



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:48 AM UTC

PDB ID : 6H1T / pdb_00006h1t
Title : Structure of the BM3 heme domain in complex with clotrimazole
Authors : Jeffreys, L.N.; Munro, A.W.M.; Leys, D.
Deposited on : 2018-07-12
Resolution : 2.08 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

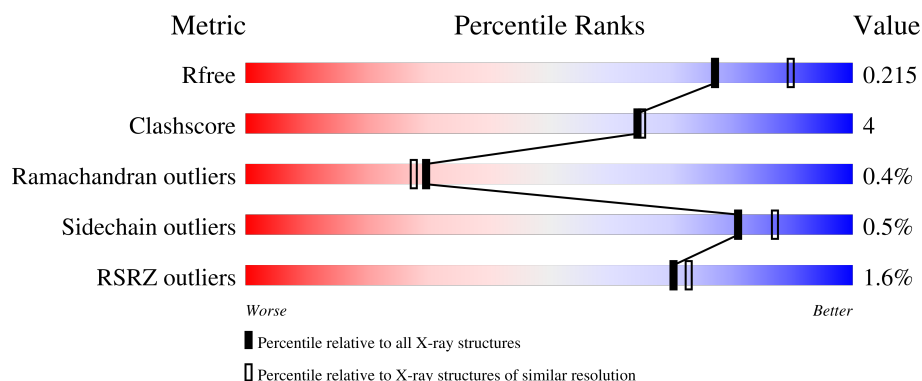
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	458	0% 93% 5%
1	B	458	2% 94% 5%
1	C	458	2% 94% 5%
1	D	458	2% 92% 6%

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
4	MPD	B	511	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16392 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.

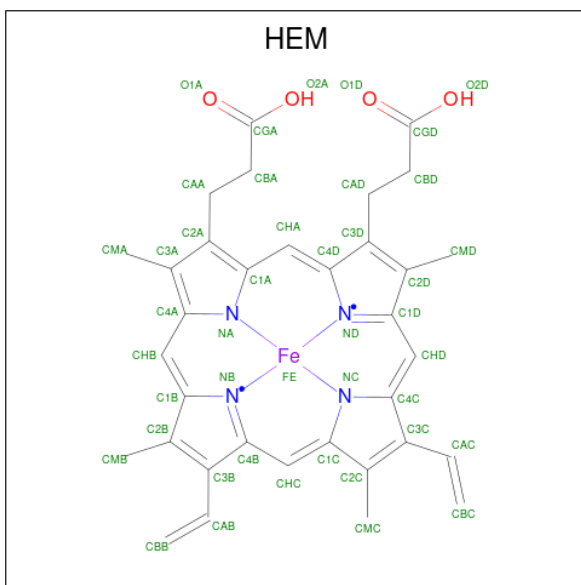
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	7	0
			3729	2383	634	695	17			
1	B	456	Total	C	N	O	S	0	2	0
			3691	2358	627	689	17			
1	C	456	Total	C	N	O	S	0	4	0
			3700	2363	629	691	17			
1	D	456	Total	C	N	O	S	0	5	0
			3710	2370	630	693	17			

There are 8 discrepancies between the modelled and reference sequences:

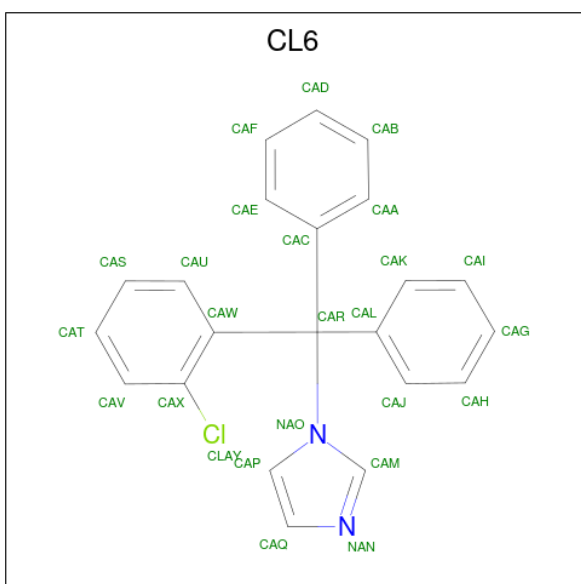
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	ALA	engineered mutation	UNP A0A1Q8UP87
A	87	VAL	PHE	engineered mutation	UNP A0A1Q8UP87
B	82	PHE	ALA	engineered mutation	UNP A0A1Q8UP87
B	87	VAL	PHE	engineered mutation	UNP A0A1Q8UP87
C	82	PHE	ALA	engineered mutation	UNP A0A1Q8UP87
C	87	VAL	PHE	engineered mutation	UNP A0A1Q8UP87
D	82	PHE	ALA	engineered mutation	UNP A0A1Q8UP87
D	87	VAL	PHE	engineered mutation	UNP A0A1Q8UP87

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



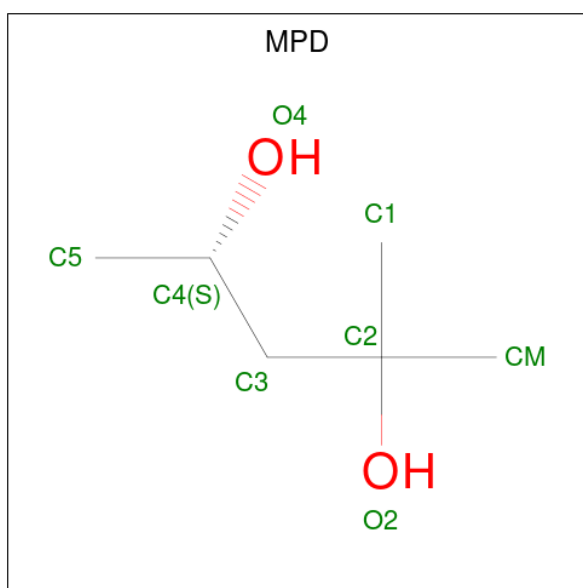
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1-[(2-CHLOROPHENYL)(DIPHENYL)METHYL]-1H-IMIDAZOLE (CCD ID: CL6) (formula: C₂₂H₁₇ClN₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



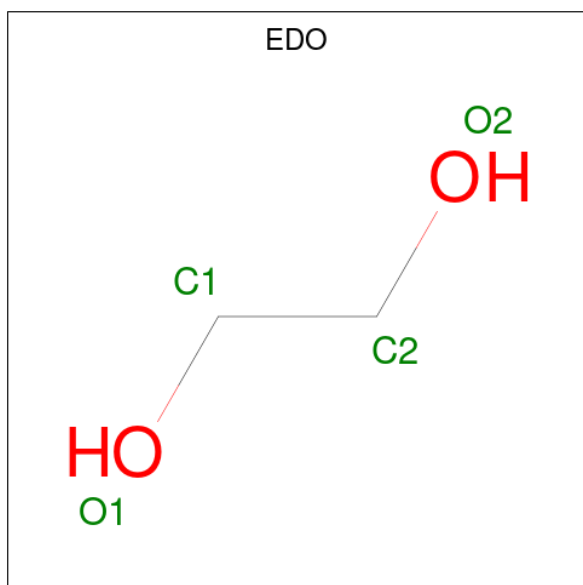
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



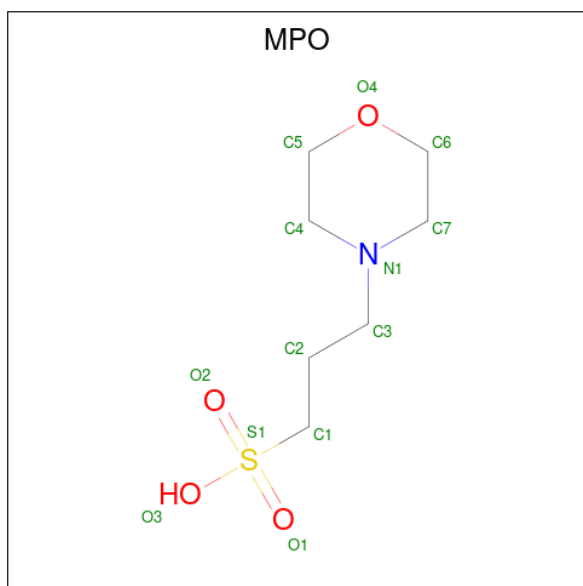
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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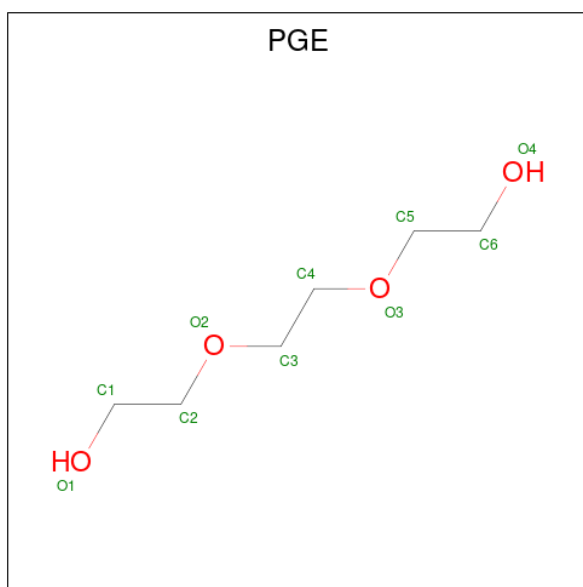
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



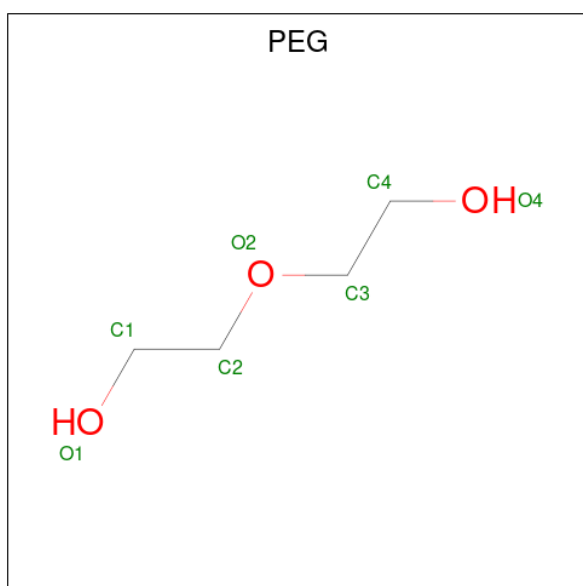
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			7	4	3		

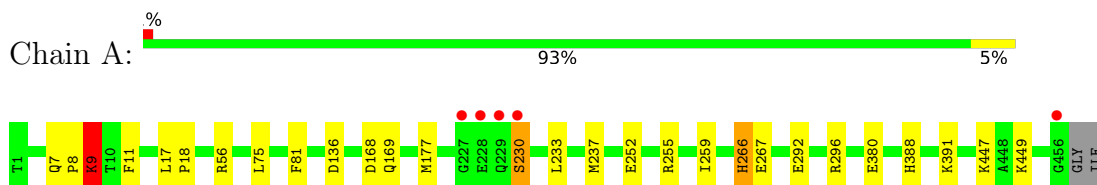
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	278	Total 278	O 278	0	0
9	B	275	Total 275	O 275	0	0
9	C	265	Total 265	O 265	0	0
9	D	279	Total 279	O 279	0	0

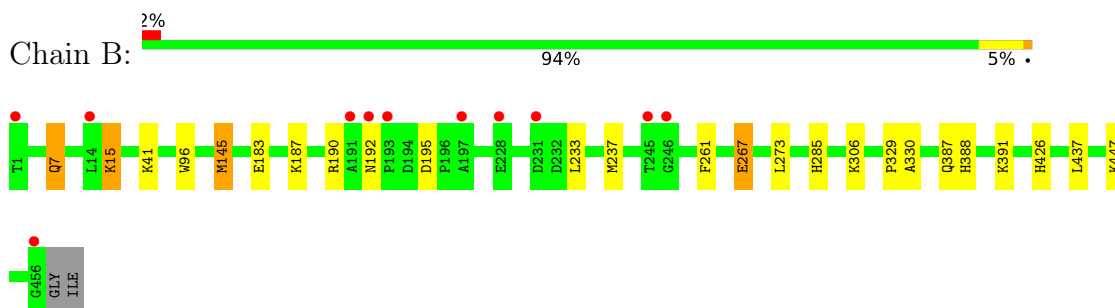
3 Residue-property plots

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.

