



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:55 PM UTC

PDB ID : 9IY1 / pdb_00009iy1
Title : P450 BS beta mutant F46A
Authors : Gong, P.Q.; Gao, X.
Deposited on : 2024-07-29
Resolution : 2.29 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

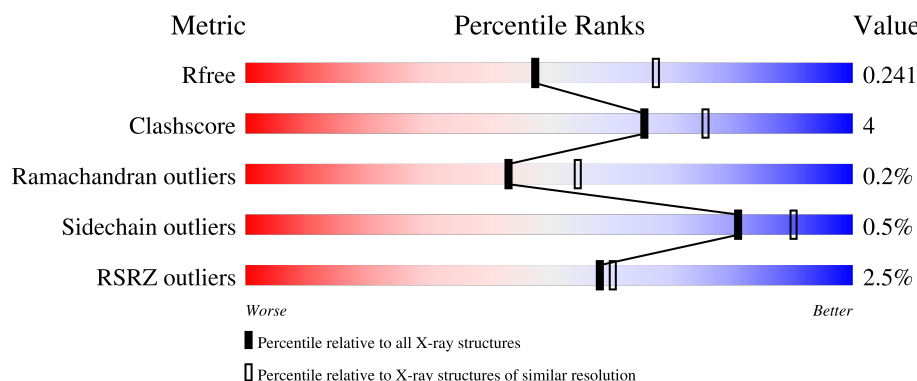
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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.



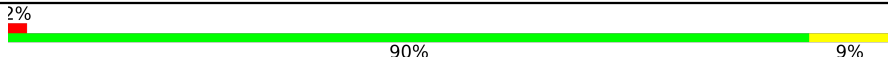
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	416	3% 89% 11%
1	B	416	3% 90% 10%
1	C	416	2% 91% 8%
1	D	416	3% 88% 12%
1	E	416	2% 91% 8%

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Mol	Chain	Length	Quality of chain
1	F	416	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '90%', and a small yellow segment at the end labeled '9%'.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21795 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.

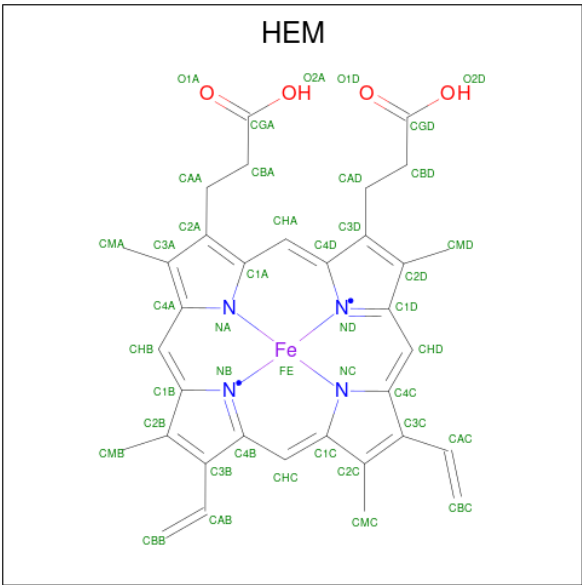
- Molecule 1 is a protein called Fatty-acid peroxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3367	2139	600	609	19			
1	B	415	Total	C	N	O	S	0	0	0
			3367	2139	600	609	19			
1	C	414	Total	C	N	O	S	0	0	0
			3357	2133	598	607	19			
1	D	416	Total	C	N	O	S	0	0	0
			3375	2144	601	610	20			
1	E	414	Total	C	N	O	S	0	0	0
			3359	2135	598	607	19			
1	F	415	Total	C	N	O	S	0	0	0
			3367	2139	600	609	19			

There are 6 discrepancies between the modelled and reference sequences:

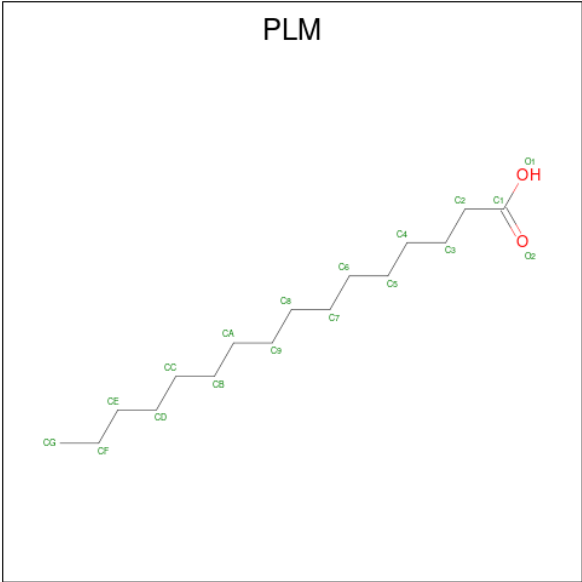
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ALA	PHE	engineered mutation	UNP O31440
B	46	ALA	PHE	engineered mutation	UNP O31440
C	46	ALA	PHE	engineered mutation	UNP O31440
D	46	ALA	PHE	engineered mutation	UNP O31440
E	46	ALA	PHE	engineered mutation	UNP O31440
F	46	ALA	PHE	engineered mutation	UNP O31440

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		
3	E	1	Total	C	O	0	0
			18	16	2		
3	F	1	Total	C	O	0	0
			18	16	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



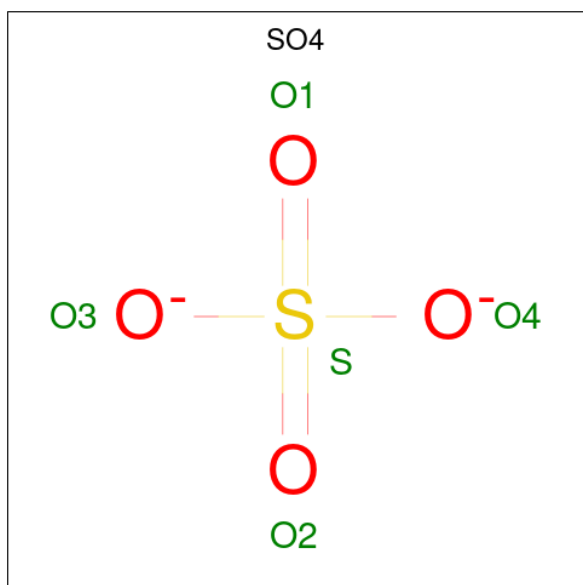
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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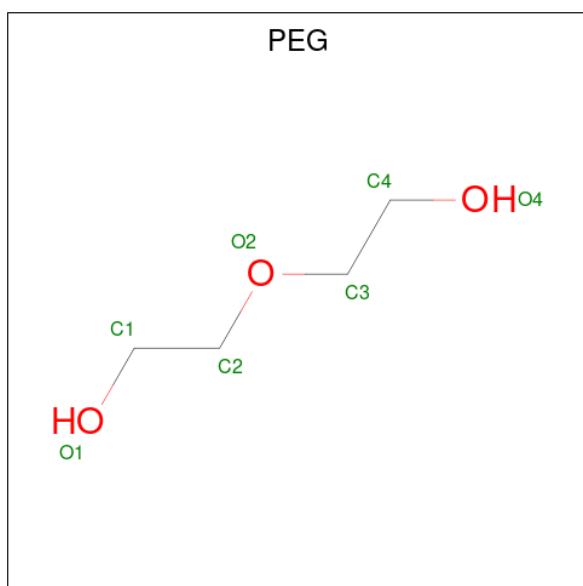
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0

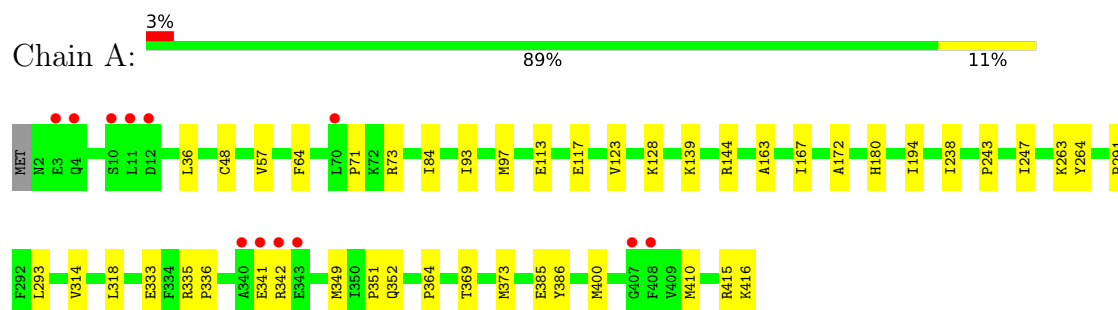
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	139	Total O 139 139	0	0
7	B	175	Total O 175 175	0	0
7	C	195	Total O 195 195	0	0
7	D	127	Total O 127 127	0	0
7	E	147	Total O 147 147	0	0
7	F	169	Total O 169 169	0	0

