Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 05:19 pm GMT

PDB ID	:	6ZFT
Title	:	Crystal structure of bovine cytochrome bc1 in complex with quinolone inhibitor CK-2-68
Authors	:	Amporndanai, K.; O'Neill, P.M.; Hong, W.D.; Amewu, R.K.; Pidathala, C.; Berry, N.G.; Biagini, G.A.; Leung, S.C.; Hasnain, S.S.; Antonyuk, S.V.
Deposited on	:	2020-06-17
Resolution	:	3.30 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 ⓘ 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 ⓘ) were used in the production of this report:

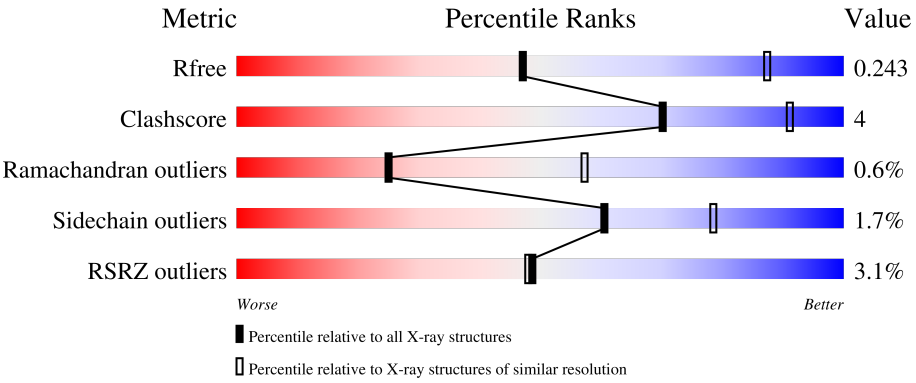
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	444	2% 90% 9%
2	B	420	% 89% 9%
3	C	378	89% 11%
4	D	239	6% 91% 9%

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Mol	Chain	Length	Quality of chain
5	E	196	7% 92% 7%
6	F	99	% 95%
7	G	74	84% 16%
8	H	65	3% 95% 5%
9	I	46	39% 78% 20%
10	J	59	2% 97%

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
11	PG4	A	503	-	-	X	-
11	PG4	C	407	-	-	-	X
13	CDL	E	203	-	-	-	X
17	PEE	C	409	X	-	-	-
17	PEE	D	503	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 16262 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3391	2121	600	650	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	THR	ALA	conflict	UNP P31800

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3108	1951	551	599	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			2996	2007	471	500	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1876	1201	321	339	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1474	923	258	286	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			848	537	156	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	406	116	97	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	65	Total	C	N	O	S	0	0	0
			517	313	92	107	5			

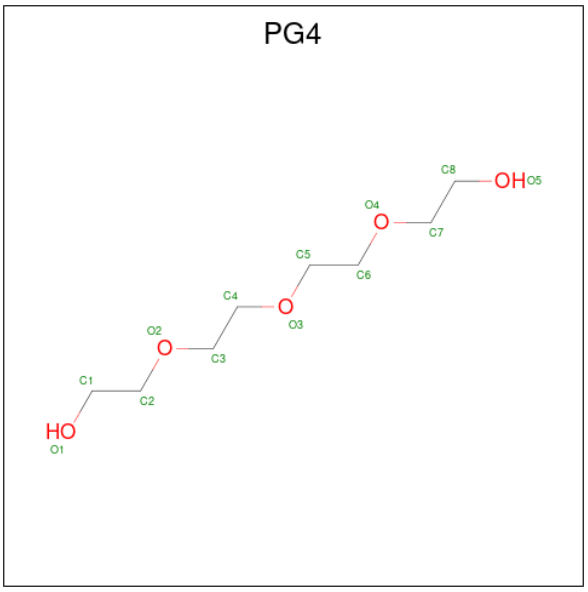
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			324	201	58	64	1			

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

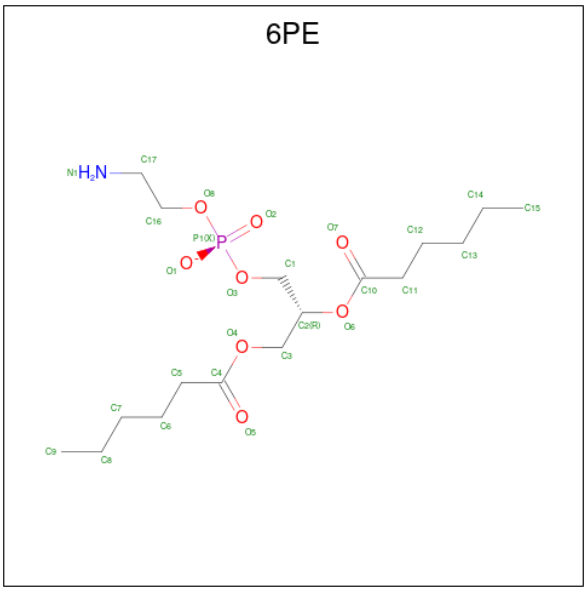
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



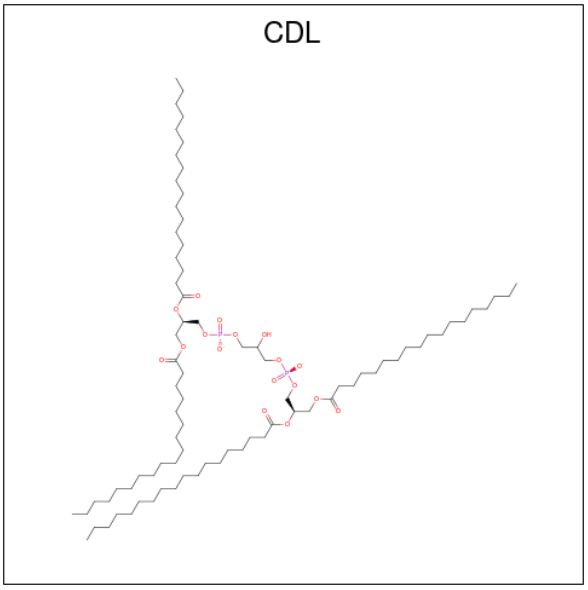
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 13 8 5	0	0
11	A	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0

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



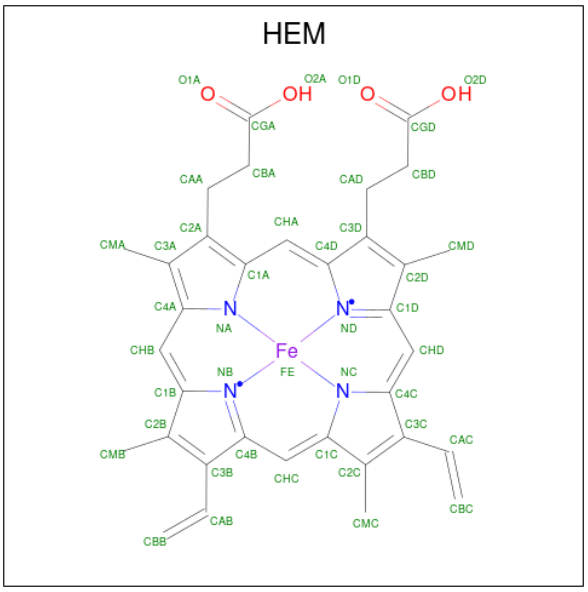
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

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



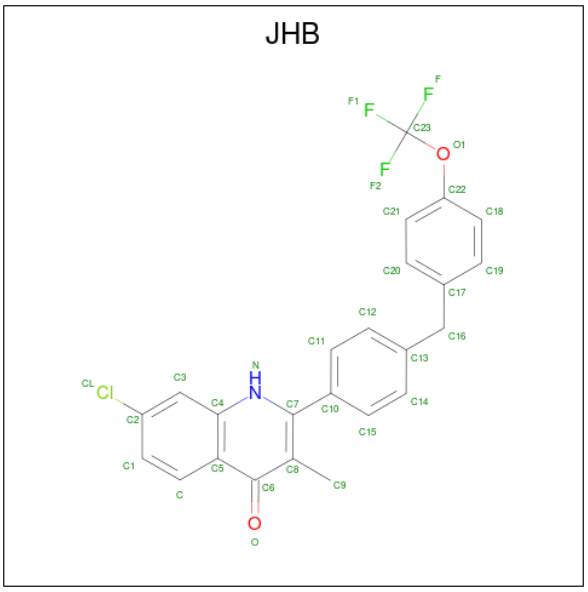
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	O	P	0	0
			34	17	15	2		
13	C	1	Total	C	O	P	0	0
			44	25	17	2		
13	D	1	Total	C	O	P	0	0
			54	35	17	2		
13	E	1	Total	C	O	P	0	0
			60	41	17	2		

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



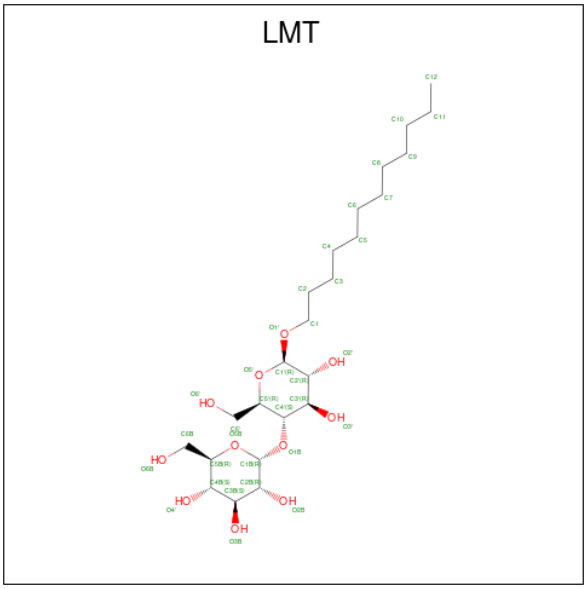
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is 7-chloranyl-3-methyl-2-[4-[[4-(trifluoromethyloxy)phenyl]methyl]phenyl]-1 { H}-quinolin-4-one (three-letter code: JHB) (formula: $C_{24}H_{17}ClF_3NO_2$) (labeled as "Ligand of Interest" by depositor).



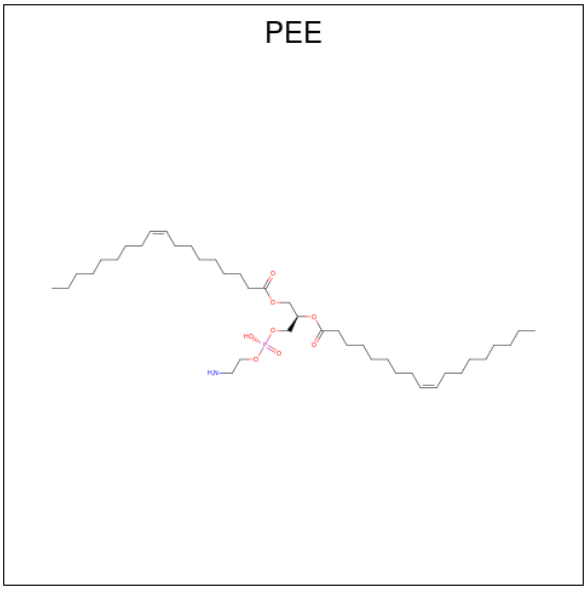
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	C	1	Total	C	Cl	F	N	O	0	0
			31	24	1	3	1	2		

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

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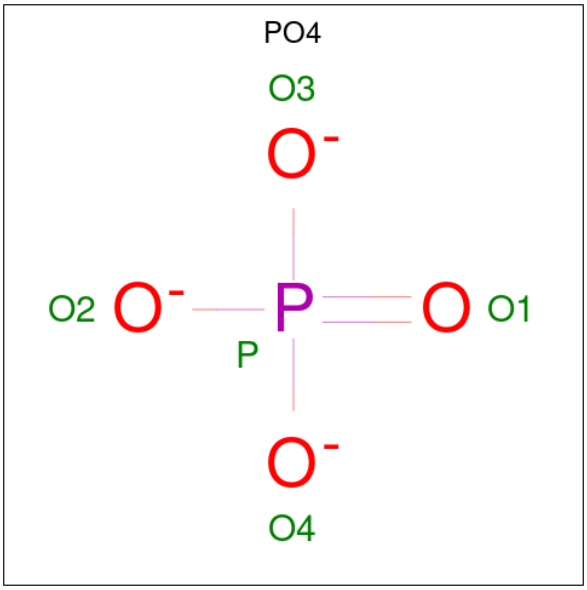
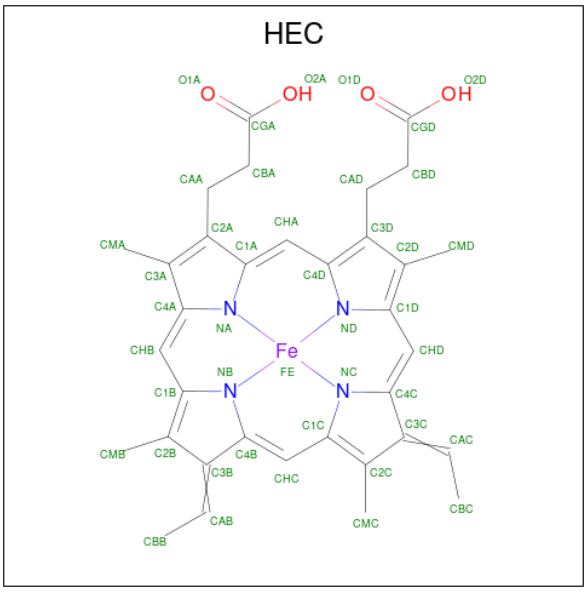
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total C N O P 37 27 1 8 1	0	0

- Molecule 18 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



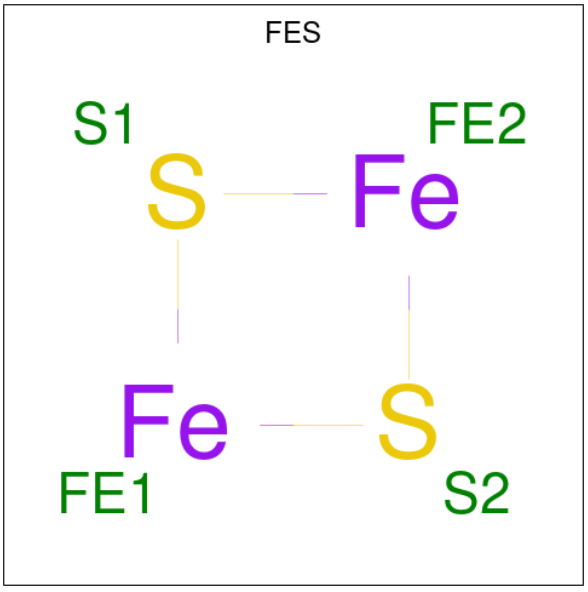
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	1	Total O P 5 4 1	0	0
18	F	1	Total O P 5 4 1	0	0
18	G	1	Total O P 5 4 1	0	0
18	G	1	Total O P 5 4 1	0	0
18	G	1	Total O P 5 4 1	0	0
18	H	1	Total O P 5 4 1	0	0

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



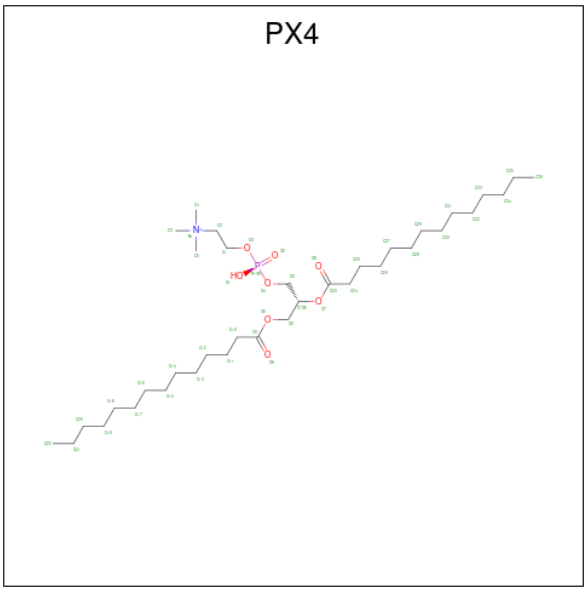
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	E	1	Total	C	N	O	P	0	0
			37	27	1	8	1		

- Molecule 22 is water.