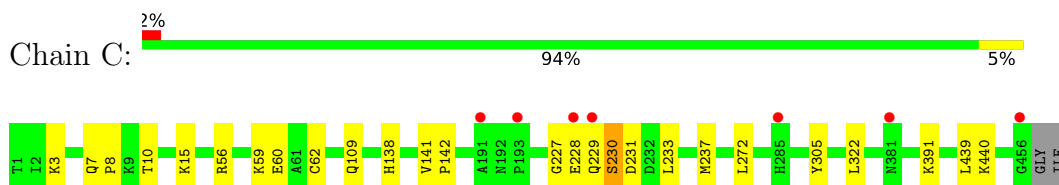
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



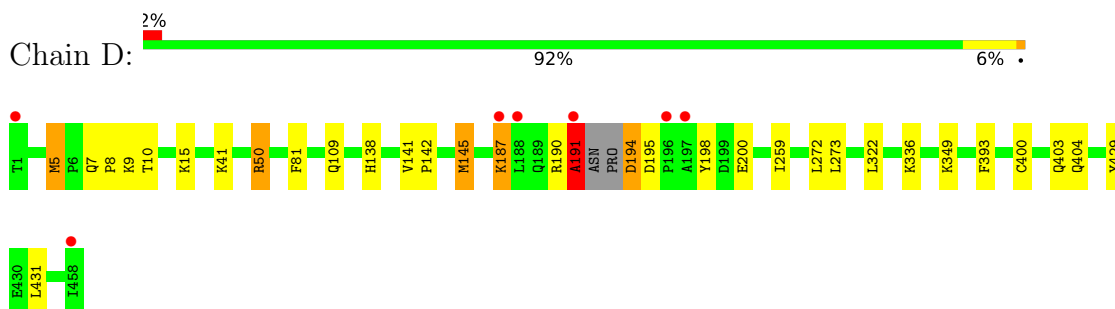
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.41Å 70.75Å 209.64Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	48.32 – 2.08 48.32 – 2.08	Depositor EDS
% Data completeness (in resolution range)	91.6 (48.32-2.08) 91.6 (48.32-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.167 , 0.207 0.174 , 0.215	Depositor DCC
R_{free} test set	6344 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16392	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MPO, PEG, HEM, EDO, CL6, PGE, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.06	0/3827	0.82	5/5174 (0.1%)
1	B	1.04	0/3779	0.83	5/5110 (0.1%)
1	C	1.00	0/3789	0.76	0/5123
1	D	1.23	2/3800 (0.1%)	0.84	3/5136 (0.1%)
All	All	1.09	2/15195 (0.0%)	0.81	13/20543 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	191	ALA	C-N	40.71	1.90	1.33
1	D	50	ARG	CZ-NH1	5.16	1.40	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	MET	CG-SD-CE	11.46	126.12	100.90
1	D	191	ALA	CA-C-N	11.36	143.24	121.54
1	D	191	ALA	C-N-CA	11.36	143.24	121.54
1	A	17	LEU	CA-C-N	-9.91	109.45	120.45
1	A	17	LEU	C-N-CA	-9.91	109.45	120.45
1	A	9	LYS	CB-CA-C	6.01	119.92	109.65
1	D	145	MET	CG-SD-CE	5.71	113.45	100.90
1	B	267	GLU	N-CA-C	5.62	117.08	111.07
1	A	266	HIS	N-CA-C	5.61	119.45	111.99
1	B	96	TRP	CA-CB-CG	-5.26	103.61	113.60
1	B	329	PRO	N-CA-C	5.19	120.43	114.20
1	B	267	GLU	CB-CA-C	-5.16	102.78	110.88
1	A	9	LYS	N-CA-CB	-5.12	102.44	109.97

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	3729	0	3708	25	0
1	B	3691	0	3668	29	0
1	C	3700	0	3668	15	0
1	D	3710	0	3688	29	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	25	0	17	4	0
3	B	25	0	17	2	0
3	C	25	0	17	2	0
3	D	25	0	17	2	0
4	A	32	0	56	2	0
4	B	16	0	28	11	0
4	C	16	0	28	3	0
4	D	16	0	28	1	0
5	A	16	0	24	0	0
5	B	20	0	30	0	0
5	C	12	0	18	0	0
5	D	12	0	18	0	0
6	B	13	0	14	0	0
6	D	13	0	15	0	0
7	B	10	0	14	0	0
7	C	10	0	14	0	0
8	D	7	0	10	0	0
9	A	278	0	0	1	0
9	B	275	0	0	3	0
9	C	265	0	0	3	0
9	D	279	0	0	1	0
All	All	16392	0	15217	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (119) 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)
1:D:191:ALA:C	1:D:194:ASP:N	1.90	1.29
1:D:145:MET:HE2	1:D:273:LEU:HD13	1.22	1.14
1:A:9:LYS:NZ	1:A:11:PHE:CE1	2.19	1.10
1:B:145:MET:HE3	1:B:273:LEU:HD13	1.35	1.05
1:D:109:GLN:HE22	1:D:404:GLN:HE22	1.15	0.92
1:A:267[B]:GLU:OE2	4:A:504:MPD:O2	1.86	0.92
1:A:177:MET:HE1	1:A:259[B]:ILE:HD11	1.54	0.89
1:D:145:MET:CE	1:D:273:LEU:HD13	2.02	0.88
1:B:145:MET:HE2	1:B:273:LEU:HB3	1.56	0.86
1:B:267:GLU:HB2	9:B:702:HOH:O	1.76	0.83
1:D:145:MET:HE2	1:D:273:LEU:CD1	2.07	0.82
1:D:194:ASP:HA	1:D:198:TYR:HD2	1.48	0.78
1:A:9:LYS:NZ	1:A:11:PHE:CD1	2.50	0.78
1:B:267:GLU:CG	4:B:511:MPD:H12	2.14	0.77
1:B:267:GLU:HG3	4:B:511:MPD:H12	1.67	0.77
1:D:194:ASP:HA	1:D:198:TYR:CD2	2.21	0.76
4:B:503:MPD:HM2	4:B:503:MPD:H52	1.67	0.75
1:B:267:GLU:CG	4:B:511:MPD:C1	2.67	0.72
1:B:267:GLU:CD	4:B:511:MPD:H12	2.16	0.71
1:B:306:LYS:HD3	9:B:704:HOH:O	1.91	0.69
1:A:177:MET:CE	1:A:259[B]:ILE:HD11	2.23	0.68
1:D:9:LYS:HZ3	1:D:10:THR:C	2.03	0.67
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.76	0.66
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.78	0.65
1:D:109:GLN:HE22	1:D:404:GLN:NE2	1.92	0.64
1:D:109:GLN:NE2	1:D:404:GLN:HE22	1.93	0.63
1:D:10:THR:HG23	1:D:15:LYS:HA	1.79	0.63
1:B:267:GLU:CD	4:B:511:MPD:C1	2.72	0.62
1:B:145:MET:CE	1:B:273:LEU:HB3	2.30	0.62
3:D:502:CL6:CAK	3:D:502:CL6:HAE	2.29	0.62
1:D:9:LYS:NZ	1:D:10:THR:O	2.23	0.62
1:A:9:LYS:NZ	1:A:11:PHE:CZ	2.67	0.61
1:A:177:MET:HE1	1:A:259[B]:ILE:CD1	2.29	0.61
1:A:266:HIS:NE2	1:A:267[A]:GLU:HG2	2.16	0.61
1:C:230:SER:OG	1:C:231:ASP:N	2.34	0.61
1:B:187:LYS:HG2	1:B:190:ARG:HH21	1.66	0.61
1:B:145:MET:CE	1:B:273:LEU:HD13	2.21	0.60
4:B:503:MPD:HM2	4:B:503:MPD:C5	2.31	0.60
1:C:109:GLN:NE2	1:C:305:TYR:OH	2.35	0.60
1:A:136:ASP:OD1	1:A:447:LYS:NZ	2.35	0.59
1:B:437:LEU:HD22	4:B:503:MPD:H13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:CL6:CAK	3:B:502:CL6:HAE	2.33	0.59
1:B:233:LEU:HG	1:B:237:MET:HE3	1.84	0.58
1:D:9:LYS:NZ	1:D:10:THR:C	2.62	0.58
1:B:267:GLU:HG3	4:B:511:MPD:C1	2.30	0.57
3:C:502:CL6:CAK	3:C:502:CL6:HAE	2.32	0.57
1:B:183:GLU:OE2	1:B:190:ARG:NH2	2.38	0.57
1:A:56[B]:ARG:NH1	9:A:602:HOH:O	2.30	0.56
1:C:233:LEU:HG	1:C:237:MET:HE3	1.87	0.56
4:C:503:MPD:H52	4:C:503:MPD:O2	2.06	0.56
1:A:11:PHE:HD2	1:A:18:PRO:HD2	1.69	0.56
1:B:267:GLU:OE2	4:B:511:MPD:H12	2.06	0.56
1:A:233:LEU:HG	1:A:237:MET:HE3	1.89	0.55
1:C:10:THR:HG23	1:C:15:LYS:HA	1.90	0.54
1:D:400:CYS:O	1:D:403[B]:GLN:HG3	2.09	0.52
1:D:138:HIS:HE1	9:D:638:HOH:O	1.91	0.52
1:C:227:GLY:O	1:C:229:GLN:N	2.39	0.52
1:A:255:ARG:HE	4:A:505:MPD:H51	1.77	0.50
1:B:285:HIS:H	1:B:285:HIS:CD2	2.30	0.50
1:A:75:LEU:HD21	3:A:502:CL6:HAH	1.92	0.50
1:B:187:LYS:HG2	1:B:190:ARG:NH2	2.27	0.49
2:D:501:HEM:HBA2	3:D:502:CL6:CAG	2.43	0.49
1:D:393:PHE:CG	1:D:403[B]:GLN:HG2	2.47	0.49
1:B:145:MET:HE3	1:B:273:LEU:CD1	2.24	0.48
1:A:9:LYS:HE3	1:A:9:LYS:HB3	1.48	0.48
3:A:502:CL6:HAA	3:A:502:CL6:CAK	2.43	0.48
1:D:190:ARG:NE	1:D:194:ASP:OD1	2.48	0.47
1:C:272:LEU:HD13	1:C:322:LEU:HG	1.97	0.47
1:D:5:MET:HE1	1:D:50:ARG:HD3	1.95	0.47
1:C:59:LYS:HG3	1:C:60:GLU:N	2.30	0.46
1:C:138:HIS:HE1	9:C:617:HOH:O	1.98	0.46
1:C:56:ARG:NH1	9:C:616:HOH:O	2.48	0.46
1:A:81:PHE:O	1:A:259[A]:ILE:HD11	2.15	0.46
1:C:3:LYS:NZ	9:C:610:HOH:O	2.43	0.46
1:D:7:GLN:HG3	1:D:8:PRO:HD2	1.97	0.46
1:D:200:GLU:HA	1:D:200:GLU:OE1	2.16	0.46
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.98	0.45
1:C:231:ASP:CG	1:C:231:ASP:O	2.58	0.45
1:D:400:CYS:HB3	1:D:403[B]:GLN:HG3	1.97	0.45
1:D:141:VAL:HB	1:D:142:PRO:HD3	1.98	0.45
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.99	0.45
1:B:330:ALA:O	4:B:503:MPD:H31	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.47	0.45
4:D:504:MPD:O4	4:D:504:MPD:H13	2.16	0.45
2:A:501:HEM:HBA2	3:A:502:CL6:CAG	2.47	0.44
3:B:502:CL6:HAJ	3:B:502:CL6:CAX	2.48	0.44
1:D:81:PHE:O	1:D:259:ILE:HD11	2.17	0.44
1:A:11:PHE:CE2	1:A:18:PRO:HB2	2.52	0.44
1:D:5:MET:HG2	1:D:41:LYS:HB2	1.99	0.44
1:A:11:PHE:CD2	1:A:18:PRO:HD2	2.52	0.44
4:C:503:MPD:H4	4:C:503:MPD:H13	1.69	0.43
1:A:7:GLN:HG3	1:A:8:PRO:HD2	1.99	0.43
1:B:7:GLN:NE2	1:B:41:LYS:O	2.52	0.43
2:C:501:HEM:HBB2	2:C:501:HEM:CMB	2.49	0.43
1:B:306:LYS:HE2	1:B:306:LYS:HB2	1.93	0.43
1:C:141:VAL:HB	1:C:142:PRO:HD3	2.01	0.42
1:D:187:LYS:HA	1:D:187:LYS:HE2	2.00	0.42
1:C:7:GLN:HG3	1:C:8:PRO:HD2	2.00	0.42
1:B:192:ASN:ND2	9:B:612:HOH:O	2.51	0.42
1:A:292:GLU:OE1	1:A:296:ARG:NH1	2.52	0.42
1:C:62:CYS:SG	1:C:391:LYS:HE2	2.60	0.42
1:A:169[B]:GLN:H	1:A:169[B]:GLN:HG3	1.59	0.42
2:C:501:HEM:HBA2	3:C:502:CL6:CAG	2.50	0.42
1:D:400:CYS:HB3	1:D:403[B]:GLN:CG	2.50	0.41
1:A:266:HIS:CD2	1:A:267[A]:GLU:HG2	2.55	0.41
1:A:252[A]:GLU:H	1:A:252[A]:GLU:CD	2.28	0.41
1:A:449:LYS:HD2	1:A:449:LYS:C	2.46	0.41
4:C:503:MPD:O2	4:C:503:MPD:C5	2.67	0.41
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	2.03	0.41
1:B:192:ASN:ND2	1:B:195:ASP:HB2	2.36	0.41
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.51	0.41
1:B:426:HIS:CD2	1:B:447:LYS:HE3	2.56	0.41
1:D:272:LEU:HD13	1:D:322:LEU:HG	2.03	0.41
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.57	0.41
3:A:502:CL6:CLAY	3:A:502:CL6:CAJ	3.06	0.40
1:C:439:LEU:O	1:C:440:LYS:HD3	2.21	0.40
1:B:233:LEU:HD21	1:B:261:PHE:CD1	2.56	0.40
1:D:336:LYS:O	1:D:349:LYS:HD2	2.20	0.40
1:D:429:TYR:CE2	1:D:431:LEU:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	461/458 (101%)	448 (97%)	12 (3%)	1 (0%)	43	44
1	B	456/458 (100%)	446 (98%)	9 (2%)	1 (0%)	43	44
1	C	457/458 (100%)	442 (97%)	13 (3%)	2 (0%)	30	28
1	D	459/458 (100%)	443 (96%)	13 (3%)	3 (1%)	18	14
All	All	1833/1832 (100%)	1779 (97%)	47 (3%)	7 (0%)	30	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	230	SER
1	D	191	ALA
1	D	194	ASP
1	D	195	ASP
1	B	15	LYS
1	C	228	GLU
1	A	230	SER

