



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 01:30 PM BST

PDB ID : 6ZFS
Title : Crystal structure of bovine cytochrome bc1 in complex with quinolone inhibitor WDH-1U-4
Authors : Amporndanai, K.; O'Neill, P.M.; Hong, W.D.; Amewu, R.K.; Pidathala, C.; Berry, N.G.; Biagini, G.A.; Leung, S.C.; Hasnain, S.S.; Antonyuk, S.V.
Deposited on : 2020-06-17
Resolution : 3.50 Å(reported)

This is a 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

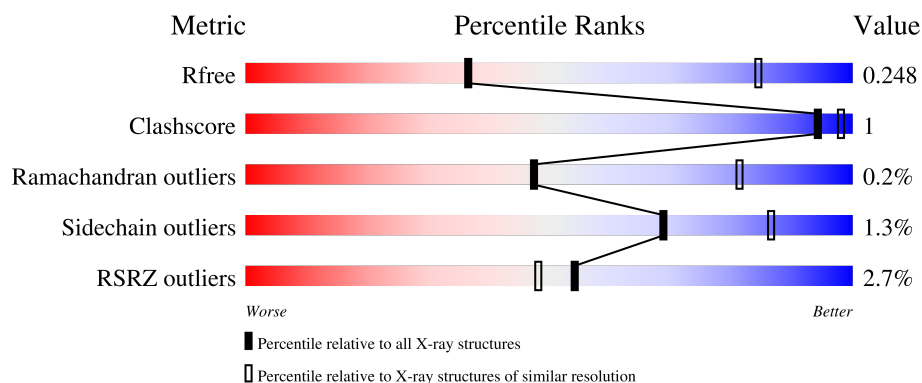
1 Overall quality at a glance

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.



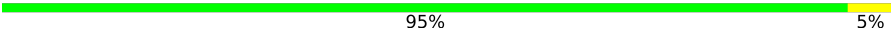

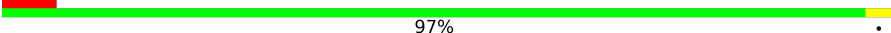

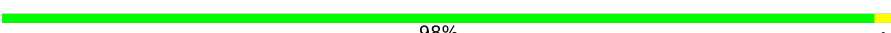
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	<div> <div>6%</div> <div>97%</div> <div>..</div> </div>
2	B	420	<div> <div>96%</div> <div>..</div> </div>
3	C	378	<div> <div>95%</div> <div>5%</div> </div>
4	D	239	<div> <div>7%</div> <div>95%</div> <div>5%</div> </div>
5	E	196	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	99	 95% 5%
7	G	75	 % 92% 8%
8	H	64	 6% 97% .
9	I	46	 4% 85% 15%
10	J	59	 98% .

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
12	PO4	A	502	-	-	-	X
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			

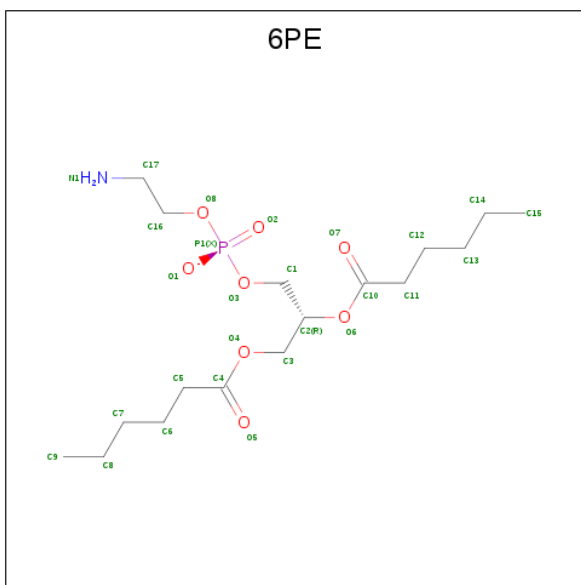
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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.

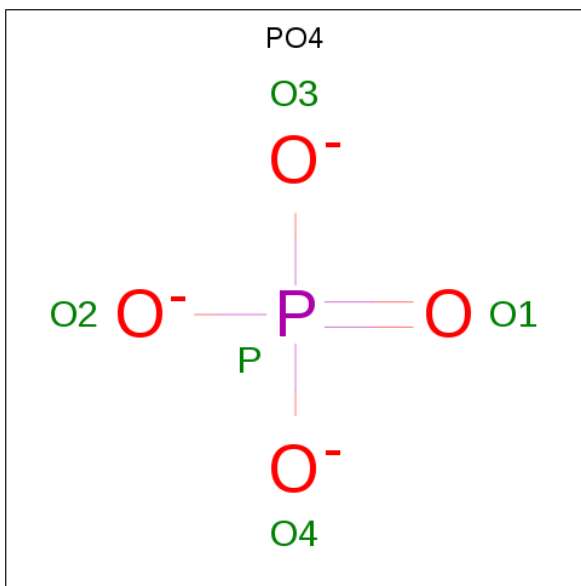
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			478	314	81	83			

- Molecule 11 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 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 (three-letter code: PO4) (formula: O_4P).



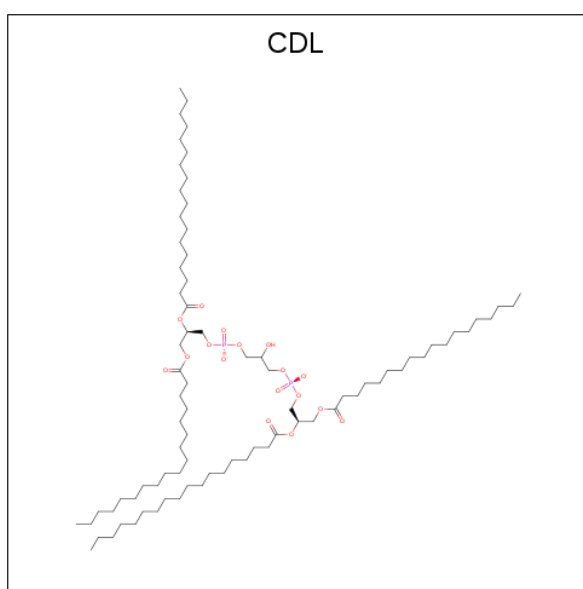
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total 5	O 4	P 1	0	0
12	D	1	Total 5	O 4	P 1	0	0
12	E	1	Total 5	O 4	P 1	0	0

Continued on next page...

Continued from previous page...

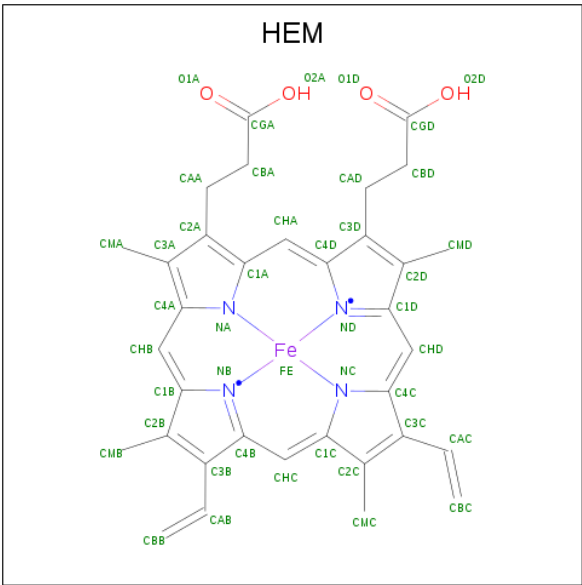
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	F	1	Total	O	P	0	0
			5	4	1		
12	G	1	Total	O	P	0	0
			5	4	1		
12	G	1	Total	O	P	0	0
			5	4	1		
12	G	1	Total	O	P	0	0
			5	4	1		

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



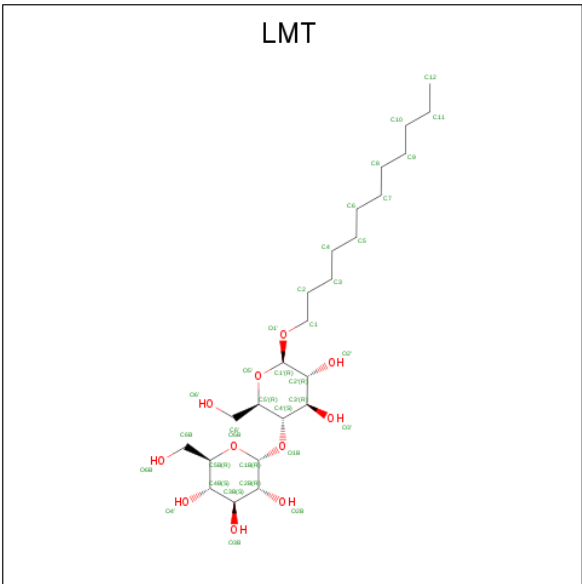
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			34	17	15	2		
13	C	1	Total	C	O	P	0	0
			44	25	17	2		
13	D	1	Total	C	O	P	0	0
			54	35	17	2		
13	E	1	Total	C	O	P	0	0
			48	30	16	2		
13	G	1	Total	C	O	P	0	0
			23	9	12	2		

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

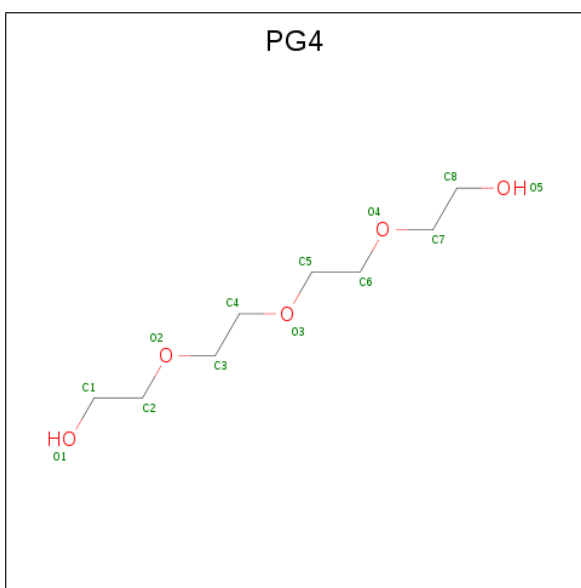


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

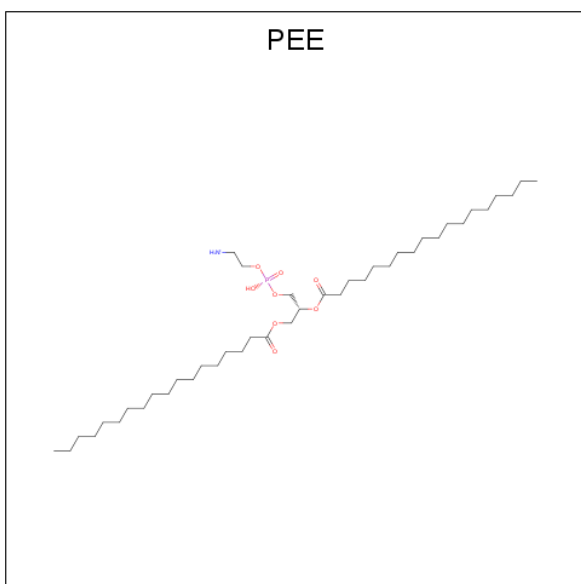


- Molecule 16 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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 (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



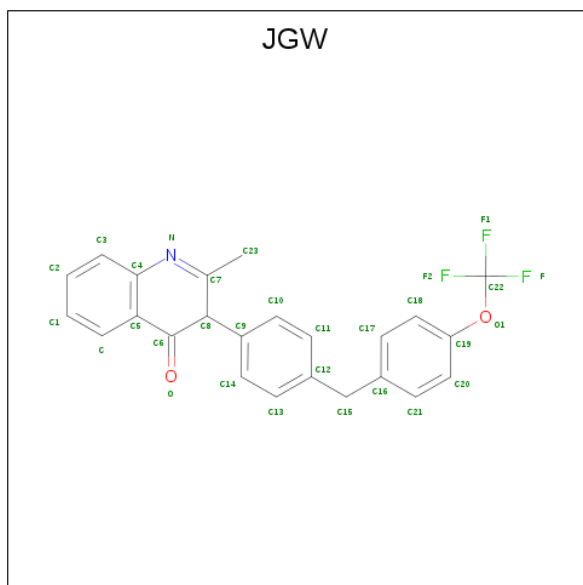
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

Continued on next page...

Continued from previous page...

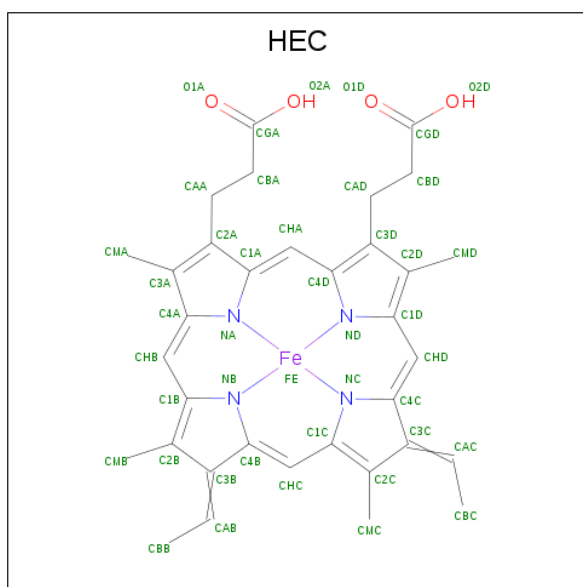
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	E	1	Total	C	N	O	P	0	0
			39	29	1	8	1		

- Molecule 18 is 2-methyl-3-[4-[[4-(trifluoromethoxy)phenyl]methyl]phenyl]-3 {H}-quinolin-4-one (three-letter code: JGW) (formula: C₂₄H₁₈F₃NO₂) (labeled as "Ligand of Interest" by depositor).