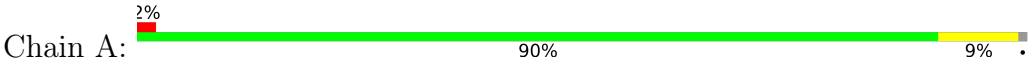
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	3	Total	O	0	0
			3	3		
22	B	1	Total	O	0	0
			1	1		
22	C	4	Total	O	0	0
			4	4		
22	D	2	Total	O	0	0
			2	2		
22	F	1	Total	O	0	0
			1	1		

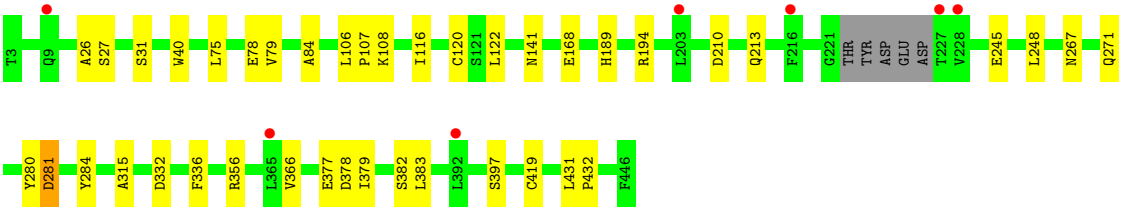
3 Residue-property plots (i)

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

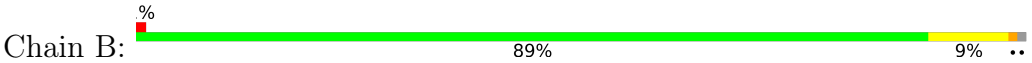
Chain A:

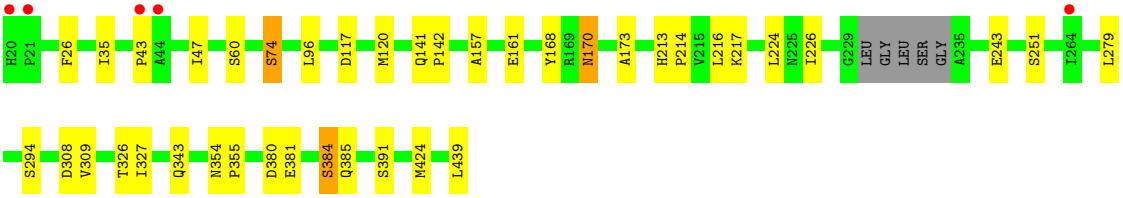




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

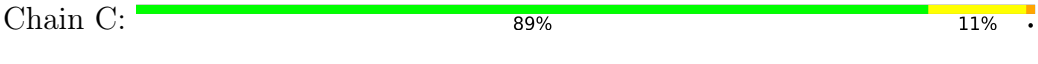
Chain B:

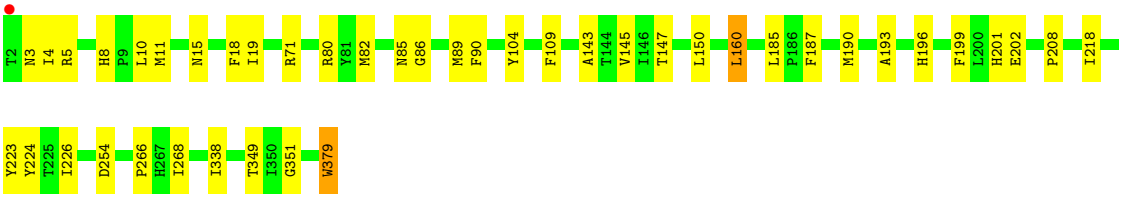




• Molecule 3: Cytochrome b

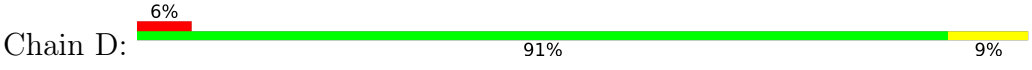
Chain C:

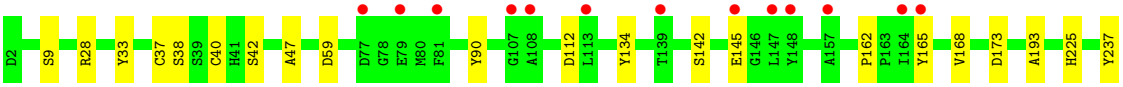




• Molecule 4: Cytochrome c1, heme protein, mitochondrial

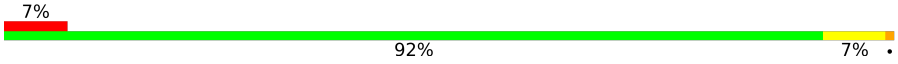
Chain D:





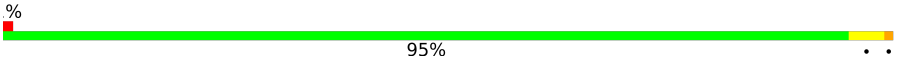
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



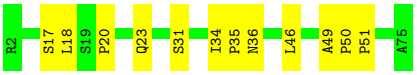
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:



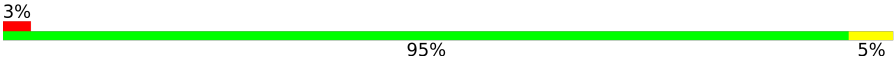
• Molecule 7: Cytochrome b-c1 complex subunit 8

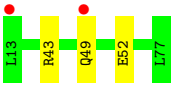
Chain G:



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

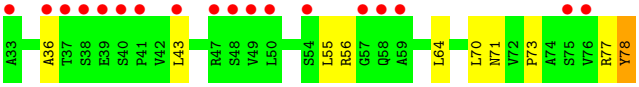
Chain H:





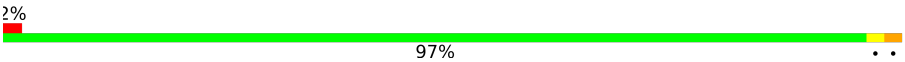
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

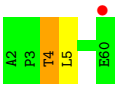
Chain I:



• Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	212.36Å 212.36Å 345.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.92 – 3.30 91.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	69.5 (60.92-3.30) 69.5 (91.95-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.214 , 0.244 0.217 , 0.243	Depositor DCC
R_{free} test set	2445 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	89.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	16262	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 3.78% 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: PEE, LMT, PO4, PX4, FES, HEM, CDL, HEC, JHB, PG4, 6PE

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	0.71	0/3462	0.79	0/4700
2	B	0.70	0/3165	0.80	0/4296
3	C	0.67	0/3092	0.74	0/4231
4	D	0.66	0/1935	0.76	0/2632
5	E	0.71	0/1507	0.79	0/2044
6	F	0.68	0/867	0.77	0/1168
7	G	0.66	0/641	0.77	0/868
8	H	0.70	0/522	0.78	0/704
9	I	0.79	0/328	0.95	0/447
10	J	0.66	0/500	0.75	0/675
All	All	0.69	0/16019	0.78	0/21765

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
2	B	0	1
8	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	ASN	Peptide

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Mol	Chain	Res	Type	Group
8	H	49	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3391	0	3286	30	0
2	B	3108	0	3067	24	0
3	C	2996	0	3058	22	0
4	D	1876	0	1806	14	0
5	E	1474	0	1401	5	0
6	F	848	0	814	5	0
7	G	620	0	624	7	0
8	H	517	0	482	1	0
9	I	324	0	327	8	0
10	J	487	0	487	1	0
11	A	26	0	36	9	0
11	C	26	0	36	0	0
12	A	23	0	19	1	0
13	C	78	0	56	2	0
13	D	54	0	52	1	0
13	E	60	0	64	0	0
14	C	86	0	60	6	0
15	C	31	0	0	3	0
16	C	35	0	46	0	0
17	C	40	0	54	0	0
17	D	37	0	48	1	0
18	C	5	0	0	0	0
18	F	5	0	0	0	0
18	G	15	0	0	0	0
18	H	5	0	0	0	0
19	D	43	0	32	5	0
20	E	4	0	0	0	0
21	E	37	0	51	0	0
22	A	3	0	0	1	0
22	B	1	0	0	0	0
22	C	4	0	0	0	0
22	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	1	0	0	0	0
All	All	16262	0	15906	114	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 4.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:CYS:SG	19:D:501:HEC:CAB	2.19	1.29
4:D:37:CYS:SG	19:D:501:HEC:C3B	2.54	0.94
4:D:37:CYS:SG	19:D:501:HEC:CBB	2.59	0.91
1:A:432:PRO:CG	11:A:503:PG4:H51	2.10	0.82
4:D:37:CYS:SG	19:D:501:HEC:HBB3	2.19	0.82
1:A:336:PHE:HA	11:A:503:PG4:H81	1.61	0.81
1:A:332:ASP:OD1	11:A:503:PG4:H52	1.81	0.80
14:C:403:HEM:HMC2	14:C:403:HEM:HBC2	1.70	0.74
1:A:432:PRO:HG3	11:A:503:PG4:H51	1.73	0.70
1:A:336:PHE:CZ	3:C:3:ASN:HB3	2.28	0.69
8:H:43:ARG:NH1	8:H:52:GLU:OE1	2.26	0.68
6:F:27:ASN:HD22	6:F:27:ASN:H	1.46	0.64
1:A:432:PRO:HB3	11:A:503:PG4:H51	1.80	0.63
1:A:432:PRO:CB	11:A:503:PG4:H51	2.29	0.62
5:E:52:LYS:O	5:E:56:SER:HB2	1.99	0.62
2:B:380:ASP:O	2:B:384:SER:HB2	2.02	0.59
1:A:336:PHE:HA	11:A:503:PG4:C8	2.33	0.58
3:C:71:ARG:NH2	4:D:193:ALA:O	2.36	0.58
3:C:193:ALA:O	3:C:196:HIS:HB3	2.05	0.57
4:D:33:TYR:CE2	4:D:38:SER:HB3	2.40	0.57
2:B:170:ASN:O	2:B:173:ALA:HB3	2.06	0.56
14:C:402:HEM:HMB1	14:C:402:HEM:HBB2	1.87	0.56
3:C:201:HIS:NE2	15:C:404:JHB:O	2.39	0.56
7:G:18:LEU:O	7:G:23:GLN:NE2	2.38	0.56
14:C:403:HEM:HMB1	14:C:403:HEM:HBB2	1.88	0.55
14:C:402:HEM:HMC1	14:C:402:HEM:HBC2	1.89	0.55
4:D:40:CYS:SG	19:D:501:HEC:HBC3	2.46	0.55
2:B:279:LEU:HA	2:B:294:SER:HB3	1.89	0.55
3:C:143:ALA:O	3:C:147:THR:OG1	2.14	0.53
2:B:157:ALA:O	2:B:161:GLU:HG2	2.10	0.52
3:C:223:TYR:O	3:C:226:ILE:HG22	2.10	0.52
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:502:6PE:H4	13:C:401:CDL:H512	1.92	0.51
3:C:379:TRP:CZ2	6:F:33:ARG:HD3	2.46	0.50
2:B:354:ASN:N	2:B:355:PRO:HD2	2.25	0.50
3:C:150:LEU:HD23	3:C:160:LEU:HD13	1.93	0.50
14:C:403:HEM:HBB2	14:C:403:HEM:CMB	2.41	0.49
1:A:366:VAL:HG21	2:B:43:PRO:HB2	1.94	0.49
14:C:403:HEM:HBC2	14:C:403:HEM:CMC	2.42	0.49
1:A:141:ASN:ND2	1:A:168:GLU:OE1	2.42	0.48
5:E:144:CYS:O	5:E:146:PRO:HD3	2.14	0.48
9:I:78:TYR:CD1	9:I:78:TYR:OXT	2.66	0.48
2:B:26:PHE:CZ	2:B:391:SER:HA	2.48	0.48
1:A:284:TYR:CZ	9:I:71:ASN:O	2.67	0.48
3:C:15:ASN:HA	3:C:19:ILE:HD12	1.95	0.47
2:B:243:GLU:HA	2:B:424:MET:O	2.15	0.47
2:B:294:SER:OG	2:B:343:GLN:NE2	2.48	0.47
15:C:404:JHB:C19	15:C:404:JHB:C14	2.87	0.47
4:D:42:SER:OG	4:D:112:ASP:OD2	2.25	0.47
3:C:187:PHE:O	3:C:190:MET:HB3	2.14	0.47
6:F:27:ASN:H	6:F:27:ASN:ND2	2.12	0.46
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.50	0.46
2:B:381:GLU:OE2	2:B:385:GLN:NE2	2.38	0.46
1:A:78:GLU:OE2	1:A:108:LYS:HE2	2.14	0.46
1:A:210:ASP:O	1:A:213:GLN:HB2	2.16	0.46
7:G:46:LEU:HD12	7:G:46:LEU:O	2.16	0.46
1:A:378:ASP:O	1:A:382:SER:HB2	2.16	0.45
2:B:326:THR:O	2:B:326:THR:OG1	2.32	0.45
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.99	0.45
2:B:224:LEU:C	2:B:226:ILE:HD12	2.37	0.45
5:E:140:THR:HG21	5:E:179:ASN:O	2.16	0.45
1:A:281:ASP:OD1	1:A:281:ASP:C	2.56	0.45
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.98	0.44
3:C:4:ILE:O	3:C:4:ILE:HG23	2.17	0.44
4:D:28:ARG:NH1	4:D:173:ASP:OD2	2.50	0.44
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.00	0.44
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.88	0.44
1:A:332:ASP:OD1	11:A:503:PG4:C5	2.57	0.44
3:C:218:ILE:HD11	3:C:224:TYR:CE2	2.52	0.44
5:E:58:PHE:O	5:E:61:SER:HB3	2.18	0.44
3:C:201:HIS:CE1	15:C:404:JHB:O	2.71	0.43
2:B:439:LEU:HD12	2:B:439:LEU:HA	1.90	0.43
3:C:8:HIS:HB3	3:C:11:MET:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.54	0.43
1:A:26:ALA:HB1	1:A:379:ILE:CG2	2.49	0.43
2:B:47:ILE:HD13	2:B:120:MET:HE2	2.00	0.43
7:G:34:ILE:N	7:G:35:PRO:HD2	2.34	0.43
6:F:25:GLY:HA2	6:F:27:ASN:HD21	1.83	0.43
4:D:134:TYR:CE2	4:D:162:PRO:HA	2.53	0.43
3:C:338:ILE:HG21	3:C:351:GLY:CA	2.49	0.42
1:A:432:PRO:HA	11:A:503:PG4:H12	2.01	0.42
7:G:49:ALA:N	7:G:50:PRO:CD	2.83	0.42
1:A:189:HIS:O	1:A:194:ARG:HD3	2.19	0.42
2:B:308:ASP:OD1	9:I:56:ARG:HD2	2.19	0.42
2:B:213:HIS:HB3	2:B:214:PRO:HD3	2.01	0.42
17:D:503:PEE:H24	5:E:50:ALA:HB1	2.01	0.42
1:A:79:VAL:HG13	1:A:84:ALA:HB3	2.00	0.42
2:B:309:VAL:O	9:I:56:ARG:NH1	2.49	0.42
1:A:267:ASN:O	1:A:271:GLN:HG2	2.20	0.42
2:B:96:LEU:HB3	9:I:70:LEU:HD12	2.02	0.42
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.55	0.42
1:A:245:GLU:HG3	1:A:248:LEU:HG	2.02	0.42
9:I:64:LEU:HD22	9:I:77:ARG:O	2.19	0.42
1:A:356:ARG:NH2	22:A:601:HOH:O	2.51	0.41
9:I:36:ALA:HB2	9:I:73:PRO:HD2	2.02	0.41
2:B:141:GLN:N	2:B:142:PRO:CD	2.83	0.41
3:C:82:MET:O	3:C:86:GLY:N	2.53	0.41
3:C:5:ARG:NH1	13:C:401:CDL:OB3	2.54	0.41
4:D:237:TYR:OH	6:F:57:ASP:OD1	2.21	0.41
4:D:165:TYR:CZ	4:D:168:VAL:HG23	2.55	0.41
4:D:47:ALA:HA	4:D:90:TYR:HA	2.02	0.41
3:C:85:ASN:O	3:C:89:MET:HG2	2.20	0.41
1:A:75:LEU:HD21	1:A:116:ILE:HG12	2.03	0.41
1:A:379:ILE:O	1:A:383:LEU:HD23	2.20	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.03	0.41
2:B:213:HIS:N	2:B:214:PRO:CD	2.84	0.41
3:C:8:HIS:CE1	3:C:10:LEU:HB2	2.56	0.41
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.56	0.41
13:D:502:CDL:PB2	7:G:36:ASN:HD22	2.44	0.41
1:A:120:CYS:O	1:A:122:LEU:HG	2.21	0.41
3:C:145:VAL:HG21	3:C:268:ILE:HD12	2.03	0.41
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.03	0.40
3:C:199:PHE:O	3:C:202:GLU:HB2	2.20	0.40
10:J:4:THR:OG1	10:J:5:LEU:N	2.55	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	435/444 (98%)	410 (94%)	23 (5%)	2 (0%)	29 61
2	B	411/420 (98%)	388 (94%)	22 (5%)	1 (0%)	47 77
3	C	376/378 (100%)	353 (94%)	21 (6%)	2 (0%)	29 61
4	D	237/239 (99%)	217 (92%)	18 (8%)	2 (1%)	19 51
5	E	194/196 (99%)	176 (91%)	14 (7%)	4 (2%)	7 31
6	F	97/99 (98%)	95 (98%)	2 (2%)	0	100 100
7	G	72/74 (97%)	72 (100%)	0	0	100 100
8	H	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
9	I	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6 29
10	J	57/59 (97%)	54 (95%)	3 (5%)	0	100 100
All	All	1986/2020 (98%)	1864 (94%)	110 (6%)	12 (1%)	25 57