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	407/401 (102%)	403 (99%)	4 (1%)	68	75
1	B	402/401 (100%)	400 (100%)	2 (0%)	81	87
1	C	403/401 (100%)	403 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/401 (101%)	402 (100%)	2 (0%)	81	87
All	All	1616/1604 (101%)	1608 (100%)	8 (0%)	81	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	168	ASP
1	A	230	SER
1	A	380	GLU
1	B	7	GLN
1	B	15	LYS
1	D	5	MET
1	D	187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	229	GLN
1	A	319	ASN
1	B	70	ASN
1	B	204	GLN
1	B	239	ASN
1	B	283	ASN
1	B	285	HIS
1	C	70	ASN
1	C	109	GLN
1	C	169	GLN
1	C	204	GLN
1	D	70	ASN
1	D	92	HIS
1	D	138	HIS
1	D	204	GLN
1	D	239	ASN
1	D	310	GLN
1	D	404	GLN

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 ⓘ

38 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	$\# Z > 2$
5	EDO	A	510	-	3,3,3	0.32	0	2,2,2	0.85	0
5	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.43	0
5	EDO	D	508	-	3,3,3	0.51	0	2,2,2	0.56	0
3	CL6	C	502	2	28,28,28	2.04	6 (21%)	39,39,39	2.41	10 (25%)
6	MPO	D	505	-	13,13,13	2.19	2 (15%)	17,17,17	1.49	3 (17%)
3	CL6	D	502	2	28,28,28	1.65	4 (14%)	39,39,39	1.78	8 (20%)
5	EDO	C	506	-	3,3,3	0.41	0	2,2,2	0.44	0
5	EDO	B	508	-	3,3,3	0.82	0	2,2,2	0.41	0
4	MPD	D	504	-	7,7,7	1.18	1 (14%)	9,10,10	2.66	5 (55%)
4	MPD	A	504	-	7,7,7	1.52	1 (14%)	9,10,10	2.33	4 (44%)
5	EDO	A	509	-	3,3,3	0.31	0	2,2,2	0.43	0
6	MPO	B	504	-	13,13,13	2.58	2 (15%)	17,17,17	1.75	5 (29%)
5	EDO	B	505	-	3,3,3	0.35	0	2,2,2	0.48	0
7	PGE	C	508	-	9,9,9	0.51	0	8,8,8	0.40	0
5	EDO	B	509	-	3,3,3	0.40	0	2,2,2	0.37	0
5	EDO	D	506	-	3,3,3	0.61	0	2,2,2	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	505	-	3,3,3	0.33	0	2,2,2	0.73	0
2	HEM	C	501	3,1	50,50,50	1.50	7 (14%)	67,82,82	1.38	8 (11%)
5	EDO	B	506	-	3,3,3	0.49	0	2,2,2	0.71	0
5	EDO	C	507	-	3,3,3	0.54	0	2,2,2	0.29	0
2	HEM	D	501	3,1	50,50,50	1.55	10 (20%)	67,82,82	1.30	12 (17%)
2	HEM	A	501	3,1	50,50,50	1.56	11 (22%)	67,82,82	1.17	7 (10%)
4	MPD	B	503	-	7,7,7	0.73	0	9,10,10	0.90	1 (11%)
7	PGE	B	510	-	9,9,9	0.57	0	8,8,8	0.43	0
4	MPD	B	511	-	7,7,7	0.92	0	9,10,10	1.07	1 (11%)
4	MPD	C	504	-	7,7,7	0.38	0	9,10,10	0.83	0
4	MPD	D	503	-	7,7,7	0.53	0	9,10,10	0.59	0
4	MPD	A	503	-	7,7,7	0.79	0	9,10,10	0.69	0
3	CL6	A	502	2	28,28,28	1.54	3 (10%)	39,39,39	2.35	7 (17%)
5	EDO	D	507	-	3,3,3	0.37	0	2,2,2	0.29	0
3	CL6	B	502	2	28,28,28	1.83	5 (17%)	39,39,39	2.26	10 (25%)
4	MPD	C	503	-	7,7,7	0.95	0	9,10,10	2.90	6 (66%)
8	PEG	D	509	-	6,6,6	0.73	0	5,5,5	0.47	0
2	HEM	B	501	3,1	50,50,50	1.59	8 (16%)	67,82,82	1.24	8 (11%)
4	MPD	A	506	-	7,7,7	0.41	0	9,10,10	0.53	0
5	EDO	B	507	-	3,3,3	0.28	0	2,2,2	0.92	0
4	MPD	A	505	-	7,7,7	0.68	0	9,10,10	0.84	0
5	EDO	A	508	-	3,3,3	0.40	0	2,2,2	0.71	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
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-
5	EDO	D	508	-	-	0/1/1/1	-
3	CL6	C	502	2	-	0/24/24/24	0/4/4/4
6	MPO	D	505	-	-	1/7/15/15	0/1/1/1
3	CL6	D	502	2	-	0/24/24/24	0/4/4/4
5	EDO	C	506	-	-	1/1/1/1	-
5	EDO	B	508	-	-	1/1/1/1	-
4	MPD	D	504	-	-	0/5/5/5	-
4	MPD	A	504	-	-	1/5/5/5	-
5	EDO	A	509	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPO	B	504	-	-	5/7/15/15	0/1/1/1
5	EDO	B	505	-	-	1/1/1/1	-
7	PGE	C	508	-	-	3/7/7/7	-
5	EDO	B	509	-	-	1/1/1/1	-
5	EDO	D	506	-	-	0/1/1/1	-
5	EDO	C	505	-	-	1/1/1/1	-
2	HEM	C	501	3,1	-	2/14/54/54	-
5	EDO	B	506	-	-	1/1/1/1	-
5	EDO	C	507	-	-	0/1/1/1	-
2	HEM	D	501	3,1	-	4/14/54/54	-
2	HEM	A	501	3,1	-	2/14/54/54	-
4	MPD	B	503	-	-	1/5/5/5	-
7	PGE	B	510	-	-	3/7/7/7	-
4	MPD	B	511	-	-	1/5/5/5	-
4	MPD	C	504	-	-	3/5/5/5	-
4	MPD	D	503	-	-	1/5/5/5	-
4	MPD	A	503	-	-	2/5/5/5	-
3	CL6	A	502	2	-	0/24/24/24	0/4/4/4
5	EDO	D	507	-	-	0/1/1/1	-
3	CL6	B	502	2	-	0/24/24/24	0/4/4/4
4	MPD	C	503	-	-	2/5/5/5	-
8	PEG	D	509	-	-	2/4/4/4	-
2	HEM	B	501	3,1	-	4/14/54/54	-
4	MPD	A	506	-	-	2/5/5/5	-
5	EDO	B	507	-	-	1/1/1/1	-
4	MPD	A	505	-	-	0/5/5/5	-
5	EDO	A	508	-	-	0/1/1/1	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	MPO	O1-S1	6.81	1.64	1.45
3	C	502	CL6	CAX-CAW	6.47	1.49	1.39
6	D	505	MPO	C1-S1	-6.28	1.68	1.77
6	B	504	MPO	C1-S1	-6.15	1.69	1.77
3	A	502	CL6	CAX-CAW	5.25	1.47	1.39
3	B	502	CL6	CAX-CAW	5.22	1.47	1.39
3	D	502	CL6	CAX-CAW	4.74	1.47	1.39
6	D	505	MPO	O3-S1	4.58	1.64	1.47
2	C	501	HEM	FE-NC	4.53	2.10	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NC	4.43	2.09	1.95
2	C	501	HEM	C1B-NB	-4.36	1.32	1.40
3	C	502	CL6	CAR-CAW	-4.36	1.50	1.54
3	B	502	CL6	CAP-NAO	-4.36	1.34	1.38
2	A	501	HEM	C1B-NB	-4.13	1.33	1.40
2	B	501	HEM	C1C-NC	-3.82	1.32	1.39
3	A	502	CL6	CAP-NAO	-3.78	1.34	1.38
2	D	501	HEM	C4D-C3D	3.77	1.51	1.45
3	D	502	CL6	CAR-NAO	3.75	1.54	1.50
3	C	502	CL6	CAR-NAO	3.73	1.54	1.50
2	B	501	HEM	FE-NB	3.71	2.06	1.94
2	A	501	HEM	FE-NB	3.70	2.06	1.94
2	A	501	HEM	C4D-C3D	3.68	1.51	1.45
2	C	501	HEM	FE-NB	3.60	2.06	1.94
2	D	501	HEM	FE-NB	3.53	2.05	1.94
2	B	501	HEM	C1B-NB	-3.49	1.34	1.40
2	B	501	HEM	C4B-NB	-3.32	1.32	1.38
2	D	501	HEM	C4B-NB	-3.24	1.32	1.38
2	D	501	HEM	FE-NC	3.19	2.05	1.95
3	D	502	CL6	CAP-NAO	-3.14	1.35	1.38
2	B	501	HEM	C4D-ND	-3.04	1.35	1.40
2	D	501	HEM	FE-NA	3.01	2.05	1.95
4	A	504	MPD	O2-C2	-2.96	1.37	1.44
2	D	501	HEM	C1B-NB	-2.94	1.35	1.40
3	C	502	CL6	CAP-NAO	-2.87	1.35	1.38
2	A	501	HEM	C1D-C2D	2.70	1.50	1.44
2	A	501	HEM	C3B-C4B	2.66	1.50	1.44
2	A	501	HEM	C3C-C4C	-2.59	1.41	1.46
2	C	501	HEM	CBD-CGD	2.59	1.56	1.50
3	A	502	CL6	CAR-NAO	-2.54	1.47	1.50
2	D	501	HEM	C1D-C2D	2.51	1.49	1.44
2	C	501	HEM	C1A-NA	-2.42	1.35	1.39
4	D	504	MPD	O2-C2	-2.37	1.38	1.44
2	B	501	HEM	C1D-C2D	2.35	1.49	1.44
2	D	501	HEM	C4D-ND	-2.33	1.36	1.40
3	C	502	CL6	CAI-CAK	2.29	1.42	1.38
3	B	502	CL6	CAM-NAN	2.26	1.38	1.32
3	B	502	CL6	CAA-CAC	2.26	1.43	1.39
3	B	502	CL6	CAF-CAE	2.25	1.42	1.38
2	A	501	HEM	O1A-CGA	2.22	1.29	1.22
2	B	501	HEM	C4D-C3D	2.18	1.48	1.45
2	C	501	HEM	FE-NA	2.17	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	CL6	CAA-CAC	2.12	1.42	1.39
2	D	501	HEM	C3D-C2D	-2.08	1.32	1.36
3	D	502	CL6	CAR-CAW	-2.05	1.52	1.54
2	D	501	HEM	C4A-NA	-2.05	1.35	1.39
2	A	501	HEM	O2D-CGD	-2.04	1.24	1.30
2	A	501	HEM	C3D-C2D	-2.03	1.32	1.36
2	C	501	HEM	C1C-NC	-2.02	1.35	1.39
2	A	501	HEM	C1D-ND	-2.01	1.34	1.38
2	A	501	HEM	FE-NC	2.00	2.01	1.95

