



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:28 PM UTC

PDB ID : 6ZFU / pdb_00006zfu
Title : Crystal structure of bovine cytochrome bc1 in complex with quinolone inhibitor RKA066
Authors : Ampornnanai, 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 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

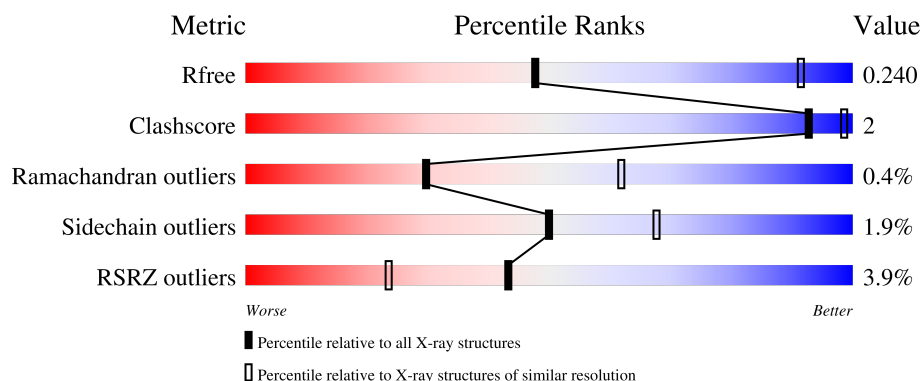
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	
6	F	99	
7	G	74	
8	H	65	
9	I	46	
10	J	59	

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	-	-	-

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.

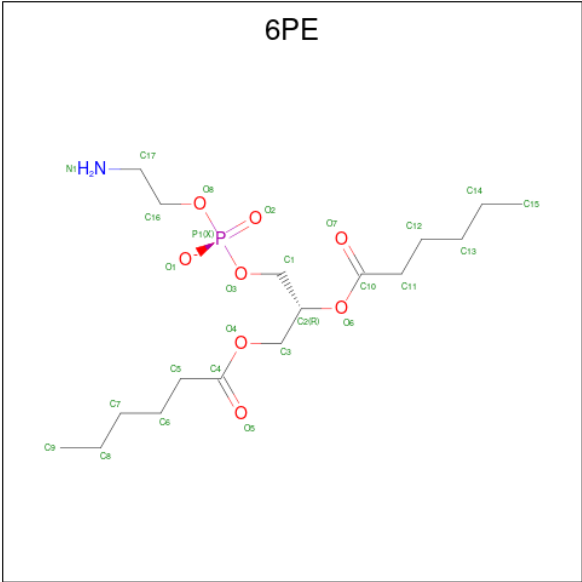
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			480	314	83	83			

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



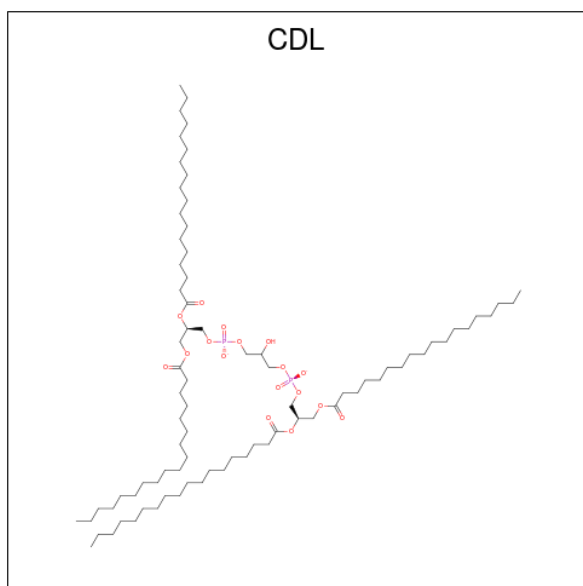
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			13	8	5		
11	C	1	Total	C	O	0	0
			13	8	5		
11	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: 6PE) (formula: C₁₇H₃₃NO₈P).



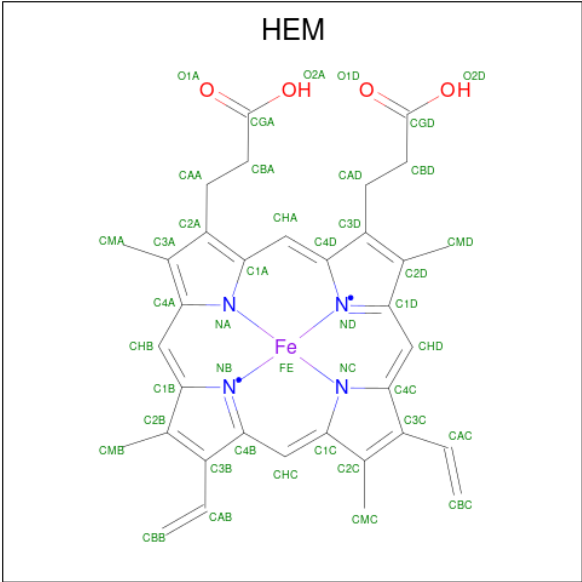
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

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



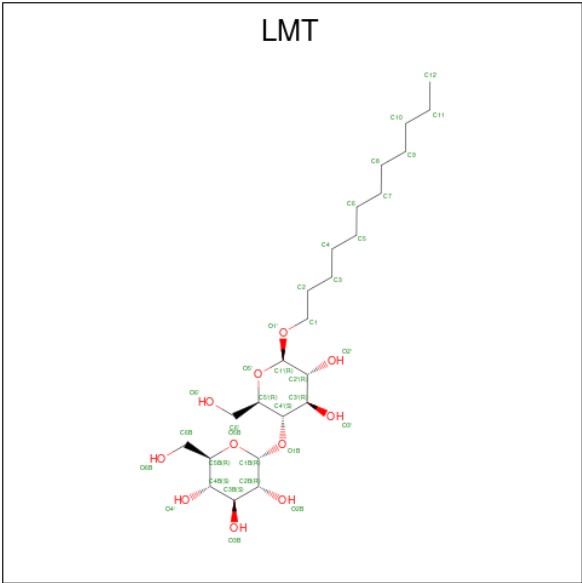
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			34	17	15	2		
13	C	1	Total	C	O	P	0	0
			44	25	17	2		
13	D	1	Total	C	O	P	0	0
			54	35	17	2		
13	E	1	Total	C	O	P	0	0
			60	41	17	2		

- 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 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

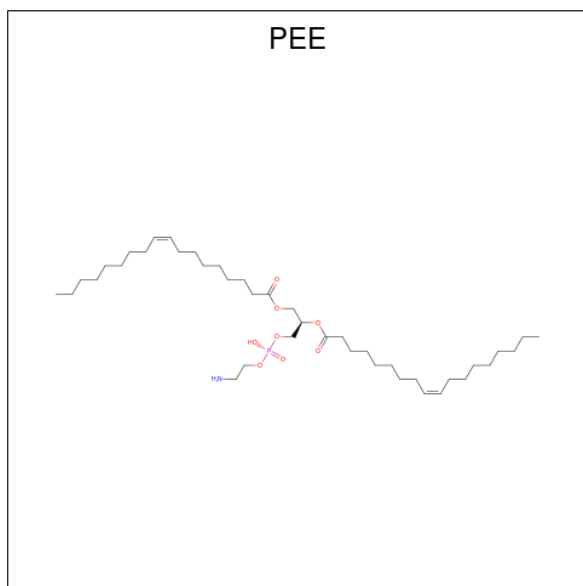
- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

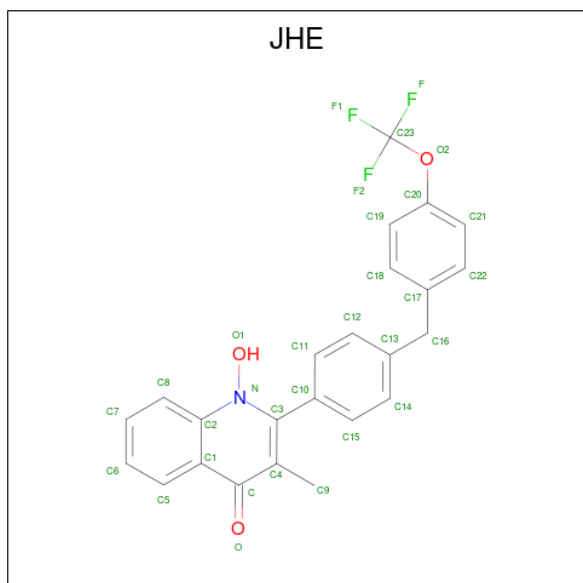
- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:

C₄₁H₇₈NO₈P).



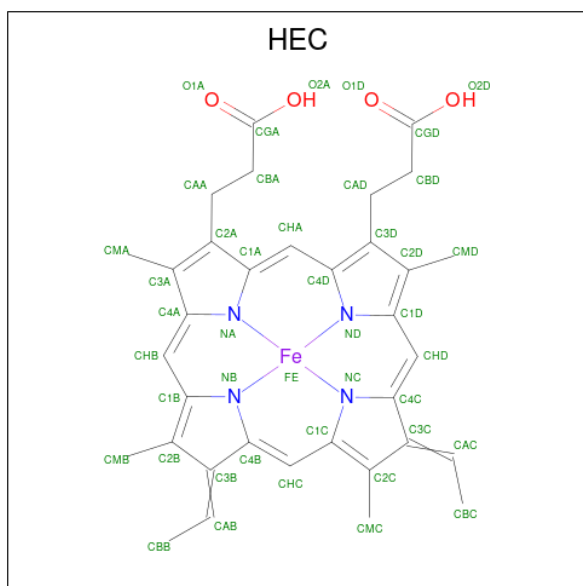
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
16	E	1	Total	C	N	O	P	0	0
			41	31	1	8	1		

- Molecule 17 is 3-methyl-1-oxidanyl-2-[4-[[4-(trifluoromethoxy)phenyl]methyl]phenyl]quinolin-4-one (CCD ID: JHE) (formula: C₂₄H₁₈F₃NO₃) (labeled as "Ligand of Interest" by depositor).



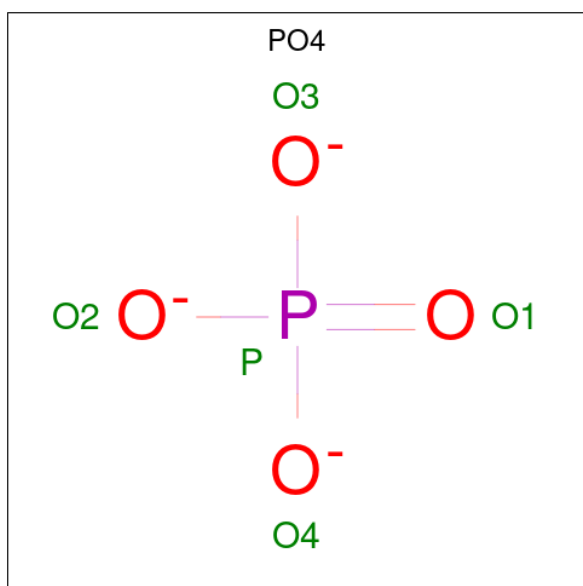
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	F	N	O	0	0
			31	24	3	1	3		

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



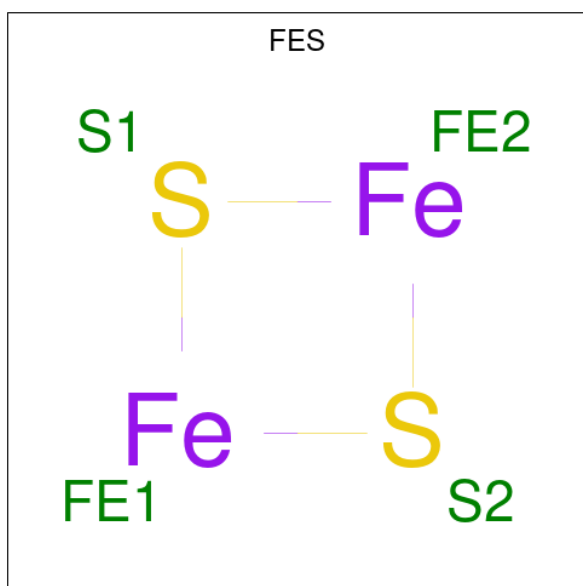
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



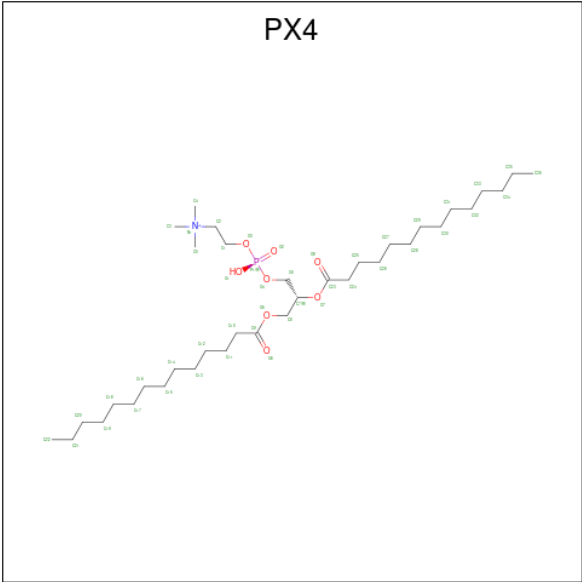
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total O P 5 4 1	0	0
19	F	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0

- 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: $\text{C}_{36}\text{H}_{73}\text{NO}_8\text{P}$).



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		

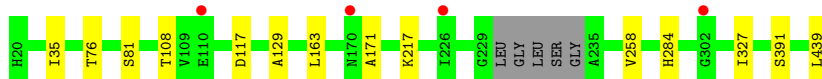
3 Residue-property plots [i](#)

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.

