Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2026 – 03:02 am BST

PDB ID	:	6ZFT / pdb_00006zft
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:

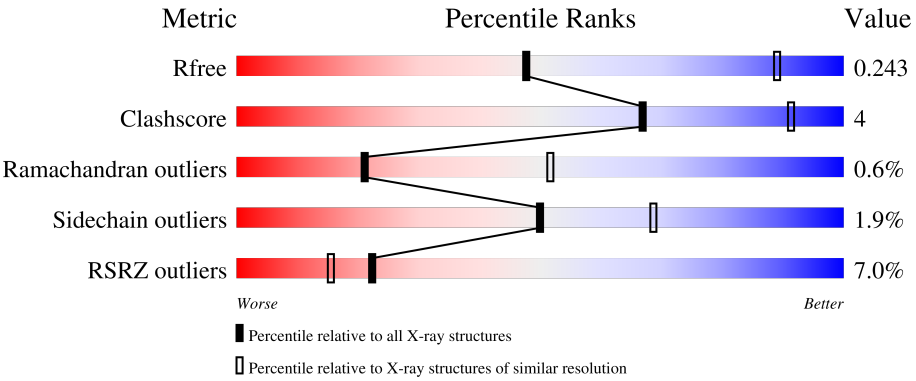
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	5% 88% 10% ·
2	B	420	5% 89% 9% ··
3	C	378	6% 89% 10% ·
4	D	239	6% 91% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	196	16% 92% 7%
6	F	99	2% 94% 5%
7	G	74	5% 84% 15%
8	H	65	5% 89% 11%
9	I	46	48% 76% 22%
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	-
17	PEE	C	409	X	-	-	-
17	PEE	D	503	X	-	-	-
19	HEC	D	501	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			

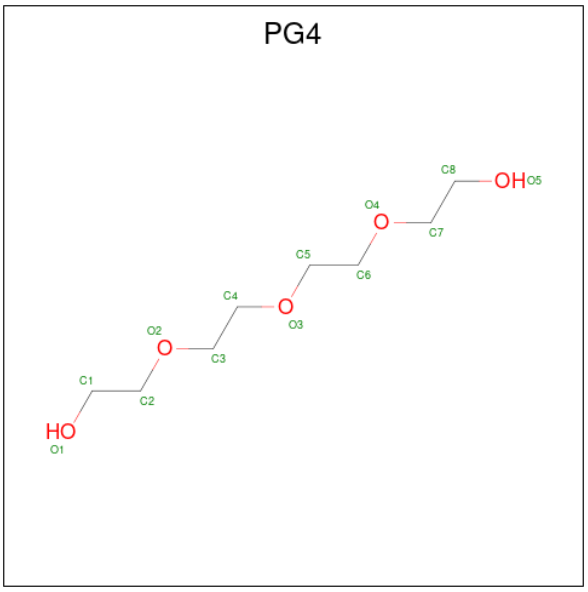
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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.

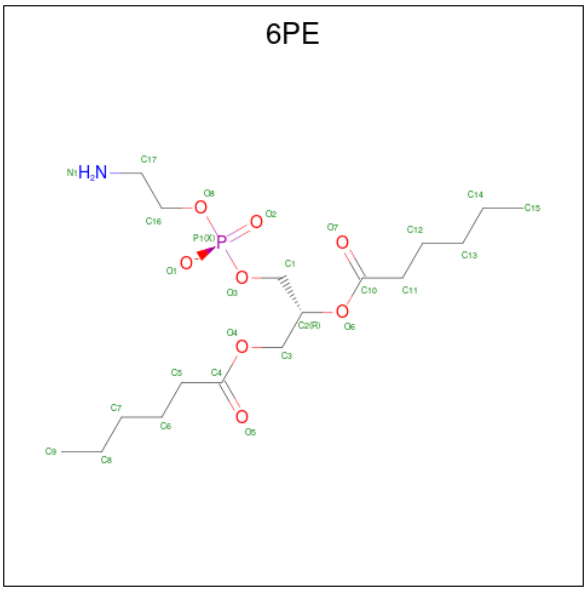
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



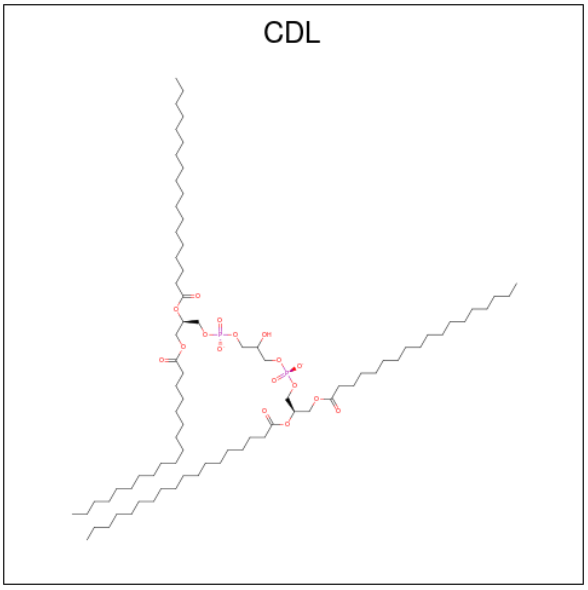
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 13 8 5	0	0
11	A	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0

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



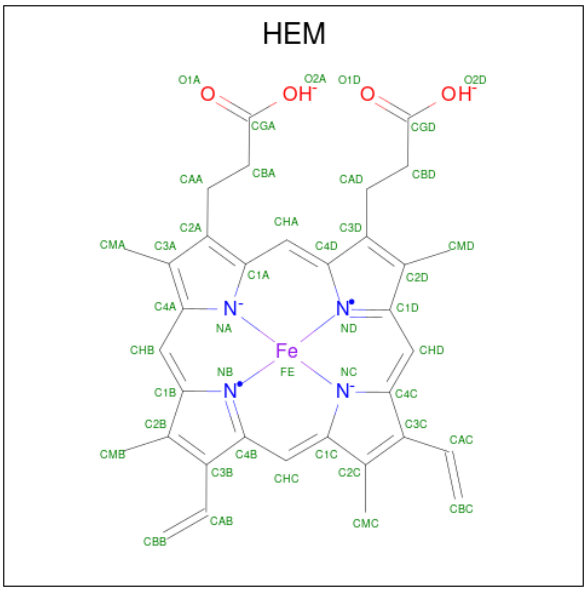
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

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



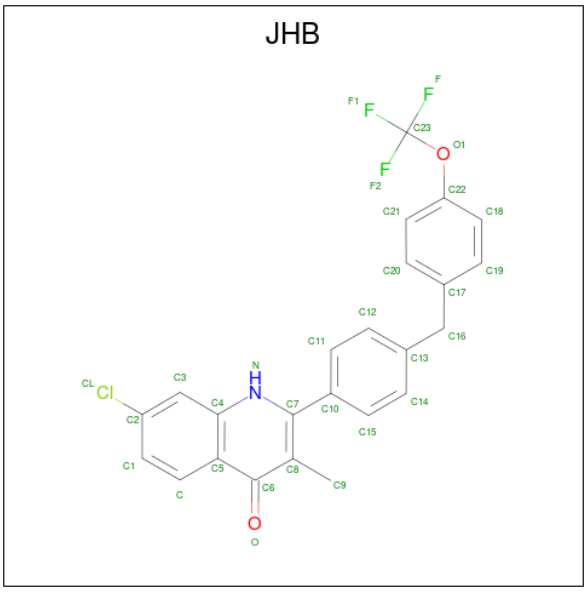
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	O	P		0	0
			34	17	15	2			
13	C	1	Total	C	O	P		0	0
			44	25	17	2			
13	D	1	Total	C	O	P		0	0
			54	35	17	2			
13	E	1	Total	C	O	P		0	0
			60	41	17	2			

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



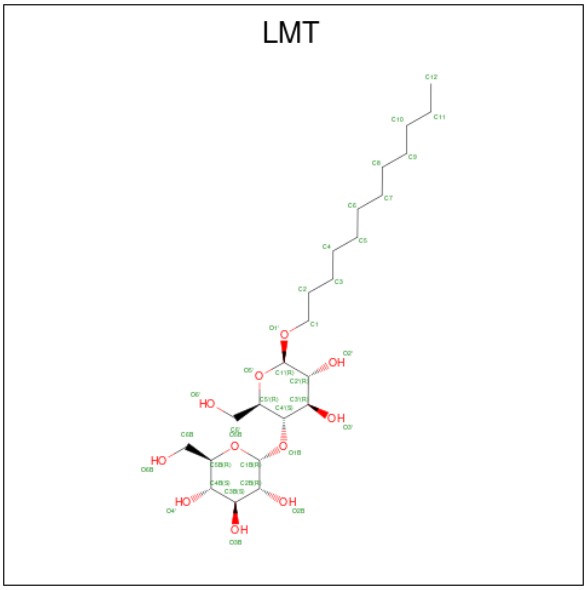
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



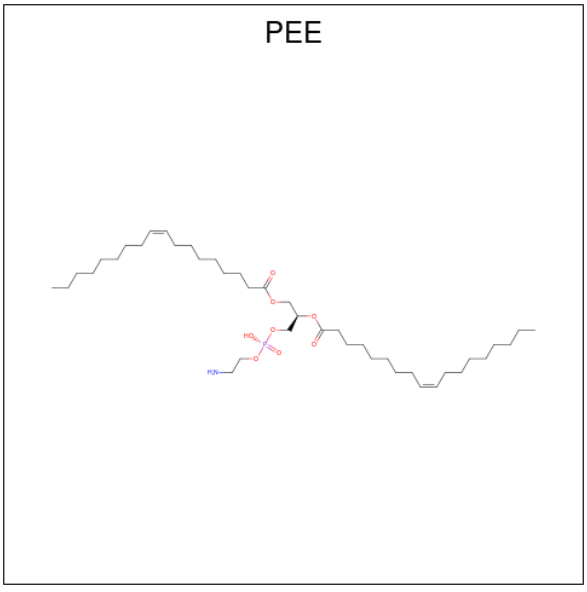
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	C	1	Total	C	Cl	F	N	O	0	0
			31	24	1	3	1	2		

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (CCD ID: 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 (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



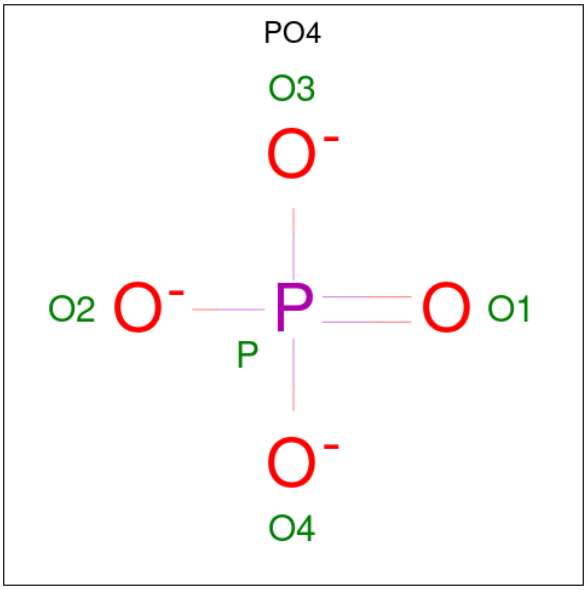
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

Continued on next page...

Continued from previous page...

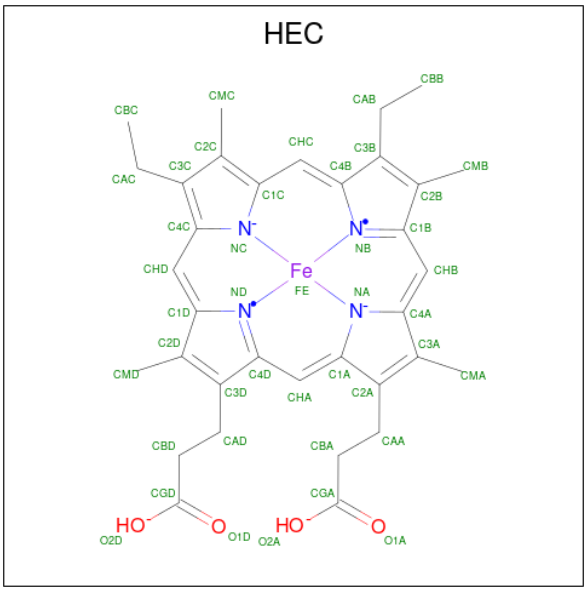
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	N	O	P	0	0
			37	27	1	8	1		

- Molecule 18 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



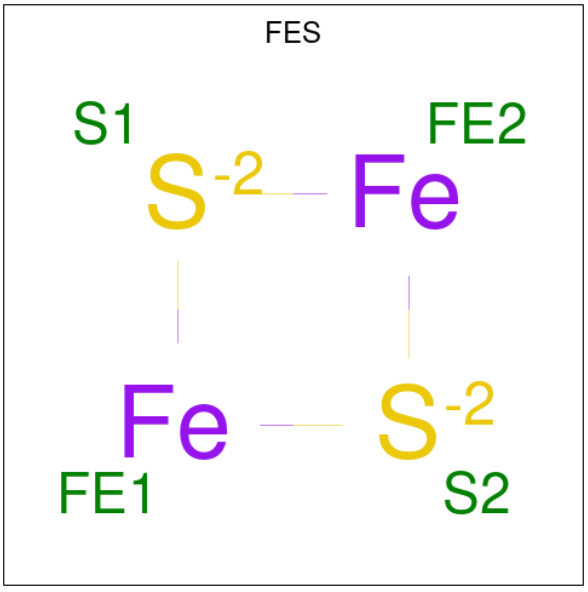
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	O	P		0	0
			5	4	1			
18	F	1	Total	O	P		0	0
			5	4	1			
18	G	1	Total	O	P		0	0
			5	4	1			
18	G	1	Total	O	P		0	0
			5	4	1			
18	G	1	Total	O	P		0	0
			5	4	1			
18	H	1	Total	O	P		0	0
			5	4	1			

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



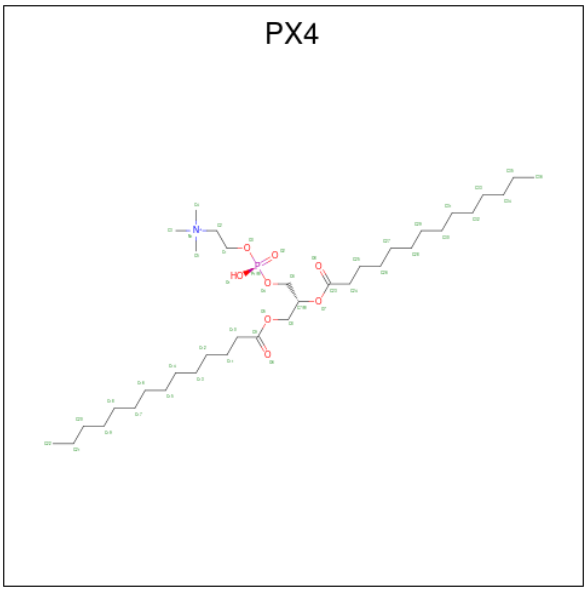
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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 (CCD ID: 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		

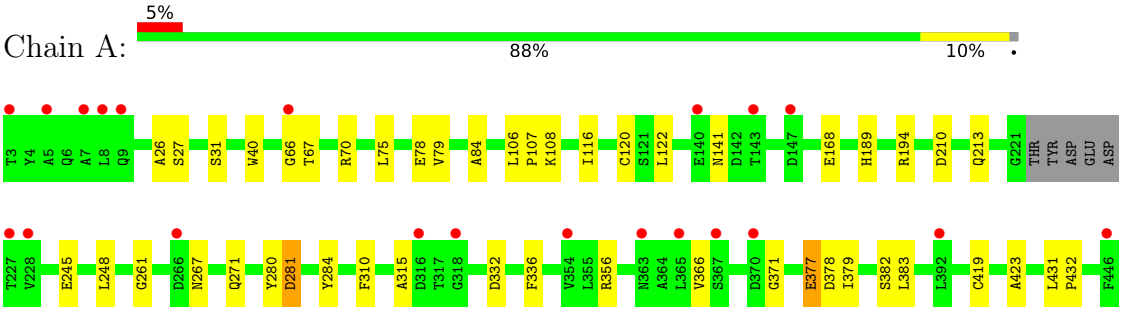
- Molecule 22 is water.