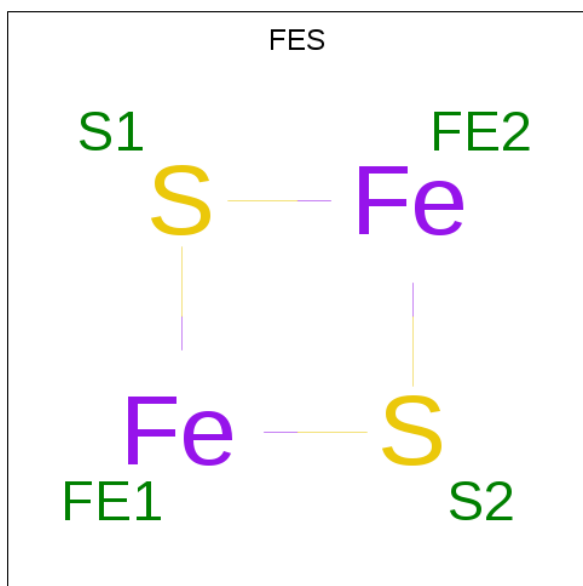
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	F	N	O	0	0
			30	24	3	1	2		

- Molecule 19 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



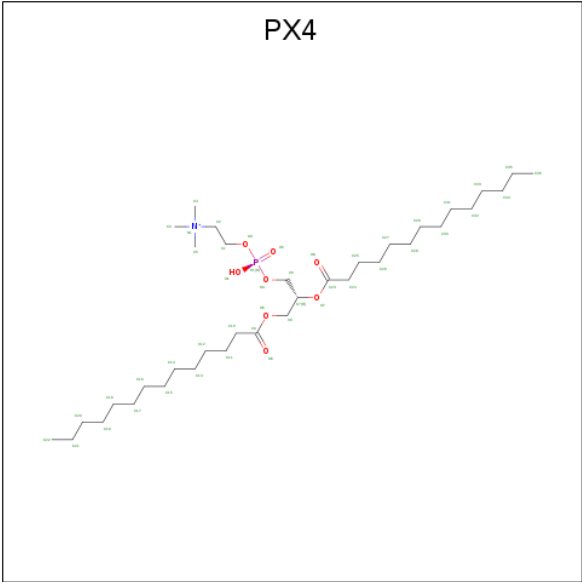
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



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

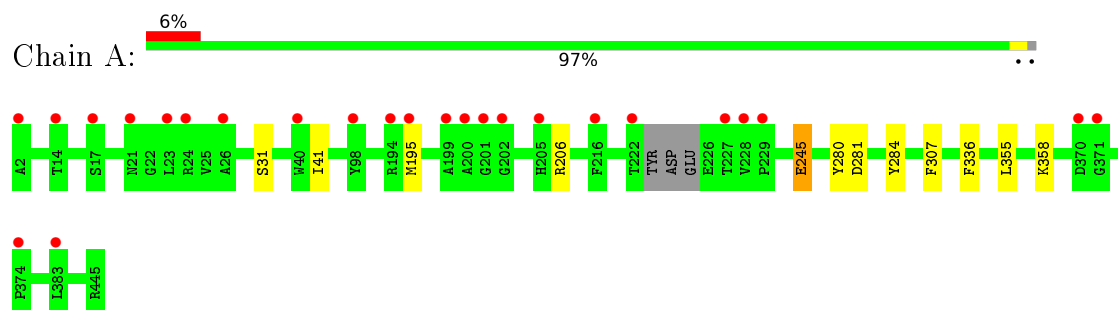
- Molecule 22 is water.

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

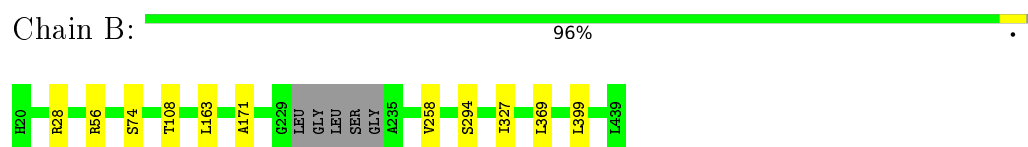
3 Residue-property plots [i](#)

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.

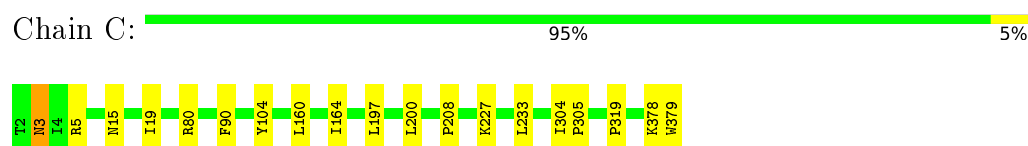
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



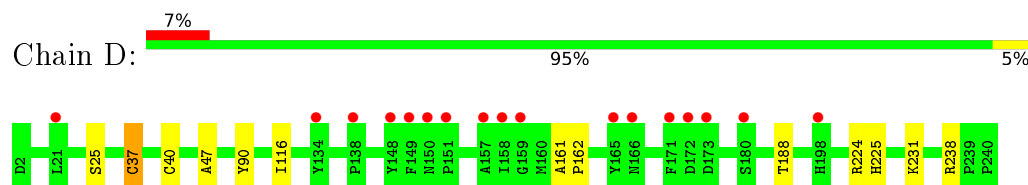
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 3: Cytochrome b

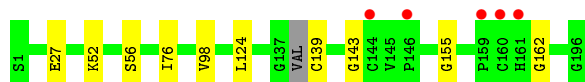


- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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





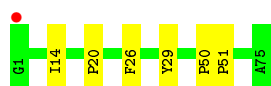
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F: 95% 5%



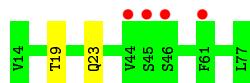
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G: 92% 8%



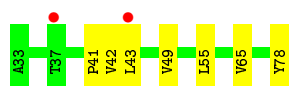
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H: 97% 6%



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

Chain I: 85% 15% 4%



- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J: 98%



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 , 0.248	Depositor DCC
R_{free} test set	2800 reflections (5.09%)	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)	0.30 , 93.7	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	0.85	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: 6PE, FES, CDL, PEE, LMT, PX4, HEC, PG4, HEM, JGW, PO4

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	0.44	0/3435	0.67	0/4663
2	B	0.43	0/3173	0.64	0/4304
3	C	0.45	0/3092	0.62	0/4231
4	D	0.44	0/1908	0.65	0/2597
5	E	0.47	0/1527	0.65	0/2064
6	F	0.46	0/878	0.69	0/1181
7	G	0.51	0/645	0.66	0/873
8	H	0.41	0/515	0.71	0/694
9	I	0.57	0/329	0.86	0/449
10	J	0.47	0/491	0.64	0/664
All	All	0.45	0/15993	0.66	0/21720

There are no bond length outliers.

There are no bond angle outliers.

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	6	0
2	B	3116	0	3089	4	0
3	C	2996	0	3058	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1849	0	1732	12	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	6	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
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	43	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 1.

All (43) 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
4:D:116:ILE:HG12	19:D:501:HEC:HMA3	1.73	0.71
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: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
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
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
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
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
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
5:E:52:LYS:O	5:E:56:SER:HB2	2.20	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
4:D:161:ALA:O	4:D:162:PRO:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5	E	191/196 (97%)	179 (94%)	9 (5%)	3 (2%)	9	43
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%)	6	36
10	J	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
All	All	1985/2020 (98%)	1909 (96%)	72 (4%)	4 (0%)	47	81

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%)	346 (99%)	4 (1%)	73	88
2	B	325/329 (99%)	321 (99%)	4 (1%)	71	87
3	C	325/326 (100%)	319 (98%)	6 (2%)	59	81
4	D	187/204 (92%)	185 (99%)	2 (1%)	73	88
5	E	163/168 (97%)	160 (98%)	3 (2%)	59	81
6	F	88/91 (97%)	87 (99%)	1 (1%)	73	88
7	G	65/66 (98%)	65 (100%)	0	100	100
8	H	56/61 (92%)	56 (100%)	0	100	100
9	I	35/38 (92%)	33 (94%)	2 (6%)	20	53
10	J	47/49 (96%)	47 (100%)	0	100	100
All	All	1641/1701 (96%)	1619 (99%)	22 (1%)	69	86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	206	ARG
1	A	245	GLU
1	A	281	ASP
2	B	28	ARG
2	B	74	SER
2	B	108	THR
2	B	294	SER
3	C	3	ASN
3	C	80	ARG
3	C	90	PHE
3	C	227	LYS
3	C	233	LEU
3	C	379	TRP
4	D	37	CYS
4	D	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	27	GLU
5	E	124	LEU
5	E	139	CYS
6	F	71	ARG
9	I	65	VAL
9	I	78	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	189	HIS
2	B	290	ASN
2	B	400	GLN
2	B	412	ASN
3	C	3	ASN
3	C	15	ASN
4	D	121	HIS
4	D	225	HIS
7	G	12	HIS
8	H	23	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
13	CDL	D	503	-	53,53,99	1.34	4 (7%)	59,65,111	1.15	5 (8%)
12	PO4	E	203	-	4,4,4	0.86	0	6,6,6	0.72	0
14	HEM	C	401	3	27,50,50	0.84	1 (3%)	17,82,82	1.15	1 (5%)
17	PEE	C	406	-	39,39,50	1.11	2 (5%)	42,44,55	1.12	3 (7%)
13	CDL	G	101	-	22,22,99	1.22	1 (4%)	26,30,111	1.06	2 (7%)
12	PO4	A	502	-	4,4,4	0.98	0	6,6,6	0.37	0
14	HEM	C	402	3	27,50,50	0.91	2 (7%)	17,82,82	1.22	2 (11%)
17	PEE	E	204	-	38,38,50	1.17	2 (5%)	41,43,55	1.07	2 (4%)
21	PX4	E	202	-	36,36,45	1.34	2 (5%)	42,44,53	1.18	4 (9%)
16	PG4	C	404	-	12,12,12	0.52	0	11,11,11	0.48	0
19	HEC	D	501	4	26,50,50	2.71	12 (46%)	18,82,82	2.46	5 (27%)
18	JGW	C	407	-	32,33,33	1.72	4 (12%)	44,48,48	1.50	5 (11%)
13	CDL	A	503	-	33,33,99	1.24	2 (6%)	37,43,111	1.27	3 (8%)
15	LMT	C	403	-	36,36,36	0.63	0	47,47,47	0.98	2 (4%)
12	PO4	G	102	-	4,4,4	0.91	0	6,6,6	0.46	0
12	PO4	G	103	-	4,4,4	0.82	0	6,6,6	0.47	0
12	PO4	G	104	-	4,4,4	0.90	0	6,6,6	0.56	0
13	CDL	C	405	-	43,43,99	1.53	4 (9%)	49,55,111	1.33	6 (12%)
11	6PE	A	501	-	22,22,26	1.52	2 (9%)	25,27,31	1.29	2 (8%)
13	CDL	E	205	-	47,47,99	1.14	3 (6%)	52,58,111	1.16	5 (9%)
12	PO4	D	502	-	4,4,4	0.90	0	6,6,6	0.42	0
20	FES	E	201	5	0,4,4	0.00	-	-	-	-
12	PO4	F	501	-	4,4,4	0.96	0	6,6,6	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FES	E	201	5	-	-	0/1/1/1
14	HEM	C	402	3	-	0/6/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	A	503	-	-	15/41/41/110	-
17	PEE	E	204	-	1/1/4/4	23/42/42/54	-
15	LMT	C	403	-	-	9/21/61/61	0/2/2/2
21	PX4	E	202	-	-	21/40/40/49	-
16	PG4	C	404	-	-	5/10/10/10	-
13	CDL	G	101	-	-	14/25/25/110	-
19	HEC	D	501	4	-	0/6/54/54	-
13	CDL	C	405	-	-	18/52/52/110	-
13	CDL	D	503	-	-	24/63/63/110	-
17	PEE	C	406	-	1/1/4/4	19/43/43/54	-
14	HEM	C	401	3	-	1/6/54/54	-
11	6PE	A	501	-	-	12/26/26/30	-
18	JGW	C	407	-	1/1/4/4	3/13/29/29	0/3/4/4
13	CDL	E	205	-	-	33/55/55/110	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	501	HEC	C3C-C2C	7.67	1.48	1.40
18	C	407	JGW	C5-C4	7.64	1.50	1.40
19	D	501	HEC	C3B-C2B	6.68	1.47	1.40
13	C	405	CDL	OA6-CA5	5.53	1.47	1.35
13	C	405	CDL	OB6-CB5	5.33	1.49	1.34
13	D	503	CDL	OA8-CA7	5.16	1.48	1.33
13	D	503	CDL	OB6-CB5	4.97	1.48	1.34
11	A	501	6PE	O6-C10	4.92	1.48	1.34
21	E	202	PX4	O7-C23	4.90	1.48	1.34
13	G	101	CDL	OB8-CB7	4.90	1.47	1.33
21	E	202	PX4	O5-C9	4.76	1.47	1.33
17	E	204	PEE	O2-C10	4.71	1.47	1.34
13	A	503	CDL	OB8-CB7	4.66	1.47	1.33
13	E	205	CDL	OB6-CB5	4.62	1.47	1.34
13	C	405	CDL	OB8-CB7	4.60	1.46	1.33
17	C	406	PEE	O3-C30	4.53	1.46	1.33
13	D	503	CDL	OA6-CA5	4.45	1.46	1.34
11	A	501	6PE	O4-C4	4.41	1.46	1.33
17	E	204	PEE	O3-C30	4.34	1.46	1.33
13	E	205	CDL	OA8-CA7	4.28	1.45	1.33
17	C	406	PEE	O2-C10	4.26	1.46	1.34
13	A	503	CDL	OB6-CB5	4.13	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	501	HEC	C2A-C3A	3.49	1.48	1.37
19	D	501	HEC	C3D-C2D	3.41	1.47	1.37
19	D	501	HEC	C3C-C4C	3.19	1.48	1.43
19	D	501	HEC	C3B-C4B	3.18	1.48	1.43
19	D	501	HEC	C4A-C3A	3.17	1.49	1.42
19	D	501	HEC	C1A-C2A	3.03	1.49	1.42
19	D	501	HEC	C1C-CHC	2.79	1.48	1.41
13	E	205	CDL	OB8-CB7	2.78	1.47	1.33
13	C	405	CDL	OA8-CA7	2.74	1.46	1.33
14	C	401	HEM	C4D-C3D	2.69	1.48	1.42
14	C	402	HEM	C4D-C3D	2.66	1.48	1.42
13	D	503	CDL	OB8-CB7	2.60	1.46	1.33
18	C	407	JGW	C9-C8	-2.57	1.50	1.53
19	D	501	HEC	C1D-CHD	2.51	1.48	1.41
14	C	402	HEM	C3B-C2B	-2.45	1.37	1.40
18	C	407	JGW	O1-C22	2.41	1.45	1.31
18	C	407	JGW	C4-N	-2.23	1.35	1.39
19	D	501	HEC	C1B-CHB	2.19	1.47	1.41
19	D	501	HEC	C4D-CHA	2.15	1.47	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	501	HEC	C1D-C2D-C3D	-5.49	103.17	107.00
18	C	407	JGW	C9-C8-C7	5.20	123.03	111.45
18	C	407	JGW	C9-C8-C6	5.19	119.25	111.37
19	D	501	HEC	CMB-C2B-C3B	4.87	131.54	125.82
13	A	503	CDL	OB6-CB5-C51	4.55	121.31	111.50
21	E	202	PX4	O7-C23-C24	4.49	121.18	111.50
19	D	501	HEC	CMC-C2C-C3C	4.35	130.94	125.82
13	E	205	CDL	OB6-CB5-C51	4.33	120.84	111.50
13	C	405	CDL	OA6-CA5-C11	4.33	119.05	111.09
11	A	501	6PE	O6-C10-C11	4.25	120.66	111.50
17	E	204	PEE	O2-C10-C11	4.23	120.61	111.50
13	D	503	CDL	OB6-CB5-C51	3.98	120.07	111.50
13	A	503	CDL	OB8-CB7-C71	3.78	121.30	111.38
17	C	406	PEE	O3-C30-C31	3.66	123.40	111.91
13	C	405	CDL	OB8-CB7-C71	3.49	122.86	111.91
13	D	503	CDL	OA8-CA7-C31	3.44	122.70	111.91
15	C	403	LMT	C1B-O5B-C5B	3.21	119.99	113.69
14	C	402	HEM	CAD-CBD-CGD	3.20	118.04	112.67
13	G	101	CDL	OB8-CB7-C71	3.12	119.56	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	E	202	PX4	O5-C9-C10	3.03	121.43	111.91
13	D	503	CDL	OA6-CA5-C11	3.02	118.01	111.50
17	C	406	PEE	O2-C10-C11	3.00	117.97	111.50
19	D	501	HEC	CAA-CBA-CGA	-2.92	107.77	112.67
13	C	405	CDL	CA6-OA8-CA7	2.86	124.29	117.10
13	E	205	CDL	CB6-OB8-CB7	2.80	124.15	117.10
13	D	503	CDL	OA8-CA7-OA9	-2.79	116.54	123.59
13	C	405	CDL	OB6-CB5-C51	2.75	118.46	110.80
13	E	205	CDL	OA8-CA7-C31	2.68	120.32	111.91
21	E	202	PX4	O5-C9-O6	-2.64	116.93	123.59
17	E	204	PEE	O3-C30-C31	2.56	119.94	111.91
13	C	405	CDL	OB8-CB7-OB9	-2.53	117.21	123.59
18	C	407	JGW	C16-C15-C12	-2.50	104.92	113.84
18	C	407	JGW	C23-C7-N	-2.46	116.18	119.71
11	A	501	6PE	O4-C4-C5	2.44	119.56	111.91
14	C	401	HEM	CBA-CAA-C2A	-2.36	108.13	112.49
14	C	402	HEM	CMC-C2C-C3C	2.35	129.07	124.68
17	C	406	PEE	C2-O2-C10	-2.32	112.08	117.79
13	D	503	CDL	OB8-CB7-C71	2.27	122.30	112.38
13	G	101	CDL	OA4-PA1-OA3	2.26	119.51	110.68
13	C	405	CDL	OA8-CA7-C31	2.25	122.20	112.38
21	E	202	PX4	O7-C23-O8	-2.22	118.34	123.70
13	A	503	CDL	OB6-CB5-OB7	-2.21	118.36	123.70
13	E	205	CDL	OA8-CA7-OA9	-2.21	118.02	123.59
15	C	403	LMT	C2'-C3'-C4'	2.19	114.69	109.68
18	C	407	JGW	C11-C10-C9	-2.19	119.00	121.20
19	D	501	HEC	C4C-C3C-C2C	-2.08	104.11	106.35
13	E	205	CDL	OB8-CB7-C71	2.08	121.43	112.38