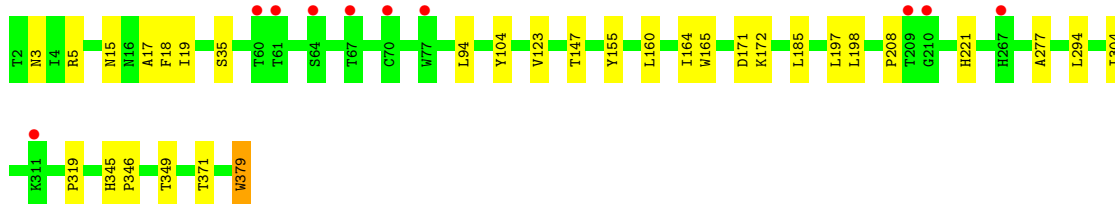
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



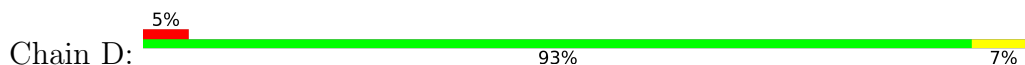
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 3: Cytochrome b

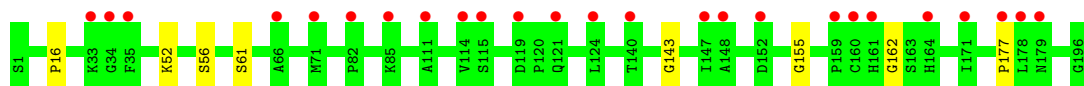


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

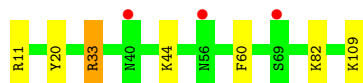


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

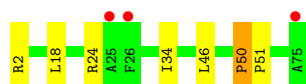
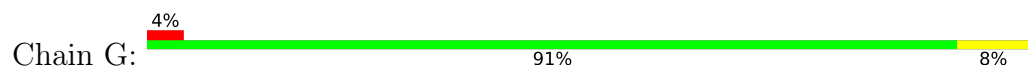




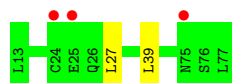
- Molecule 6: Cytochrome b-c1 complex subunit 7



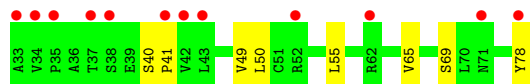
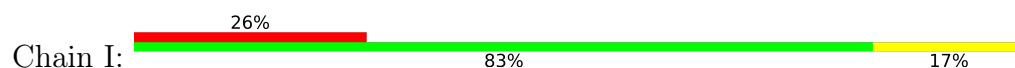
- Molecule 7: Cytochrome b-c1 complex subunit 8



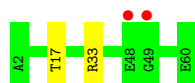
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



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



- Molecule 10: Cytochrome b-c1 complex subunit 9



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, PX4, PO4, HEM, 6PE, PG4, FES, JHE, LMT, 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

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	310	PHE	N-CA-C	5.50	122.52	110.80
9	I	40	SER	CB-CA-C	5.47	116.03	109.31
7	G	50	PRO	N-CA-C	5.36	117.24	110.70
1	A	315	ALA	CB-CA-C	-5.29	102.81	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	ALA	N-CA-C	5.17	117.00	109.30
2	B	391	SER	N-CA-C	5.13	114.91	108.45
1	A	263	ALA	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:B:163:LEU:HD11	2:B:258:VAL:HG22	1.88	0.56
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.89	0.55
5:E:16:PRO:HD3	7:G:24:ARG:HD3	1.89	0.55
4:D:37:CYS:SG	18:D:501:HEC:C3B	2.95	0.55
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.91	0.52
14:C:402:HEM:HMB1	14:C:402:HEM:HBB2	1.92	0.51
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.92	0.50
1:A:80:GLU:HG2	2:B:284:HIS:HB2	1.93	0.50
3:C:15:ASN:HA	3:C:19:ILE:HD12	1.93	0.49
3:C:197:LEU:HD21	14:C:402:HEM:HMA3	1.92	0.49
4:D:37:CYS:SG	18:D:501:HEC:HBB3	2.52	0.49
5:E:52:LYS:O	5:E:56:SER:HB2	2.12	0.49
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.48	0.49
4:D:211:MET:HG3	16:E:203:PEE:H15	1.97	0.47
3:C:171:ASP:CG	3:C:172:LYS:H	2.22	0.47
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.46
4:D:37:CYS:SG	18:D:501:HEC:CBB	3.05	0.45
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.51	0.45
3:C:379:TRP:CZ2	6:F:33:ARG:HD3	2.51	0.45
1:A:79:VAL:HG11	1:A:86:LEU:HB2	1.99	0.45
14:C:402:HEM:HBB2	14:C:402:HEM:CMB	2.46	0.44
4:D:42:SER:HB3	4:D:93:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:401:HEM:HBC2	14:C:401:HEM:CMC	2.48	0.44
3:C:17:ALA:C	3:C:18:PHE:HD2	2.25	0.44
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.53	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.00	0.43
1:A:436:ARG:NH1	3:C:221:HIS:O	2.51	0.43
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.52	0.43
3:C:94:LEU:HD11	3:C:123:VAL:HG11	2.01	0.43
3:C:319:PRO:HD2	6:F:20:TYR:CE2	2.54	0.42
12:A:502:6PE:H4	13:A:503:CDL:H512	2.01	0.42
4:D:116:ILE:HG12	18:D:501:HEC:HMA3	2.01	0.42
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.48	0.42
13:E:204:CDL:H132	13:E:204:CDL:H172	2.02	0.41
9:I:49:VAL:HG11	9:I:55:LEU:HD13	2.02	0.41
2:B:76:THR:HG23	2:B:81:SER:HA	2.02	0.41
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.54	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.02	0.41
12:A:502:6PE:H28	13:A:503:CDL:HB31	2.03	0.41
3:C:160:LEU:O	3:C:164:ILE:HG12	2.21	0.41
1:A:41:ILE:HG12	1:A:195:MET:HG2	2.03	0.40
3:C:345:HIS:HA	3:C:346:PRO:HA	1.91	0.40
13:A:503:CDL:OB3	3:C:5:ARG:NH1	2.54	0.40
3:C:147:THR:HG21	3:C:165:TRP:NE1	2.37	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	171	ALA
3	C	155	TYR
5	E	162	GLY
9	I	41	PRO
5	E	155	GLY
5	E	143	GLY
5	E	177	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

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

Mol	Chain	Res	Type
1	A	104	LYS
1	A	184	GLU
1	A	245	GLU
1	A	366	VAL
1	A	377	GLU
2	B	108	THR
2	B	117	ASP
2	B	439	LEU
3	C	35	SER
3	C	185	LEU
3	C	198	LEU
3	C	349	THR
3	C	371	THR
3	C	379	TRP
4	D	3	LEU
4	D	214	LEU
5	E	61	SER
6	F	11	ARG
6	F	33	ARG
6	F	44	LYS
6	F	82	LYS
6	F	109	LYS
7	G	2	ARG
7	G	18	LEU
7	G	46	LEU
8	H	27	LEU
8	H	39	LEU
9	I	50	LEU
9	I	65	VAL
9	I	78	TYR
10	J	17	THR
10	J	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	159	GLN
1	A	165	GLN
1	A	240	GLN
1	A	267	ASN
1	A	271	GLN
1	A	311	ASN
2	B	143	GLN
2	B	158	HIS
2	B	290	ASN
2	B	343	GLN
2	B	400	GLN
2	B	401	GLN
3	C	15	ASN
3	C	54	HIS
3	C	345	HIS
4	D	6	HIS
4	D	105	ASN
4	D	181	GLN
4	D	225	HIS
5	E	122	HIS
5	E	149	ASN
6	F	38	HIS
6	F	79	GLN
7	G	12	HIS
8	H	23	GLN
8	H	63	HIS
10	J	57	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 ⓘ