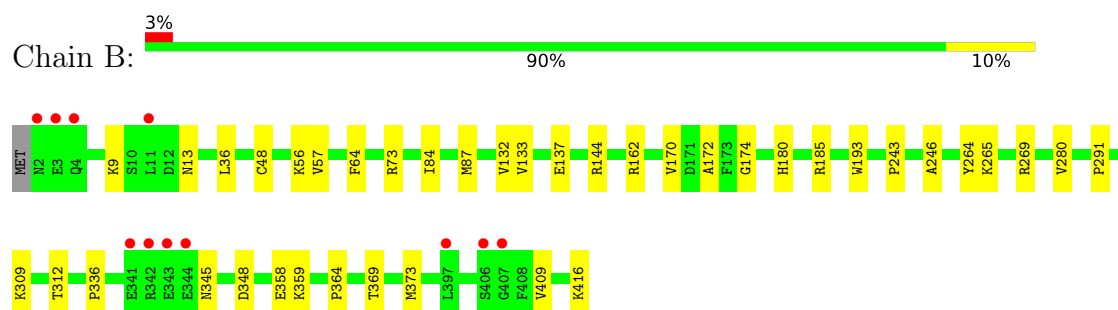
3 Residue-property plots [i](#)

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.

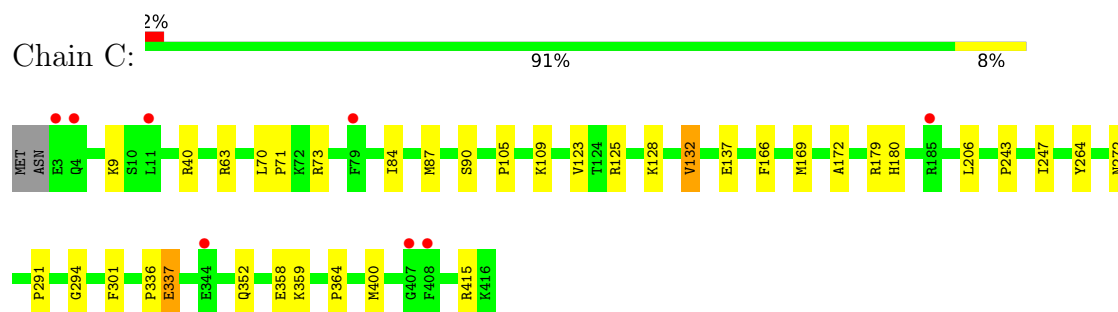
- Molecule 1: Fatty-acid peroxygenase



- Molecule 1: Fatty-acid peroxygenase

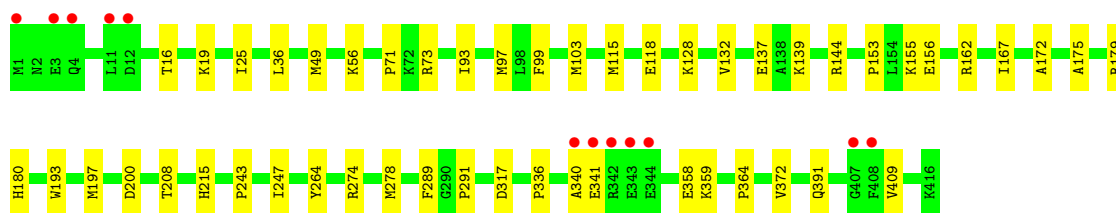


- Molecule 1: Fatty-acid peroxygenase

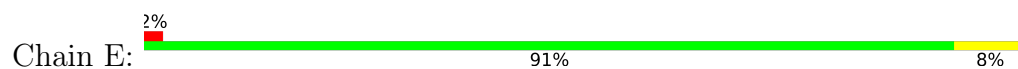


- Molecule 1: Fatty-acid peroxygenase

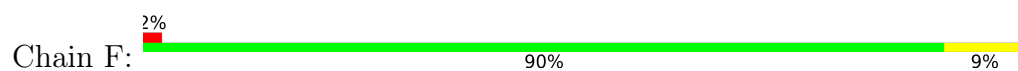




• Molecule 1: Fatty-acid peroxygenase



• Molecule 1: Fatty-acid peroxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.42Å 190.11Å 226.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 2.29 49.49 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.49-2.29) 97.4 (49.49-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.240 0.198 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21795	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PLM, SO4, HEM, PEG

