wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2026 – 04:50 am BST

PDB ID	:	6ZFU / pdb_00006zfu
Title	:	Crystal structure of bovine cytochrome bc1 in complex with quinolone inhibitor RKA066
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	:	3.50 Å(reported)

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

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

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

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

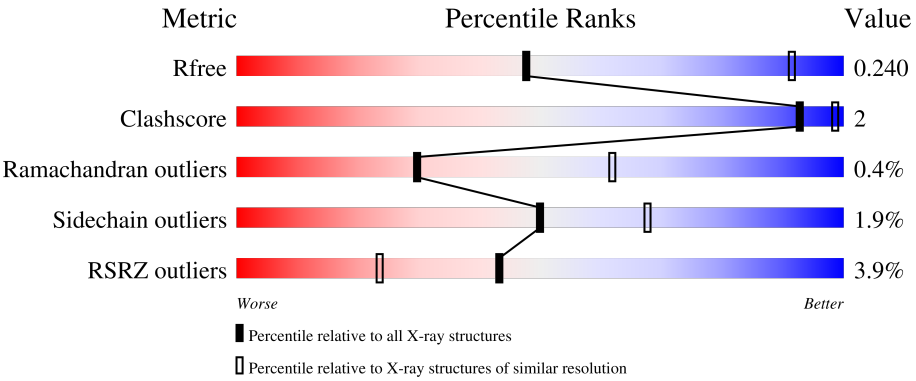
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	96% .
2	B	420	95% . .
3	C	378	3% 92% 8%
4	D	239	5% 93% 7%

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Mol	Chain	Length	Quality of chain
5	E	196	13% 96%
6	F	99	3% 93% 6%
7	G	74	4% 91% 8%
8	H	65	5% 97%
9	I	46	26% 83% 17%
10	J	59	3% 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
16	PEE	C	407	X	-	-	-
16	PEE	E	203	X	-	-	-
18	HEC	D	501	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 16290 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	444	Total	C	N	O	S	0	0	0
			3417	2133	603	661	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLU	ASP	conflict	UNP P31800
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
			3106	1952	550	597	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
			2990	2004	468	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
			1872	1198	321	338	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
			1509	950	263	288	8			

- 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
			859	545	157	155	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
			616	403	115	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
			507	307	93	102	5			

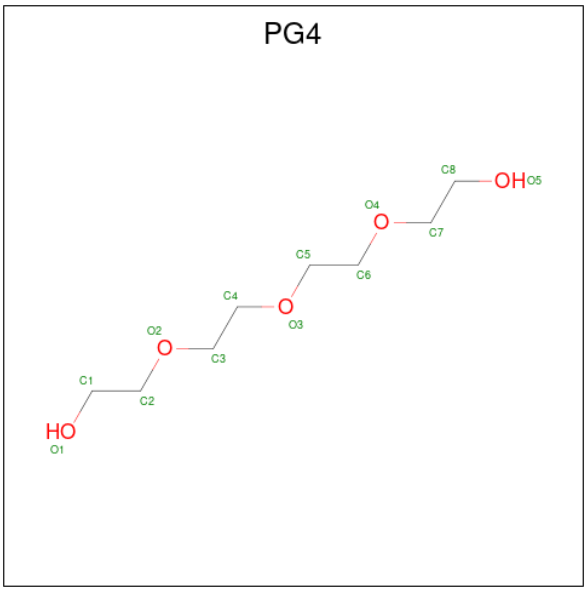
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			332	206	61	64	1			

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

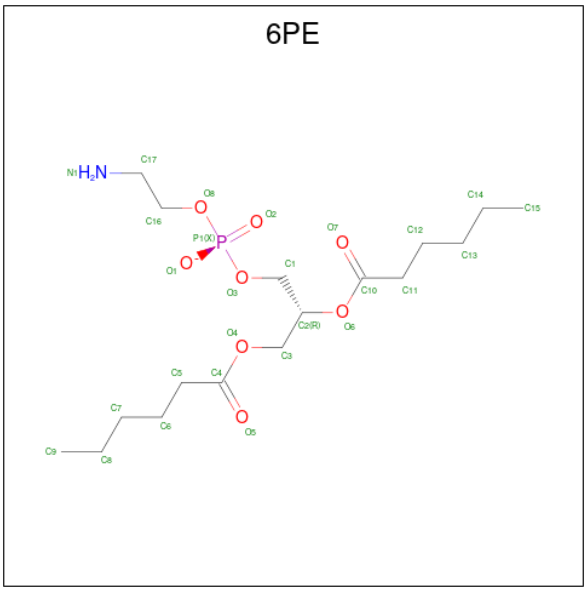
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			480	314	83	83			

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



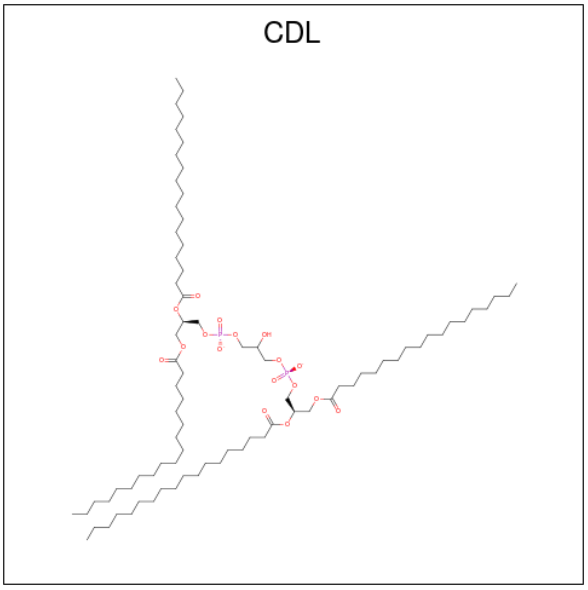
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0
11	C	1	Total C O 13 8 5	0	0

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



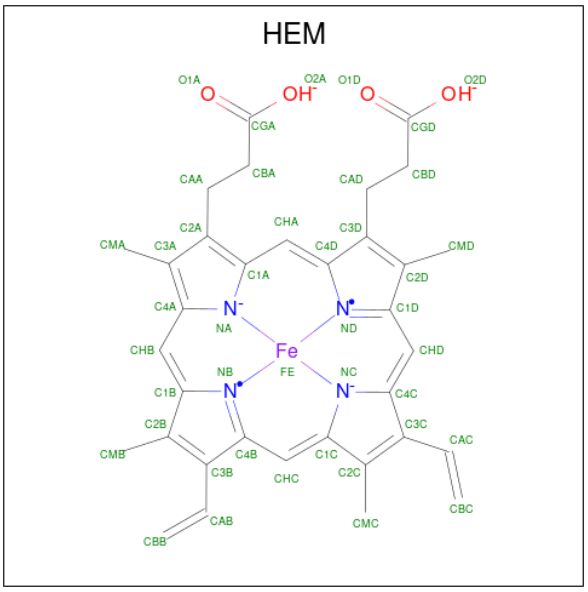
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

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



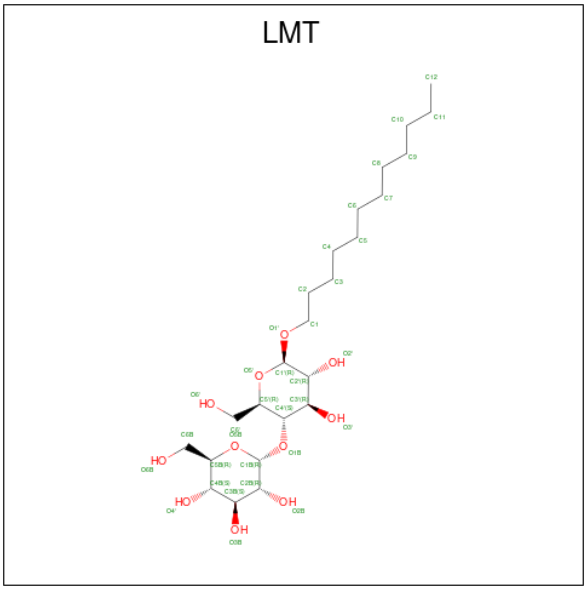
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	O	P		0	0
			34	17	15	2			
13	C	1	Total	C	O	P		0	0
			44	25	17	2			
13	D	1	Total	C	O	P		0	0
			54	35	17	2			
13	E	1	Total	C	O	P		0	0
			60	41	17	2			

- 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		

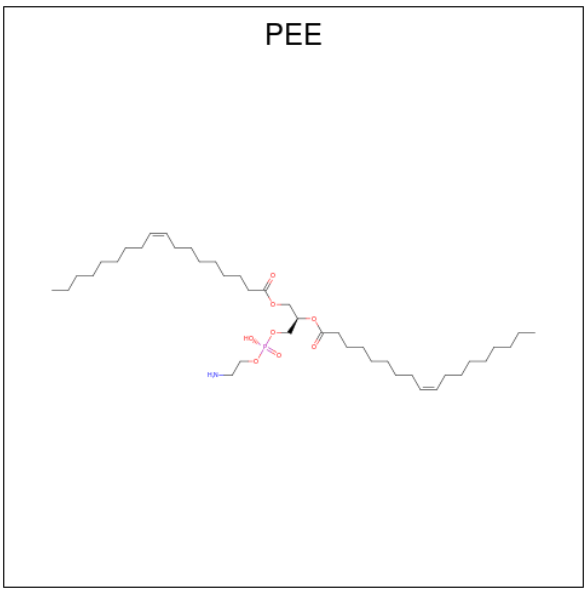
- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

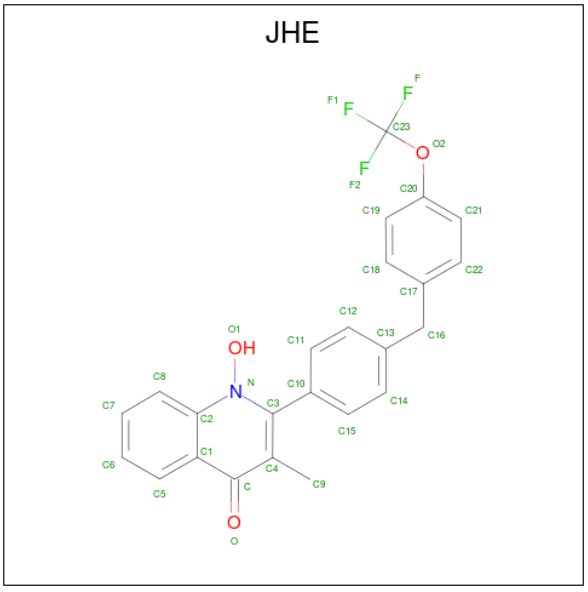
- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:

$C_{41}H_{78}NO_8P$).



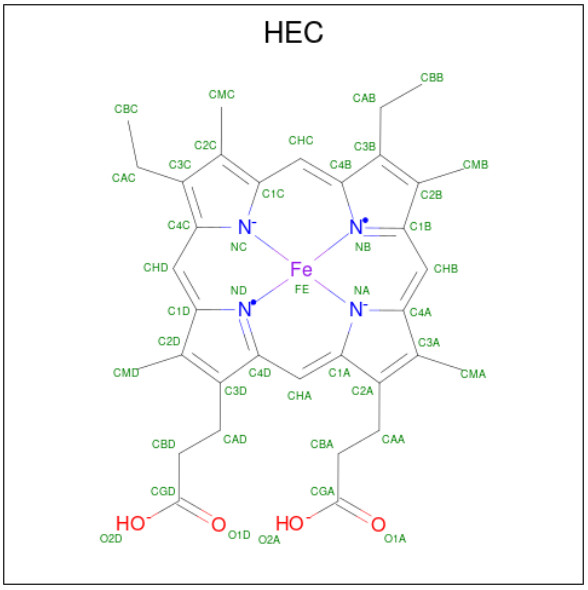
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
16	E	1	Total	C	N	O	P	0	0
			41	31	1	8	1		

- Molecule 17 is 3-methyl-1-oxidanyl-2-[4-[[4-(trifluoromethyloxy)phenyl]methyl]phenyl]quinolin-4-one (CCD ID: JHE) (formula: $C_{24}H_{18}F_3NO_3$) (labeled as "Ligand of Interest" by depositor).