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	CL6	NAO-CAM-NAN	-8.71	107.89	112.36
3	C	502	CL6	CAP-NAO-CAM	8.15	110.75	106.03
3	A	502	CL6	NAO-CAM-NAN	-8.14	108.19	112.36
3	B	502	CL6	CAP-NAO-CAM	8.04	110.69	106.03
3	A	502	CL6	CAP-NAO-CAM	7.01	110.09	106.03
3	B	502	CL6	NAO-CAM-NAN	-6.55	109.00	112.36
3	A	502	CL6	CAC-CAR-CAW	-6.41	102.71	111.85
2	C	501	HEM	CHC-C4B-NB	4.69	129.47	124.42
3	D	502	CL6	CAC-CAR-CAW	-4.65	105.22	111.85
4	A	504	MPD	O2-C2-CM	4.33	121.47	107.99
4	C	503	MPD	O2-C2-C1	4.32	121.44	107.99
3	D	502	CL6	CAP-NAO-CAM	4.24	108.48	106.03
4	C	503	MPD	O2-C2-C3	-4.23	93.46	109.27
3	D	502	CL6	NAO-CAM-NAN	-4.17	110.22	112.36
6	B	504	MPO	O1-S1-C1	4.14	112.99	106.73
3	D	502	CL6	CAU-CAW-CAX	-4.13	112.11	116.51
3	B	502	CL6	CAC-CAR-CAW	-4.11	105.99	111.85
4	D	504	MPD	CM-C2-C3	-4.06	92.69	110.20
3	C	502	CL6	CAC-CAR-CAW	-3.82	106.40	111.85
2	B	501	HEM	CHD-C1D-ND	3.67	128.38	124.42
4	C	503	MPD	O2-C2-CM	3.67	119.41	107.99
4	A	504	MPD	O2-C2-C1	3.59	119.19	107.99
4	D	504	MPD	CM-C2-C1	3.57	118.62	110.63
4	D	504	MPD	O2-C2-CM	3.55	119.06	107.99
2	D	501	HEM	C1B-NB-C4B	3.47	109.32	105.21
2	C	501	HEM	C4B-C3B-C2B	-3.44	104.12	107.28
4	C	503	MPD	CM-C2-C3	-3.37	95.66	110.20
3	B	502	CL6	CAU-CAW-CAX	-3.33	112.97	116.51
3	B	502	CL6	CAR-CAW-CAX	3.33	125.50	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CHD-C1D-ND	3.20	127.87	124.42
6	D	505	MPO	O2-S1-C1	3.16	111.51	106.73
2	A	501	HEM	C1B-NB-C4B	3.09	108.87	105.21
3	A	502	CL6	CAF-CAE-CAC	3.01	123.82	120.75
6	D	505	MPO	O1-S1-C1	2.96	111.20	106.73
4	D	504	MPD	O2-C2-C1	2.92	117.09	107.99
2	D	501	HEM	CHC-C4B-NB	2.91	127.55	124.42
2	C	501	HEM	C1B-NB-C4B	2.88	108.62	105.21
6	B	504	MPO	C5-C4-N1	-2.87	105.76	110.12
4	D	504	MPD	O2-C2-C3	-2.86	98.58	109.27
2	B	501	HEM	CHD-C1D-C2D	-2.82	120.57	125.03
3	B	502	CL6	CAB-CAA-CAC	2.81	123.61	120.75
4	C	503	MPD	C1-C2-C3	-2.81	98.10	110.20
2	C	501	HEM	CHD-C1D-C2D	-2.80	120.61	125.03
3	C	502	CL6	CAU-CAW-CAX	-2.79	113.54	116.51
3	C	502	CL6	CAT-CAS-CAU	2.76	123.64	120.24
2	B	501	HEM	CHC-C4B-NB	2.74	127.37	124.42
2	A	501	HEM	CHC-C4B-NB	2.71	127.34	124.42
2	A	501	HEM	CHA-C4D-ND	2.71	127.72	124.37
2	B	501	HEM	C4C-C3C-C2C	-2.70	104.47	106.81
3	C	502	CL6	CAH-CAG-CAI	-2.67	116.22	119.87
2	D	501	HEM	CAD-C3D-C4D	2.60	129.23	124.70
2	D	501	HEM	CHB-C1B-NB	2.60	127.58	124.37
3	C	502	CL6	CAG-CAH-CAJ	2.54	123.38	120.24
6	B	504	MPO	C6-O4-C5	2.54	118.09	109.88
3	B	502	CL6	CAI-CAK-CAL	2.53	123.33	120.75
4	A	504	MPD	O2-C2-C3	-2.52	99.84	109.27
2	B	501	HEM	CMD-C2D-C1D	2.50	128.94	125.03
2	B	501	HEM	C1B-NB-C4B	2.49	108.16	105.21
4	C	503	MPD	CM-C2-C1	2.49	116.20	110.63
3	A	502	CL6	CAG-CAH-CAJ	2.47	123.29	120.24
3	B	502	CL6	CAD-CAF-CAE	2.40	123.20	120.24
3	B	502	CL6	CAS-CAU-CAW	2.33	124.18	119.99
3	D	502	CL6	CAR-CAW-CAX	2.30	124.65	122.74
2	D	501	HEM	CMD-C2D-C1D	2.29	128.62	125.03
2	D	501	HEM	CHA-C4D-ND	2.29	127.20	124.37
6	D	505	MPO	C7-N1-C4	2.29	113.77	108.84
2	A	501	HEM	CHD-C1D-C2D	-2.28	121.43	125.03
3	C	502	CL6	CAW-CAX-CLAY	-2.27	118.96	121.70
2	D	501	HEM	C4B-C3B-C2B	-2.27	105.20	107.28
3	D	502	CL6	CAU-CAW-CAR	2.26	123.00	120.97
2	A	501	HEM	C4B-C3B-C2B	-2.24	105.22	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	MPD	CM-C2-C1	-2.20	105.70	110.63
6	B	504	MPO	O2-S1-C1	2.18	110.02	106.73
2	C	501	HEM	O2D-CGD-CBD	2.18	120.89	114.00
3	C	502	CL6	CAR-CAW-CAX	2.17	124.54	122.74
3	D	502	CL6	CAS-CAT-CAV	-2.16	117.58	120.24
3	C	502	CL6	CAI-CAK-CAL	2.13	122.92	120.75
6	B	504	MPO	O2-S1-O1	-2.13	106.91	113.82
2	D	501	HEM	C4C-NC-C1C	2.11	109.26	105.82
2	B	501	HEM	CHA-C4D-ND	2.10	126.97	124.37
2	A	501	HEM	CMB-C2B-C1B	2.09	128.29	125.03
2	D	501	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
4	A	504	MPD	C1-C2-C3	-2.08	101.23	110.20
3	B	502	CL6	CAW-CAR-NAO	2.08	109.31	106.35
2	D	501	HEM	CBD-CAD-C3D	-2.07	106.81	112.53
2	C	501	HEM	C4C-CHD-C1D	-2.06	121.64	126.02
2	D	501	HEM	CAD-C3D-C2D	-2.06	124.01	127.87
3	A	502	CL6	CAS-CAU-CAW	2.06	123.69	119.99
4	B	511	MPD	O4-C4-C5	-2.06	100.60	109.45
3	A	502	CL6	CAH-CAG-CAI	-2.05	117.06	119.87
3	D	502	CL6	CAT-CAS-CAU	2.04	122.76	120.24
2	A	501	HEM	CHD-C1D-ND	2.03	126.61	124.42
2	C	501	HEM	C3B-C2B-C1B	2.03	107.93	106.41
2	B	501	HEM	CHA-C4D-C3D	-2.03	121.49	125.23
2	D	501	HEM	C2D-C1D-ND	2.00	112.22	109.90

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	MPD	C2-C3-C4-O4
4	A	503	MPD	C2-C3-C4-C5
4	C	503	MPD	C2-C3-C4-O4
4	C	503	MPD	C2-C3-C4-C5
6	B	504	MPO	C2-C1-S1-O1
6	B	504	MPO	C2-C1-S1-O2
6	D	505	MPO	C1-C2-C3-N1
8	D	509	PEG	C4-C3-O2-C2
6	B	504	MPO	C2-C3-N1-C7
6	B	504	MPO	C2-C1-S1-O3
6	B	504	MPO	C2-C3-N1-C4
7	B	510	PGE	O2-C3-C4-O3
7	C	508	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	508	EDO	O1-C1-C2-O2
7	C	508	PGE	C4-C3-O2-C2
4	B	503	MPD	O2-C2-C3-C4
4	D	503	MPD	C2-C3-C4-O4
5	B	505	EDO	O1-C1-C2-O2
4	A	506	MPD	C2-C3-C4-C5
5	B	507	EDO	O1-C1-C2-O2
5	C	506	EDO	O1-C1-C2-O2
8	D	509	PEG	C1-C2-O2-C3
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D
5	A	507	EDO	O1-C1-C2-O2
5	C	505	EDO	O1-C1-C2-O2
2	B	501	HEM	CAA-CBA-CGA-O2A
7	C	508	PGE	O2-C3-C4-O3
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAD-CBD-CGD-O1D
5	B	506	EDO	O1-C1-C2-O2
5	B	509	EDO	O1-C1-C2-O2
2	B	501	HEM	CAA-CBA-CGA-O1A
4	C	504	MPD	O2-C2-C3-C4
7	B	510	PGE	O1-C1-C2-O2
4	A	506	MPD	C2-C3-C4-O4
4	B	511	MPD	C2-C3-C4-O4
2	B	501	HEM	CAD-CBD-CGD-O2D
5	A	510	EDO	O1-C1-C2-O2
4	A	504	MPD	C1-C2-C3-C4
4	C	504	MPD	C1-C2-C3-C4
4	C	504	MPD	CM-C2-C3-C4
7	B	510	PGE	C1-C2-O2-C3

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	CL6	2	0
3	D	502	CL6	2	0

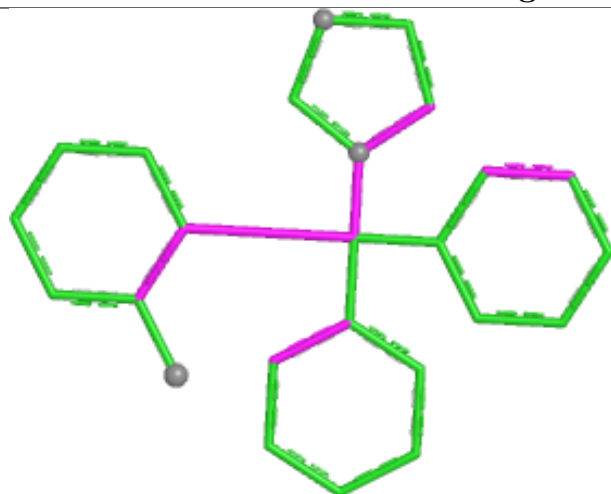
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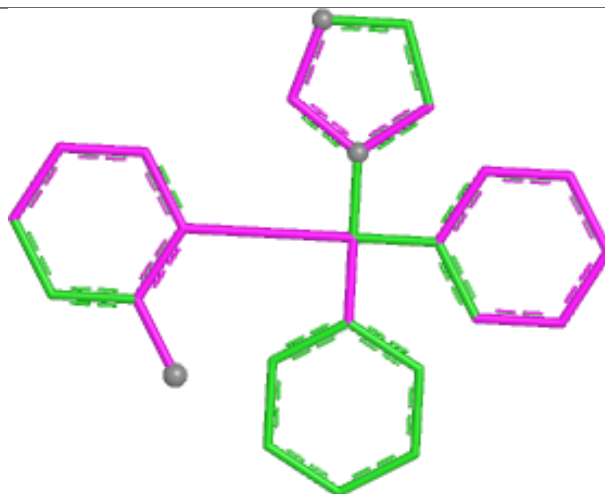
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	MPD	1	0
4	A	504	MPD	1	0
2	C	501	HEM	3	0
2	D	501	HEM	3	0
2	A	501	HEM	1	0
4	B	503	MPD	4	0
4	B	511	MPD	7	0
3	A	502	CL6	4	0
3	B	502	CL6	2	0
4	C	503	MPD	3	0
2	B	501	HEM	2	0
4	A	505	MPD	1	0

