1
4	D	192	TRP	2.1
1	A	192	ALA	2.1
10	J	60	GLU	2.1
5	E	146	PRO	2.1
6	F	19	TRP	2.1
5	E	102	THR	2.1
11	K	2	LEU	2.1
3	C	228	ASP	2.1
4	D	147	LEU	2.1
9	I	25	ALA	2.1
4	D	170	GLU	2.1
1	A	222	THR	2.1
4	D	189	PHE	2.1
6	F	70	MET	2.0
3	C	362	ILE	2.0
9	I	60	ALA	2.0
11	K	8	PRO	2.0
4	D	81	PHE	2.0
5	E	95	PRO	2.0
7	G	66	PHE	2.0
3	C	268	ILE	2.0
4	D	228	SER	2.0
5	E	110	ALA	2.0
2	B	303	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

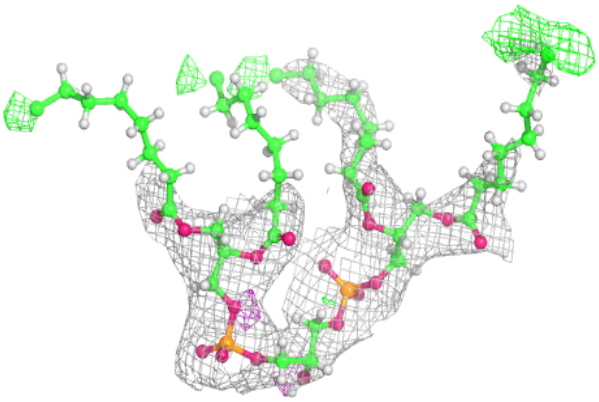
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

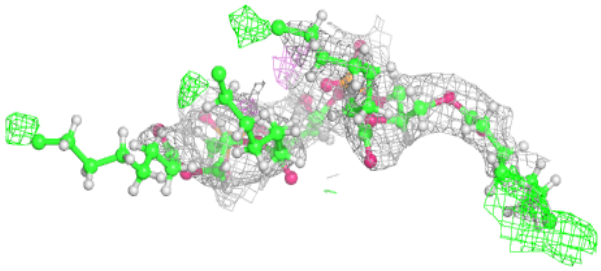
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	CDL	D	1002	60/100	0.60	0.47	101,128,156,157	0
13	CDL	C	1006	60/100	0.68	0.47	96,125,150,151	0
18	CL	C	1007	1/1	0.80	0.37	72,72,72,72	0
21	PX4	J	101	46/46	0.80	0.44	93,123,139,141	0
12	6PE	K	101	27/27	0.84	0.41	116,141,166,166	0
16	8PE	C	1004	47/47	0.84	0.44	63,103,131,135	0
17	PEF	C	1005	47/47	0.88	0.34	86,110,131,133	0
12	6PE	A	501	27/27	0.89	0.31	76,107,131,131	0
13	CDL	A	502	60/100	0.91	0.30	88,114,138,139	0
15	PQU	C	1003	28/28	0.92	0.25	111,119,141,147	0
19	HEC	D	1001	43/43	0.94	0.27	130,149,179,185	0
14	HEM	C	1001	43/43	0.96	0.25	85,102,121,133	0
14	HEM	C	1002	43/43	0.97	0.28	66,82,101,107	0
20	FES	E	1001	4/4	0.99	0.15	118,126,126,132	0

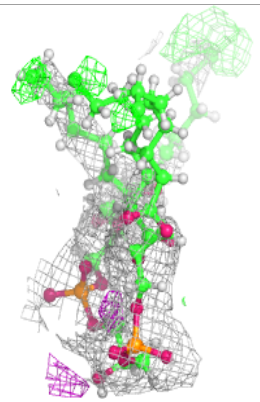
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL D 1002:

