



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:49 PM UTC

PDB ID : 6ZFS / pdb_00006zfs
Title : Crystal structure of bovine cytochrome bc1 in complex with quinolone inhibitor WDH-1U-4
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:

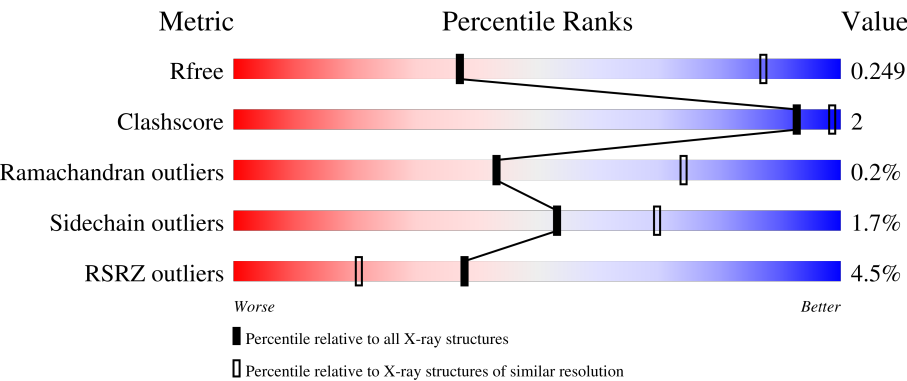
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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 $\leq 5\%$. 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	95%
2	B	420	% 95%
3	C	378	4% 94% 5%
4	D	239	9% 93% 6%

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Mol	Chain	Length	Quality of chain
5	E	196	
6	F	99	
7	G	75	
8	H	64	
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
17	PEE	C	406	X	-	-	-
17	PEE	E	204	X	-	-	-
18	JGW	C	407	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 16241 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	441	Total	C	N	O	S	0	0	0
			3365	2100	599	646	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
			3116	1957	553	599	7			

- Molecule 3 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1849	1181	319	334	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	195	Total	C	N	O	S	0	0	0
			1495	937	261	289	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	75	Total	C	N	O	S	0	0	0
			624	408	117	98	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			510	307	94	104	5			

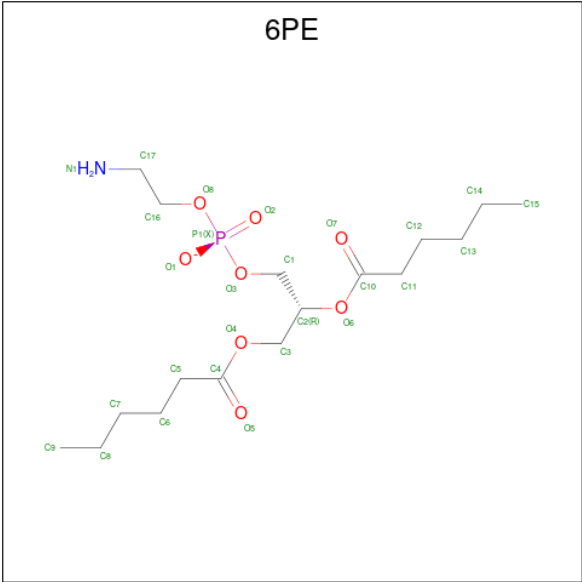
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			325	200	60	64	1			

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

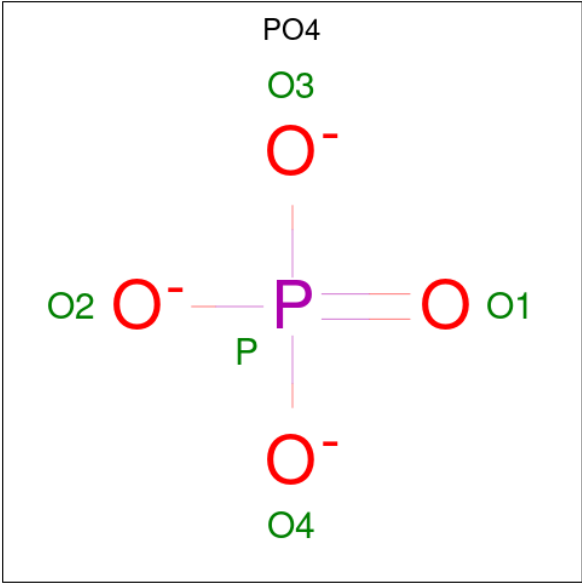
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			478	314	81	83			

- Molecule 11 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: 6PE) (formula: C₁₇H₃₃NO₈P).



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

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



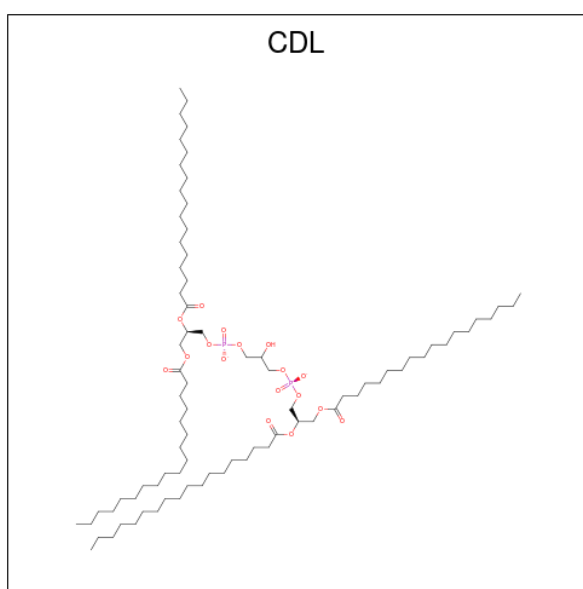
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	E	1	Total	O	P	0	0
			5	4	1		

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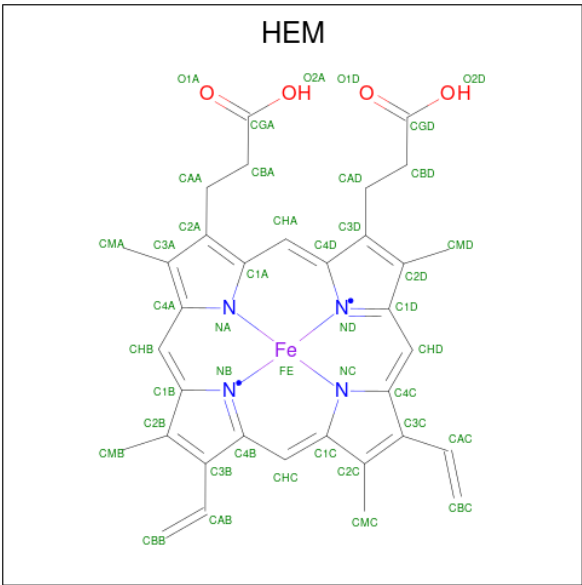
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	F	1	Total	O	P	0	0
			5	4	1		
12	G	1	Total	O	P	0	0
			5	4	1		
12	G	1	Total	O	P	0	0
			5	4	1		
12	G	1	Total	O	P	0	0
			5	4	1		

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



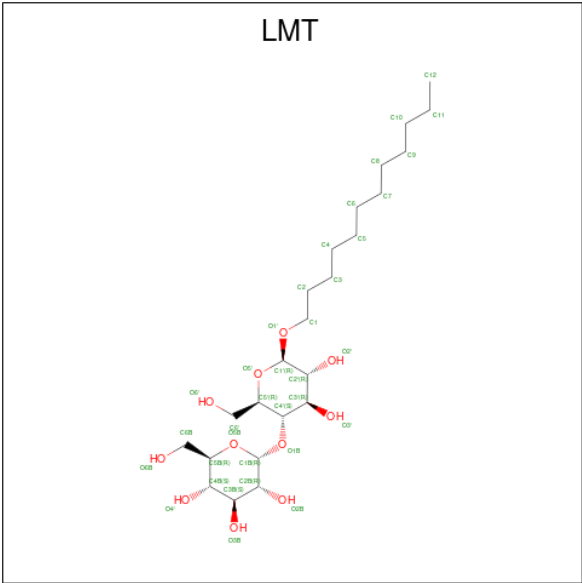
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			34	17	15	2		
13	C	1	Total	C	O	P	0	0
			44	25	17	2		
13	D	1	Total	C	O	P	0	0
			54	35	17	2		
13	E	1	Total	C	O	P	0	0
			48	30	16	2		
13	G	1	Total	C	O	P	0	0
			23	9	12	2		

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



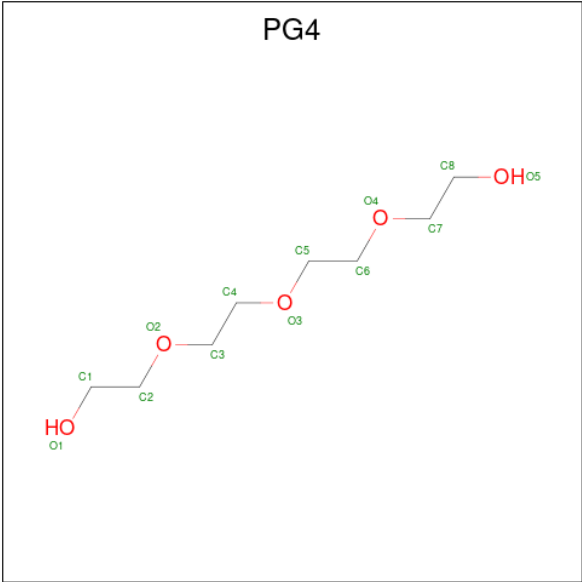
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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



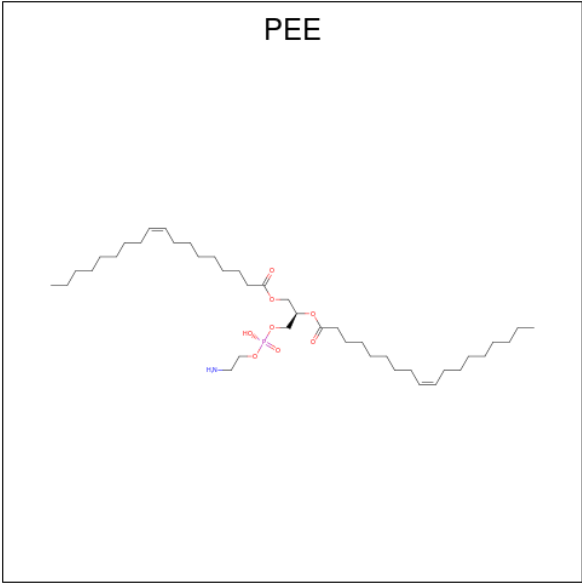
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O		
			35	24	11	0	0

- Molecule 16 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



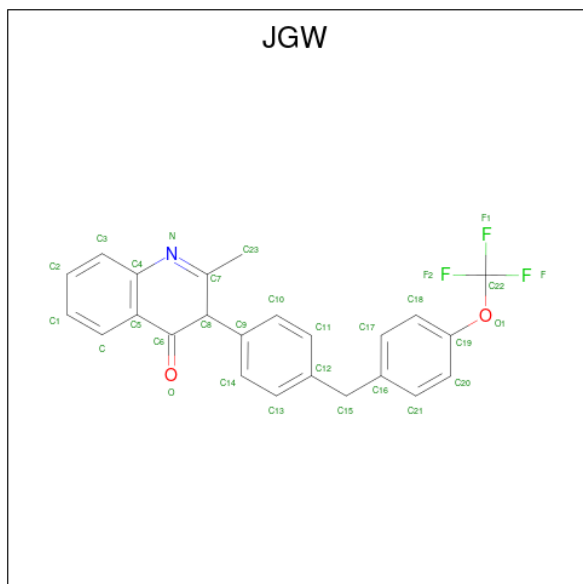
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			13	8	5		

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



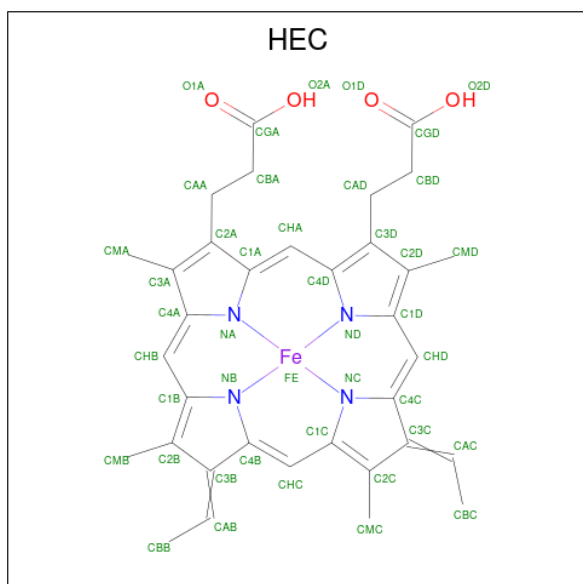
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
17	E	1	Total	C	N	O	P	0	0
			39	29	1	8	1		

- Molecule 18 is 2-methyl-3-[4-[[4-(trifluoromethoxy)phenyl]methyl]phenyl]-3 {H}-quinolin-4-one (CCD ID: JGW) (formula: $C_{24}H_{18}F_3NO_2$) (labeled as "Ligand of Interest" by depositor).



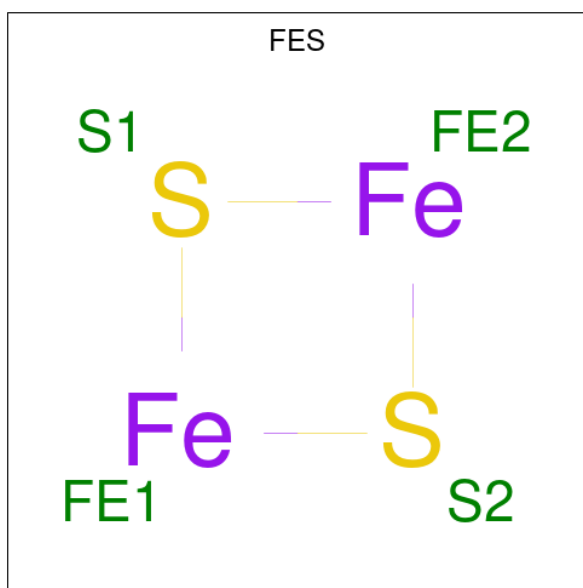
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	F	N	O	0	0
			30	24	3	1	2		

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



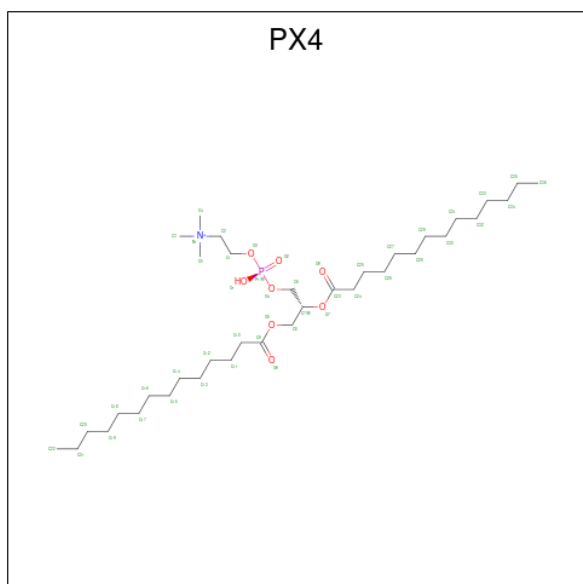
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 21 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: $\text{C}_{36}\text{H}_{73}\text{NO}_8\text{P}$).