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

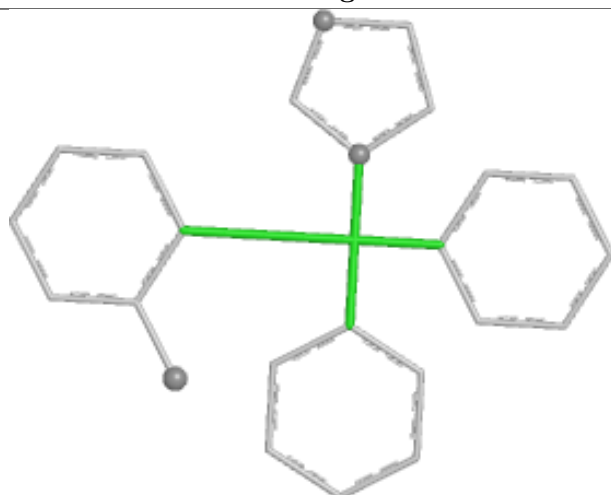
Ligand CL6 C 502



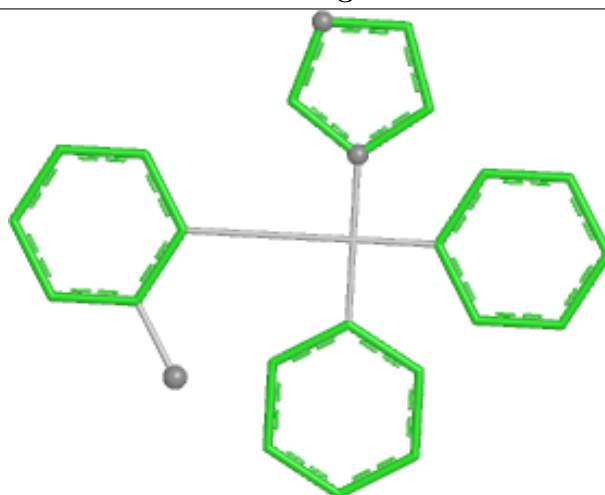
Bond lengths



Bond angles

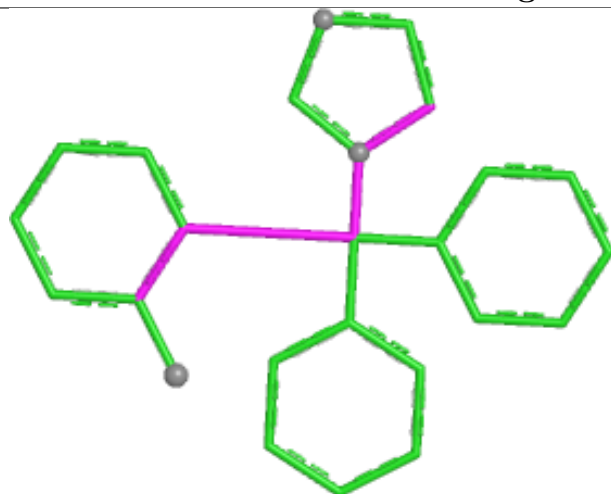


Torsions

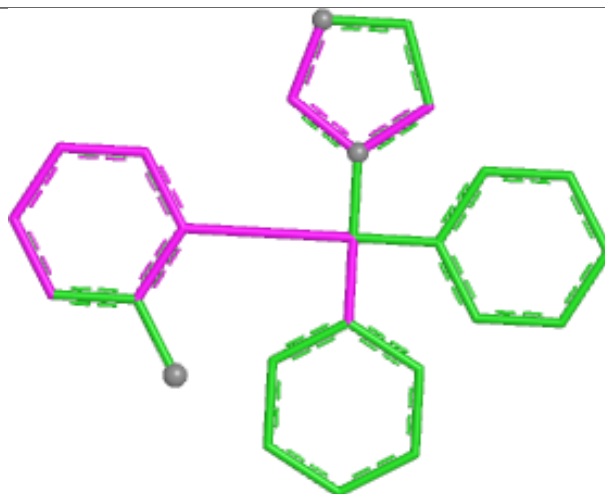


Rings

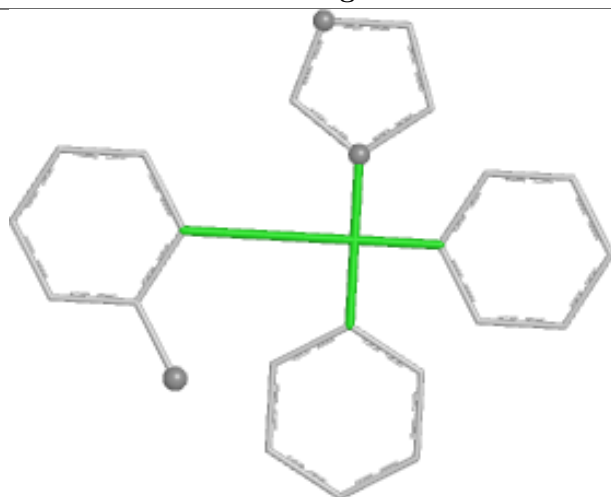
Ligand CL6 D 502



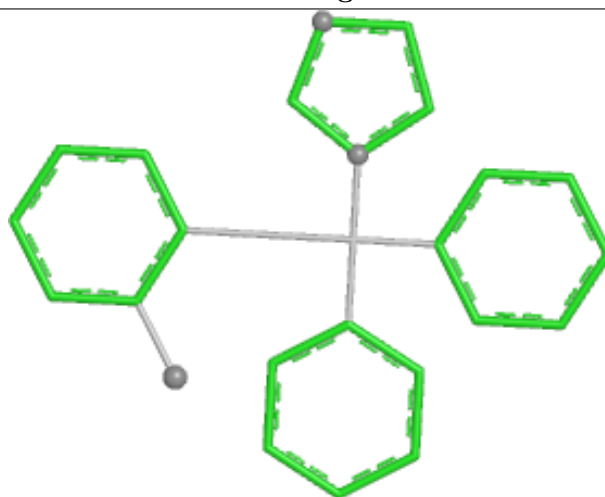
Bond lengths



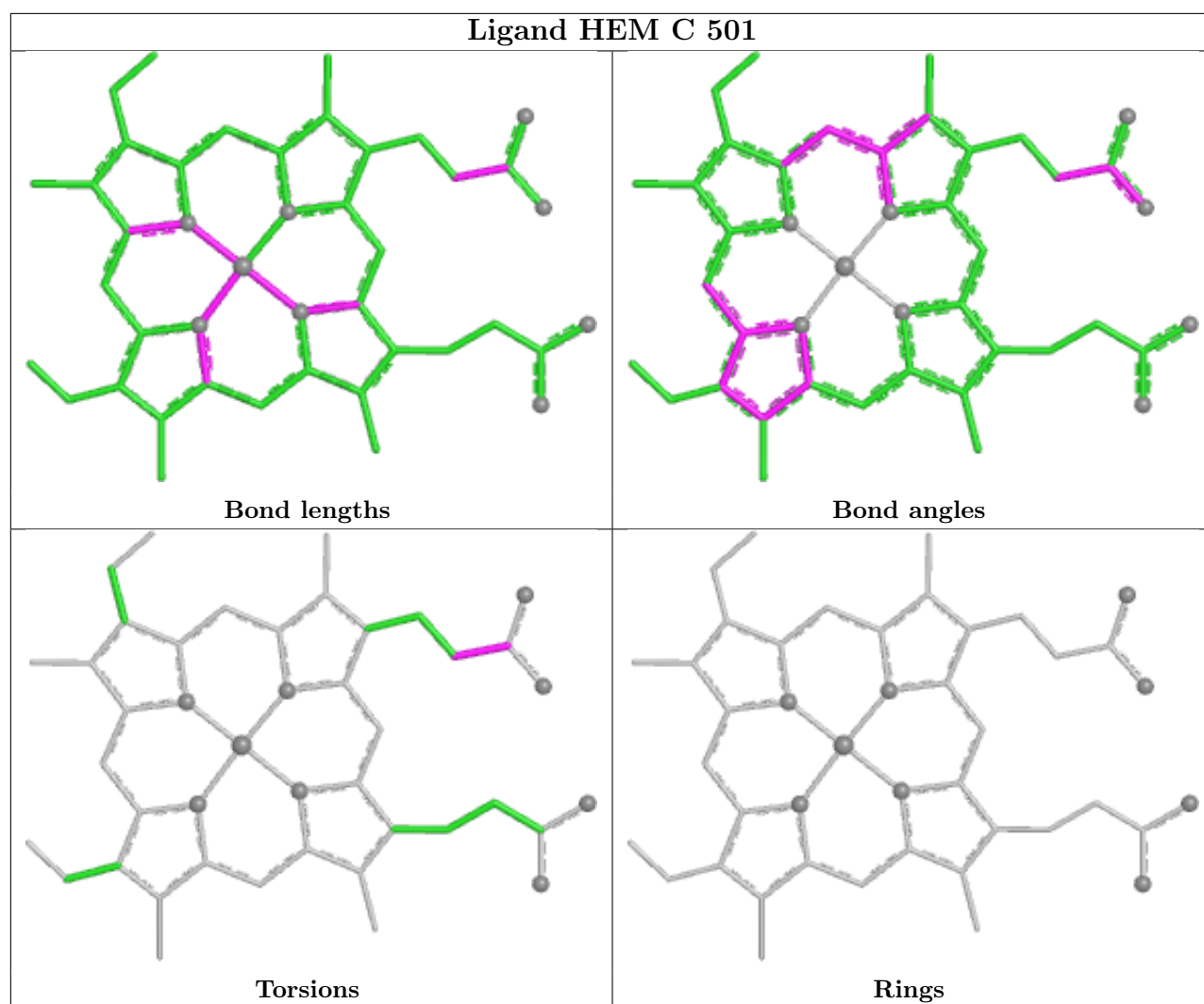
Bond angles

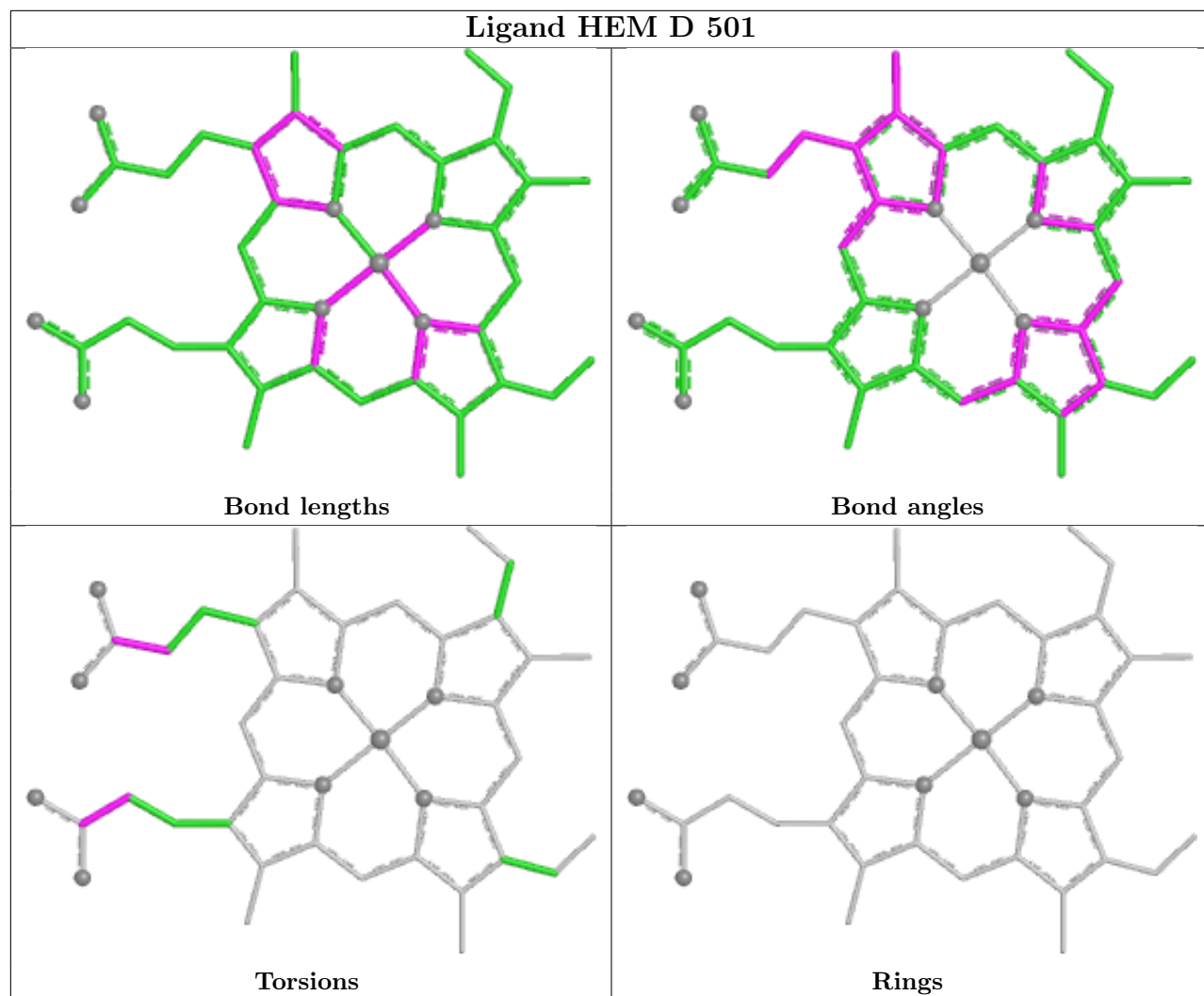


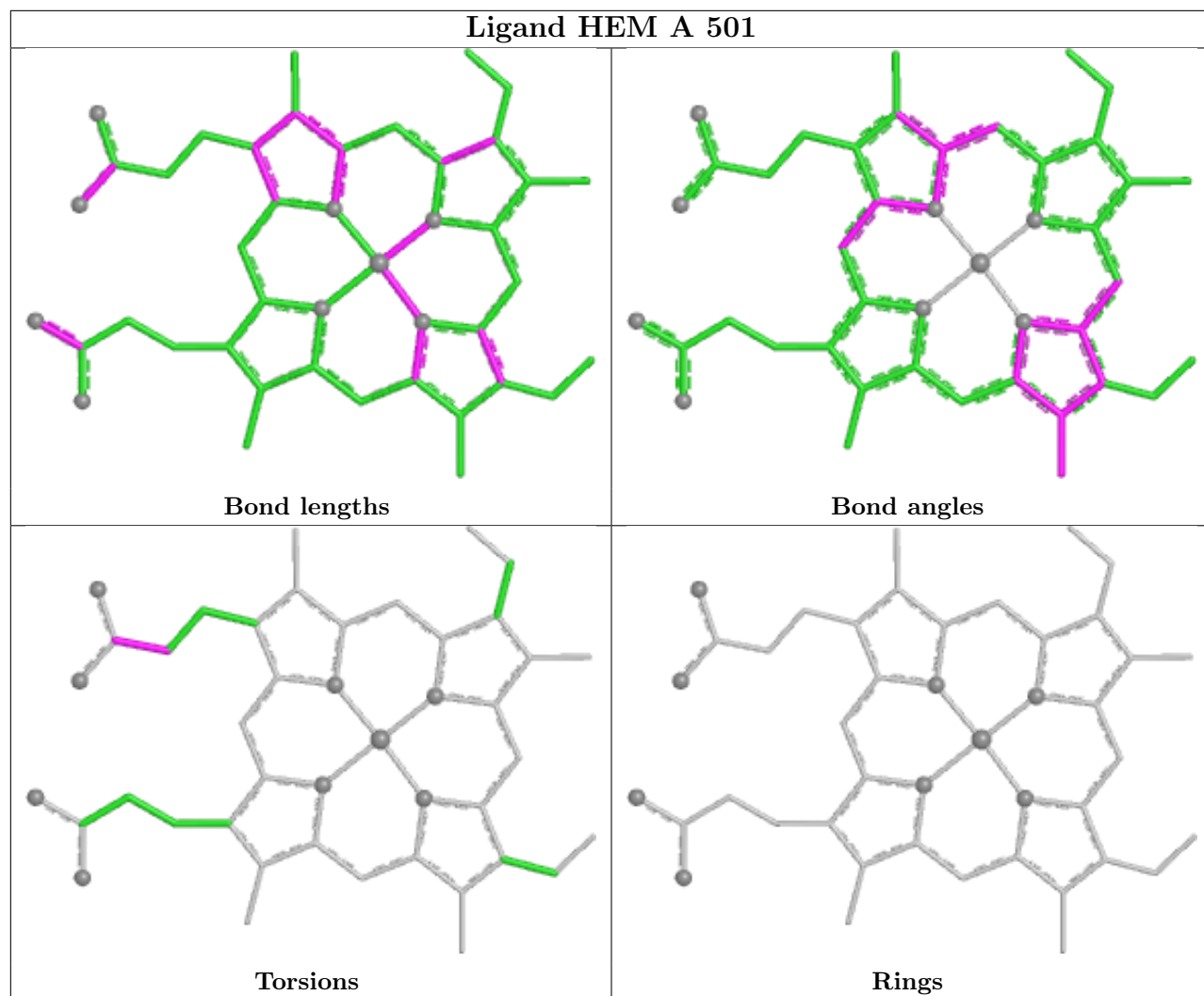