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		

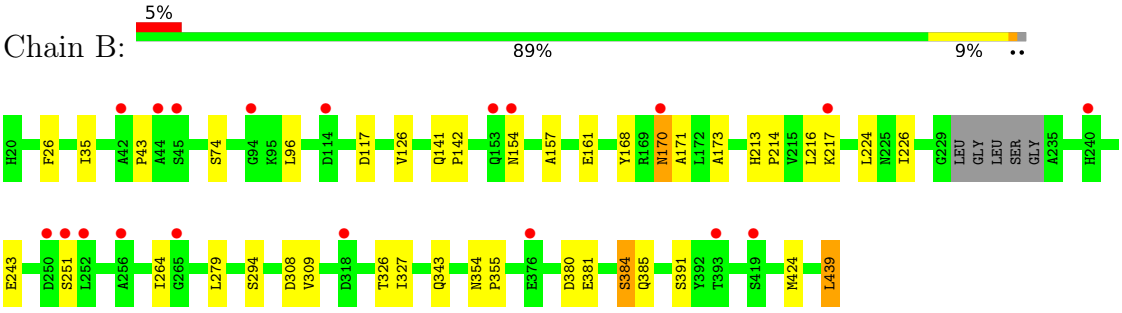
3 Residue-property plots (i)

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.

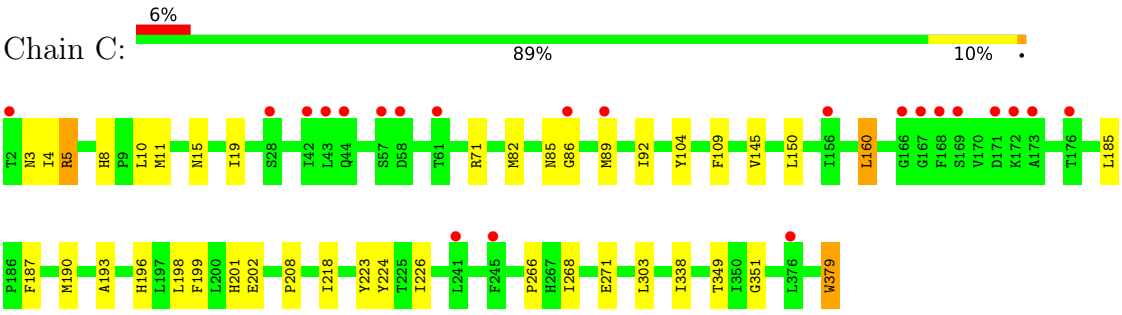
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



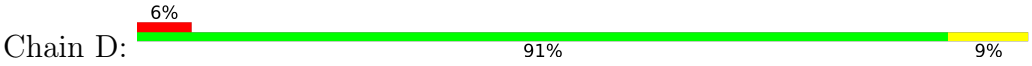
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

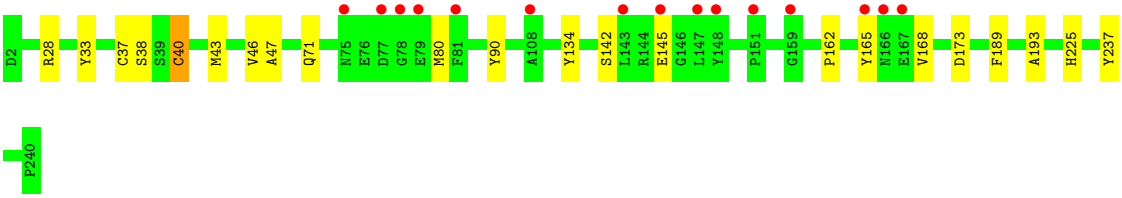


• Molecule 3: Cytochrome b

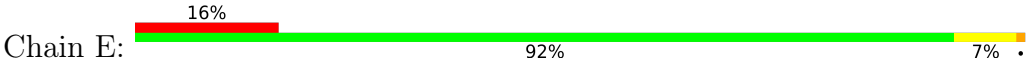


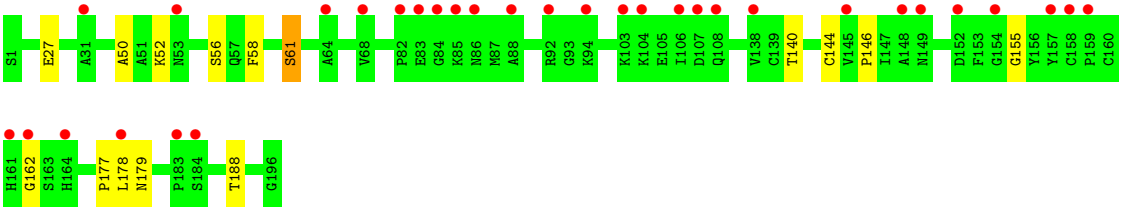
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



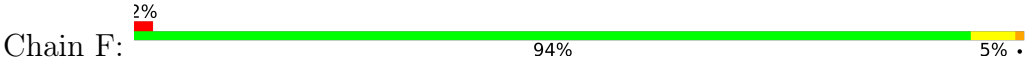


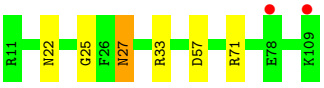
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



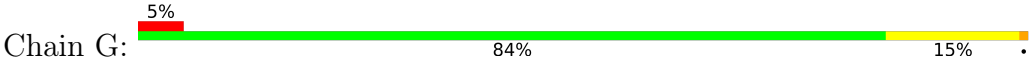


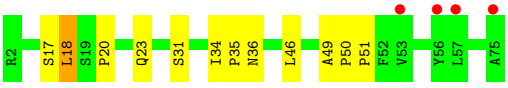
• Molecule 6: Cytochrome b-c1 complex subunit 7



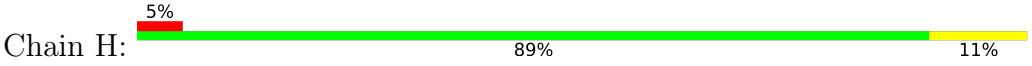


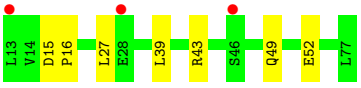
• Molecule 7: Cytochrome b-c1 complex subunit 8



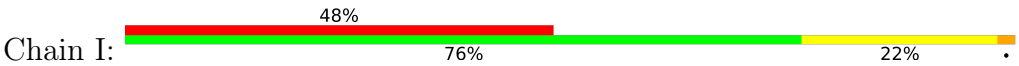


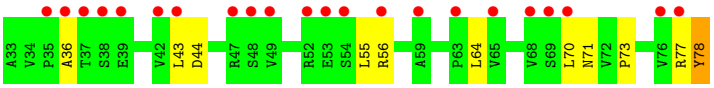
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



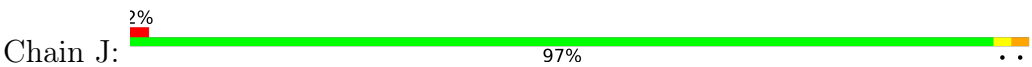


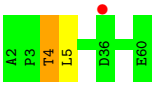
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial





• Molecule 10: Cytochrome b-c1 complex subunit 9




A2
P3
T4
L5
D36
E60

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 60.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	69.5 (60.92-3.30) 69.5 (60.92-3.30)	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 (3.51%)	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)	0.27 , 65.5	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	0.89	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: PO4, JHB, CDL, HEC, 6PE, PG4, PX4, LMT, PEE, HEM, FES

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	1.08	0/3462	1.52	6/4700 (0.1%)
2	B	1.09	0/3165	1.54	0/4296
3	C	1.02	0/3092	1.53	2/4231 (0.0%)
4	D	1.03	0/1935	1.47	0/2632
5	E	1.11	0/1507	1.52	0/2044
6	F	1.00	0/867	1.54	0/1168
7	G	1.03	0/641	1.46	0/868
8	H	1.06	0/522	1.60	0/704
9	I	1.25	0/328	1.67	1/447 (0.2%)
10	J	1.01	0/500	1.60	0/675
All	All	1.06	0/16019	1.53	9/21765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	44	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	423	ALA	CA-C-N	5.70	125.53	121.65
1	A	423	ALA	C-N-CA	5.70	125.53	121.65
1	A	66	GLY	CA-C-O	-5.58	118.59	122.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	371	GLY	CA-C-O	-5.52	118.42	122.23
3	C	92	ILE	N-CA-C	-5.38	105.08	110.30
1	A	261	GLY	CA-C-O	-5.27	118.65	122.45
1	A	310	PHE	CA-CB-CG	5.10	118.90	113.80
3	C	5	ARG	N-CA-C	-5.01	106.85	113.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	ASN	Peptide
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	31	0
2	B	3108	0	3067	24	0
3	C	2996	0	3058	21	0
4	D	1876	0	1806	17	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	2	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	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
22	F	1	0	0	0	0
All	All	16262	0	15906	118	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 (118) 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
14:C:402:HEM:HBB2	14:C:402:HEM:HMB2	1.78	0.64
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
4:D:237:TYR:OH	6:F:57:ASP:OD1	2.21	0.59
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.84	0.58
1:A:336:PHE:HA	11:A:503:PG4:C8	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:B:224:LEU:C	2:B:226:ILE:HD12	2.37	0.50
3:C:150:LEU:HD23	3:C:160:LEU:HD13	1.93	0.50
1:A:281:ASP:OD1	1:A:281:ASP:C	2.56	0.49
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
4:D:40:CYS:SG	19:D:501:HEC:HMC1	2.52	0.48
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.99	0.45
5:E:140:THR:HG21	5:E:179:ASN:O	2.16	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
8:H:15:ASP:O	8:H:16:PRO:C	2.61	0.43
1:A:67:THR:HG1	1:A:70:ARG:H	1.66	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
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
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
4:D:71:GLN:HE21	4:D:80:MET:HE3	1.84	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
2:B:170:ASN:CG	2:B:171:ALA:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.56	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%)	24 55
2	B	411/420 (98%)	388 (94%)	22 (5%)	1 (0%)	43 71
3	C	376/378 (100%)	353 (94%)	21 (6%)	2 (0%)	24 55
4	D	237/239 (99%)	217 (92%)	18 (8%)	2 (1%)	16 45
5	E	194/196 (99%)	176 (91%)	14 (7%)	4 (2%)	5 26
6	F	97/99 (98%)	95 (98%)	2 (2%)	0	100 100
7	G	72/74 (97%)	72 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	H	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
9	I	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5 25
10	J	57/59 (97%)	54 (95%)	3 (5%)	0	100 100
All	All	1986/2020 (98%)	1864 (94%)	110 (6%)	12 (1%)	21 52

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%)	65 76
2	B	323/329 (98%)	316 (98%)	7 (2%)	45 66
3	C	325/326 (100%)	318 (98%)	7 (2%)	45 66
4	D	198/204 (97%)	197 (100%)	1 (0%)	81 83
5	E	155/168 (92%)	152 (98%)	3 (2%)	50 68
6	F	85/91 (93%)	82 (96%)	3 (4%)	32 58
7	G	65/66 (98%)	62 (95%)	3 (5%)	24 53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	59/62 (95%)	57 (97%)	2 (3%)	32 59
9	I	35/38 (92%)	34 (97%)	1 (3%)	37 62
10	J	49/49 (100%)	48 (98%)	1 (2%)	48 68
All	All	1656/1703 (97%)	1624 (98%)	32 (2%)	50 68