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

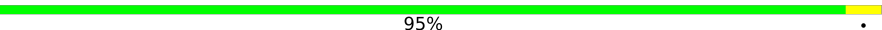
- Molecule 22 is water.

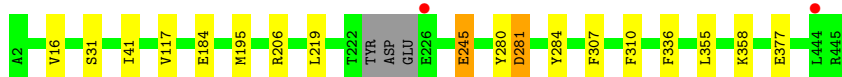
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	10	Total O 10 10	0	0
22	B	5	Total O 5 5	0	0
22	C	8	Total O 8 8	0	0
22	D	3	Total O 3 3	0	0
22	E	4	Total O 4 4	0	0
22	F	4	Total O 4 4	0	0
22	G	1	Total O 1 1	0	0
22	J	1	Total O 1 1	0	0

3 Residue-property plots

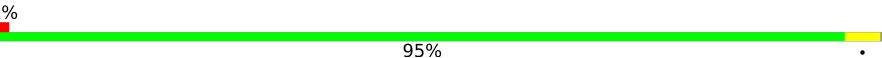
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 

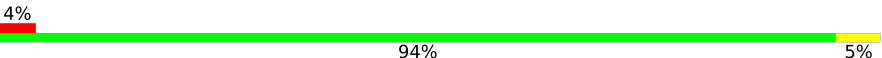


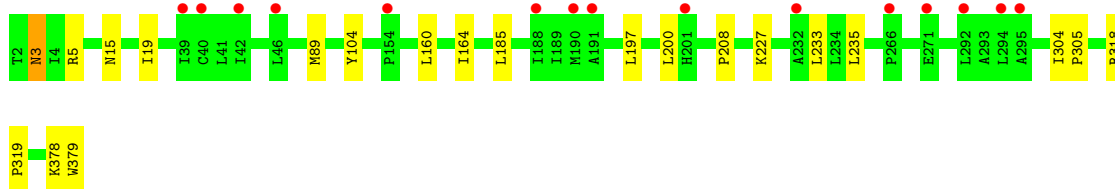
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 

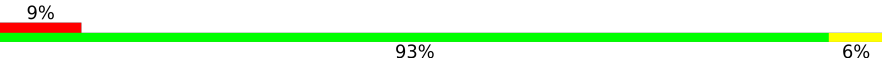


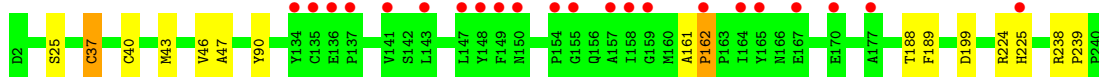
- Molecule 3: Cytochrome b

Chain C: 

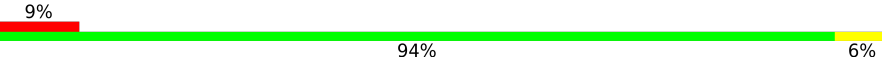


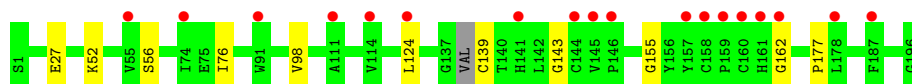
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 

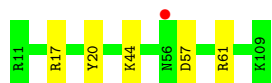


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 



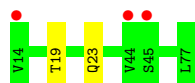
- Molecule 6: Cytochrome b-c1 complex subunit 7



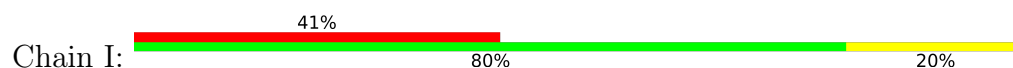
- Molecule 7: Cytochrome b-c1 complex subunit 8



- 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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	209.56Å 209.56Å 343.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.74 – 3.50 90.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (90.74-3.50) 97.0 (90.74-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.217 , 0.246 0.221 , 0.249	Depositor DCC
R_{free} test set	2800 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	87.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 112.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16241	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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

5.1 Standard geometry

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

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	0.58	0/3435	1.01	0/4663
2	B	0.57	0/3173	0.98	2/4304 (0.0%)
3	C	0.58	0/3092	1.03	2/4231 (0.0%)
4	D	0.63	1/1908 (0.1%)	1.05	3/2597 (0.1%)
5	E	0.67	0/1527	1.00	1/2064 (0.0%)
6	F	0.55	0/878	1.02	0/1181
7	G	0.66	0/645	1.03	0/873
8	H	0.55	0/515	1.04	0/694
9	I	0.96	1/329 (0.3%)	1.18	1/449 (0.2%)
10	J	0.61	0/491	1.04	0/664
All	All	0.61	2/15993 (0.0%)	1.02	9/21720 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	239	PRO	CA-C	5.81	1.56	1.52
9	I	62	ARG	CA-C	5.38	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	162	PRO	N-CA-C	-8.06	100.87	110.70
5	E	177	PRO	CB-CA-C	-7.23	99.64	111.56
4	D	162	PRO	CB-CA-C	6.80	119.22	110.92
3	C	318	ARG	CA-C-N	5.92	125.40	119.24
3	C	318	ARG	C-N-CA	5.92	125.40	119.24
9	I	69	SER	N-CA-C	5.55	115.61	108.34
4	D	239	PRO	O-C-N	5.35	123.67	121.15
2	B	129	ALA	N-CA-C	5.16	116.98	109.30
2	B	170	ASN	N-CA-C	5.03	121.51	110.80

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	3365	0	3217	9	0
2	B	3116	0	3089	5	0
3	C	2996	0	3058	11	0
4	D	1849	0	1732	13	0
5	E	1495	0	1458	2	0
6	F	859	0	838	3	0
7	G	624	0	630	5	0
8	H	510	0	467	1	0
9	I	325	0	325	3	0
10	J	478	0	467	1	0
11	A	23	0	19	0	0
12	A	5	0	0	0	0
12	D	5	0	0	0	0
12	E	5	0	0	0	0
12	F	5	0	0	0	0
12	G	15	0	0	0	0
13	A	34	0	24	0	0
13	C	44	0	32	0	0
13	D	54	0	52	0	0
13	E	48	0	46	0	0
13	G	23	0	13	0	0
14	C	86	0	60	5	0
15	C	35	0	46	0	0
16	C	13	0	18	0	0
17	C	40	0	54	0	0
17	E	39	0	55	0	0
18	C	30	0	0	0	0
19	D	43	0	32	5	0
20	E	4	0	0	0	0
21	E	37	0	51	1	0
22	A	10	0	0	0	0
22	B	5	0	0	0	0
22	C	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D	3	0	0	0	0
22	E	4	0	0	0	0
22	F	4	0	0	0	0
22	G	1	0	0	0	0
22	J	1	0	0	0	0
All	All	16241	0	15783	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:37:CYS:SG	19:D:501:HEC:CAB	2.36	1.13
4:D:37:CYS:SG	19:D:501:HEC:CBB	2.57	0.93
4:D:37:CYS:SG	19:D:501:HEC:HBB3	2.11	0.90
14:C:401:HEM:HMC1	14:C:401:HEM:HBC2	1.79	0.64
4:D:37:CYS:SG	19:D:501:HEC:C3B	2.88	0.62
2:B:163:LEU:HD11	2:B:258:VAL:HG22	1.84	0.60
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.42	0.55
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.44	0.53
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.89	0.53
1:A:336:PHE:CZ	3:C:3:ASN:HB3	2.45	0.51
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.94	0.50
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.93	0.49
4:D:40:CYS:SG	19:D:501:HEC:HBC3	2.52	0.48
14:C:401:HEM:HMB1	14:C:401:HEM:HBB2	1.95	0.48
3:C:197:LEU:HD21	14:C:402:HEM:HMA3	1.96	0.48
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.48
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.49	0.47
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.49	0.47
8:H:19:THR:HG22	8:H:23:GLN:HE21	1.80	0.47
1:A:41:ILE:HG12	1:A:195:MET:HG2	1.96	0.46
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.51	0.46
4:D:224:ARG:HH21	7:G:26:PHE:HA	1.80	0.45
3:C:200:LEU:CD2	14:C:402:HEM:HAA1	2.46	0.45
4:D:161:ALA:O	4:D:162:PRO:C	2.59	0.45
3:C:378:LYS:HE3	6:F:17:ARG:HD3	1.98	0.45
1:A:355:LEU:HA	1:A:358:LYS:HD3	1.98	0.44
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.98	0.44
7:G:26:PHE:HB3	7:G:29:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:304:ILE:HB	3:C:305:PRO:HD3	1.99	0.44
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.99	0.43
2:B:101:THR:C	2:B:176:LEU:HD21	2.43	0.43
14:C:401:HEM:HBB2	14:C:401:HEM:CMB	2.49	0.43
3:C:319:PRO:HD2	6:F:20:TYR:CE2	2.53	0.43
2:B:369:LEU:HD11	2:B:399:LEU:HD11	2.01	0.43
21:E:202:PX4:H12	10:J:17:THR:HG23	2.01	0.43
1:A:245:GLU:O	1:A:245:GLU:HG3	2.19	0.42
4:D:238:ARG:HG3	7:G:14:ILE:HD12	2.01	0.42
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.00	0.42
4:D:43:MET:HE3	4:D:46:VAL:HG21	2.00	0.42
3:C:15:ASN:HA	3:C:19:ILE:HD12	2.02	0.42
3:C:5:ARG:HE	3:C:15:ASN:ND2	2.18	0.42
3:C:89:MET:HE2	3:C:235:LEU:HD12	2.01	0.41
5:E:52:LYS:O	5:E:56:SER:HB2	2.20	0.41
1:A:281:ASP:OD1	1:A:281:ASP:C	2.63	0.41
1:A:310:PHE:CD1	1:A:310:PHE:C	2.98	0.41
4:D:25:SER:HB3	4:D:188:THR:HG21	2.03	0.41
6:F:57:ASP:HB3	6:F:61:ARG:HH12	1.86	0.41
3:C:160:LEU:O	3:C:164:ILE:HG12	2.21	0.40
9:I:42:VAL:HG12	9:I:43:LEU:HG	2.04	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	437/444 (98%)	419 (96%)	18 (4%)	0	100	100
2	B	411/420 (98%)	398 (97%)	13 (3%)	0	100	100
3	C	376/378 (100%)	363 (96%)	13 (4%)	0	100	100
4	D	237/239 (99%)	226 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	191/196 (97%)	179 (94%)	9 (5%)	3 (2%)	7	36
6	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
7	G	73/75 (97%)	73 (100%)	0	0	100	100
8	H	62/64 (97%)	57 (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	1985/2020 (98%)	1909 (96%)	72 (4%)	4 (0%)	43	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	162	GLY
9	I	41	PRO
5	E	155	GLY
5	E	143	GLY

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	350/369 (95%)	342 (98%)	8 (2%)	44	64
2	B	325/329 (99%)	320 (98%)	5 (2%)	57	71
3	C	325/326 (100%)	320 (98%)	5 (2%)	57	71
4	D	187/204 (92%)	185 (99%)	2 (1%)	65	74
5	E	163/168 (97%)	160 (98%)	3 (2%)	51	69
6	F	88/91 (97%)	87 (99%)	1 (1%)	65	74
7	G	65/66 (98%)	64 (98%)	1 (2%)	57	71
8	H	56/61 (92%)	56 (100%)	0	100	100
9	I	35/38 (92%)	33 (94%)	2 (6%)	18	45
10	J	47/49 (96%)	46 (98%)	1 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1641/1701 (96%)	1613 (98%)	28 (2%)	53 70

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

Mol	Chain	Res	Type
1	A	16	VAL
1	A	31	SER
1	A	184	GLU
1	A	206	ARG
1	A	219	LEU
1	A	245	GLU
1	A	281	ASP
1	A	377	GLU
2	B	74	SER
2	B	108	THR
2	B	126	VAL
2	B	264	ILE
2	B	294	SER
3	C	3	ASN
3	C	185	LEU
3	C	227	LYS
3	C	233	LEU
3	C	379	TRP
4	D	37	CYS
4	D	199	ASP
5	E	27	GLU
5	E	124	LEU
5	E	139	CYS
6	F	44	LYS
7	G	18	LEU
9	I	65	VAL
9	I	78	TYR
10	J	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	165	GLN
1	A	213	GLN
1	A	240	GLN

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	271	GLN
1	A	311	ASN
1	A	328	HIS
1	A	339	GLN
2	B	158	HIS
2	B	290	ASN
2	B	400	GLN
2	B	401	GLN
2	B	412	ASN
3	C	3	ASN
3	C	15	ASN
3	C	54	HIS
3	C	159	ASN
3	C	345	HIS
4	D	6	HIS
4	D	105	ASN
4	D	121	HIS
4	D	181	GLN
4	D	225	HIS
5	E	108	GLN
5	E	122	HIS
6	F	38	HIS
6	F	79	GLN
7	G	12	HIS
8	H	23	GLN
8	H	67	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