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 (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	6PE	C1-O3-P1-O1
11	A	501	6PE	C11-C10-O6-C2
11	A	501	6PE	O8-C16-C17-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	C11-CA5-OA6-CA4
13	C	405	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	CB2-OB2-PB2-OB3
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	CB2-OB2-PB2-OB3
13	E	205	CDL	CB2-OB2-PB2-OB5
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-O1P
17	C	406	PEE	C4-O4P-P-O2P
17	C	406	PEE	C4-O4P-P-O3P
17	E	204	PEE	O4P-C4-C5-N
17	E	204	PEE	C4-O4P-P-O1P
21	E	202	PX4	C24-C23-O7-C7
13	E	205	CDL	CB4-CB6-OB8-CB7
21	E	202	PX4	O6-C9-O5-C8
13	C	405	CDL	OA7-CA5-OA6-CA4
13	D	503	CDL	OB9-CB7-OB8-CB6
13	A	503	CDL	OB7-CB5-OB6-CB4
13	D	503	CDL	C31-CA7-OA8-CA6
13	E	205	CDL	C71-CB7-OB8-CB6
17	C	406	PEE	C31-C30-O3-C3
13	C	405	CDL	C31-CA7-OA8-CA6
13	D	503	CDL	C71-CB7-OB8-CB6
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	C	406	PEE	O5-C30-O3-C3
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	D	503	CDL	C51-CB5-OB6-CB4
15	C	403	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	405	CDL	CB4-CB3-OB5-PB2
17	E	204	PEE	O5-C30-O3-C3
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	D	503	CDL	OA5-CA3-CA4-OA6
16	C	404	PG4	O2-C3-C4-O3
13	E	205	CDL	O1-C1-CA2-OA2
13	G	101	CDL	O1-C1-CB2-OB2
13	E	205	CDL	OB9-CB7-OB8-CB6
13	D	503	CDL	CA5-C11-C12-C13
13	E	205	CDL	CB5-C51-C52-C53
21	E	202	PX4	C9-C10-C11-C12
13	C	405	CDL	OA9-CA7-OA8-CA6
16	C	404	PG4	O4-C7-C8-O5
13	A	503	CDL	CB5-C51-C52-C53
17	E	204	PEE	C10-C11-C12-C13
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
11	A	501	6PE	C1-O3-P1-O8
13	E	205	CDL	CA2-OA2-PA1-OA5
13	A	503	CDL	OA5-CA3-CA4-CA6
18	C	407	JGW	F-C22-O1-C19
15	C	403	LMT	C7-C8-C9-C10
13	E	205	CDL	CA3-CA4-CA6-OA8
17	C	406	PEE	C13-C14-C15-C16
17	C	406	PEE	C31-C32-C33-C34
13	E	205	CDL	C33-C34-C35-C36
13	E	205	CDL	C53-C54-C55-C56
17	E	204	PEE	C15-C16-C17-C18
21	E	202	PX4	C18-C19-C20-C21
15	C	403	LMT	C3-C4-C5-C6
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	D	503	CDL	C11-C12-C13-C14
21	E	202	PX4	C13-C14-C15-C16
13	D	503	CDL	C51-C52-C53-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	403	LMT	C11-C10-C9-C8
21	E	202	PX4	C17-C18-C19-C20
13	E	205	CDL	C51-C52-C53-C54
11	A	501	6PE	C4-C5-C6-C7
13	E	205	CDL	C32-C33-C34-C35
13	E	205	CDL	CB2-C1-CA2-OA2
17	C	406	PEE	C11-C12-C13-C14
17	E	204	PEE	O4-C10-O2-C2
17	C	406	PEE	C10-C11-C12-C13
11	A	501	6PE	C5-C4-O4-C3
17	E	204	PEE	C23-C24-C25-C26
17	C	406	PEE	C32-C33-C34-C35
21	E	202	PX4	C12-C13-C14-C15
13	C	405	CDL	C51-CB5-OB6-CB4
17	E	204	PEE	C11-C10-O2-C2
13	C	405	CDL	OB7-CB5-OB6-CB4
13	E	205	CDL	C52-C53-C54-C55
15	C	403	LMT	O5B-C5B-C6B-O6B
13	E	205	CDL	C51-CB5-OB6-CB4
13	D	503	CDL	CB2-OB2-PB2-OB5
13	C	405	CDL	CB7-C71-C72-C73
13	D	503	CDL	OA5-CA3-CA4-CA6
13	E	205	CDL	C31-C32-C33-C34
17	C	406	PEE	C18-C19-C20-C21
11	A	501	6PE	O5-C4-O4-C3
13	D	503	CDL	CA3-CA4-CA6-OA8
13	C	405	CDL	C71-CB7-OB8-CB6
21	E	202	PX4	C24-C25-C26-C27
18	C	407	JGW	F1-C22-O1-C19
21	E	202	PX4	C10-C11-C12-C13
17	E	204	PEE	C14-C15-C16-C17
13	D	503	CDL	CB6-CB4-OB6-CB5
17	E	204	PEE	O2-C2-C3-O3
13	C	405	CDL	OB9-CB7-OB8-CB6
13	G	101	CDL	CA2-C1-CB2-OB2
17	E	204	PEE	C24-C25-C26-C27
18	C	407	JGW	F2-C22-O1-C19
13	A	503	CDL	OB5-CB3-CB4-CB6
13	D	503	CDL	OB5-CB3-CB4-CB6
17	C	406	PEE	O3P-C1-C2-C3
17	E	204	PEE	C30-C31-C32-C33
17	C	406	PEE	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	E	202	PX4	C16-C17-C18-C19
11	A	501	6PE	C2-C1-O3-P1
21	E	202	PX4	C14-C15-C16-C17
13	D	503	CDL	C54-C55-C56-C57
13	C	405	CDL	CB2-OB2-PB2-OB5
15	C	403	LMT	C4-C5-C6-C7
17	E	204	PEE	C12-C13-C14-C15
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	C23-C24-C25-C26
11	A	501	6PE	O6-C2-C3-O4
13	D	503	CDL	OA6-CA4-CA6-OA8
13	A	503	CDL	C51-C52-C53-C54
13	E	205	CDL	C55-C56-C57-C58
13	E	205	CDL	OB7-CB5-OB6-CB4
17	C	406	PEE	C16-C17-C18-C19
17	E	204	PEE	O3P-C1-C2-C3
17	C	406	PEE	C15-C16-C17-C18
17	E	204	PEE	O3P-C1-C2-O2
16	C	404	PG4	C6-C5-O3-C4
16	C	404	PG4	C4-C3-O2-C2
13	E	205	CDL	C34-C35-C36-C37
16	C	404	PG4	C1-C2-O2-C3
13	E	205	CDL	C36-C37-C38-C39
13	G	101	CDL	C71-CB7-OB8-CB6
13	C	405	CDL	CA3-OA5-PA1-OA4
13	D	503	CDL	CB2-OB2-PB2-OB4
13	E	205	CDL	CA2-OA2-PA1-OA3
13	E	205	CDL	CB3-OB5-PB2-OB4
13	C	405	CDL	OB5-CB3-CB4-CB6
13	D	503	CDL	C31-C32-C33-C34
17	E	204	PEE	C5-C4-O4P-P
13	A	503	CDL	O1-C1-CA2-OA2
11	A	501	6PE	C1-C2-C3-O4
21	E	202	PX4	O3-C1-C2-N1
13	A	503	CDL	CA4-CA3-OA5-PA1
13	G	101	CDL	C1-CA2-OA2-PA1
13	C	405	CDL	C71-C72-C73-C74
13	G	101	CDL	OB9-CB7-OB8-CB6
21	E	202	PX4	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	E	204	PEE	C1-O3P-P-O4P
15	C	403	LMT	C5-C6-C7-C8
17	E	204	PEE	C1-C2-C3-O3
17	E	204	PEE	C3-C2-O2-C10
17	E	204	PEE	C4-O4P-P-O3P
13	D	503	CDL	C12-C13-C14-C15
14	C	401	HEM	C3D-CAD-CBD-CGD
21	E	202	PX4	C11-C10-C9-O5
21	E	202	PX4	O4-C6-C7-O7
13	D	503	CDL	OB6-CB4-CB6-OB8
21	E	202	PX4	C1-C2-N1-C4
13	E	205	CDL	CA7-C31-C32-C33
17	E	204	PEE	C31-C32-C33-C34
13	D	503	CDL	CB5-C51-C52-C53
21	E	202	PX4	C11-C10-C9-O6
13	A	503	CDL	CB2-OB2-PB2-OB3
13	A	503	CDL	CB3-OB5-PB2-OB3
13	G	101	CDL	CB2-OB2-PB2-OB3
21	E	202	PX4	C6-O4-P1-O2
13	E	205	CDL	C32-C31-CA7-OA8
13	C	405	CDL	O1-C1-CA2-OA2
17	C	406	PEE	O3-C30-C31-C32
11	A	501	6PE	O4-C4-C5-C6
13	G	101	CDL	C72-C71-CB7-OB8
15	C	403	LMT	C2-C1-O1'-C1'
17	C	406	PEE	O5-C30-C31-C32