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	281	ASP
1	A	377	GLU
1	A	419	CYS
2	B	117	ASP
2	B	126	VAL
2	B	154	ASN
2	B	251	SER
2	B	264	ILE
2	B	384	SER
2	B	439	LEU
3	C	160	LEU
3	C	185	LEU
3	C	198	LEU
3	C	271	GLU
3	C	303	LEU
3	C	349	THR
3	C	379	TRP
4	D	40	CYS
5	E	27	GLU
5	E	61	SER
5	E	178	LEU
6	F	22	ASN
6	F	27	ASN
6	F	71	ARG
7	G	17	SER
7	G	18	LEU
7	G	31	SER
8	H	27	LEU
8	H	39	LEU
9	I	78	TYR
10	J	4	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	165	GLN
1	A	252	HIS
1	A	267	ASN
1	A	271	GLN
1	A	311	ASN
1	A	328	HIS
1	A	368	HIS
2	B	20	HIS
2	B	192	HIS
2	B	343	GLN
2	B	351	ASN
2	B	412	ASN
3	C	68	HIS
3	C	263	ASN
3	C	322	GLN
4	D	6	HIS
4	D	50	HIS
4	D	71	GLN
4	D	105	ASN
5	E	57	GLN
6	F	27	ASN
6	F	38	HIS
6	F	79	GLN
8	H	23	GLN
8	H	67	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides 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	$\#\|Z\| > 2$
12	6PE	A	502	-	22,22,26	0.41	0	25,27,31	0.65	0
18	PO4	G	102	-	4,4,4	0.66	0	6,6,6	0.43	0
20	FES	E	201	5	0,4,4	-	-	-		
16	LMT	C	405	-	36,36,36	0.73	1 (2%)	47,47,47	1.42	7 (14%)
17	PEE	C	409	-	39,39,50	0.69	1 (2%)	42,44,55	0.63	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
13	CDL	E	203	-	59,59,99	0.38	0	65,71,111	0.61	1 (1%)
18	PO4	G	103	-	4,4,4	0.46	0	6,6,6	0.56	0
11	PG4	C	407	-	12,12,12	0.30	0	11,11,11	0.15	0
13	CDL	C	408	-	43,43,99	0.49	0	49,55,111	0.84	2 (4%)
18	PO4	H	101	-	4,4,4	0.76	0	6,6,6	0.37	0
21	PX4	E	202	-	36,36,45	0.42	0	42,44,53	0.68	1 (2%)
15	JHB	C	404	-	34,34,34	2.00	5 (14%)	48,50,50	1.29	4 (8%)
14	HEM	C	403	3	50,50,50	1.55	9 (18%)	66,82,82	1.53	13 (19%)
14	HEM	C	402	3	50,50,50	1.61	10 (20%)	66,82,82	1.52	10 (15%)
13	CDL	D	502	-	53,53,99	0.42	0	59,65,111	0.59	0
13	CDL	C	401	-	33,33,99	0.51	0	37,43,111	0.81	1 (2%)
18	PO4	C	410	-	4,4,4	0.74	0	6,6,6	0.41	0
18	PO4	F	501	-	4,4,4	0.63	0	6,6,6	0.47	0
11	PG4	A	501	-	12,12,12	0.23	0	11,11,11	0.14	0
19	HEC	D	501	4	50,50,50	2.83	29 (58%)	68,82,82	2.55	32 (47%)
17	PEE	D	503	-	36,36,50	0.79	1 (2%)	39,41,55	0.67	1 (2%)
18	PO4	G	101	-	4,4,4	0.73	0	6,6,6	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	6PE	A	502	-	-	13/26/26/30	-
13	CDL	D	502	-	-	25/63/63/110	-
17	PEE	C	409	-	1/1/4/8	17/43/43/54	-
13	CDL	C	401	-	-	21/41/41/110	-
11	PG4	A	503	-	-	6/10/10/10	-
13	CDL	C	408	-	-	21/52/52/110	-
11	PG4	A	501	-	-	6/10/10/10	-
11	PG4	C	406	-	-	5/10/10/10	-
13	CDL	E	203	-	-	34/69/69/110	-
14	HEM	C	403	3	-	4/14/54/54	-
21	PX4	E	202	-	-	21/40/40/49	-
19	HEC	D	501	4	1/1/3/7	7/14/54/54	-
17	PEE	D	503	-	1/1/4/8	23/40/40/54	-
20	FES	E	201	5	-	-	0/1/1/1
11	PG4	C	407	-	-	4/10/10/10	-
15	JHB	C	404	-	-	0/13/13/13	0/4/4/4
14	HEM	C	402	3	-	6/14/54/54	-
16	LMT	C	405	-	-	11/21/61/61	0/2/2/2

All (56) 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
15	C	404	JHB	C7-C8	6.57	1.51	1.37
19	D	501	HEC	FE-ND	5.18	2.10	1.94
19	D	501	HEC	C2A-C3A	5.14	1.47	1.36
19	D	501	HEC	CHB-C4A	4.97	1.48	1.38
19	D	501	HEC	FE-NB	4.85	2.09	1.94
19	D	501	HEC	CHA-C1A	4.85	1.47	1.38
19	D	501	HEC	C3D-C2D	4.64	1.46	1.36
19	D	501	HEC	CHC-C4B	4.62	1.47	1.38
14	C	402	HEM	FE-NB	4.56	2.09	1.94
14	C	403	HEM	FE-NB	4.44	2.08	1.94
19	D	501	HEC	C3B-C2B	4.28	1.45	1.36
19	D	501	HEC	FE-NA	4.10	2.09	1.95
19	D	501	HEC	CHC-C1C	4.01	1.48	1.39
19	D	501	HEC	FE-NC	4.01	2.08	1.95
19	D	501	HEC	CHD-C1D	3.93	1.46	1.38
17	D	503	PEE	C18-C19	3.83	1.54	1.31
14	C	402	HEM	FE-NC	3.73	2.07	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	403	HEM	C1B-NB	-3.70	1.33	1.40
19	D	501	HEC	CHB-C1B	3.64	1.47	1.39
17	C	409	PEE	C18-C19	3.54	1.52	1.31
19	D	501	HEC	C4B-NB	-3.54	1.34	1.40
19	D	501	HEC	CHD-C4C	3.53	1.47	1.39
14	C	402	HEM	C1B-NB	-3.51	1.34	1.40
19	D	501	HEC	C3C-C2C	3.45	1.48	1.38
14	C	403	HEM	FE-NC	3.39	2.06	1.95
19	D	501	HEC	CHA-C4D	3.35	1.46	1.39
14	C	402	HEM	C4D-ND	-3.15	1.34	1.40
19	D	501	HEC	C1D-ND	-3.07	1.35	1.40
14	C	403	HEM	C4B-NB	-3.04	1.32	1.38
16	C	405	LMT	O1'-C1'	2.88	1.45	1.40
14	C	402	HEM	C4D-C3D	2.72	1.49	1.45
15	C	404	JHB	O1-C23	2.64	1.46	1.31
19	D	501	HEC	C1A-C2A	2.61	1.49	1.45
19	D	501	HEC	C1C-C2C	2.60	1.49	1.43
19	D	501	HEC	C4A-NA	-2.58	1.34	1.39
15	C	404	JHB	C3-C2	2.54	1.42	1.38
14	C	402	HEM	C3B-C4B	2.43	1.49	1.44
14	C	403	HEM	C4D-ND	-2.38	1.36	1.40
19	D	501	HEC	C1C-NC	-2.38	1.35	1.39
19	D	501	HEC	C4D-C3D	2.37	1.49	1.45
19	D	501	HEC	C4C-NC	-2.34	1.35	1.39
14	C	403	HEM	C1C-NC	-2.32	1.35	1.39
14	C	403	HEM	C1C-C2C	-2.31	1.40	1.45
14	C	402	HEM	C3C-C4C	-2.27	1.42	1.46
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	C1B-NB	-2.21	1.34	1.38
19	D	501	HEC	C4A-C3A	2.19	1.49	1.45
19	D	501	HEC	C4B-C3B	2.15	1.48	1.45
14	C	402	HEM	C1D-ND	-2.08	1.34	1.38
19	D	501	HEC	C1A-NA	-2.05	1.35	1.39
19	D	501	HEC	C1D-C2D	2.04	1.48	1.44
14	C	403	HEM	C1D-ND	-2.04	1.34	1.38
14	C	403	HEM	C1D-C2D	2.01	1.48	1.44
14	C	402	HEM	C1C-NC	-2.01	1.35	1.39

All (72) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	501	HEC	C3D-C4D-ND	6.06	116.23	110.36
19	D	501	HEC	C1B-C2B-C3B	-5.65	101.01	106.96
19	D	501	HEC	C2A-C1A-NA	5.54	115.71	110.32
19	D	501	HEC	C2B-C1B-NB	5.44	116.40	109.88
19	D	501	HEC	C2D-C1D-ND	5.35	116.18	109.84
16	C	405	LMT	C1B-O5B-C5B	4.56	122.64	113.69
19	D	501	HEC	CBB-CAB-C3B	4.35	124.43	112.43
14	C	402	HEM	CHC-C4B-NB	4.35	129.15	124.42
19	D	501	HEC	C1A-C2A-C3A	-4.24	101.60	107.13
19	D	501	HEC	C1C-C2C-C3C	-4.22	101.89	106.83
14	C	403	HEM	CHC-C4B-NB	4.21	129.00	124.42
14	C	403	HEM	C1B-NB-C4B	4.05	109.26	105.07
19	D	501	HEC	C1D-C2D-C3D	-3.97	102.78	106.96
16	C	405	LMT	C1'-O5'-C5'	3.93	121.41	113.69
19	D	501	HEC	CBC-CAC-C3C	3.83	122.99	112.43
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
19	D	501	HEC	C3C-C4C-NC	3.48	114.04	110.15
14	C	403	HEM	C4C-NC-C1C	3.46	108.74	105.35
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
19	D	501	HEC	CHB-C1B-C2B	-3.25	119.90	124.98
19	D	501	HEC	C4D-C3D-C2D	-3.25	102.16	106.90
14	C	402	HEM	CAD-C3D-C4D	3.22	130.29	124.66
19	D	501	HEC	CAC-C3C-C2C	3.15	131.91	126.86
14	C	403	HEM	CHA-C4D-ND	3.08	128.17	124.37
19	D	501	HEC	C2C-C1C-NC	3.05	114.73	110.08
14	C	403	HEM	CHD-C1D-ND	3.05	127.73	124.42
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
19	D	501	HEC	C3B-C4B-NB	2.97	113.47	110.17
19	D	501	HEC	CMC-C2C-C3C	2.93	131.95	125.61
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	2.87	127.91	124.37
14	C	402	HEM	CHD-C1D-ND	2.84	127.51	124.42
19	D	501	HEC	CAD-C3D-C4D	2.84	129.62	124.66
19	D	501	HEC	CHA-C4D-C3D	-2.83	120.69	124.84
14	C	402	HEM	C4C-NC-C1C	2.77	108.06	105.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	501	HEC	CMA-C3A-C4A	2.75	129.56	124.71
14	C	402	HEM	CHD-C4C-NC	2.71	127.37	124.44
19	D	501	HEC	C3A-C4A-NA	2.69	114.65	109.69
19	D	501	HEC	CHA-C1A-C2A	-2.67	120.60	124.94
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
19	D	501	HEC	CMD-C2D-C1D	2.60	129.00	125.04
19	D	501	HEC	CAA-C2A-C1A	2.58	129.75	124.89
13	E	203	CDL	CB2-C1-CA2	2.53	120.25	112.79
14	C	402	HEM	CHB-C1B-NB	2.49	127.45	124.37
19	D	501	HEC	CBD-CAD-C3D	-2.48	105.75	112.63
14	C	402	HEM	CMD-C2D-C1D	2.44	128.76	125.04
19	D	501	HEC	CAA-CBA-CGA	-2.42	108.39	113.60
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
19	D	501	HEC	C1D-ND-C4D	-2.36	102.64	105.07
14	C	402	HEM	O2D-CGD-CBD	2.36	121.60	114.03
16	C	405	LMT	C3'-C4'-C5'	-2.33	105.59	110.93
19	D	501	HEC	CHD-C1D-C2D	-2.25	120.48	126.73
19	D	501	HEC	C4A-C3A-C2A	-2.16	103.79	106.94
19	D	501	HEC	CHC-C1C-C2C	-2.15	121.16	127.24
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
13	C	401	CDL	CB2-C1-CA2	2.11	118.98	112.79
14	C	403	HEM	CHD-C4C-NC	2.10	126.71	124.44
17	D	503	PEE	O2-C10-C11	2.09	116.01	111.50
19	D	501	HEC	CMB-C2B-C3B	2.08	131.75	126.12
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
19	D	501	HEC	CHD-C4C-C3C	-2.03	120.92	125.36
14	C	403	HEM	C1A-CHA-C4D	-2.02	121.56	126.34

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	C	409	PEE	C2
17	D	503	PEE	C2
19	D	501	HEC	NA

All (224) 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
21	E	202	PX4	C1-O3-P1-O2
21	E	202	PX4	C24-C23-O7-C7
13	C	408	CDL	C11-CA5-OA6-CA4
19	D	501	HEC	C2B-C3B-CAB-CBB
19	D	501	HEC	C4B-C3B-CAB-CBB
19	D	501	HEC	C4C-C3C-CAC-CBC
13	D	502	CDL	OB9-CB7-OB8-CB6
19	D	501	HEC	C2C-C3C-CAC-CBC
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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
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
14	C	402	HEM	C2A-CAA-CBA-CGA
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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

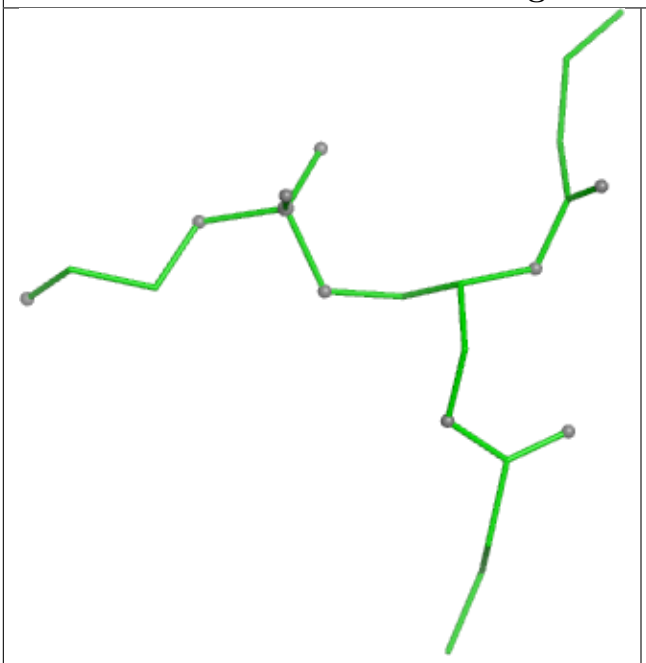
There are no ring outliers.

9 monomers are involved in 28 short contacts:

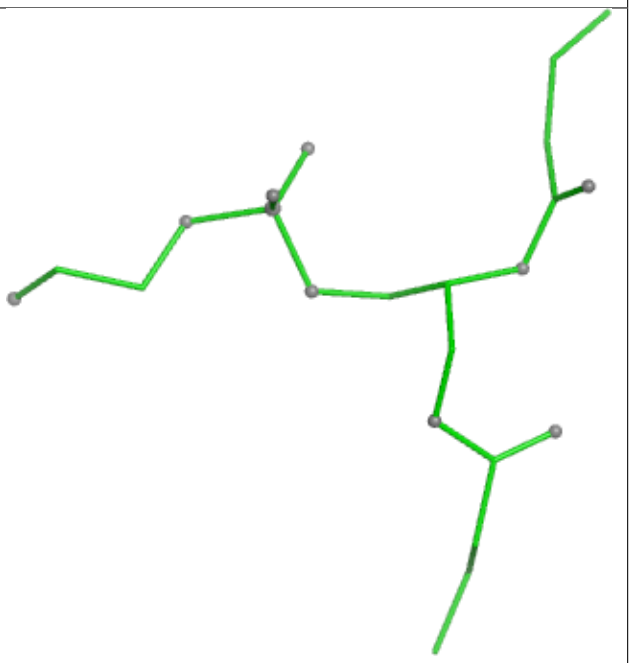
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	502	6PE	1	0
11	A	503	PG4	9	0
15	C	404	JHB	3	0
14	C	403	HEM	4	0
14	C	402	HEM	2	0
13	D	502	CDL	1	0
13	C	401	CDL	2	0
19	D	501	HEC	6	0
17	D	503	PEE	1	0

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.