23 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
17	PEE	E	204	-	38,38,50	1.33	3 (7%)	41,43,55	1.13	2 (4%)
21	PX4	E	202	-	36,36,45	1.35	2 (5%)	42,44,53	1.20	4 (9%)
12	PO4	G	103	-	4,4,4	0.87	0	6,6,6	0.50	0
12	PO4	G	102	-	4,4,4	0.95	0	6,6,6	0.49	0
12	PO4	D	502	-	4,4,4	0.95	0	6,6,6	0.45	0
15	LMT	C	403	-	36,36,36	0.63	0	47,47,47	0.99	2 (4%)
14	HEM	C	402	3	50,50,50	1.53	9 (18%)	67,82,82	1.25	7 (10%)
18	JGW	C	407	-	32,33,33	1.76	5 (15%)	44,48,48	1.75	5 (11%)
19	HEC	D	501	4	46,50,50	2.68	24 (52%)	58,82,82	2.19	19 (32%)
11	6PE	A	501	-	22,22,26	1.52	2 (9%)	25,27,31	1.31	2 (8%)
12	PO4	F	501	-	4,4,4	1.00	0	6,6,6	0.50	0
12	PO4	E	203	-	4,4,4	0.91	0	6,6,6	0.75	0
12	PO4	G	104	-	4,4,4	0.94	0	6,6,6	0.59	0
16	PG4	C	404	-	12,12,12	0.53	0	11,11,11	0.47	0
17	PEE	C	406	-	39,39,50	1.28	3 (7%)	42,44,55	1.19	3 (7%)
13	CDL	C	405	-	43,43,99	1.55	4 (9%)	49,55,111	1.34	6 (12%)
13	CDL	G	101	-	22,22,99	1.23	1 (4%)	25,30,111	0.98	2 (8%)
13	CDL	A	503	-	33,33,99	1.25	2 (6%)	37,43,111	1.25	3 (8%)
13	CDL	D	503	-	53,53,99	1.35	4 (7%)	59,65,111	1.17	5 (8%)
13	CDL	E	205	-	47,47,99	1.15	3 (6%)	52,58,111	1.18	5 (9%)
14	HEM	C	401	3	50,50,50	1.54	7 (14%)	67,82,82	1.38	9 (13%)
12	PO4	A	502	-	4,4,4	1.03	0	6,6,6	0.40	0
20	FES	E	201	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	JGW	C	407	-	1/1/4/4	3/13/29/29	0/3/4/4
17	PEE	E	204	-	1/1/4/8	23/42/42/54	-
17	PEE	C	406	-	1/1/4/8	15/43/43/54	-
14	HEM	C	402	3	-	4/14/54/54	-
13	CDL	C	405	-	-	17/52/52/110	-
21	PX4	E	202	-	-	20/40/40/49	-
13	CDL	G	101	-	-	13/25/25/110	-
13	CDL	A	503	-	-	14/41/41/110	-
19	HEC	D	501	4	-	4/14/54/54	-
11	6PE	A	501	-	-	11/26/26/30	-
13	CDL	D	503	-	-	25/63/63/110	-
13	CDL	E	205	-	-	33/55/55/110	-
14	HEM	C	401	3	-	5/14/54/54	-
16	PG4	C	404	-	-	5/10/10/10	-
20	FES	E	201	5	-	-	0/1/1/1
15	LMT	C	403	-	-	8/21/61/61	0/2/2/2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	407	JGW	C5-C4	7.63	1.50	1.40
13	C	405	CDL	OA6-CA5	5.65	1.47	1.35
13	C	405	CDL	OB6-CB5	5.33	1.49	1.34
14	C	402	HEM	FE-NB	5.31	2.11	1.94
14	C	401	HEM	FE-NB	5.23	2.11	1.94
19	D	501	HEC	C2A-C3A	5.21	1.48	1.36
13	D	503	CDL	OA8-CA7	5.18	1.48	1.33
13	D	503	CDL	OB6-CB5	4.96	1.48	1.34
19	D	501	HEC	CHC-C4B	4.95	1.48	1.38
11	A	501	6PE	O6-C10	4.92	1.48	1.34
13	G	101	CDL	OB8-CB7	4.91	1.47	1.33
21	E	202	PX4	O7-C23	4.90	1.48	1.34
19	D	501	HEC	CHB-C4A	4.84	1.47	1.38
21	E	202	PX4	O5-C9	4.77	1.47	1.33
19	D	501	HEC	CHD-C4C	4.76	1.47	1.38
17	E	204	PEE	O2-C10	4.71	1.47	1.34
19	D	501	HEC	CAC-C3C	4.67	1.50	1.35
13	A	503	CDL	OB8-CB7	4.67	1.47	1.33
19	D	501	HEC	CAB-C3B	4.66	1.50	1.35
13	E	205	CDL	OB6-CB5	4.62	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	405	CDL	OB8-CB7	4.61	1.46	1.33
19	D	501	HEC	CHA-C1A	4.58	1.47	1.38
17	C	406	PEE	O3-C30	4.54	1.46	1.33
13	D	503	CDL	OA6-CA5	4.45	1.46	1.34
11	A	501	6PE	O4-C4	4.42	1.46	1.33
17	E	204	PEE	O3-C30	4.35	1.46	1.33
13	E	205	CDL	OA8-CA7	4.29	1.45	1.33
17	C	406	PEE	O2-C10	4.26	1.46	1.34
19	D	501	HEC	CHC-C1C	4.15	1.48	1.39
13	A	503	CDL	OB6-CB5	4.14	1.46	1.34
14	C	401	HEM	FE-NC	3.99	2.08	1.95
17	C	406	PEE	C18-C19	3.92	1.53	1.31
14	C	402	HEM	FE-NC	3.91	2.08	1.95
17	E	204	PEE	C18-C19	3.89	1.53	1.31
19	D	501	HEC	CHD-C1D	3.81	1.48	1.39
19	D	501	HEC	CHB-C1B	3.42	1.47	1.39
19	D	501	HEC	C3D-C2D	3.40	1.47	1.38
19	D	501	HEC	CHA-C4D	3.37	1.47	1.39
19	D	501	HEC	C1C-C2C	3.15	1.50	1.43
14	C	401	HEM	C1B-NB	-2.94	1.35	1.40
19	D	501	HEC	C1D-C2D	2.93	1.50	1.43
14	C	402	HEM	C1B-NB	-2.91	1.35	1.40
13	E	205	CDL	OB8-CB7	2.86	1.47	1.33
13	C	405	CDL	OA8-CA7	2.81	1.46	1.33
14	C	401	HEM	C3B-C4B	2.68	1.50	1.44
13	D	503	CDL	OB8-CB7	2.66	1.46	1.33
14	C	401	HEM	C4D-ND	-2.62	1.35	1.40
18	C	407	JGW	O1-C22	2.58	1.45	1.31
14	C	402	HEM	C4B-NB	-2.57	1.33	1.38
18	C	407	JGW	C9-C8	-2.55	1.50	1.53
14	C	402	HEM	C4D-ND	-2.55	1.35	1.40
19	D	501	HEC	C4B-NB	-2.50	1.34	1.39
19	D	501	HEC	C4D-C3D	2.48	1.49	1.44
19	D	501	HEC	C1A-C2A	2.41	1.49	1.45
19	D	501	HEC	C1B-NB	-2.36	1.35	1.39
19	D	501	HEC	C4A-NA	-2.36	1.35	1.39
19	D	501	HEC	C1B-C2B	2.35	1.48	1.43
18	C	407	JGW	C4-N	-2.32	1.35	1.39
19	D	501	HEC	C3C-C2C	2.25	1.48	1.41
19	D	501	HEC	C4A-C3A	2.23	1.49	1.45
19	D	501	HEC	C1D-ND	-2.22	1.35	1.39
18	C	407	JGW	O-C6	2.13	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	401	HEM	C4D-C3D	2.13	1.48	1.45
14	C	401	HEM	C4B-NB	-2.12	1.34	1.38
14	C	402	HEM	C4D-C3D	2.09	1.48	1.45
14	C	402	HEM	C3B-C4B	2.08	1.49	1.44
14	C	402	HEM	C1C-C2C	-2.07	1.41	1.45
14	C	402	HEM	C1D-ND	-2.05	1.34	1.38
19	D	501	HEC	C1A-NA	-2.04	1.35	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	407	JGW	O-C6-C8	-8.39	122.66	126.92
19	D	501	HEC	C2A-C1A-NA	6.03	116.14	110.32
19	D	501	HEC	C3D-C4D-ND	6.00	116.81	110.15
13	A	503	CDL	OB6-CB5-C51	4.54	121.31	111.48
21	E	202	PX4	O7-C23-C24	4.48	121.18	111.48
13	C	405	CDL	OA6-CA5-C11	4.47	119.05	111.09
13	E	205	CDL	OB6-CB5-C51	4.32	120.84	111.48
11	A	501	6PE	O6-C10-C11	4.24	120.66	111.48
17	E	204	PEE	O2-C10-C11	4.22	120.61	111.48
18	C	407	JGW	C9-C8-C6	4.11	119.25	111.46
19	D	501	HEC	C2B-C1B-NB	4.04	116.61	110.14
13	D	503	CDL	OB6-CB5-C51	3.97	120.07	111.48
19	D	501	HEC	C1A-C2A-C3A	-3.91	101.96	107.11
14	C	402	HEM	CHC-C4B-NB	3.84	128.56	124.42
17	C	406	PEE	O3-C30-C31	3.79	123.40	111.83
14	C	401	HEM	CHC-C4B-NB	3.70	128.41	124.42
13	C	405	CDL	OB8-CB7-C71	3.62	122.86	111.83
13	D	503	CDL	OA8-CA7-C31	3.56	122.70	111.83
19	D	501	HEC	C2D-C1D-ND	3.43	115.64	110.14
19	D	501	HEC	C4D-C3D-C2D	-3.41	101.59	106.87
13	A	503	CDL	OB8-CB7-C71	3.34	121.30	111.15
19	D	501	HEC	C2C-C1C-NC	3.24	115.34	110.14
15	C	403	LMT	C1B-O5B-C5B	3.21	119.99	113.72
19	D	501	HEC	C1D-C2D-C3D	-3.18	103.17	106.82
19	D	501	HEC	C3A-C4A-NA	3.15	115.47	109.64
21	E	202	PX4	O5-C9-C10	3.15	121.43	111.83
14	C	401	HEM	CHD-C1D-ND	3.08	127.73	124.42
13	D	503	CDL	OA6-CA5-C11	3.02	118.01	111.48
17	C	406	PEE	O2-C10-C11	3.00	117.97	111.48
14	C	402	HEM	O2D-CGD-CBD	2.98	123.42	114.00
14	C	401	HEM	CHD-C4C-NC	2.94	127.66	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	405	CDL	CA6-OA8-CA7	2.92	124.29	117.08
13	E	205	CDL	CB6-OB8-CB7	2.86	124.15	117.08
13	D	503	CDL	OA8-CA7-OA9	-2.83	116.54	123.63
14	C	401	HEM	C1B-NB-C4B	2.83	108.56	105.21
13	E	205	CDL	OA8-CA7-C31	2.78	120.32	111.83
13	G	101	CDL	OB8-CB7-C71	2.77	119.56	111.15
14	C	401	HEM	CHB-C1B-NB	2.71	127.72	124.37
19	D	501	HEC	C4A-C3A-C2A	-2.69	102.99	106.97
21	E	202	PX4	O5-C9-O6	-2.68	116.93	123.63
17	E	204	PEE	O3-C30-C31	2.66	119.94	111.83
14	C	401	HEM	CHD-C1D-C2D	-2.62	120.88	125.03
19	D	501	HEC	CAD-C3D-C4D	2.60	130.01	124.94
18	C	407	JGW	C16-C15-C12	-2.58	104.92	113.76
13	C	405	CDL	OB8-CB7-OB9	-2.57	117.21	123.63
14	C	401	HEM	CHA-C4D-ND	2.56	127.54	124.37
11	A	501	6PE	O4-C4-C5	2.53	119.56	111.83
18	C	407	JGW	C23-C7-N	-2.46	116.18	119.71
19	D	501	HEC	CHB-C4A-NA	-2.42	121.82	124.45
17	C	406	PEE	C2-O2-C10	-2.39	112.08	117.80
14	C	402	HEM	CHD-C1D-ND	2.38	126.99	124.42
19	D	501	HEC	CHA-C1A-C2A	-2.38	121.11	124.86
14	C	402	HEM	C1B-NB-C4B	2.34	107.98	105.21
13	D	503	CDL	OB8-CB7-C71	2.34	122.30	112.38
13	C	405	CDL	OA8-CA7-C31	2.32	122.20	112.38
14	C	402	HEM	CHA-C4D-ND	2.31	127.23	124.37
21	E	202	PX4	O7-C23-O8	-2.29	118.34	123.70
13	A	503	CDL	OB6-CB5-OB7	-2.28	118.36	123.70
13	E	205	CDL	OA8-CA7-OA9	-2.24	118.02	123.63
13	G	101	CDL	OA4-PA1-OA3	2.23	119.51	110.83
19	D	501	HEC	CAA-CBA-CGA	-2.22	107.77	113.67
15	C	403	LMT	C2'-C3'-C4'	2.21	114.69	109.68
19	D	501	HEC	CMD-C2D-C1D	2.20	128.76	125.42
18	C	407	JGW	C11-C10-C9	-2.19	119.00	121.18
19	D	501	HEC	CMA-C3A-C4A	2.16	128.53	124.73
19	D	501	HEC	O2D-CGD-CBD	2.15	120.78	114.00
19	D	501	HEC	CHB-C1B-C2B	-2.14	121.22	127.43
13	E	205	CDL	OB8-CB7-C71	2.13	121.43	112.38
19	D	501	HEC	CMB-C2B-C3B	2.12	131.54	126.55
14	C	401	HEM	O2D-CGD-CBD	2.10	120.62	114.00
13	C	405	CDL	OB6-CB5-C51	2.05	118.46	110.93
14	C	402	HEM	O2D-CGD-O1D	-2.04	118.10	123.33
14	C	401	HEM	CHB-C1B-C2B	-2.02	121.21	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	402	HEM	CHA-C4D-C3D	-2.02	121.50	125.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	C	406	PEE	C2
17	E	204	PEE	C2
18	C	407	JGW	C8

All (200) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	6PE	C1-O3-P1-O1
11	A	501	6PE	C1-O3-P1-O8
11	A	501	6PE	C11-C10-O6-C2
11	A	501	6PE	O8-C16-C17-N1
13	A	503	CDL	CA3-OA5-PA1-OA2
13	A	503	CDL	CA3-OA5-PA1-OA3
13	A	503	CDL	CA3-OA5-PA1-OA4
13	A	503	CDL	C51-CB5-OB6-CB4
13	C	405	CDL	CA3-OA5-PA1-OA2
13	C	405	CDL	CA3-OA5-PA1-OA4
13	C	405	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	CB2-OB2-PB2-OB5
13	E	205	CDL	O1-C1-CB2-OB2
13	E	205	CDL	CA2-C1-CB2-OB2
13	E	205	CDL	C1-CA2-OA2-PA1
13	E	205	CDL	CA2-OA2-PA1-OA5
13	E	205	CDL	CB2-OB2-PB2-OB3
13	E	205	CDL	CB3-OB5-PB2-OB3
13	G	101	CDL	CA2-OA2-PA1-OA3
13	G	101	CDL	CA2-OA2-PA1-OA4
13	G	101	CDL	CA2-OA2-PA1-OA5
17	C	406	PEE	C4-O4P-P-O3P
17	C	406	PEE	C4-O4P-P-O2P
17	C	406	PEE	C4-O4P-P-O1P
17	E	204	PEE	C4-O4P-P-O1P
17	E	204	PEE	O4P-C4-C5-N
21	E	202	PX4	C24-C23-O7-C7
13	C	405	CDL	C11-CA5-OA6-CA4
13	E	205	CDL	CB4-CB6-OB8-CB7