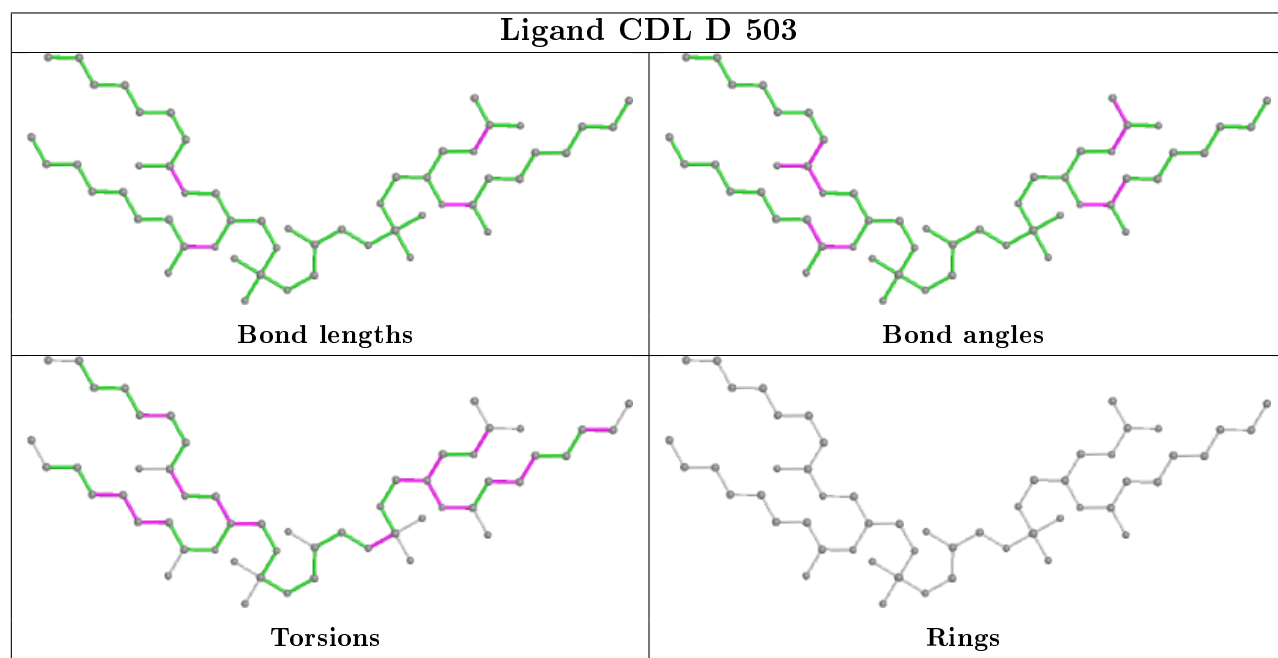
There are no ring outliers.

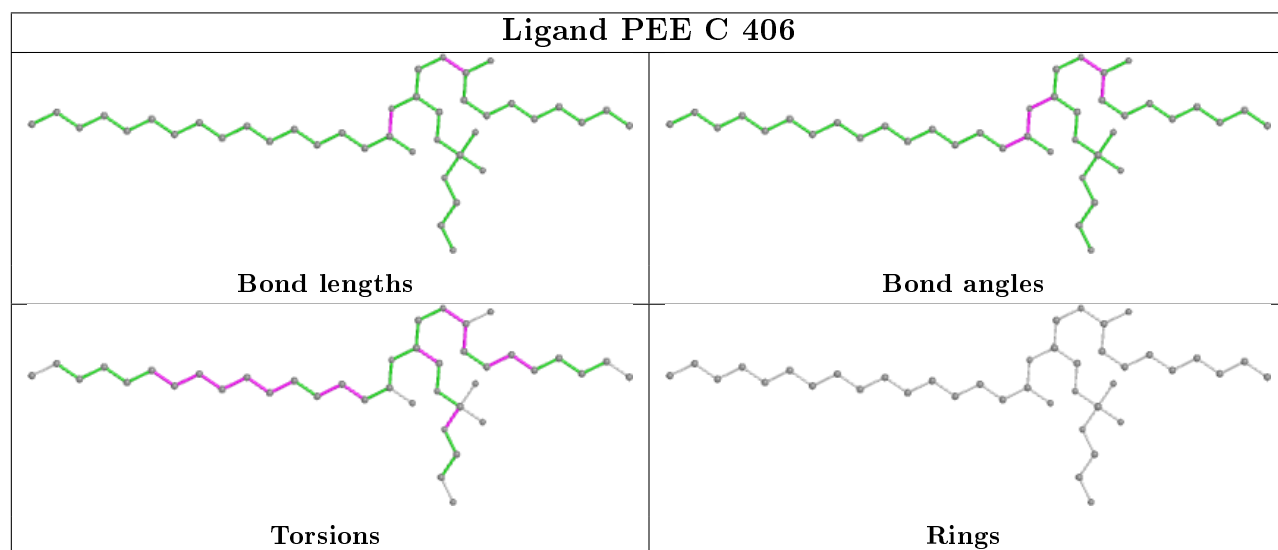
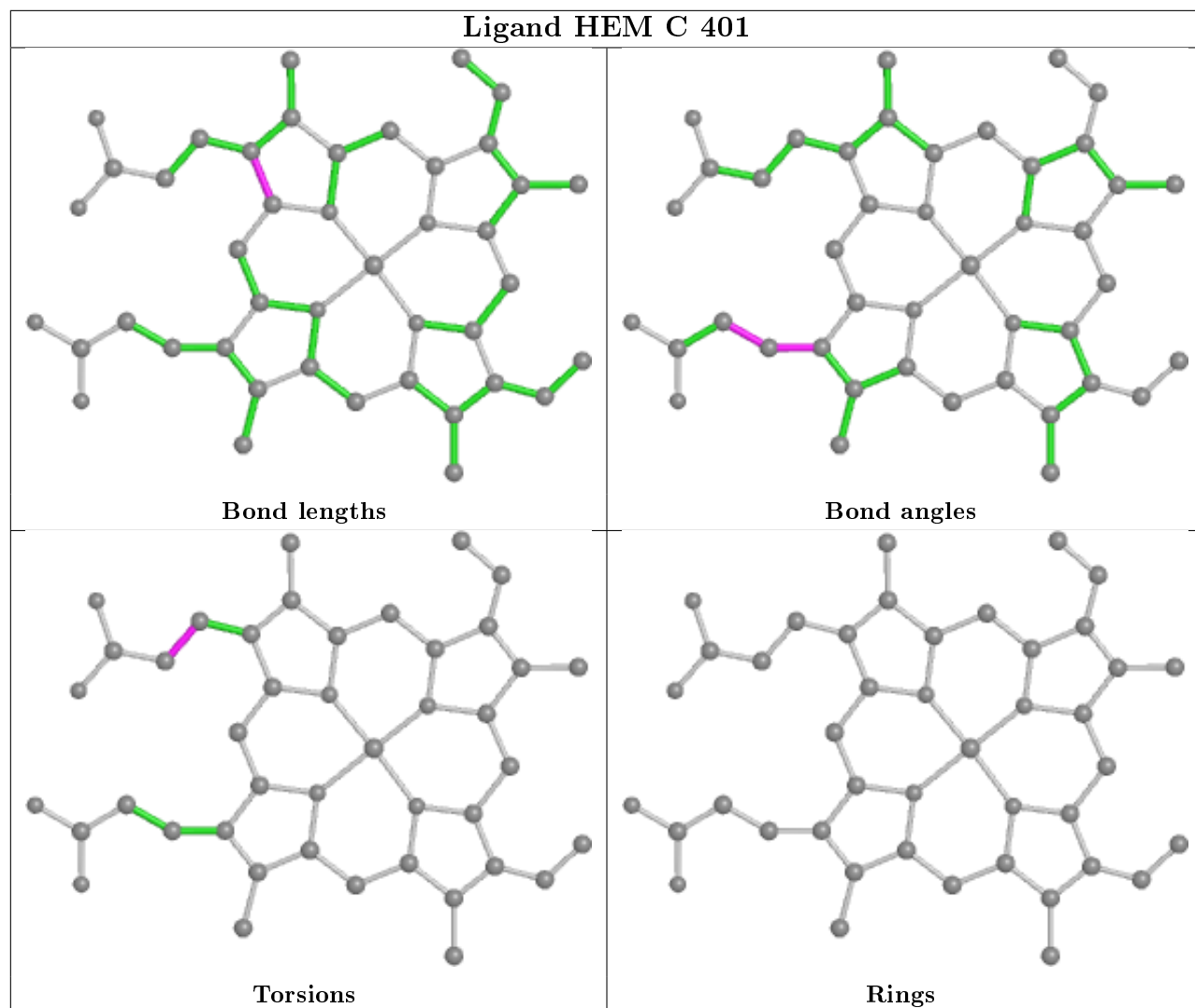
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	401	HEM	3	0
14	C	402	HEM	2	0
21	E	202	PX4	1	0
19	D	501	HEC	6	0

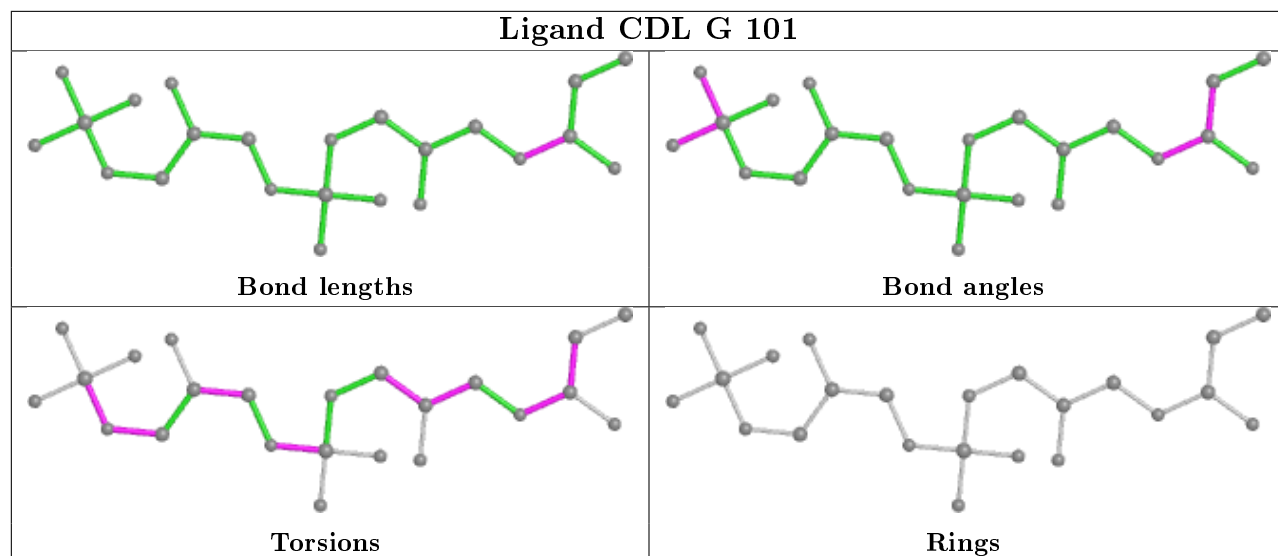
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