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	0.09	0/3449	0.25	0/4652
1	B	0.09	0/3449	0.25	0/4652
1	C	0.09	0/3439	0.26	0/4638
1	D	0.09	0/3457	0.25	0/4662
1	E	0.09	0/3441	0.25	0/4641
1	F	0.09	0/3449	0.25	0/4652
All	All	0.09	0/20684	0.25	0/27897

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3367	0	3316	27	0
1	B	3367	0	3316	29	0
1	C	3357	0	3303	26	0
1	D	3375	0	3328	32	0
1	E	3359	0	3310	24	0
1	F	3367	0	3316	24	0
2	A	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	5	0
2	C	43	0	30	7	0
2	D	43	0	30	6	0
2	E	43	0	30	3	0
2	F	43	0	30	3	0
3	A	18	0	31	0	0
3	B	18	0	31	1	0
3	C	18	0	31	0	0
3	D	18	0	31	0	0
3	E	18	0	31	0	0
3	F	18	0	31	0	0
4	A	42	0	56	1	0
4	B	12	0	16	0	0
4	C	24	0	32	2	0
4	D	24	0	32	0	0
4	E	18	0	24	1	0
4	F	30	0	40	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	15	0	0	0	0
5	E	5	0	0	0	0
5	F	20	0	0	0	0
6	B	14	0	20	2	0
6	C	21	0	30	2	0
6	D	14	0	20	2	0
6	F	21	0	30	0	0
7	A	139	0	0	1	0
7	B	175	0	0	3	0
7	C	195	0	0	0	0
7	D	127	0	0	0	0
7	E	147	0	0	2	0
7	F	169	0	0	0	0
All	All	21795	0	20555	156	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 (156) 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:A:247:ILE:HD11	2:A:501:HEM:HBB1	1.62	0.79
1:C:352:GLN:HG2	2:C:501:HEM:HBC2	1.64	0.78
1:A:352:GLN:HG2	2:A:501:HEM:HBC2	1.65	0.76
1:D:247:ILE:HD11	2:D:501:HEM:HBB1	1.68	0.75
1:B:358:GLU:HG2	1:B:359:LYS:HG3	1.70	0.73
1:C:247:ILE:HD11	2:C:501:HEM:HBB1	1.71	0.71
1:D:358:GLU:HG2	1:D:359:LYS:HG3	1.75	0.67
1:E:330:HIS:HB3	1:E:333:GLU:HG3	1.77	0.67
1:A:139:LYS:HG2	1:A:163:ALA:HB1	1.77	0.66
1:F:140:GLU:OE2	1:F:160:LYS:NZ	2.29	0.64
1:E:243:PRO:HB2	2:E:501:HEM:C2C	2.32	0.64
1:B:162:ARG:HH22	6:B:503:PEG:H21	1.64	0.63
1:D:162:ARG:HH22	6:D:505:PEG:H21	1.64	0.62
1:C:125:ARG:NH2	1:C:137:GLU:OE1	2.28	0.61
1:F:385:GLU:OE2	1:F:416:LYS:NZ	2.34	0.61
1:A:333:GLU:OE1	1:A:335:ARG:NH2	2.34	0.60
1:C:123:VAL:HG11	1:C:415:ARG:HG3	1.84	0.60
1:A:349:MET:HE3	1:A:351:PRO:HG3	1.83	0.60
1:C:243:PRO:HB2	2:C:501:HEM:C3B	2.37	0.59
1:A:71:PRO:HB2	1:A:73:ARG:HG2	1.83	0.59
1:B:193:TRP:HB2	6:B:503:PEG:H12	1.83	0.59
1:C:358:GLU:HG2	1:C:359:LYS:HG3	1.85	0.59
1:E:139:LYS:HE2	1:E:167:ILE:HG13	1.85	0.59