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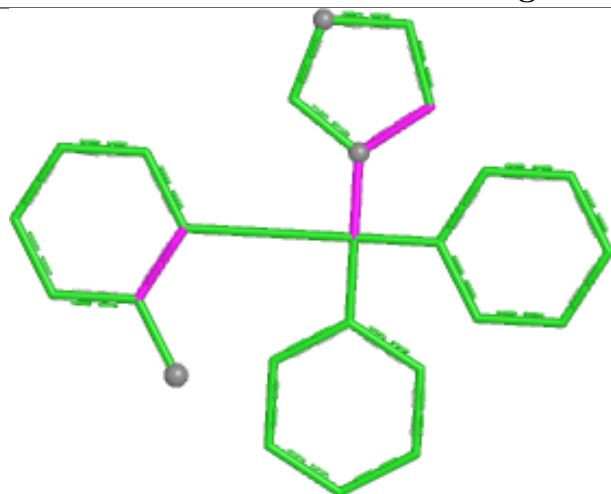
Rings



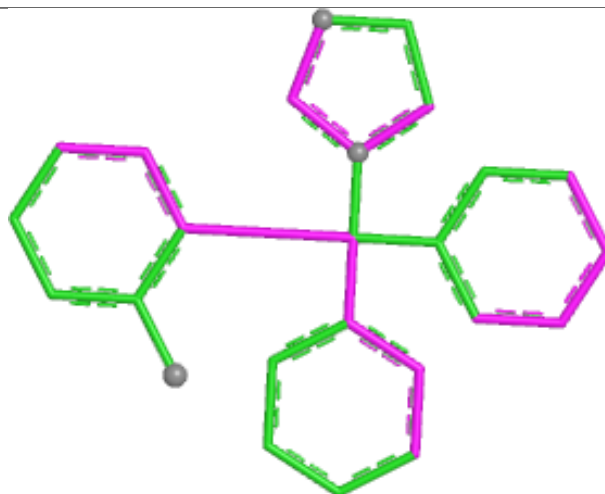




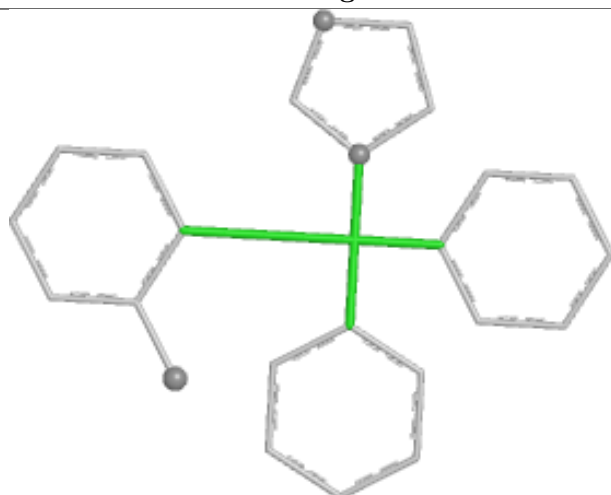
Ligand CL6 A 502



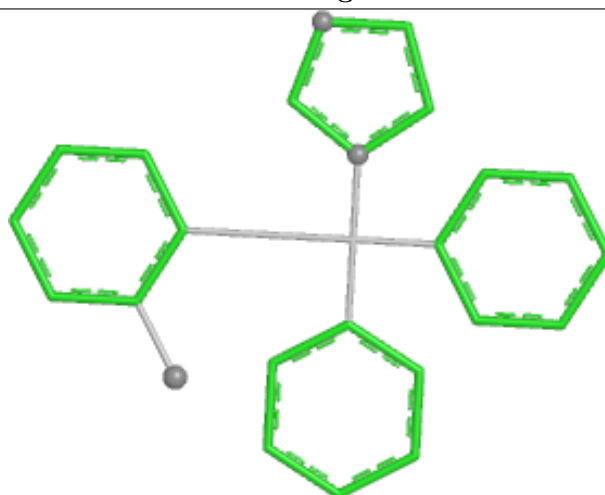
Bond lengths



Bond angles

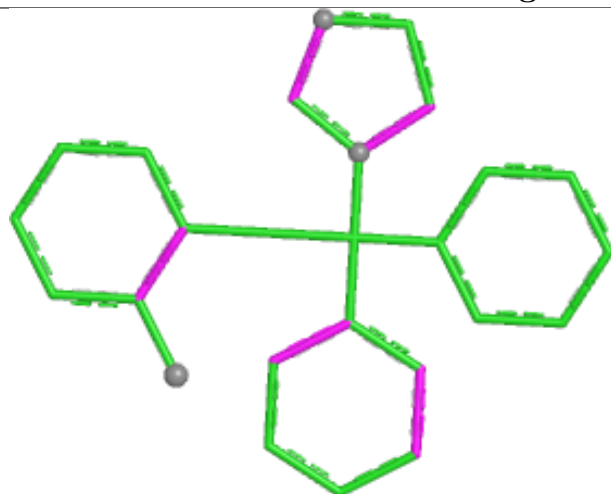


Torsions

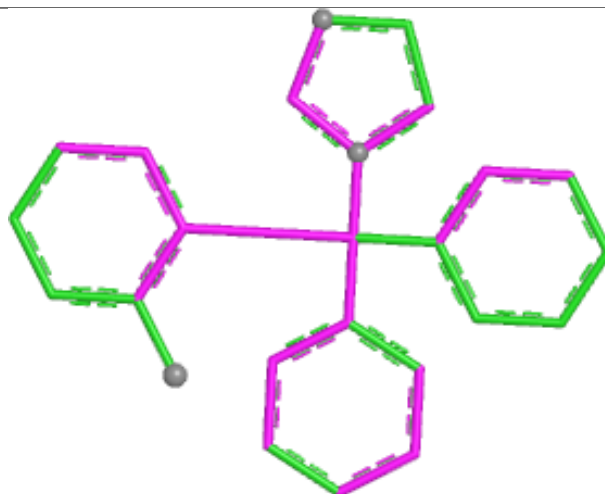


Rings

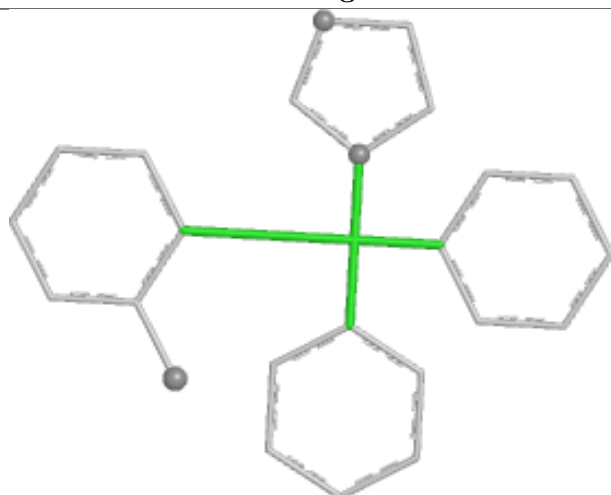
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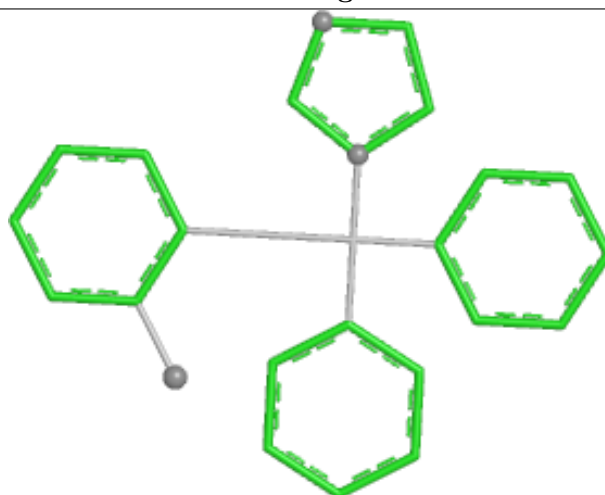
Bond lengths