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
11	PG4	A	501	-	12,12,12	0.56	0	11,11,11	0.38	0
19	PO4	G	103	-	4,4,4	0.89	0	6,6,6	0.60	0
20	FES	E	201	-	0,4,4	-	-	-	-	-
18	HEC	D	501	4	46,50,50	2.68	25 (54%)	58,82,82	2.20	17 (29%)
14	HEM	C	402	3	50,50,50	1.56	9 (18%)	67,82,82	1.22	9 (13%)
17	JHE	C	408	-	34,34,34	1.97	5 (14%)	46,50,50	1.15	3 (6%)
16	PEE	E	203	-	40,40,50	1.28	3 (7%)	43,45,55	1.12	2 (4%)
13	CDL	D	503	-	53,53,99	1.41	4 (7%)	59,65,111	1.24	6 (10%)
11	PG4	C	405	-	12,12,12	0.50	0	11,11,11	0.42	0
12	6PE	A	502	-	22,22,26	1.54	2 (9%)	25,27,31	1.42	3 (12%)
13	CDL	A	503	-	33,33,99	1.29	2 (6%)	37,43,111	1.31	4 (10%)
15	LMT	C	403	-	36,36,36	0.83	1 (2%)	47,47,47	1.23	5 (10%)
14	HEM	C	401	3	50,50,50	1.61	9 (18%)	67,82,82	1.36	12 (17%)
19	PO4	G	102	-	4,4,4	0.96	0	6,6,6	0.54	0
19	PO4	G	101	-	4,4,4	0.78	0	6,6,6	0.88	0
16	PEE	C	407	-	39,39,50	1.26	3 (7%)	42,44,55	1.17	2 (4%)
13	CDL	C	406	-	43,43,99	1.59	4 (9%)	49,55,111	1.54	7 (14%)
19	PO4	F	501	-	4,4,4	0.93	0	6,6,6	0.46	0
11	PG4	C	404	-	12,12,12	0.70	0	11,11,11	0.63	0
13	CDL	E	204	-	59,59,99	1.27	4 (6%)	65,71,111	1.20	7 (10%)
19	PO4	D	502	-	4,4,4	1.11	0	6,6,6	0.38	0
21	PX4	E	202	-	36,36,45	1.33	2 (5%)	42,44,53	1.22	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
11	PG4	A	501	-	-	6/10/10/10	-
17	JHE	C	408	-	-	2/13/13/13	0/4/4/4
16	PEE	E	203	-	1/1/4/8	27/44/44/54	-
16	PEE	C	407	-	1/1/4/8	17/43/43/54	-
18	HEC	D	501	4	-	2/14/54/54	-
20	FES	E	201	-	-	-	0/1/1/1
13	CDL	A	503	-	-	17/41/41/110	-
13	CDL	C	406	-	-	16/52/52/110	-
13	CDL	D	503	-	-	24/63/63/110	-
14	HEM	C	401	3	-	5/14/54/54	-
15	LMT	C	403	-	-	9/21/61/61	0/2/2/2
11	PG4	C	404	-	-	5/10/10/10	-
14	HEM	C	402	3	-	2/14/54/54	-
11	PG4	C	405	-	-	5/10/10/10	-
13	CDL	E	204	-	-	35/69/69/110	-
12	6PE	A	502	-	-	12/26/26/30	-
21	PX4	E	202	-	-	14/40/40/49	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	408	JHE	C3-C4	7.78	1.49	1.36
17	C	408	JHE	C1-C2	5.95	1.50	1.41
13	C	406	CDL	OA6-CA5	5.73	1.47	1.35
14	C	402	HEM	FE-NB	5.72	2.12	1.94
14	C	401	HEM	FE-NB	5.67	2.12	1.94
13	D	503	CDL	OA8-CA7	5.55	1.49	1.33
13	C	406	CDL	OB6-CB5	5.47	1.49	1.34
13	E	204	CDL	OA6-CA5	5.11	1.48	1.34
18	D	501	HEC	CHC-C4B	5.10	1.48	1.38
18	D	501	HEC	C2A-C3A	5.08	1.47	1.36
21	E	202	PX4	O7-C23	5.01	1.48	1.34
13	D	503	CDL	OB6-CB5	4.97	1.48	1.34
18	D	501	HEC	CHB-C4A	4.80	1.47	1.38
13	C	406	CDL	OB8-CB7	4.80	1.47	1.33
18	D	501	HEC	CHD-C4C	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	203	PEE	O2-C10	4.70	1.47	1.34
18	D	501	HEC	CAC-C3C	4.69	1.50	1.35
13	A	503	CDL	OB8-CB7	4.68	1.47	1.33
12	A	502	6PE	O6-C10	4.67	1.47	1.34
12	A	502	6PE	O4-C4	4.65	1.46	1.33
21	E	202	PX4	O5-C9	4.62	1.46	1.33
18	D	501	HEC	CAB-C3B	4.61	1.50	1.35
13	D	503	CDL	OA6-CA5	4.61	1.47	1.34
13	E	204	CDL	OA8-CA7	4.54	1.46	1.33
16	C	407	PEE	O3-C30	4.53	1.46	1.33
13	E	204	CDL	OB6-CB5	4.52	1.47	1.34
18	D	501	HEC	CHA-C1A	4.51	1.47	1.38
13	A	503	CDL	OB6-CB5	4.32	1.46	1.34
16	E	203	PEE	O3-C30	4.31	1.45	1.33
18	D	501	HEC	CHC-C1C	4.27	1.49	1.39
14	C	402	HEM	FE-NC	4.18	2.08	1.95
16	C	407	PEE	O2-C10	4.12	1.45	1.34
14	C	401	HEM	FE-NC	3.98	2.08	1.95
16	E	203	PEE	C18-C19	3.79	1.53	1.31
16	C	407	PEE	C18-C19	3.77	1.53	1.31
18	D	501	HEC	CHD-C1D	3.74	1.47	1.39
18	D	501	HEC	C3D-C2D	3.56	1.48	1.38
18	D	501	HEC	CHA-C4D	3.55	1.47	1.39
18	D	501	HEC	CHB-C1B	3.41	1.47	1.39
18	D	501	HEC	C1C-C2C	3.05	1.50	1.43
14	C	402	HEM	C1B-NB	-3.01	1.35	1.40
13	C	406	CDL	OA8-CA7	2.93	1.47	1.33
15	C	403	LMT	O1'-C1'	2.87	1.45	1.40
18	D	501	HEC	C1D-C2D	2.85	1.49	1.43
17	C	408	JHE	O1-N	2.82	1.43	1.39
14	C	401	HEM	C1B-NB	-2.81	1.35	1.40
14	C	402	HEM	C4D-ND	-2.80	1.35	1.40
13	E	204	CDL	OB8-CB7	2.80	1.46	1.33
14	C	401	HEM	C4D-ND	-2.77	1.35	1.40
14	C	401	HEM	C3B-C4B	2.75	1.50	1.44
13	D	503	CDL	OB8-CB7	2.65	1.46	1.33
18	D	501	HEC	C4D-C3D	2.59	1.49	1.44
17	C	408	JHE	C3-N	2.54	1.42	1.38
18	D	501	HEC	C4B-NB	-2.42	1.35	1.39
17	C	408	JHE	O2-C23	2.42	1.44	1.31
18	D	501	HEC	C4A-NA	-2.40	1.35	1.39
14	C	401	HEM	C4B-NB	-2.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	501	HEC	C1B-C2B	2.32	1.48	1.43
18	D	501	HEC	C1A-C2A	2.30	1.49	1.45
18	D	501	HEC	C3C-C2C	2.27	1.48	1.41
14	C	401	HEM	C4D-C3D	2.14	1.48	1.45
14	C	402	HEM	C4B-NB	-2.13	1.34	1.38
14	C	402	HEM	C3B-C4B	2.12	1.49	1.44
18	D	501	HEC	C1D-ND	-2.09	1.35	1.39
18	D	501	HEC	C1B-NB	-2.08	1.35	1.39
18	D	501	HEC	C4C-NC	-2.06	1.35	1.39
14	C	401	HEM	C1D-ND	-2.06	1.34	1.38
14	C	402	HEM	C1D-ND	-2.04	1.34	1.38
14	C	402	HEM	FE-ND	-2.02	1.88	1.94
18	D	501	HEC	C4A-C3A	2.02	1.49	1.45
14	C	402	HEM	C1D-C2D	2.02	1.48	1.44
14	C	401	HEM	FE-ND	-2.01	1.88	1.94
18	D	501	HEC	C1A-NA	-2.00	1.35	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	501	HEC	C2A-C1A-NA	6.39	116.49	110.32
13	C	406	CDL	OA6-CA5-C11	6.27	122.27	111.09
18	D	501	HEC	C3D-C4D-ND	5.62	116.38	110.15
12	A	502	6PE	O6-C10-C11	4.59	121.40	111.48
21	E	202	PX4	O7-C23-C24	4.52	121.25	111.48
13	A	503	CDL	OB6-CB5-C51	4.44	121.09	111.48
18	D	501	HEC	C2B-C1B-NB	4.40	117.19	110.14
17	C	408	JHE	C2-N-C3	-4.38	123.12	126.68
16	E	203	PEE	O2-C10-C11	4.38	120.95	111.48
18	D	501	HEC	C1A-C2A-C3A	-4.13	101.67	107.11
13	D	503	CDL	OB6-CB5-C51	4.08	120.31	111.48
16	C	407	PEE	O3-C30-C31	3.98	123.96	111.83
13	A	503	CDL	OB8-CB7-C71	3.96	123.16	111.15
13	E	204	CDL	OA6-CA5-C11	3.88	119.87	111.48
13	E	204	CDL	OB6-CB5-C51	3.85	119.82	111.48
15	C	403	LMT	O1B-C4'-C3'	3.84	116.99	107.23
13	D	503	CDL	OA8-CA7-C31	3.83	123.50	111.83
15	C	403	LMT	C1B-O5B-C5B	3.76	121.06	113.72
14	C	402	HEM	CHC-C4B-NB	3.66	128.36	124.42
13	C	406	CDL	OB8-CB7-C71	3.60	122.81	111.83
18	D	501	HEC	C2D-C1D-ND	3.55	115.84	110.14
18	D	501	HEC	C1D-C2D-C3D	-3.46	102.85	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	E	202	PX4	O5-C9-C10	3.30	121.90	111.83
18	D	501	HEC	C3A-C4A-NA	3.24	115.63	109.64
18	D	501	HEC	C4D-C3D-C2D	-3.18	101.95	106.87
14	C	401	HEM	CHB-C1B-NB	3.17	128.28	124.37
13	D	503	CDL	OA6-CA5-C11	3.14	118.28	111.48
14	C	401	HEM	CHC-C4B-NB	3.07	127.73	124.42
18	D	501	HEC	C2C-C1C-NC	3.04	115.02	110.14
13	D	503	CDL	OA8-CA7-OA9	-3.01	116.11	123.63
13	E	204	CDL	OA8-CA7-C31	2.93	120.78	111.83
13	C	406	CDL	OB6-CB5-C51	2.86	121.44	110.93
21	E	202	PX4	O5-C9-O6	-2.84	116.53	123.63
13	E	204	CDL	CA6-OA8-CA7	2.80	127.35	117.12
15	C	403	LMT	C1'-O5'-C5'	2.78	119.14	113.72
13	C	406	CDL	OA8-CA7-C31	2.77	124.14	112.38
13	C	406	CDL	CA6-OA8-CA7	2.75	123.86	117.08
12	A	502	6PE	O4-C4-C5	2.70	120.06	111.83
12	A	502	6PE	O6-C10-O7	-2.65	117.50	123.70
13	E	204	CDL	CB6-OB8-CB7	2.60	123.50	117.08
14	C	401	HEM	CHD-C4C-NC	2.57	127.25	124.45
13	A	503	CDL	OB6-CB5-OB7	-2.57	117.69	123.70
14	C	402	HEM	CHA-C4D-ND	2.57	127.55	124.37
18	D	501	HEC	C4A-C3A-C2A	-2.55	103.20	106.97
14	C	401	HEM	CAD-C3D-C4D	2.53	129.11	124.70
16	C	407	PEE	O2-C10-C11	2.50	116.88	111.48
13	A	503	CDL	OB8-CB7-OB9	-2.50	117.39	123.63
17	C	408	JHE	C9-C4-C	2.49	121.26	116.68
21	E	202	PX4	O7-C23-O8	-2.48	117.91	123.70
14	C	401	HEM	C1B-NB-C4B	2.45	108.11	105.21
14	C	402	HEM	O2D-CGD-CBD	2.44	121.71	114.00
13	E	204	CDL	OB8-CB7-C71	2.41	122.61	112.38
14	C	401	HEM	CHD-C1D-ND	2.41	127.01	124.42
18	D	501	HEC	CHB-C1B-C2B	-2.40	120.47	127.43
16	E	203	PEE	O3-C30-C31	2.39	119.13	111.83
14	C	401	HEM	CHB-C1B-C2B	-2.39	120.16	126.95
18	D	501	HEC	CHA-C1A-C2A	-2.36	121.14	124.86
14	C	401	HEM	CHA-C4D-ND	2.32	127.24	124.37
13	D	503	CDL	OB8-CB7-C71	2.32	122.20	112.38
17	C	408	JHE	C2-C1-C	-2.31	119.18	121.38
15	C	403	LMT	O5'-C5'-C6'	2.30	112.13	106.44
13	D	503	CDL	CA6-OA8-CA7	2.29	125.50	117.12
14	C	402	HEM	CMD-C2D-C1D	2.28	128.60	125.03
14	C	401	HEM	CMD-C2D-C1D	2.21	128.49	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	501	HEC	CAD-C3D-C4D	2.21	129.26	124.94
18	D	501	HEC	CMB-C2B-C3B	2.21	131.74	126.55
14	C	402	HEM	CHA-C4D-C3D	-2.19	121.20	125.23
13	C	406	CDL	OB8-CB7-OB9	-2.17	118.20	123.63
18	D	501	HEC	CHC-C4B-NB	-2.17	122.09	124.45
13	E	204	CDL	OB6-CB5-OB7	-2.14	118.69	123.70
14	C	402	HEM	CHD-C1D-ND	2.14	126.72	124.42
14	C	401	HEM	O2D-CGD-CBD	2.13	120.74	114.00
14	C	402	HEM	CAD-C3D-C4D	2.12	128.40	124.70
18	D	501	HEC	O2D-CGD-CBD	2.06	120.52	114.00
15	C	403	LMT	C1B-O1B-C4'	-2.06	113.11	117.98
14	C	402	HEM	O2A-CGA-CBA	2.05	120.49	114.00
21	E	202	PX4	O5-C8-C7	2.05	114.30	108.40
14	C	402	HEM	C1B-NB-C4B	2.04	107.62	105.21
14	C	401	HEM	CHA-C4D-C3D	-2.03	121.48	125.23
18	D	501	HEC	CHB-C4A-NA	-2.01	122.26	124.45
13	C	406	CDL	OA6-CA5-OA7	-2.01	119.11	122.99
14	C	401	HEM	CBA-CAA-C2A	-2.01	106.98	112.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	407	PEE	C2
16	E	203	PEE	C2