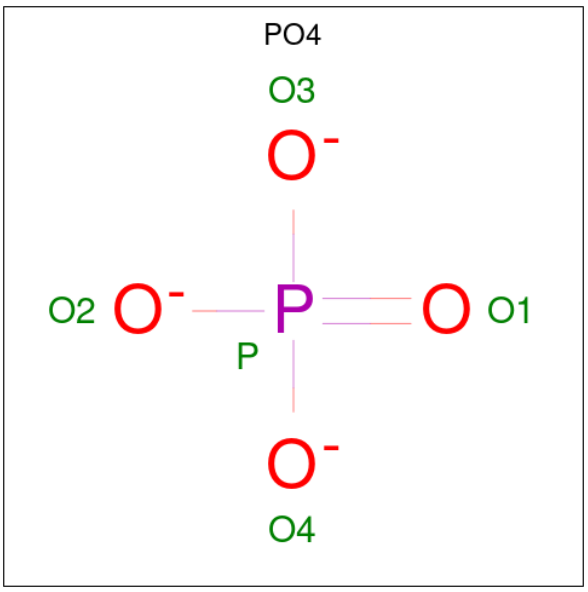
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	F	N	O	0	0
			31	24	3	1	3		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



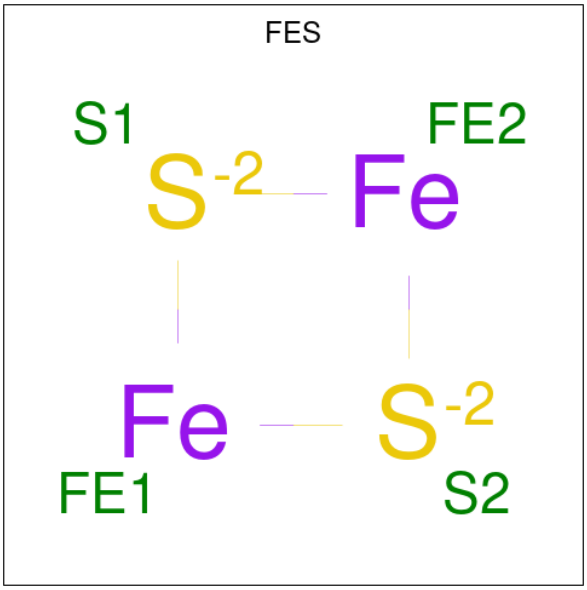
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 19 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



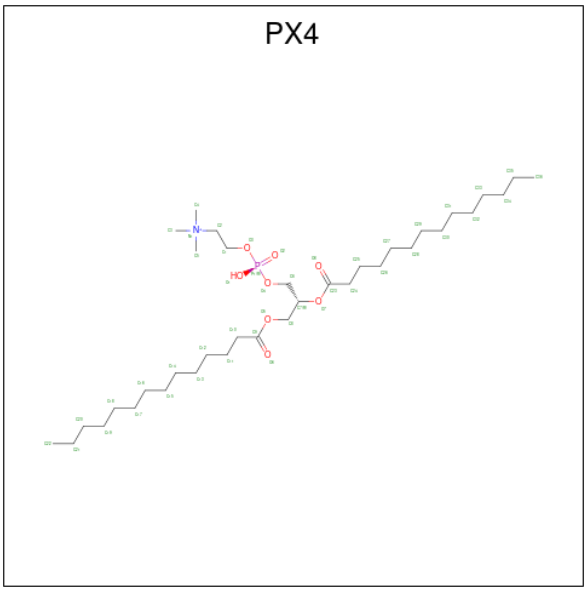
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total O P 5 4 1	0	0
19	F	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0

- 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 4 2 2	0	0

- 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	C	1	Total	O	0	0
			1	1		
22	G	1	Total	O	0	0
			1	1		
22	I	1	Total	O	0	0
			1	1		

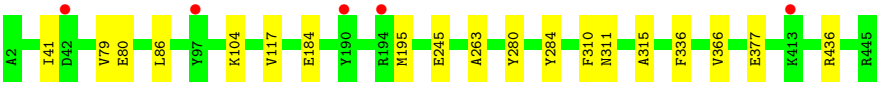
3 Residue-property plots (i)

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

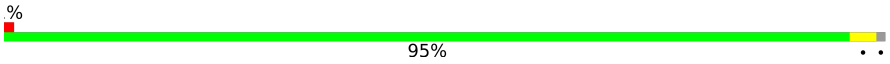
Chain A:

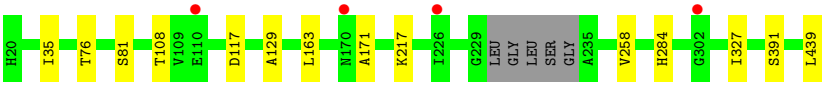




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

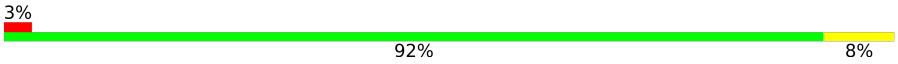
Chain B:



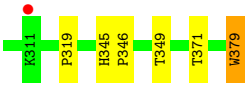


• Molecule 3: Cytochrome b

Chain C:

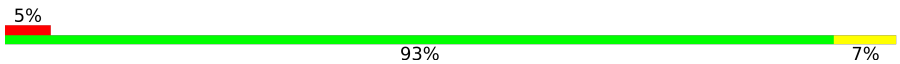






• Molecule 4: Cytochrome c1, heme protein, mitochondrial

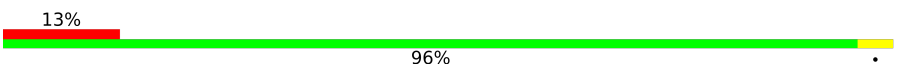
Chain D:

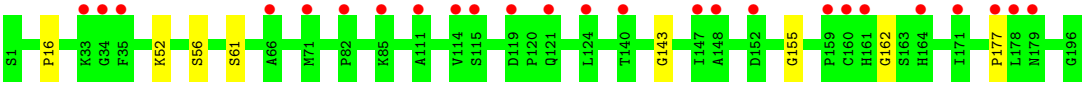




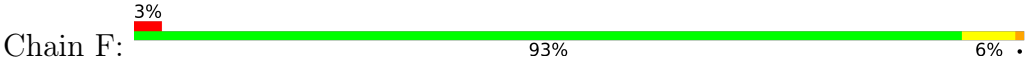
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

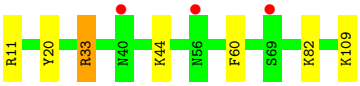
Chain E:



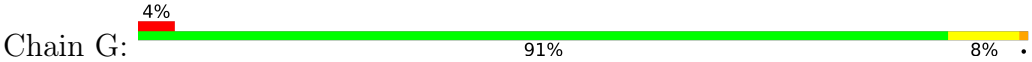


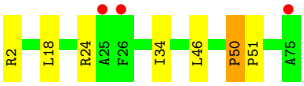
• Molecule 6: Cytochrome b-c1 complex subunit 7





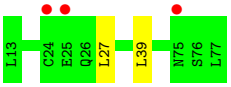
• Molecule 7: Cytochrome b-c1 complex subunit 8



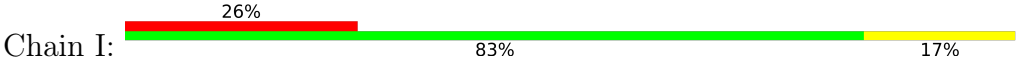


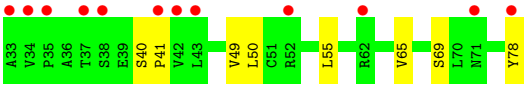
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial





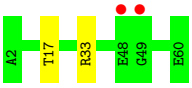
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial





• Molecule 10: Cytochrome b-c1 complex subunit 9





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	210.74Å 210.74Å 343.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	89.85 – 3.50 89.85 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.85-3.50) 99.9 (89.85-3.50)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.221 , 0.238 0.225 , 0.240	Depositor DCC
R_{free} test set	2925 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	96.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 146.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	16290	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: PX4, PG4, FES, PO4, PEE, LMT, HEM, JHE, CDL, 6PE, HEC

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	0.63	0/3488	1.03	5/4738 (0.1%)
2	B	0.64	0/3163	1.01	2/4292 (0.0%)
3	C	0.64	1/3086 (0.0%)	1.05	0/4224
4	D	0.66	0/1931	1.03	2/2627 (0.1%)
5	E	0.72	0/1542	1.01	0/2085
6	F	0.61	0/878	1.02	0/1181
7	G	0.74	1/637 (0.2%)	1.11	1/864 (0.1%)
8	H	0.65	0/512	1.09	0/692
9	I	1.02	0/336	1.28	2/457 (0.4%)
10	J	0.69	0/493	1.07	0/667
All	All	0.66	2/16066 (0.0%)	1.04	12/21827 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	304	ILE	CA-CB	6.41	1.57	1.54
7	G	34	ILE	CA-CB	5.59	1.56	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	ALA	N-CA-C	10.41	122.32	110.97
4	D	162	PRO	N-CA-C	-8.78	99.99	110.70
1	A	311	ASN	N-CA-C	6.63	119.31	111.02
9	I	69	SER	N-CA-C	6.07	116.29	108.34
4	D	97	ASN	N-CA-C	5.70	113.14	108.07

There are no chirality outliers.

There are no planarity outliers.

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	3417	0	3296	7	0
2	B	3106	0	3074	5	0
3	C	2990	0	3047	15	0
4	D	1872	0	1785	13	0
5	E	1509	0	1495	2	0
6	F	859	0	838	3	0
7	G	616	0	613	2	0
8	H	507	0	468	0	0
9	I	332	0	345	2	0
10	J	480	0	467	0	0
11	A	13	0	18	0	0
11	C	26	0	36	0	0
12	A	23	0	19	2	0
13	A	34	0	24	3	0
13	C	44	0	32	0	0
13	D	54	0	52	0	0
13	E	60	0	64	1	0
14	C	86	0	60	6	0
15	C	35	0	46	0	0
16	C	40	0	54	0	0
16	E	41	0	59	1	0
17	C	31	0	0	0	0
18	D	43	0	32	5	0
19	D	5	0	0	0	0
19	F	5	0	0	0	0
19	G	15	0	0	0	0
20	E	4	0	0	0	0
21	E	37	0	51	0	0
22	A	3	0	0	0	0
22	C	1	0	0	0	0
22	G	1	0	0	0	0
22	I	1	0	0	0	0
All	All	16290	0	15975	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 49 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:211:MET:HA	4:D:211:MET:HE2	1.62	0.82
4:D:37:CYS:SG	18:D:501:HEC:CAB	2.74	0.75
1:A:336:PHE:CZ	3:C:3:ASN:HB3	2.24	0.73
14:C:402:HEM:HMC2	14:C:402:HEM:HBC2	1.79	0.65
14:C:401:HEM:HMC1	14:C:401:HEM:HBC2	1.80	0.64

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	442/444 (100%)	424 (96%)	18 (4%)	0	100 100
2	B	411/420 (98%)	399 (97%)	11 (3%)	1 (0%)	43 74
3	C	376/378 (100%)	363 (96%)	12 (3%)	1 (0%)	36 67
4	D	237/239 (99%)	225 (95%)	12 (5%)	0	100 100
5	E	194/196 (99%)	179 (92%)	11 (6%)	4 (2%)	5 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%)	43 (98%)	0	1 (2%)	5 30
10	J	57/59 (97%)	55 (96%)	2 (4%)	0	100 100
All	All	1993/2020 (99%)	1913 (96%)	73 (4%)	7 (0%)	30 62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	171	ALA

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Mol	Chain	Res	Type
3	C	155	TYR
5	E	162	GLY
9	I	41	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	363/369 (98%)	358 (99%)	5 (1%)	59	71
2	B	323/329 (98%)	320 (99%)	3 (1%)	70	76
3	C	324/326 (99%)	318 (98%)	6 (2%)	50	68
4	D	194/204 (95%)	192 (99%)	2 (1%)	68	75
5	E	166/168 (99%)	165 (99%)	1 (1%)	78	79
6	F	88/91 (97%)	83 (94%)	5 (6%)	18	45
7	G	64/66 (97%)	61 (95%)	3 (5%)	23	49
8	H	56/62 (90%)	54 (96%)	2 (4%)	31	57
9	I	37/38 (97%)	34 (92%)	3 (8%)	11	35
10	J	47/49 (96%)	45 (96%)	2 (4%)	26	51
All	All	1662/1702 (98%)	1630 (98%)	32 (2%)	50	68

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	65	VAL
9	I	78	TYR
3	C	371	THR
3	C	349	THR
10	J	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	54	HIS
10	J	57	HIS
4	D	105	ASN
7	G	12	HIS
4	D	6	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	LMT	C	403	-	36,36,36	0.82	1 (2%)	47,47,47	1.21	4 (8%)
19	PO4	F	501	-	4,4,4	0.88	0	6,6,6	0.43	0
11	PG4	C	405	-	12,12,12	0.49	0	11,11,11	0.43	0
13	CDL	E	204	-	59,59,99	1.27	4 (6%)	65,71,111	1.18	7 (10%)
19	PO4	G	101	-	4,4,4	0.74	0	6,6,6	0.84	0
12	6PE	A	502	-	22,22,26	1.54	2 (9%)	25,27,31	1.40	3 (12%)
14	HEM	C	401	3	50,50,50	1.60	7 (14%)	66,82,82	1.43	13 (19%)
11	PG4	C	404	-	12,12,12	0.69	0	11,11,11	0.63	0
16	PEE	E	203	-	40,40,50	1.28	3 (7%)	43,45,55	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	HEC	D	501	4	50,50,50	2.94	28 (56%)	68,82,82	2.69	31 (45%)
14	HEM	C	402	3	50,50,50	1.55	7 (14%)	66,82,82	1.29	10 (15%)
20	FES	E	201	-	0,4,4	-	-	-		
11	PG4	A	501	-	12,12,12	0.56	0	11,11,11	0.39	0
13	CDL	D	503	-	53,53,99	1.40	4 (7%)	59,65,111	1.22	6 (10%)
13	CDL	C	406	-	43,43,99	1.58	4 (9%)	49,55,111	1.55	6 (12%)
19	PO4	G	102	-	4,4,4	0.91	0	6,6,6	0.50	0
16	PEE	C	407	-	39,39,50	1.25	3 (7%)	42,44,55	1.15	2 (4%)
17	JHE	C	408	-	34,34,34	2.39	5 (14%)	44,50,50	1.03	3 (6%)
19	PO4	D	502	-	4,4,4	1.07	0	6,6,6	0.36	0
13	CDL	A	503	-	33,33,99	1.28	2 (6%)	37,43,111	1.35	4 (10%)
19	PO4	G	103	-	4,4,4	0.85	0	6,6,6	0.57	0
21	PX4	E	202	-	36,36,45	1.33	2 (5%)	42,44,53	1.20	5 (11%)