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	315	ALA
4	D	145	GLU
5	E	177	PRO
4	D	142	SER
5	E	162	GLY
3	C	109	PHE
9	I	43	LEU
2	B	74	SER
5	E	188	THR
3	C	266	PRO
5	E	155	GLY

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	362/370 (98%)	358 (99%)	4 (1%)	73 85
2	B	323/329 (98%)	318 (98%)	5 (2%)	65 81
3	C	325/326 (100%)	317 (98%)	8 (2%)	47 72
4	D	198/204 (97%)	196 (99%)	2 (1%)	76 86
5	E	155/168 (92%)	152 (98%)	3 (2%)	57 77
6	F	85/91 (93%)	83 (98%)	2 (2%)	49 73
7	G	65/66 (98%)	63 (97%)	2 (3%)	40 67
8	H	59/62 (95%)	59 (100%)	0	100 100
9	I	35/38 (92%)	34 (97%)	1 (3%)	42 69
10	J	49/49 (100%)	48 (98%)	1 (2%)	55 76
All	All	1656/1703 (97%)	1628 (98%)	28 (2%)	60 78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	281	ASP
1	A	397	SER
1	A	419	CYS
2	B	60	SER
2	B	74	SER
2	B	117	ASP
2	B	251	SER
2	B	384	SER
3	C	18	PHE
3	C	80	ARG
3	C	90	PHE
3	C	160	LEU
3	C	185	LEU
3	C	254	ASP
3	C	349	THR

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Mol	Chain	Res	Type
3	C	379	TRP
4	D	9	SER
4	D	59	ASP
5	E	27	GLU
5	E	61	SER
5	E	178	LEU
6	F	27	ASN
6	F	71	ARG
7	G	17	SER
7	G	31	SER
9	I	78	TYR
10	J	4	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	252	HIS
1	A	271	GLN
1	A	311	ASN
1	A	328	HIS
4	D	71	GLN
5	E	57	GLN
6	F	27	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
18	PO4	G	101	-	4,4,4	0.73	0	6,6,6	0.41	0
11	PG4	C	407	-	12,12,12	0.30	0	11,11,11	0.15	0
18	PO4	F	501	-	4,4,4	0.63	0	6,6,6	0.47	0
11	PG4	A	503	-	12,12,12	0.44	0	11,11,11	0.33	0
11	PG4	C	406	-	12,12,12	0.27	0	11,11,11	0.22	0
18	PO4	H	101	-	4,4,4	0.76	0	6,6,6	0.37	0
13	CDL	E	203	-	59,59,99	0.38	0	65,71,111	0.61	1 (1%)
13	CDL	C	408	-	43,43,99	0.49	0	49,55,111	0.84	2 (4%)
20	FES	E	201	5	0,4,4	-	-	-		
18	PO4	C	410	-	4,4,4	0.74	0	6,6,6	0.41	0
19	HEC	D	501	4	32,50,50	2.25	11 (34%)	24,82,82	2.46	6 (25%)
18	PO4	G	103	-	4,4,4	0.46	0	6,6,6	0.56	0
15	JHB	C	404	-	34,34,34	2.00	5 (14%)	48,50,50	1.29	4 (8%)
11	PG4	A	501	-	12,12,12	0.23	0	11,11,11	0.14	0
21	PX4	E	202	-	36,36,45	0.42	0	42,44,53	0.68	1 (2%)
14	HEM	C	403	3	41,50,50	1.37	6 (14%)	45,82,82	1.70	10 (22%)
16	LMT	C	405	-	36,36,36	0.73	1 (2%)	47,47,47	1.42	7 (14%)
12	6PE	A	502	-	22,22,26	0.41	0	25,27,31	0.65	0
17	PEE	D	503	-	36,36,50	0.79	1 (2%)	39,41,55	0.67	1 (2%)
17	PEE	C	409	-	39,39,50	0.69	1 (2%)	42,44,55	0.63	0
13	CDL	D	502	-	53,53,99	0.42	0	59,65,111	0.59	0
18	PO4	G	102	-	4,4,4	0.66	0	6,6,6	0.43	0
14	HEM	C	402	3	41,50,50	1.40	7 (17%)	45,82,82	1.70	8 (17%)
13	CDL	C	401	-	33,33,99	0.51	0	37,43,111	0.81	1 (2%)

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
19	HEC	D	501	4	-	3/10/54/54	-
11	PG4	C	407	-	-	4/10/10/10	-
14	HEM	C	403	3	-	4/12/54/54	-
15	JHB	C	404	-	-	0/13/13/13	0/4/4/4
16	LMT	C	405	-	-	11/21/61/61	0/2/2/2
12	6PE	A	502	-	-	13/26/26/30	-
17	PEE	D	503	-	1/1/4/8	23/40/40/54	-
11	PG4	A	503	-	-	6/10/10/10	-
11	PG4	C	406	-	-	5/10/10/10	-
21	PX4	E	202	-	-	21/40/40/49	-
14	HEM	C	402	3	-	6/12/54/54	-
13	CDL	E	203	-	-	34/69/69/110	-
13	CDL	C	408	-	-	21/52/52/110	-
17	PEE	C	409	-	1/1/4/8	17/43/43/54	-
11	PG4	A	501	-	-	6/10/10/10	-
20	FES	E	201	5	-	-	0/1/1/1
13	CDL	D	502	-	-	25/63/63/110	-
13	CDL	C	401	-	-	21/41/41/110	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	404	JHB	C5-C4	7.02	1.52	1.41
19	D	501	HEC	C3C-C2C	6.99	1.48	1.40
15	C	404	JHB	C7-C8	6.57	1.51	1.37
19	D	501	HEC	C2B-C3B	4.86	1.45	1.40
17	D	503	PEE	C18-C19	3.83	1.54	1.31
14	C	403	HEM	C1B-NB	-3.70	1.33	1.40
17	C	409	PEE	C18-C19	3.54	1.52	1.31
14	C	402	HEM	C1B-NB	-3.51	1.34	1.40
19	D	501	HEC	C2A-C3A	3.37	1.47	1.37
19	D	501	HEC	C2A-C1A	3.22	1.49	1.42
14	C	402	HEM	C4D-ND	-3.15	1.34	1.40
19	D	501	HEC	C4B-C3B	3.14	1.48	1.43
19	D	501	HEC	C3A-C4A	3.12	1.49	1.42
14	C	403	HEM	C4B-NB	-3.04	1.32	1.38
19	D	501	HEC	C3D-C2D	3.01	1.46	1.37
16	C	405	LMT	O1'-C1'	2.88	1.45	1.40
14	C	402	HEM	C4D-C3D	2.72	1.49	1.45
19	D	501	HEC	C1C-CHC	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	404	JHB	O1-C23	2.64	1.46	1.31
19	D	501	HEC	C3C-C4C	2.59	1.47	1.43
15	C	404	JHB	C3-C2	2.54	1.42	1.38
14	C	402	HEM	FE-NB	2.45	2.09	1.96
14	C	402	HEM	C3B-C4B	2.43	1.49	1.44
14	C	403	HEM	C4D-ND	-2.38	1.36	1.40
14	C	403	HEM	FE-NB	2.38	2.08	1.96
19	D	501	HEC	C1B-CHB	2.35	1.47	1.41
15	C	404	JHB	C2-CL	2.26	1.79	1.74
14	C	402	HEM	C4B-NB	-2.26	1.34	1.38
19	D	501	HEC	C4D-CHA	2.12	1.46	1.41
14	C	402	HEM	C1D-ND	-2.08	1.34	1.38
14	C	403	HEM	C1D-ND	-2.04	1.34	1.38
14	C	403	HEM	C1D-C2D	2.01	1.48	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	501	HEC	C1D-C2D-C3D	-6.06	102.78	107.00
19	D	501	HEC	CMC-C2C-C3C	5.21	131.95	125.82
19	D	501	HEC	CMB-C2B-C3B	5.04	131.75	125.82
16	C	405	LMT	C1B-O5B-C5B	4.56	122.64	113.69
14	C	402	HEM	CHC-C4B-NB	4.34	129.15	124.43
14	C	403	HEM	CHC-C4B-NB	4.20	129.00	124.43
14	C	403	HEM	C1B-NB-C4B	4.05	109.26	105.07
19	D	501	HEC	CBD-CAD-C3D	-4.03	105.75	112.62
16	C	405	LMT	C1'-O5'-C5'	3.93	121.41	113.69
16	C	405	LMT	C1-O1'-C1'	3.76	120.08	113.84
14	C	402	HEM	C1B-NB-C4B	3.74	108.94	105.07
15	C	404	JHB	C5-C4-N	3.68	122.39	119.49
15	C	404	JHB	C13-C16-C17	-3.60	100.98	113.84
15	C	404	JHB	C4-C5-C6	-3.29	117.58	120.36
15	C	404	JHB	C10-C7-N	3.26	120.27	115.68
14	C	402	HEM	CAD-C3D-C4D	3.22	130.29	124.66
14	C	403	HEM	CHA-C4D-ND	3.06	128.17	124.38
14	C	403	HEM	CHD-C1D-ND	3.03	127.73	124.43
14	C	403	HEM	O2A-CGA-O1A	-3.03	115.74	123.30
14	C	402	HEM	CHD-C1D-C2D	-3.00	120.30	124.98
21	E	202	PX4	O7-C23-C24	2.93	117.81	111.50
16	C	405	LMT	O1B-C1B-C2B	2.89	115.60	108.10
14	C	403	HEM	CHB-C1B-NB	2.86	127.91	124.38
14	C	402	HEM	CHD-C1D-ND	2.83	127.51	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	403	HEM	CHA-C4D-C3D	-2.66	120.33	125.33
14	C	403	HEM	O2A-CGA-CBA	2.61	122.41	114.03
13	E	203	CDL	CB2-C1-CA2	2.53	120.25	112.79
14	C	402	HEM	CHB-C1B-NB	2.48	127.45	124.38
14	C	402	HEM	CMD-C2D-C1D	2.44	128.76	125.04
13	C	408	CDL	OB6-CB5-C51	2.40	117.49	110.80
13	C	408	CDL	O1-C1-CB2	2.37	117.85	109.56
14	C	402	HEM	O2D-CGD-CBD	2.36	121.60	114.03
19	D	501	HEC	CBA-CAA-C2A	2.34	116.56	112.60
16	C	405	LMT	C3'-C4'-C5'	-2.33	105.59	110.93
16	C	405	LMT	O5B-C5B-C4B	2.12	113.55	109.69
14	C	403	HEM	CAD-C3D-C4D	2.12	128.37	124.66
19	D	501	HEC	C4C-C3C-C2C	-2.11	104.08	106.35
13	C	401	CDL	CB2-C1-CA2	2.11	118.98	112.79
17	D	503	PEE	O2-C10-C11	2.09	116.01	111.50
16	C	405	LMT	O1B-C4'-C3'	2.07	112.78	107.28
14	C	403	HEM	O2D-CGD-CBD	2.03	120.56	114.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	C	409	PEE	C2
17	D	503	PEE	C2