All (198) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	502	6PE	C1-O3-P1-O1
12	A	502	6PE	C1-O3-P1-O8
12	A	502	6PE	C11-C10-O6-C2
12	A	502	6PE	O8-C16-C17-N1
13	A	503	CDL	CA3-OA5-PA1-OA2
13	A	503	CDL	CA3-OA5-PA1-OA4
13	A	503	CDL	CB2-OB2-PB2-OB3
13	A	503	CDL	C51-CB5-OB6-CB4
13	C	406	CDL	CA3-OA5-PA1-OA2
13	C	406	CDL	CA3-OA5-PA1-OA4
13	C	406	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	CB2-OB2-PB2-OB5
13	E	204	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
13	E	204	CDL	CB3-OB5-PB2-OB3
13	E	204	CDL	C51-CB5-OB6-CB4
15	C	403	LMT	C2-C1-O1'-C1'
16	C	407	PEE	C4-O4P-P-O3P
16	C	407	PEE	C4-O4P-P-O2P
16	C	407	PEE	C4-O4P-P-O1P
16	E	203	PEE	C4-O4P-P-O1P
16	E	203	PEE	O4P-C4-C5-N
21	E	202	PX4	C6-O4-P1-O1
21	E	202	PX4	C24-C23-O7-C7
13	C	406	CDL	C11-CA5-OA6-CA4
13	C	406	CDL	OA7-CA5-OA6-CA4
12	A	502	6PE	O7-C10-O6-C2
13	A	503	CDL	OB7-CB5-OB6-CB4
13	D	503	CDL	OB7-CB5-OB6-CB4
13	E	204	CDL	OB7-CB5-OB6-CB4
21	E	202	PX4	O8-C23-O7-C7
13	D	503	CDL	C31-CA7-OA8-CA6
16	C	407	PEE	C31-C30-O3-C3
16	E	203	PEE	C31-C30-O3-C3
21	E	202	PX4	C10-C9-O5-C8
13	D	503	CDL	OB9-CB7-OB8-CB6
13	D	503	CDL	C71-CB7-OB8-CB6
13	D	503	CDL	OA9-CA7-OA8-CA6
16	C	407	PEE	O5-C30-O3-C3
21	E	202	PX4	O6-C9-O5-C8
13	C	406	CDL	C31-CA7-OA8-CA6
13	E	204	CDL	O1-C1-CB2-OB2
13	D	503	CDL	C51-CB5-OB6-CB4
13	E	204	CDL	CB4-CB6-OB8-CB7
16	E	203	PEE	O5-C30-O3-C3
11	C	404	PG4	O2-C3-C4-O3
15	C	403	LMT	O5'-C1'-O1'-C1
16	C	407	PEE	C17-C18-C19-C20
13	A	503	CDL	OA5-CA3-CA4-CA6
13	E	204	CDL	C71-CB7-OB8-CB6
15	C	403	LMT	C2'-C1'-O1'-C1
13	A	503	CDL	OA5-CA3-CA4-OA6
11	C	405	PG4	O2-C3-C4-O3
13	D	503	CDL	OA5-CA3-CA4-OA6
13	C	406	CDL	OA9-CA7-OA8-CA6
13	D	503	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	A	501	PG4	O1-C1-C2-O2
13	A	503	CDL	CB5-C51-C52-C53
13	E	204	CDL	OA7-CA5-OA6-CA4
11	C	404	PG4	O3-C5-C6-O4
13	E	204	CDL	C11-CA5-OA6-CA4
13	E	204	CDL	CB4-CB3-OB5-PB2
21	E	202	PX4	C12-C13-C14-C15
15	C	403	LMT	C4-C5-C6-C7
16	C	407	PEE	C31-C32-C33-C34
13	E	204	CDL	OB9-CB7-OB8-CB6
16	E	203	PEE	C11-C10-O2-C2
13	D	503	CDL	C51-C52-C53-C54
12	A	502	6PE	C4-C5-C6-C7
13	C	406	CDL	C71-CB7-OB8-CB6
13	E	204	CDL	C35-C36-C37-C38
16	C	407	PEE	C13-C14-C15-C16
11	A	501	PG4	O2-C3-C4-O3
16	C	407	PEE	C14-C15-C16-C17
16	E	203	PEE	C13-C14-C15-C16
13	E	204	CDL	C31-CA7-OA8-CA6
13	E	204	CDL	C54-C55-C56-C57
13	E	204	CDL	C51-C52-C53-C54
13	E	204	CDL	OA9-CA7-OA8-CA6
16	E	203	PEE	C10-C11-C12-C13
12	A	502	6PE	C5-C4-O4-C3
15	C	403	LMT	C11-C10-C9-C8
13	C	406	CDL	C51-CB5-OB6-CB4
13	C	406	CDL	OB7-CB5-OB6-CB4
16	E	203	PEE	O4-C10-O2-C2
13	C	406	CDL	OB9-CB7-OB8-CB6
13	D	503	CDL	C11-C12-C13-C14
16	C	407	PEE	C10-C11-C12-C13
16	E	203	PEE	C23-C24-C25-C26
13	C	406	CDL	CB4-CB3-OB5-PB2
11	A	501	PG4	O4-C7-C8-O5
11	C	404	PG4	O1-C1-C2-O2
13	E	204	CDL	CA2-C1-CB2-OB2
16	E	203	PEE	C15-C16-C17-C18
13	A	503	CDL	OB5-CB3-CB4-CB6
13	D	503	CDL	OA5-CA3-CA4-CA6
12	A	502	6PE	O5-C4-O4-C3
12	A	502	6PE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	C	407	PEE	C11-C12-C13-C14
21	E	202	PX4	C13-C14-C15-C16
15	C	403	LMT	O5B-C5B-C6B-O6B
13	E	204	CDL	CA5-C11-C12-C13
13	D	503	CDL	CB6-CB4-OB6-CB5
13	D	503	CDL	C53-C54-C55-C56
13	E	204	CDL	C12-C13-C14-C15
13	D	503	CDL	C54-C55-C56-C57
21	E	202	PX4	C24-C25-C26-C27
16	E	203	PEE	C24-C25-C26-C27
13	C	406	CDL	OB5-CB3-CB4-CB6
16	E	203	PEE	C14-C15-C16-C17
15	C	403	LMT	C6-C7-C8-C9
16	E	203	PEE	C34-C35-C36-C37
21	E	202	PX4	C11-C12-C13-C14
13	E	204	CDL	CA3-CA4-CA6-OA8
16	C	407	PEE	O3P-C1-C2-O2
12	A	502	6PE	C2-C1-O3-P1
13	E	204	CDL	C31-C32-C33-C34
16	E	203	PEE	O2-C2-C3-O3
11	C	405	PG4	C6-C5-O3-C4
13	D	503	CDL	OB5-CB3-CB4-CB6
16	C	407	PEE	O3P-C1-C2-C3
11	C	404	PG4	C3-C4-O3-C5
16	E	203	PEE	C31-C32-C33-C34
11	C	404	PG4	C4-C3-O2-C2
16	E	203	PEE	O3P-C1-C2-O2
12	A	502	6PE	C1-C2-C3-O4
13	D	503	CDL	CA3-CA4-CA6-OA8
13	E	204	CDL	C13-C14-C15-C16
13	D	503	CDL	OA6-CA4-CA6-OA8
13	E	204	CDL	C53-C54-C55-C56
11	C	405	PG4	C1-C2-O2-C3
16	C	407	PEE	C32-C33-C34-C35
21	E	202	PX4	O3-C1-C2-N1
16	E	203	PEE	C12-C13-C14-C15
16	E	203	PEE	O3P-C1-C2-C3
13	C	406	CDL	OB5-CB3-CB4-OB6
13	D	503	CDL	OB5-CB3-CB4-OB6
12	A	502	6PE	O6-C2-C3-O4
13	D	503	CDL	OB6-CB4-CB6-OB8
11	C	405	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
13	D	503	CDL	C31-C32-C33-C34
13	A	503	CDL	CA3-OA5-PA1-OA3
13	A	503	CDL	CB2-OB2-PB2-OB5
13	A	503	CDL	CB3-OB5-PB2-OB2
13	C	406	CDL	CB2-OB2-PB2-OB5
13	D	503	CDL	CB2-OB2-PB2-OB4
13	E	204	CDL	CA2-OA2-PA1-OA3
13	E	204	CDL	CB2-OB2-PB2-OB3
13	E	204	CDL	CB3-OB5-PB2-OB4
16	E	203	PEE	C1-O3P-P-O1P
14	C	401	HEM	C3D-CAD-CBD-CGD
16	E	203	PEE	C3-C2-O2-C10
16	E	203	PEE	C16-C17-C18-C19
13	A	503	CDL	OB5-CB3-CB4-OB6
13	E	204	CDL	C1-CA2-OA2-PA1
11	A	501	PG4	C5-C6-O4-C7
16	E	203	PEE	C18-C19-C20-C21
15	C	403	LMT	C3-C4-C5-C6
15	C	403	LMT	O5B-C1B-O1B-C4'
16	C	407	PEE	C15-C16-C17-C18
14	C	402	HEM	CAA-CBA-CGA-O2A
14	C	402	HEM	CAA-CBA-CGA-O1A
21	E	202	PX4	C9-C10-C11-C12
13	E	204	CDL	OA5-CA3-CA4-OA6
13	E	204	CDL	CA7-C31-C32-C33
13	E	204	CDL	C34-C35-C36-C37
14	C	401	HEM	CAA-CBA-CGA-O2A
13	A	503	CDL	CA4-CA3-OA5-PA1
18	D	501	HEC	CAA-CBA-CGA-O2A
13	E	204	CDL	CB5-C51-C52-C53
16	E	203	PEE	C17-C18-C19-C20
14	C	401	HEM	CAA-CBA-CGA-O1A
13	C	406	CDL	CB7-C71-C72-C73
16	E	203	PEE	C32-C33-C34-C35
14	C	401	HEM	CAD-CBD-CGD-O2D
11	A	501	PG4	C1-C2-O2-C3
18	D	501	HEC	CAA-CBA-CGA-O1A
16	E	203	PEE	C5-C4-O4P-P
14	C	401	HEM	CAD-CBD-CGD-O1D
13	A	503	CDL	O1-C1-CA2-OA2
13	E	204	CDL	C32-C31-CA7-OA8
11	C	405	PG4	C3-C4-O3-C5

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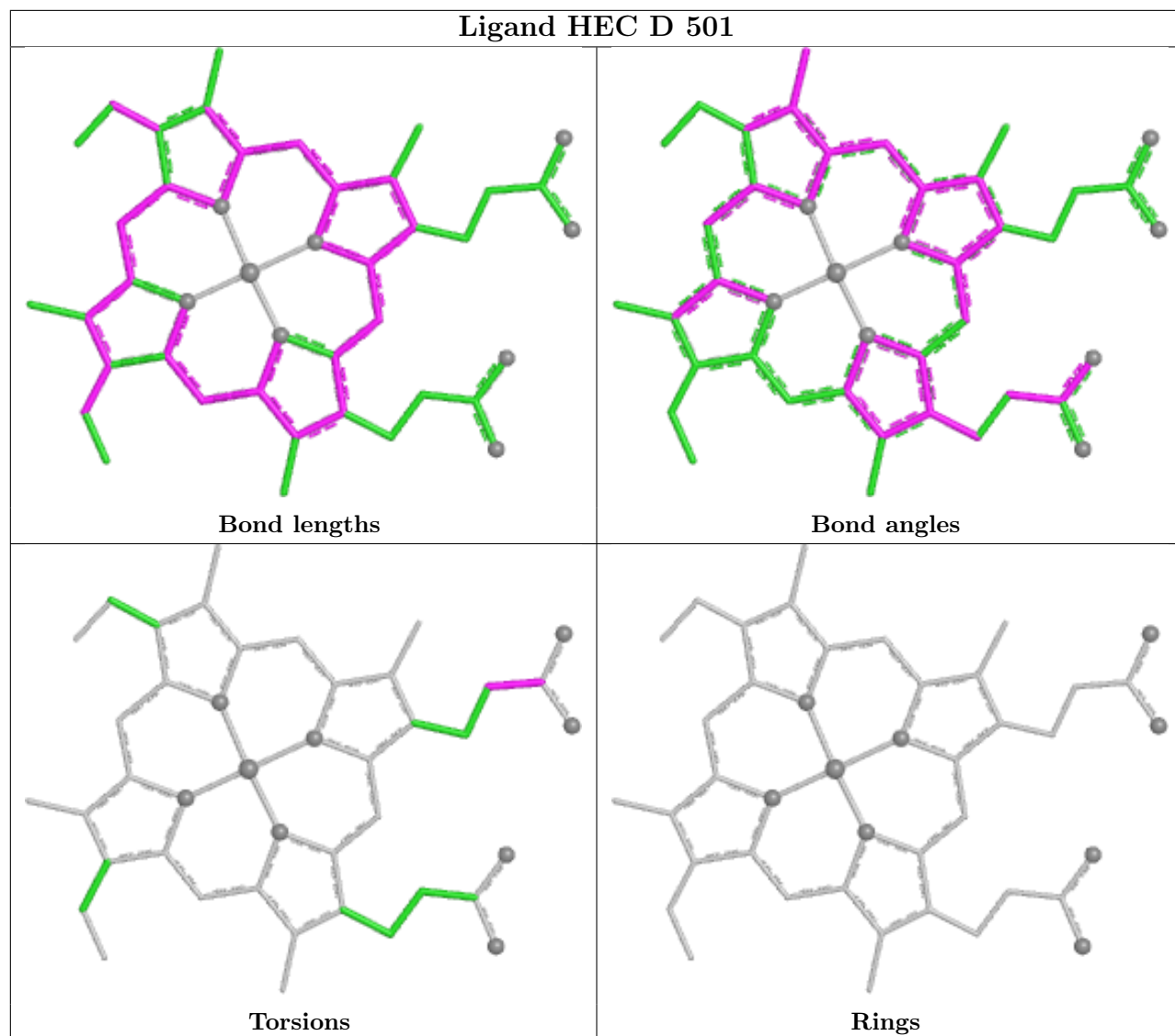
Mol	Chain	Res	Type	Atoms
13	D	503	CDL	CB3-CB4-CB6-OB8
16	E	203	PEE	C33-C34-C35-C36
17	C	408	JHE	C21-C20-O2-C23
13	A	503	CDL	C72-C71-CB7-OB9
21	E	202	PX4	C11-C10-C9-O5
21	E	202	PX4	C14-C15-C16-C17
11	A	501	PG4	C8-C7-O4-C6
13	A	503	CDL	C72-C71-CB7-OB8
16	E	203	PEE	C11-C12-C13-C14
13	E	204	CDL	OA6-CA4-CA6-OA8
13	E	204	CDL	C55-C56-C57-C58
13	E	204	CDL	C32-C31-CA7-OA9
16	C	407	PEE	C30-C31-C32-C33
16	C	407	PEE	O3-C30-C31-C32
17	C	408	JHE	C19-C20-O2-C23
21	E	202	PX4	C11-C10-C9-O6

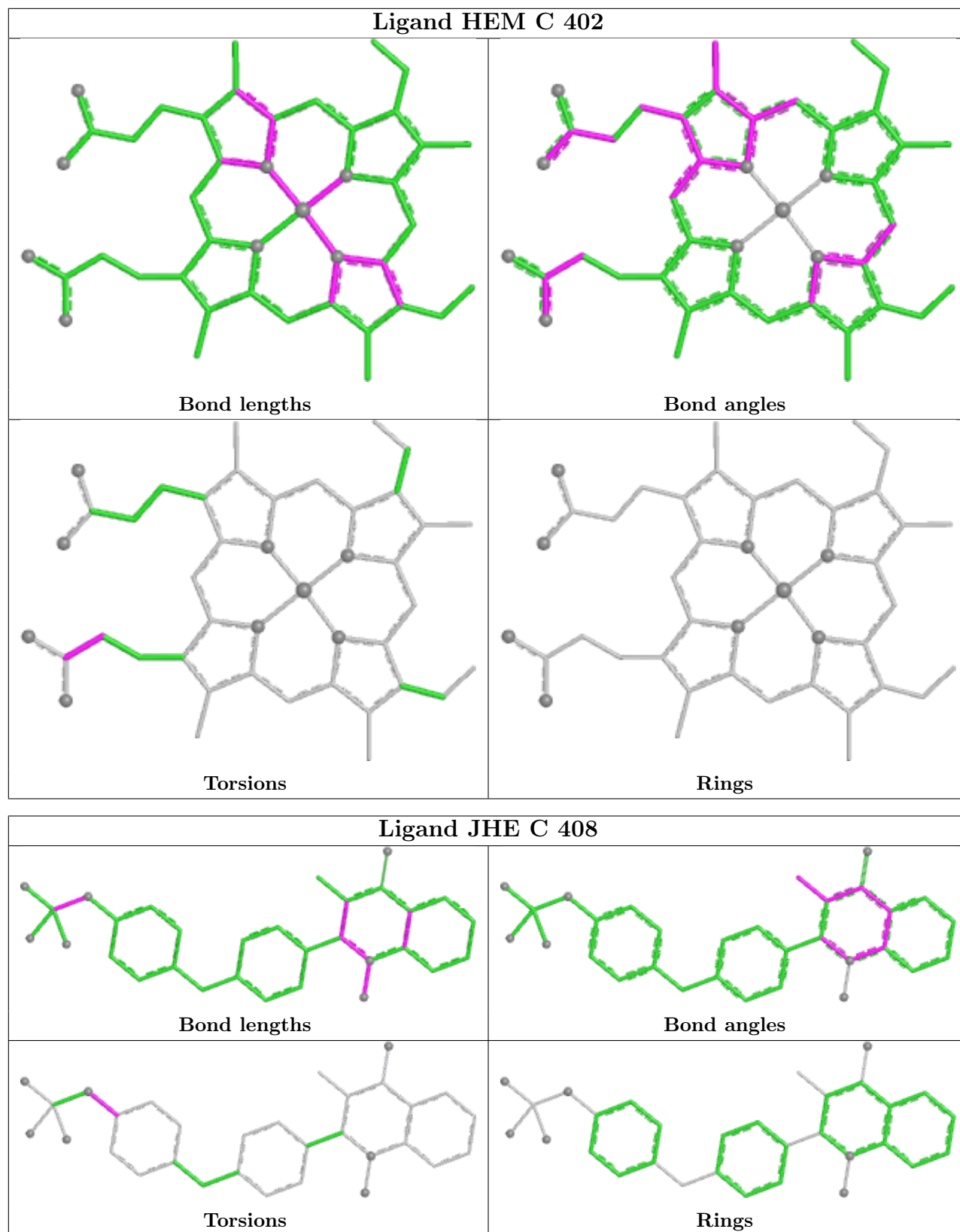
There are no ring outliers.