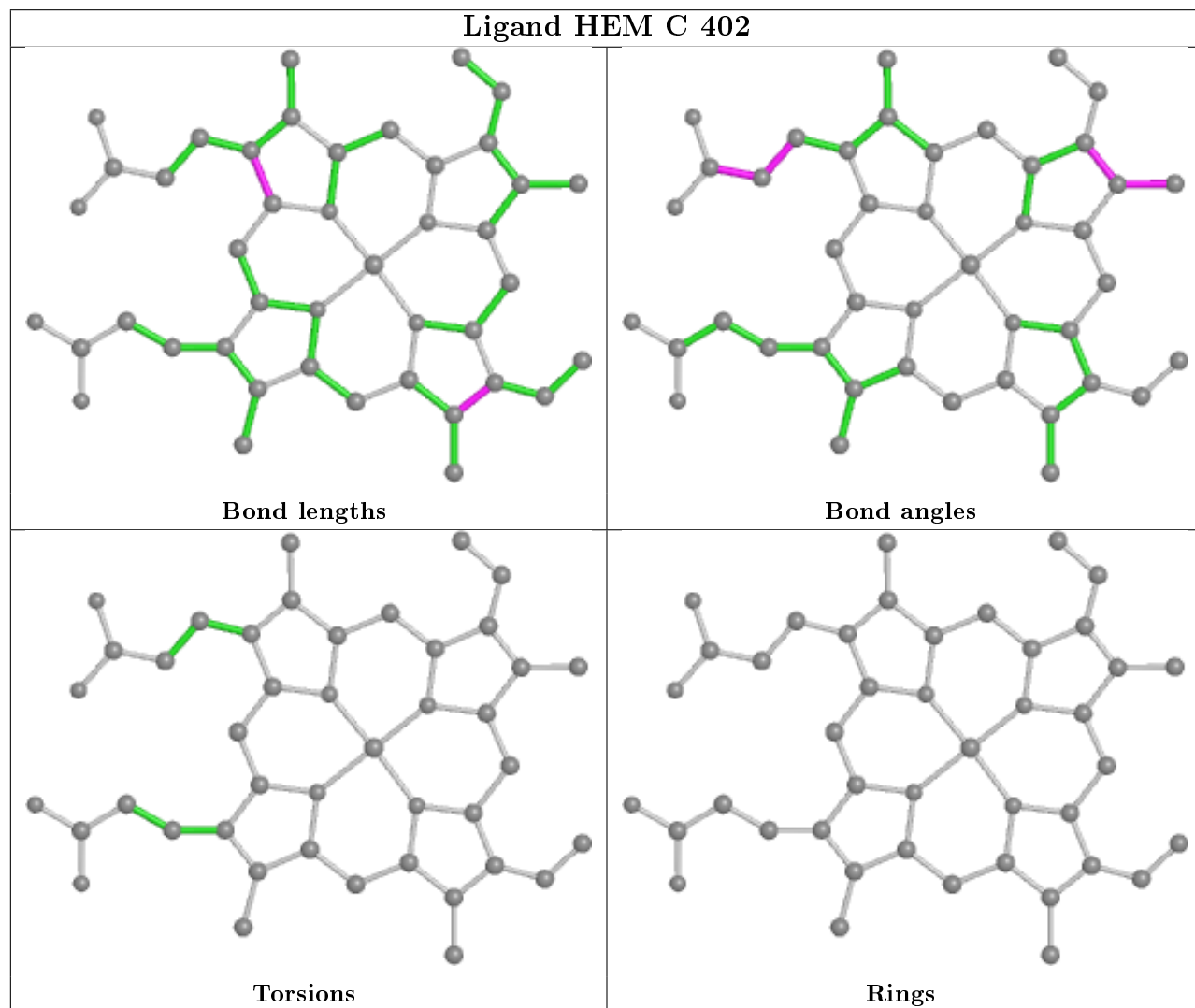


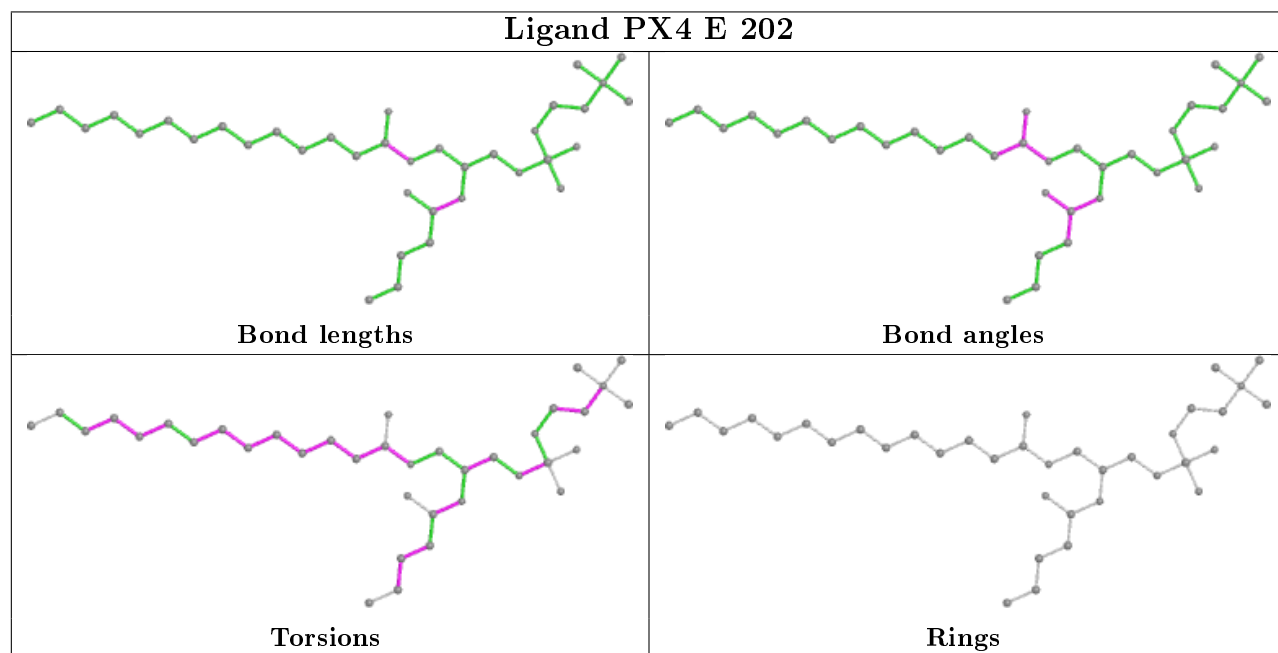
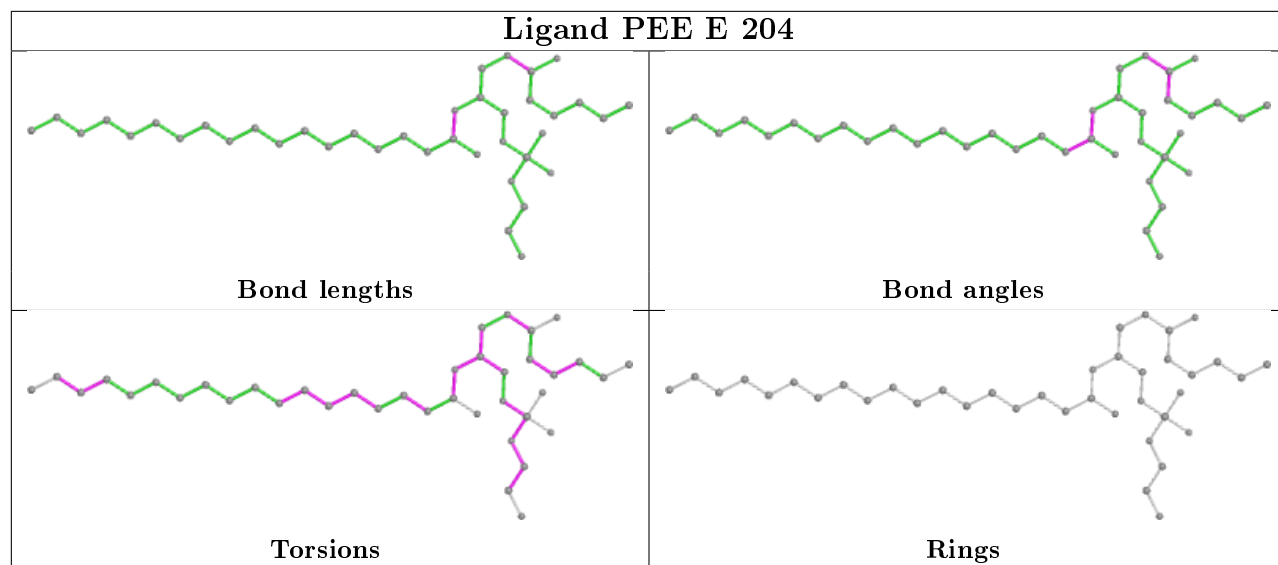


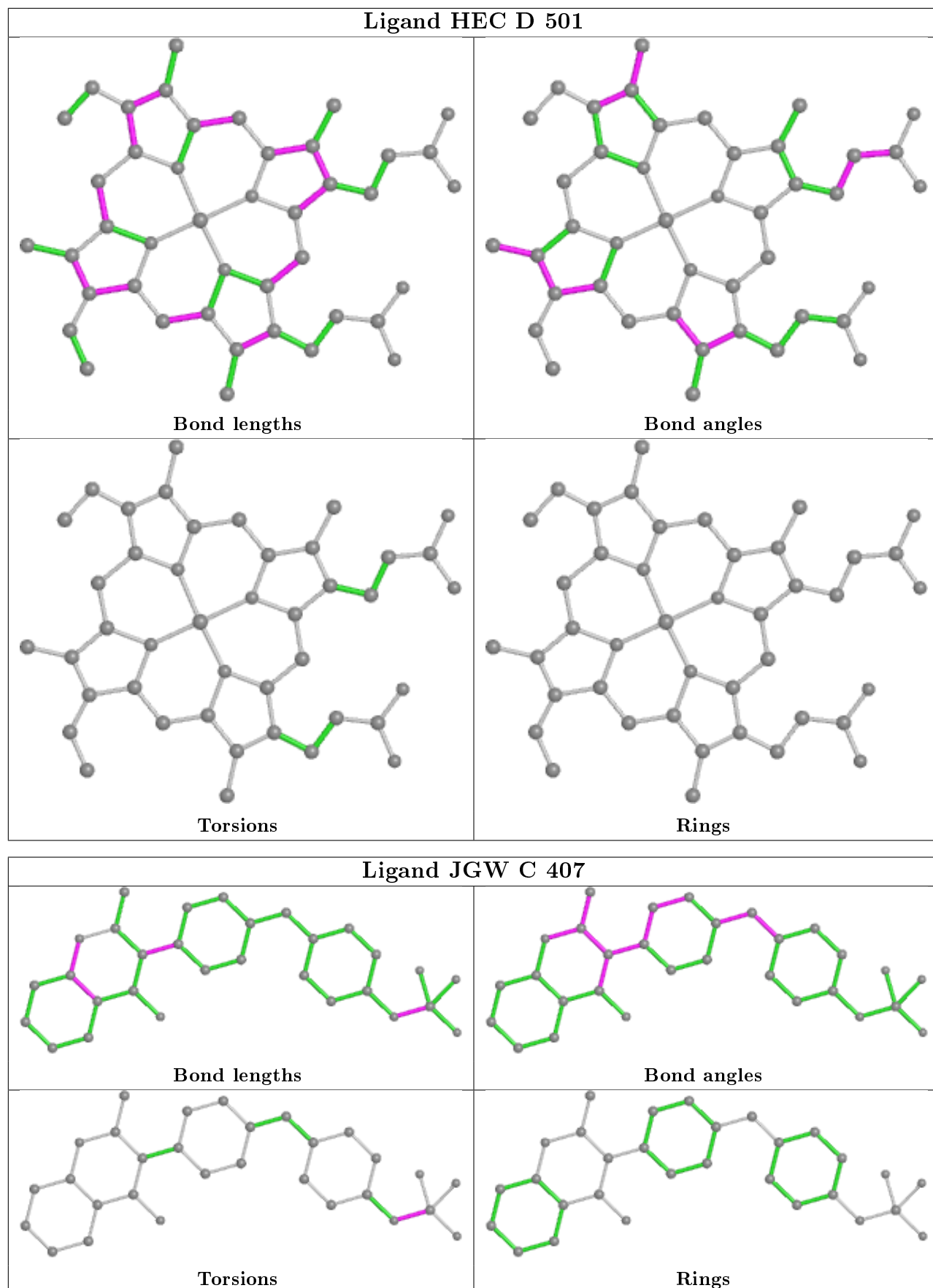
Ligand CDL G 101

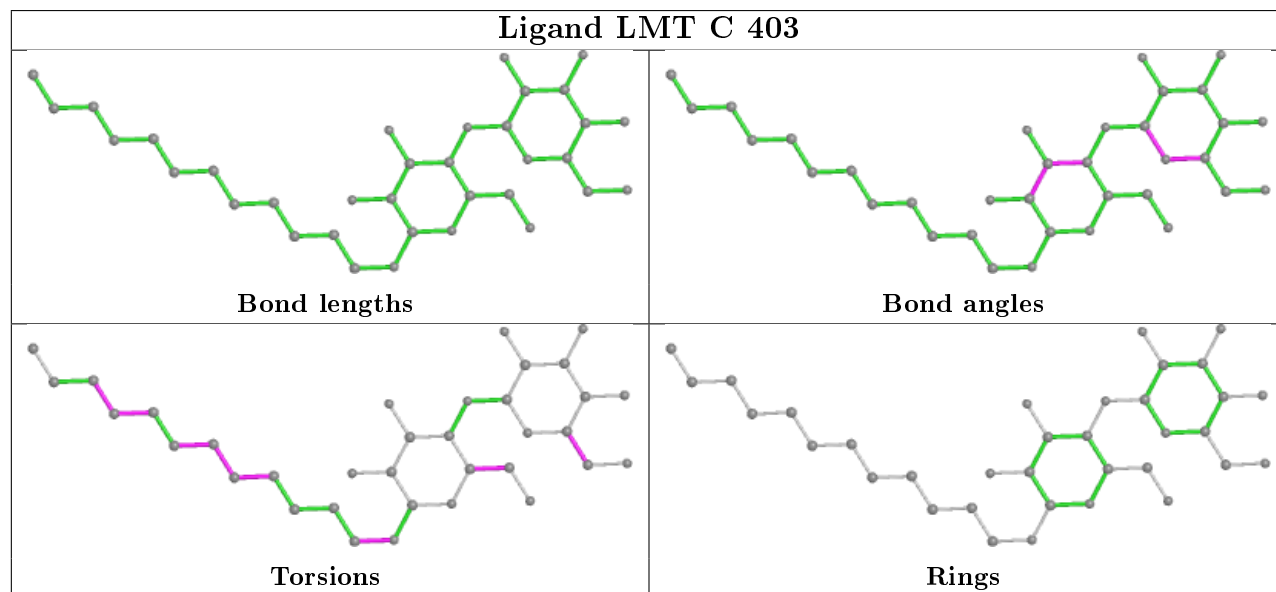
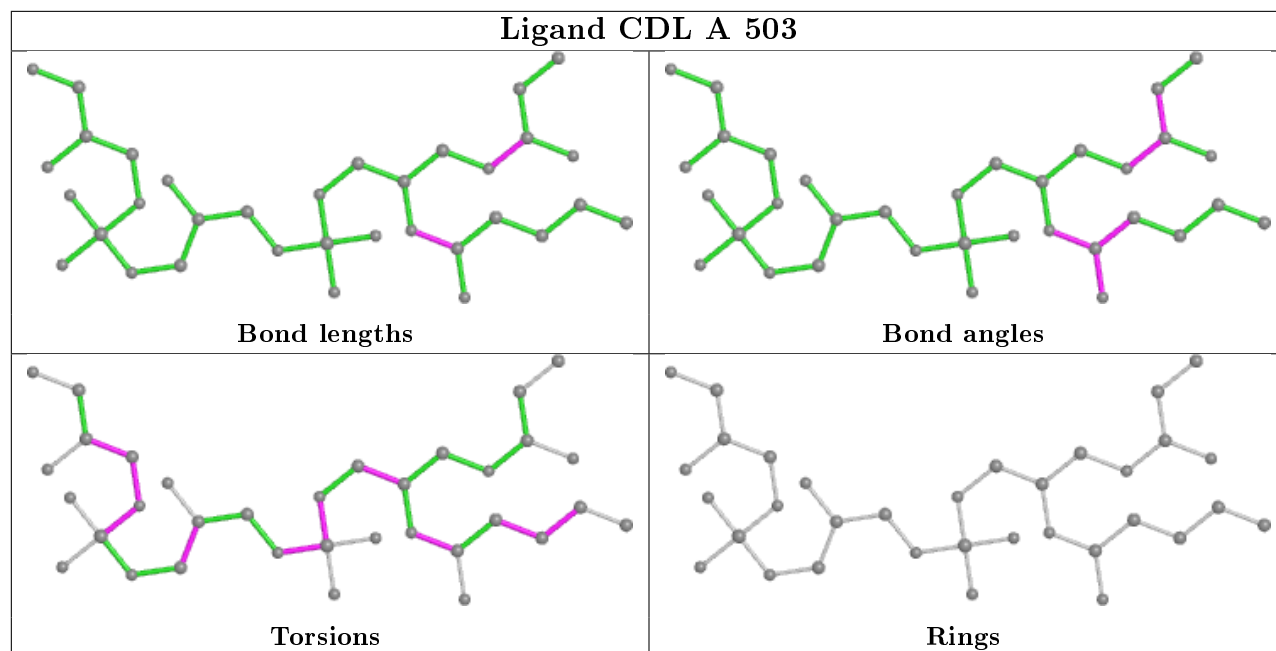