1:E:342:ARG:HG2	4:E:504:GOL:H31	1.84	0.58
1:B:133:VAL:HG22	1:B:409:VAL:HG22	1.85	0.58
1:A:385:GLU:HG2	1:A:416:LYS:HD3	1.85	0.57
1:E:125:ARG:NH2	7:E:602:HOH:O	2.36	0.57
1:D:289:PHE:HB3	2:D:501:HEM:HBC1	1.87	0.57
1:B:174:GLY:HA2	3:B:502:PLM:HF2	1.87	0.56
1:D:243:PRO:HB2	2:D:501:HEM:C3B	2.40	0.56
1:D:264:TYR:CZ	1:D:336:PRO:HD2	2.41	0.56
1:B:243:PRO:HB2	2:B:501:HEM:C2C	2.40	0.56
1:D:200:ASP:OD1	1:F:73:ARG:NH1	2.35	0.56
1:F:133:VAL:HG22	1:F:409:VAL:HG22	1.88	0.56
1:F:243:PRO:HB2	2:F:501:HEM:C2C	2.40	0.55
1:C:90:SER:H	4:C:507:GOL:H11	1.72	0.55
1:A:144:ARG:NH2	7:A:602:HOH:O	2.40	0.55
1:A:243:PRO:HB2	2:A:501:HEM:C3B	2.42	0.54
1:D:243:PRO:HB2	2:D:501:HEM:C2B	2.42	0.54
1:E:179:ARG:NH2	1:E:400:MET:O	2.40	0.54
1:B:144:ARG:NH2	7:B:603:HOH:O	2.38	0.54
1:A:369:THR:O	1:A:373:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:VAL:HG11	1:E:415:ARG:HG2	1.91	0.53
1:E:231:ARG:NH2	7:E:601:HOH:O	2.33	0.53
1:B:264:TYR:CZ	1:B:336:PRO:HD2	2.44	0.53
1:E:264:TYR:CZ	1:E:336:PRO:HD2	2.44	0.53
1:F:243:PRO:HB2	2:F:501:HEM:C3C	2.44	0.53
1:B:243:PRO:HB2	2:B:501:HEM:C3C	2.44	0.52
1:F:132:VAL:HG13	1:F:137:GLU:HG3	1.92	0.52
6:C:510:PEG:H42	1:E:204:GLY:HA3	1.91	0.51
1:A:264:TYR:CZ	1:A:336:PRO:HD2	2.45	0.51
1:F:99:PHE:O	1:F:103:MET:HG3	2.11	0.51
1:F:139:LYS:HE3	1:F:167:ILE:HG13	1.93	0.51
1:A:93:ILE:O	1:A:97:MET:HG2	2.11	0.51
1:A:57:VAL:HG12	1:A:64:PHE:HE2	1.75	0.51
1:A:342:ARG:HD2	1:A:342:ARG:C	2.36	0.50
1:B:144:ARG:HG2	1:C:128:LYS:HD2	1.93	0.50
1:E:364:PRO:HD2	2:E:501:HEM:C1D	2.46	0.50
1:E:385:GLU:HG2	1:E:416:LYS:HG2	1.92	0.50
1:D:118:GLU:OE2	1:E:128:LYS:NZ	2.41	0.50
1:B:265:LYS:HE2	1:B:269:ARG:NH2	2.27	0.49
1:A:123:VAL:HG11	1:A:415:ARG:HG3	1.93	0.49
1:F:115:MET:HG3	1:F:372:VAL:HG13	1.94	0.49
1:B:369:THR:HG21	2:B:501:HEM:HAB	1.93	0.49
1:E:132:VAL:HG13	1:E:137:GLU:HG3	1.95	0.49
1:C:40:ARG:HG2	6:C:510:PEG:H32	1.95	0.49
1:F:264:TYR:CZ	1:F:336:PRO:HD2	2.47	0.49
1:C:179:ARG:NH2	1:C:400:MET:O	2.46	0.49
1:C:243:PRO:HB2	2:C:501:HEM:C2B	2.48	0.49
1:A:139:LYS:HE2	1:A:167:ILE:HG13	1.95	0.48
1:D:115:MET:HG3	1:D:372:VAL:HG13	1.95	0.48
1:D:139:LYS:HE3	1:D:167:ILE:HG13	1.94	0.48