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	502	6PE	C1-O3-P1-O1
12	A	502	6PE	C11-C10-O6-C2
12	A	502	6PE	O8-C16-C17-N1
13	C	401	CDL	CB2-OB2-PB2-OB3
13	C	401	CDL	CB3-OB5-PB2-OB4
13	C	408	CDL	CA3-OA5-PA1-OA4
13	D	502	CDL	OA5-CA3-CA4-OA6
13	D	502	CDL	CB2-OB2-PB2-OB4
13	E	203	CDL	CA2-OA2-PA1-OA3
13	E	203	CDL	CB3-OB5-PB2-OB3
13	E	203	CDL	C51-CB5-OB6-CB4
16	C	405	LMT	C2-C1-O1'-C1'
17	C	409	PEE	C4-O4P-P-O2P
17	D	503	PEE	C1-O3P-P-O2P
17	D	503	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
21	E	202	PX4	C1-O3-P1-O2
21	E	202	PX4	C24-C23-O7-C7
13	C	408	CDL	C11-CA5-OA6-CA4
13	D	502	CDL	OB9-CB7-OB8-CB6
12	A	502	6PE	O7-C10-O6-C2
13	C	401	CDL	OB7-CB5-OB6-CB4
13	E	203	CDL	OB7-CB5-OB6-CB4
21	E	202	PX4	O8-C23-O7-C7
13	C	401	CDL	C51-CB5-OB6-CB4
13	C	408	CDL	OA7-CA5-OA6-CA4
13	C	408	CDL	C31-CA7-OA8-CA6
21	E	202	PX4	O6-C9-O5-C8
17	C	409	PEE	C31-C30-O3-C3
13	D	502	CDL	C71-CB7-OB8-CB6
17	C	409	PEE	C17-C18-C19-C20
13	D	502	CDL	OB7-CB5-OB6-CB4
17	C	409	PEE	O5-C30-O3-C3
13	C	401	CDL	O1-C1-CA2-OA2
13	D	502	CDL	O1-C1-CA2-OA2
13	D	502	CDL	O1-C1-CB2-OB2
13	D	502	CDL	C31-CA7-OA8-CA6
13	D	502	CDL	C51-CB5-OB6-CB4
21	E	202	PX4	C10-C9-O5-C8
13	D	502	CDL	OA9-CA7-OA8-CA6
11	C	407	PG4	O2-C3-C4-O3
16	C	405	LMT	O5B-C5B-C6B-O6B
11	A	501	PG4	O2-C3-C4-O3
13	C	401	CDL	CA2-C1-CB2-OB2
16	C	405	LMT	C4B-C5B-C6B-O6B
11	A	503	PG4	O2-C3-C4-O3
11	C	406	PG4	O2-C3-C4-O3
13	C	408	CDL	OA9-CA7-OA8-CA6
13	C	408	CDL	CB7-C71-C72-C73
13	D	502	CDL	CA5-C11-C12-C13
13	E	203	CDL	CB4-CB3-OB5-PB2
13	E	203	CDL	CA5-C11-C12-C13
11	A	501	PG4	O1-C1-C2-O2
11	C	407	PG4	O1-C1-C2-O2
13	C	401	CDL	CB5-C51-C52-C53
13	C	401	CDL	OA5-CA3-CA4-OA6
11	C	406	PG4	O3-C5-C6-O4
13	E	203	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
12	A	502	6PE	C1-O3-P1-O8
13	C	401	CDL	CA3-OA5-PA1-OA2
13	C	401	CDL	CB2-OB2-PB2-OB5
13	C	408	CDL	CA3-OA5-PA1-OA2
13	D	502	CDL	CB2-OB2-PB2-OB5
17	C	409	PEE	C4-O4P-P-O3P
17	D	503	PEE	C1-O3P-P-O4P
13	C	408	CDL	C71-CB7-OB8-CB6
13	C	401	CDL	OA5-CA3-CA4-CA6
13	E	203	CDL	OA7-CA5-OA6-CA4
11	C	406	PG4	O1-C1-C2-O2
13	E	203	CDL	C31-CA7-OA8-CA6
17	D	503	PEE	C30-C31-C32-C33
17	C	409	PEE	C31-C32-C33-C34
13	E	203	CDL	C53-C54-C55-C56
21	E	202	PX4	C14-C15-C16-C17
13	E	203	CDL	C52-C53-C54-C55
13	E	203	CDL	C51-C52-C53-C54
16	C	405	LMT	C5-C6-C7-C8
17	C	409	PEE	C32-C33-C34-C35
16	C	405	LMT	C2'-C1'-O1'-C1
17	C	409	PEE	C13-C14-C15-C16
17	C	409	PEE	C14-C15-C16-C17
21	E	202	PX4	C16-C17-C18-C19
13	C	408	CDL	OB9-CB7-OB8-CB6
13	D	502	CDL	C51-C52-C53-C54
13	D	502	CDL	C53-C54-C55-C56
21	E	202	PX4	C13-C14-C15-C16
16	C	405	LMT	O5'-C1'-O1'-C1
16	C	405	LMT	C4-C5-C6-C7
13	E	203	CDL	C15-C16-C17-C18
16	C	405	LMT	C7-C8-C9-C10
21	E	202	PX4	C12-C13-C14-C15
13	E	203	CDL	CA7-C31-C32-C33
13	E	203	CDL	OA9-CA7-OA8-CA6
21	E	202	PX4	C18-C19-C20-C21
17	D	503	PEE	C31-C30-O3-C3
21	E	202	PX4	C17-C18-C19-C20
13	C	408	CDL	OB7-CB5-OB6-CB4
13	C	408	CDL	C51-CB5-OB6-CB4
17	D	503	PEE	C11-C10-O2-C2
12	A	502	6PE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	D	503	PEE	O4-C10-O2-C2
11	A	503	PG4	O4-C7-C8-O5
17	D	503	PEE	O5-C30-O3-C3
13	E	203	CDL	C54-C55-C56-C57
17	C	409	PEE	C11-C12-C13-C14
13	E	203	CDL	C71-CB7-OB8-CB6
16	C	405	LMT	C6-C7-C8-C9
17	D	503	PEE	C13-C14-C15-C16
13	D	502	CDL	C11-C12-C13-C14
13	C	401	CDL	CB3-OB5-PB2-OB2
12	A	502	6PE	C2-C1-O3-P1
13	C	401	CDL	OB5-CB3-CB4-CB6
13	D	502	CDL	OA5-CA3-CA4-CA6
13	D	502	CDL	OB5-CB3-CB4-CB6
16	C	405	LMT	C1-C2-C3-C4
13	D	502	CDL	CA3-CA4-CA6-OA8
17	D	503	PEE	C34-C35-C36-C37
13	D	502	CDL	C54-C55-C56-C57
17	D	503	PEE	C15-C16-C17-C18
17	C	409	PEE	C10-C11-C12-C13
21	E	202	PX4	C24-C25-C26-C27
11	A	503	PG4	O3-C5-C6-O4
13	C	401	CDL	C71-CB7-OB8-CB6
13	C	408	CDL	O1-C1-CA2-OA2
13	C	401	CDL	OB9-CB7-OB8-CB6
13	E	203	CDL	CB5-C51-C52-C53
13	C	408	CDL	C75-C76-C77-C78
13	E	203	CDL	CA2-C1-CB2-OB2
13	E	203	CDL	C13-C14-C15-C16
17	C	409	PEE	O3P-C1-C2-C3
17	D	503	PEE	C14-C15-C16-C17
13	C	408	CDL	C71-C72-C73-C74
13	C	408	CDL	CB4-CB3-OB5-PB2
13	E	203	CDL	CA3-CA4-CA6-OA8
13	D	502	CDL	C31-C32-C33-C34
13	C	408	CDL	OB5-CB3-CB4-OB6
17	C	409	PEE	O3P-C1-C2-O2
13	E	203	CDL	OA6-CA4-CA6-OA8
17	D	503	PEE	O2-C2-C3-O3
13	E	203	CDL	C35-C36-C37-C38
13	E	203	CDL	C1-CA2-OA2-PA1
13	E	203	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
13	C	408	CDL	OB5-CB3-CB4-CB6
17	D	503	PEE	O3P-C1-C2-C3
13	E	203	CDL	C17-C18-C19-C20
13	D	502	CDL	CB6-CB4-OB6-CB5
11	A	503	PG4	C1-C2-O2-C3
11	A	501	PG4	C1-C2-O2-C3
11	A	501	PG4	C3-C4-O3-C5
11	A	501	PG4	C8-C7-O4-C6
11	A	501	PG4	C5-C6-O4-C7
11	A	503	PG4	C8-C7-O4-C6
12	A	502	6PE	O6-C2-C3-O4
17	D	503	PEE	C19-C20-C21-C22
21	E	202	PX4	C10-C11-C12-C13
11	C	406	PG4	C4-C3-O2-C2
21	E	202	PX4	C1-O3-P1-O4
13	C	401	CDL	CA3-OA5-PA1-OA3
13	C	401	CDL	CB2-OB2-PB2-OB4
13	C	401	CDL	CB3-OB5-PB2-OB3
13	E	203	CDL	CB3-OB5-PB2-OB4
17	C	409	PEE	C4-O4P-P-O1P
16	C	405	LMT	C11-C10-C9-C8
13	C	401	CDL	OB5-CB3-CB4-OB6
21	E	202	PX4	O3-C1-C2-N1
13	D	502	CDL	OA6-CA4-CA6-OA8
13	E	203	CDL	C32-C33-C34-C35
13	E	203	CDL	C34-C35-C36-C37
17	C	409	PEE	C30-C31-C32-C33
11	C	406	PG4	C3-C4-O3-C5
11	C	407	PG4	C6-C5-O3-C4
13	D	502	CDL	OB5-CB3-CB4-OB6
13	E	203	CDL	OA5-CA3-CA4-OA6
14	C	402	HEM	C2A-CAA-CBA-CGA
13	C	408	CDL	CB2-OB2-PB2-OB5
13	E	203	CDL	CA2-OA2-PA1-OA5
13	E	203	CDL	CB2-OB2-PB2-OB5
14	C	403	HEM	CAD-CBD-CGD-O1D
17	C	409	PEE	C15-C16-C17-C18
11	C	407	PG4	C4-C3-O2-C2
14	C	403	HEM	CAA-CBA-CGA-O1A
13	E	203	CDL	C14-C15-C16-C17
14	C	403	HEM	CAA-CBA-CGA-O2A
13	C	408	CDL	C72-C73-C74-C75

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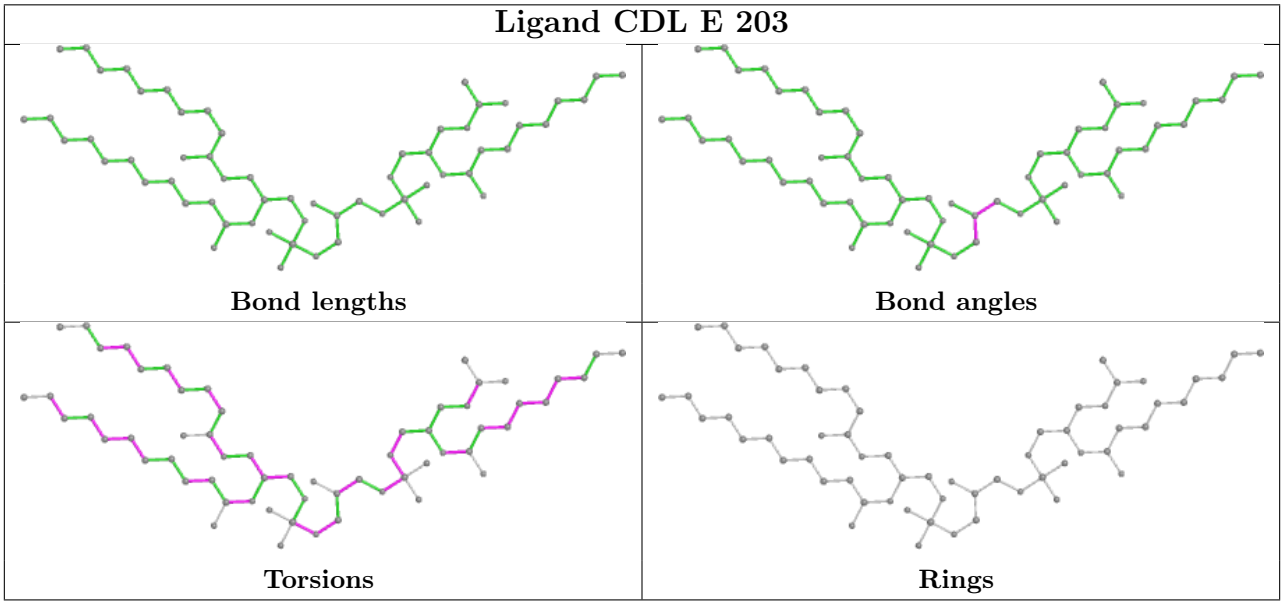
Mol	Chain	Res	Type	Atoms
17	D	503	PEE	C32-C33-C34-C35
17	D	503	PEE	C3-C2-O2-C10
13	D	502	CDL	CA2-C1-CB2-OB2
14	C	403	HEM	CAD-CBD-CGD-O2D
17	D	503	PEE	C16-C17-C18-C19
12	A	502	6PE	C1-C2-C3-O4
14	C	402	HEM	CAD-CBD-CGD-O2D
11	A	503	PG4	C6-C5-O3-C4
17	D	503	PEE	O3P-C1-C2-O2
19	D	501	HEC	CAA-CBA-CGA-O2A
21	E	202	PX4	C11-C12-C13-C14
14	C	402	HEM	CAA-CBA-CGA-O2A
12	A	502	6PE	C5-C4-O4-C3
21	E	202	PX4	O7-C23-C24-C25
19	D	501	HEC	CAA-CBA-CGA-O1A
17	D	503	PEE	C18-C19-C20-C21
14	C	402	HEM	CAD-CBD-CGD-O1D
14	C	402	HEM	CAA-CBA-CGA-O1A
12	A	502	6PE	O5-C4-O4-C3
13	C	401	CDL	CA4-CA3-OA5-PA1
21	E	202	PX4	O8-C23-C24-C25
13	D	502	CDL	CA2-OA2-PA1-OA3
13	E	203	CDL	CB2-OB2-PB2-OB3
17	D	503	PEE	C4-O4P-P-O1P
17	D	503	PEE	C5-C4-O4P-P
17	D	503	PEE	C10-C11-C12-C13
21	E	202	PX4	C11-C10-C9-O5
13	C	401	CDL	CB2-C1-CA2-OA2
21	E	202	PX4	C23-C24-C25-C26
12	A	502	6PE	O5-C4-C5-C6
12	A	502	6PE	O4-C4-C5-C6
13	C	408	CDL	C72-C71-CB7-OB8
17	C	409	PEE	C33-C34-C35-C36
21	E	202	PX4	C11-C10-C9-O6
14	C	402	HEM	C3D-CAD-CBD-CGD
13	C	408	CDL	C72-C71-CB7-OB9
19	D	501	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

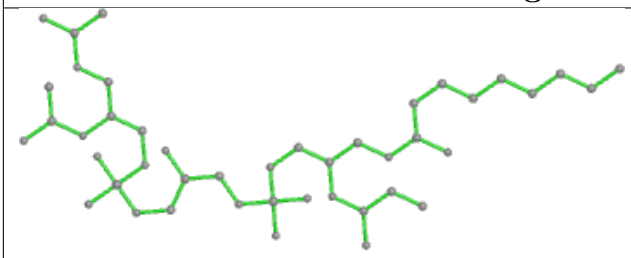
9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	503	PG4	9	0
19	D	501	HEC	5	0
15	C	404	JHB	3	0
14	C	403	HEM	4	0
12	A	502	6PE	1	0
17	D	503	PEE	1	0
13	D	502	CDL	1	0
14	C	402	HEM	2	0
13	C	401	CDL	2	0

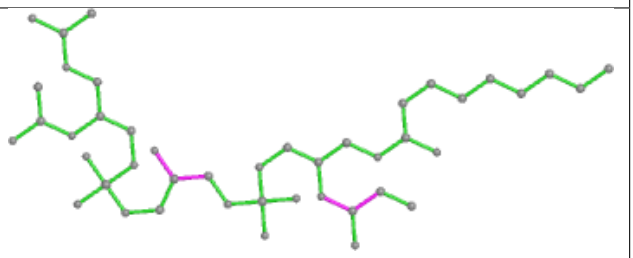
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