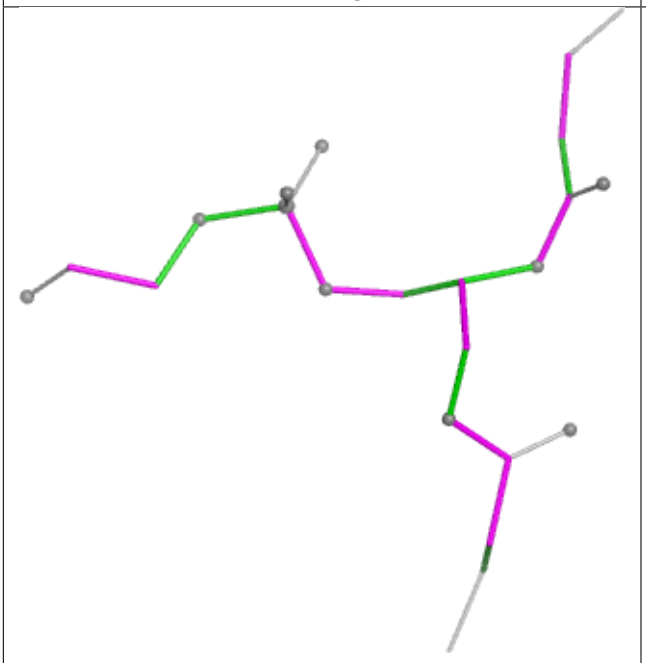
Ligand 6PE A 502



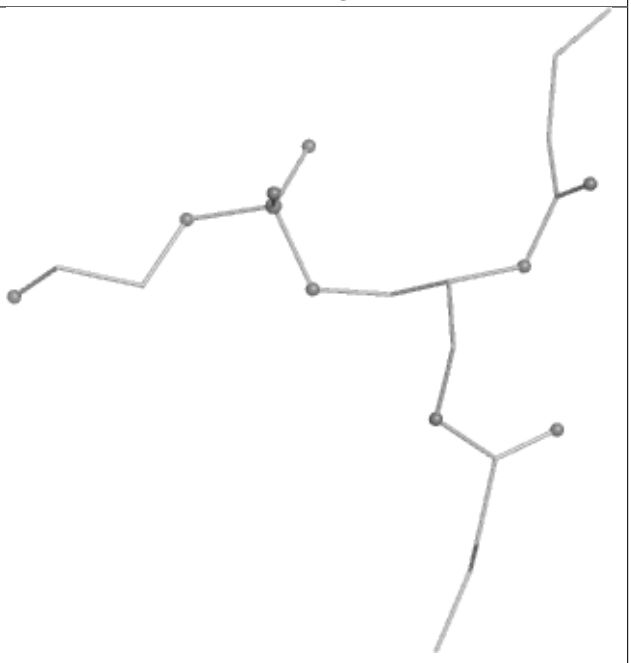
Bond lengths



Bond angles

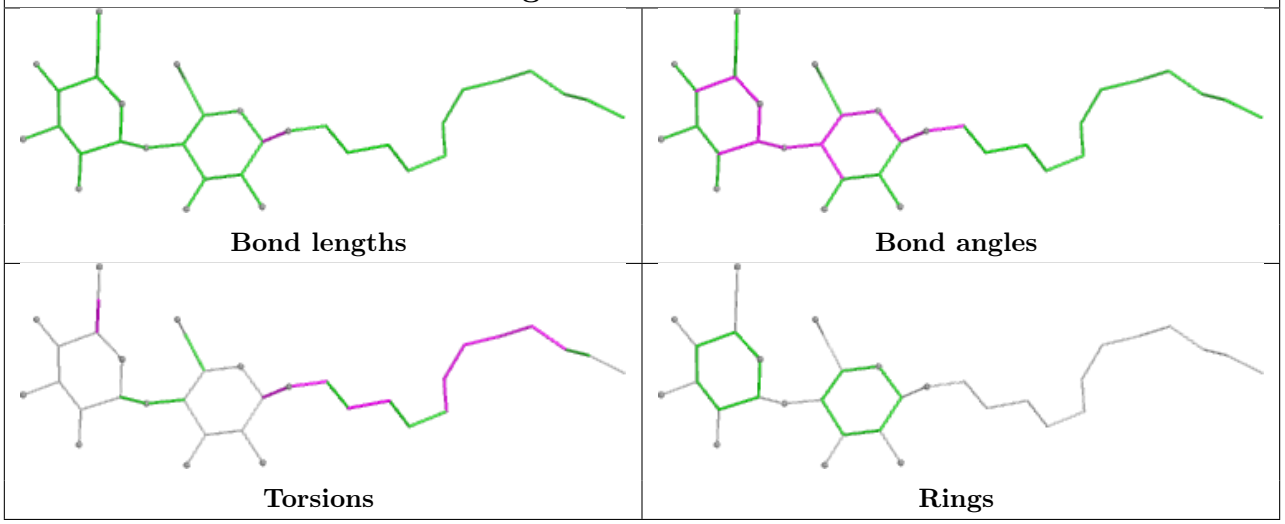


Torsions

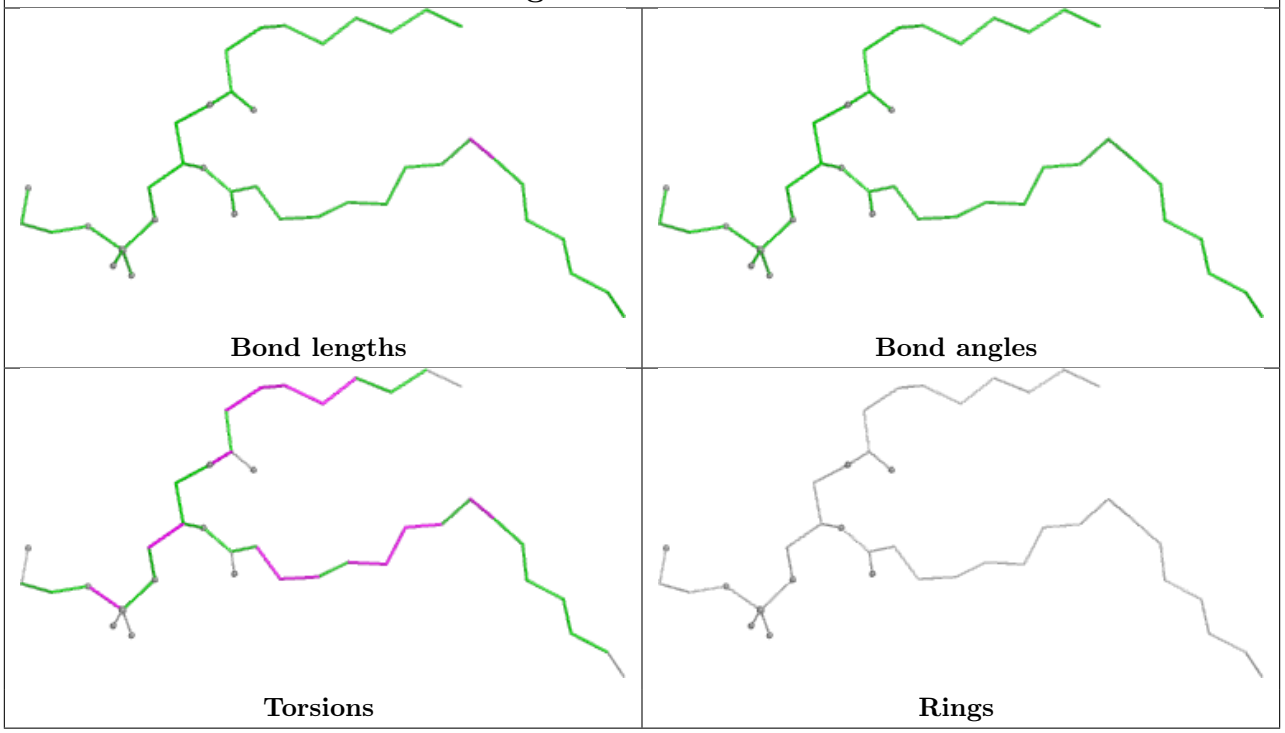


Rings

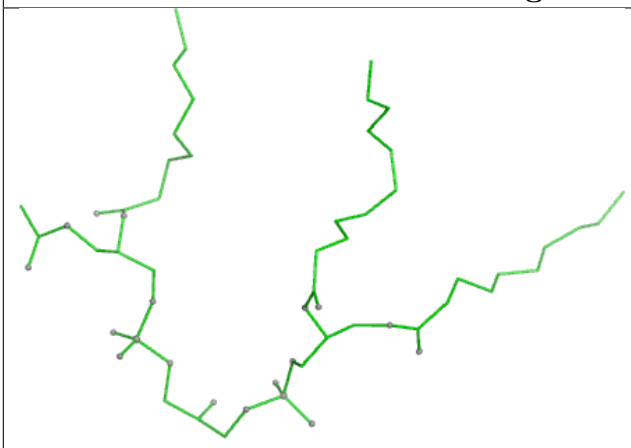
Ligand LMT C 405



Ligand PEE C 409



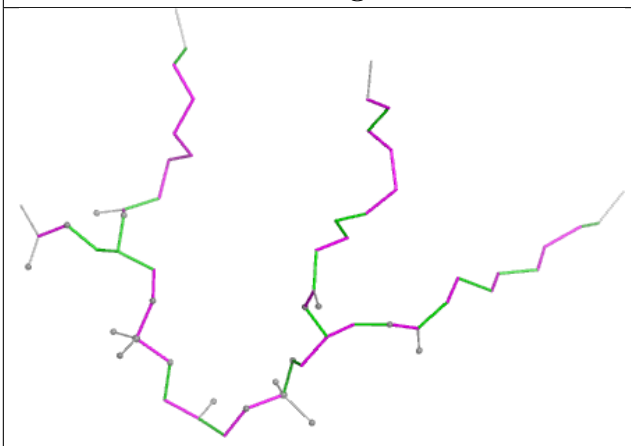
Ligand CDL E 203



Bond lengths



Bond angles

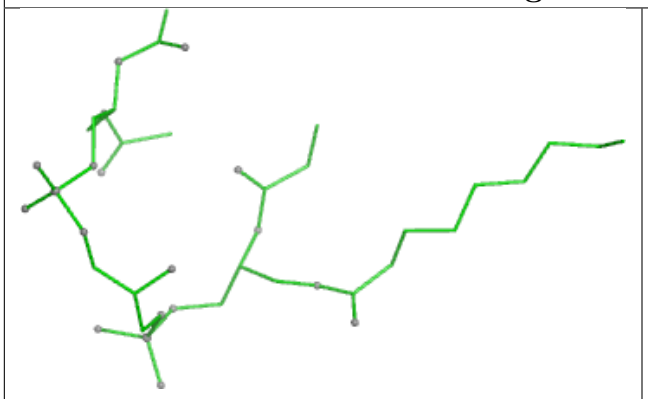


Torsions

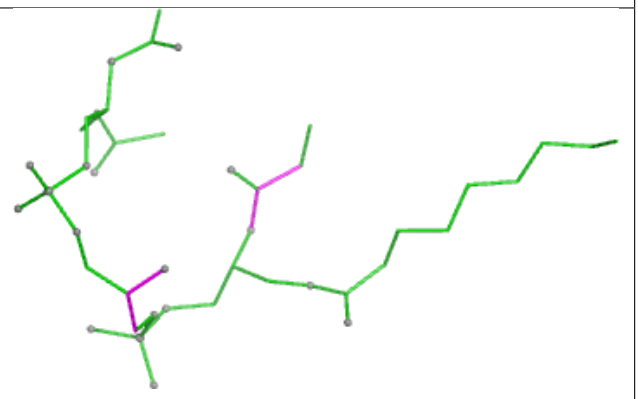


Rings

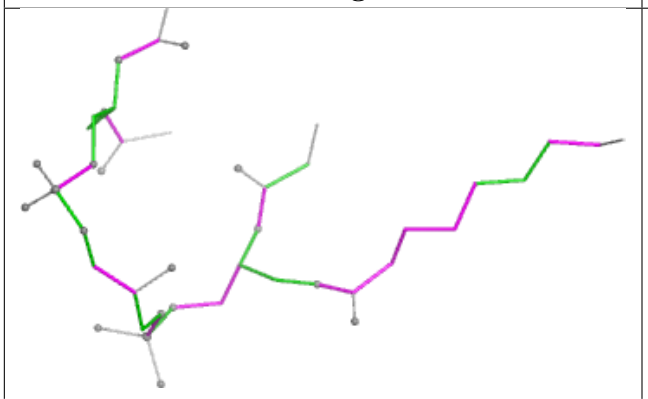
Ligand CDL C 408



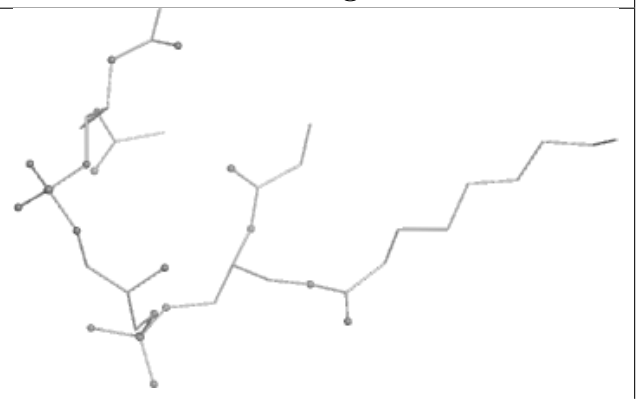
Bond lengths



Bond angles



Torsions

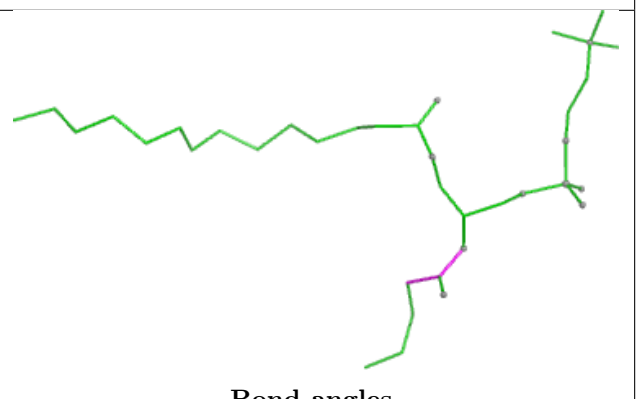


Rings

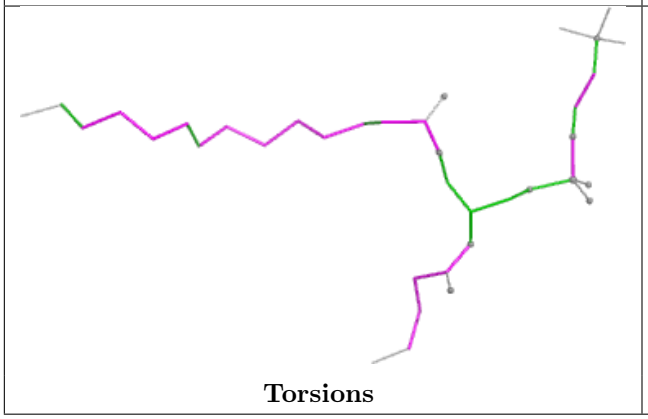
Ligand PX4 E 202



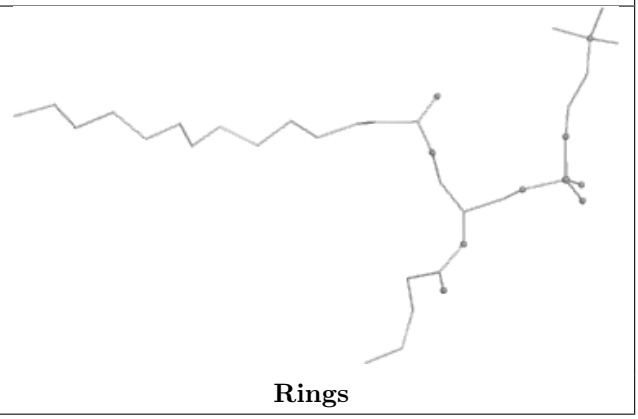
Bond lengths



Bond angles

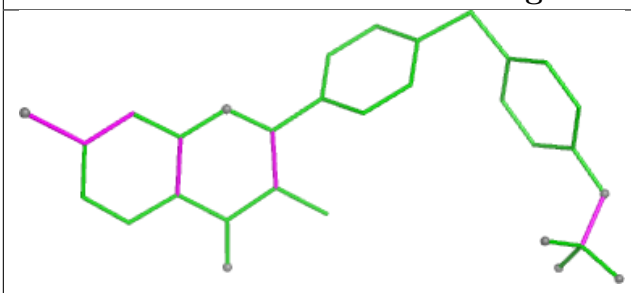


Torsions

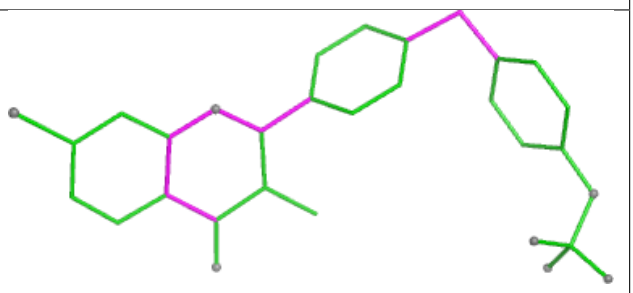


Rings

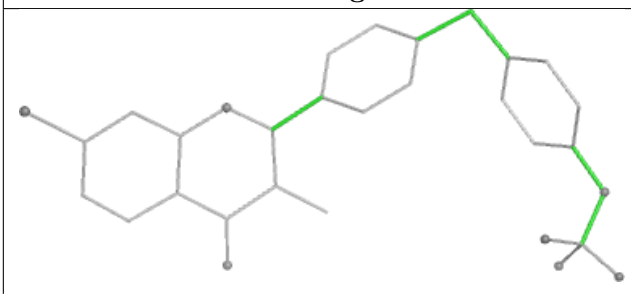
Ligand JHB C 404



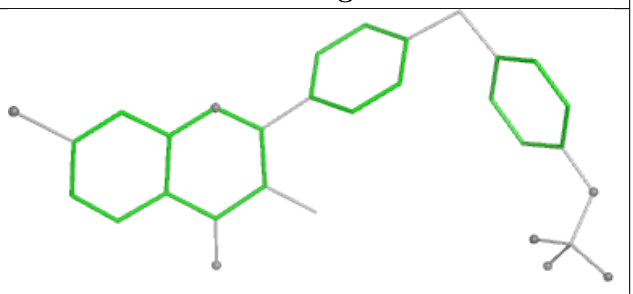
Bond lengths



Bond angles

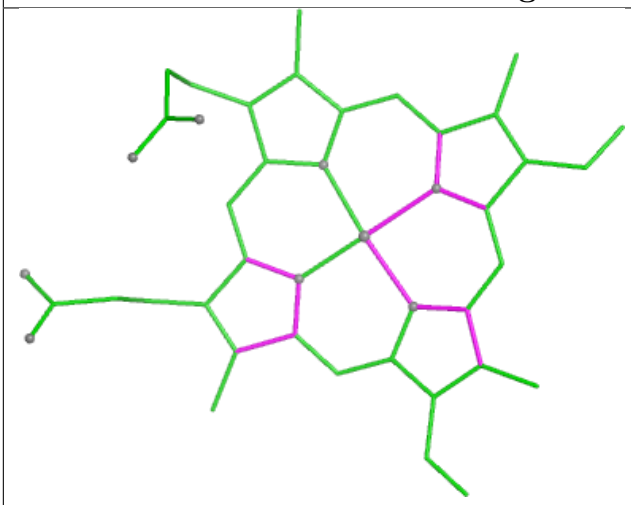


Torsions

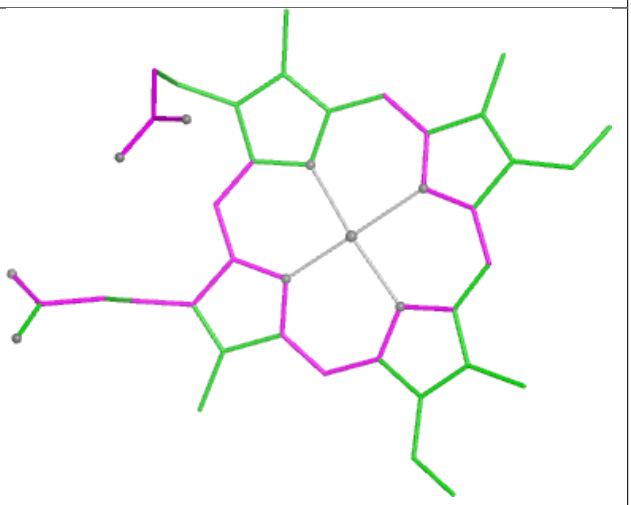


Rings

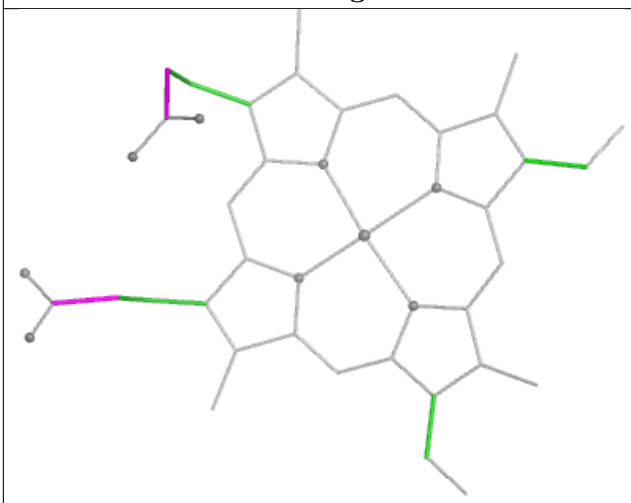
Ligand HEM C 403



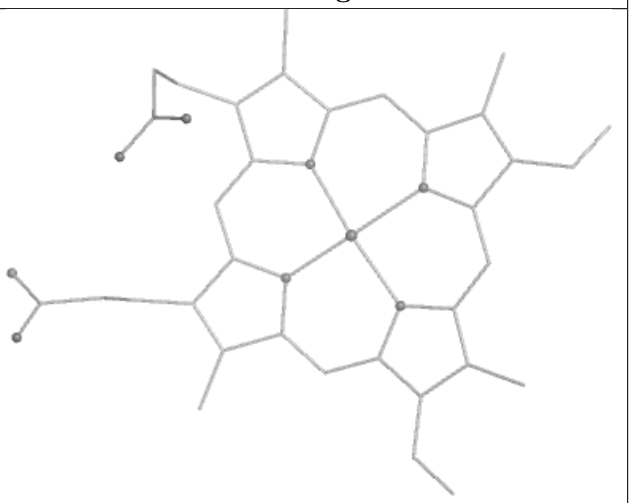
Bond lengths



Bond angles

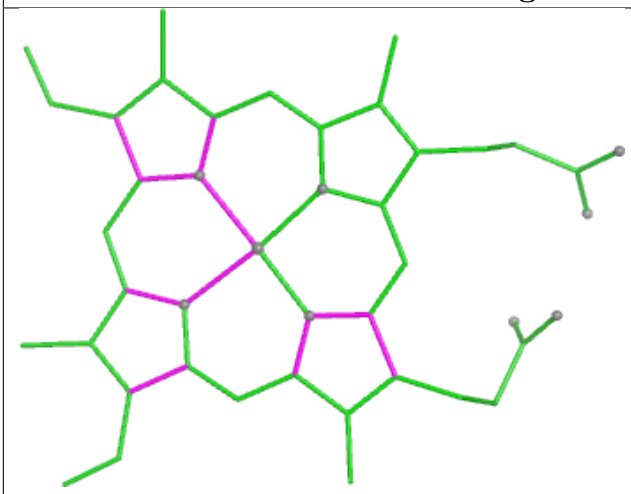


Torsions

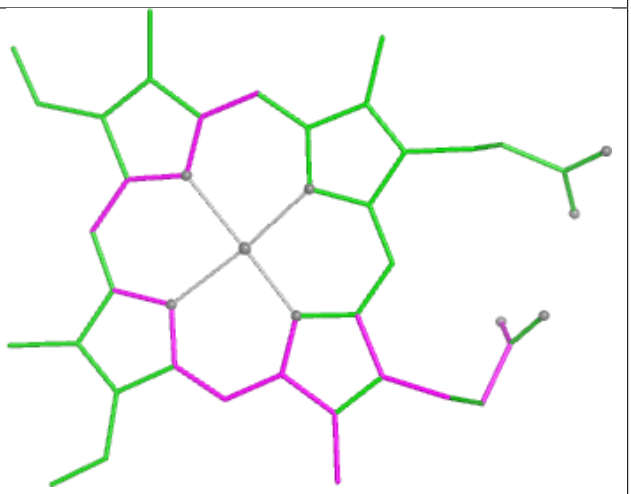


Rings

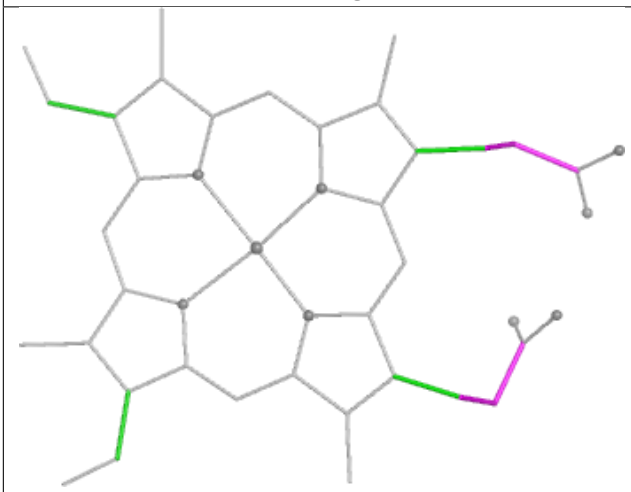
Ligand HEM C 402



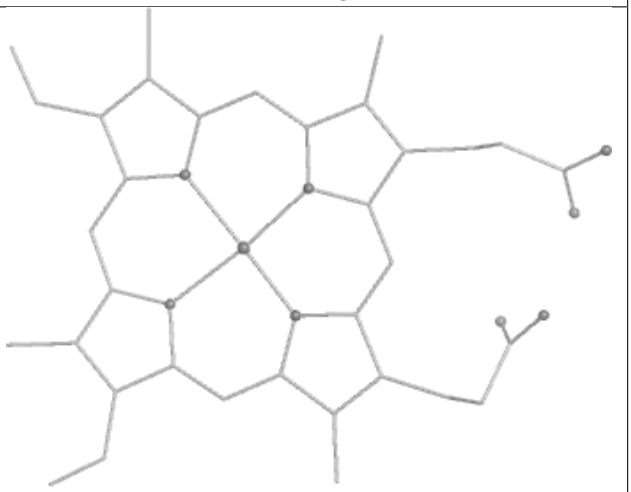
Bond lengths



Bond angles

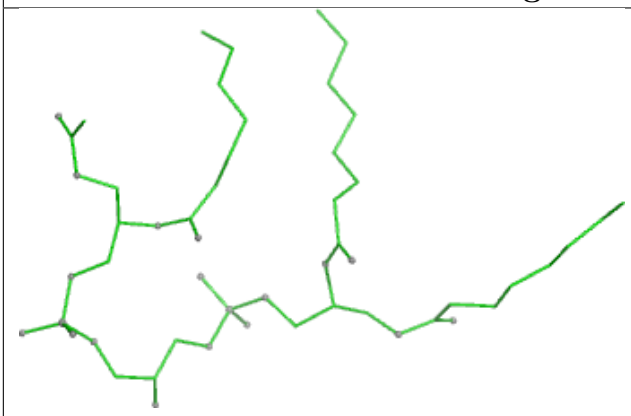


Torsions

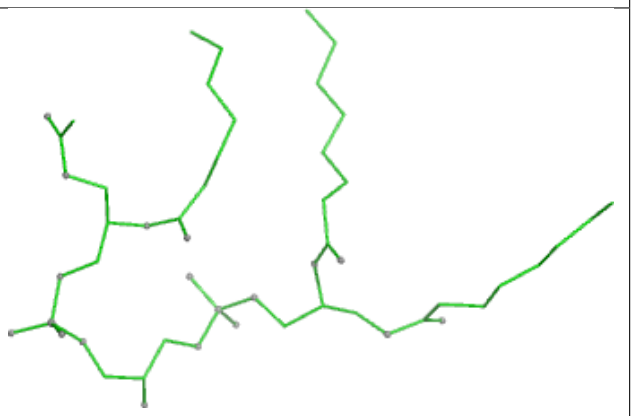


Rings

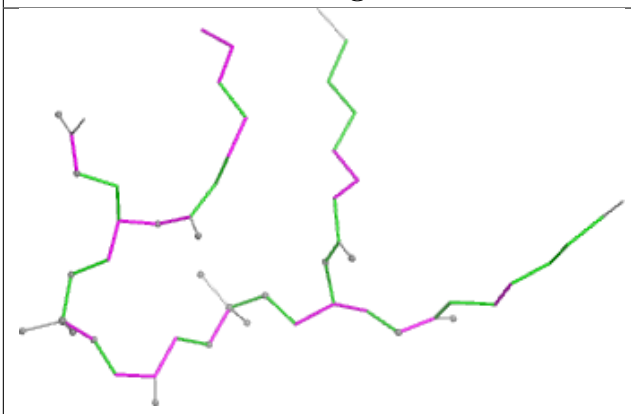
Ligand CDL D 502



Bond lengths



Bond angles

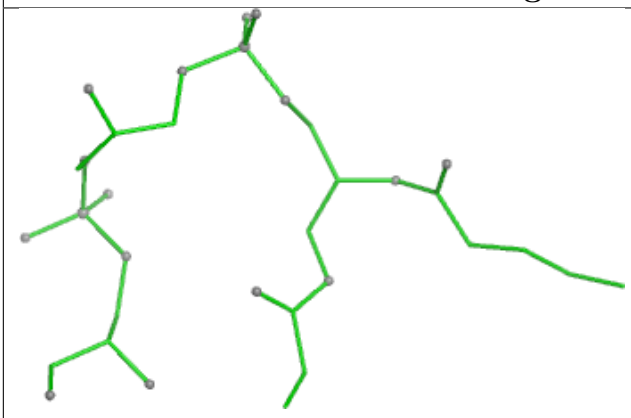


Torsions

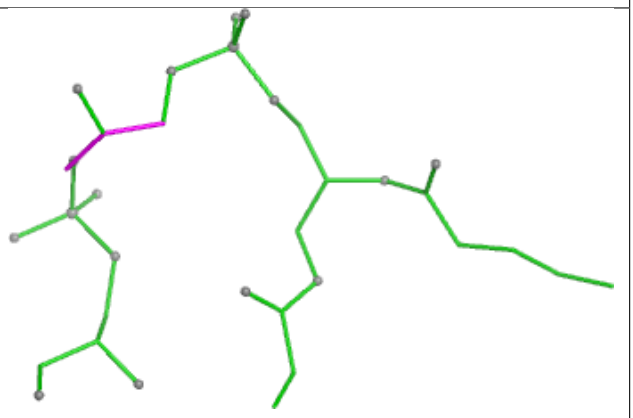


Rings

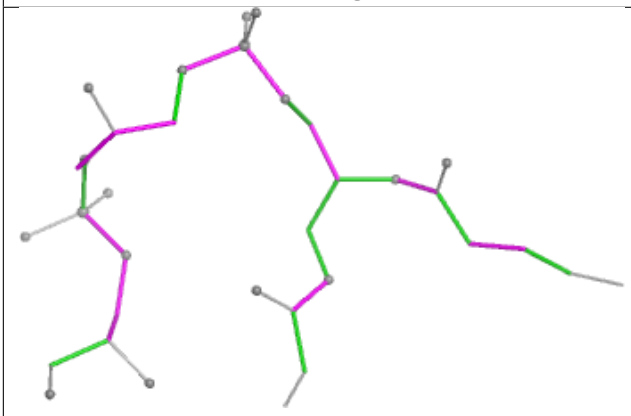
Ligand CDL C 401



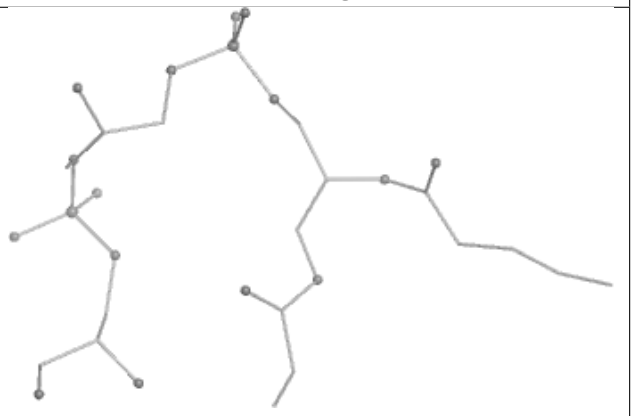
Bond lengths



Bond angles

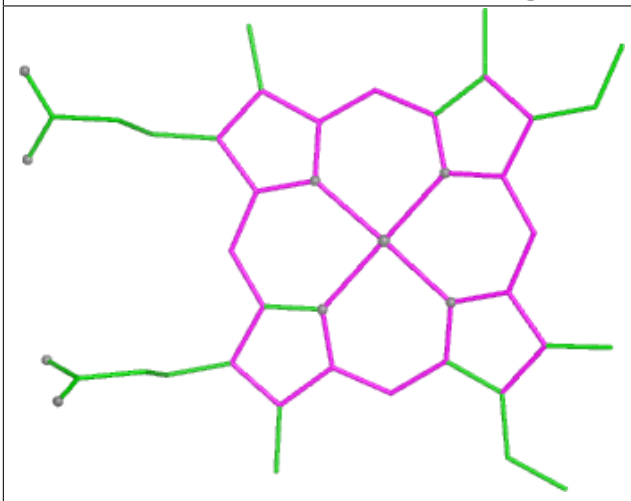


Torsions

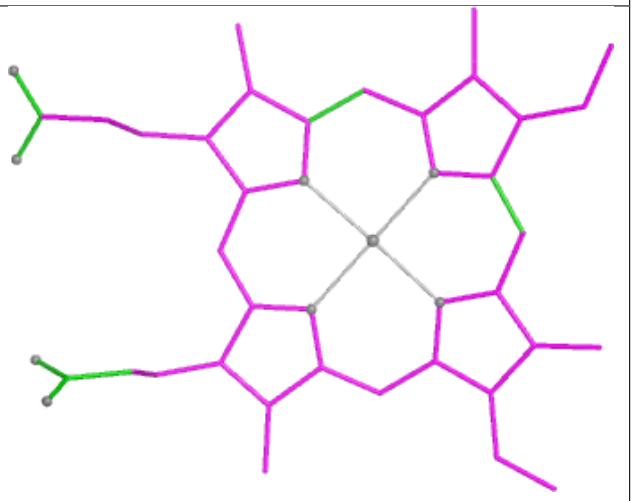


Rings

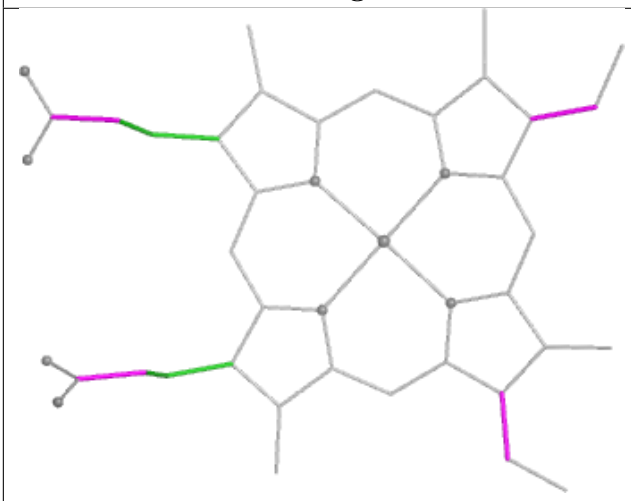
Ligand HEC D 501