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Mol	Chain	Res	Type	Atoms
21	E	202	PX4	O6-C9-O5-C8
13	A	503	CDL	OB7-CB5-OB6-CB4
13	C	405	CDL	OA7-CA5-OA6-CA4
13	D	503	CDL	C31-CA7-OA8-CA6
13	D	503	CDL	OB9-CB7-OB8-CB6
13	E	205	CDL	C71-CB7-OB8-CB6
17	C	406	PEE	C31-C30-O3-C3
13	D	503	CDL	C71-CB7-OB8-CB6
17	C	406	PEE	O5-C30-O3-C3
11	A	501	6PE	O7-C10-O6-C2
13	D	503	CDL	OB7-CB5-OB6-CB4
21	E	202	PX4	O8-C23-O7-C7
17	E	204	PEE	C31-C30-O3-C3
21	E	202	PX4	C10-C9-O5-C8
13	D	503	CDL	OA9-CA7-OA8-CA6
13	C	405	CDL	C31-CA7-OA8-CA6
13	D	503	CDL	C51-CB5-OB6-CB4
15	C	403	LMT	O5'-C5'-C6'-O6'
13	C	405	CDL	CB4-CB3-OB5-PB2
17	E	204	PEE	O5-C30-O3-C3
17	C	406	PEE	C17-C18-C19-C20
13	G	101	CDL	OB5-CB3-CB4-CB6
13	E	205	CDL	C31-CA7-OA8-CA6
13	G	101	CDL	CB3-CB4-CB6-OB8
13	E	205	CDL	O1-C1-CA2-OA2
13	G	101	CDL	O1-C1-CB2-OB2
13	D	503	CDL	OA5-CA3-CA4-OA6
13	D	503	CDL	CA5-C11-C12-C13
13	E	205	CDL	OB9-CB7-OB8-CB6
16	C	404	PG4	O2-C3-C4-O3
13	E	205	CDL	CB5-C51-C52-C53
21	E	202	PX4	C9-C10-C11-C12
13	C	405	CDL	OA9-CA7-OA8-CA6
13	A	503	CDL	OA5-CA3-CA4-OA6
13	G	101	CDL	OB5-CB3-CB4-OB6
13	E	205	CDL	OA9-CA7-OA8-CA6
15	C	403	LMT	C4'-C5'-C6'-O6'
13	E	205	CDL	OA6-CA4-CA6-OA8
13	G	101	CDL	OB6-CB4-CB6-OB8
13	A	503	CDL	CB5-C51-C52-C53
16	C	404	PG4	O4-C7-C8-O5
13	A	503	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
17	E	204	PEE	C10-C11-C12-C13
18	C	407	JGW	F-C22-O1-C19
13	E	205	CDL	CA3-CA4-CA6-OA8
15	C	403	LMT	C7-C8-C9-C10
17	C	406	PEE	C13-C14-C15-C16
17	C	406	PEE	C31-C32-C33-C34
11	A	501	6PE	C4-C5-C6-C7
13	E	205	CDL	C53-C54-C55-C56
13	E	205	CDL	CB2-C1-CA2-OA2
13	E	205	CDL	C33-C34-C35-C36
13	D	503	CDL	C51-C52-C53-C54
15	C	403	LMT	C11-C10-C9-C8
13	E	205	CDL	C51-C52-C53-C54
15	C	403	LMT	C3-C4-C5-C6
21	E	202	PX4	C18-C19-C20-C21
11	A	501	6PE	C5-C4-O4-C3
13	D	503	CDL	C11-C12-C13-C14
13	E	205	CDL	C35-C36-C37-C38
17	C	406	PEE	C14-C15-C16-C17
17	E	204	PEE	C13-C14-C15-C16
13	C	405	CDL	C51-CB5-OB6-CB4
17	E	204	PEE	C11-C10-O2-C2
17	C	406	PEE	C11-C12-C13-C14
17	E	204	PEE	O4-C10-O2-C2
13	E	205	CDL	C51-CB5-OB6-CB4
15	C	403	LMT	O5B-C5B-C6B-O6B
17	E	204	PEE	C23-C24-C25-C26
21	E	202	PX4	C13-C14-C15-C16
17	C	406	PEE	C10-C11-C12-C13
21	E	202	PX4	C17-C18-C19-C20
21	E	202	PX4	C12-C13-C14-C15
13	E	205	CDL	C32-C33-C34-C35
13	C	405	CDL	OB7-CB5-OB6-CB4
18	C	407	JGW	F1-C22-O1-C19
11	A	501	6PE	O5-C4-O4-C3
13	E	205	CDL	C52-C53-C54-C55
13	C	405	CDL	C71-CB7-OB8-CB6
13	D	503	CDL	OA5-CA3-CA4-CA6
13	C	405	CDL	CB7-C71-C72-C73
13	D	503	CDL	CA3-CA4-CA6-OA8
17	C	406	PEE	C32-C33-C34-C35
17	E	204	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	C	405	CDL	OB9-CB7-OB8-CB6
13	D	503	CDL	CB6-CB4-OB6-CB5
13	G	101	CDL	CA2-C1-CB2-OB2
21	E	202	PX4	C24-C25-C26-C27
13	E	205	CDL	C31-C32-C33-C34
17	E	204	PEE	O2-C2-C3-O3
21	E	202	PX4	C10-C11-C12-C13
17	E	204	PEE	C14-C15-C16-C17
11	A	501	6PE	C2-C1-O3-P1
13	A	503	CDL	OB5-CB3-CB4-CB6
13	D	503	CDL	OB5-CB3-CB4-CB6
17	C	406	PEE	O3P-C1-C2-C3
18	C	407	JGW	F2-C22-O1-C19
17	E	204	PEE	C24-C25-C26-C27
21	E	202	PX4	C16-C17-C18-C19
13	A	503	CDL	OB5-CB3-CB4-OB6
13	C	405	CDL	OB5-CB3-CB4-OB6
13	D	503	CDL	OB5-CB3-CB4-OB6
17	C	406	PEE	O3P-C1-C2-O2
21	E	202	PX4	C14-C15-C16-C17
11	A	501	6PE	O6-C2-C3-O4
13	D	503	CDL	OA6-CA4-CA6-OA8
13	D	503	CDL	C54-C55-C56-C57
15	C	403	LMT	C4-C5-C6-C7
17	E	204	PEE	C30-C31-C32-C33
13	E	205	CDL	C55-C56-C57-C58
17	E	204	PEE	C12-C13-C14-C15
17	E	204	PEE	O3P-C1-C2-C3
13	A	503	CDL	C51-C52-C53-C54
14	C	401	HEM	C3D-CAD-CBD-CGD
13	E	205	CDL	OB7-CB5-OB6-CB4
21	E	202	PX4	C23-C24-C25-C26
16	C	404	PG4	C6-C5-O3-C4
17	E	204	PEE	O3P-C1-C2-O2
16	C	404	PG4	C4-C3-O2-C2
17	E	204	PEE	C5-C4-O4P-P
17	C	406	PEE	C15-C16-C17-C18
16	C	404	PG4	C1-C2-O2-C3
21	E	202	PX4	O3-C1-C2-N1
13	A	503	CDL	O1-C1-CA2-OA2
13	G	101	CDL	C71-CB7-OB8-CB6
13	E	205	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
17	E	204	PEE	C16-C17-C18-C19
13	C	405	CDL	OB5-CB3-CB4-CB6
13	E	205	CDL	C36-C37-C38-C39
13	D	503	CDL	C31-C32-C33-C34
11	A	501	6PE	C1-C2-C3-O4
13	G	101	CDL	OB9-CB7-OB8-CB6
13	A	503	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	CB2-OB2-PB2-OB4
13	E	205	CDL	CA2-OA2-PA1-OA3
13	E	205	CDL	CB2-OB2-PB2-OB5
13	E	205	CDL	CB3-OB5-PB2-OB4
13	G	101	CDL	C1-CA2-OA2-PA1
13	C	405	CDL	C71-C72-C73-C74
21	E	202	PX4	C11-C12-C13-C14
15	C	403	LMT	C5-C6-C7-C8
14	C	401	HEM	CAA-CBA-CGA-O2A
13	A	503	CDL	CA4-CA3-OA5-PA1
14	C	401	HEM	CAA-CBA-CGA-O1A
17	E	204	PEE	C3-C2-O2-C10
14	C	402	HEM	CAA-CBA-CGA-O1A
14	C	402	HEM	CAA-CBA-CGA-O2A
13	D	503	CDL	C12-C13-C14-C15
17	E	204	PEE	C1-C2-C3-O3
19	D	501	HEC	CAA-CBA-CGA-O2A
14	C	401	HEM	CAD-CBD-CGD-O2D
21	E	202	PX4	O4-C6-C7-O7
14	C	401	HEM	CAD-CBD-CGD-O1D
13	D	503	CDL	OB6-CB4-CB6-OB8
17	E	204	PEE	C18-C19-C20-C21
21	E	202	PX4	C11-C10-C9-O5
19	D	501	HEC	CAA-CBA-CGA-O1A
13	G	101	CDL	C72-C71-CB7-OB8
17	E	204	PEE	C31-C32-C33-C34
21	E	202	PX4	C1-C2-N1-C4
13	E	205	CDL	CA7-C31-C32-C33
14	C	402	HEM	CAD-CBD-CGD-O1D
21	E	202	PX4	C11-C10-C9-O6
13	E	205	CDL	C32-C31-CA7-OA8
13	D	503	CDL	CB3-CB4-CB6-OB8
13	D	503	CDL	CB5-C51-C52-C53
19	D	501	HEC	CAD-CBD-CGD-O2D
13	C	405	CDL	O1-C1-CA2-OA2

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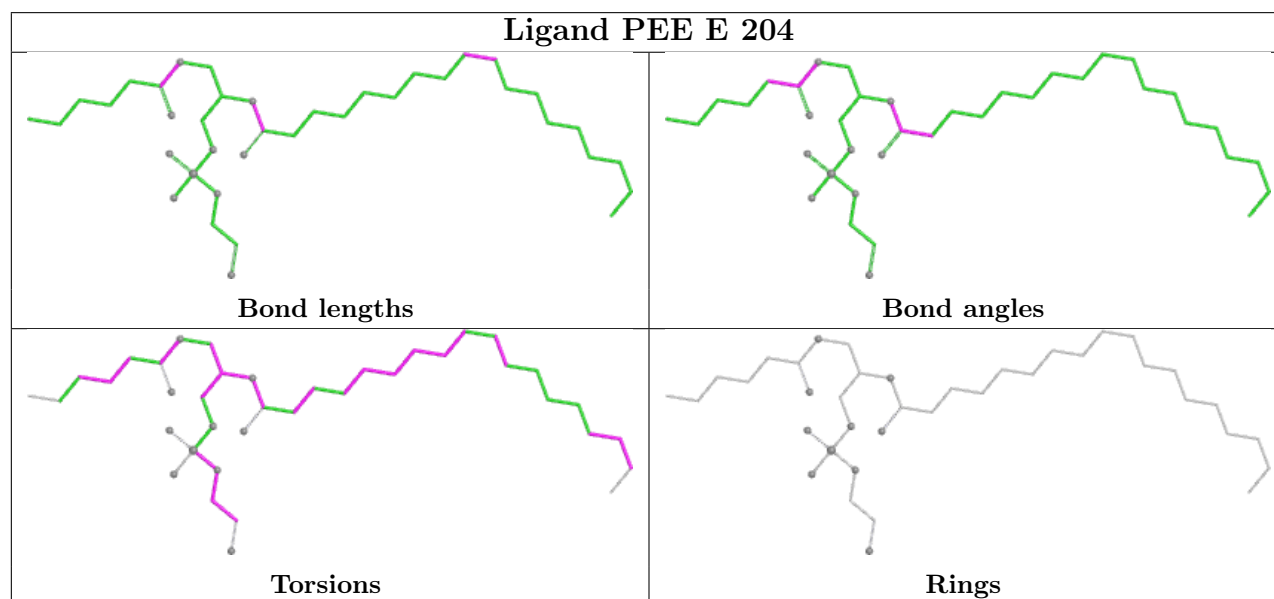
Mol	Chain	Res	Type	Atoms
14	C	402	HEM	CAD-CBD-CGD-O2D
19	D	501	HEC	CAD-CBD-CGD-O1D

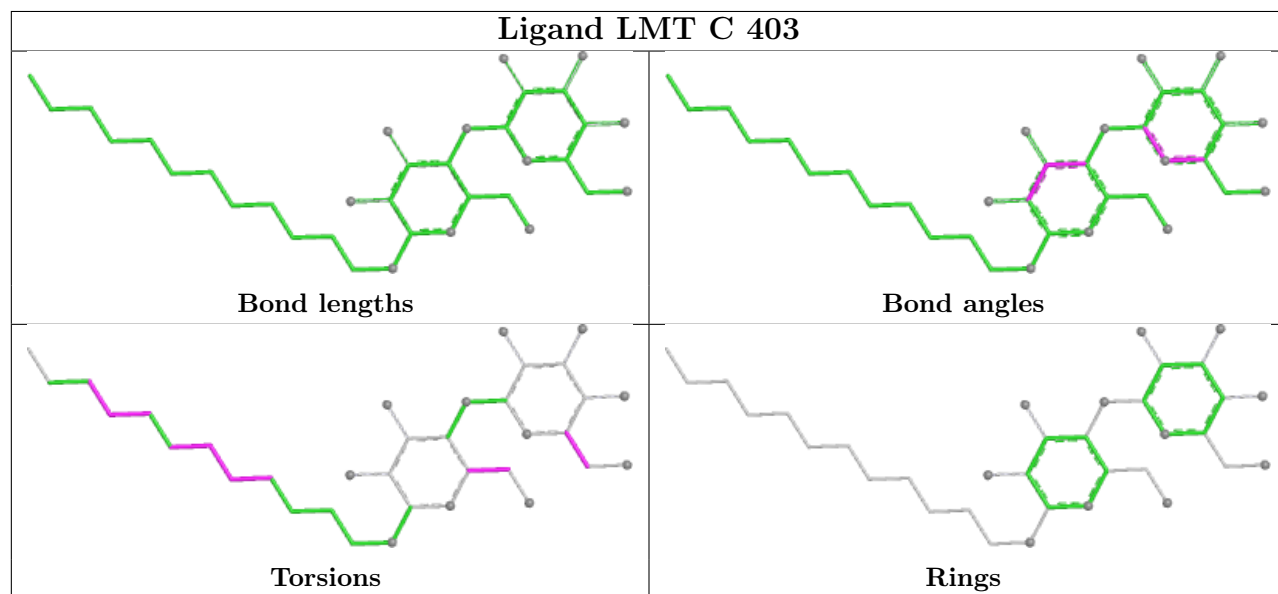
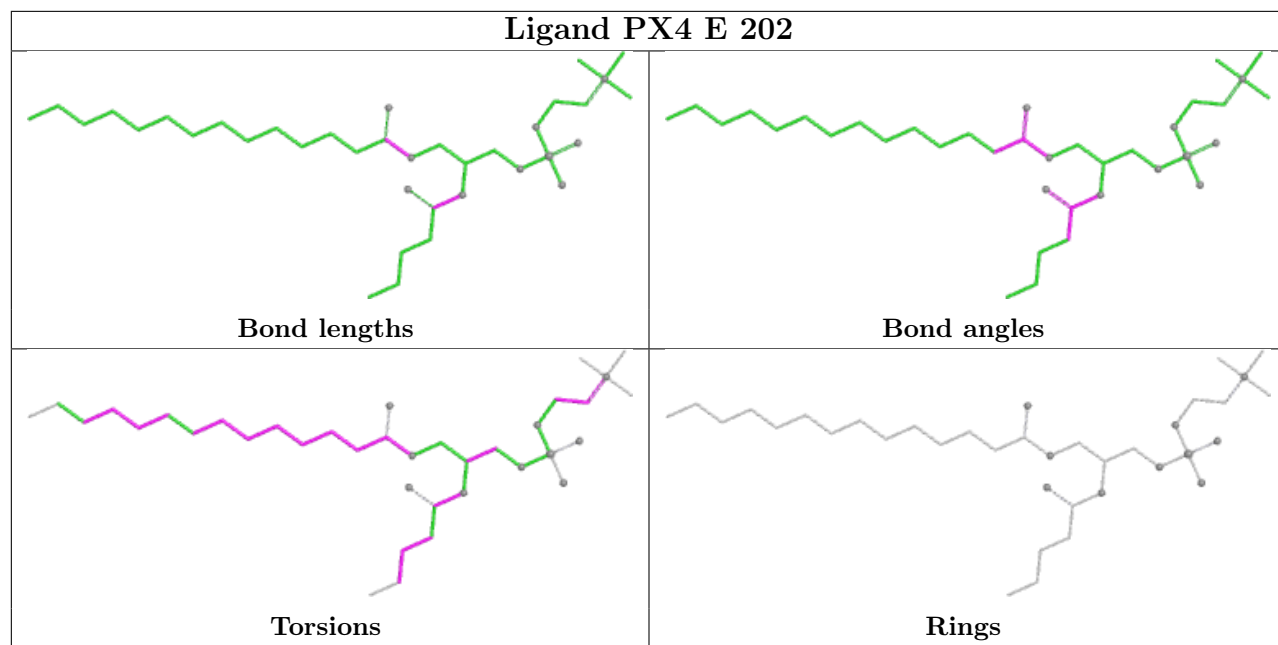
There are no ring outliers.