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
16	PEE	C	407	-	1/1/4/8	18/43/43/54	-
11	PG4	C	405	-	-	5/10/10/10	-
15	LMT	C	403	-	-	9/21/61/61	0/2/2/2
13	CDL	E	204	-	-	36/69/69/110	-
20	FES	E	201	-	-	-	0/1/1/1
11	PG4	A	501	-	-	6/10/10/10	-
13	CDL	D	503	-	-	24/63/63/110	-
17	JHE	C	408	-	-	2/13/13/13	0/4/4/4
12	6PE	A	502	-	-	12/26/26/30	-
13	CDL	C	406	-	-	16/52/52/110	-
13	CDL	A	503	-	-	18/41/41/110	-
14	HEM	C	401	3	-	5/14/54/54	-
11	PG4	C	404	-	-	5/10/10/10	-
16	PEE	E	203	-	1/1/4/8	29/44/44/54	-
18	HEC	D	501	4	1/1/3/7	6/14/54/54	-
14	HEM	C	402	3	-	4/14/54/54	-
21	PX4	E	202	-	-	15/40/40/49	-

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	408	JHE	C3-C4	11.23	1.49	1.36
17	C	408	JHE	C1-C2	5.79	1.50	1.41
14	C	402	HEM	FE-NB	5.70	2.12	1.94
14	C	401	HEM	FE-NB	5.65	2.12	1.94
13	C	406	CDL	OA6-CA5	5.61	1.47	1.35

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	501	HEC	C1B-C2B-C3B	-6.46	100.16	106.96
18	D	501	HEC	C2A-C1A-NA	6.34	116.49	110.32
18	D	501	HEC	C3D-C4D-ND	6.22	116.38	110.36
18	D	501	HEC	C2B-C1B-NB	6.10	117.19	109.88
13	C	406	CDL	OA6-CA5-C11	6.08	122.27	111.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	407	PEE	C2
16	E	203	PEE	C2
18	D	501	HEC	NA

5 of 210 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	A	503	CDL	CA3-OA5-PA1-OA4
13	A	503	CDL	CB2-OB2-PB2-OB3

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	204	CDL	1	0
12	A	502	6PE	2	0
14	C	401	HEM	2	0
16	E	203	PEE	1	0
18	D	501	HEC	5	0
14	C	402	HEM	4	0

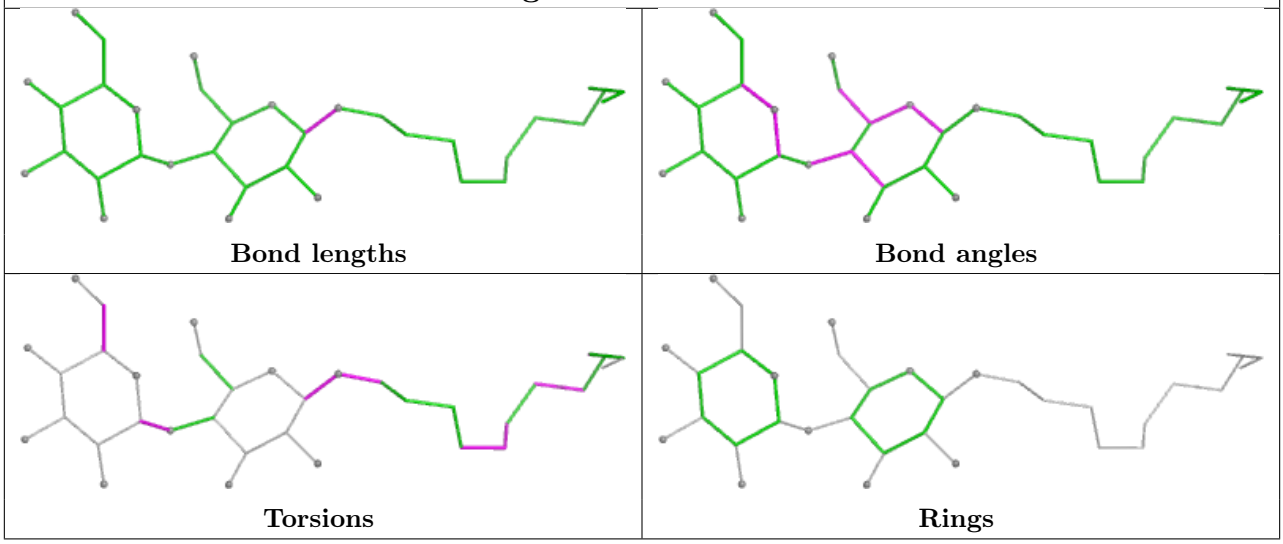
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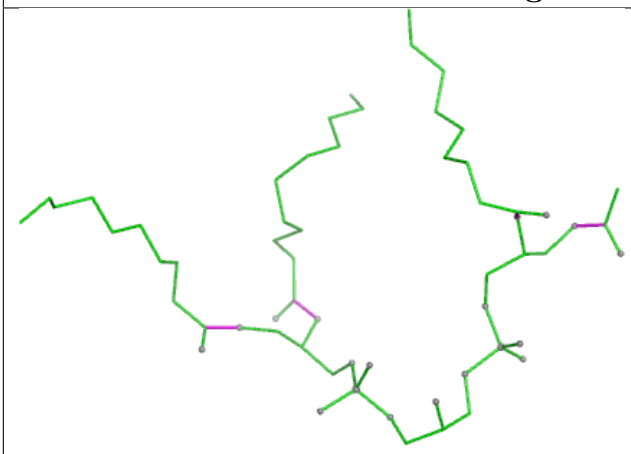
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	503	CDL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

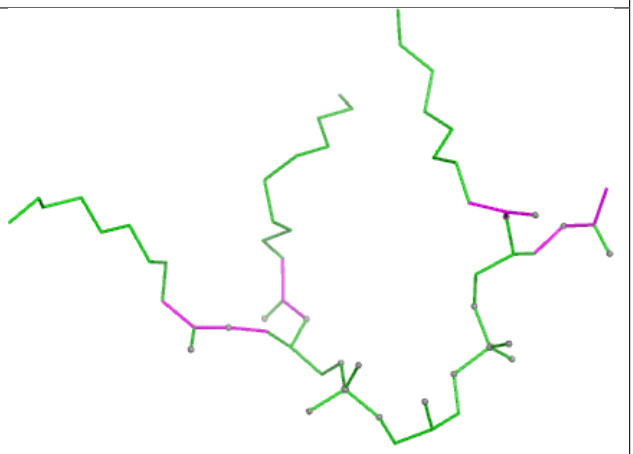
Ligand LMT C 403



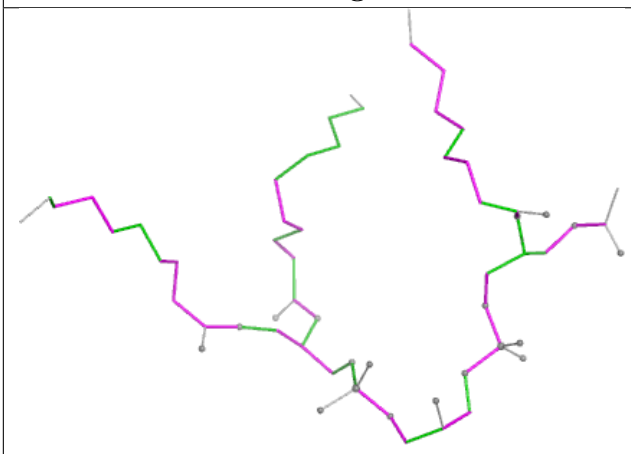
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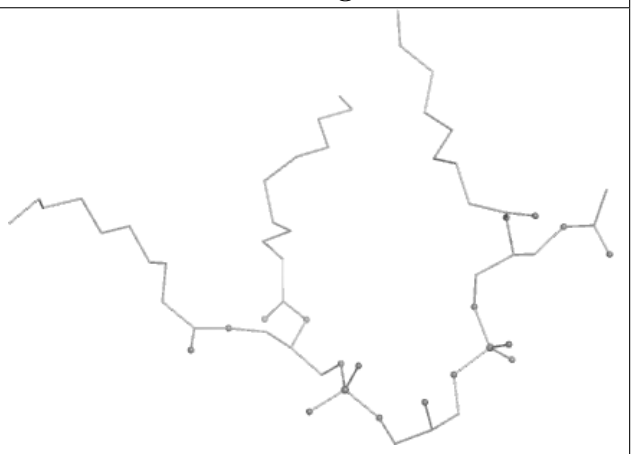
Bond lengths



Bond angles

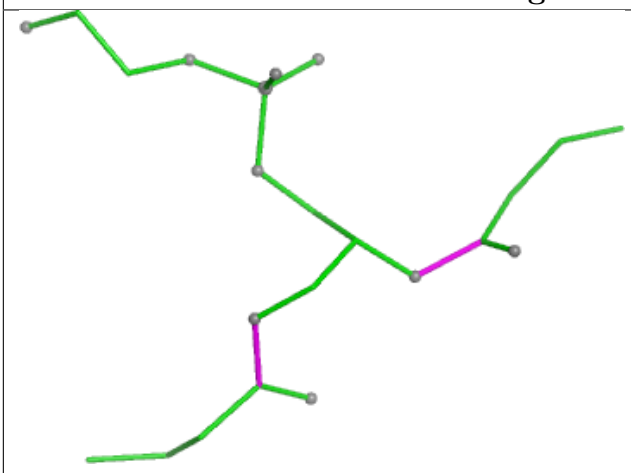


Torsions

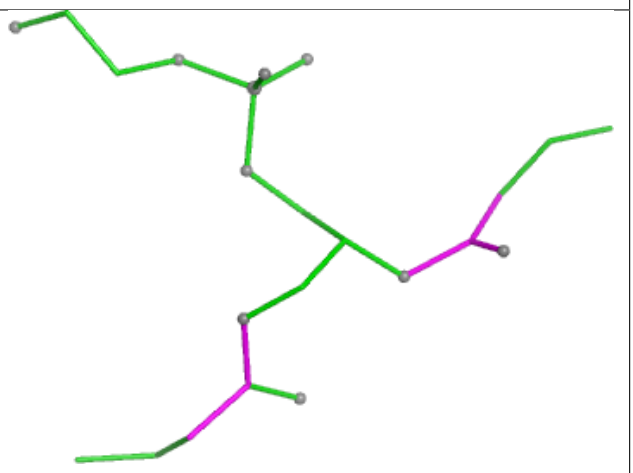


Rings

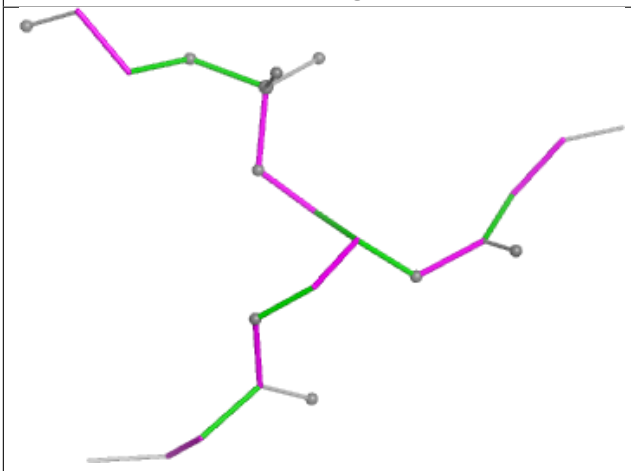
Ligand 6PE A 502



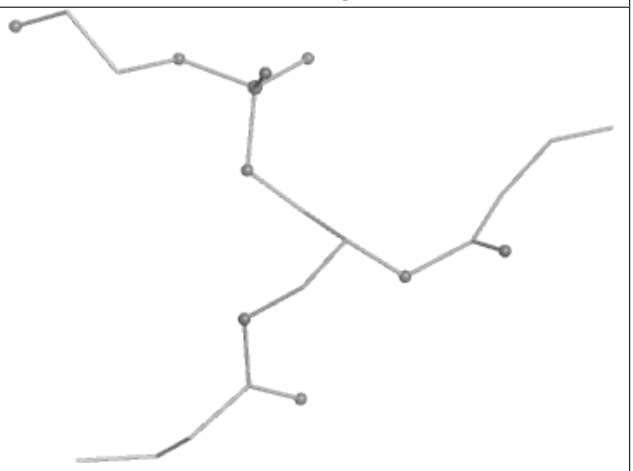
Bond lengths



Bond angles

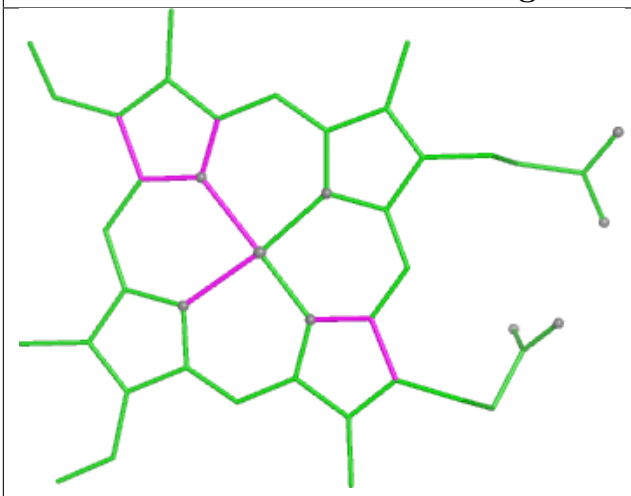


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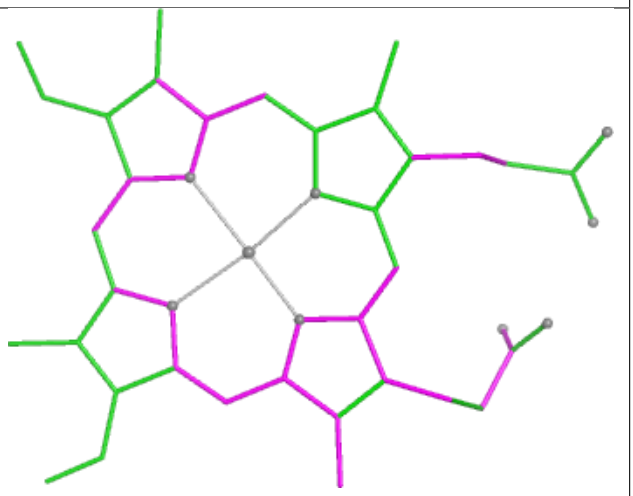