7 monomers are involved in 16 short contacts:

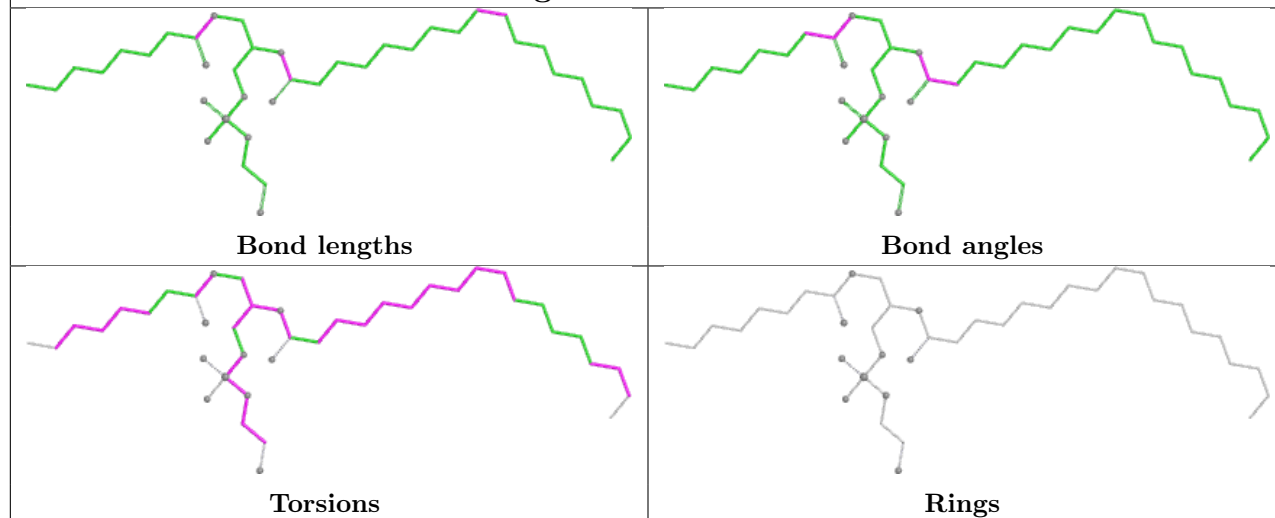
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	501	HEC	5	0
14	C	402	HEM	4	0
16	E	203	PEE	1	0
12	A	502	6PE	2	0
13	A	503	CDL	3	0
14	C	401	HEM	2	0
13	E	204	CDL	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