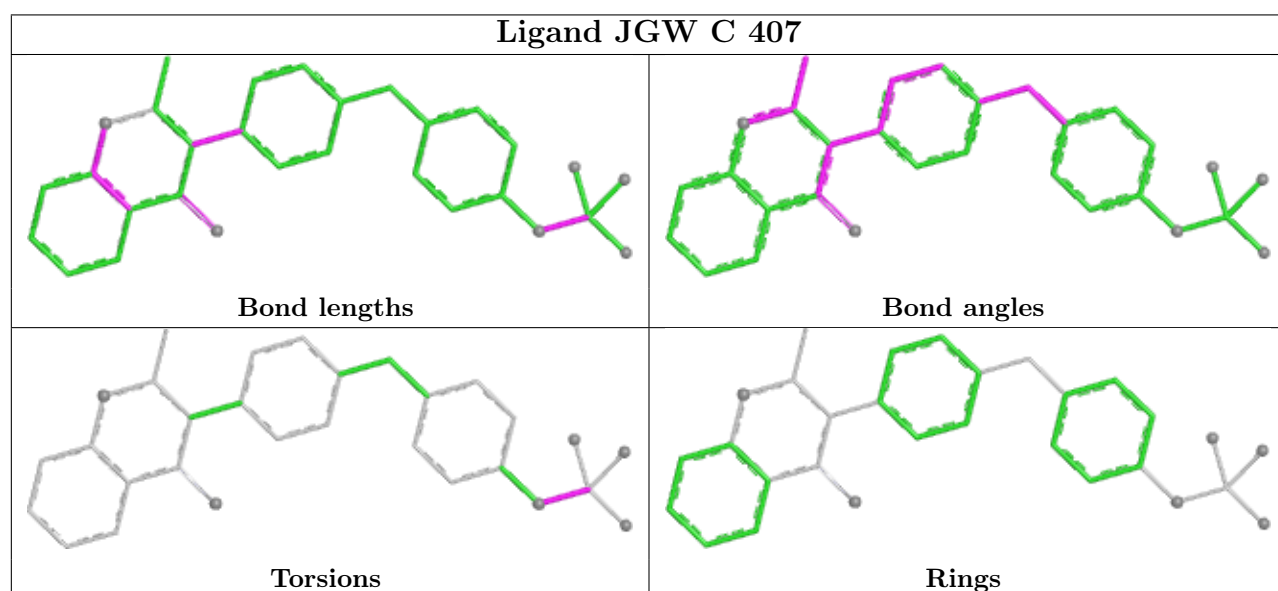
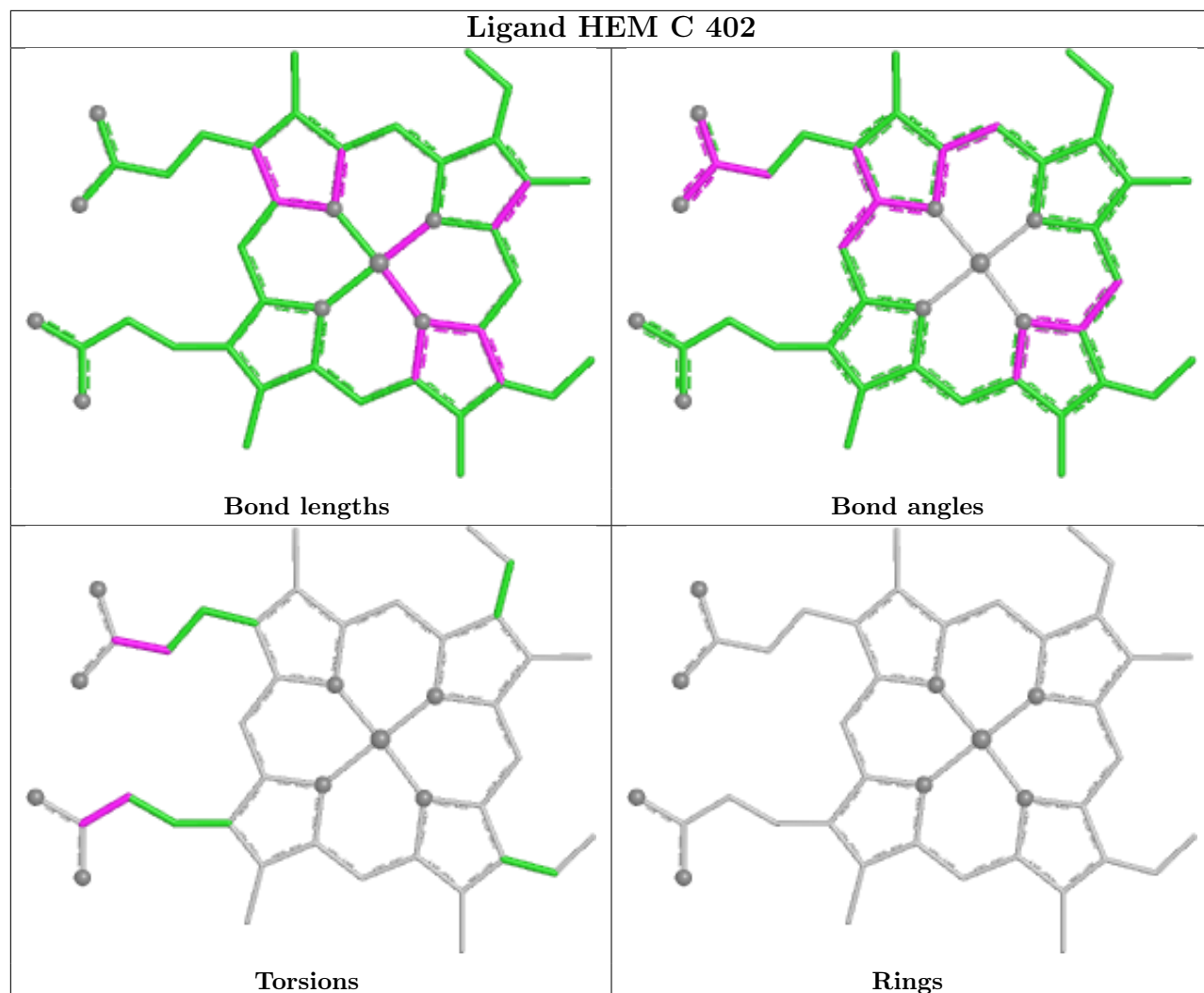
4 monomers are involved in 11 short contacts:

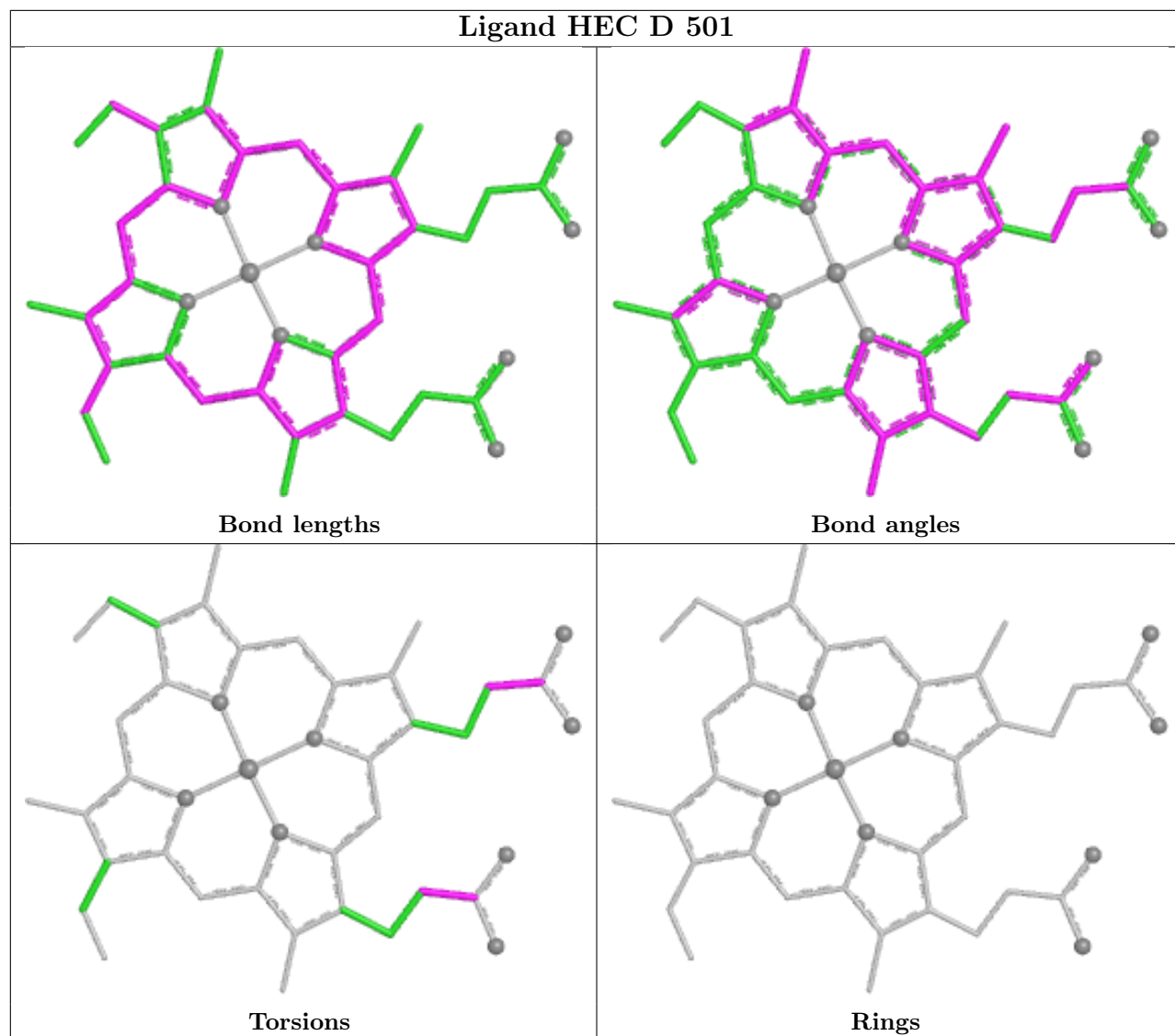
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	202	PX4	1	0
14	C	402	HEM	2	0
19	D	501	HEC	5	0
14	C	401	HEM	3	0

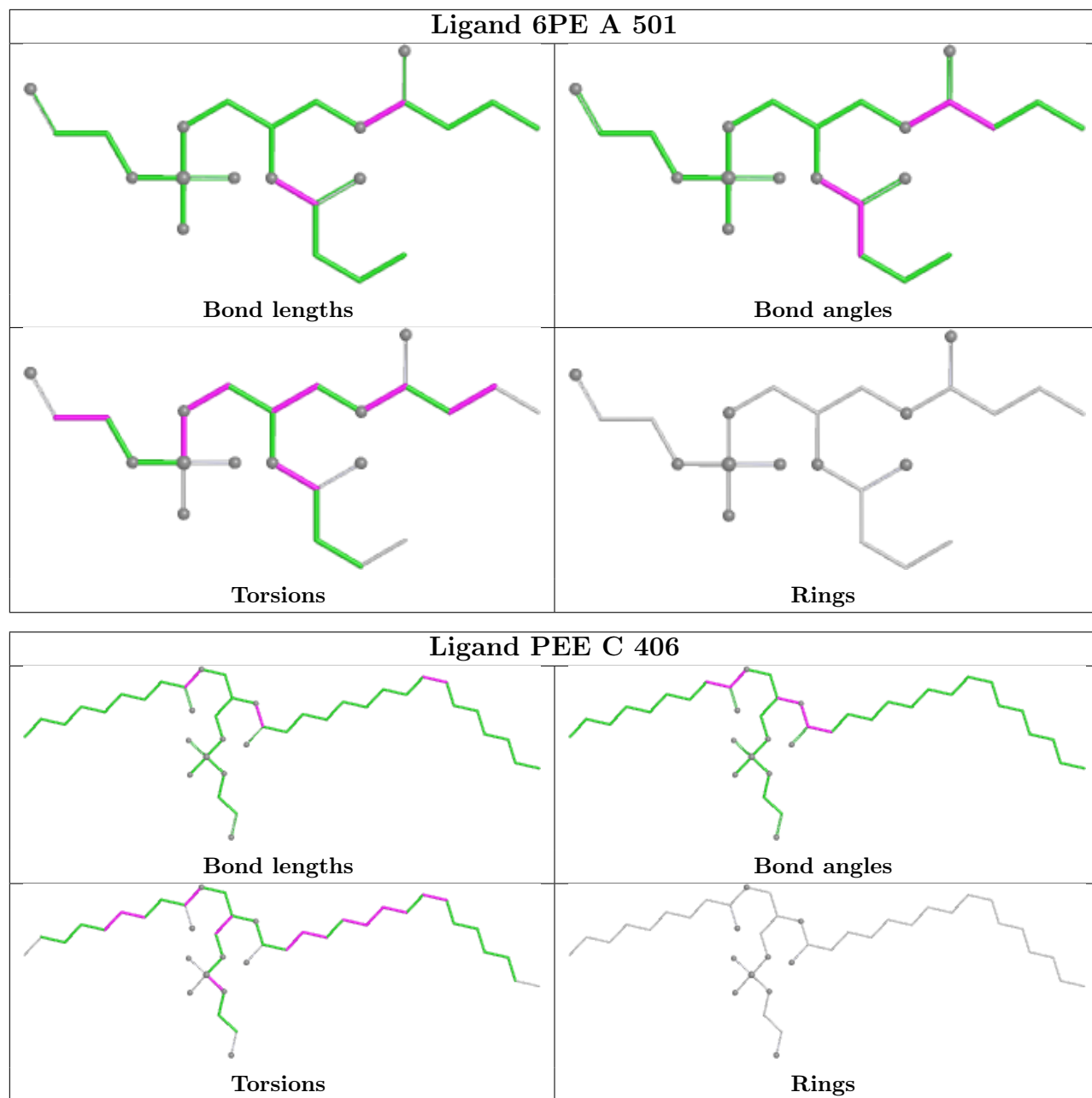
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