Rings

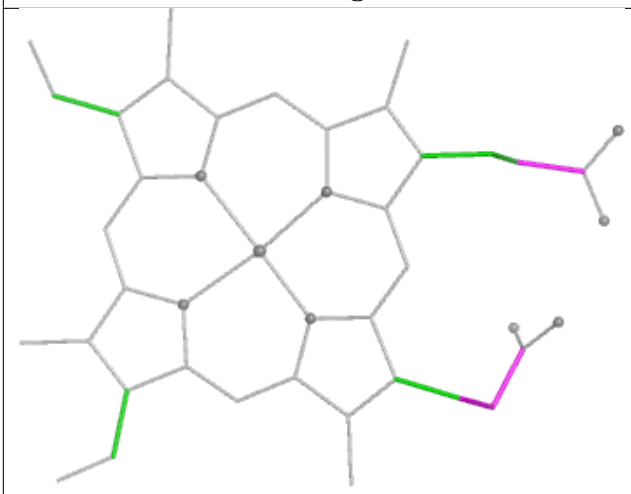
Ligand HEM C 401



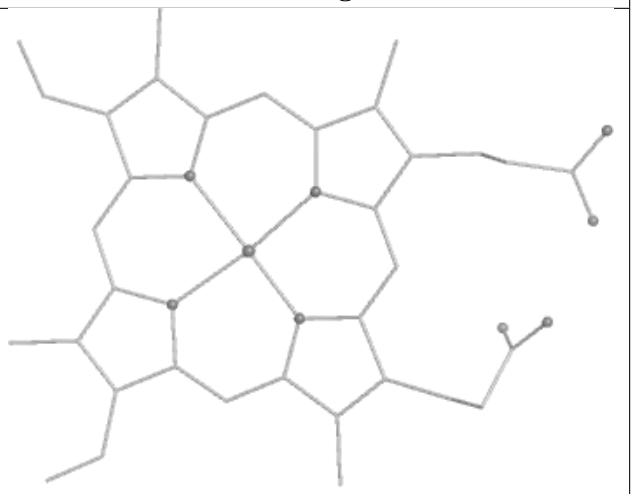
Bond lengths



Bond angles

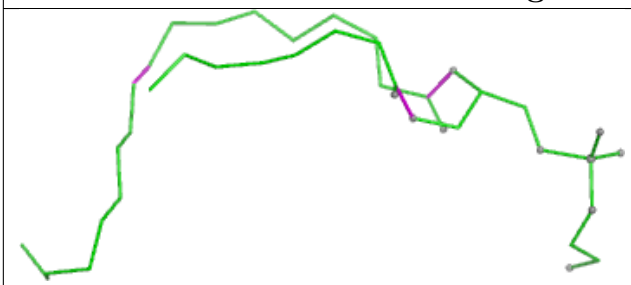


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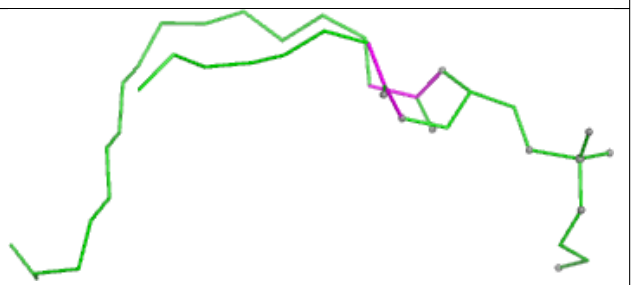