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

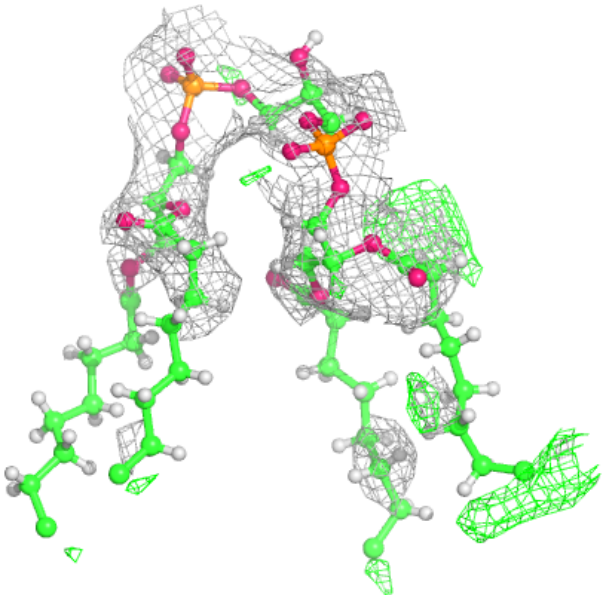


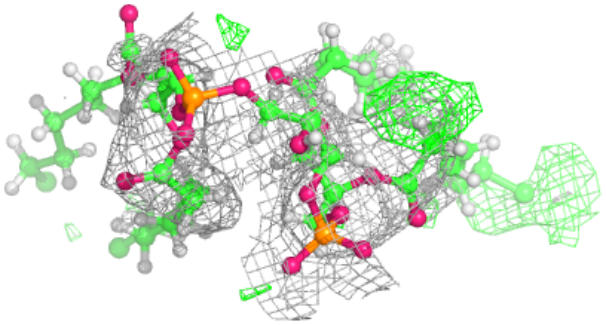


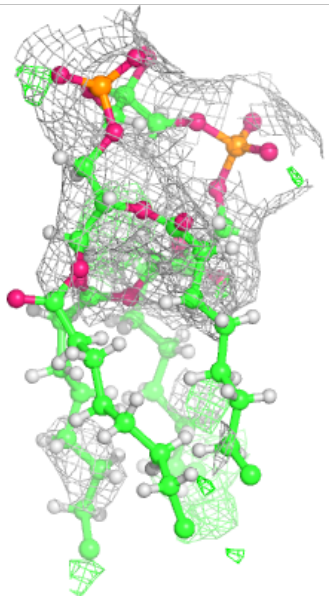


Electron density around CDL C 1006:

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

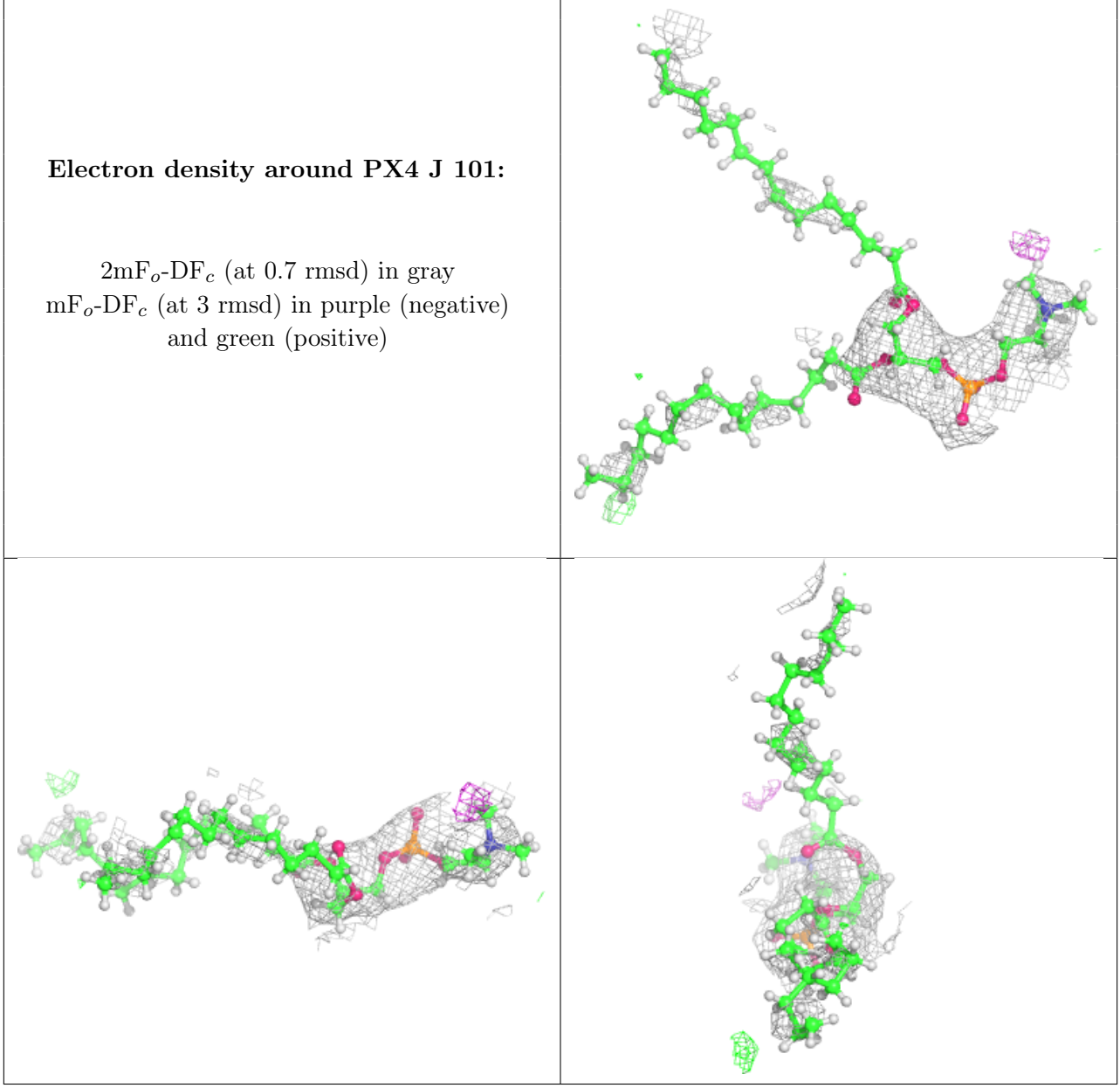






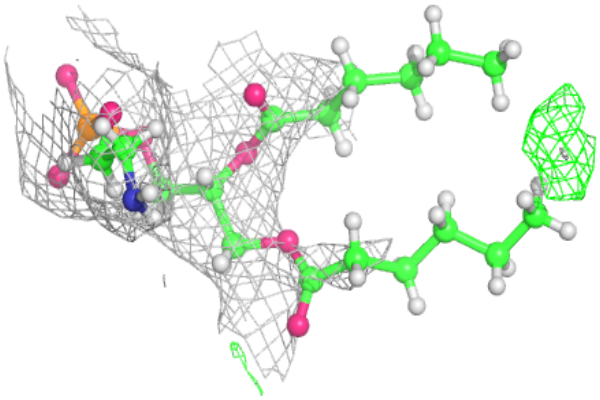
Electron density around PX4 J 101:

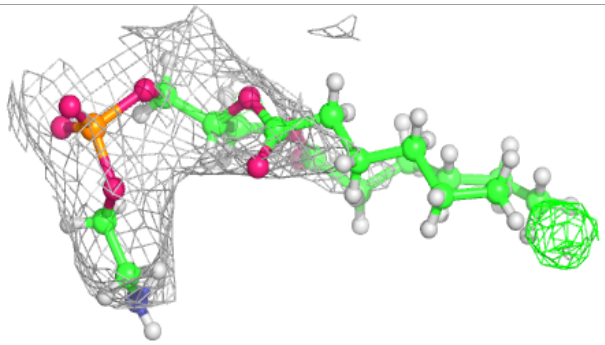
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

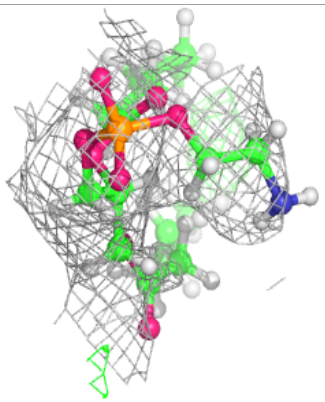


Electron density around 6PE K 101:

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

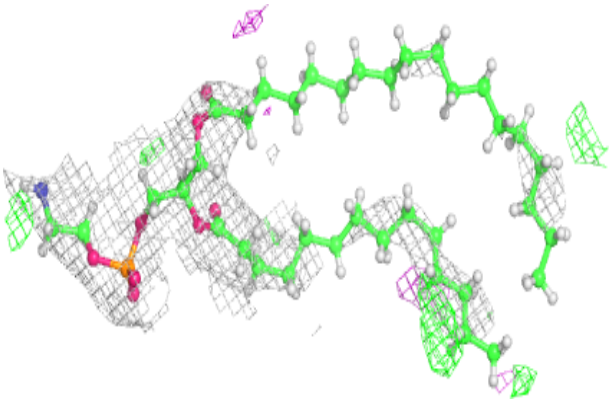


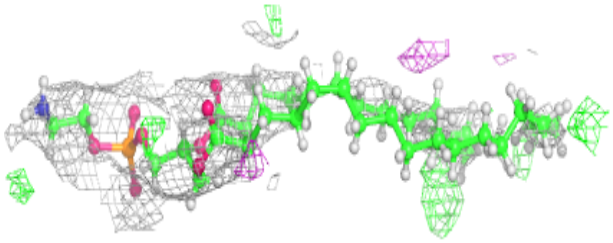


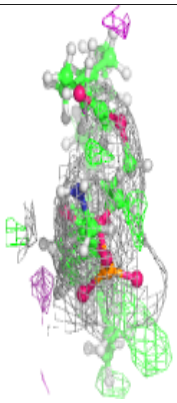


Electron density around 8PE C 1004:

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

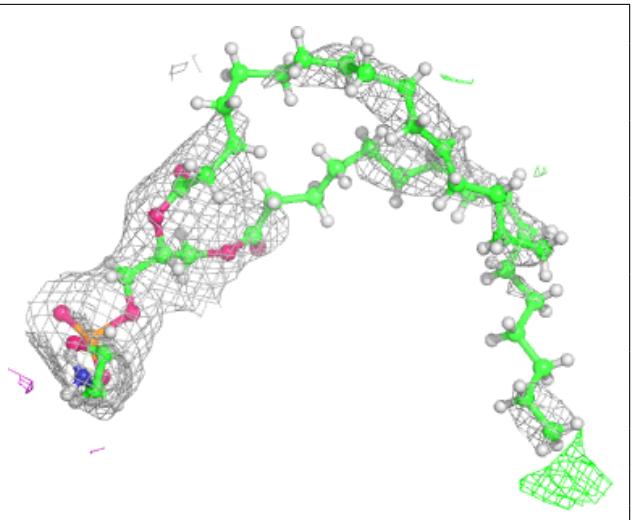


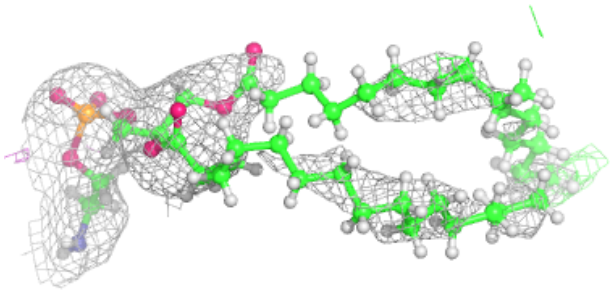


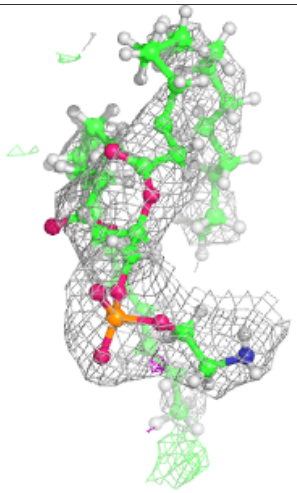


Electron density around PEF C 1005:

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

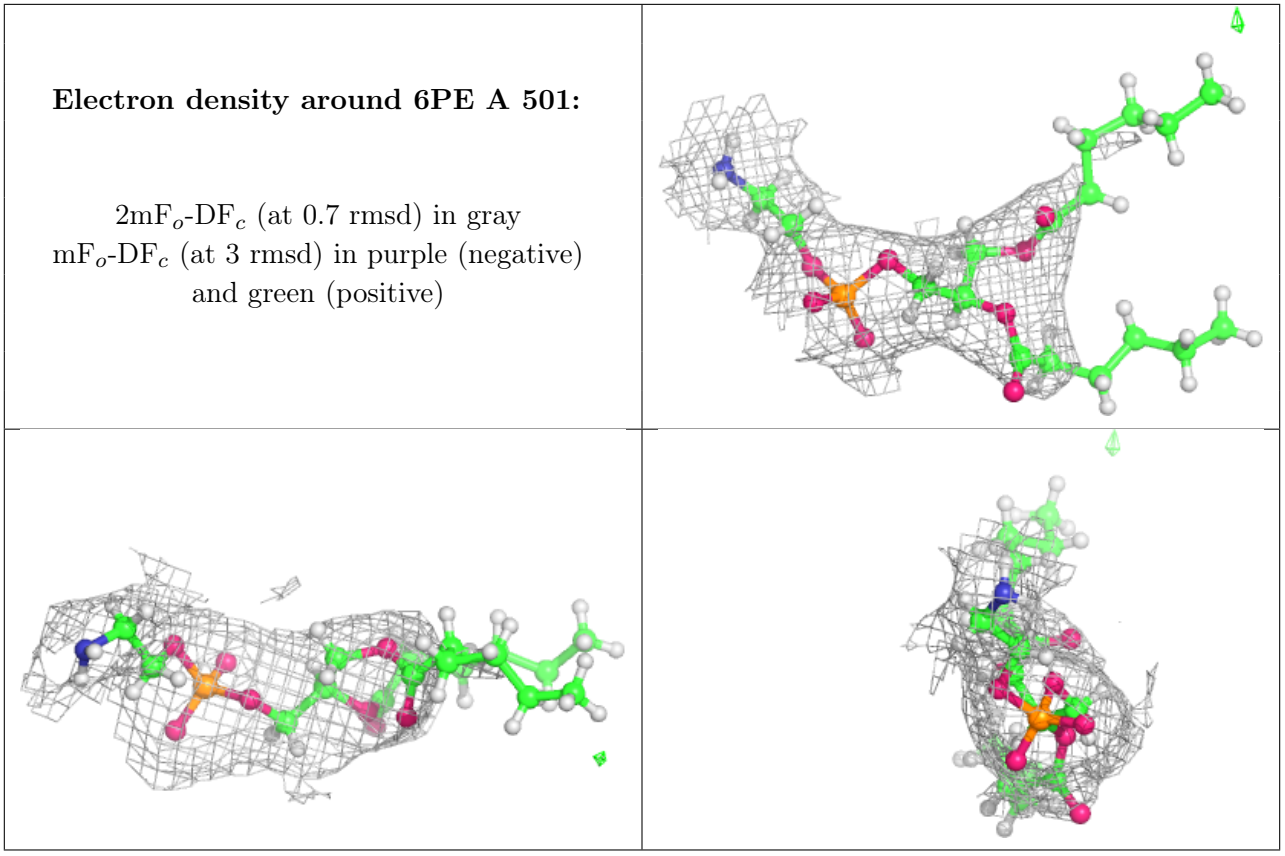






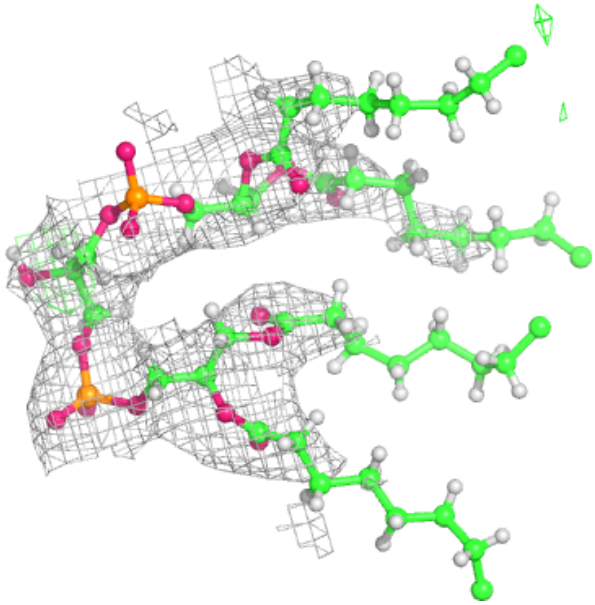
Electron density around 6PE A 501:

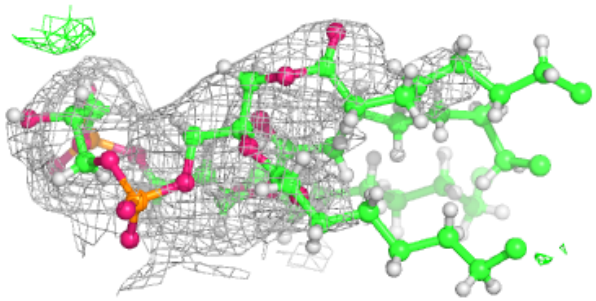
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