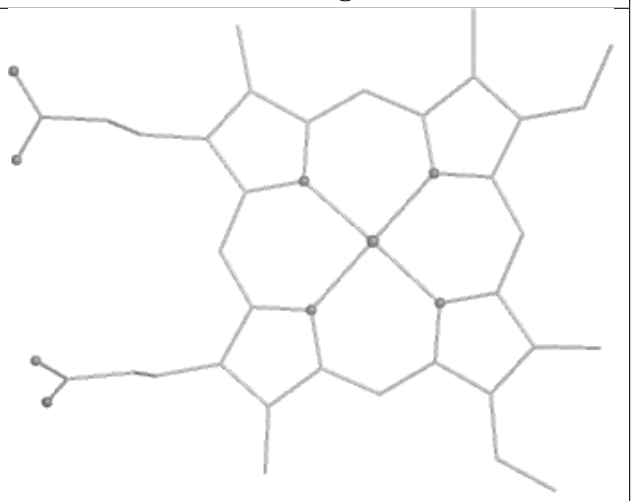
Bond lengths



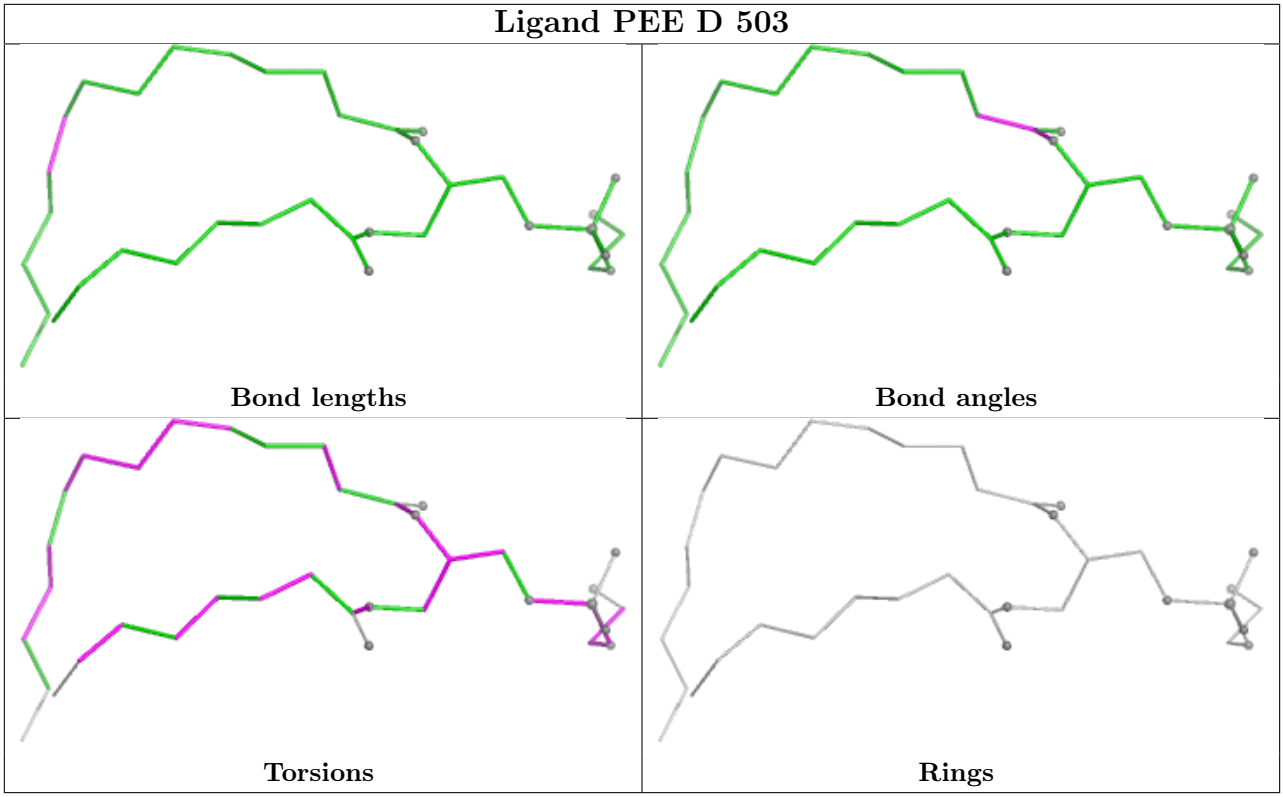
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.01	21 (4%) 35 24	72, 96, 128, 161	0
2	B	415/420 (98%)	0.08	19 (4%) 37 25	72, 98, 129, 178	0
3	C	378/378 (100%)	0.15	22 (5%) 29 19	72, 86, 116, 137	0
4	D	239/239 (100%)	0.22	15 (6%) 26 17	109, 135, 160, 186	0
5	E	196/196 (100%)	0.82	32 (16%) 4 4	82, 143, 179, 195	0
6	F	99/99 (100%)	-0.07	2 (2%) 65 46	80, 98, 141, 185	0
7	G	74/74 (100%)	0.09	4 (5%) 31 21	74, 98, 151, 157	0
8	H	65/65 (100%)	0.12	3 (4%) 37 25	143, 166, 184, 189	0
9	I	46/46 (100%)	2.20	22 (47%) 0 0	122, 144, 165, 176	0
10	J	59/59 (100%)	0.01	1 (1%) 69 50	90, 106, 151, 157	0
All	All	2010/2020 (99%)	0.20	141 (7%) 22 15	72, 104, 164, 195	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	37	THR	9.0
4	D	77	ASP	6.5
5	E	159	PRO	6.3
5	E	83	GLU	5.9
9	I	38	SER	5.4
4	D	78	GLY	5.4
1	A	228	VAL	5.1
5	E	164	HIS	4.9
9	I	42	VAL	4.9
9	I	48	SER	4.7
4	D	167	GLU	4.7
4	D	79	GLU	4.6
9	I	43	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	68	VAL	4.4
5	E	108	GLN	4.4
5	E	152	ASP	4.3
1	A	7	ALA	4.2
2	B	251	SER	4.1
3	C	172	LYS	4.0
2	B	376	GLU	3.9
1	A	367	SER	3.8
9	I	77	ARG	3.8
3	C	57	SER	3.7
1	A	446	PHE	3.7
1	A	66	GLY	3.7
5	E	82	PRO	3.7
6	F	78	GLU	3.7
1	A	363	ASN	3.6
3	C	168	PHE	3.6
9	I	63	PRO	3.5
4	D	165	TYR	3.5
3	C	43	LEU	3.5
2	B	217	LYS	3.4
5	E	94	LYS	3.4
1	A	370	ASP	3.4
4	D	81	PHE	3.4
9	I	39	GLU	3.4
5	E	157	TYR	3.4
5	E	162	GLY	3.4
1	A	140	GLU	3.3
7	G	56	TYR	3.3
2	B	250	ASP	3.3
1	A	147	ASP	3.3
1	A	3	THR	3.3
8	H	28	GLU	3.3
4	D	148	TYR	3.2
4	D	147	LEU	3.2
3	C	58	ASP	3.2
5	E	92	ARG	3.2
9	I	54	SER	3.2
5	E	158	CYS	3.2
3	C	241	LEU	3.1
9	I	35	PRO	3.1
9	I	52	ARG	3.1
4	D	75	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	9	GLN	3.0
3	C	61	THR	3.0
3	C	171	ASP	2.9
2	B	153	GLN	2.9
2	B	318	ASP	2.9
3	C	2	THR	2.9
2	B	154	ASN	2.8
9	I	69	SER	2.8
9	I	36	ALA	2.8
5	E	103	LYS	2.8
2	B	256	ALA	2.8
1	A	365	LEU	2.8
1	A	5	ALA	2.8
9	I	47	ARG	2.7
5	E	104	LYS	2.7
3	C	173	ALA	2.7
7	G	53	VAL	2.7
2	B	114	ASP	2.7
5	E	53	ASN	2.7
3	C	169	SER	2.6
9	I	70	LEU	2.6
3	C	167	GLY	2.6
5	E	178	LEU	2.6
1	A	227	THR	2.6