Rings

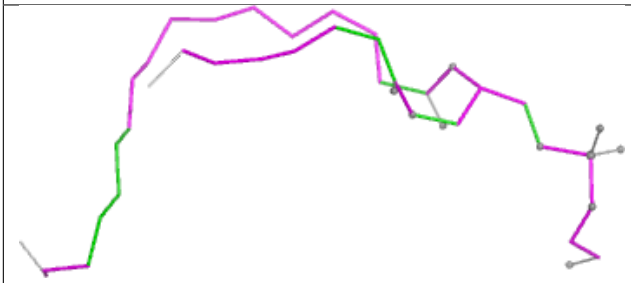
Ligand PEE E 203



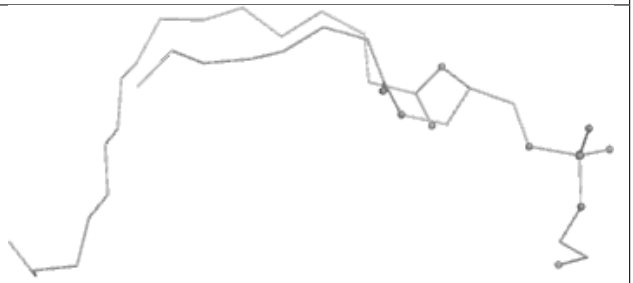
Bond lengths



Bond angles

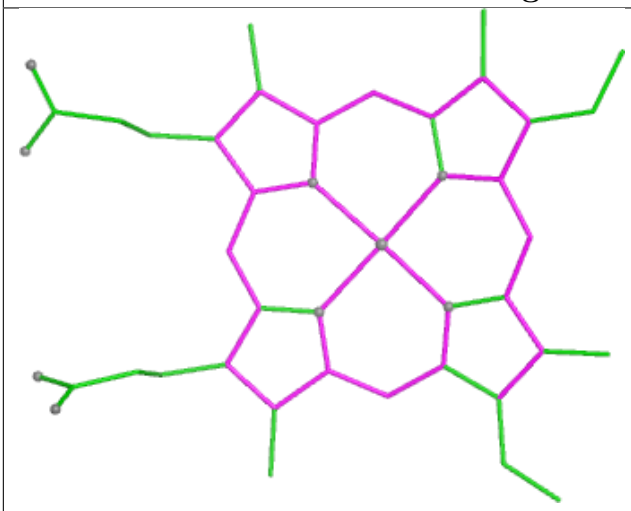


Torsions

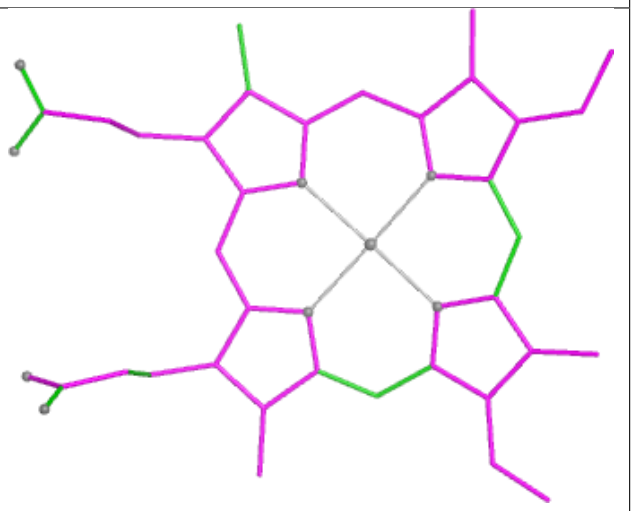


Rings

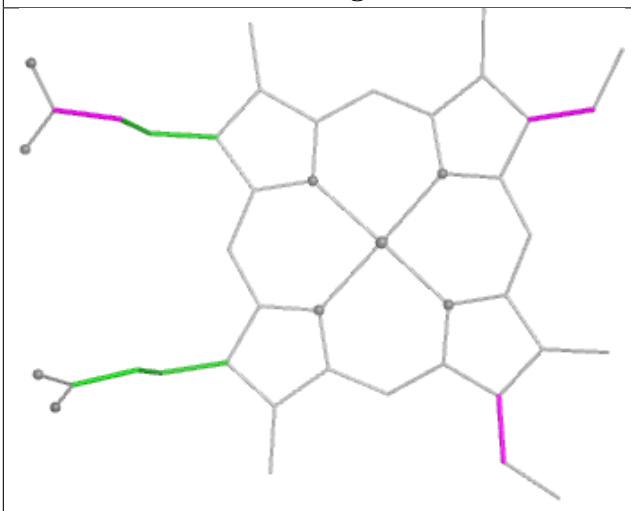
Ligand HEC D 501



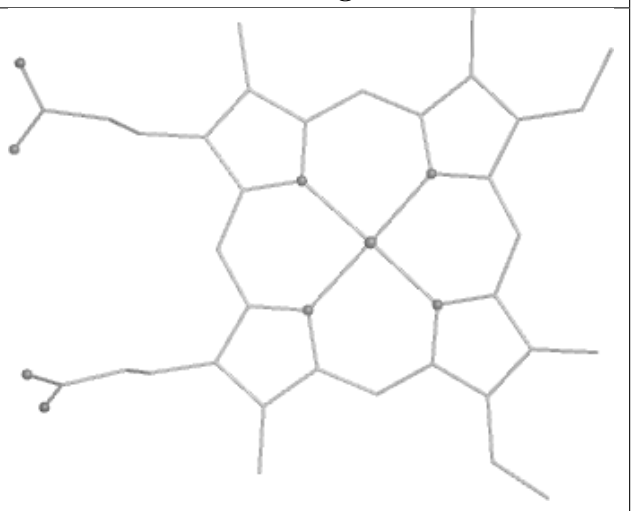
Bond lengths



Bond angles

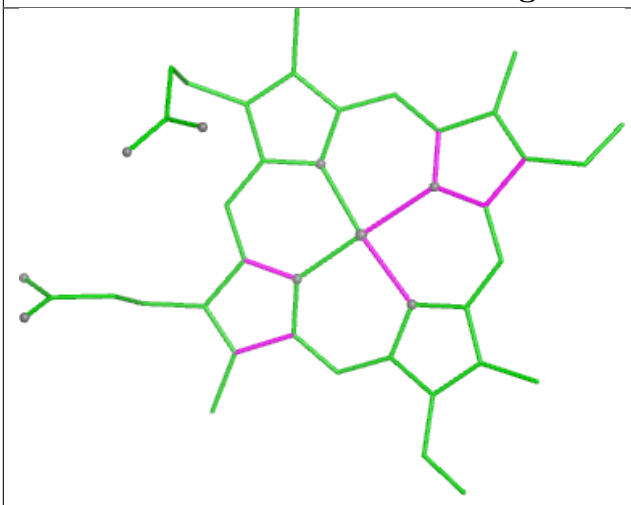


Torsions

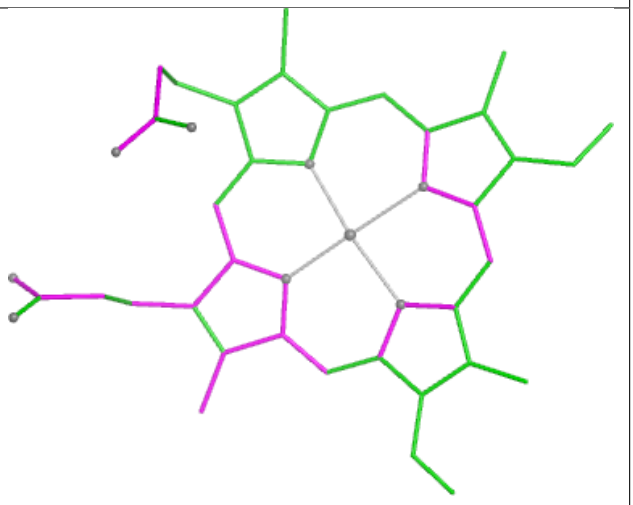


Rings

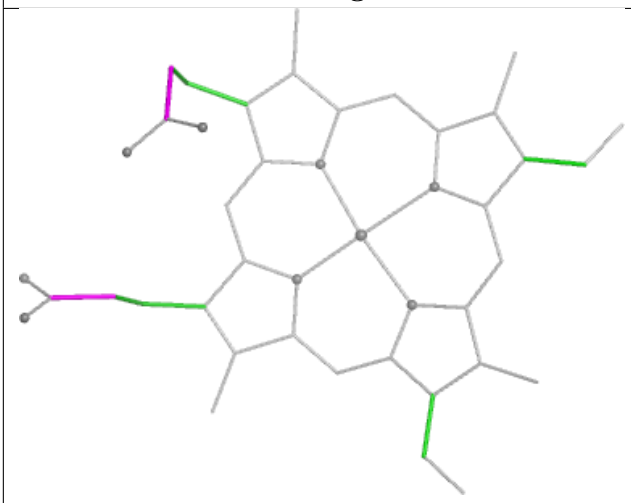
Ligand HEM C 402



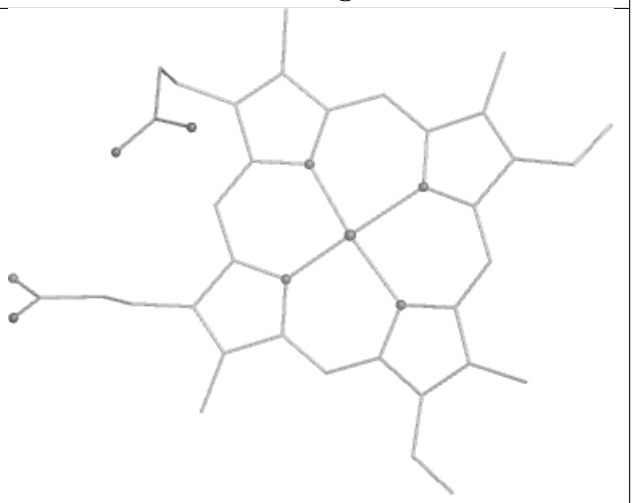
Bond lengths



Bond angles

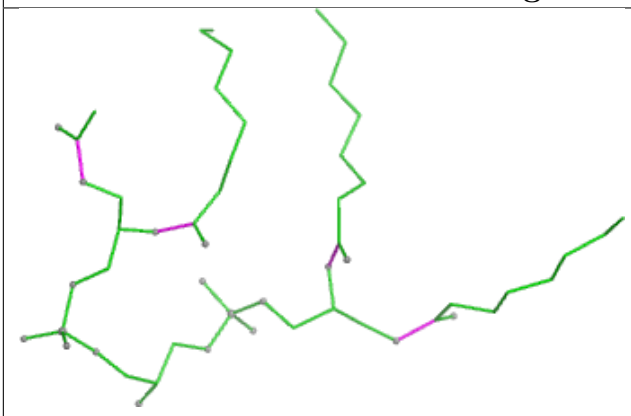


Torsions

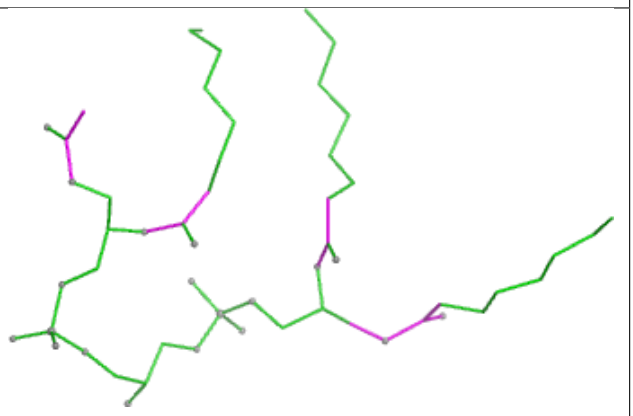


Rings

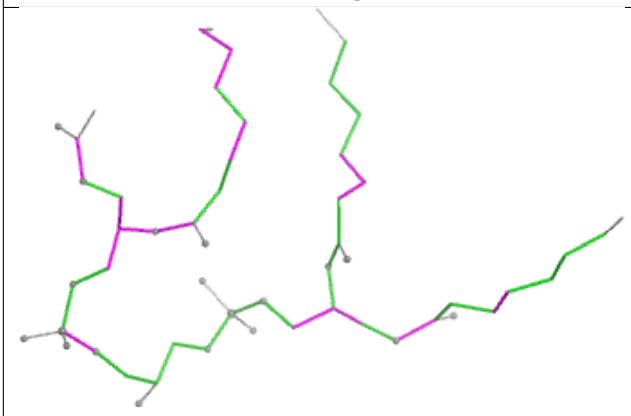
Ligand CDL D 503



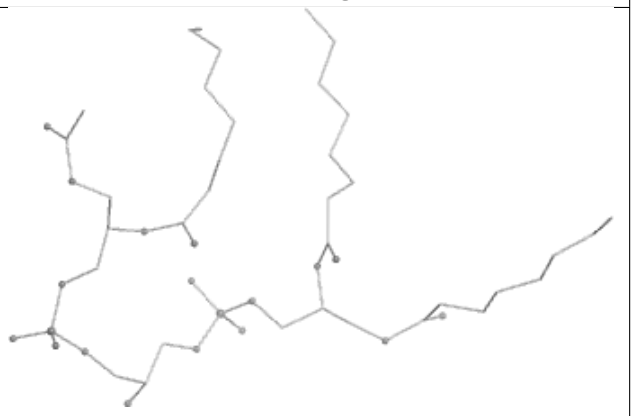
Bond lengths



Bond angles

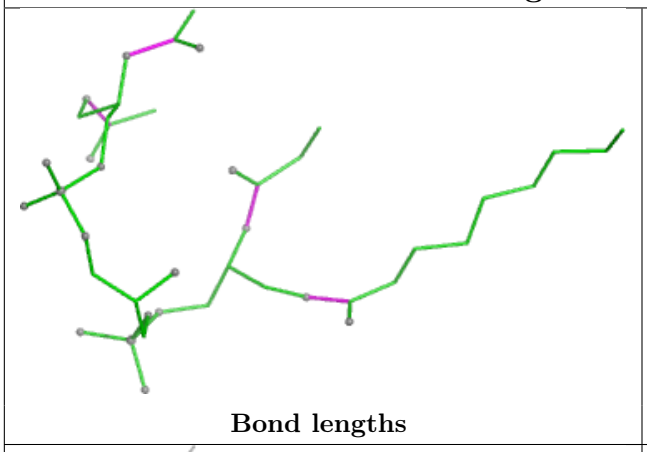


Torsions

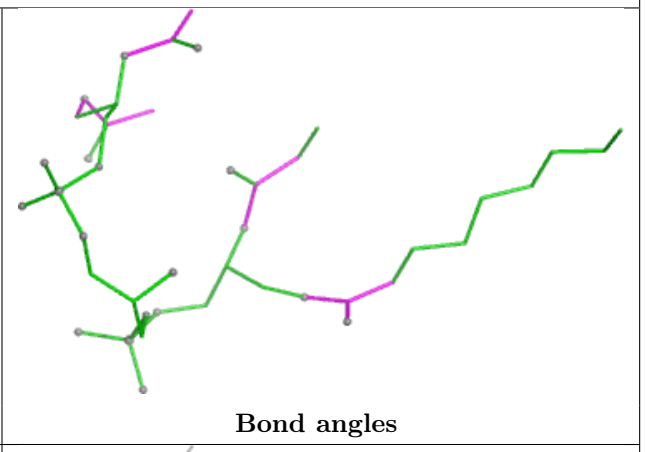


Rings

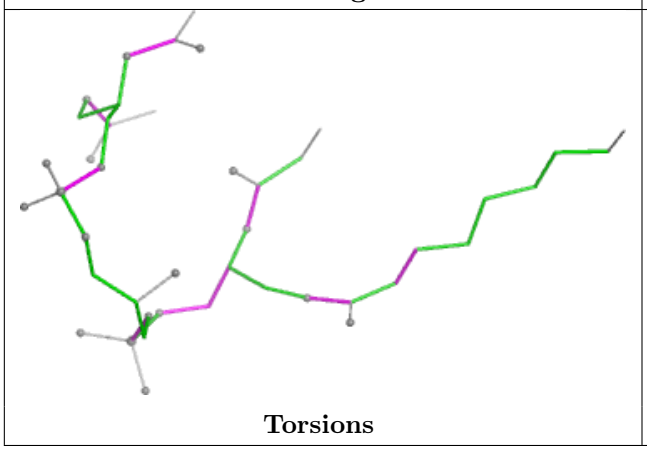
Ligand CDL C 406



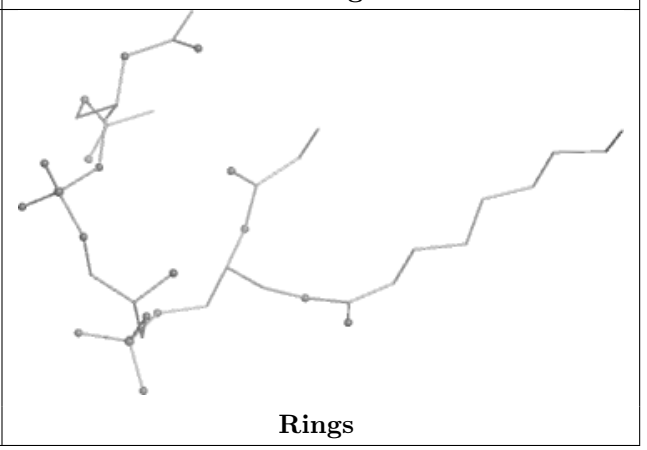
Bond lengths



Bond angles

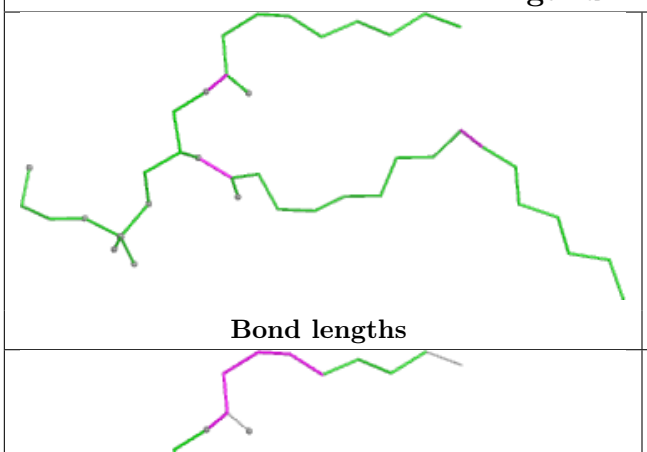


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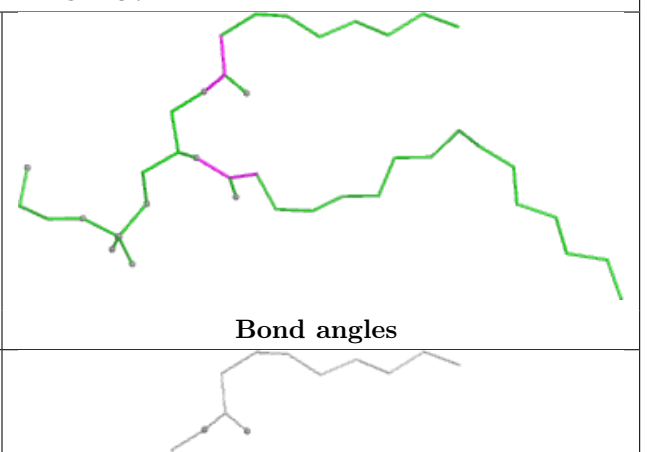