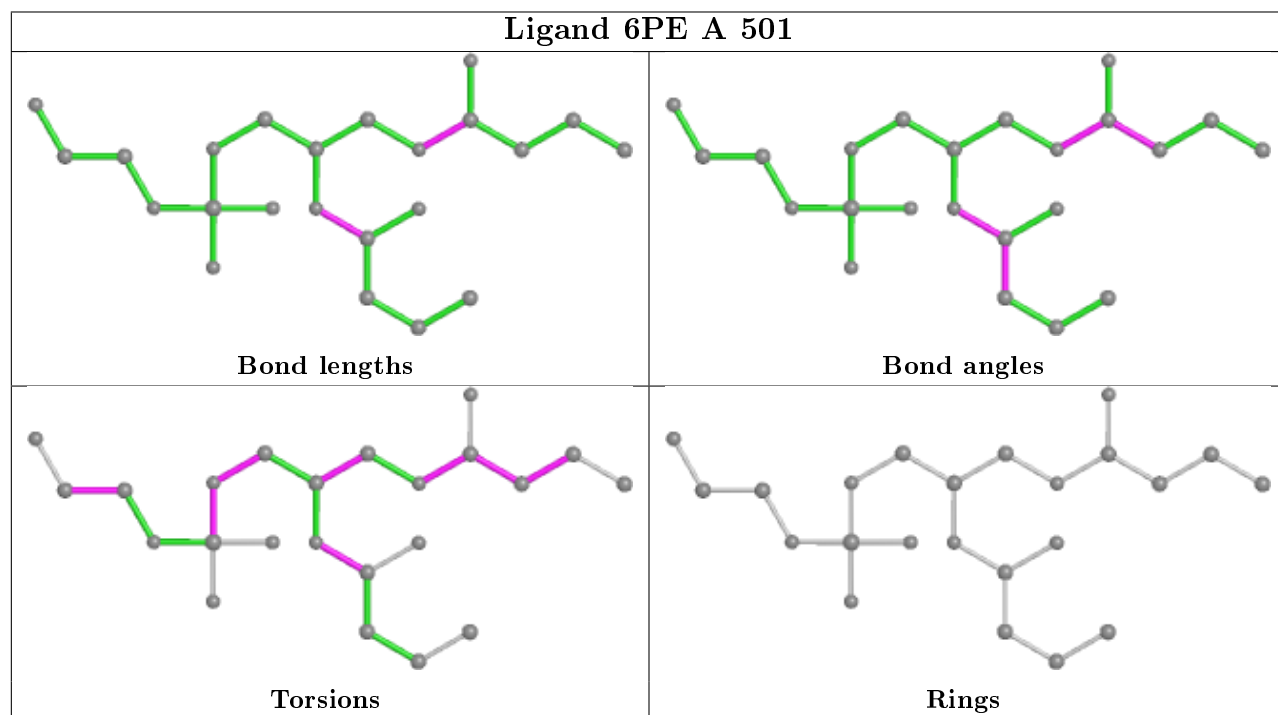
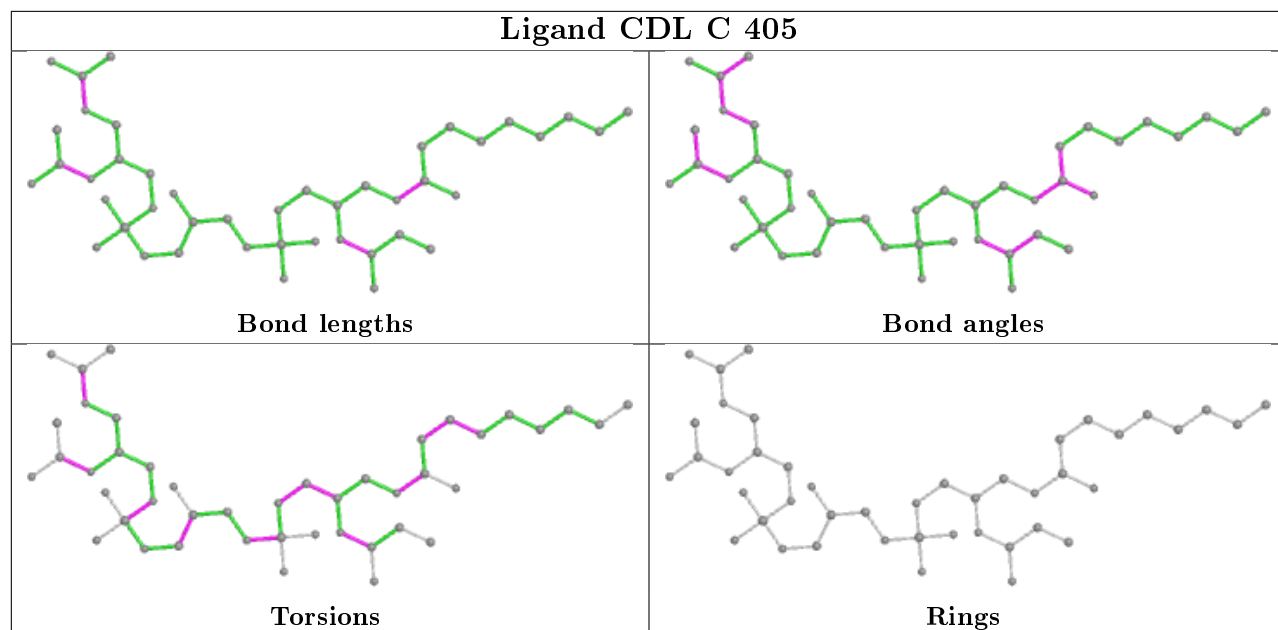
Ligand HEM C 402

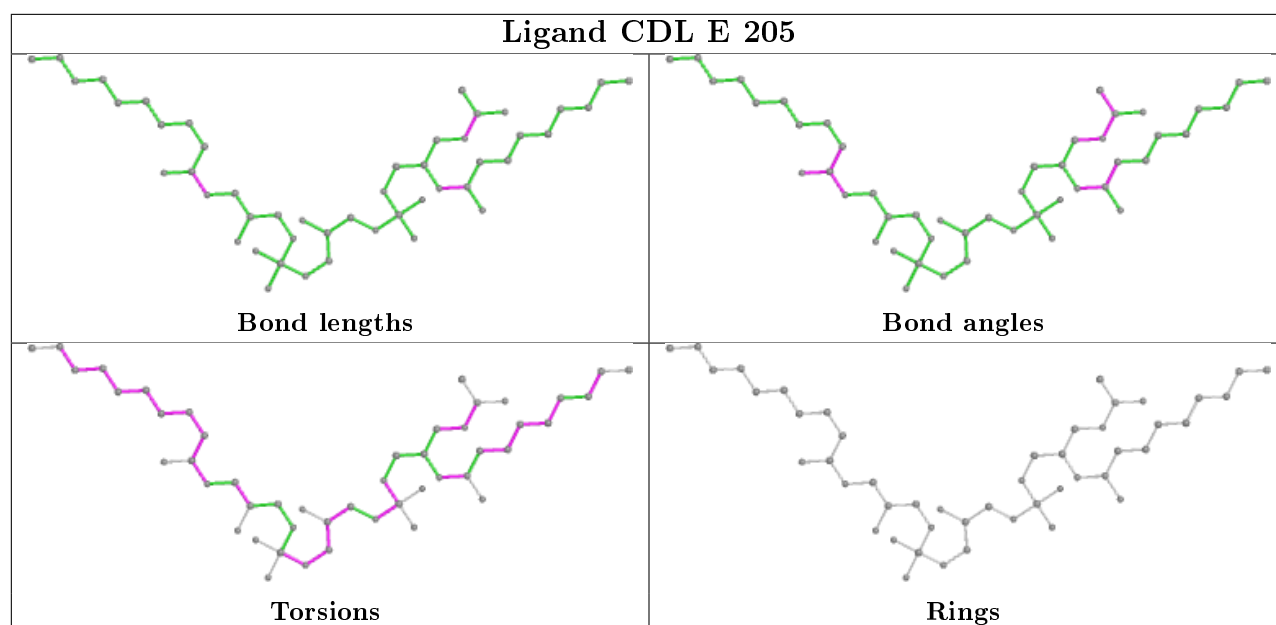












5.7 Other polymers [i](#)

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	441/444 (99%)	0.39	25 (5%) 23 21	91, 122, 152, 185	0
2	B	415/420 (98%)	-0.03	0 100 100	98, 126, 159, 220	0
3	C	378/378 (100%)	-0.19	0 100 100	90, 114, 147, 180	0
4	D	239/239 (100%)	0.47	17 (7%) 16 15	108, 147, 174, 191	0
5	E	195/196 (99%)	0.03	5 (2%) 56 49	103, 180, 222, 242	0
6	F	99/99 (100%)	-0.28	0 100 100	70, 120, 155, 199	0
7	G	75/75 (100%)	-0.24	1 (1%) 77 71	96, 123, 163, 187	0
8	H	64/64 (100%)	0.74	4 (6%) 20 18	154, 181, 197, 206	0
9	I	46/46 (100%)	0.52	2 (4%) 35 31	144, 180, 201, 204	0
10	J	59/59 (100%)	-0.12	0 100 100	114, 136, 183, 201	0
All	All	2011/2020 (99%)	0.11	54 (2%) 54 48	70, 128, 190, 242	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	149	PHE	5.4
4	D	158	ILE	3.8
4	D	148	TYR	3.7
4	D	134	TYR	3.5
4	D	180	SER	3.3
5	E	146	PRO	3.2
1	A	40	TRP	3.1
1	A	23	LEU	3.1
4	D	21	LEU	3.1
1	A	229	PRO	3.0
1	A	216	PHE	3.0
5	E	160	CYS	3.0
4	D	159	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	161	HIS	2.9
4	D	151	PRO	2.9
5	E	144	CYS	2.9
1	A	200	ALA	2.9
4	D	157	ALA	2.7
1	A	17	SER	2.7
8	H	61	PHE	2.7
1	A	222	THR	2.7
1	A	199	ALA	2.7
1	A	194	ARG	2.7
4	D	172	ASP	2.6
1	A	2	ALA	2.6
8	H	45	SER	2.6
4	D	138	PRO	2.5
1	A	383	LEU	2.5
1	A	202	GLY	2.5
8	H	44	VAL	2.5
1	A	205	HIS	2.5
4	D	165	TYR	2.4
8	H	46	SER	2.4
1	A	195	MET	2.4
9	I	43	LEU	2.4
4	D	171	PHE	2.4
1	A	21	ASN	2.3
1	A	24	ARG	2.3
1	A	26	ALA	2.3
5	E	159	PRO	2.3
4	D	166	ASN	2.2
1	A	201	GLY	2.2
1	A	371	GLY	2.1
1	A	370	ASP	2.1
1	A	98	TYR	2.1
4	D	150	ASN	2.1
1	A	228	VAL	2.1
7	G	1	GLY	2.1
4	D	198	HIS	2.1
1	A	227	THR	2.1
9	I	37	THR	2.1
4	D	173	ASP	2.0
1	A	374	PRO	2.0
1	A	14	THR	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 monosaccharides in this entry.