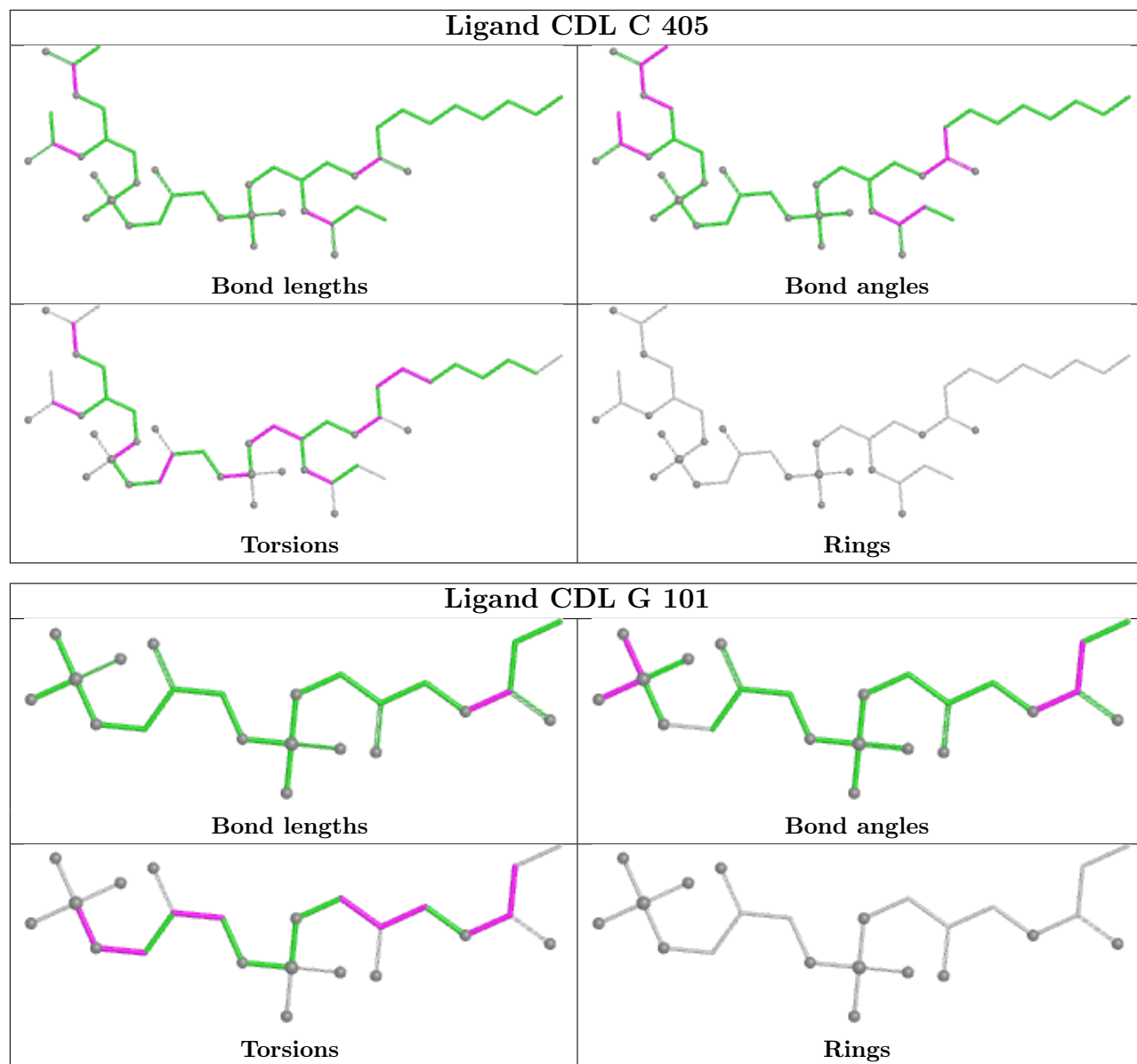


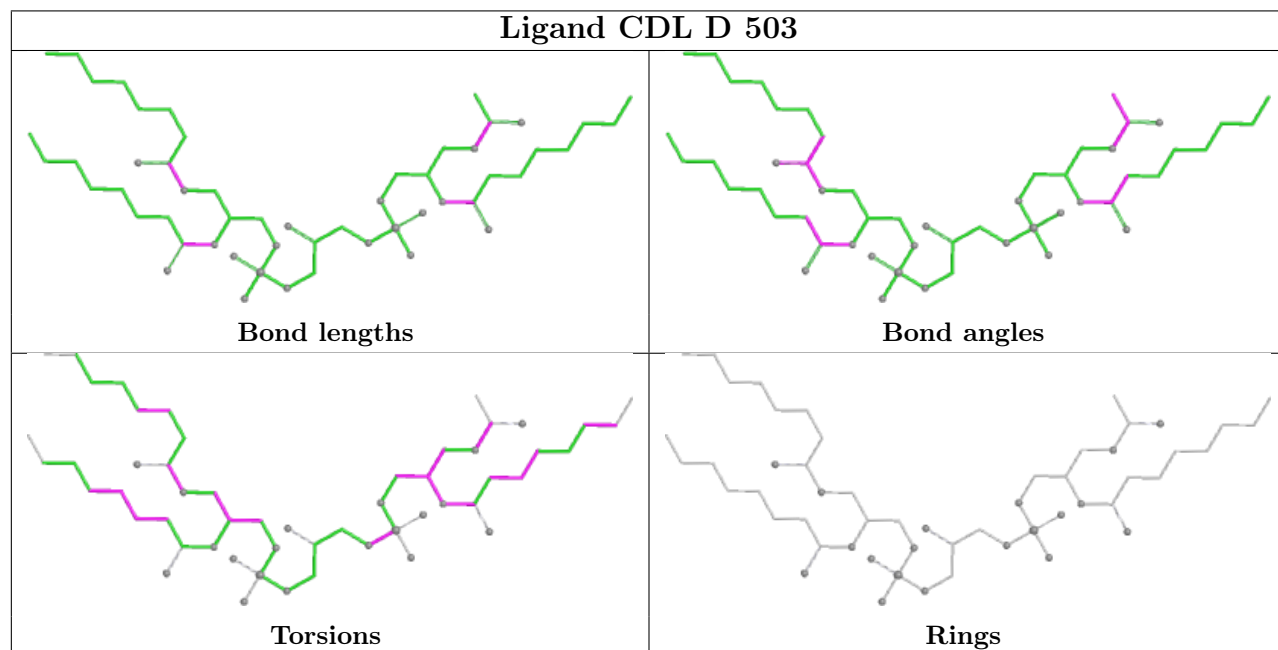
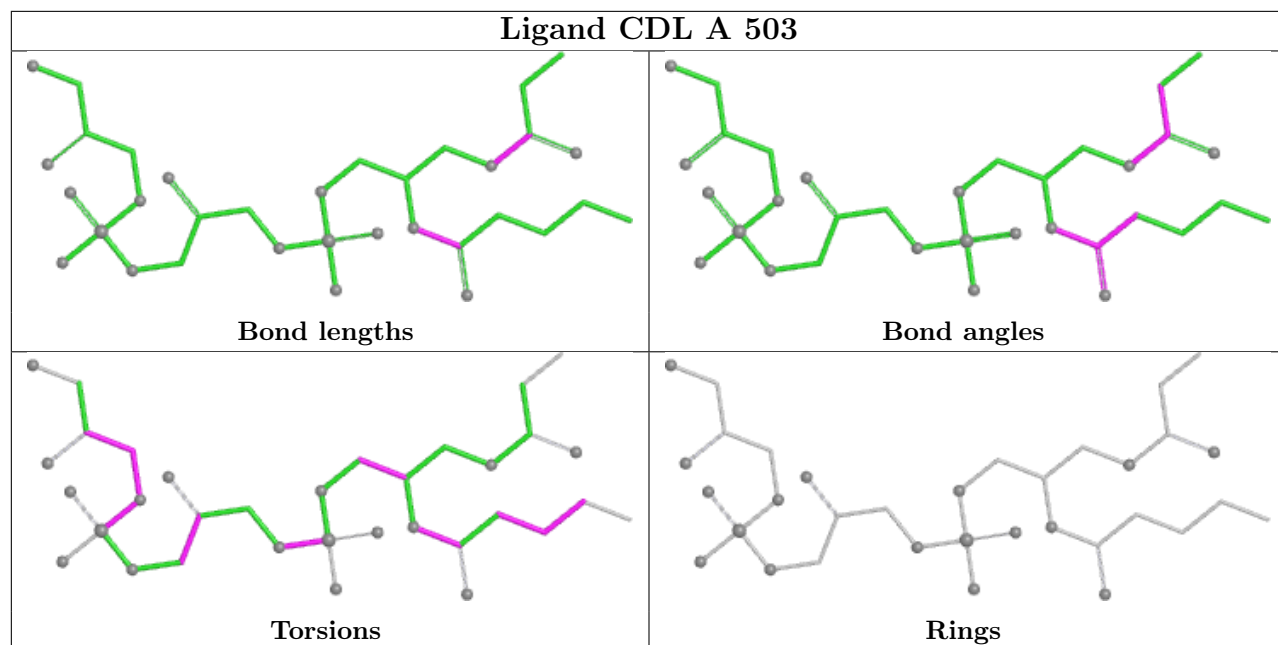


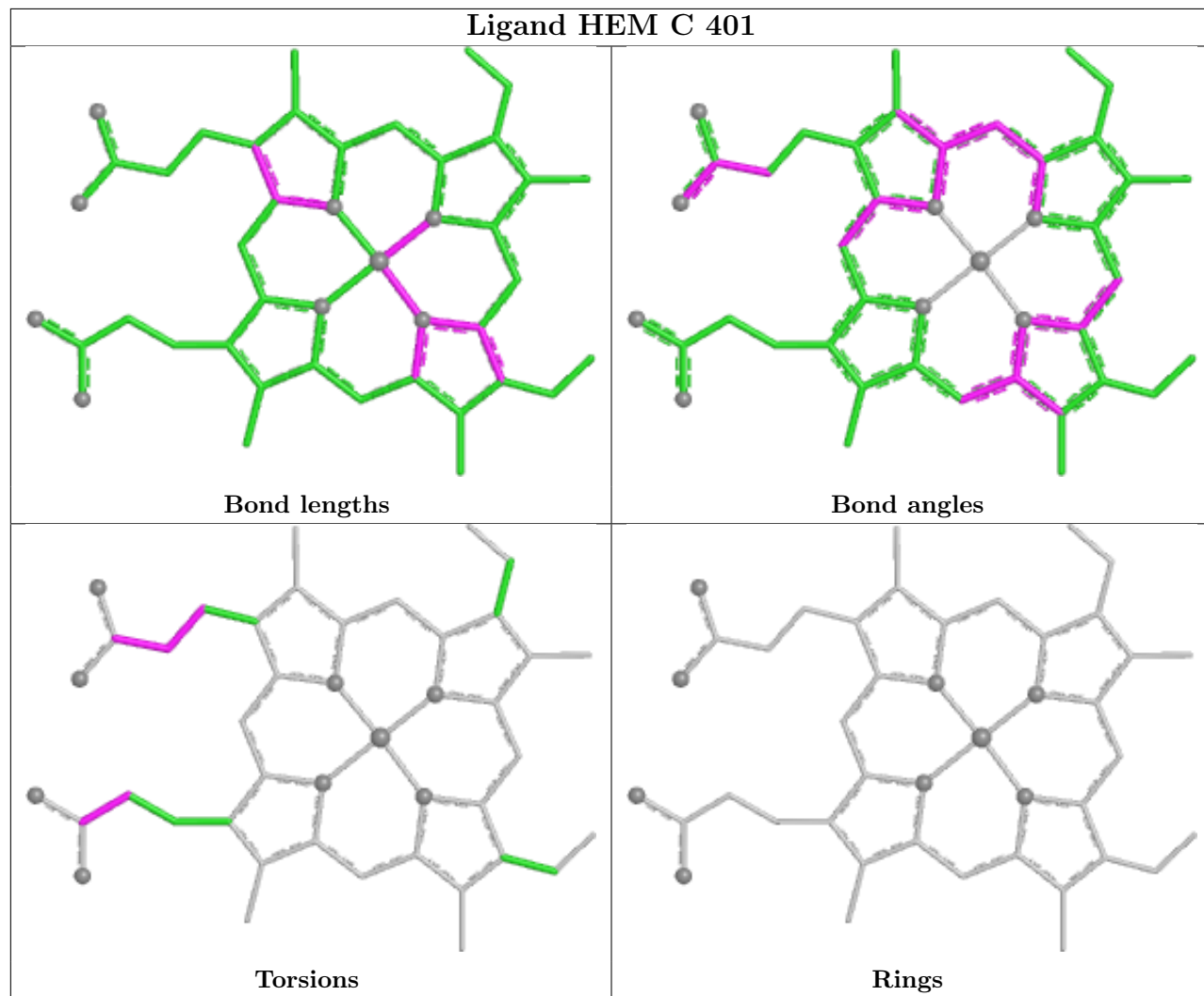
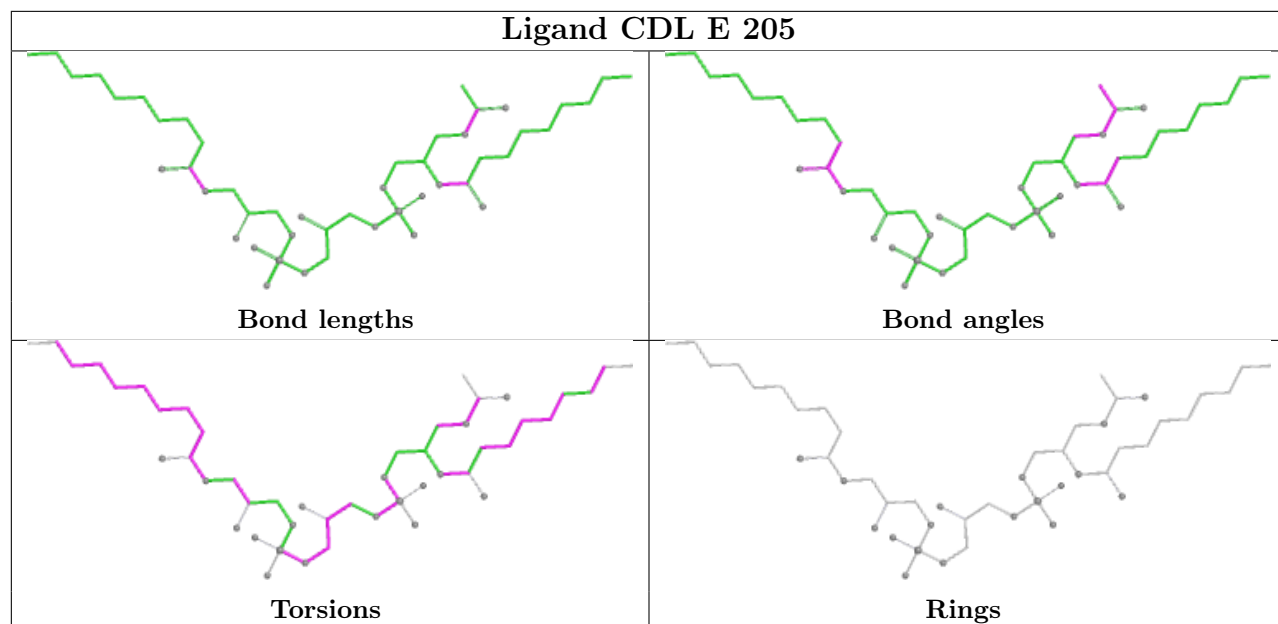