Rings

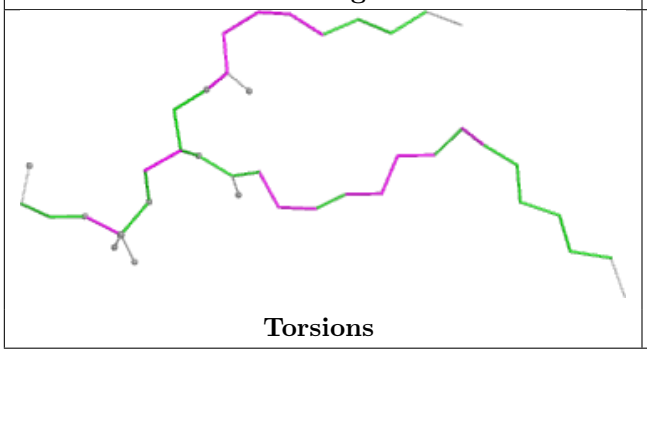
Ligand PEE C 407



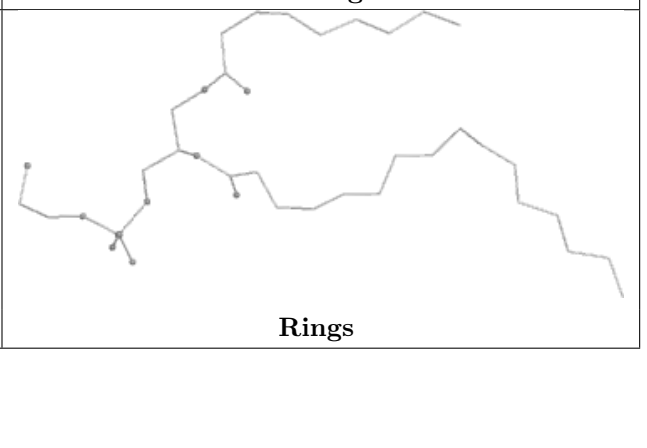
Bond lengths



Bond angles

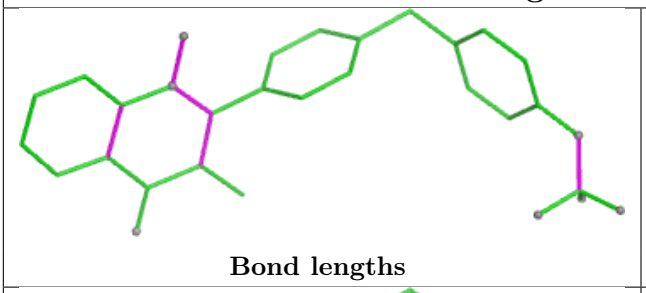


Torsions

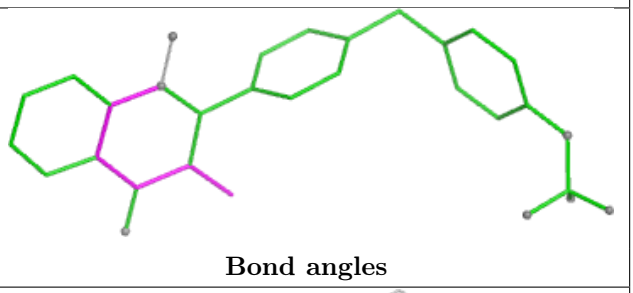


Rings

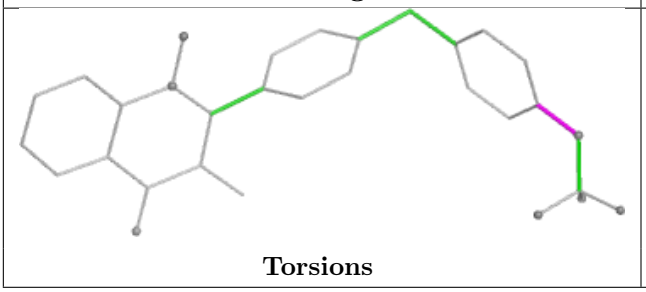
Ligand JHE C 408



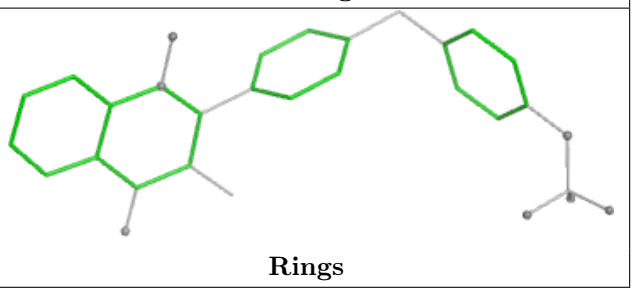
Bond lengths



Bond angles

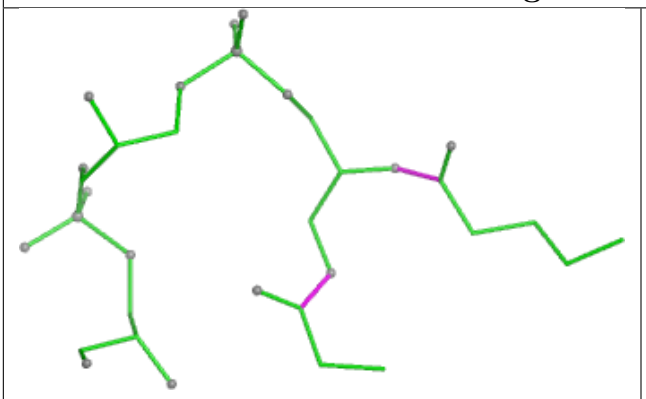


Torsions



Rings

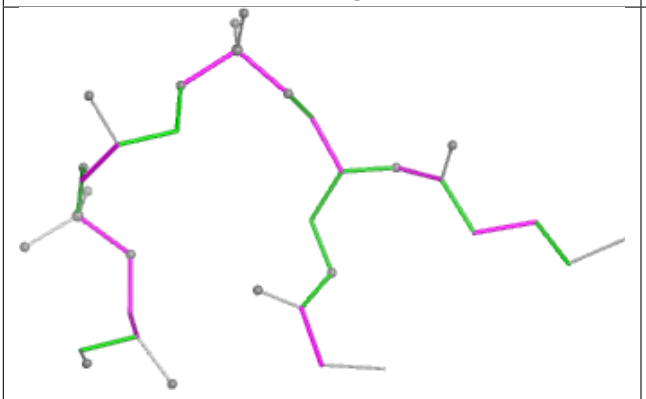
Ligand CDL A 503



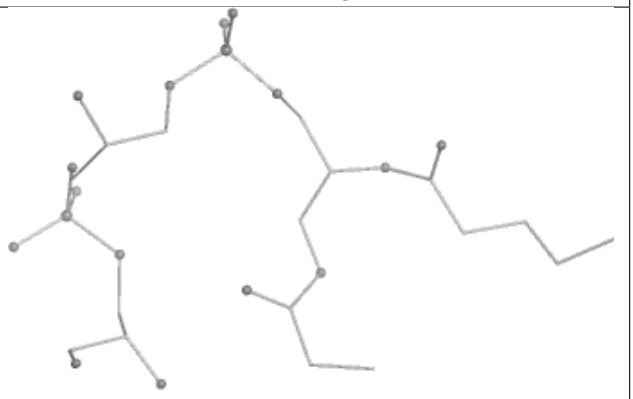
Bond lengths



Bond angles

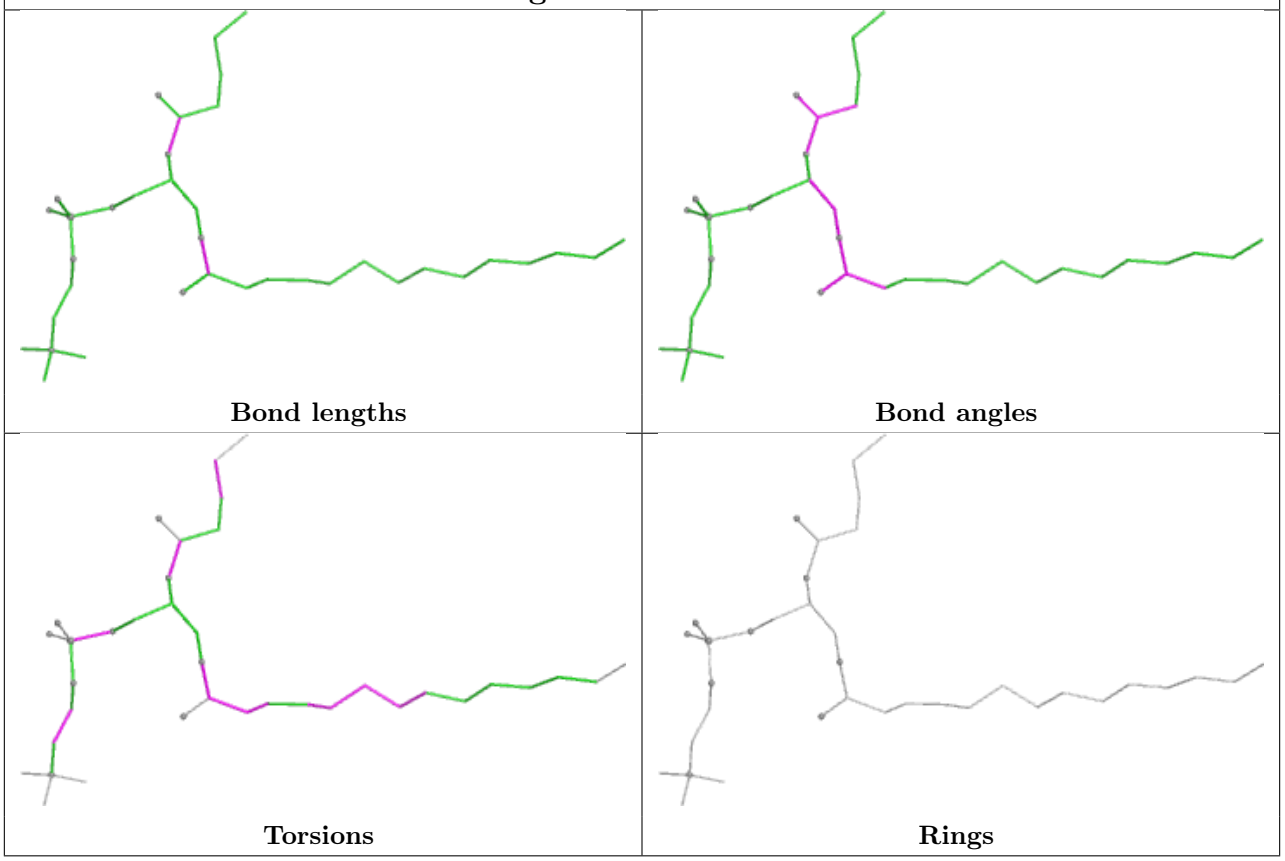


Torsions



Rings

Ligand PX4 E 202



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	444/444 (100%)	-0.09	5 (1%) 78 54	91, 128, 164, 240	0
2	B	415/420 (98%)	-0.06	4 (0%) 79 56	98, 132, 164, 226	0
3	C	378/378 (100%)	0.05	10 (2%) 57 33	88, 116, 152, 188	0
4	D	239/239 (100%)	0.36	11 (4%) 37 20	115, 154, 182, 203	0
5	E	196/196 (100%)	0.93	25 (12%) 7 6	106, 189, 242, 279	0
6	F	99/99 (100%)	0.28	3 (3%) 52 30	73, 125, 162, 198	0
7	G	74/74 (100%)	0.13	3 (4%) 41 22	99, 133, 179, 195	0
8	H	65/65 (100%)	0.73	3 (4%) 37 20	183, 200, 216, 227	0
9	I	46/46 (100%)	1.52	12 (26%) 1 2	142, 187, 205, 211	0
10	J	59/59 (100%)	0.63	2 (3%) 48 27	115, 141, 189, 209	0
All	All	2015/2020 (99%)	0.21	78 (3%) 43 23	73, 134, 205, 279	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	152	ASP	5.6
9	I	43	LEU	5.1
5	E	159	PRO	4.8
4	D	199	ASP	4.7
5	E	161	HIS	3.9

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

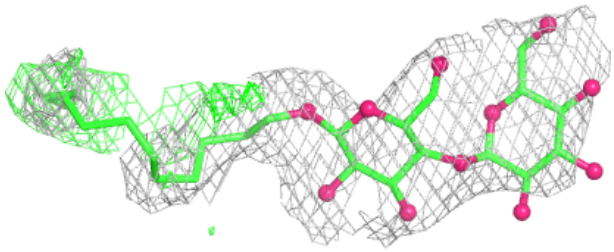
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

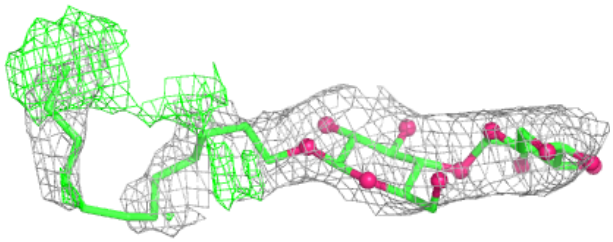
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	LMT	C	403	35/35	0.28	0.24	170,207,219,222	0
13	CDL	E	204	60/100	0.68	0.23	150,185,246,250	0
19	PO4	G	102	5/5	0.71	0.10	239,242,243,249	0
19	PO4	G	103	5/5	0.74	0.12	191,192,195,198	0
19	PO4	D	502	5/5	0.76	0.12	211,212,216,218	0
11	PG4	A	501	13/13	0.83	0.14	150,169,181,182	0
19	PO4	G	101	5/5	0.83	0.17	168,168,171,172	0
13	CDL	A	503	34/100	0.86	0.17	143,166,179,181	0
13	CDL	D	503	54/100	0.86	0.24	106,145,185,193	0
19	PO4	F	501	5/5	0.88	0.10	203,206,209,209	0
11	PG4	C	404	13/13	0.89	0.22	125,128,135,135	0
11	PG4	C	405	13/13	0.90	0.21	126,134,144,146	0
16	PEE	E	203	41/51	0.92	0.22	122,128,140,142	0
21	PX4	E	202	37/46	0.92	0.19	122,143,153,155	0
13	CDL	C	406	44/100	0.93	0.15	124,134,144,149	0
17	JHE	C	408	31/31	0.93	0.14	66,75,121,132	0
12	6PE	A	502	23/27	0.96	0.12	133,157,178,183	0
20	FES	E	201	4/4	0.96	0.06	288,291,295,306	0
16	PEE	C	407	40/51	0.96	0.13	107,113,119,123	0
14	HEM	C	402	43/43	0.97	0.09	96,100,106,110	0
18	HEC	D	501	43/43	0.98	0.11	147,155,164,168	0
14	HEM	C	401	43/43	0.99	0.07	103,106,112,114	0

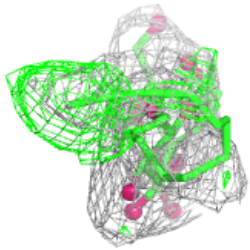
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT C 403:

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

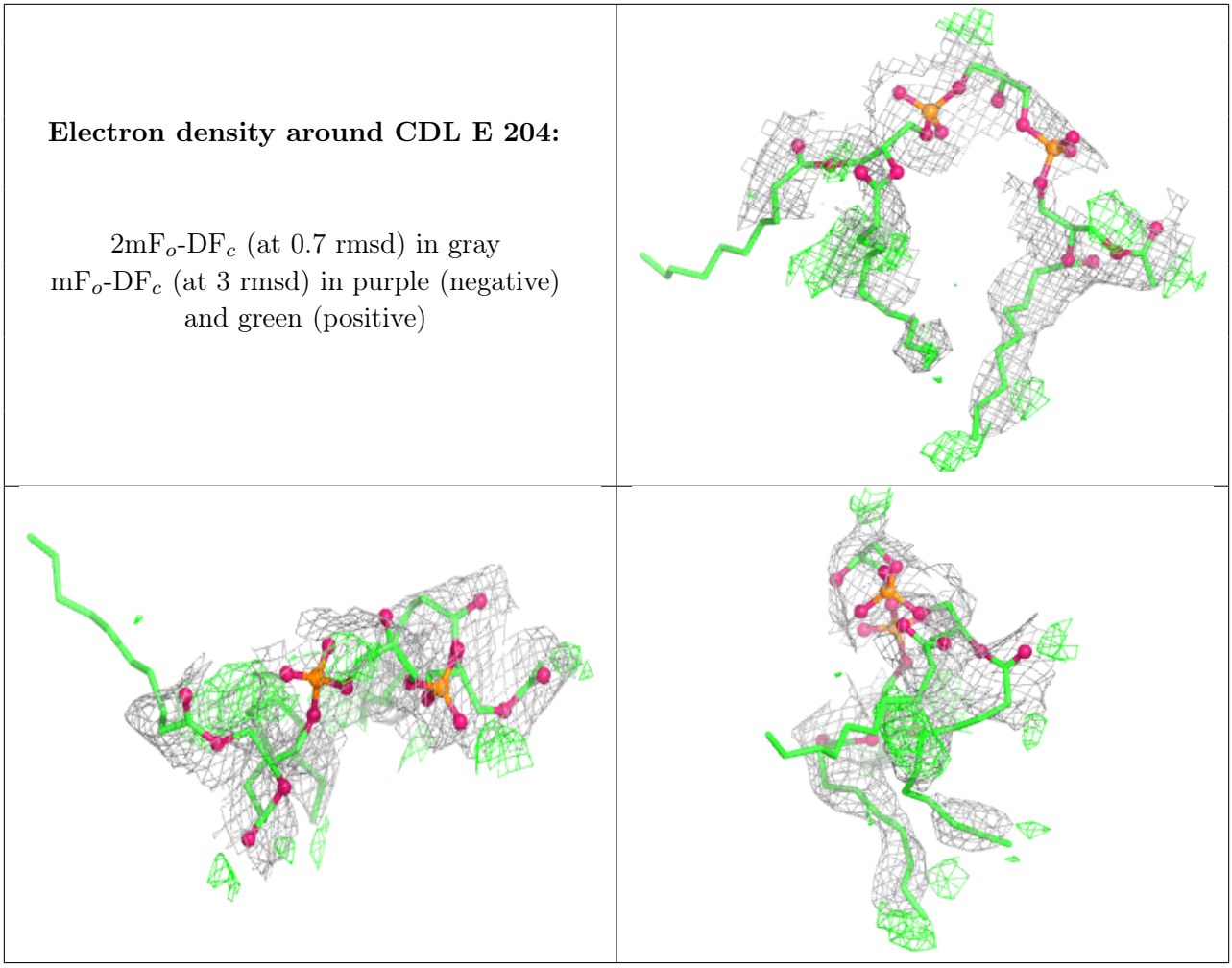






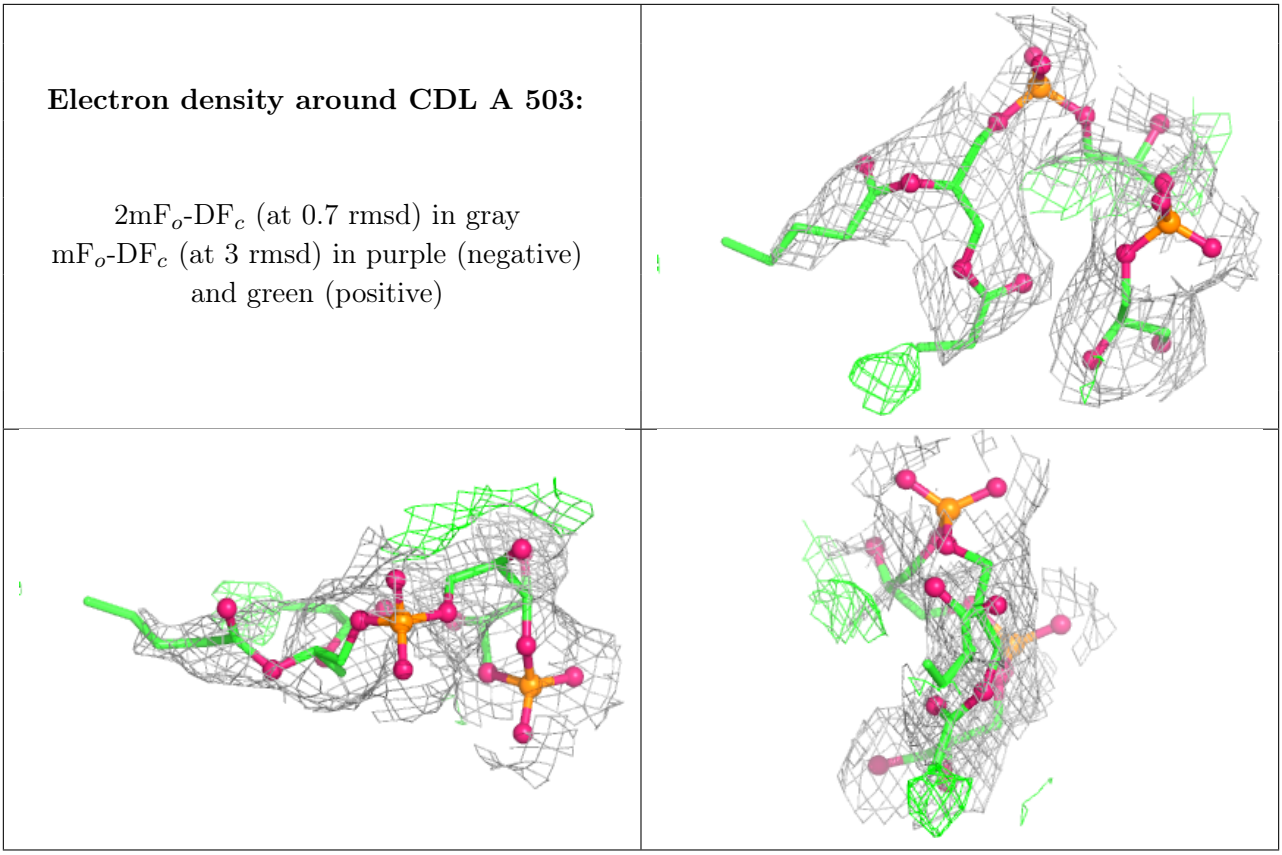
Electron density around CDL E 204:

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



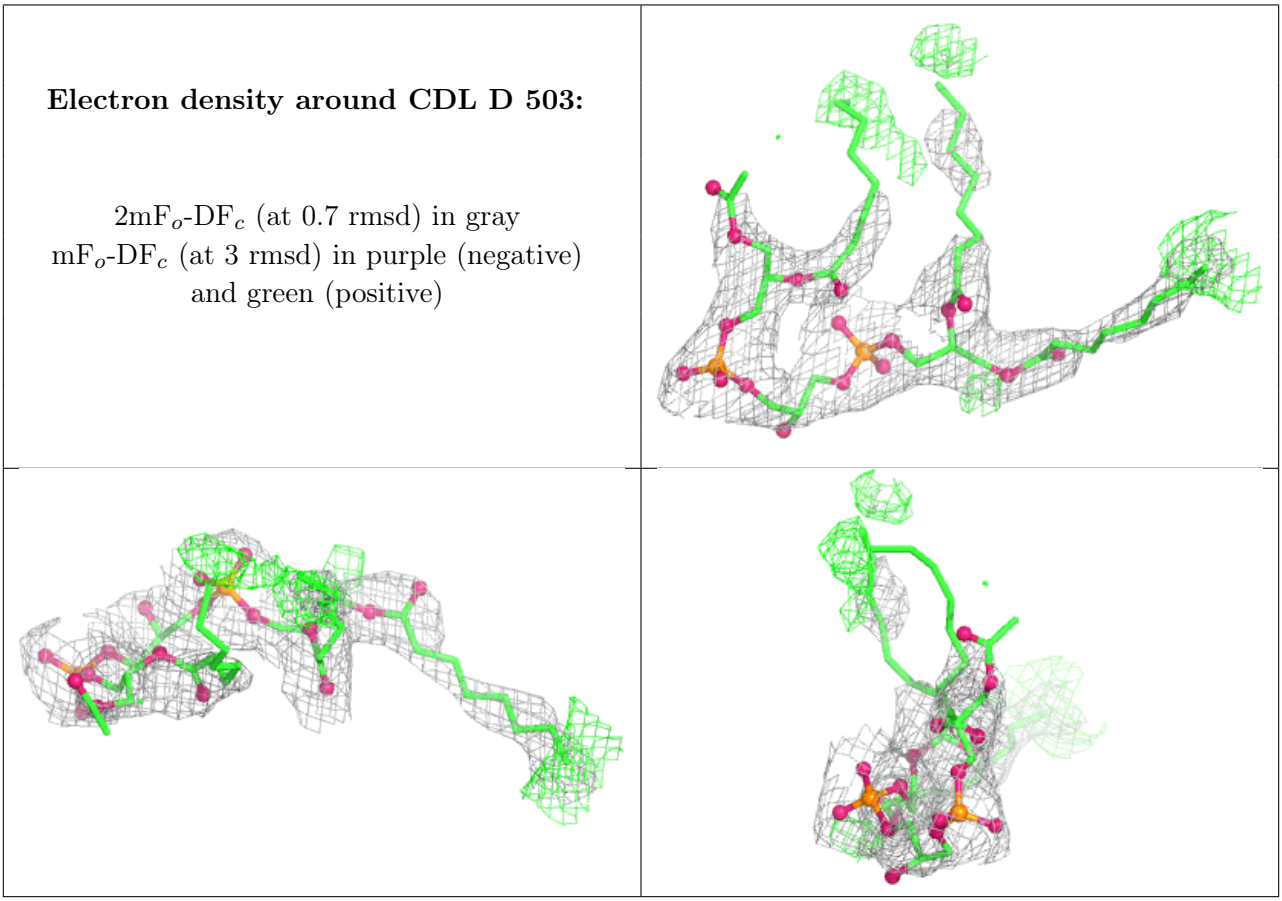
Electron density around CDL A 503:

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



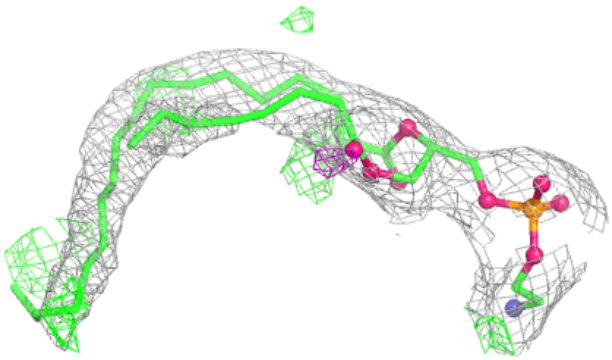
Electron density around CDL D 503:

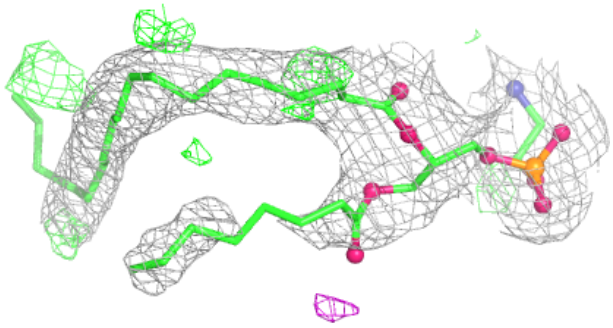
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

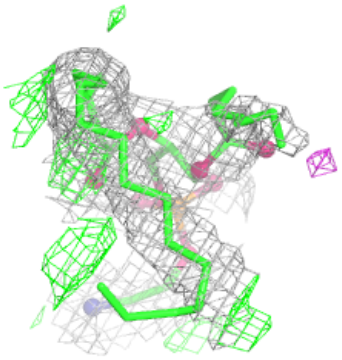


Electron density around PEE E 203:

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

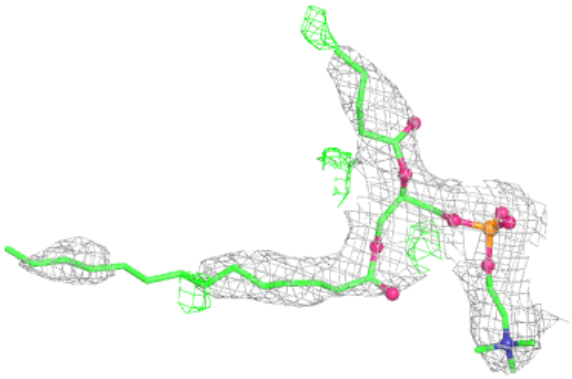


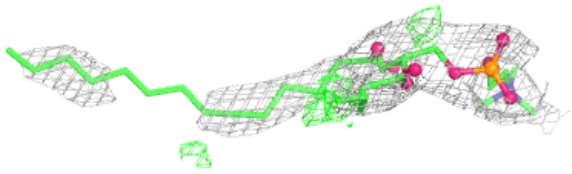


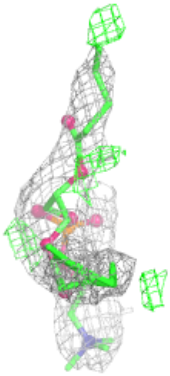


Electron density around PX4 E 202:

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

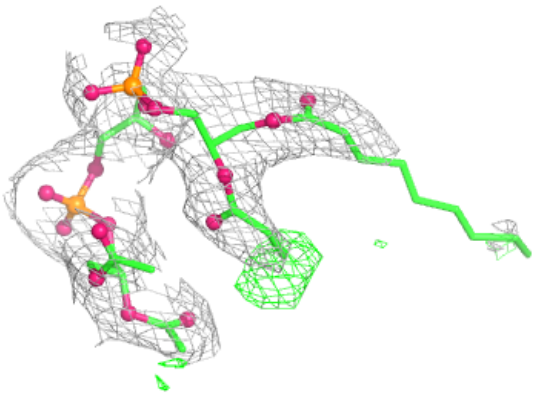


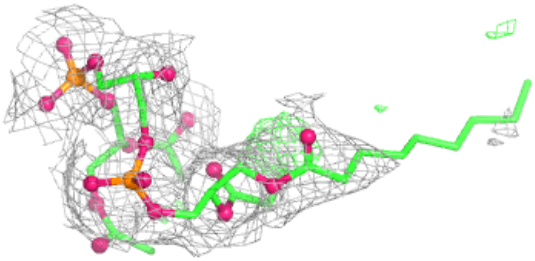


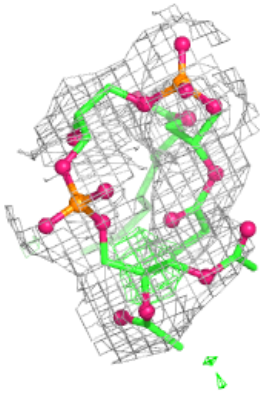


Electron density around CDL C 406:

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

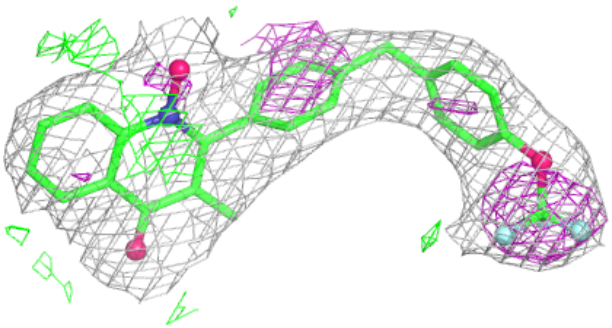


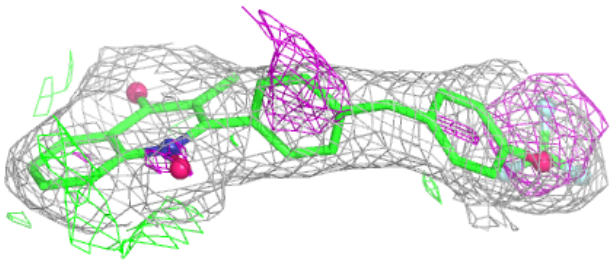


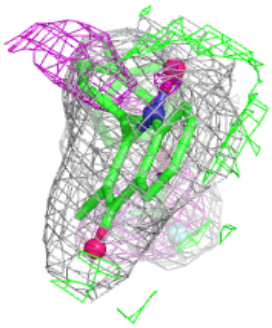


Electron density around JHE C 408:

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

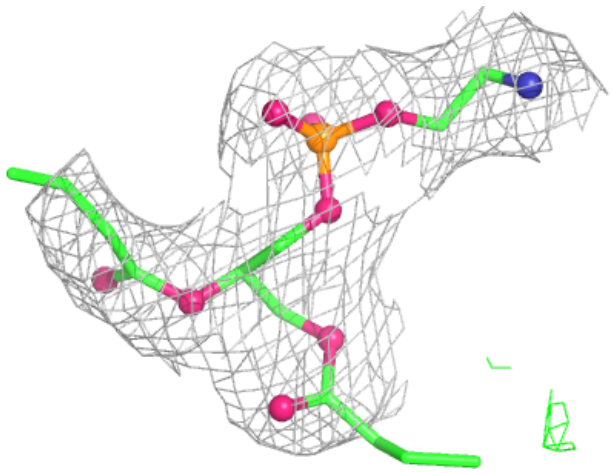


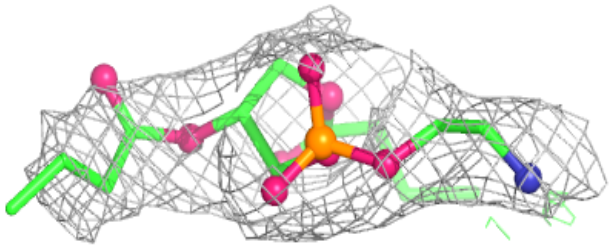


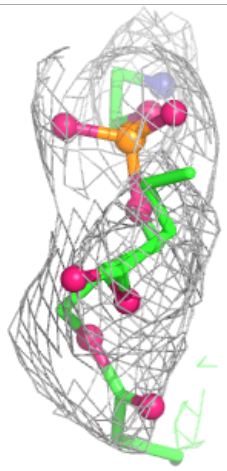


Electron density around 6PE A 502:

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

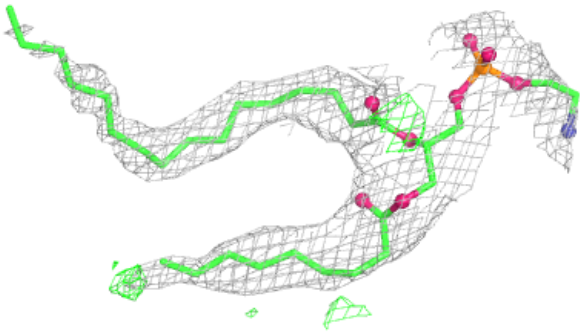


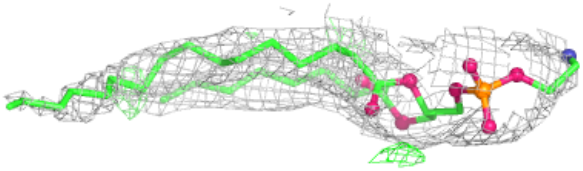




Electron density around PEE C 407:

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

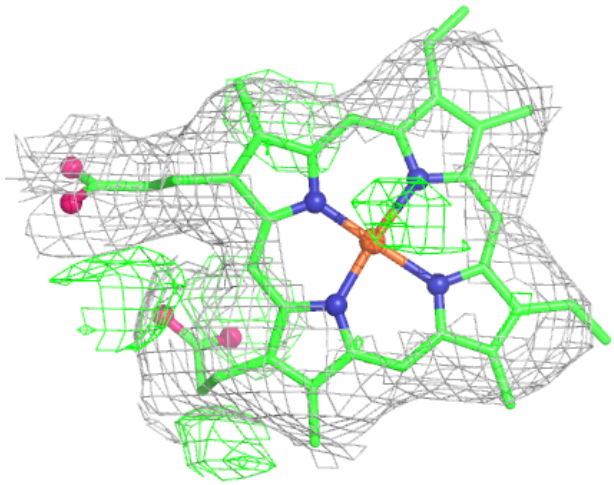


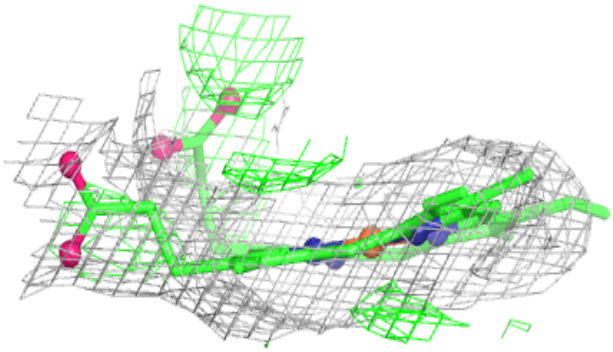


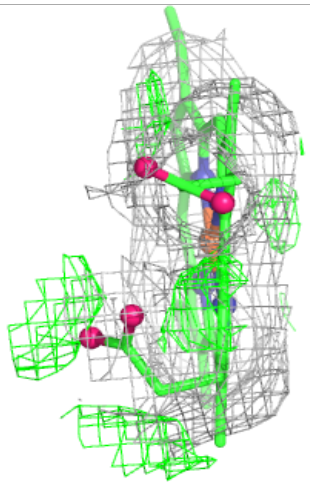


Electron density around HEM C 402:

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

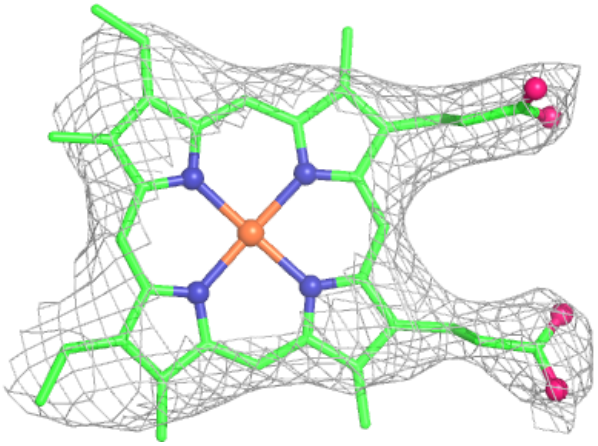


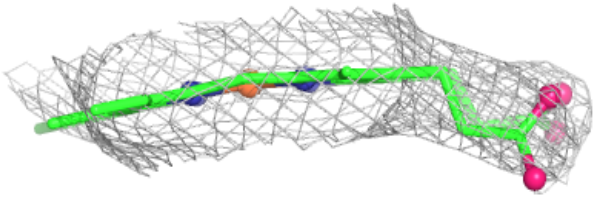


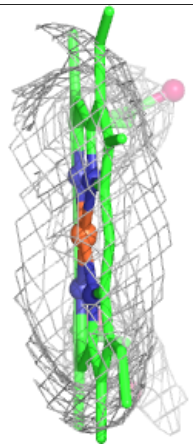


Electron density around HEC D 501:

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

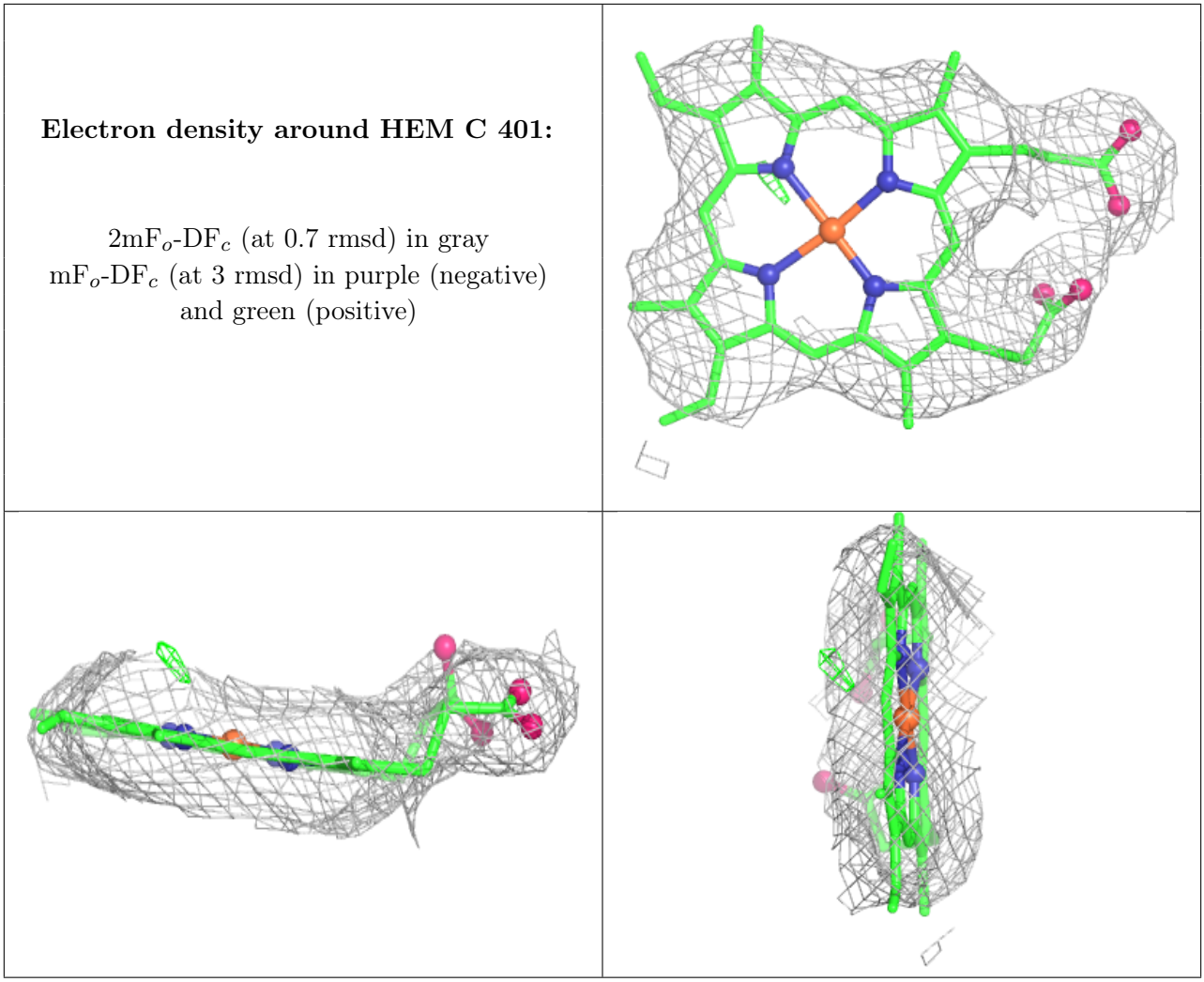






Electron density around HEM C 401:

$2mF_o$-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.