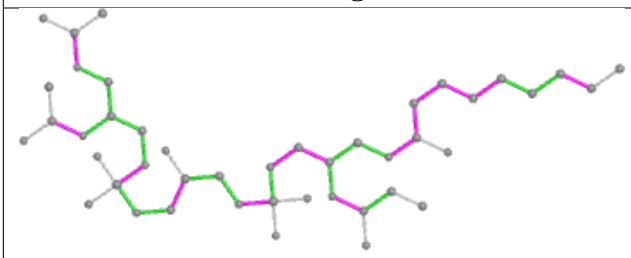
Ligand CDL C 408



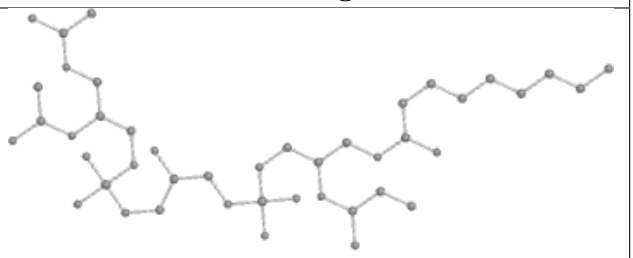
Bond lengths



Bond angles

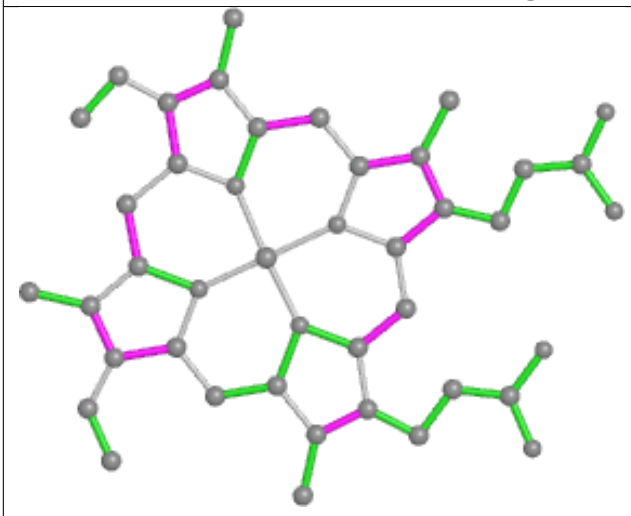


Torsions

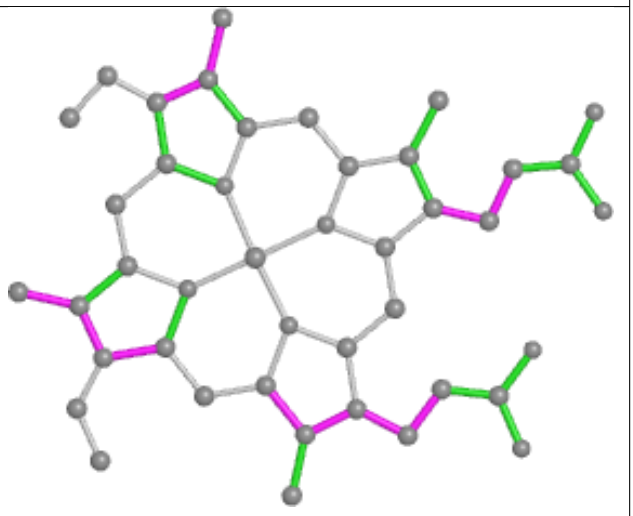


Rings

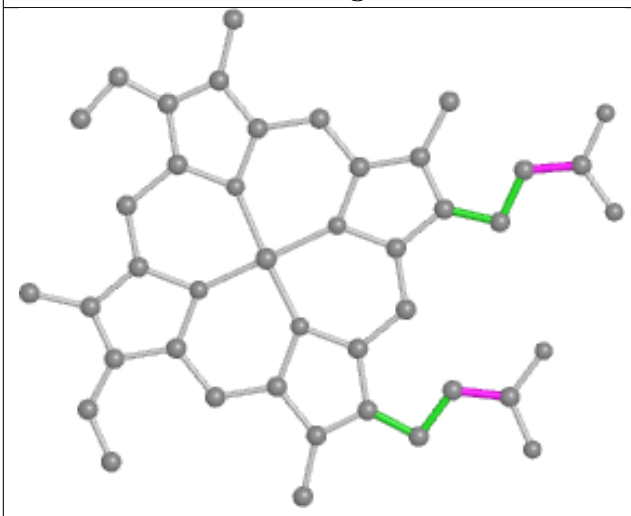
Ligand HEC D 501



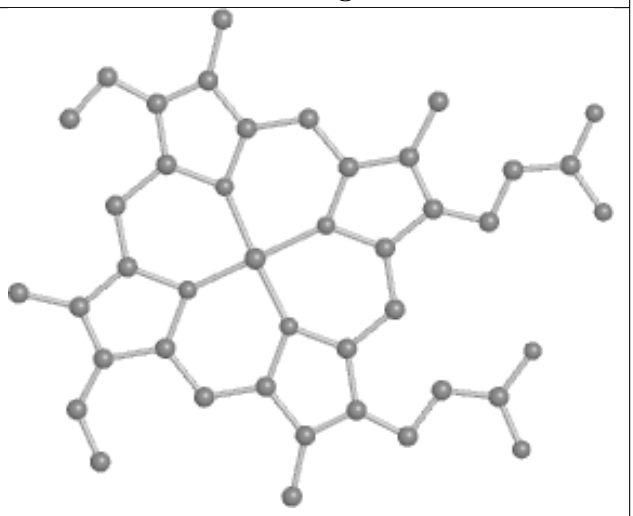
Bond lengths



Bond angles

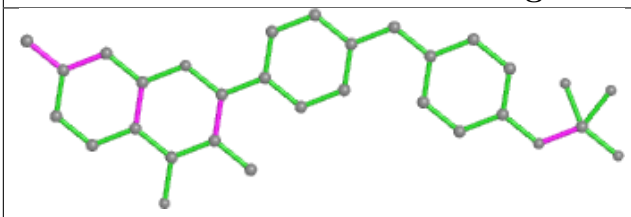


Torsions

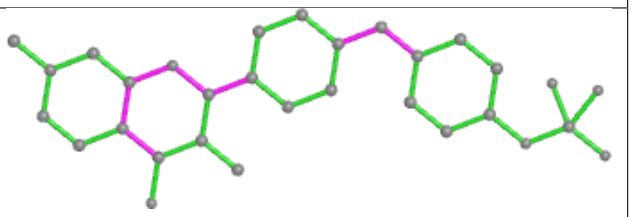


Rings

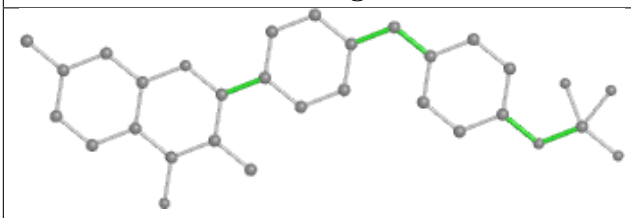
Ligand JHB C 404



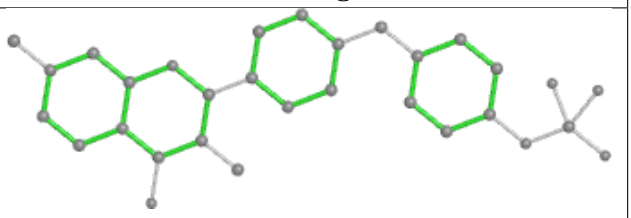
Bond lengths



Bond angles

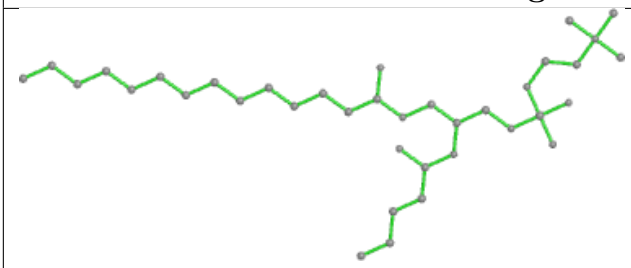


Torsions

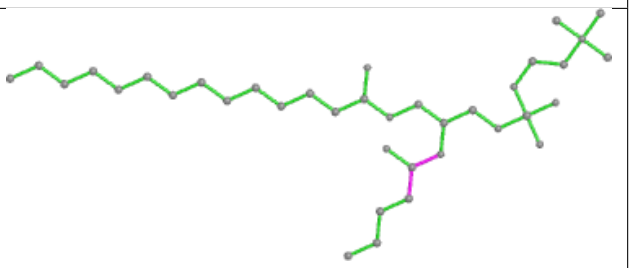


Rings

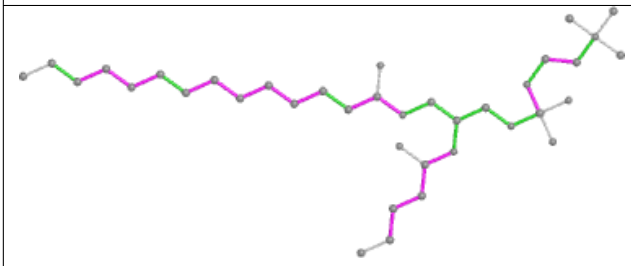
Ligand PX4 E 202



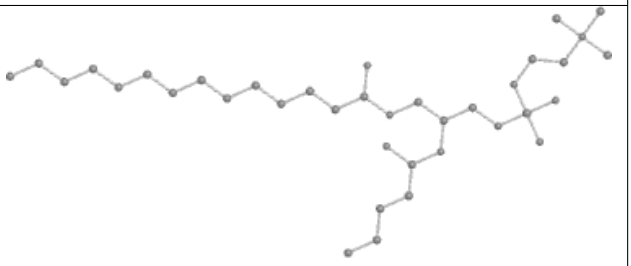
Bond lengths



Bond angles

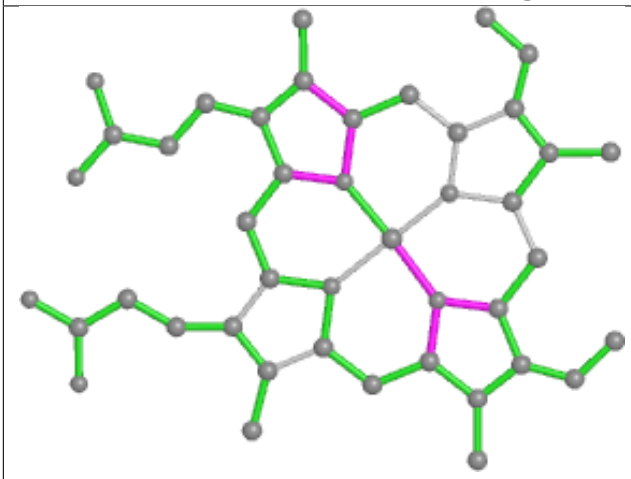


Torsions

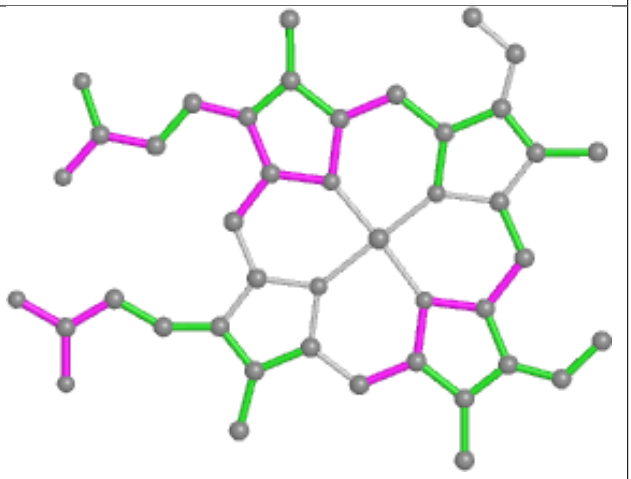


Rings

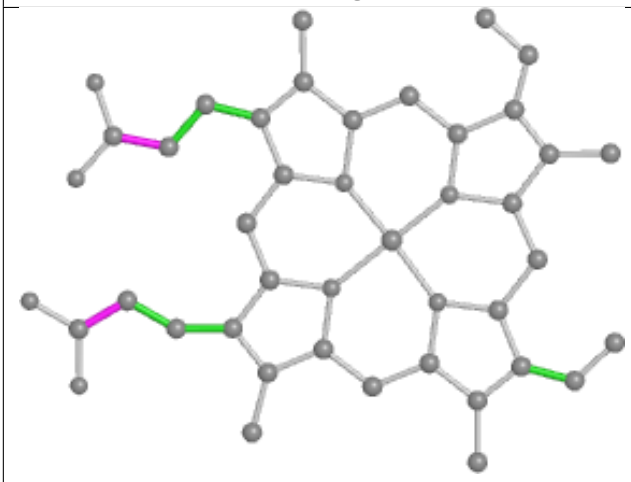
Ligand HEM C 403



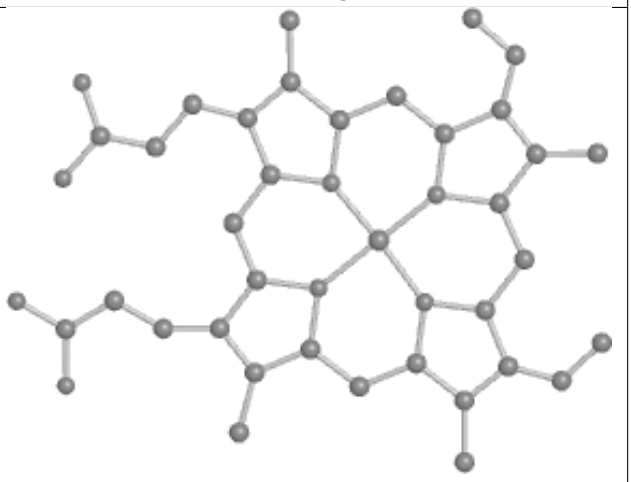
Bond lengths



Bond angles

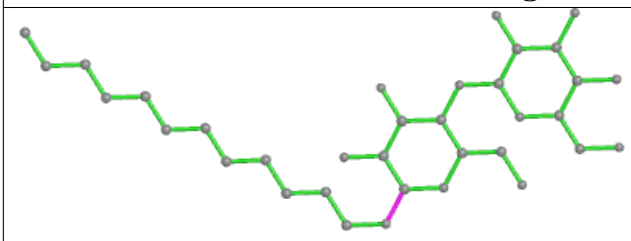


Torsions

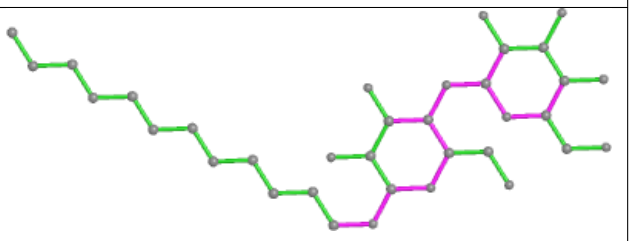


Rings

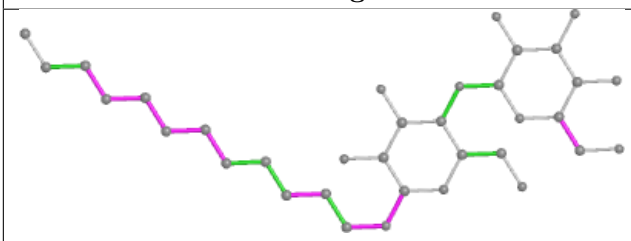
Ligand LMT C 405



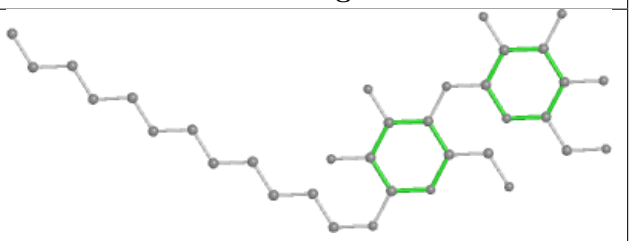
Bond lengths



Bond angles

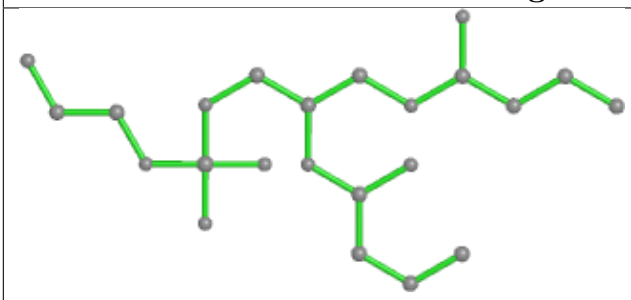


Torsions

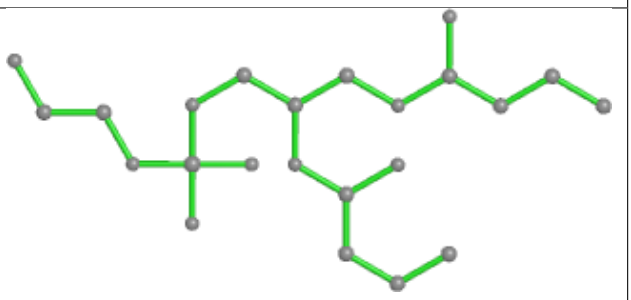


Rings

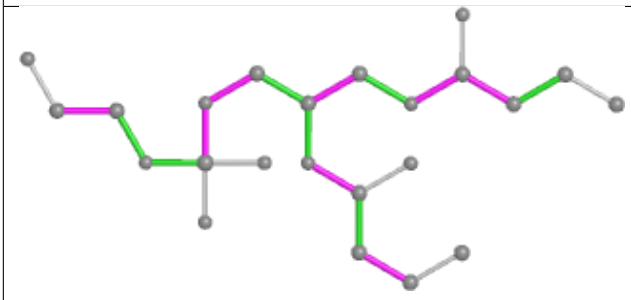
Ligand 6PE A 502



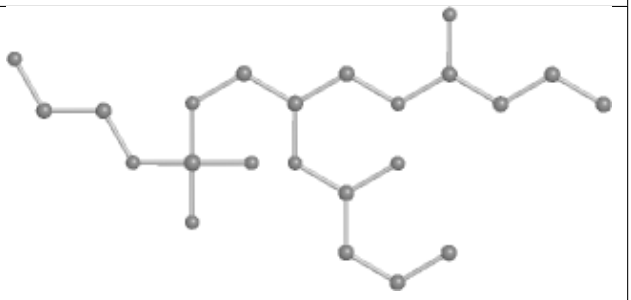
Bond lengths



Bond angles

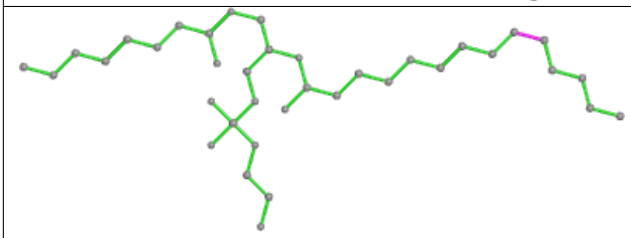


Torsions



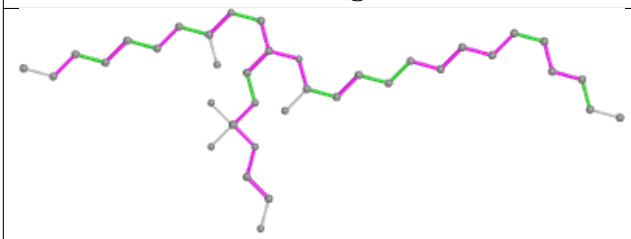
Rings

Ligand PEE D 503

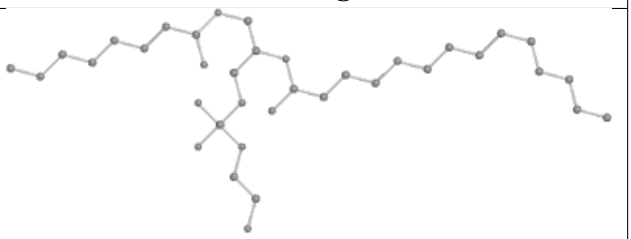


Bond lengths

Bond angles

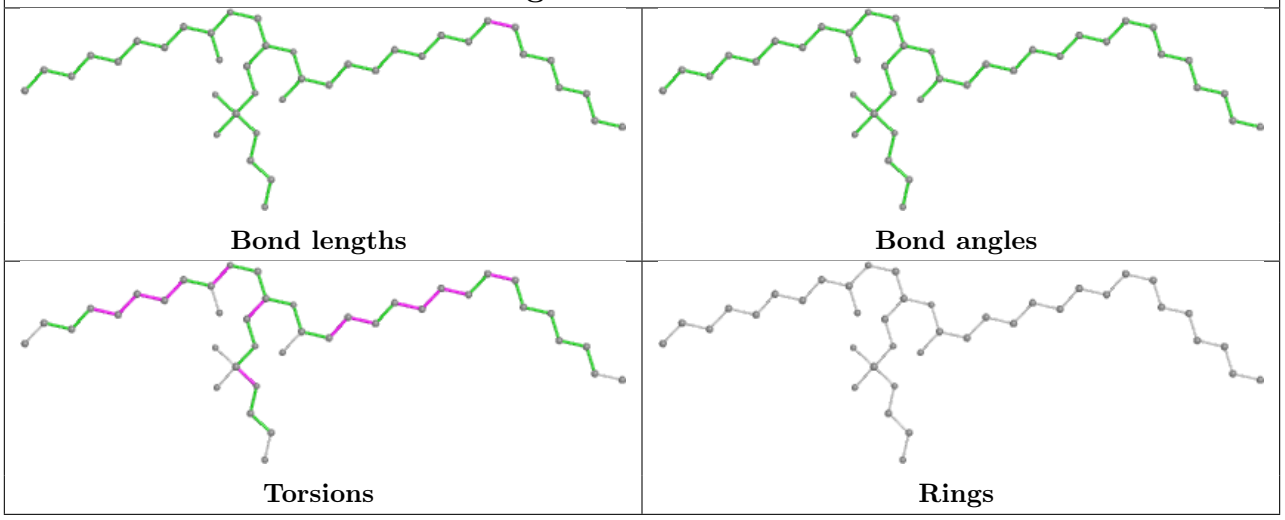


Torsions

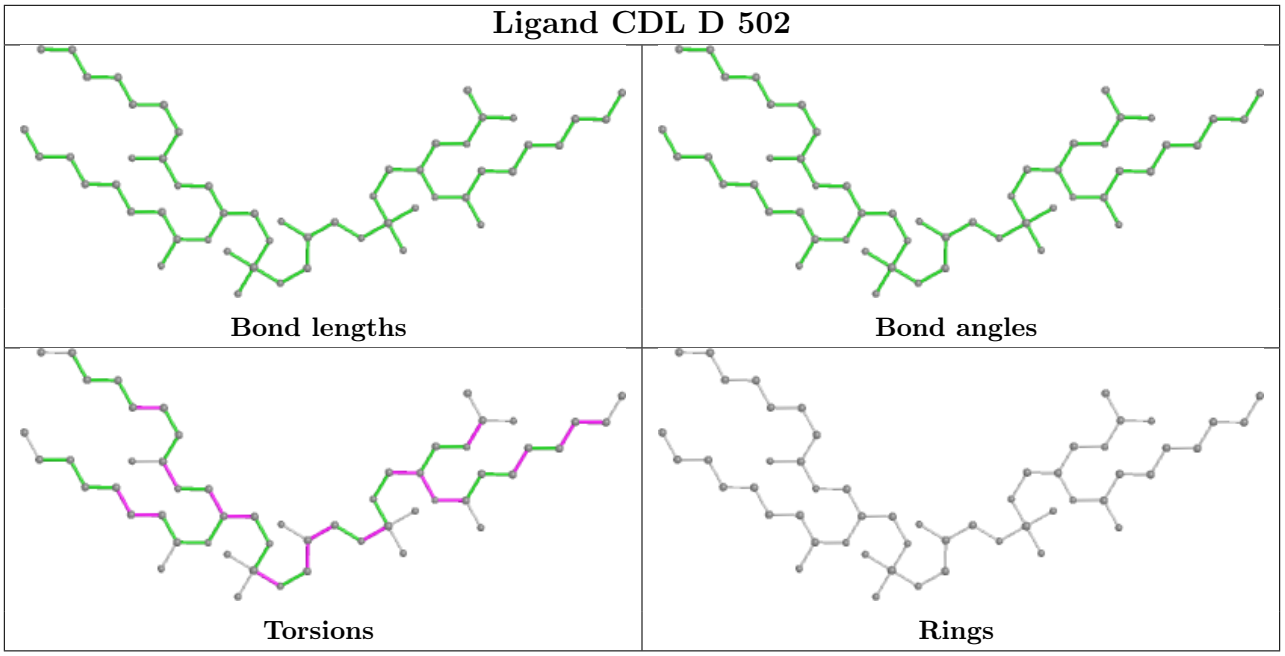


Rings

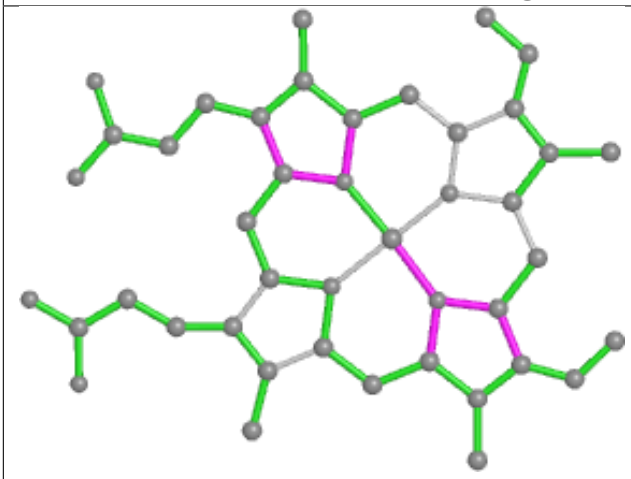
Ligand PEE C 409



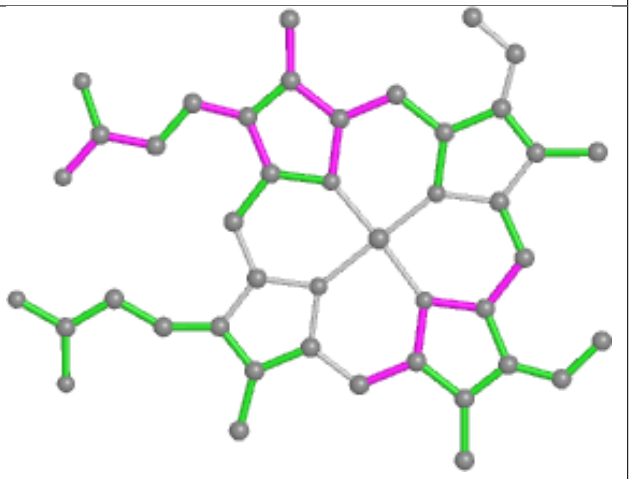
Ligand CDL D 502



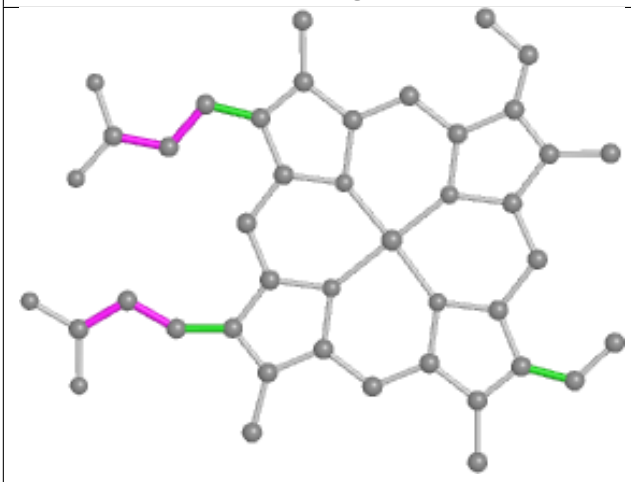
Ligand HEM C 402



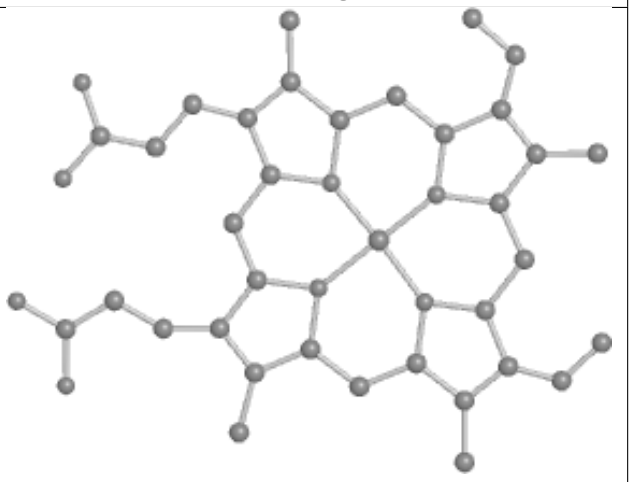
Bond lengths



Bond angles

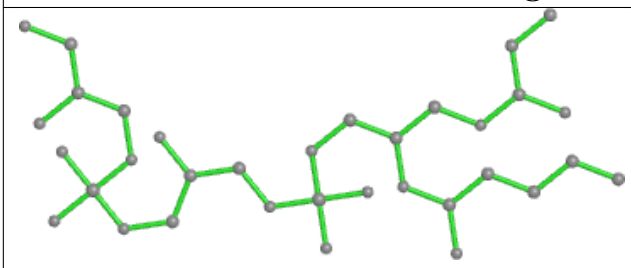


Torsions

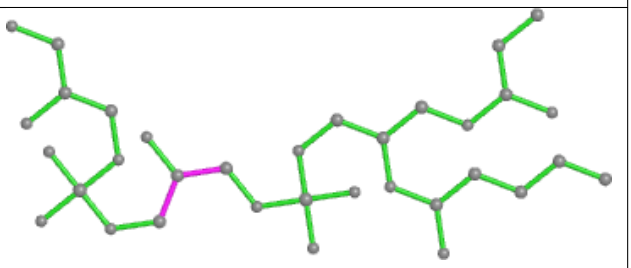


Rings

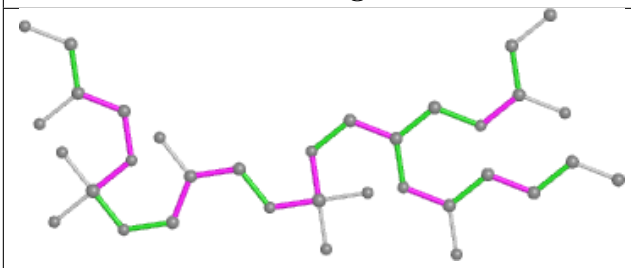
Ligand CDL C 401



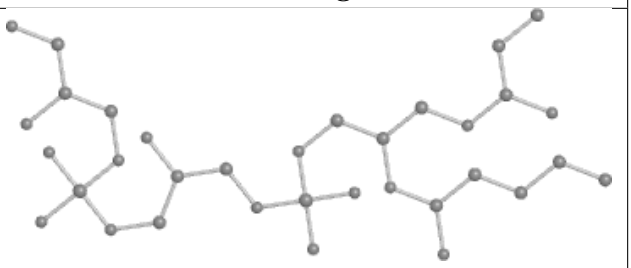
Bond lengths



Bond angles



Torsions



Rings

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	439/444 (98%)	-0.02	7 (1%) 72 70	72, 96, 128, 161	0
2	B	415/420 (98%)	-0.14	5 (1%) 79 78	72, 98, 129, 178	0
3	C	378/378 (100%)	-0.12	1 (0%) 94 94	72, 86, 116, 137	0
4	D	239/239 (100%)	0.20	14 (5%) 22 22	109, 135, 160, 186	0
5	E	196/196 (100%)	0.34	14 (7%) 16 16	82, 143, 179, 195	0
6	F	99/99 (100%)	-0.01	1 (1%) 82 82	80, 98, 141, 185	0