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	441/444 (99%)	-0.01	2 (0%) 87 68	91, 122, 152, 185	0
2	B	415/420 (98%)	-0.08	5 (1%) 76 52	98, 126, 159, 220	0
3	C	378/378 (100%)	0.26	15 (3%) 42 23	90, 114, 147, 180	0
4	D	239/239 (100%)	0.35	22 (9%) 14 9	108, 147, 174, 191	0
5	E	195/196 (99%)	0.80	18 (9%) 14 9	103, 180, 222, 242	0
6	F	99/99 (100%)	0.08	1 (1%) 79 56	70, 120, 155, 199	0
7	G	75/75 (100%)	0.28	5 (6%) 24 15	96, 123, 163, 187	0
8	H	64/64 (100%)	0.41	3 (4%) 36 20	154, 181, 197, 206	0
9	I	46/46 (100%)	1.80	19 (41%) 0 1	144, 180, 201, 204	0
10	J	59/59 (100%)	0.23	0 100 100	114, 136, 183, 201	0
All	All	2011/2020 (99%)	0.22	90 (4%) 38 20	70, 128, 190, 242	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	160	CYS	10.3
5	E	161	HIS	8.2
5	E	159	PRO	7.1
4	D	148	TYR	5.2
9	I	43	LEU	4.4
4	D	157	ALA	4.2
4	D	149	PHE	4.1
4	D	159	GLY	4.1
9	I	52	ARG	3.8
5	E	144	CYS	3.7
9	I	38	SER	3.6
9	I	33	ALA	3.6
3	C	42	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	158	ILE	3.6
6	F	56	ASN	3.5
5	E	114	VAL	3.4
9	I	42	VAL	3.3
3	C	39	ILE	3.3
9	I	41	PRO	3.3
4	D	165	TYR	3.2
3	C	295	ALA	3.2
9	I	45	LEU	3.1
4	D	137	PRO	3.1
3	C	40	CYS	3.0
7	G	8	THR	3.0
7	G	9	ARG	3.0
3	C	266	PRO	3.0
4	D	155	GLY	2.9
1	A	226	GLU	2.9
4	D	170	GLU	2.9
3	C	188	ILE	2.9
3	C	190	MET	2.9
5	E	158	CYS	2.9
5	E	146	PRO	2.8
9	I	75	SER	2.8
3	C	271	GLU	2.8
4	D	150	ASN	2.8
9	I	40	SER	2.7
5	E	145	VAL	2.7
9	I	34	VAL	2.7
7	G	10	VAL	2.6
4	D	154	PRO	2.6
3	C	294	LEU	2.6
5	E	111	ALA	2.6
4	D	167	GLU	2.6
9	I	39	GLU	2.6
4	D	141	VAL	2.6
9	I	37	THR	2.5
3	C	292	LEU	2.5
4	D	162	PRO	2.5
2	B	265	GLY	2.5
4	D	143	LEU	2.5
7	G	75	ALA	2.5
5	E	124	LEU	2.5
9	I	44	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	154	PRO	2.4
4	D	135	CYS	2.4
5	E	178	LEU	2.4
3	C	46	LEU	2.4
4	D	147	LEU	2.4
5	E	157	TYR	2.4
4	D	225	HIS	2.3
5	E	162	GLY	2.3
4	D	164	ILE	2.3
2	B	318	ASP	2.3
5	E	55	VAL	2.3
4	D	136	GLU	2.3
8	H	44	VAL	2.3
7	G	6	HIS	2.3
4	D	134	TYR	2.3
2	B	388	ALA	2.2
1	A	444	LEU	2.2
3	C	201	HIS	2.2
4	D	177	ALA	2.2
9	I	70	LEU	2.2
9	I	72	VAL	2.2
2	B	99	THR	2.2
3	C	191	ALA	2.2
9	I	76	VAL	2.2
9	I	62	ARG	2.1
3	C	232	ALA	2.1
8	H	14	VAL	2.1
9	I	73	PRO	2.1
9	I	71	ASN	2.1
5	E	74	ILE	2.1
5	E	187	PHE	2.1
5	E	91	TRP	2.1
5	E	141	HIS	2.1
2	B	28	ARG	2.0
8	H	45	SER	2.0

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

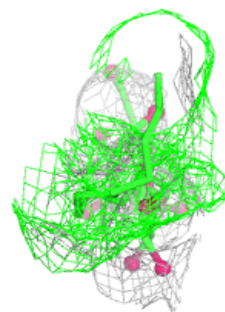
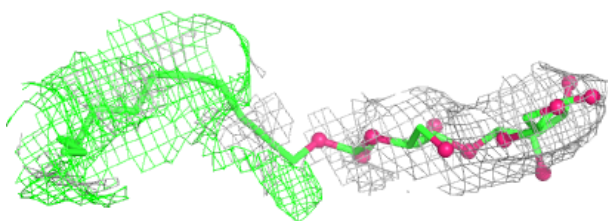
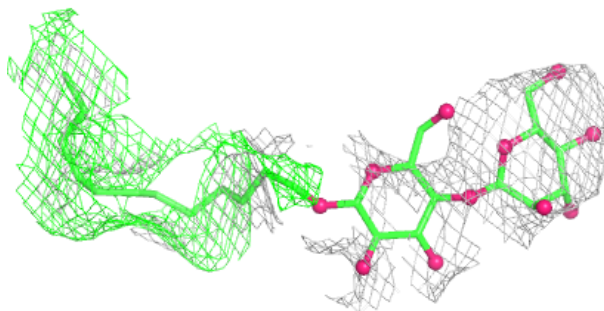
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	LMT	C	403	35/35	-0.08	0.29	179,215,223,223	0
13	CDL	G	101	23/100	0.44	0.16	141,201,207,213	0
12	PO4	E	203	5/5	0.67	0.17	205,209,210,211	0
12	PO4	D	502	5/5	0.69	0.11	200,202,207,207	0
12	PO4	G	103	5/5	0.69	0.09	214,215,217,222	0
13	CDL	E	205	48/100	0.71	0.21	147,179,222,226	0
12	PO4	G	104	5/5	0.85	0.11	185,186,188,190	0
12	PO4	G	102	5/5	0.86	0.10	156,156,160,161	0
16	PG4	C	404	13/13	0.86	0.19	119,126,136,136	0
18	JGW	C	407	30/30	0.87	0.27	111,133,186,190	0
13	CDL	A	503	34/100	0.88	0.16	150,182,190,193	0
12	PO4	A	502	5/5	0.90	0.26	129,129,132,137	0
21	PX4	E	202	37/46	0.90	0.27	132,142,151,152	0
11	6PE	A	501	23/27	0.92	0.18	141,159,170,170	0
12	PO4	F	501	5/5	0.92	0.08	171,176,178,179	0
17	PEE	E	204	39/51	0.93	0.19	117,122,128,131	0
13	CDL	C	405	44/100	0.93	0.16	121,129,141,145	0
13	CDL	D	503	54/100	0.93	0.18	105,146,183,186	0
17	PEE	C	406	40/51	0.95	0.14	103,111,116,117	0
20	FES	E	201	4/4	0.96	0.06	254,258,263,267	0
19	HEC	D	501	43/43	0.97	0.10	141,151,161,164	0
14	HEM	C	401	43/43	0.98	0.11	106,109,111,113	0
14	HEM	C	402	43/43	0.98	0.09	95,96,99,101	0

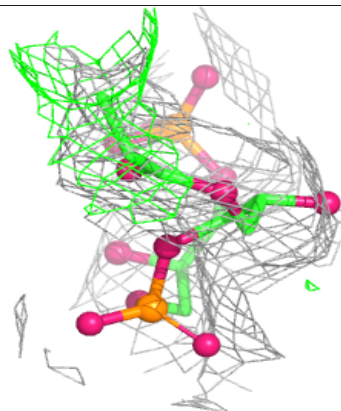
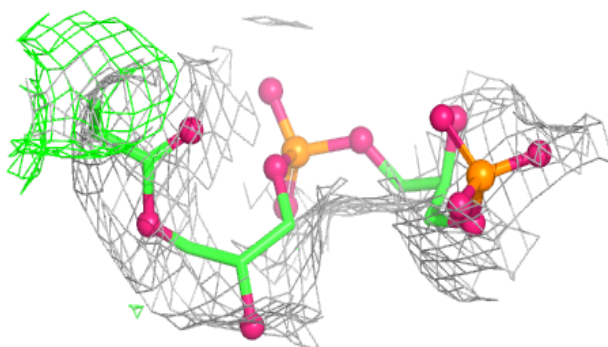
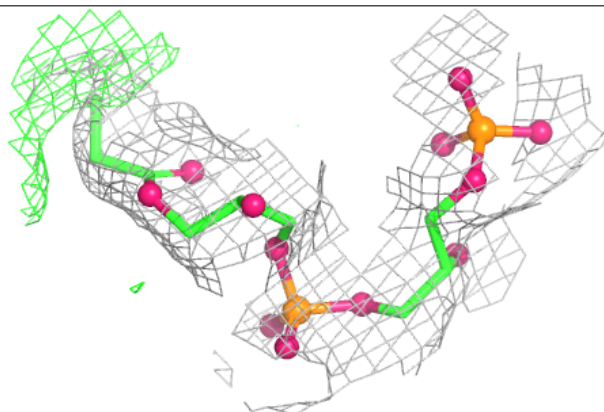
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

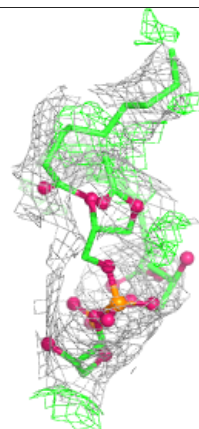
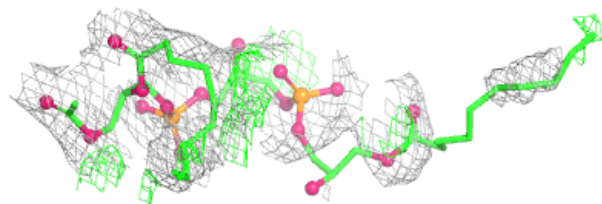
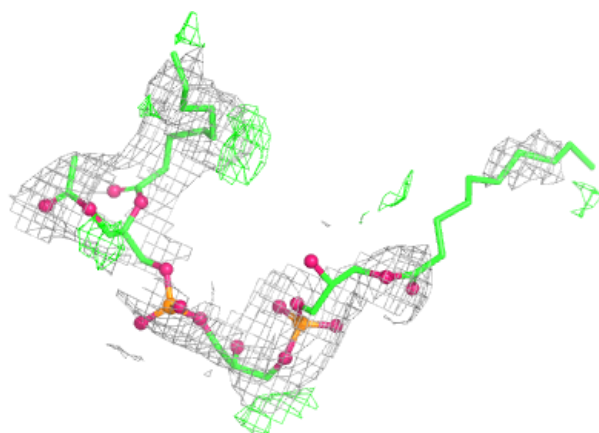
**Electron density around CDL G 101:**

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

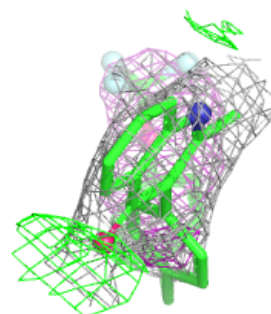
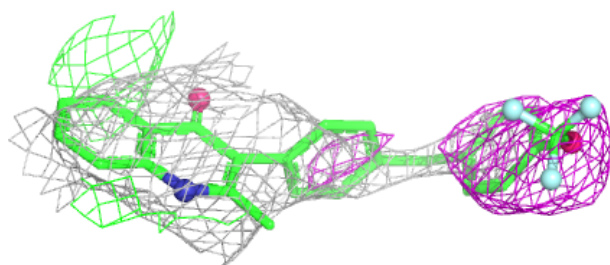
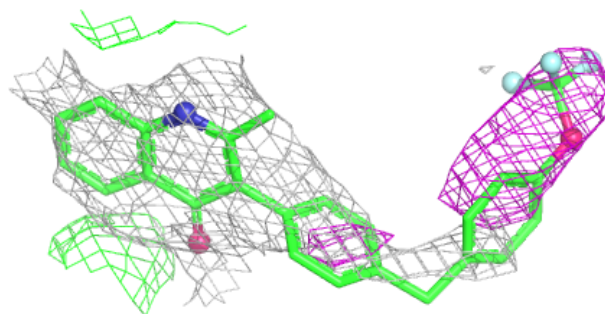


Electron density around CDL E 205:

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

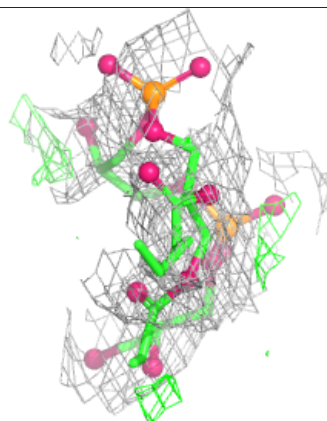
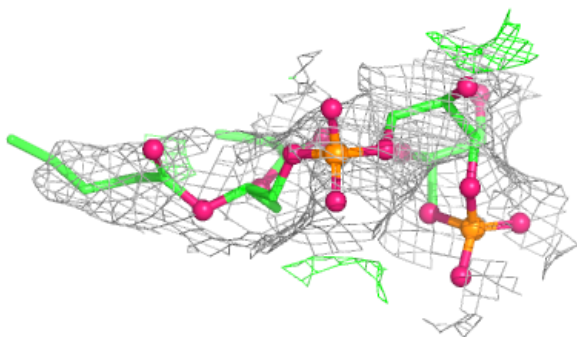
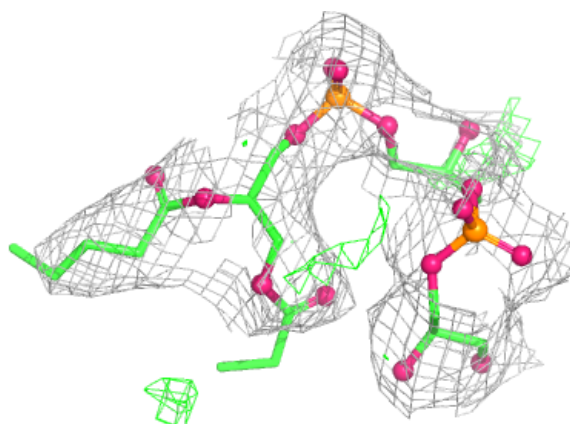
**Electron density around JGW C 407:**