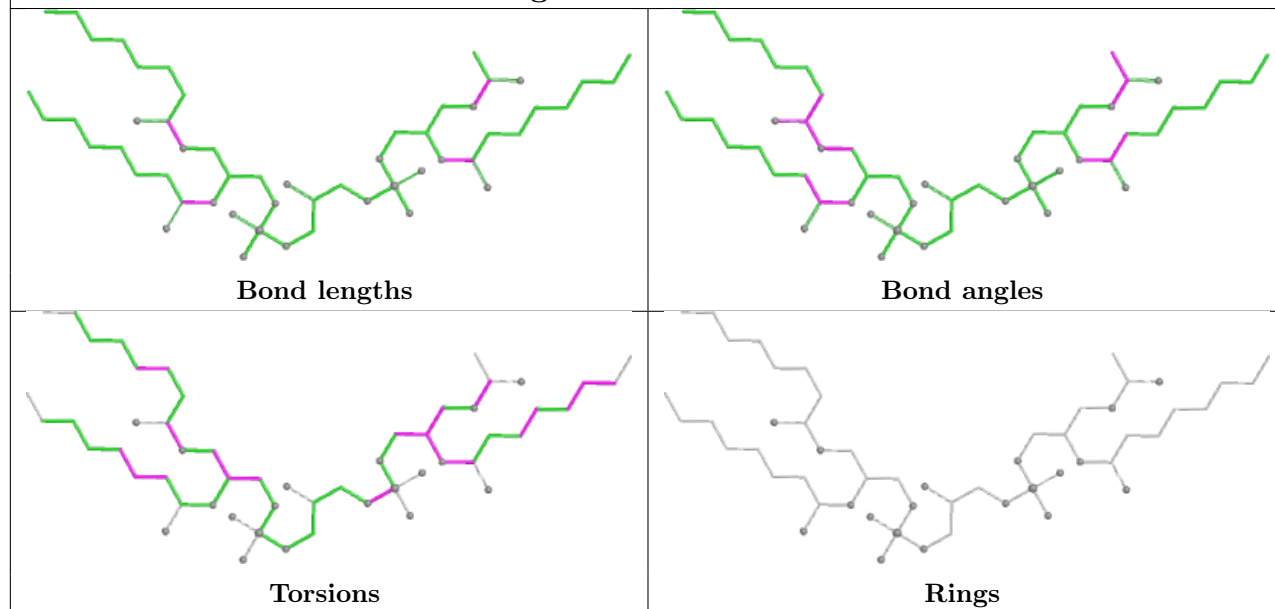




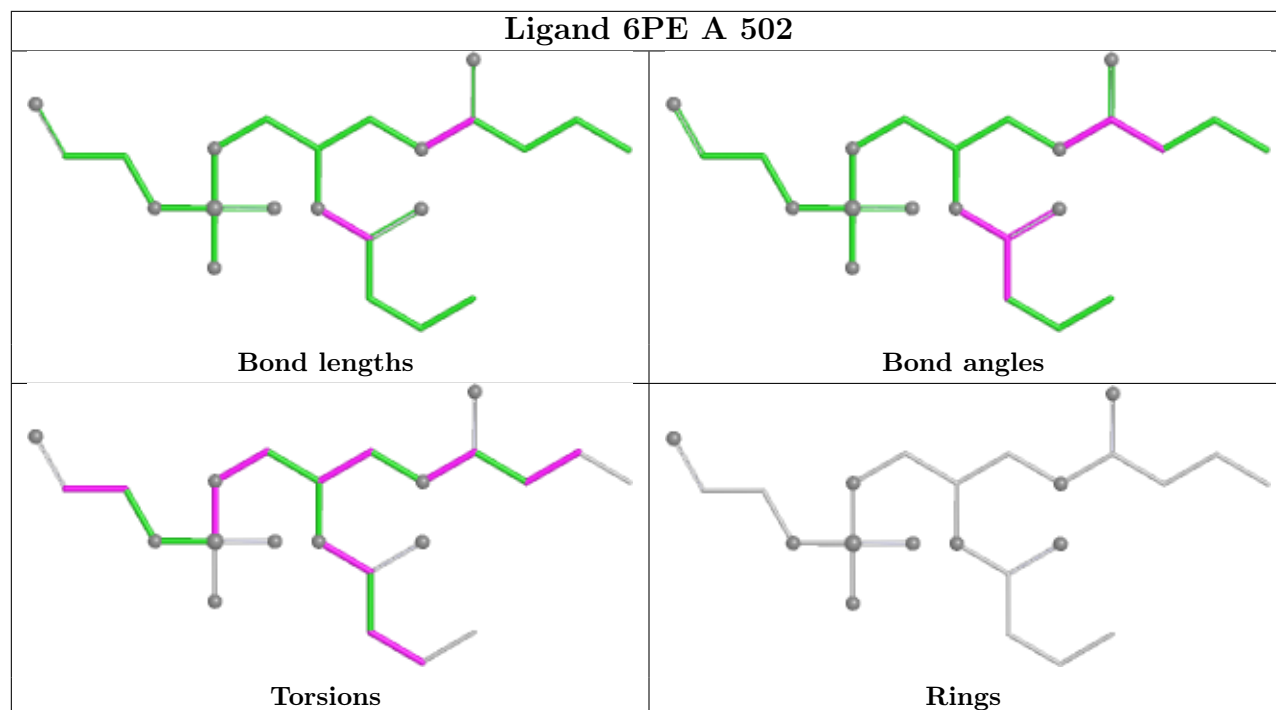
Ligand PEE E 203



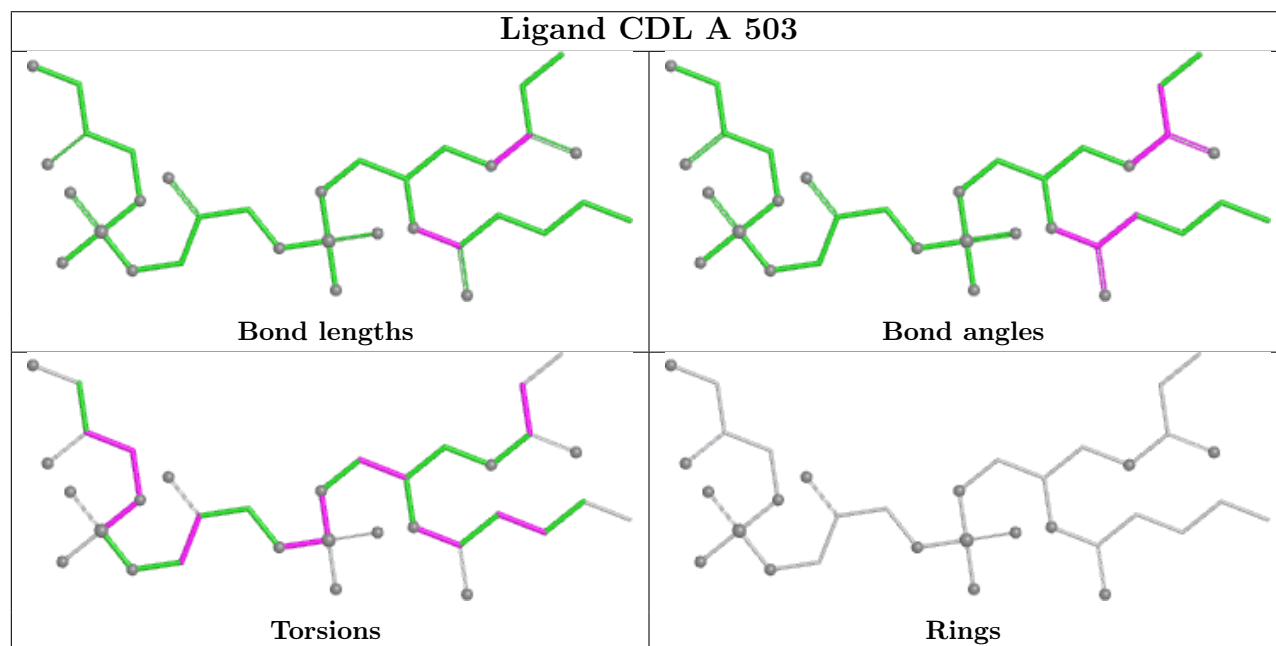
Ligand CDL D 503

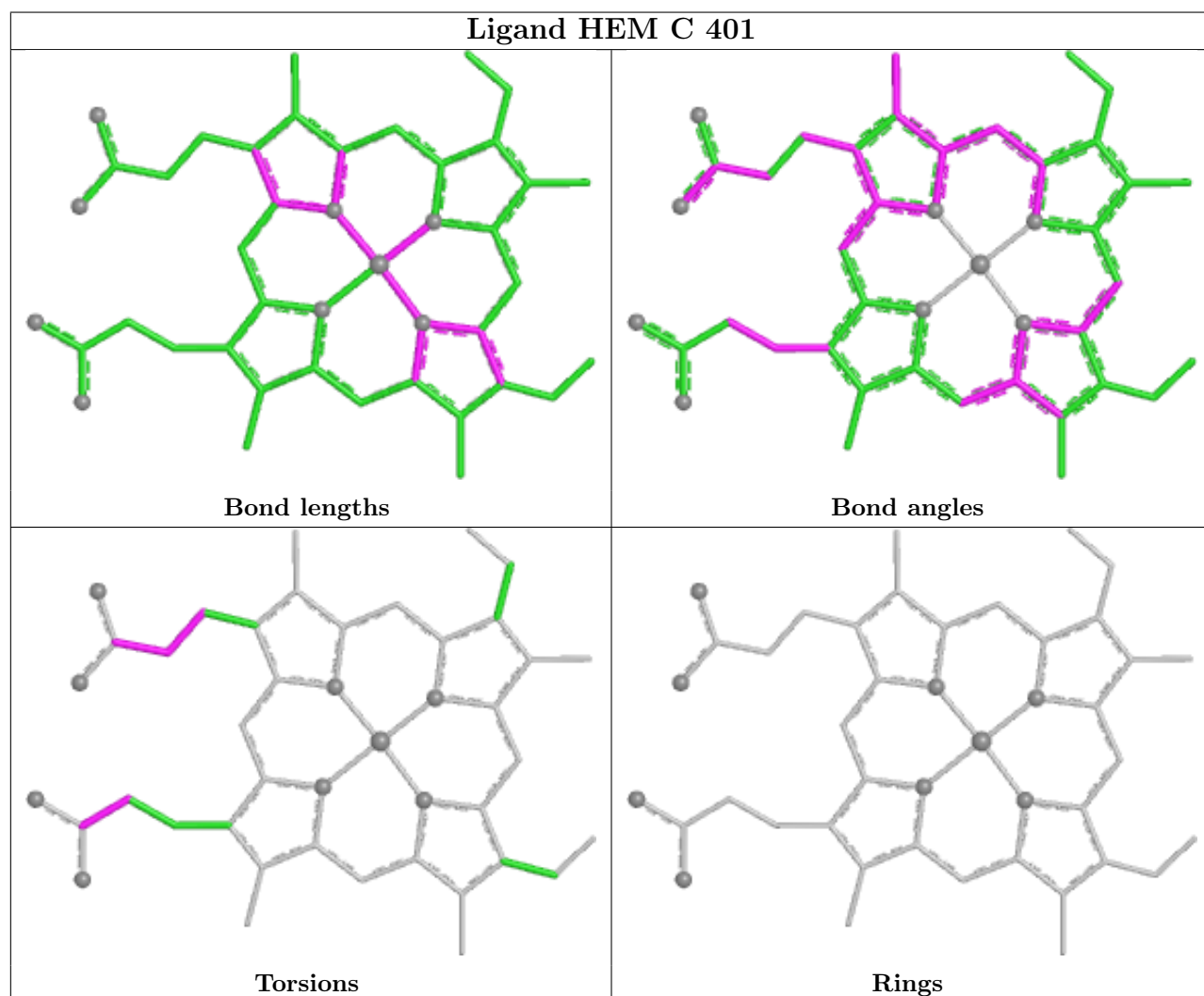
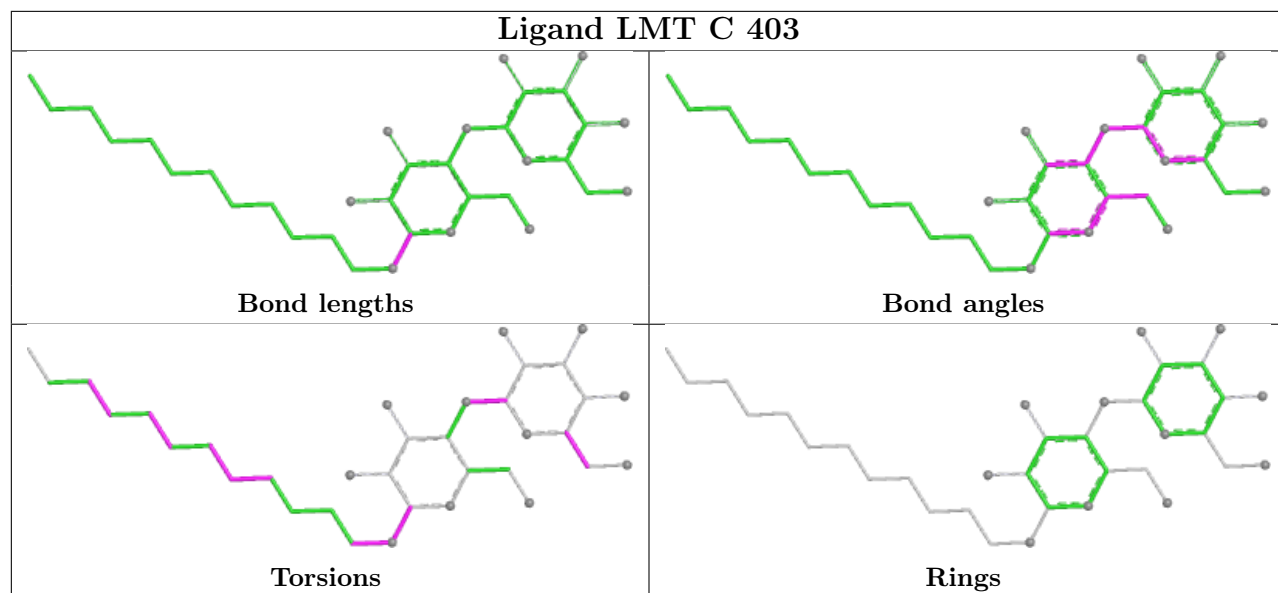


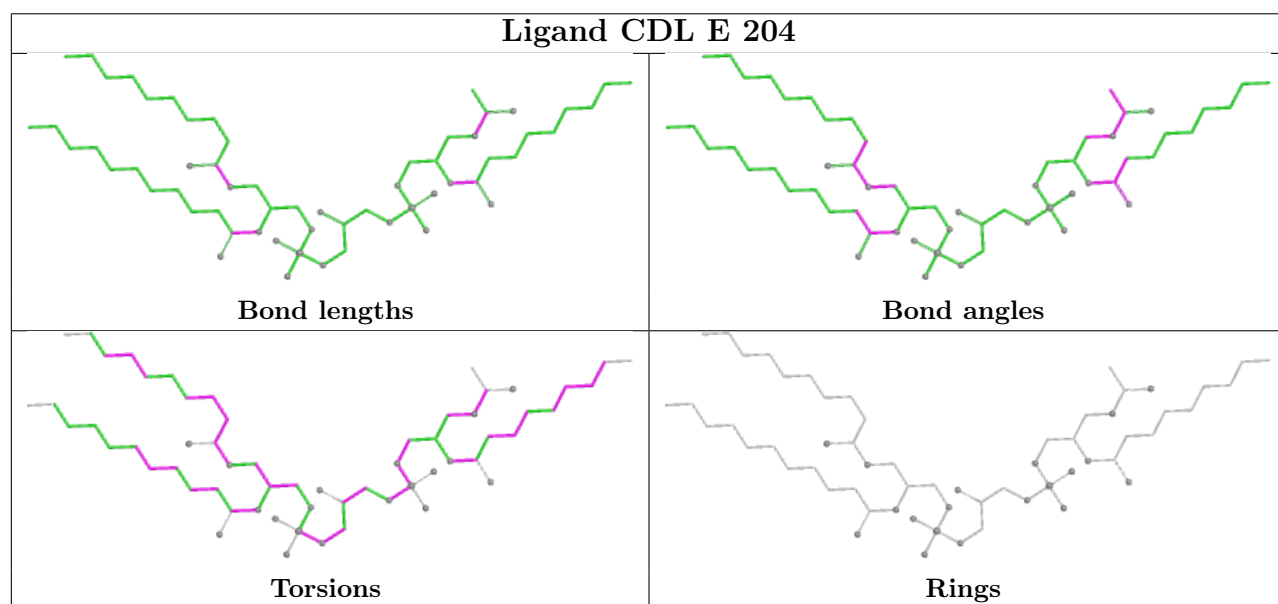
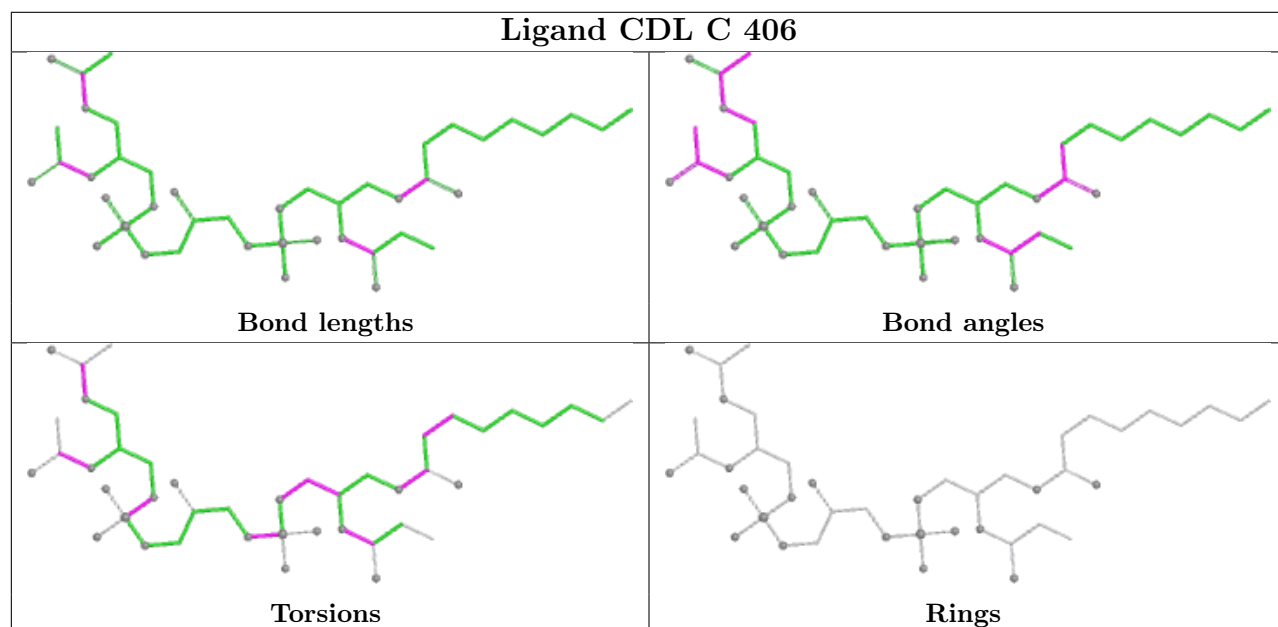
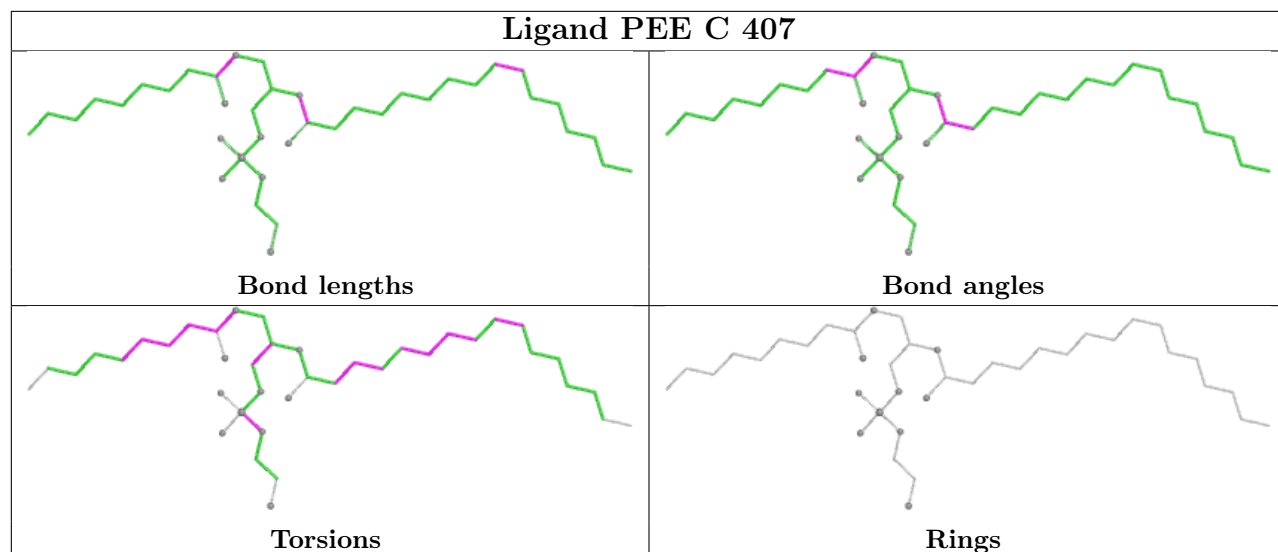
Ligand 6PE A 502

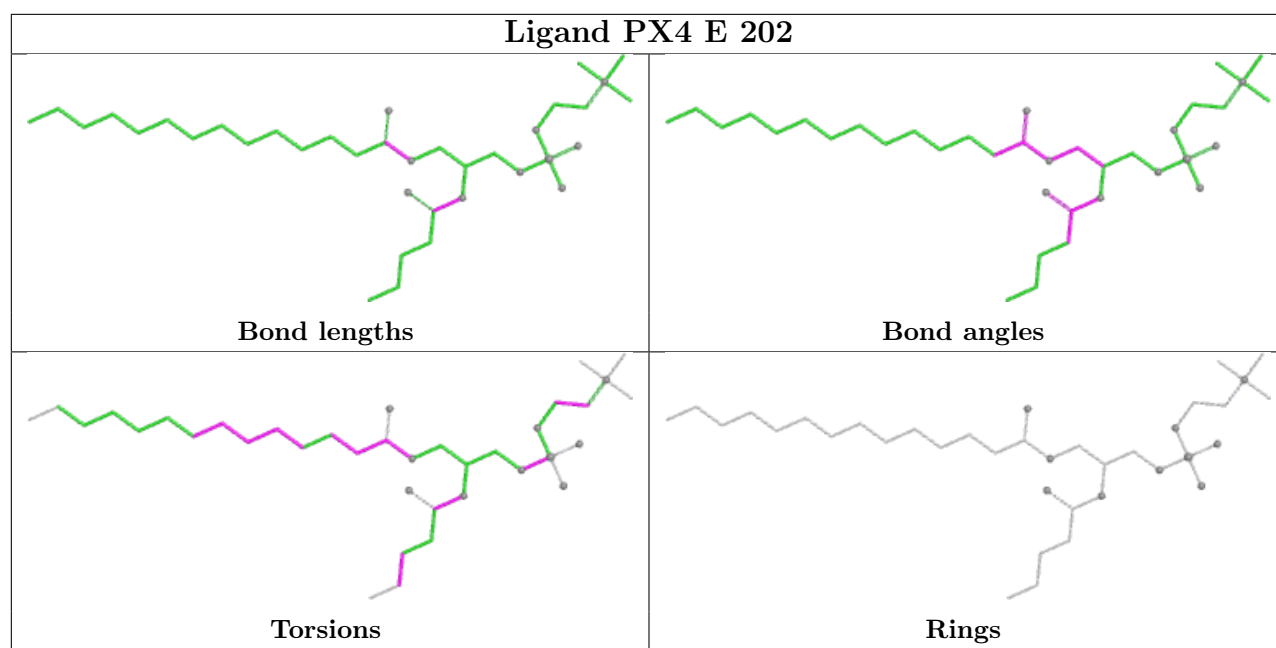


Ligand CDL A 503









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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	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