7	G	74/74 (100%)	-0.15	0 100 100	74, 98, 151, 157	0
8	H	65/65 (100%)	0.27	2 (3%) 49 48	143, 166, 184, 189	0
9	I	46/46 (100%)	1.70	18 (39%) 0 0	122, 144, 165, 176	0
10	J	59/59 (100%)	-0.10	1 (1%) 70 68	90, 106, 151, 157	0
All	All	2010/2020 (99%)	0.04	63 (3%) 49 48	72, 104, 164, 195	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	37	THR	6.0
5	E	152	ASP	5.0
5	E	159	PRO	5.0
8	H	13	LEU	4.8
5	E	163	SER	4.7
9	I	33	ALA	4.7
9	I	48	SER	4.7
5	E	162	GLY	4.2
5	E	164	HIS	4.1
9	I	38	SER	4.0
5	E	155	GLY	4.0
9	I	47	ARG	4.0
4	D	108	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
9	I	54	SER	3.8
5	E	157	TYR	3.6
9	I	36	ALA	3.3
2	B	43	PRO	3.2
2	B	20	HIS	3.2
1	A	228	VAL	3.0
9	I	39	GLU	2.9
1	A	216	PHE	2.8
9	I	76	VAL	2.8
4	D	139	THR	2.8
9	I	50	LEU	2.8
4	D	107	GLY	2.7
1	A	392	LEU	2.7
1	A	227	THR	2.7
4	D	81	PHE	2.6
5	E	86	ASN	2.6
9	I	75	SER	2.6
9	I	58	GLN	2.5
1	A	365	LEU	2.5
2	B	264	ILE	2.5
4	D	164	ILE	2.5
4	D	165	TYR	2.5
9	I	57	GLY	2.5
6	F	11	ARG	2.5
5	E	83	GLU	2.5
1	A	9	GLN	2.5
5	E	108	GLN	2.4
5	E	153	PHE	2.4
10	J	60	GLU	2.4
4	D	240	PRO	2.4
9	I	40	SER	2.3
4	D	145	GLU	2.3
1	A	203	LEU	2.3
5	E	156	TYR	2.3
9	I	59	ALA	2.3
9	I	49	VAL	2.3
8	H	49	GLN	2.2
4	D	113	LEU	2.2
9	I	41	PRO	2.2
5	E	158	CYS	2.1
4	D	147	LEU	2.1
4	D	77	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	2	THR	2.1
4	D	79	GLU	2.1
4	D	148	TYR	2.1
4	D	157	ALA	2.1
9	I	43	LEU	2.0
2	B	21	PRO	2.0
5	E	161	HIS	2.0
2	B	44	ALA	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
18	PO4	H	101	5/5	0.37	0.28	209,210,213,216	0
18	PO4	G	102	5/5	0.67	0.16	175,175,177,181	0
13	CDL	E	203	60/100	0.69	0.55	130,164,197,201	0
11	PG4	A	501	13/13	0.70	0.40	127,137,143,144	0
16	LMT	C	405	35/35	0.76	0.38	155,168,174,175	0
11	PG4	C	407	13/13	0.77	0.47	105,108,113,114	0
18	PO4	F	501	5/5	0.79	0.26	153,156,156,157	0
18	PO4	C	410	5/5	0.81	0.27	159,161,162,162	0
18	PO4	G	103	5/5	0.85	0.19	134,134,134,135	0
18	PO4	G	101	5/5	0.87	0.17	127,128,130,131	0
11	PG4	C	406	13/13	0.89	0.44	91,93,96,96	0
13	CDL	D	502	54/100	0.89	0.42	112,152,177,180	0
15	JHB	C	404	31/31	0.90	0.23	90,97,124,128	0
13	CDL	C	401	34/100	0.90	0.20	116,129,138,139	0
11	PG4	A	503	13/13	0.91	0.21	47,57,70,71	0

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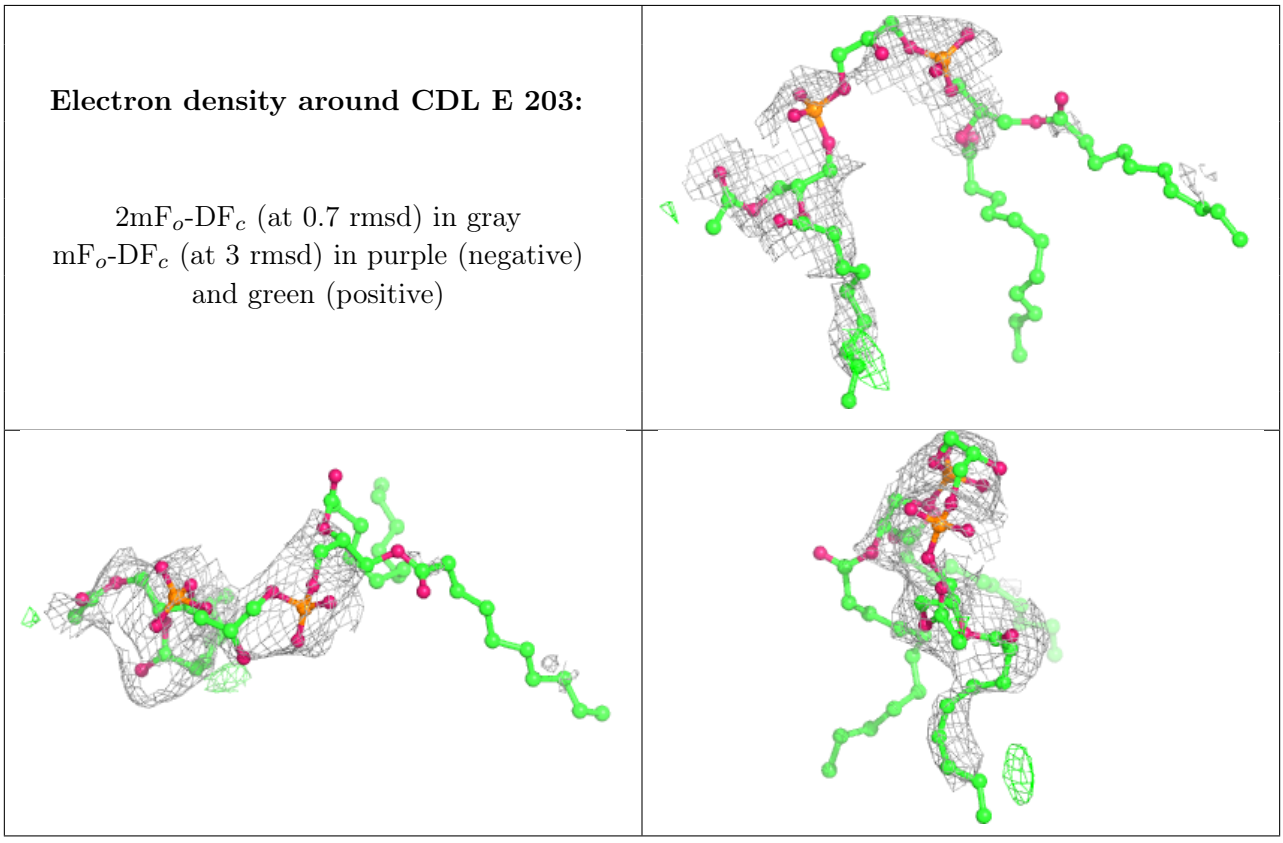
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	PEE	D	503	37/51	0.92	0.58	89,106,110,110	0
21	PX4	E	202	37/46	0.92	0.47	119,132,142,144	0
12	6PE	A	502	23/27	0.93	0.24	109,122,132,132	0
13	CDL	C	408	44/100	0.94	0.24	86,92,96,96	0
20	FES	E	201	4/4	0.95	0.08	214,214,217,220	0
17	PEE	C	409	40/51	0.96	0.28	82,84,85,85	0
19	HEC	D	501	43/43	0.98	0.30	126,132,135,138	0
14	HEM	C	402	43/43	0.98	0.27	76,77,79,79	0
14	HEM	C	403	43/43	0.98	0.23	73,73,73,74	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.