6.4 Ligands ⓘ

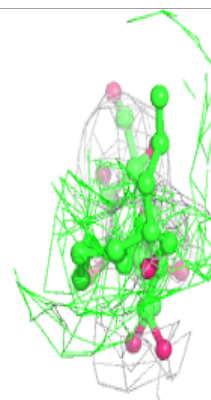
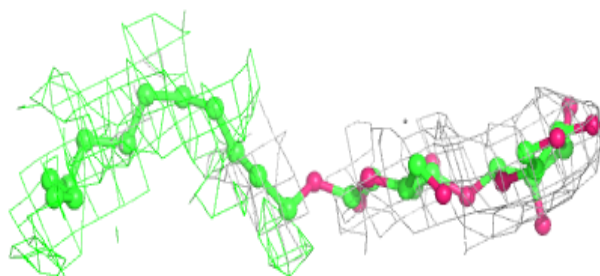
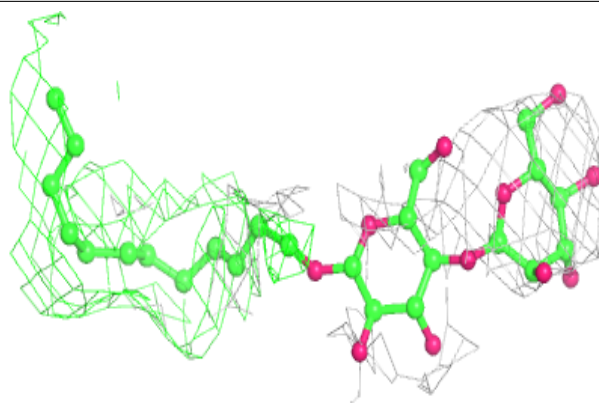
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	PO4	G	103	5/5	0.43	0.28	214,215,217,222	0
15	LMT	C	403	35/35	0.44	0.27	179,215,223,223	0
12	PO4	E	203	5/5	0.46	0.28	205,209,210,211	0
13	CDL	G	101	23/100	0.61	0.25	141,201,207,213	0
12	PO4	G	104	5/5	0.68	0.23	185,186,188,190	0
12	PO4	D	502	5/5	0.72	0.26	200,202,207,207	0
13	CDL	E	205	48/100	0.75	0.24	147,179,222,226	0
12	PO4	A	502	5/5	0.78	0.47	129,129,132,137	0
12	PO4	G	102	5/5	0.81	0.18	156,156,160,161	0
16	PG4	C	404	13/13	0.81	0.53	119,126,136,136	0
12	PO4	F	501	5/5	0.82	0.26	171,176,178,179	0
13	CDL	A	503	34/100	0.83	0.26	150,182,190,193	0
18	JGW	C	407	30/30	0.83	0.51	111,133,186,190	0
17	PEE	E	204	39/51	0.85	0.64	117,122,128,131	0
21	PX4	E	202	37/46	0.88	0.38	132,142,151,152	0
13	CDL	D	503	54/100	0.90	0.38	105,146,183,186	0
11	6PE	A	501	23/27	0.91	0.23	141,159,170,170	0
13	CDL	C	405	44/100	0.93	0.30	121,129,141,145	0
20	FES	E	201	4/4	0.94	0.17	254,258,263,267	0
17	PEE	C	406	40/51	0.94	0.35	103,111,116,117	0
14	HEM	C	402	43/43	0.97	0.28	95,96,99,101	0
19	HEC	D	501	43/43	0.97	0.42	141,151,161,164	0
14	HEM	C	401	43/43	0.98	0.33	106,109,111,113	0

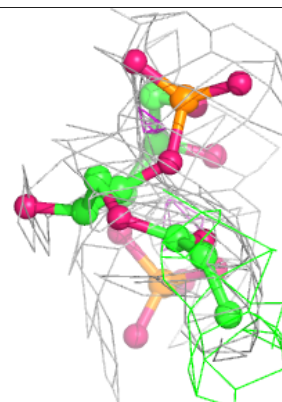
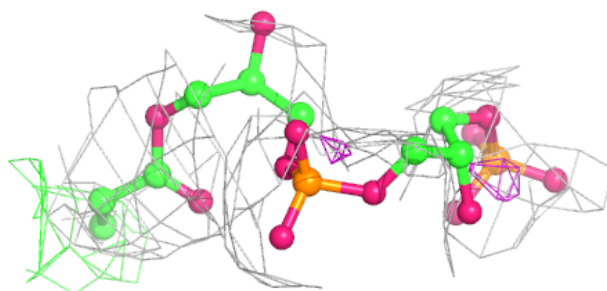
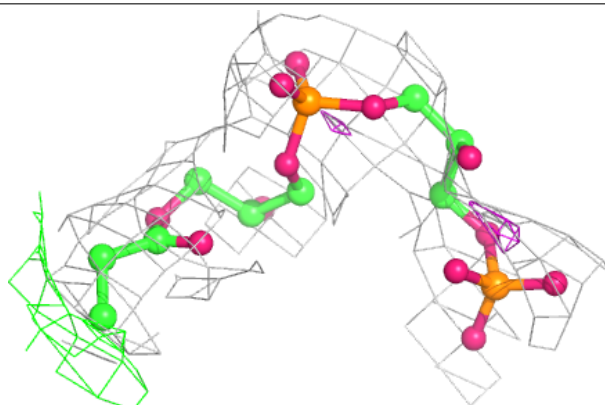
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

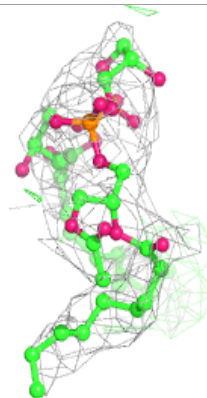
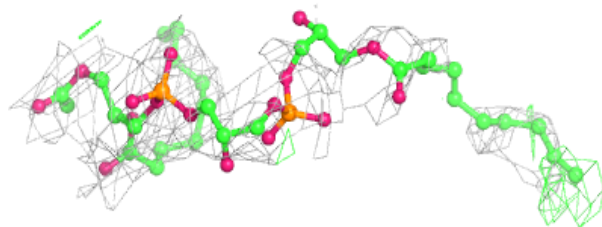
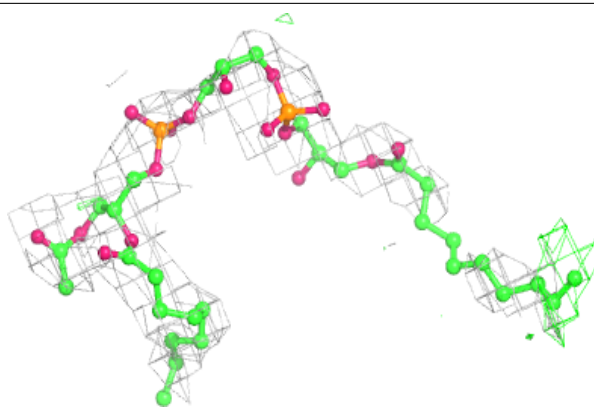
**Electron density around CDL G 101:**

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



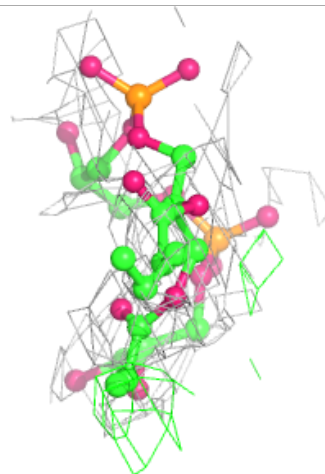
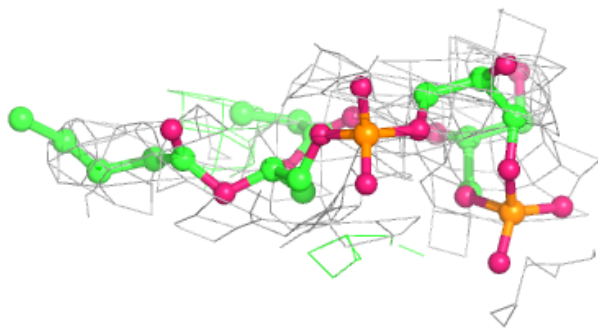
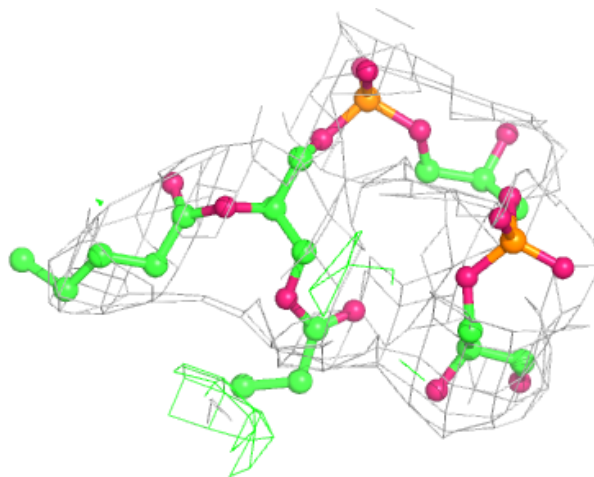
Electron density around CDL E 205:

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



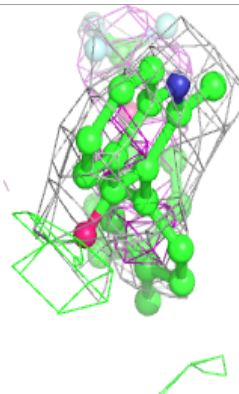
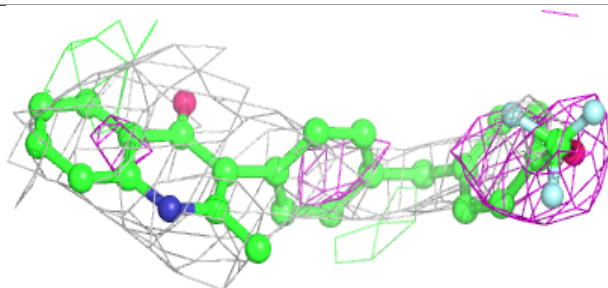
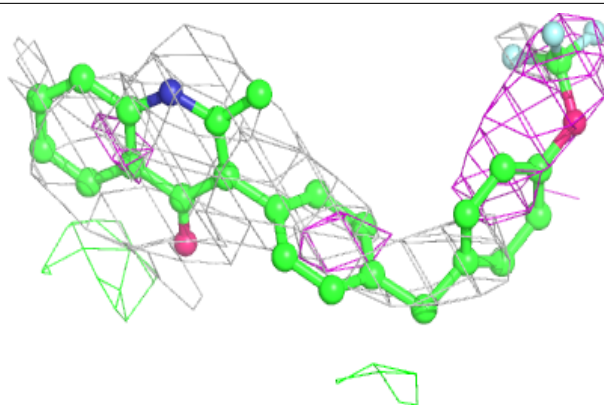
Electron density around CDL A 503:

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

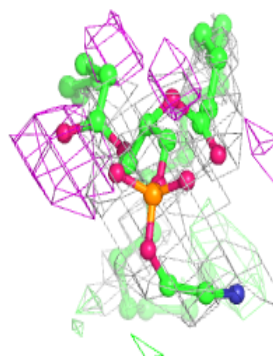
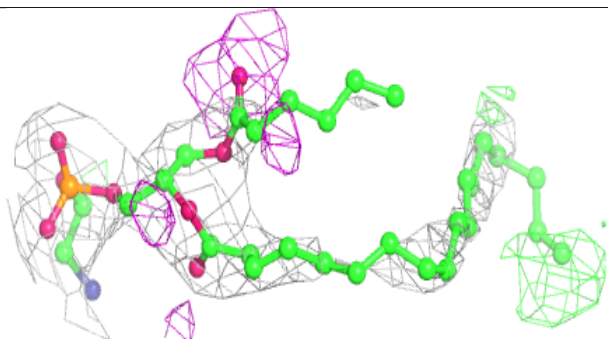
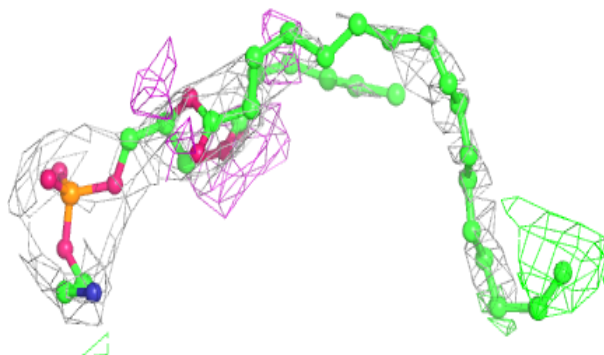


Electron density around JGW C 407:

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

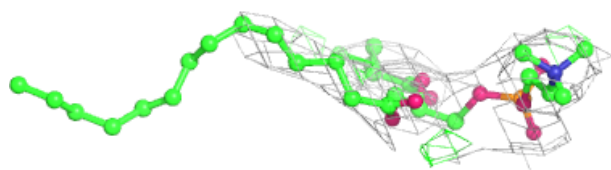
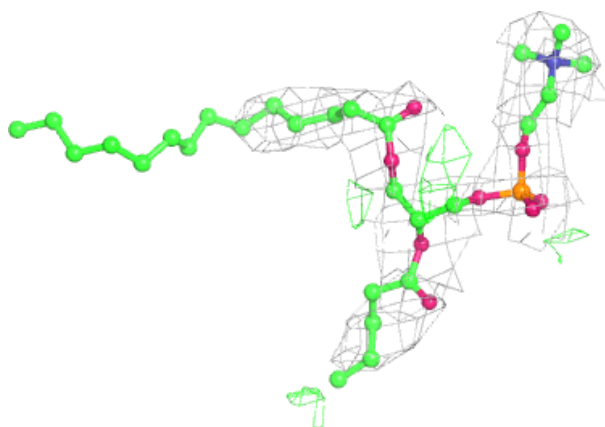
**Electron density around PEE E 204:**