2	B	44	ALA	2.6
1	A	8	LEU	2.6
1	A	143	THR	2.6
4	D	166	ASN	2.5
5	E	107	ASP	2.5
5	E	149	ASN	2.5
5	E	85	LYS	2.5
5	E	161	HIS	2.5
5	E	86	ASN	2.5
1	A	392	LEU	2.5
7	G	57	LEU	2.5
8	H	13	LEU	2.5
1	A	318	GLY	2.5
3	C	156	ILE	2.4
4	D	108	ALA	2.4
5	E	148	ALA	2.4
8	H	46	SER	2.4
4	D	151	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	86	GLY	2.4
3	C	166	GLY	2.4
9	I	65	VAL	2.4
3	C	42	ILE	2.4
2	B	240	HIS	2.3
2	B	252	LEU	2.3
2	B	419	SER	2.3
5	E	106	ILE	2.3
5	E	64	ALA	2.3
4	D	145	GLU	2.3
2	B	42	ALA	2.3
7	G	75	ALA	2.3
2	B	45	SER	2.3
3	C	44	GLN	2.3
1	A	266	ASP	2.3
4	D	159	GLY	2.2
3	C	376	LEU	2.2
5	E	138	VAL	2.2
10	J	36	ASP	2.2
5	E	183	PRO	2.2
9	I	59	ALA	2.2
2	B	170	ASN	2.2
9	I	56	ARG	2.2
2	B	393	THR	2.2
3	C	176	THR	2.2
3	C	89	MET	2.2
5	E	31	ALA	2.2
3	C	245	PHE	2.2
6	F	109	LYS	2.1
1	A	316	ASP	2.1
1	A	354	VAL	2.1
3	C	28	SER	2.1
5	E	184	SER	2.1
9	I	53	GLU	2.1
5	E	145	VAL	2.1
2	B	265	GLY	2.1
5	E	84	GLY	2.1
2	B	94	GLY	2.1
9	I	49	VAL	2.1
9	I	76	VAL	2.1
5	E	88	ALA	2.1
4	D	143	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	154	GLY	2.0
9	I	68	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 oligosaccharides 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
16	LMT	C	405	35/35	0.44	0.17	155,168,174,175	0
13	CDL	E	203	60/100	0.64	0.16	130,164,197,201	0
18	PO4	G	102	5/5	0.72	0.09	175,175,177,181	0
11	PG4	A	501	13/13	0.81	0.13	127,137,143,144	0
18	PO4	H	101	5/5	0.82	0.11	209,210,213,216	0
18	PO4	G	101	5/5	0.84	0.10	127,128,130,131	0
18	PO4	G	103	5/5	0.85	0.20	134,134,134,135	0
15	JHB	C	404	31/31	0.85	0.19	90,97,124,128	0
13	CDL	C	401	34/100	0.88	0.13	116,129,138,139	0
17	PEE	D	503	37/51	0.91	0.14	89,106,110,110	0
18	PO4	F	501	5/5	0.91	0.30	153,156,156,157	0
12	6PE	A	502	23/27	0.91	0.15	109,122,132,132	0
21	PX4	E	202	37/46	0.91	0.24	119,132,142,144	0
11	PG4	A	503	13/13	0.93	0.15	47,57,70,71	0
11	PG4	C	406	13/13	0.93	0.13	91,93,96,96	0
13	CDL	D	502	54/100	0.93	0.12	112,152,177,180	0
18	PO4	C	410	5/5	0.93	0.10	159,161,162,162	0
11	PG4	C	407	13/13	0.93	0.11	105,108,113,114	0
20	FES	E	201	4/4	0.95	0.05	214,214,217,220	0
17	PEE	C	409	40/51	0.96	0.11	82,84,85,85	0
13	CDL	C	408	44/100	0.96	0.11	86,92,96,96	0