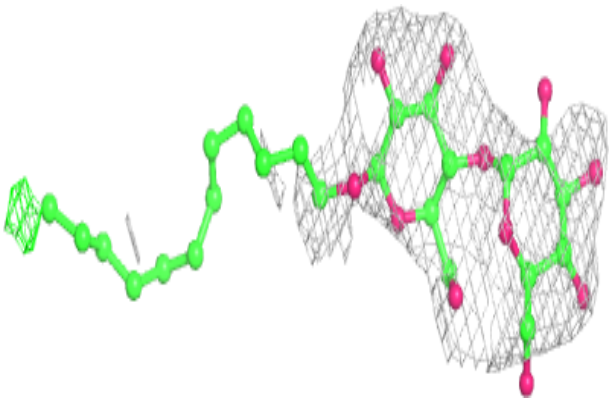
Electron density around CDL E 203:

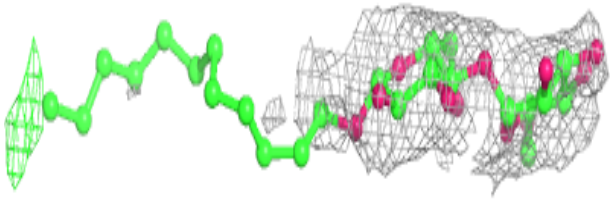
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

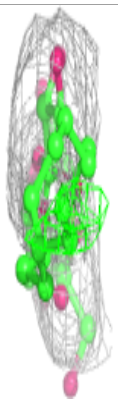


Electron density around LMT C 405:

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

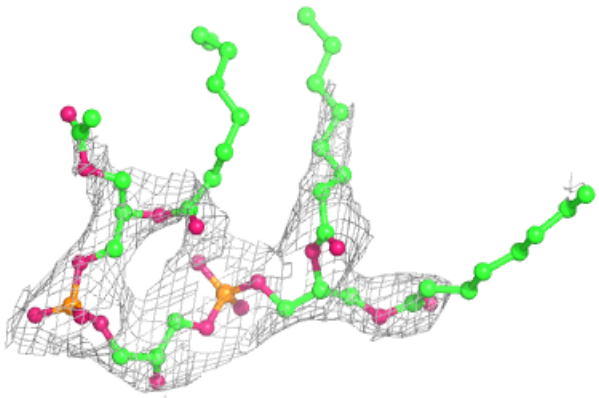


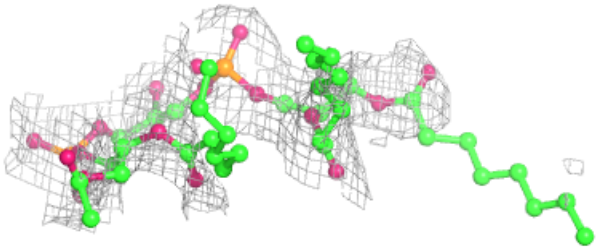


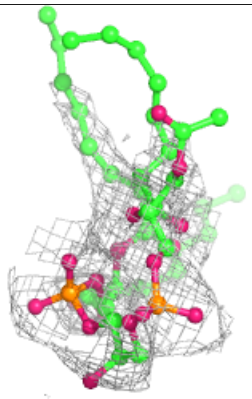


Electron density around CDL D 502:

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

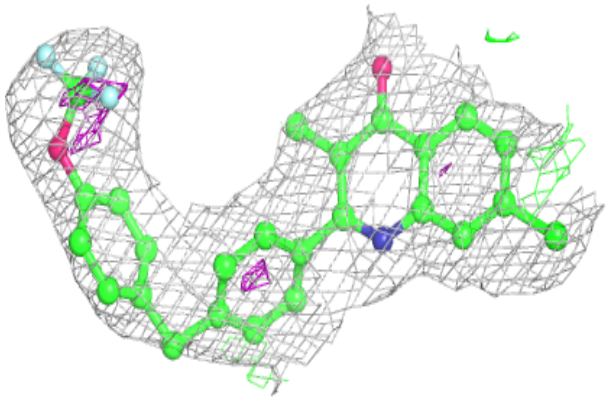


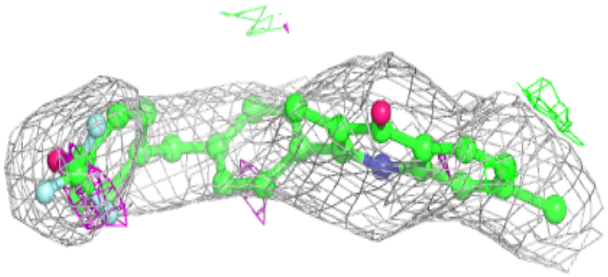


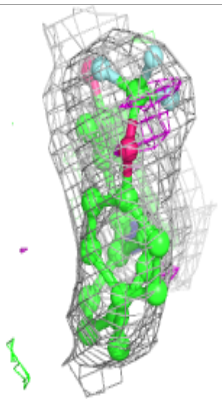


Electron density around JHB C 404:

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

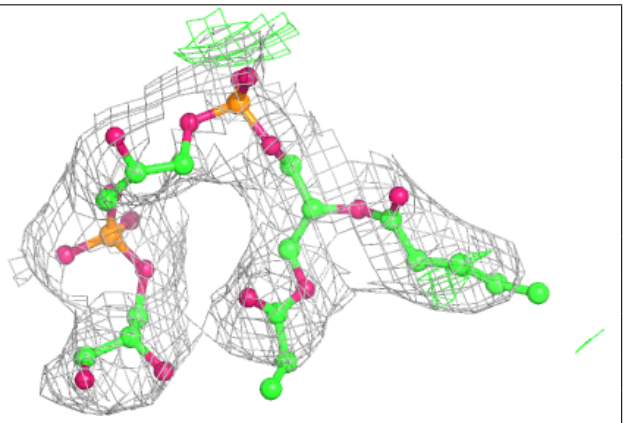


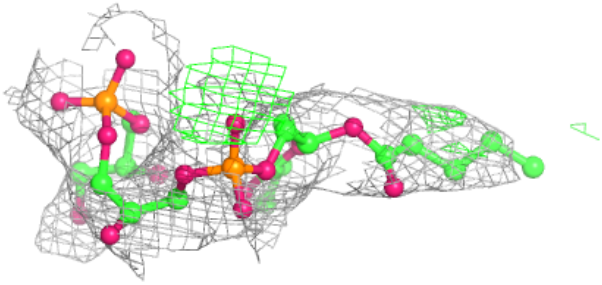


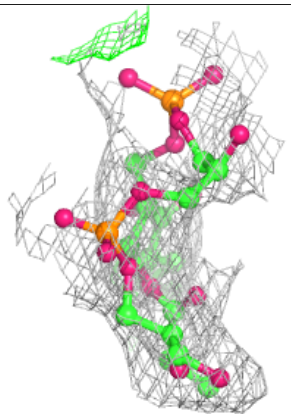


Electron density around CDL C 401:

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

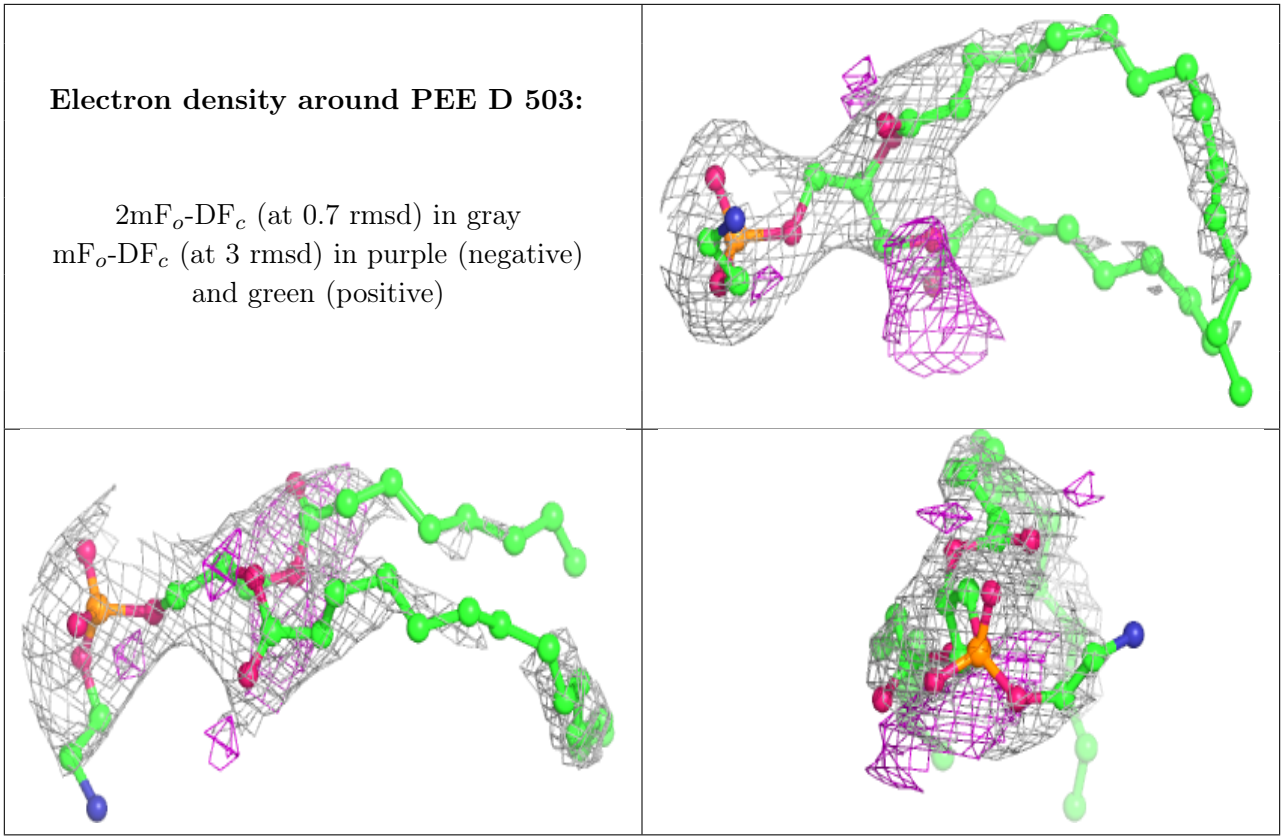






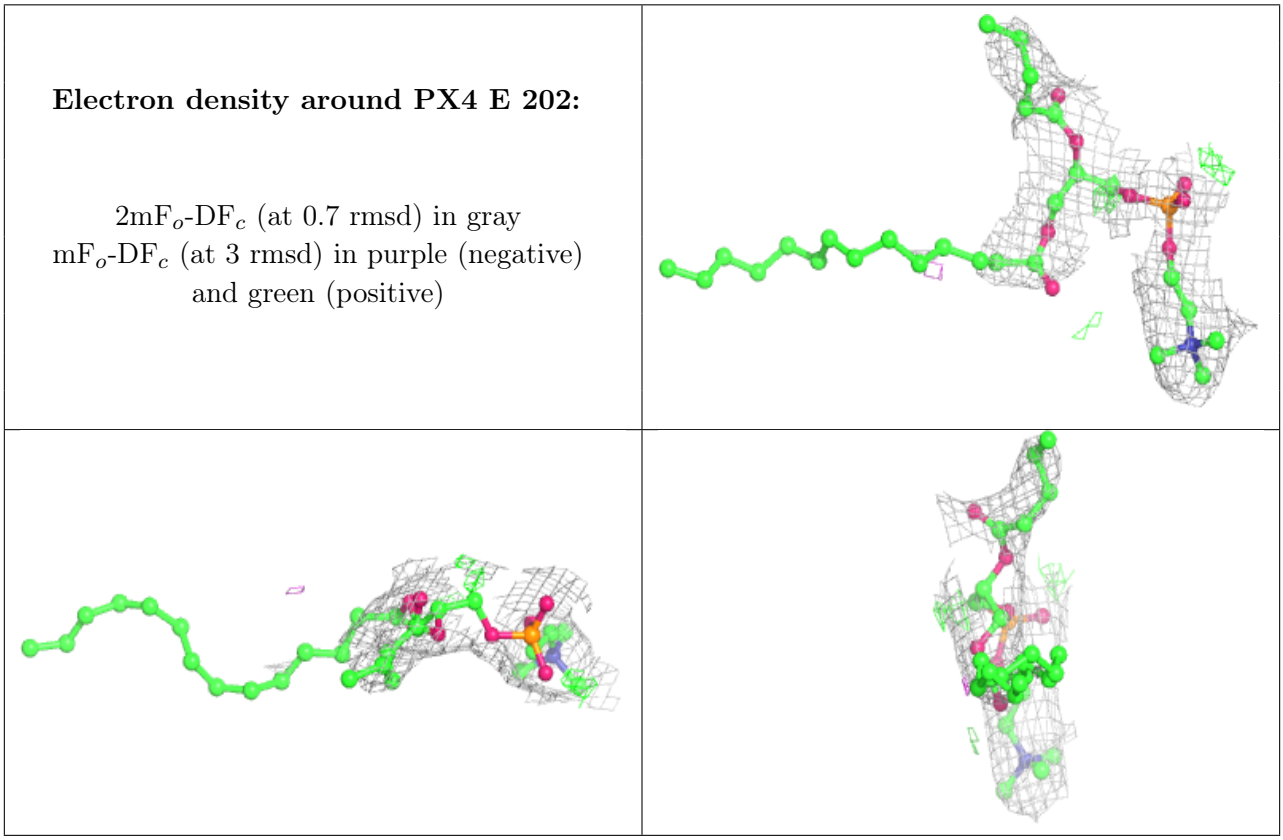
Electron density around PEE D 503:

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



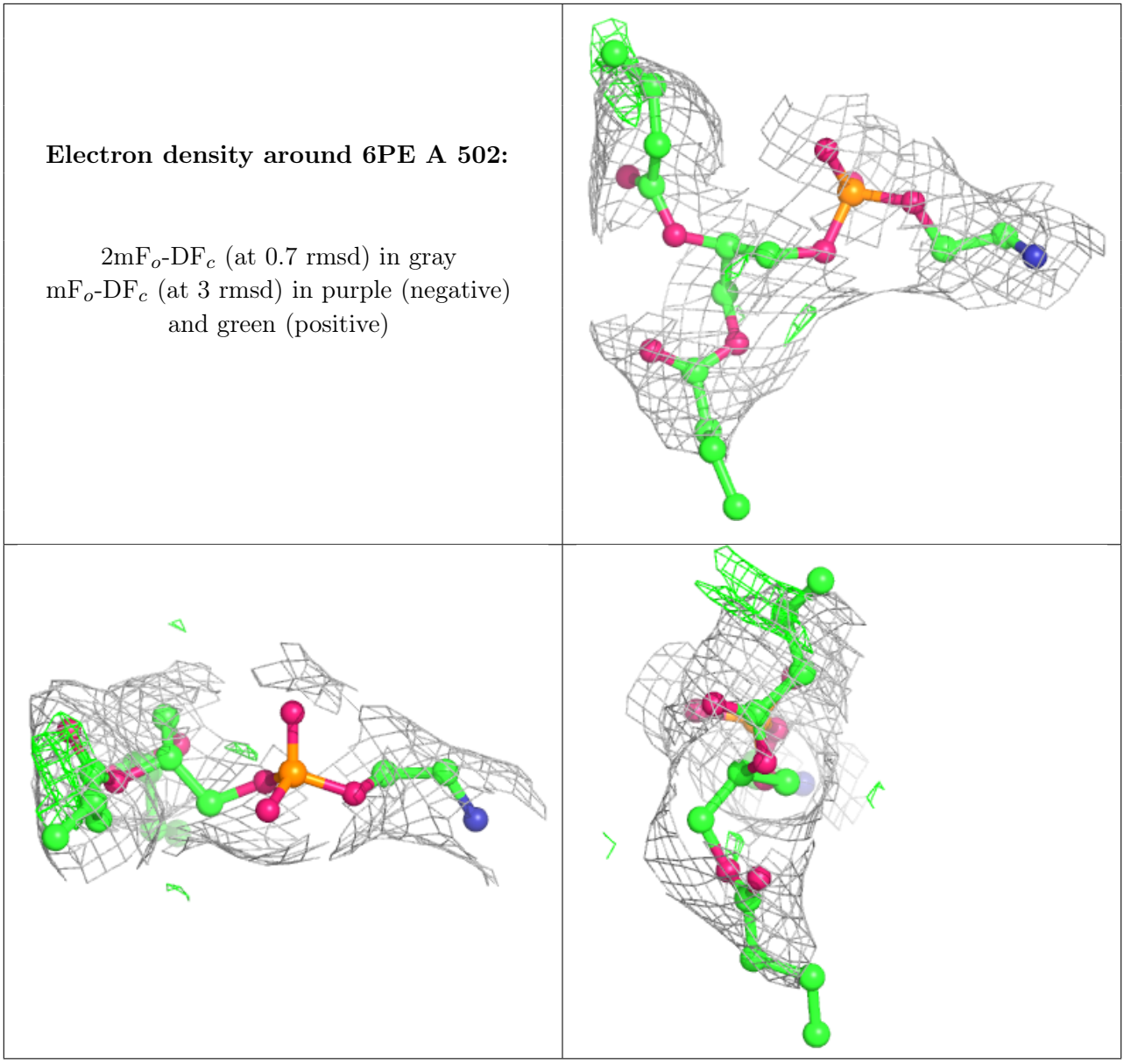
Electron density around PX4 E 202:

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



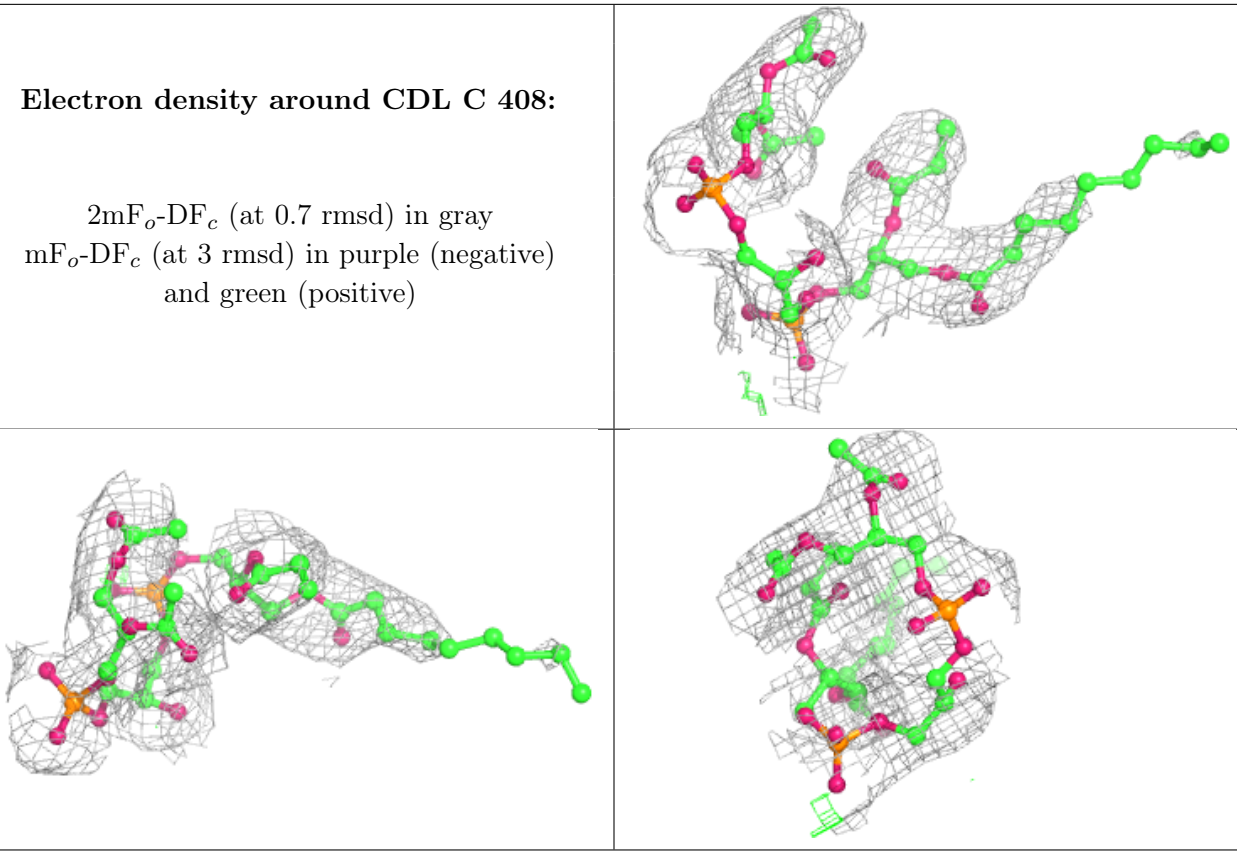
Electron density around 6PE A 502:

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



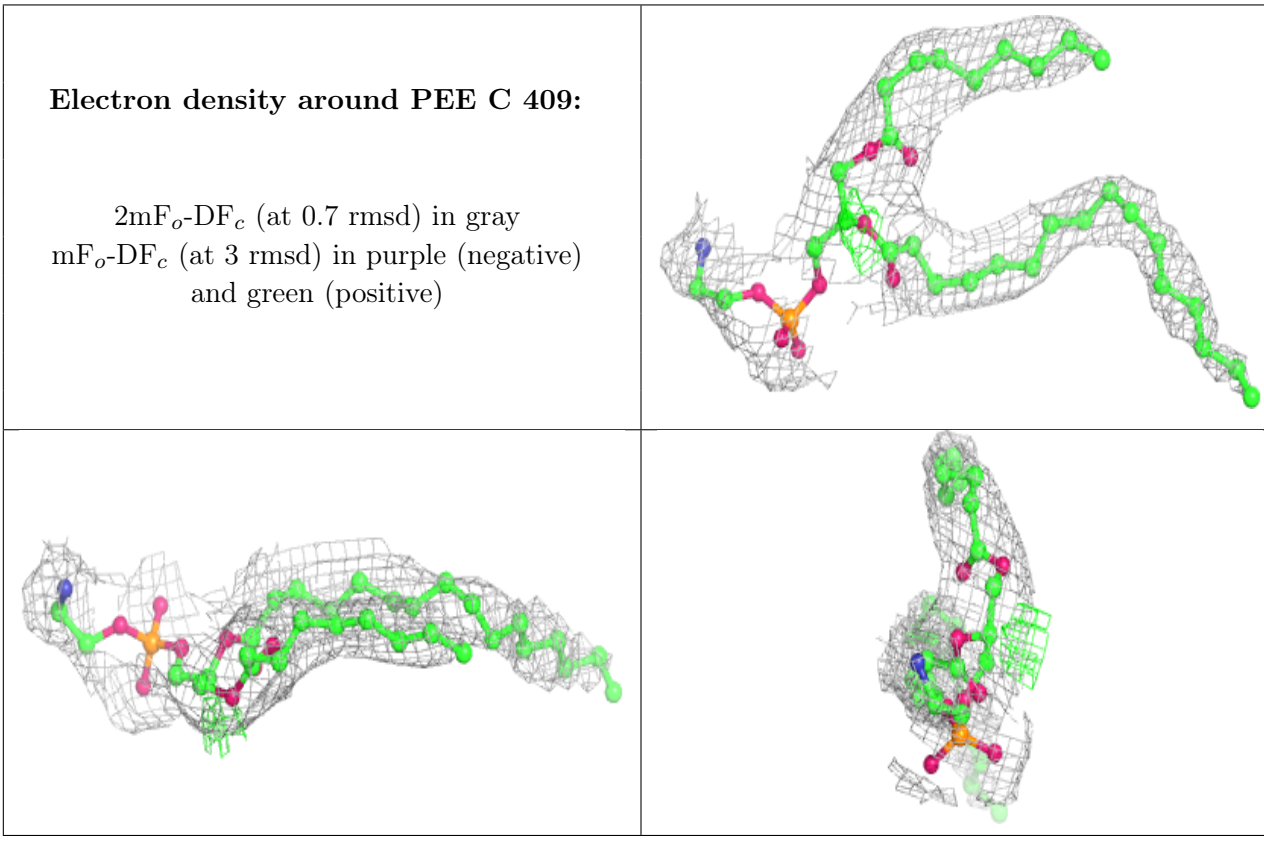
Electron density around CDL C 408:

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



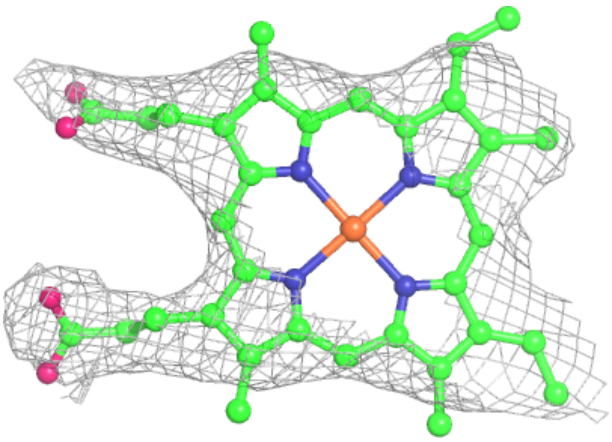
Electron density around PEE C 409:

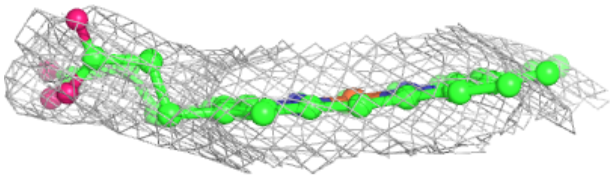
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

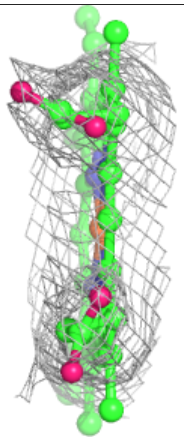


Electron density around HEC D 501:

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

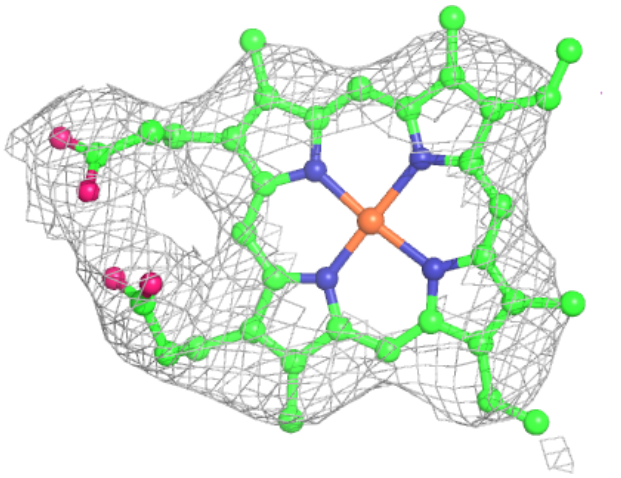


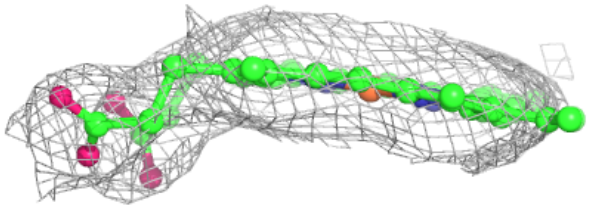


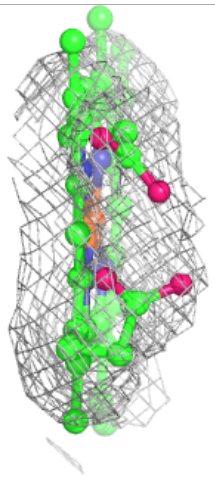


Electron density around HEM C 402:

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

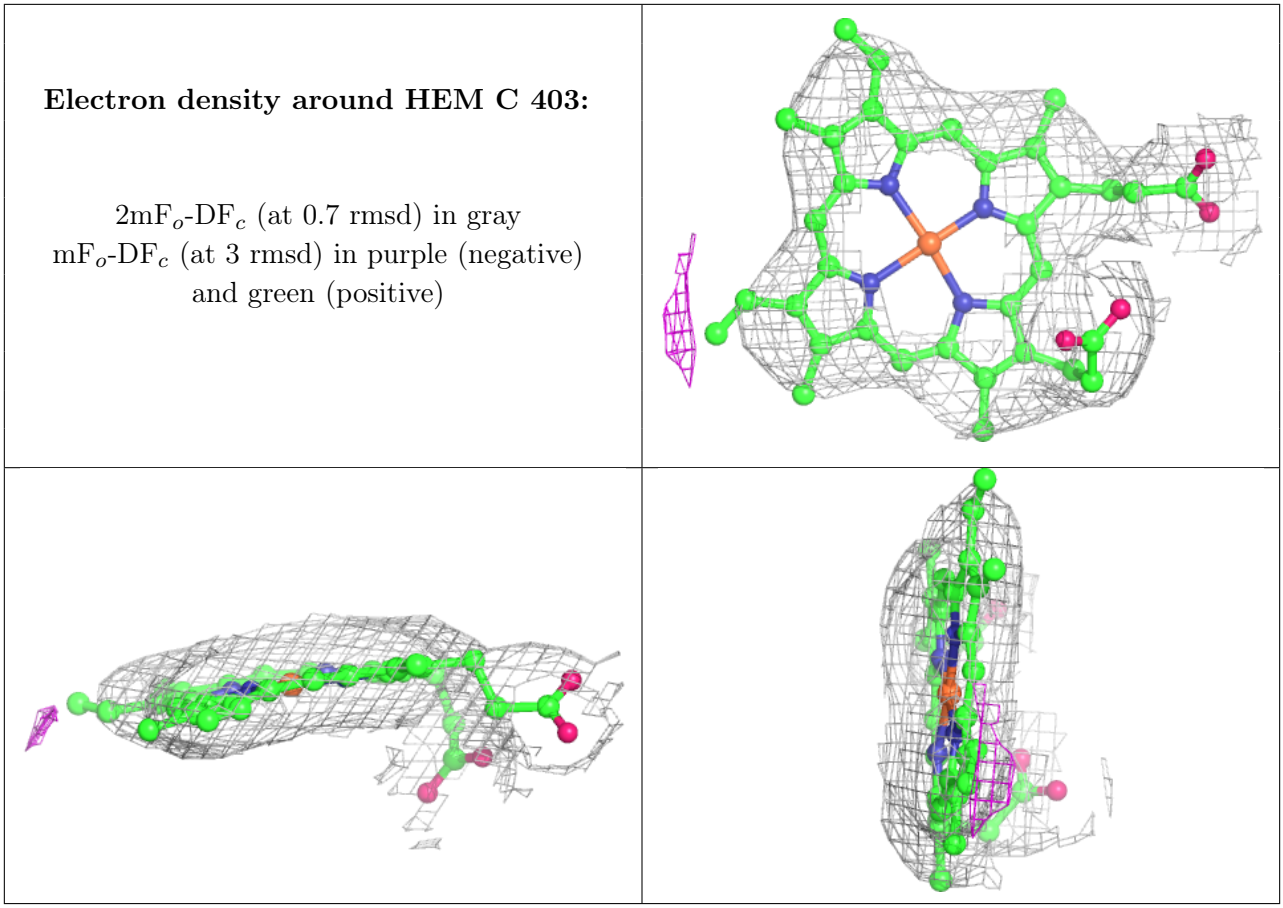






Electron density around HEM C 403:

$2mF_o$-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.