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

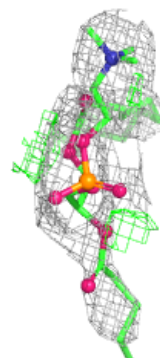
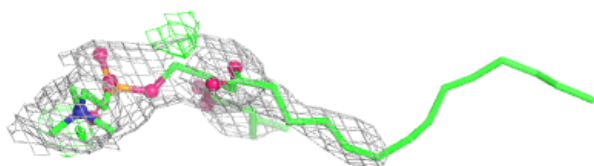
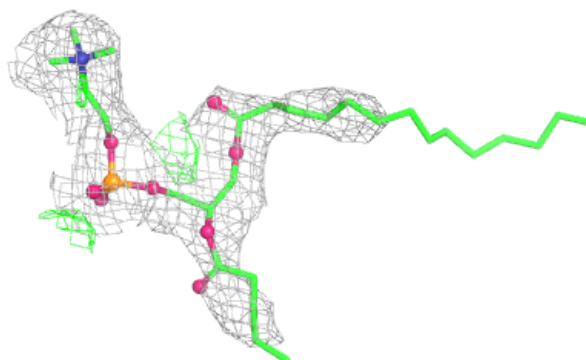


Electron density around CDL A 503:

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

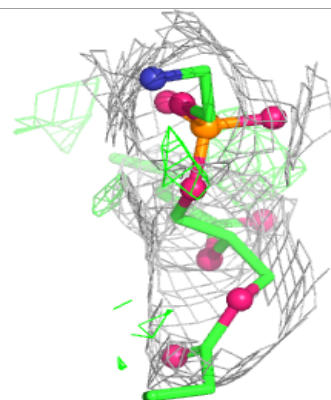
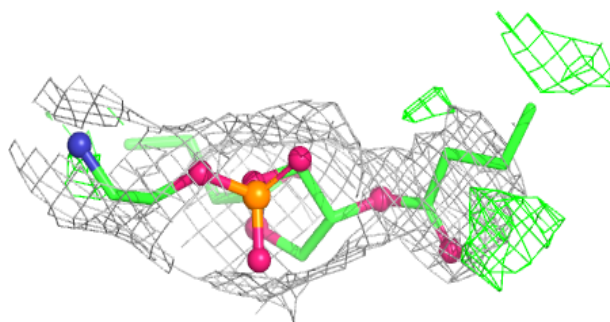
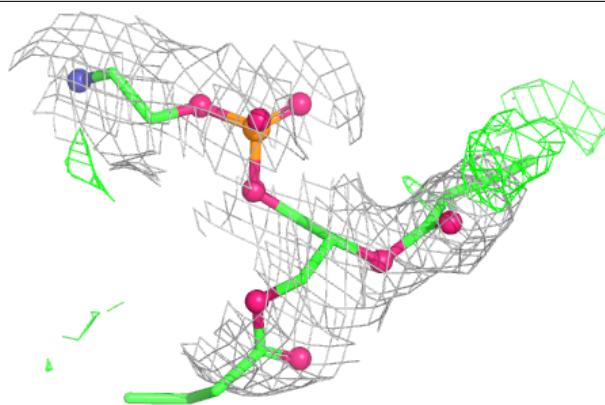
**Electron density around PX4 E 202:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

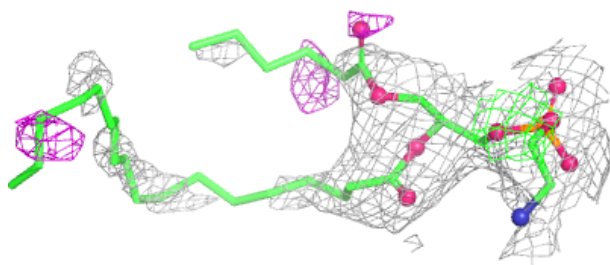
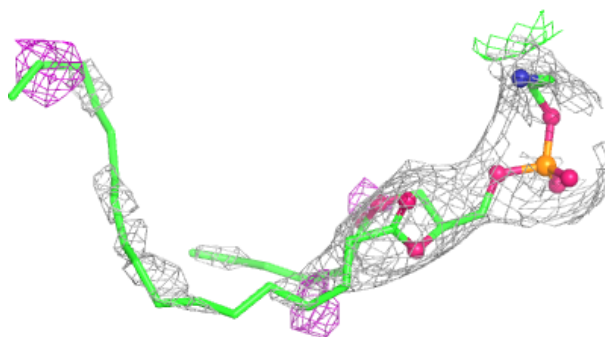


Electron density around 6PE A 501:

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

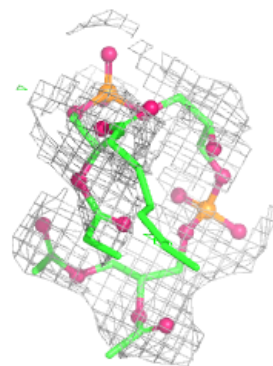
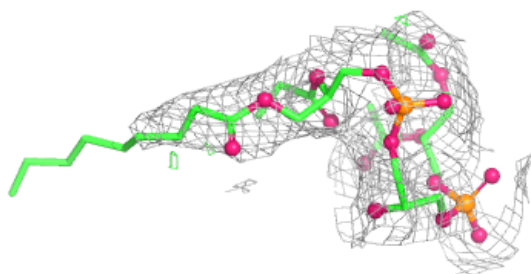
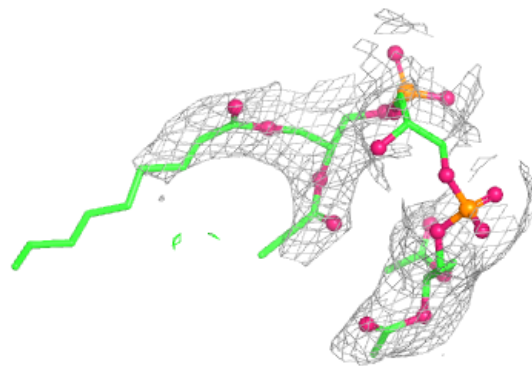
**Electron density around PEE E 204:**

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

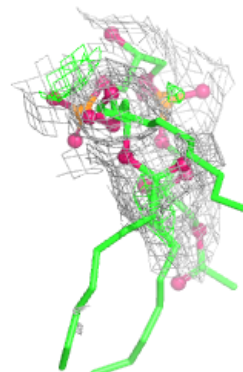
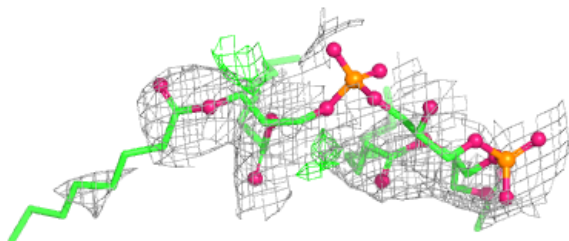
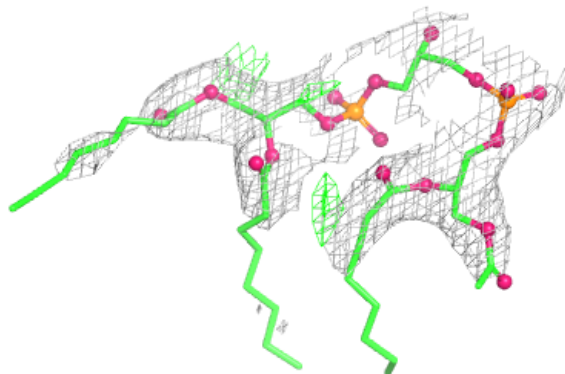


Electron density around CDL C 405:

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

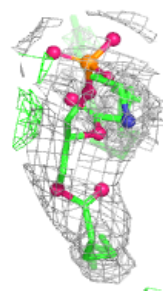
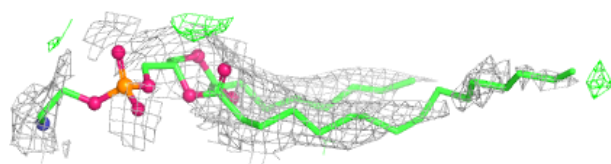
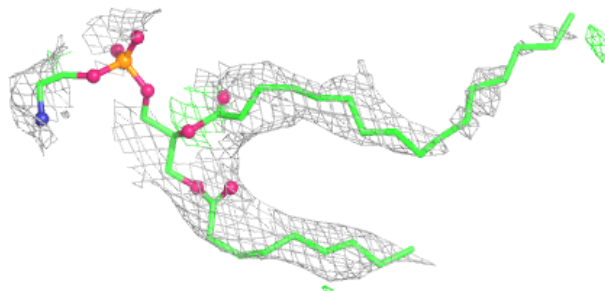
**Electron density around CDL D 503:**

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

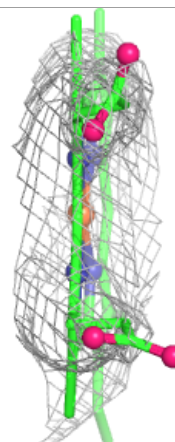
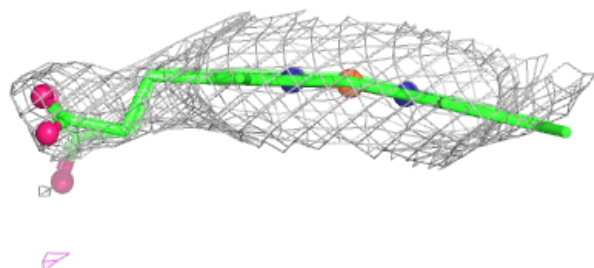
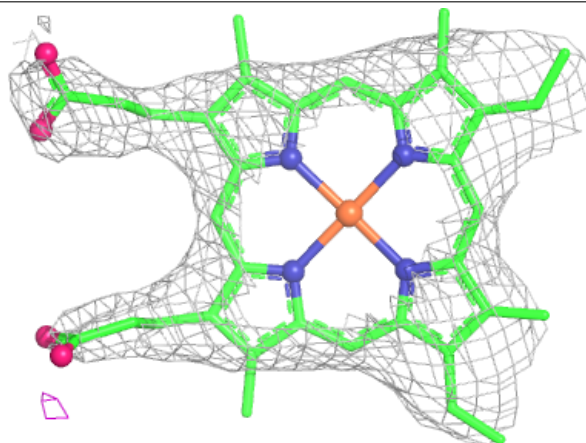


Electron density around PEE C 406:

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

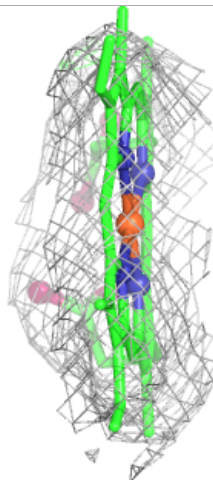
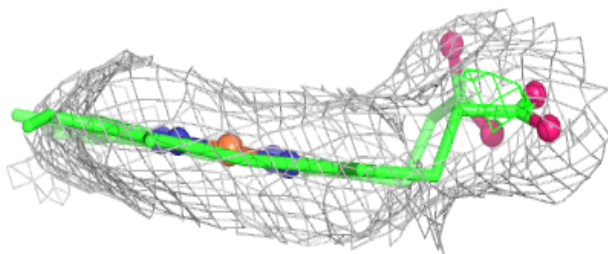
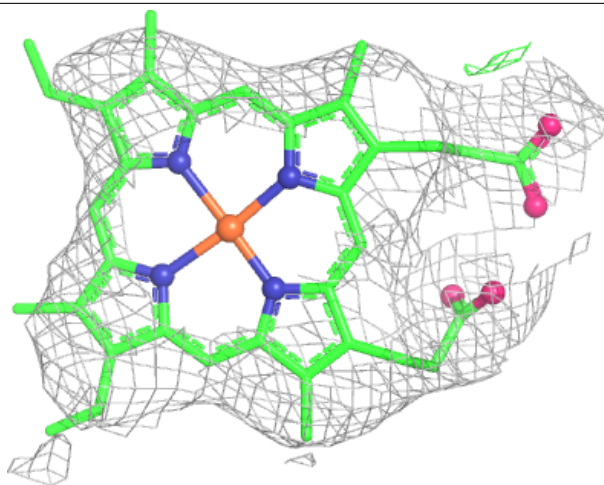
**Electron density around HEC D 501:**

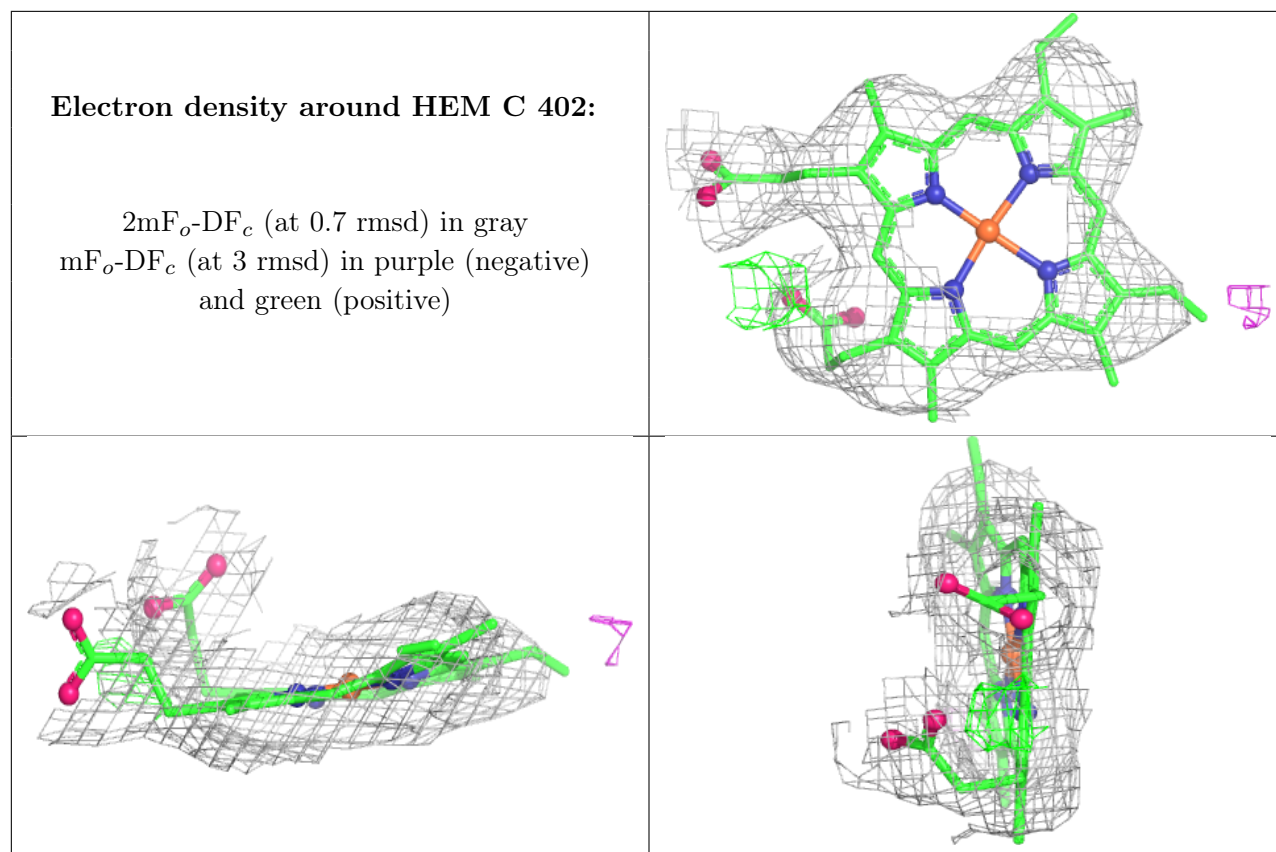
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.