Continued on next page...

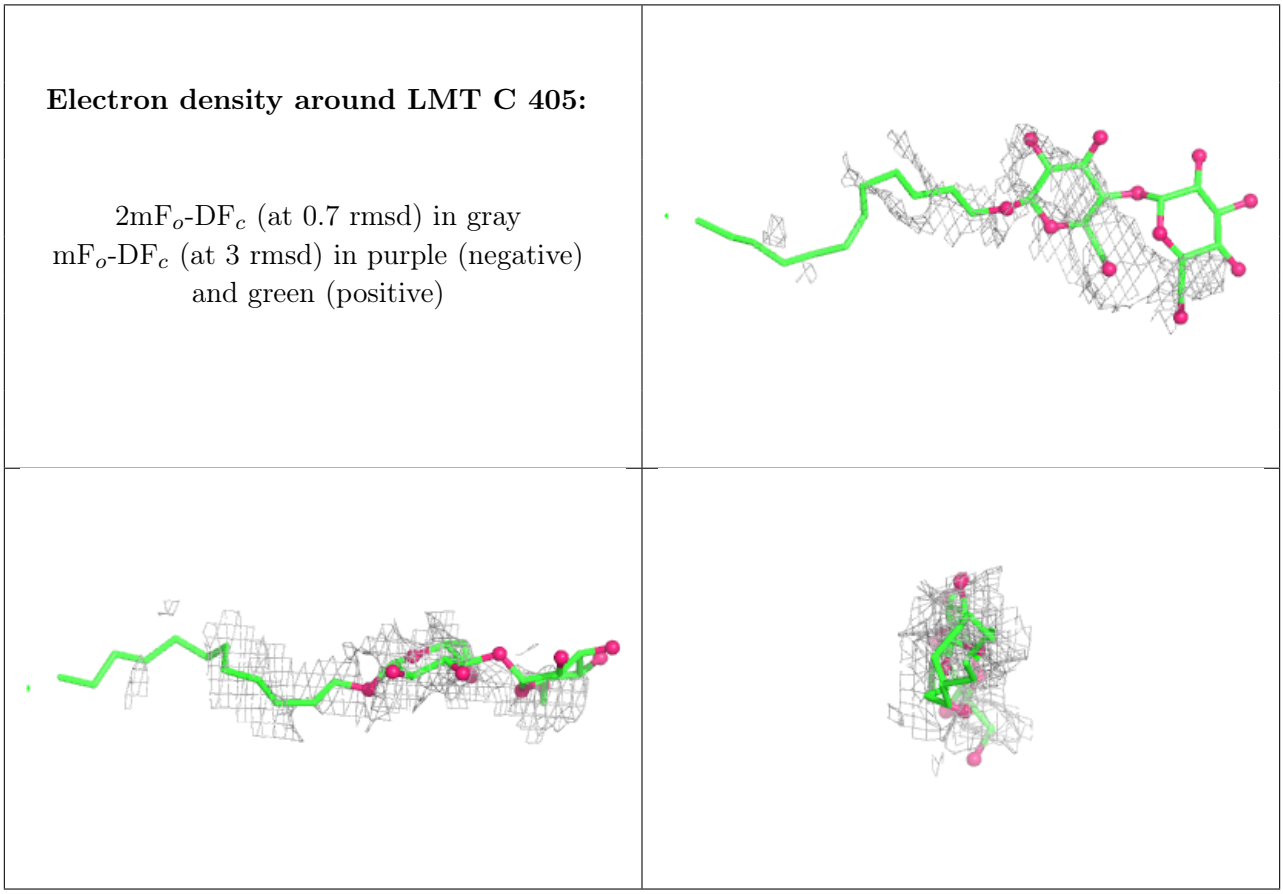
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	HEC	D	501	43/43	0.98	0.07	126,132,135,138	0
14	HEM	C	402	43/43	0.98	0.08	76,77,79,79	0
14	HEM	C	403	43/43	0.98	0.08	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.

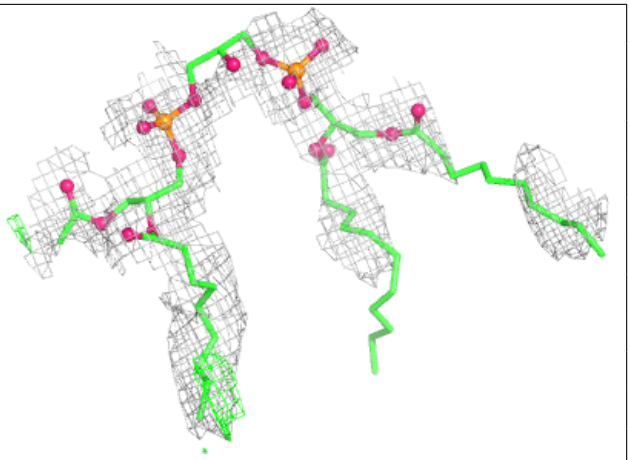
Electron density around LMT C 405:

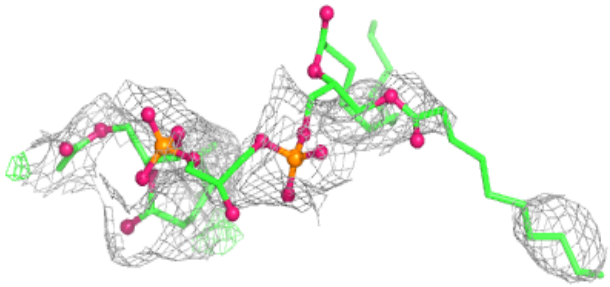
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

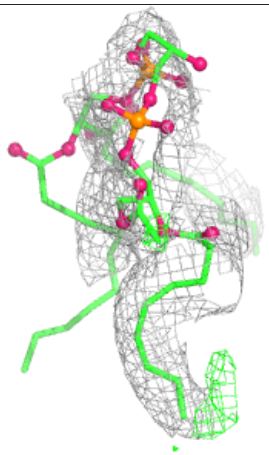


Electron density around CDL E 203:

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

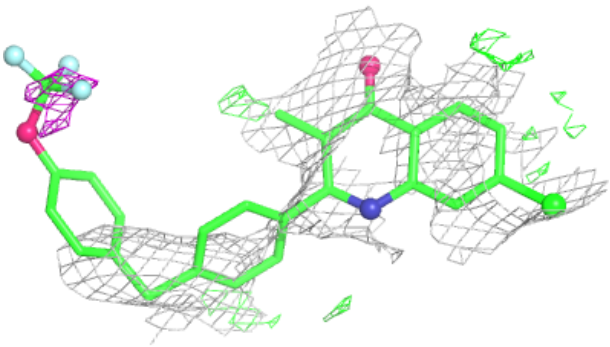


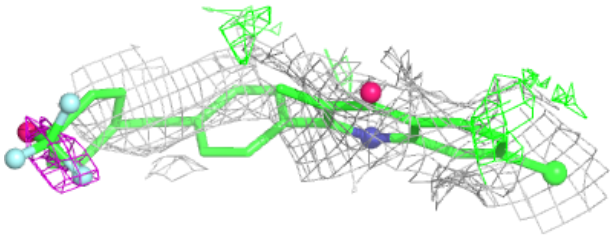


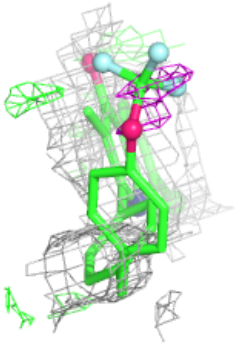


Electron density around JHB C 404:

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

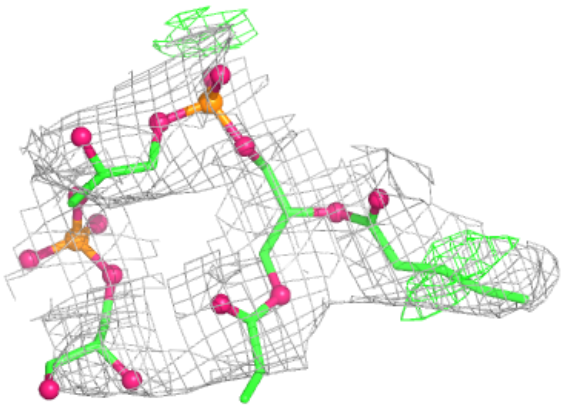


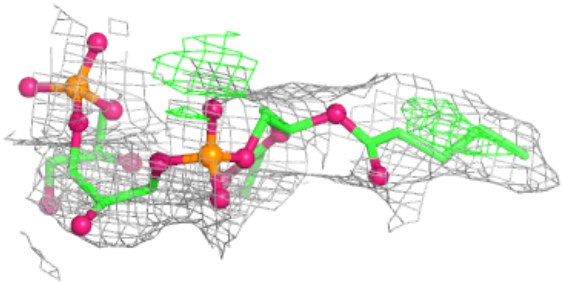


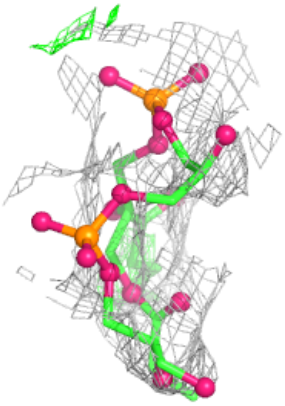


Electron density around CDL C 401:

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

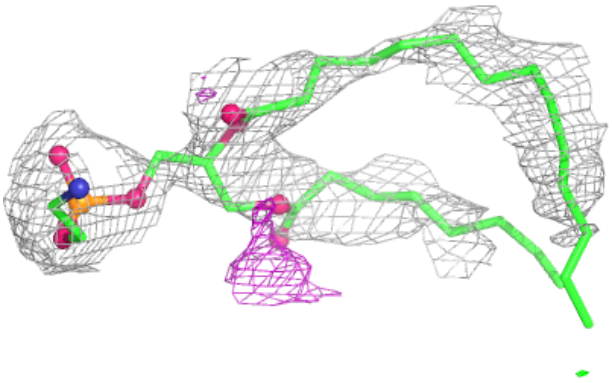


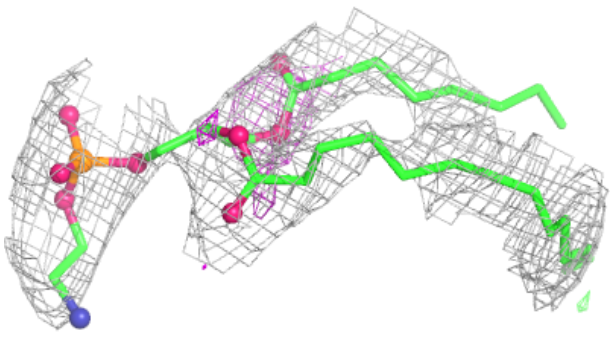


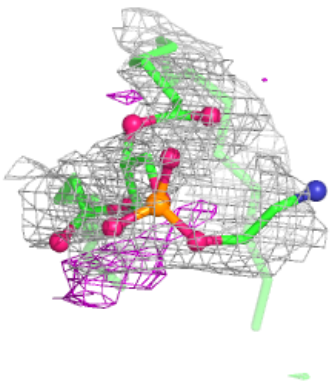


Electron density around PEE D 503:

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

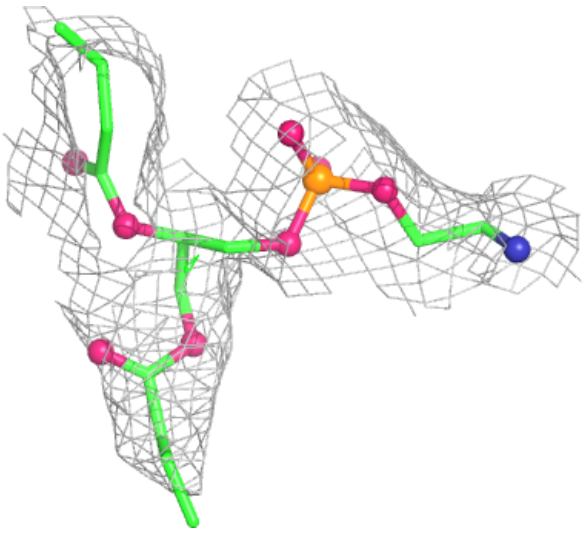


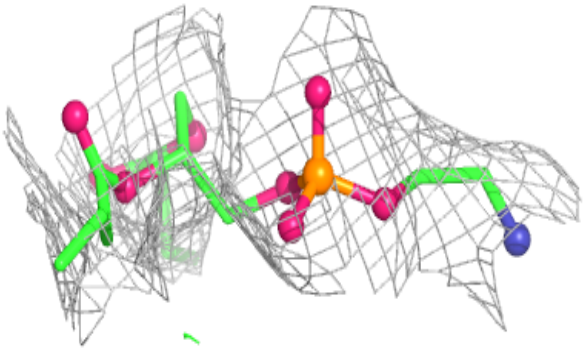


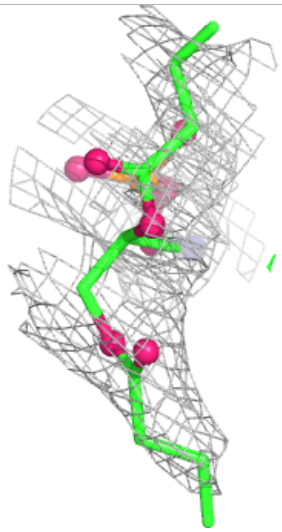


Electron density around 6PE A 502:

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

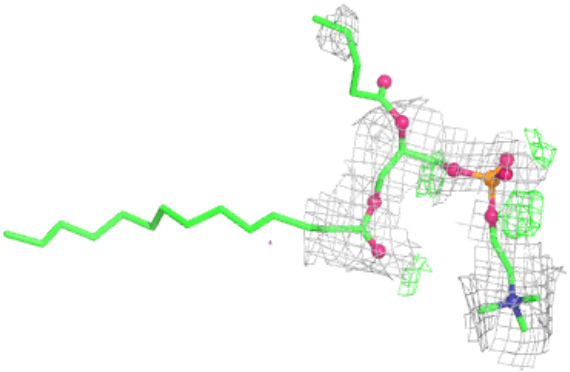




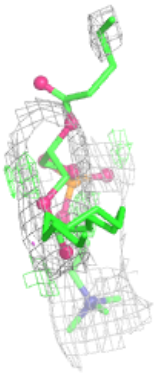


Electron density around PX4 E 202:

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

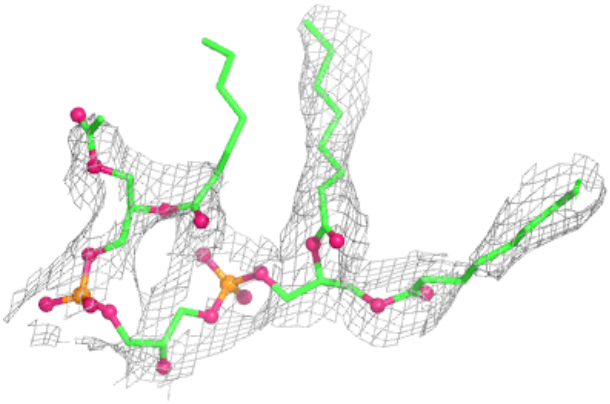


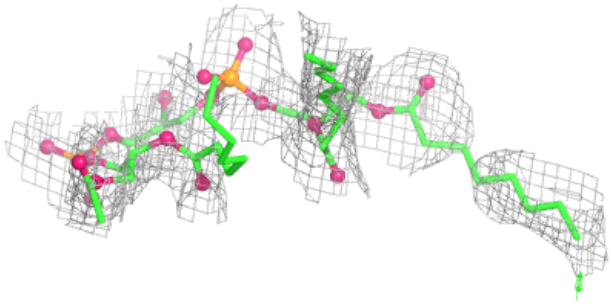


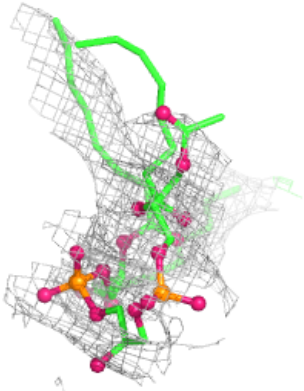


Electron density around CDL D 502:

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

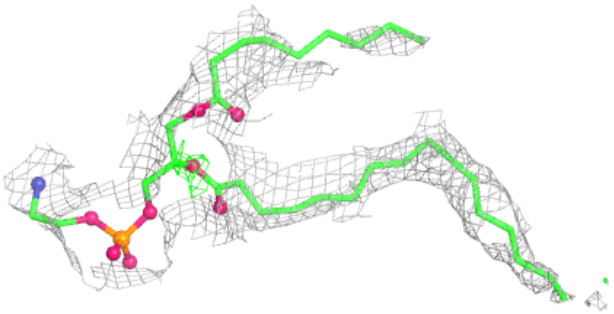


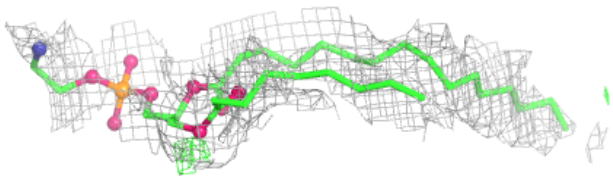


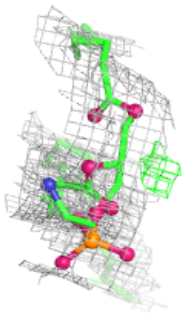


Electron density around PEE C 409:

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

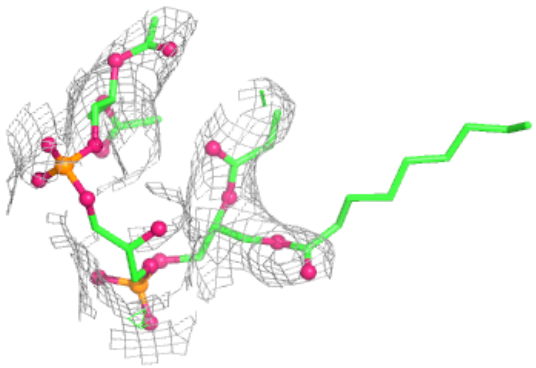


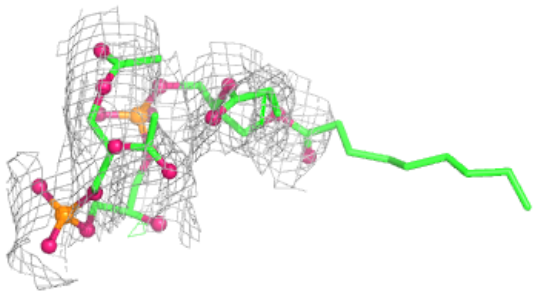




Electron density around CDL C 408:

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

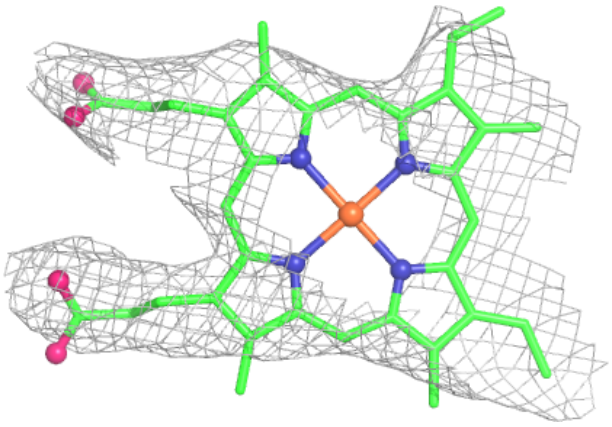


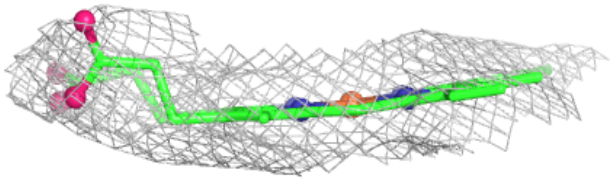


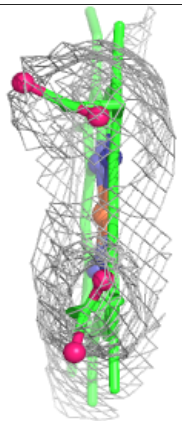


Electron density around HEC D 501:

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

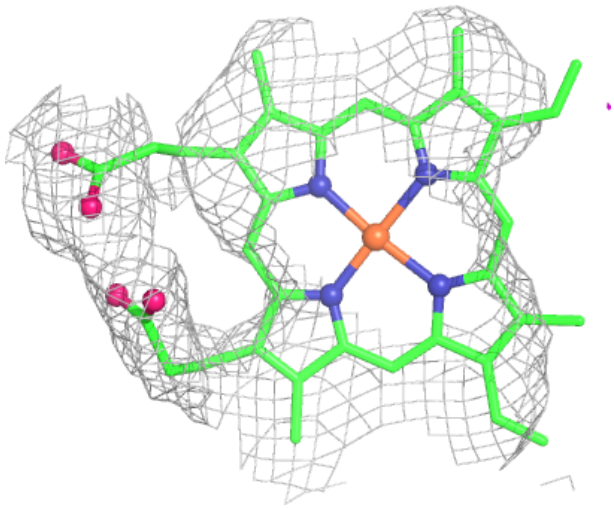


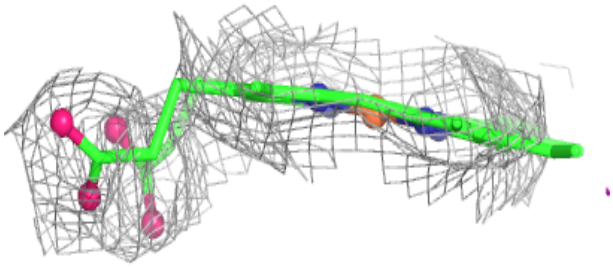


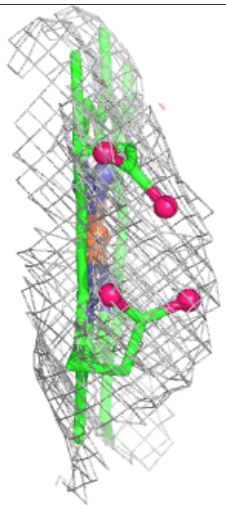


Electron density around HEM C 402:

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

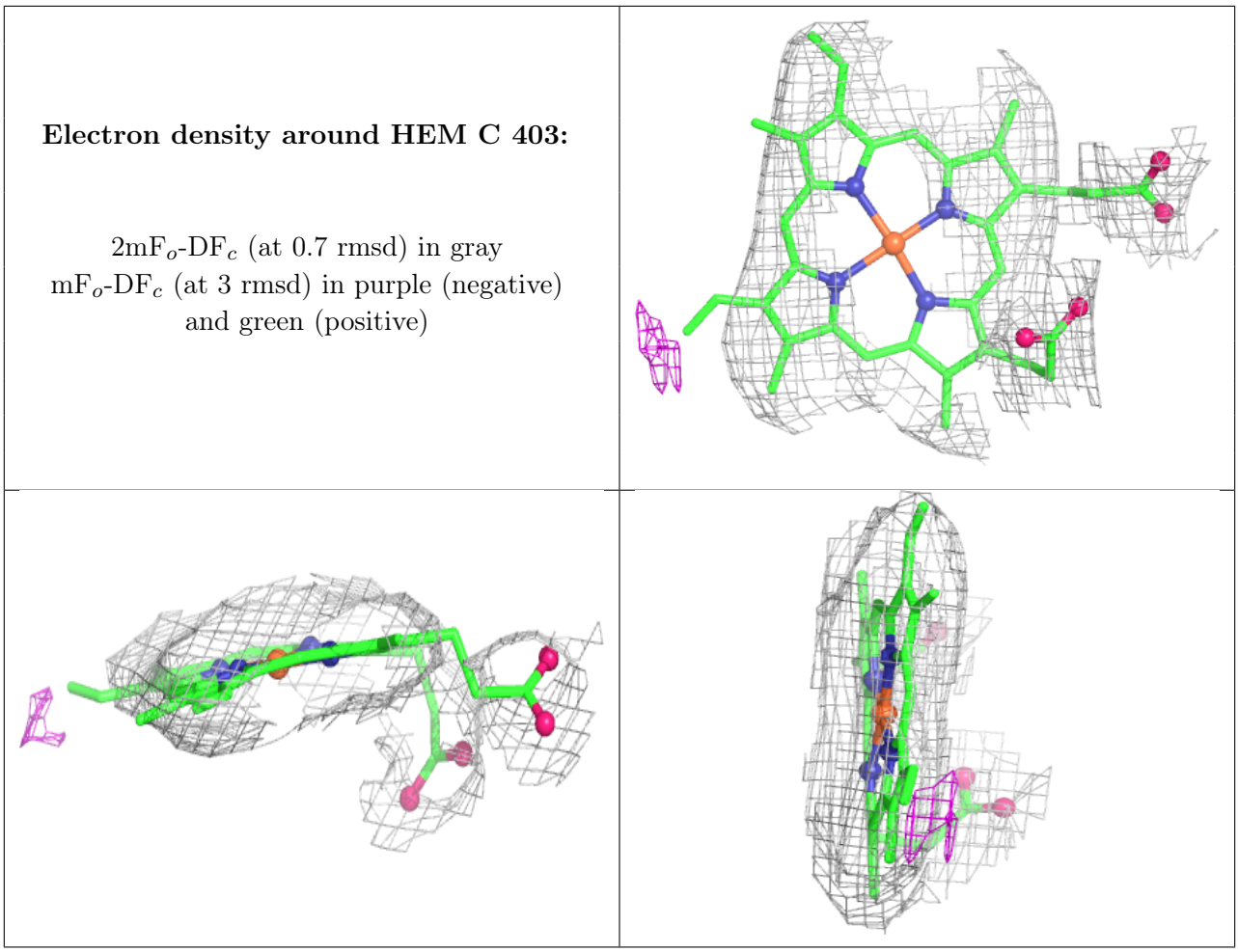






Electron density around HEM C 403:

$2mF_o$-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 (i)

There are no such residues in this entry.