All (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
5	E	115	SER	3.7
5	E	35	PHE	3.7
4	D	200	HIS	3.6
3	C	60	THR	3.5
9	I	37	THR	3.2
4	D	198	HIS	3.2
3	C	70	CYS	3.2
7	G	75	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
10	J	49	GLY	3.0
2	B	170	ASN	2.9
5	E	111	ALA	2.9
5	E	114	VAL	2.8
5	E	178	LEU	2.8
4	D	211	MET	2.8
1	A	42	ASP	2.8
5	E	179	ASN	2.8
2	B	110	GLU	2.7
4	D	121	HIS	2.7
6	F	56	ASN	2.7
5	E	148	ALA	2.6
9	I	33	ALA	2.6
5	E	119	ASP	2.6
8	H	24	CYS	2.6
3	C	210	GLY	2.6
5	E	124	LEU	2.6
4	D	45	TYR	2.6
9	I	41	PRO	2.6
5	E	164	HIS	2.5
3	C	67	THR	2.5
5	E	147	ILE	2.5
4	D	147	LEU	2.5
6	F	40	ASN	2.5
7	G	26	PHE	2.5
5	E	85	LYS	2.5
5	E	34	GLY	2.5
5	E	160	CYS	2.5
9	I	52	ARG	2.4
3	C	267	HIS	2.4
9	I	35	PRO	2.4
3	C	61	THR	2.4
1	A	190	TYR	2.4
4	D	195	GLU	2.4
2	B	302	GLY	2.3
9	I	42	VAL	2.3
7	G	25	ALA	2.3
9	I	78	TYR	2.3
5	E	121	GLN	2.3
3	C	311	LYS	2.3
9	I	34	VAL	2.3
4	D	13	SER	2.3

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Mol	Chain	Res	Type	RSRZ
10	J	48	GLU	2.3
6	F	69	SER	2.2
1	A	194	ARG	2.2
9	I	38	SER	2.2
5	E	140	THR	2.2
5	E	177	PRO	2.2
5	E	66	ALA	2.2
5	E	71	MET	2.2
3	C	77	TRP	2.2
1	A	97	TYR	2.2
5	E	171	ILE	2.2
8	H	75	ASN	2.2
9	I	62	ARG	2.1
2	B	226	ILE	2.1
9	I	71	ASN	2.1
4	D	215	LEU	2.1
3	C	64	SER	2.1
5	E	82	PRO	2.1
5	E	33	LYS	2.0
8	H	25	GLU	2.0
1	A	413	LYS	2.0
3	C	209	THR	2.0
4	D	214	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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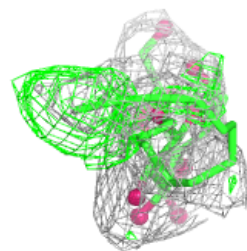
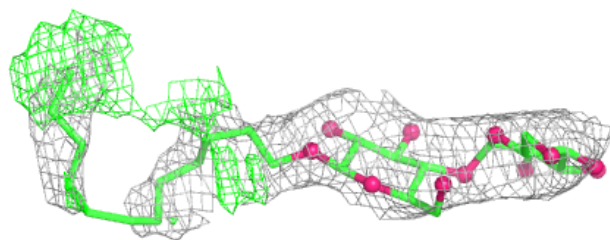
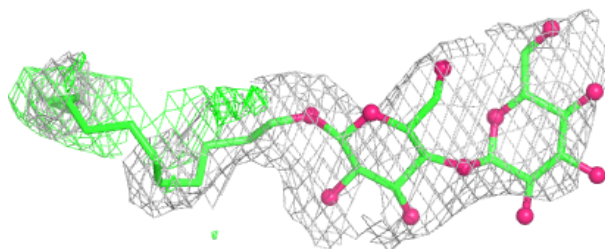
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	LMT	C	403	35/35	0.28	0.24	170,207,219,222	0
13	CDL	E	204	60/100	0.68	0.23	150,185,246,250	0
19	PO4	G	102	5/5	0.71	0.10	239,242,243,249	0
19	PO4	G	103	5/5	0.74	0.12	191,192,195,198	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.

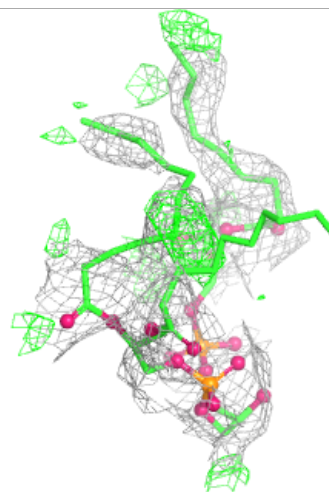
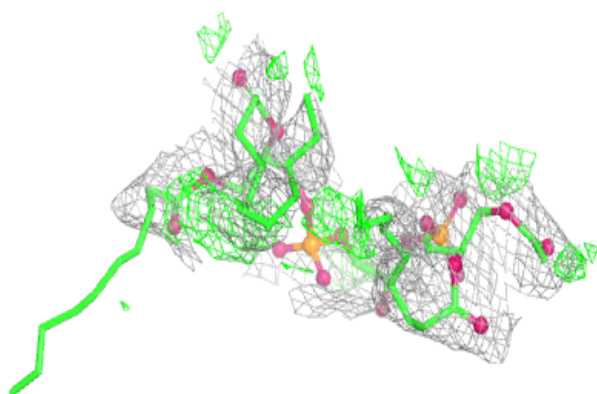
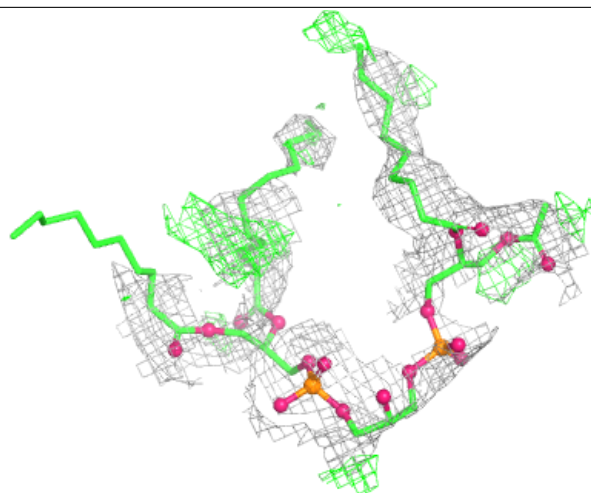
Electron density around LMT C 403:

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



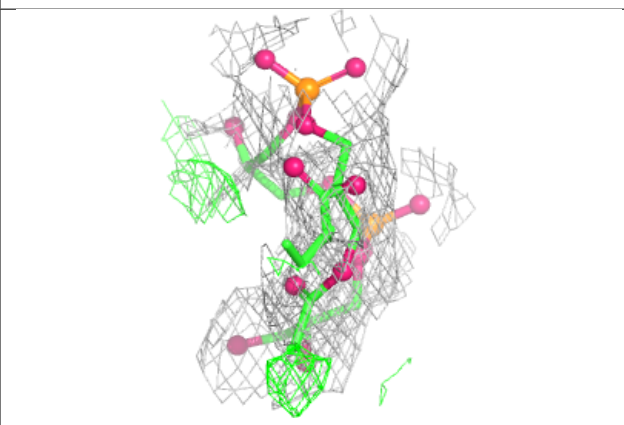
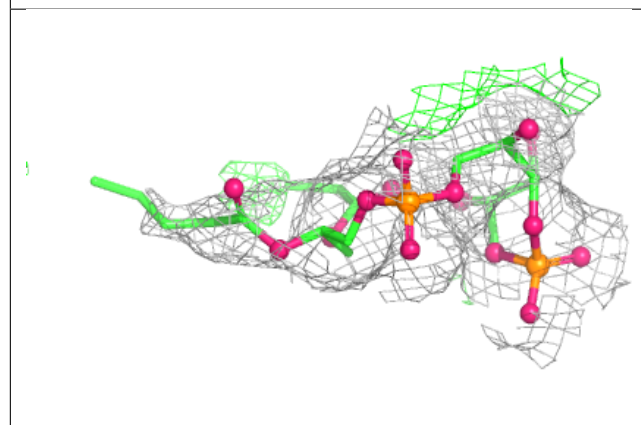
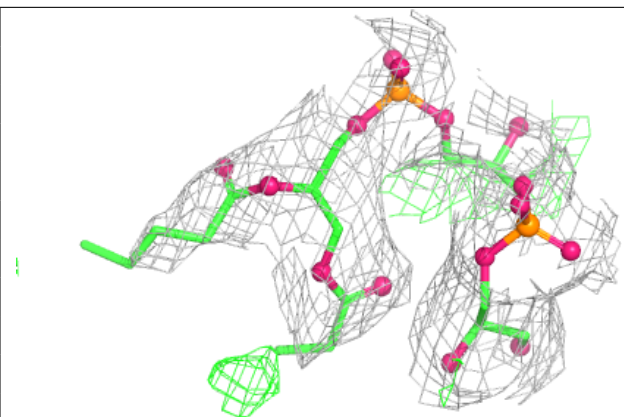
Electron density around CDL E 204:

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

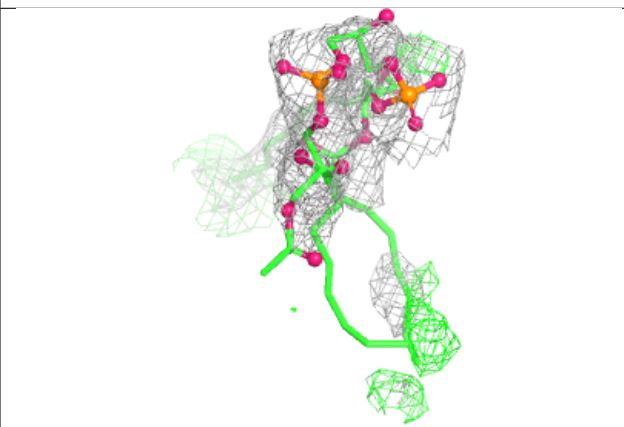
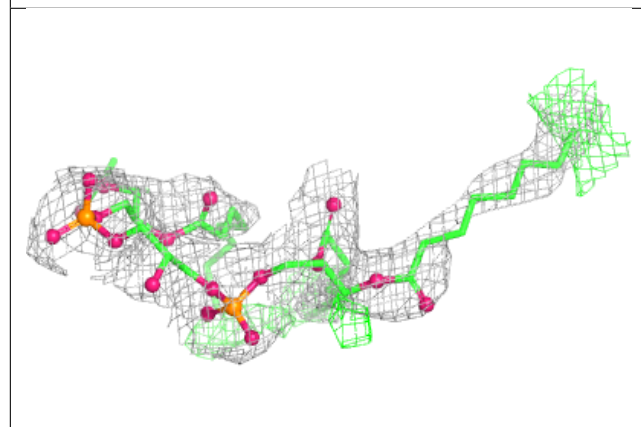
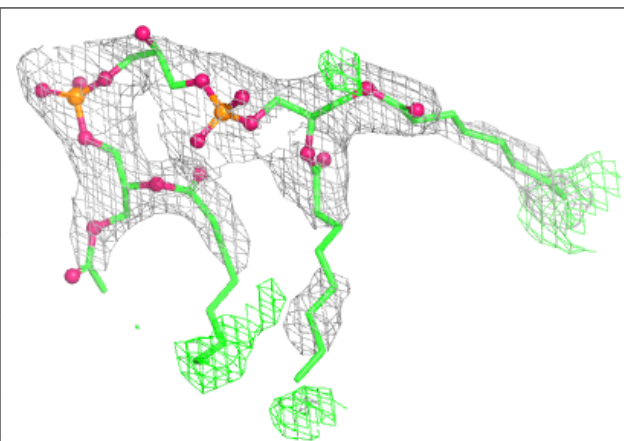


Electron density around CDL A 503:

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

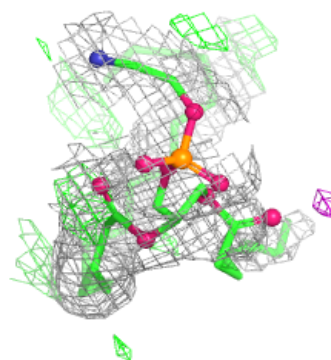
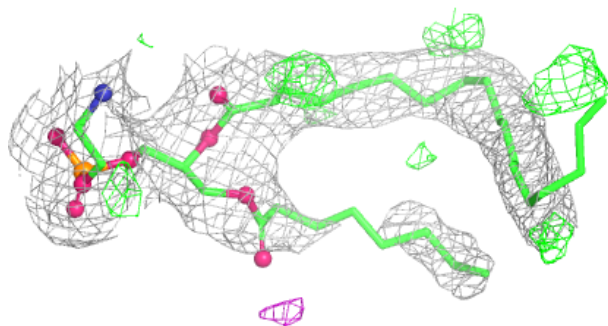
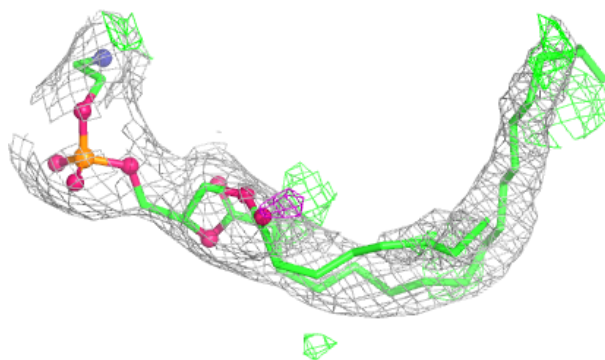
**Electron density around CDL D 503:**