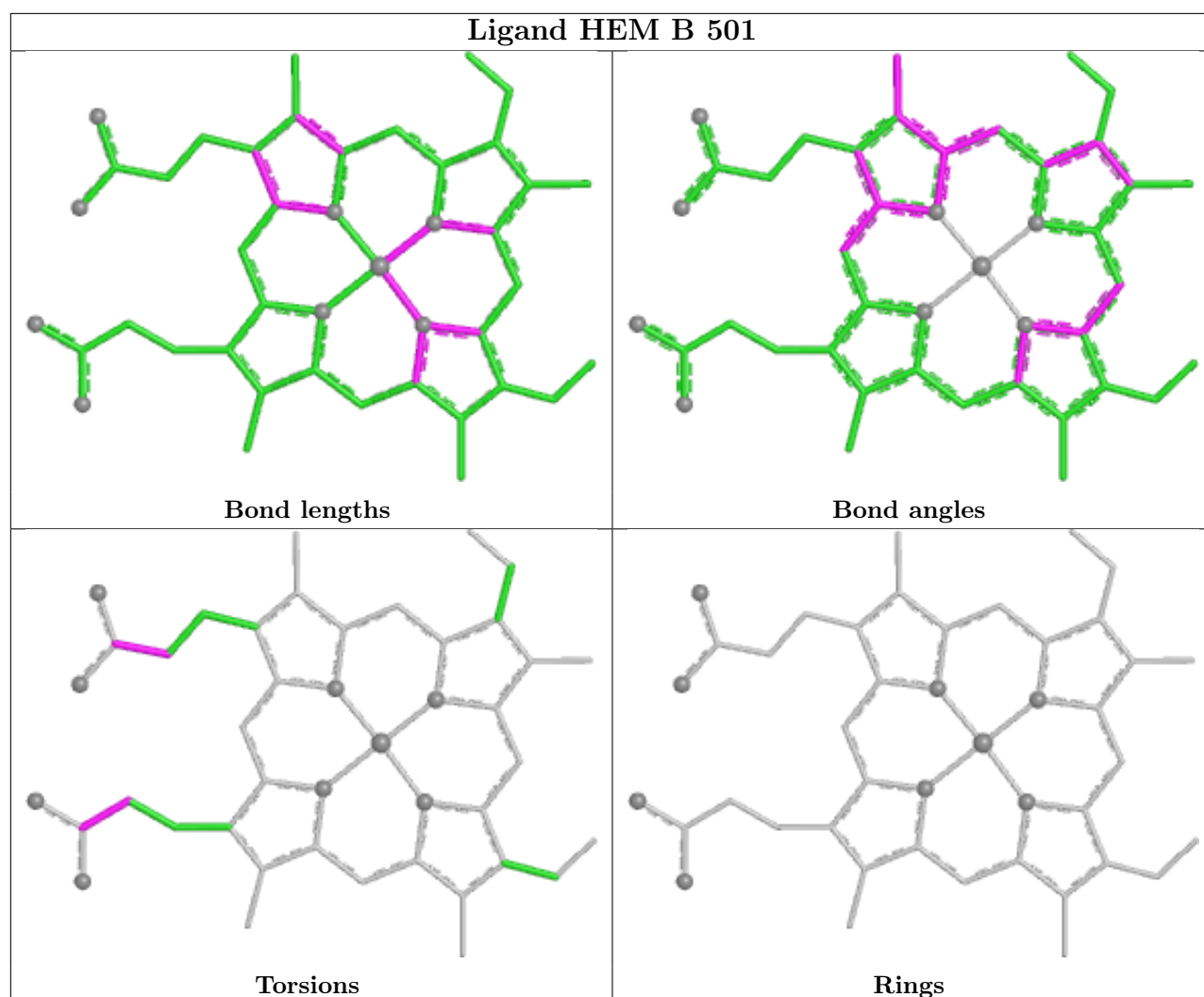
Bond angles



Torsions



Rings



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	456/458 (99%)	-0.30	5 (1%) 78 80	13, 31, 55, 117	7 (1%)
1	B	456/458 (99%)	-0.24	11 (2%) 59 62	17, 31, 66, 100	2 (0%)
1	C	456/458 (99%)	-0.20	7 (1%) 72 74	17, 33, 64, 115	3 (0%)
1	D	456/458 (99%)	-0.17	7 (1%) 72 74	12, 33, 65, 98	5 (1%)
All	All	1824/1832 (99%)	-0.23	30 (1%) 70 73	12, 32, 64, 117	17 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	GLY	4.2
1	B	14	LEU	4.2
1	B	191	ALA	4.1
1	B	456	GLY	4.0
1	D	191	ALA	3.6
1	C	456	GLY	3.4
1	A	229	GLN	3.3
1	C	285[A]	HIS	3.2
1	A	456	GLY	3.2
1	C	228	GLU	3.0
1	D	458	ILE	2.8
1	B	193	PRO	2.8
1	D	197	ALA	2.8
1	C	191	ALA	2.7
1	B	228	GLU	2.6
1	C	229	GLN	2.6
1	D	187	LYS	2.6
1	B	197	ALA	2.5
1	D	196	PRO	2.5
1	C	193	PRO	2.4
1	A	230	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	2.3
1	B	231	ASP	2.3
1	B	192	ASN	2.3
1	D	188	LEU	2.3
1	D	1	THR	2.2
1	C	381	ASN	2.2
1	B	1	THR	2.2
1	A	228	GLU	2.1
1	B	245	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	508	4/4	0.80	0.23	48,55,57,58	0
5	EDO	A	510	4/4	0.81	0.20	56,63,63,70	0
5	EDO	C	505	4/4	0.81	0.18	59,61,66,67	0
4	MPD	B	511	8/8	0.82	0.19	28,31,35,36	0
6	MPO	B	504	13/13	0.82	0.15	60,72,101,102	0
8	PEG	D	509	7/7	0.82	0.13	59,61,67,70	0
5	EDO	A	508	4/4	0.84	0.14	53,55,58,66	0
7	PGE	B	510	10/10	0.84	0.15	62,71,88,89	0
5	EDO	C	506	4/4	0.84	0.20	56,57,61,62	0
5	EDO	C	507	4/4	0.85	0.19	55,59,61,62	0
4	MPD	D	503	8/8	0.85	0.17	48,54,60,73	0
5	EDO	A	507	4/4	0.86	0.11	60,62,63,67	0
5	EDO	B	507	4/4	0.86	0.14	61,62,62,62	0
5	EDO	D	506	4/4	0.86	0.14	35,52,53,58	0

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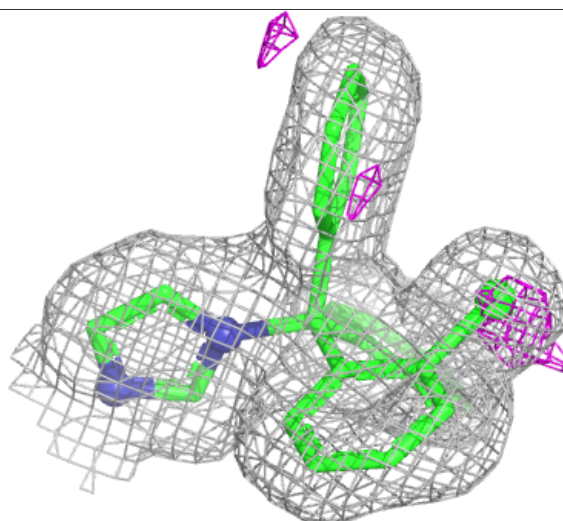
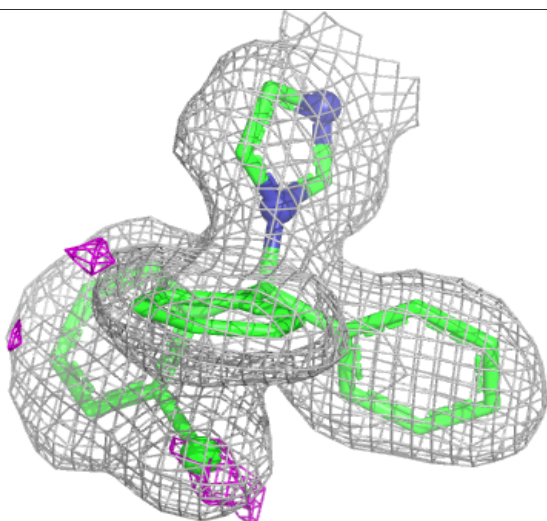
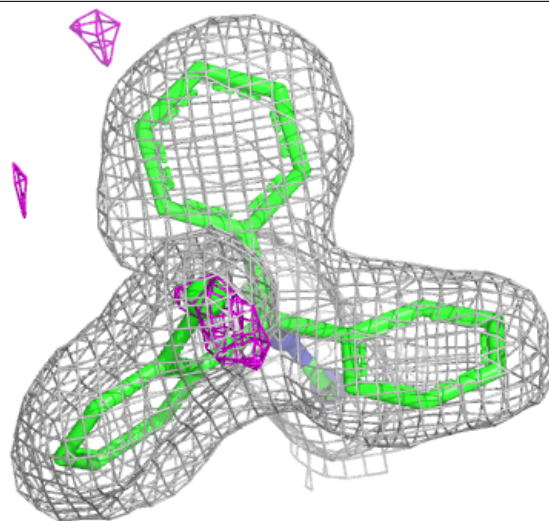
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PGE	C	508	10/10	0.87	0.13	51,63,70,73	0
4	MPD	D	504	8/8	0.87	0.16	58,72,75,75	0
5	EDO	B	506	4/4	0.88	0.20	41,49,52,58	0
5	EDO	B	509	4/4	0.88	0.17	59,64,64,65	0
4	MPD	A	506	8/8	0.88	0.17	61,72,75,80	0
5	EDO	D	508	4/4	0.88	0.15	59,59,63,65	0
4	MPD	B	503	8/8	0.89	0.17	52,55,59,59	0
4	MPD	A	505	8/8	0.89	0.17	59,61,65,67	0
4	MPD	A	504	8/8	0.90	0.16	56,59,63,64	0
5	EDO	B	505	4/4	0.90	0.14	40,48,60,77	0
6	MPO	D	505	13/13	0.90	0.12	55,65,84,98	0
4	MPD	C	503	8/8	0.91	0.14	46,54,58,62	0
5	EDO	A	509	4/4	0.92	0.11	51,54,54,56	0
4	MPD	C	504	8/8	0.93	0.12	49,55,57,65	0
4	MPD	A	503	8/8	0.93	0.11	38,43,49,52	0
5	EDO	D	507	4/4	0.93	0.10	53,57,60,63	0
3	CL6	C	502	25/25	0.95	0.07	24,27,32,36	0
3	CL6	B	502	25/25	0.97	0.05	23,26,31,35	0
3	CL6	D	502	25/25	0.97	0.06	21,28,31,36	0
3	CL6	A	502	25/25	0.98	0.04	21,23,27,32	0
2	HEM	C	501	43/43	0.99	0.05	19,22,27,31	0
2	HEM	D	501	43/43	0.99	0.04	20,24,26,27	0
2	HEM	A	501	43/43	0.99	0.04	17,20,24,28	0
2	HEM	B	501	43/43	0.99	0.05	18,22,25,31	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.

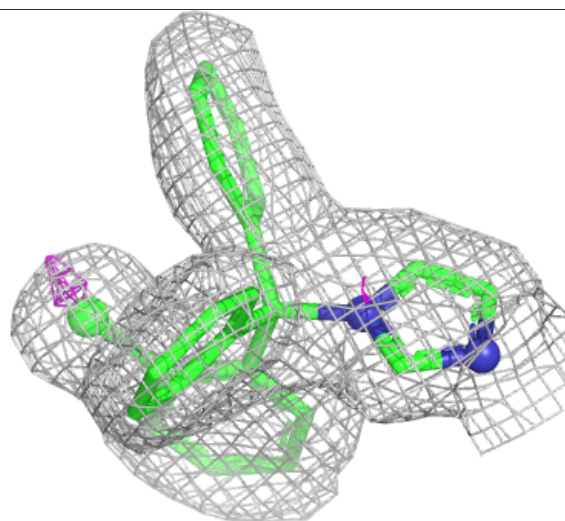
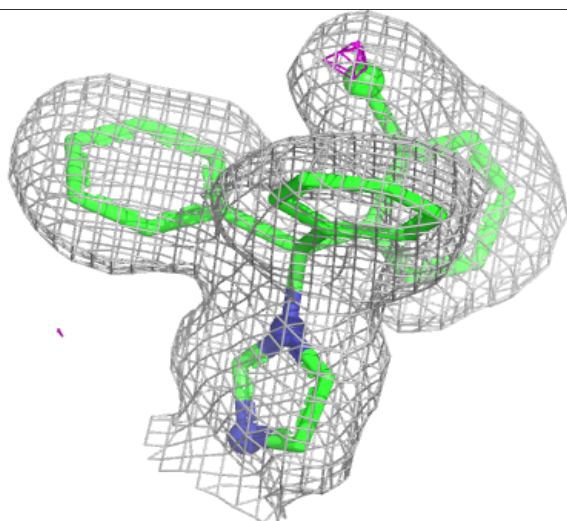
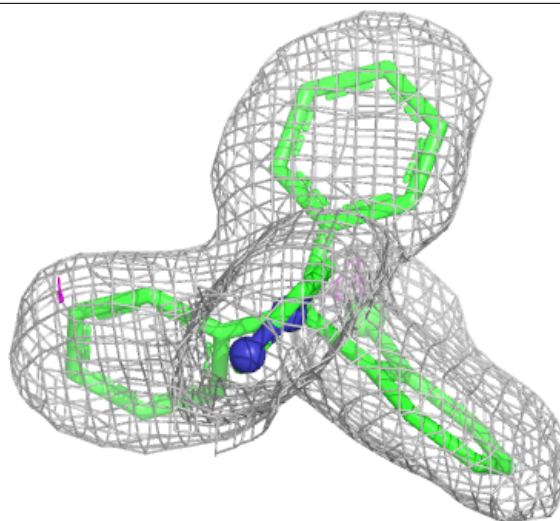
Electron density around CL6 C 502:

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



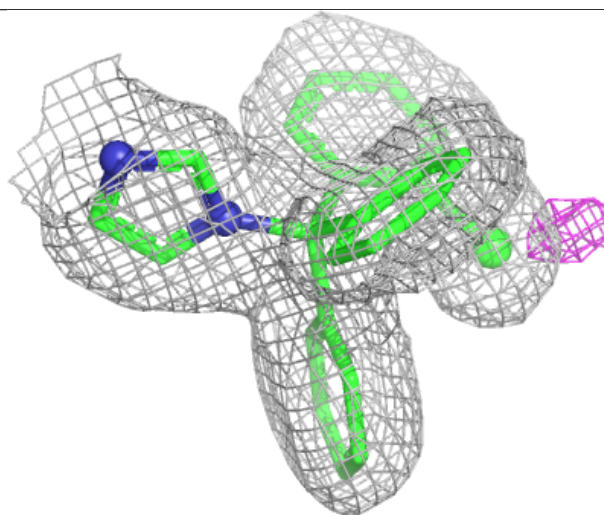
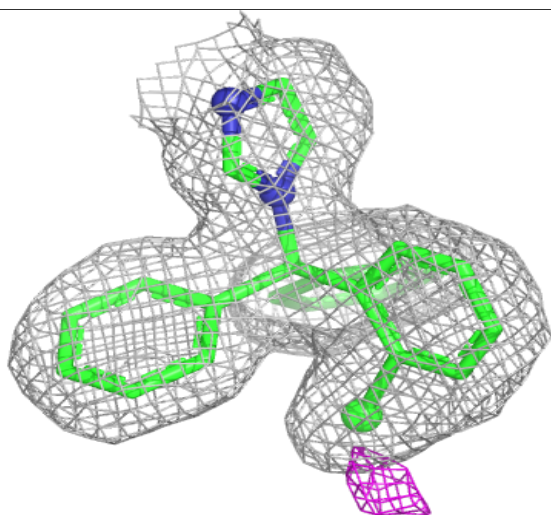
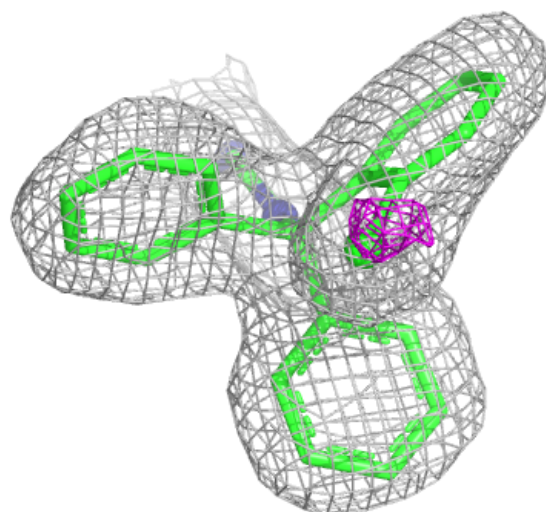
Electron density around CL6 B 502:

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



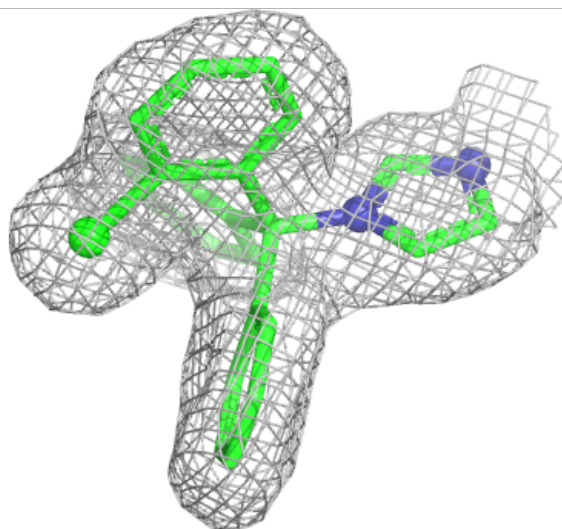
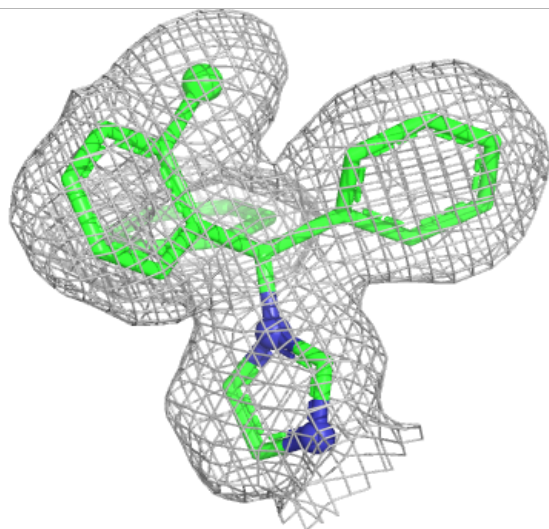
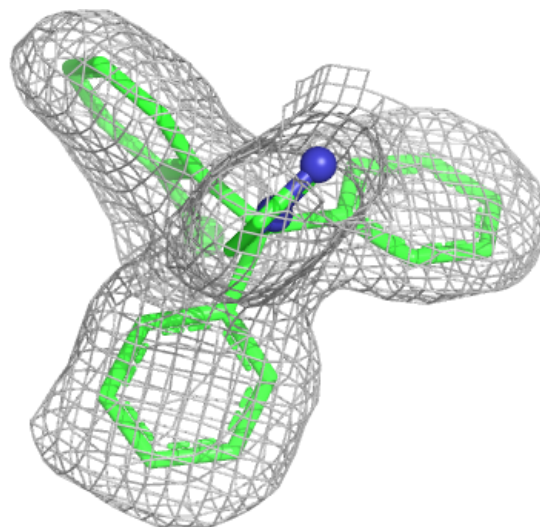
Electron density around CL6 D 502:

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



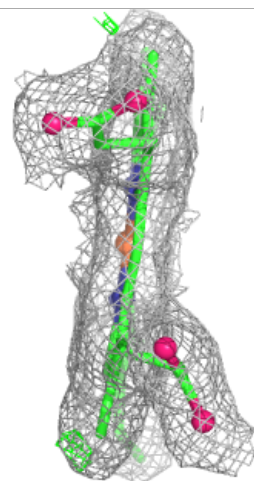
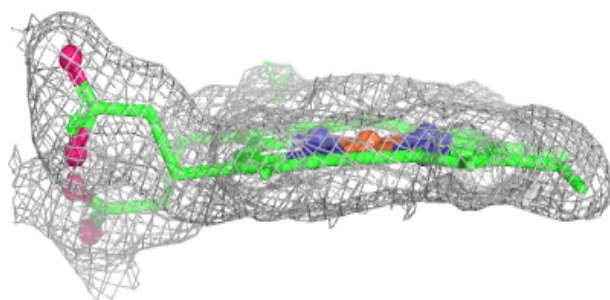
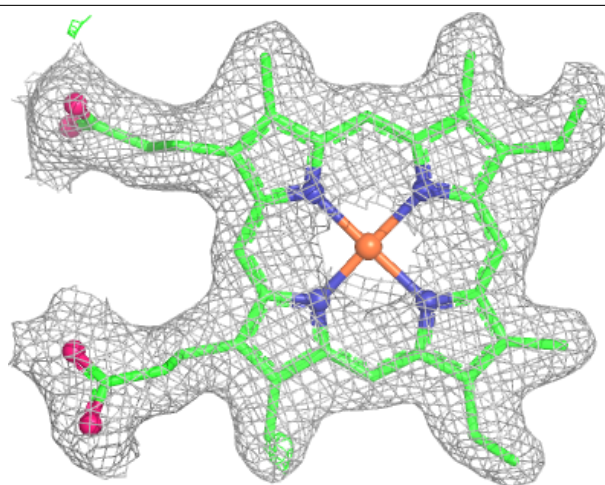
Electron density around CL6 A 502:

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



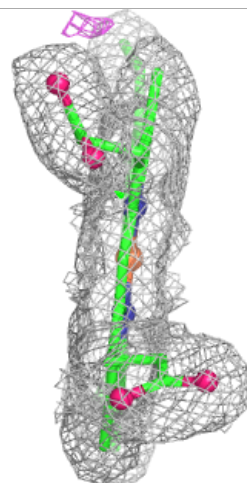
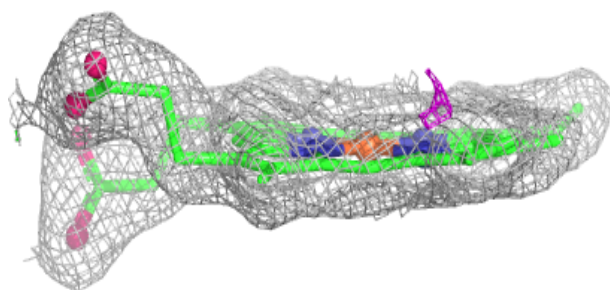
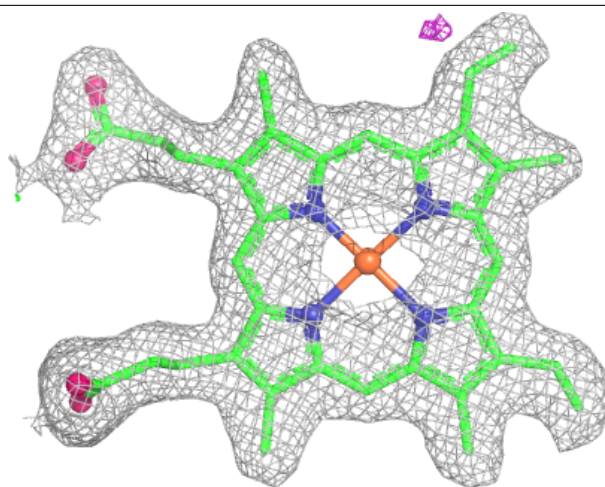
Electron density around HEM C 501:

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



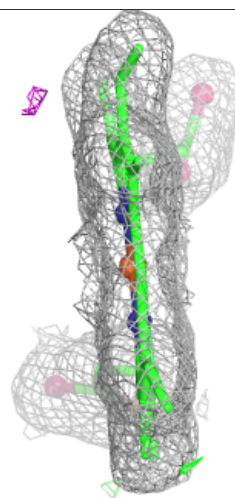
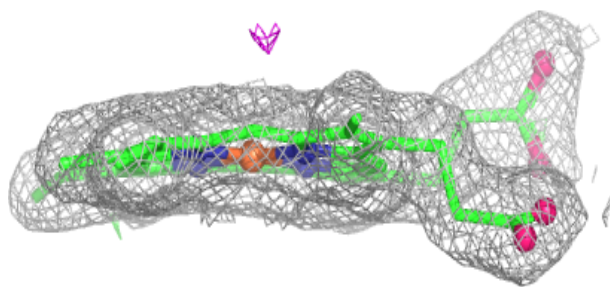
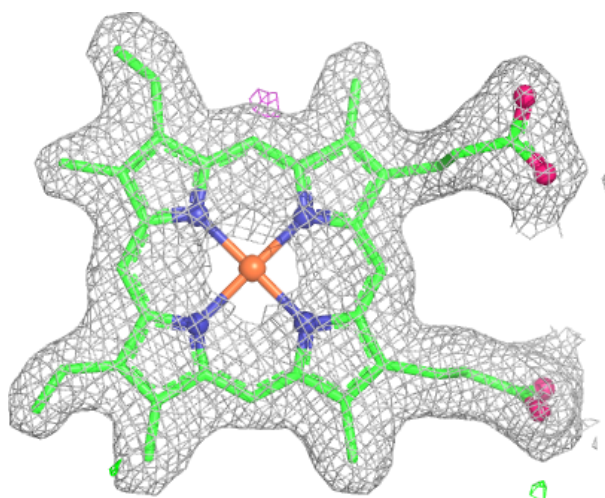
Electron density around HEM D 501:

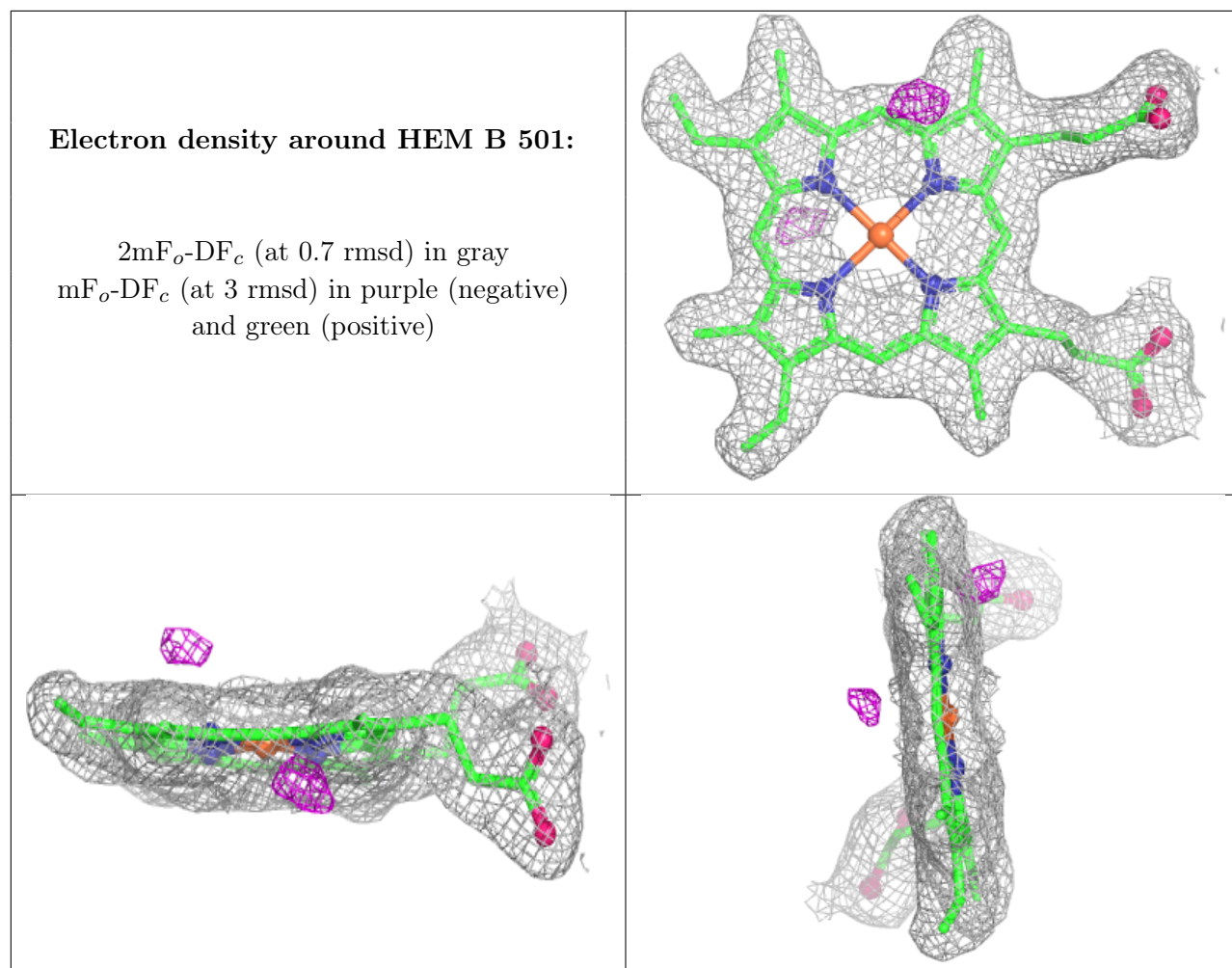
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.