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

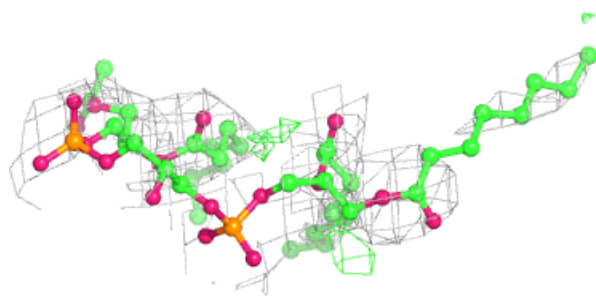
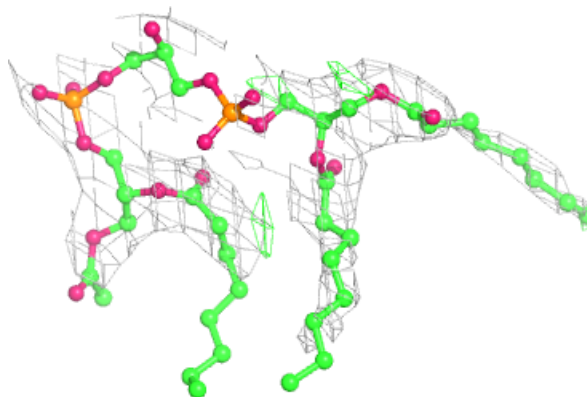


Electron density around PX4 E 202:

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

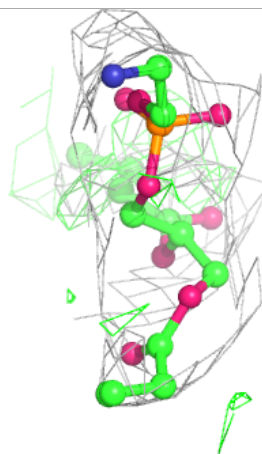
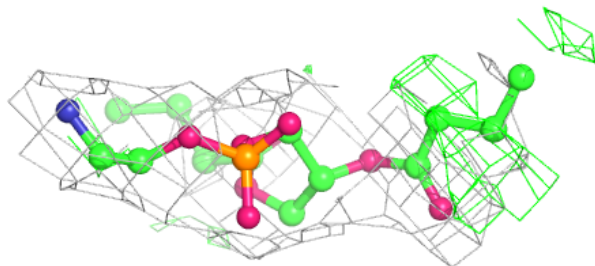
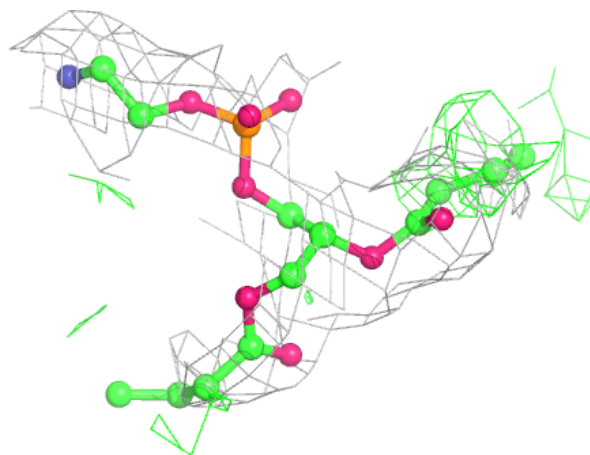
**Electron density around CDL D 503:**

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



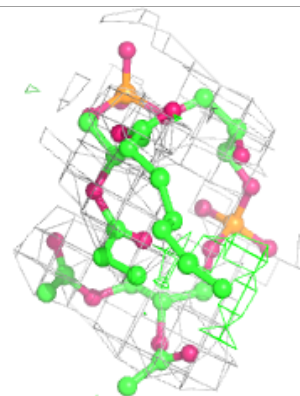
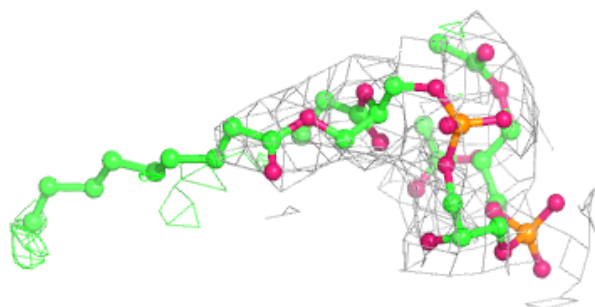
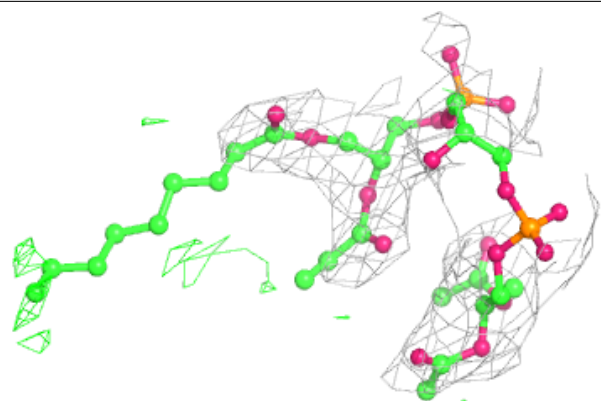
Electron density around 6PE A 501:

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

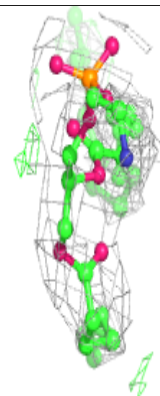
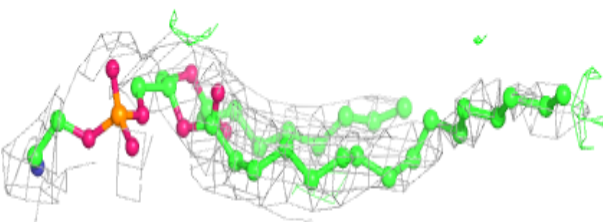
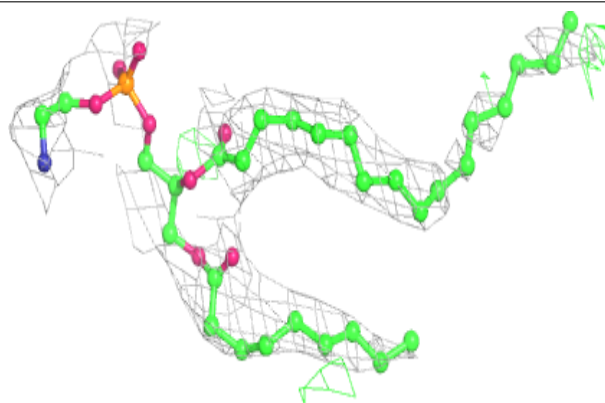


Electron density around CDL C 405:

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

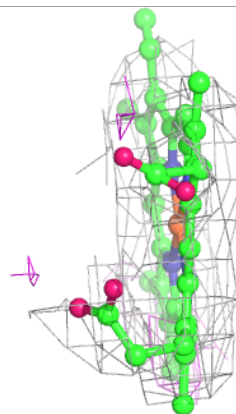
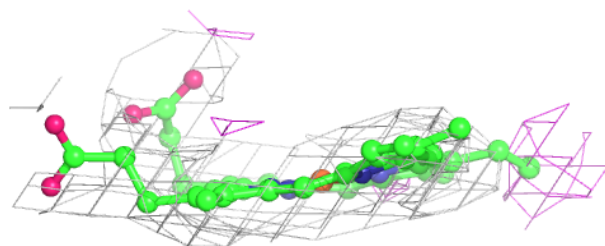
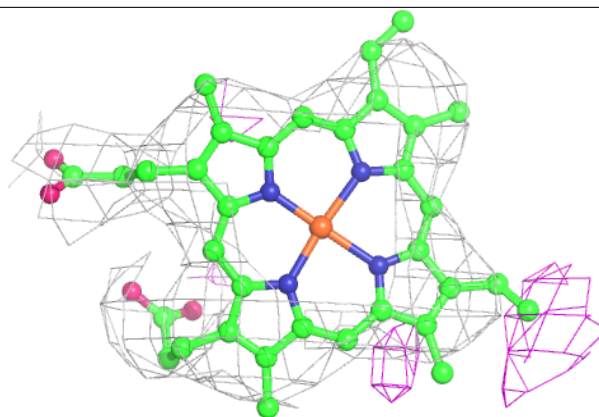
**Electron density around PEE C 406:**

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



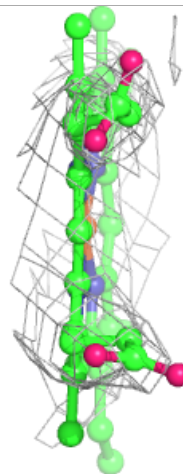
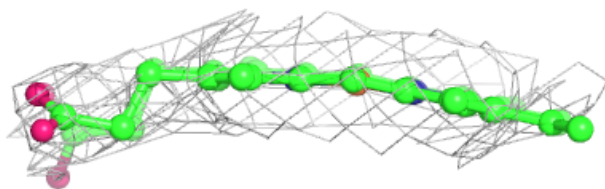
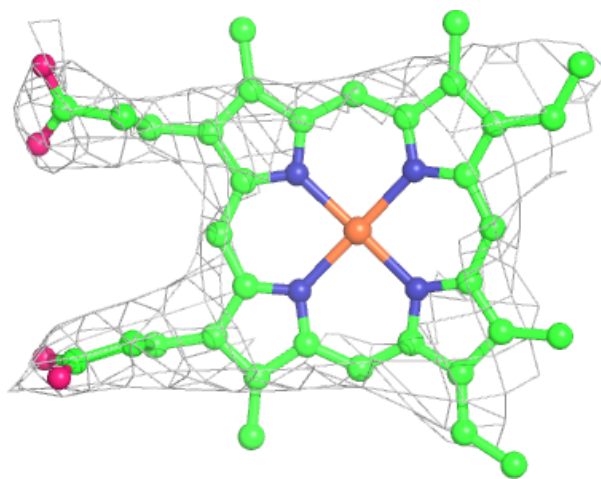
Electron density around HEM C 402:

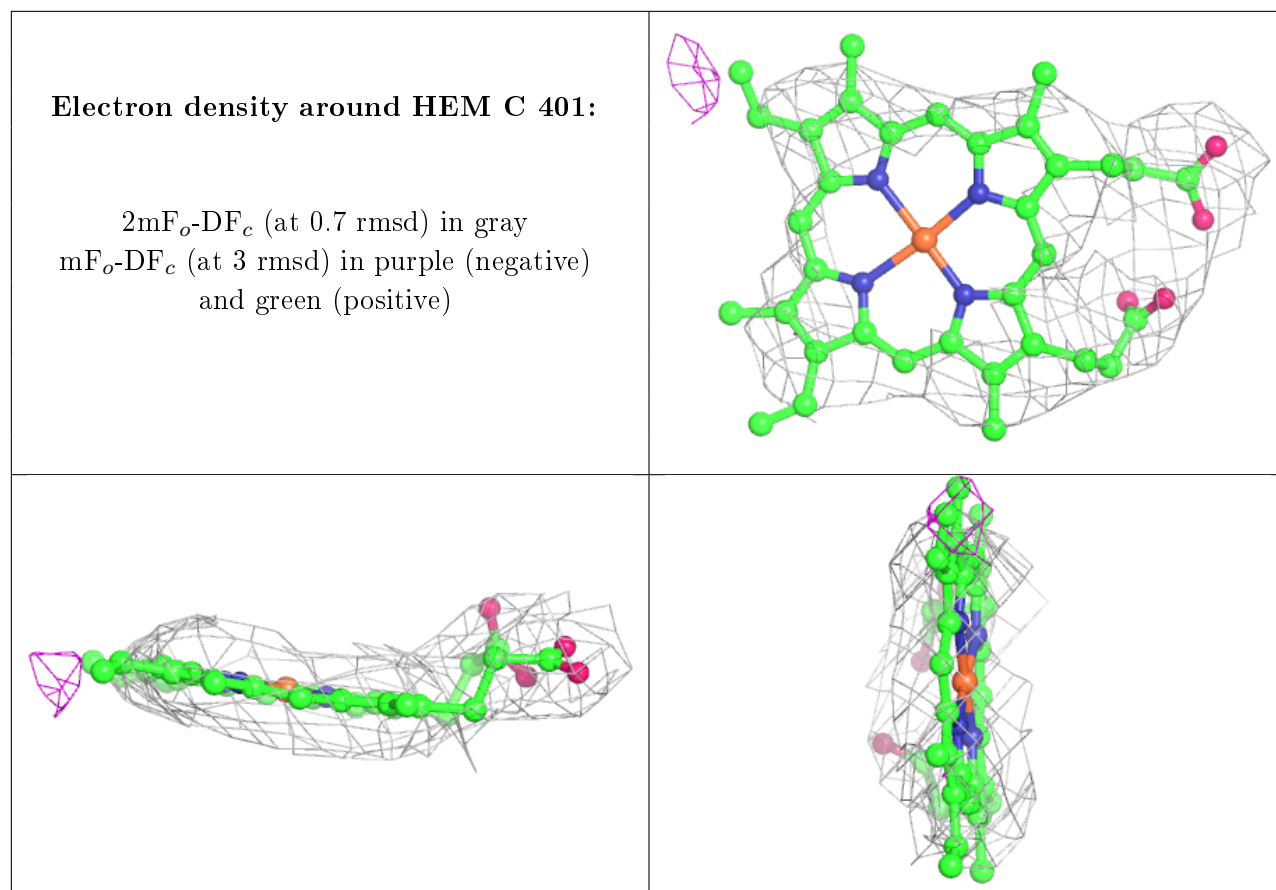
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.