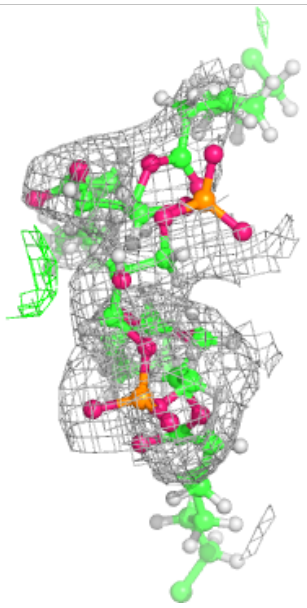


Electron density around CDL A 502:

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

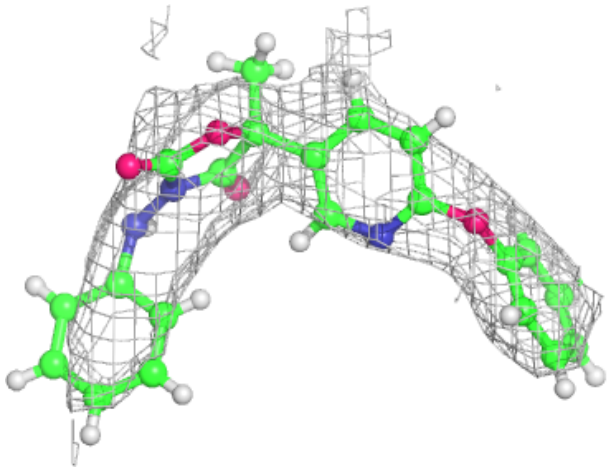


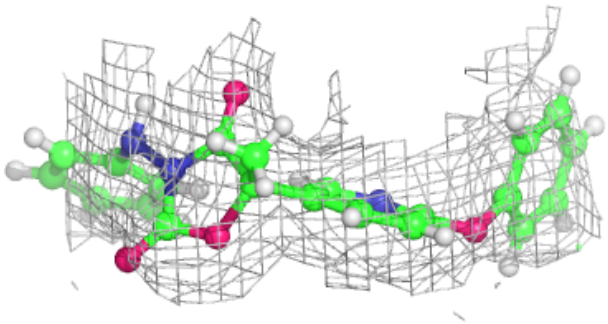


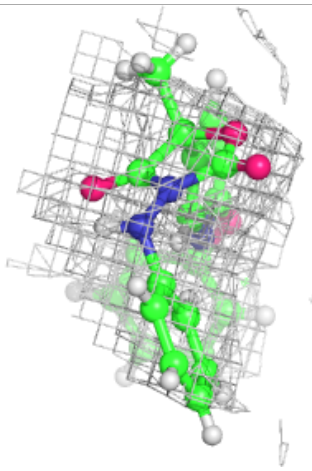


Electron density around PQU C 1003:

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

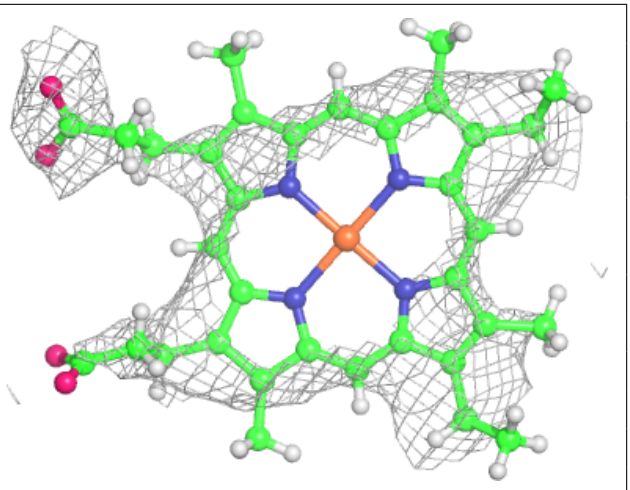


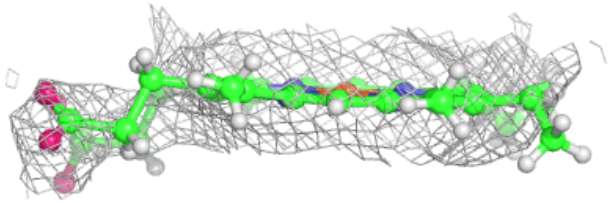


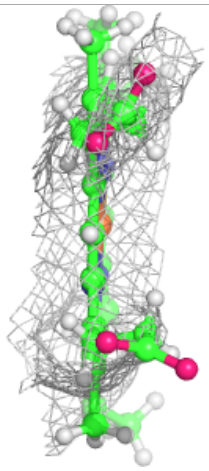


Electron density around HEC D 1001:

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

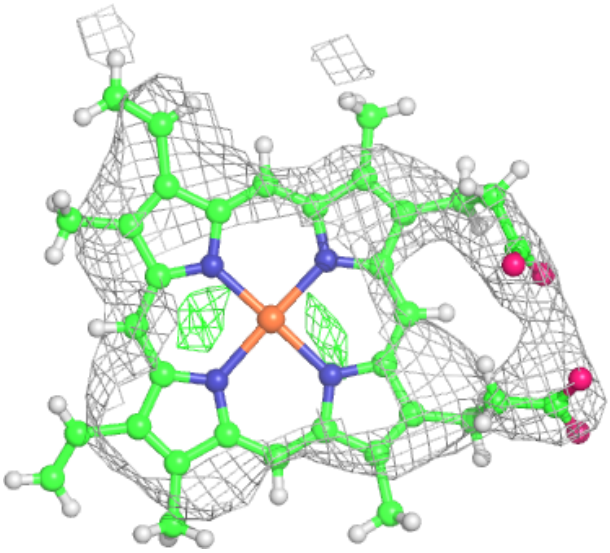


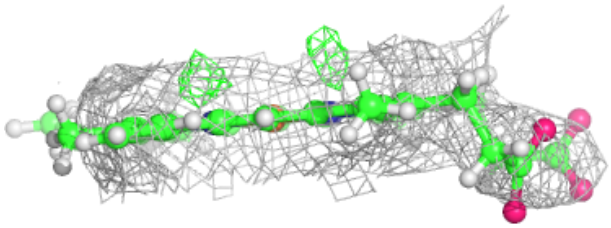


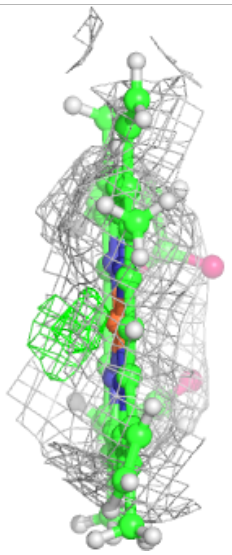


Electron density around HEM C 1001:

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

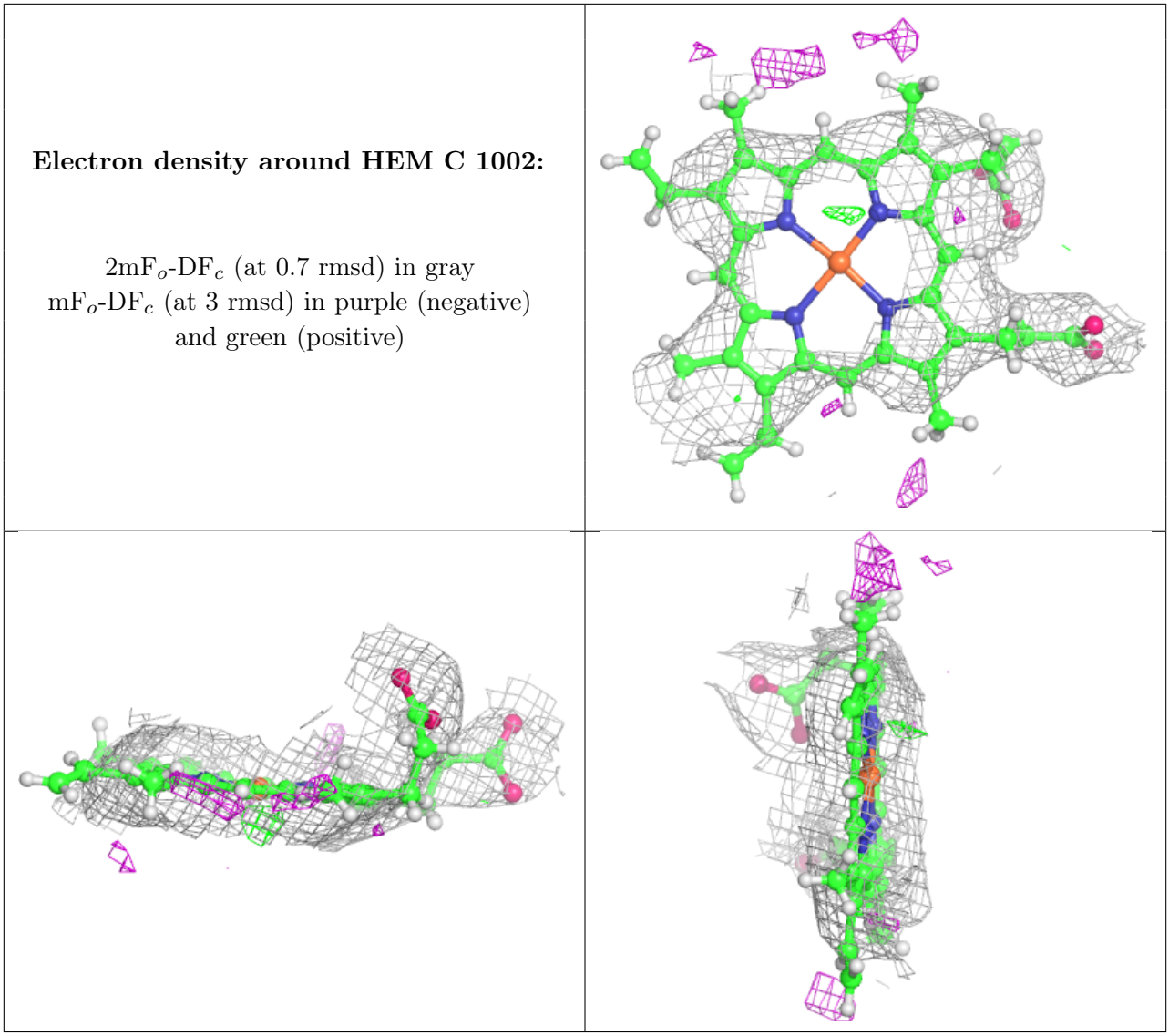






Electron density around HEM C 1002:

$2mF_o$-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.