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

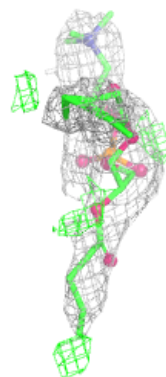
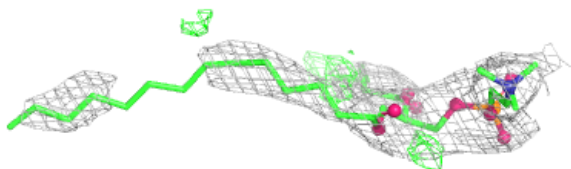
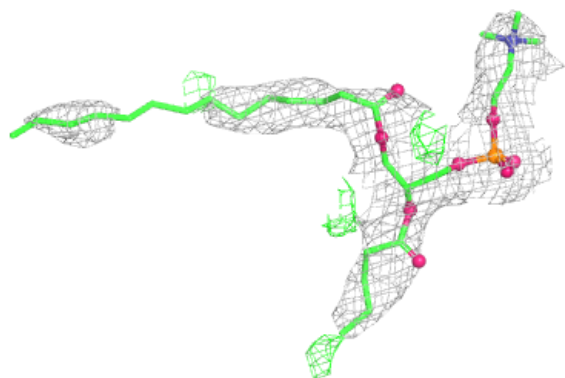


Electron density around PEE E 203:

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

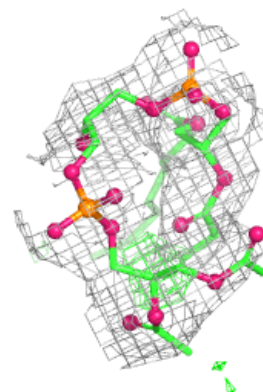
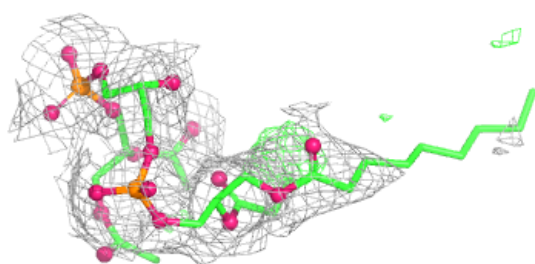
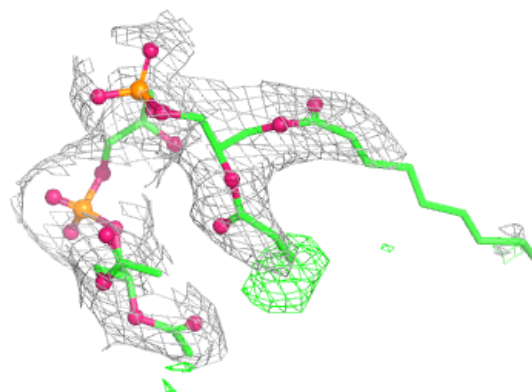
**Electron density around PX4 E 202:**

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

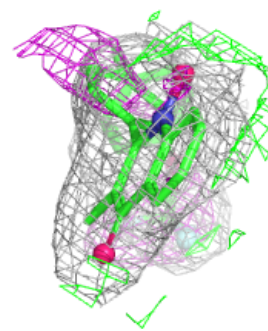
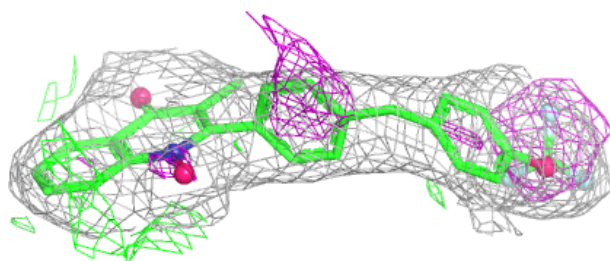
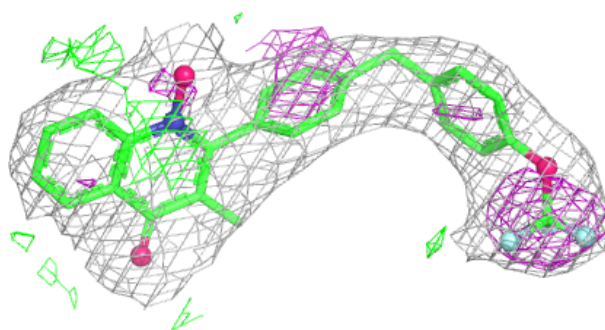


Electron density around CDL C 406:

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

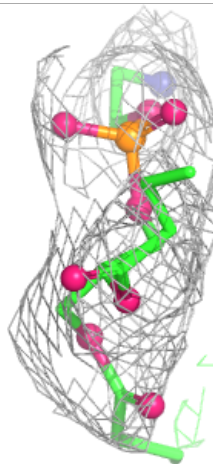
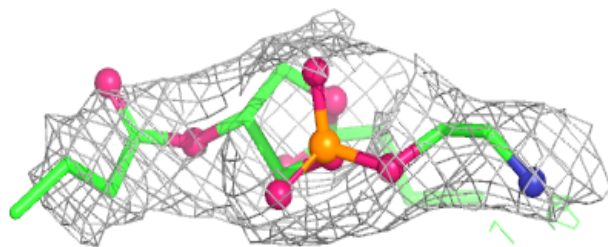
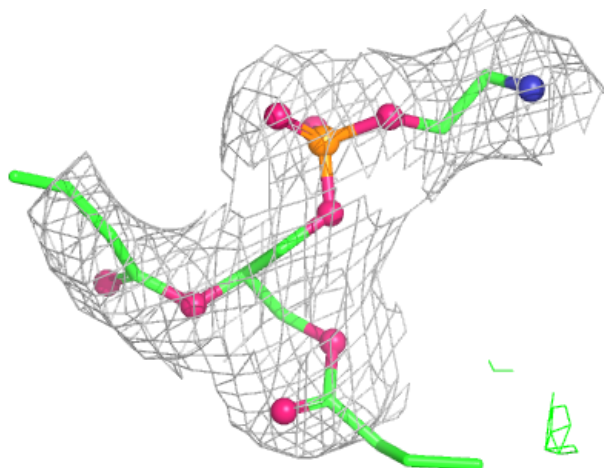
**Electron density around JHE C 408:**

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



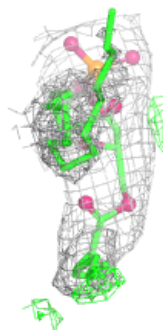
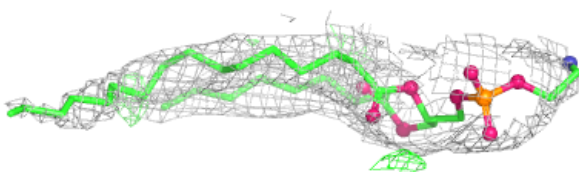
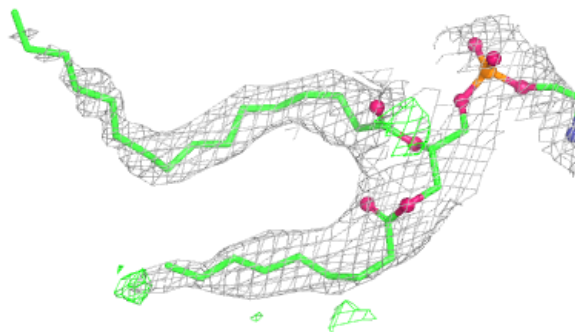
Electron density around 6PE A 502:

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



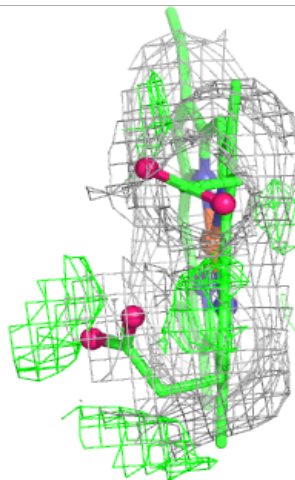
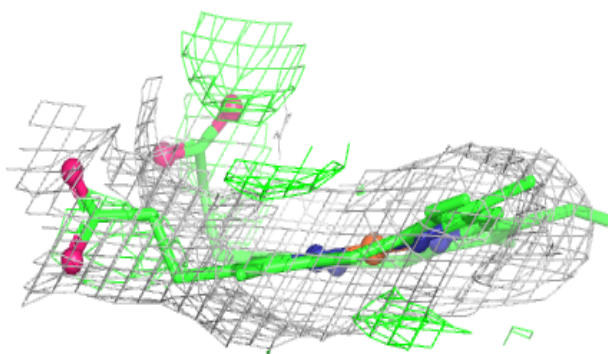
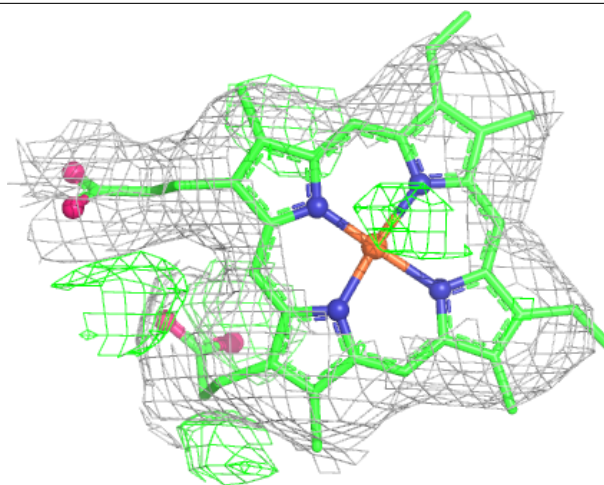
Electron density around PEE C 407:

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



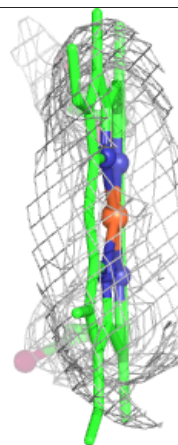
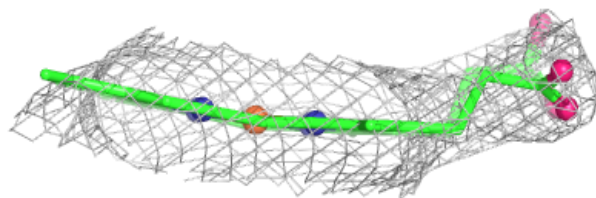
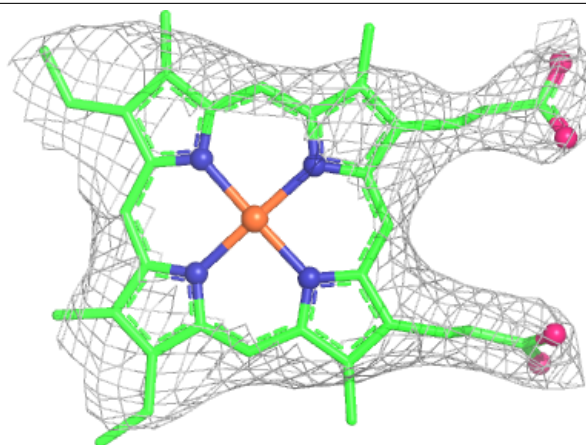
Electron density around HEM C 402:

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



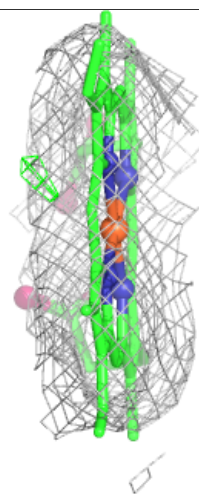
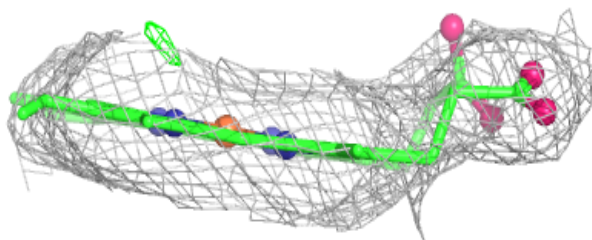
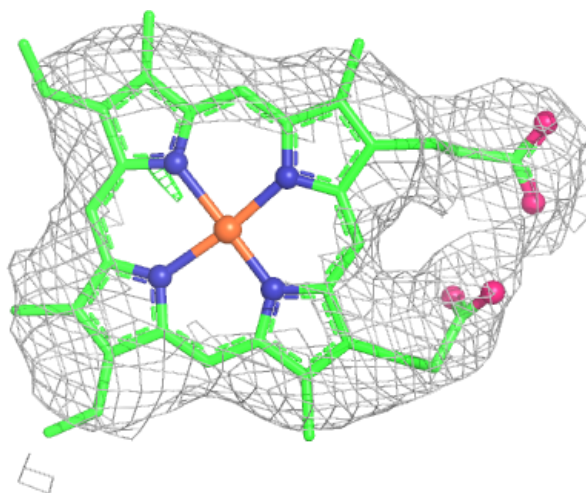
Electron density around HEC D 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.