1:C:172:ALA:HB1	1:C:180:HIS:HA	1.94	0.48
1:C:264:TYR:CZ	1:C:336:PRO:HD2	2.48	0.48
1:F:172:ALA:HB1	1:F:180:HIS:HA	1.96	0.48
1:C:166:PHE:HA	1:C:169:MET:HE3	1.96	0.48
1:B:132:VAL:HG13	1:B:137:GLU:HG3	1.95	0.48
1:B:57:VAL:HG12	1:B:64:PHE:HE2	1.79	0.47
1:D:172:ALA:HB1	1:D:180:HIS:HA	1.96	0.47
1:A:113:GLU:O	1:A:117:GLU:HG3	2.14	0.47
1:F:358:GLU:CD	1:F:358:GLU:H	2.21	0.47
1:C:9:LYS:HE2	1:C:9:LYS:HB2	1.59	0.47
1:D:71:PRO:HB2	1:D:73:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PRO:HB2	2:A:501:HEM:C2B	2.49	0.47
1:D:99:PHE:O	1:D:103:MET:HG3	2.15	0.47
1:A:364:PRO:HD2	2:A:501:HEM:C4A	2.49	0.47
1:D:93:ILE:O	1:D:97:MET:HG2	2.15	0.47
1:F:179:ARG:NH2	1:F:400:MET:O	2.48	0.47
1:A:172:ALA:HB1	1:A:180:HIS:HA	1.97	0.47
1:D:16:THR:HA	1:D:19:LYS:HG2	1.97	0.46
1:A:400:MET:HE3	1:A:400:MET:HB2	1.79	0.46
1:C:63:ARG:HD2	1:C:301:PHE:CG	2.51	0.46
1:A:263:LYS:HD3	4:A:508:GOL:H31	1.96	0.46
1:F:195:GLU:O	1:F:199:GLU:HG3	2.16	0.46
1:F:269:ARG:HH22	1:F:416:LYS:HZ1	1.63	0.46
1:A:194:ILE:HG13	1:A:238:ILE:HD11	1.98	0.46
1:B:13:ASN:ND2	7:B:609:HOH:O	2.50	0.45
1:B:73:ARG:NH1	1:F:200:ASP:OD1	2.43	0.45
1:B:172:ALA:HB1	1:B:180:HIS:HA	1.98	0.45
1:B:364:PRO:HD2	2:B:501:HEM:C1D	2.51	0.45
1:D:274:ARG:NH2	1:D:341:GLU:OE2	2.50	0.45
1:B:56:LYS:HB2	1:B:56:LYS:HE3	1.81	0.45
1:F:25:ILE:HG21	1:F:317:ASP:HB2	1.99	0.45
1:D:56:LYS:HE3	1:D:56:LYS:HB3	1.81	0.45
1:F:349:MET:HE3	1:F:351:PRO:HG3	1.99	0.45
1:D:364:PRO:HD2	2:D:501:HEM:C4A	2.51	0.45
1:E:285:ARG:HB2	1:E:349:MET:SD	2.57	0.44
1:F:5:ILE:HD12	1:F:36:LEU:HD11	1.99	0.44
1:D:144:ARG:NH1	1:D:156:GLU:OE1	2.51	0.44
1:D:155:LYS:HE3	1:D:155:LYS:HB2	1.70	0.44
1:B:84:ILE:HA	1:B:87:MET:SD	2.57	0.44
1:D:128:LYS:HD2	1:E:144:ARG:HG2	2.00	0.44
1:B:185:ARG:NH2	7:B:611:HOH:O	2.50	0.44
1:F:364:PRO:HD2	2:F:501:HEM:C1D	2.52	0.44
1:A:386:TYR:CD2	1:A:410:MET:HG2	2.52	0.44
1:D:208:THR:HB	1:D:215:HIS:HB2	2.00	0.44
1:C:364:PRO:HD2	2:C:501:HEM:C4A	2.52	0.43
1:D:36:LEU:CD1	1:D:49:MET:HB3	2.48	0.43
1:B:345:ASN:HB3	1:B:348:ASP:OD1	2.18	0.43
1:E:358:GLU:H	1:E:358:GLU:CD	2.26	0.43
1:B:280:VAL:HG13	1:B:373:MET:HE2	2.00	0.43
1:C:337:GLU:CD	1:C:337:GLU:H	2.25	0.43
1:E:169:MET:HE3	1:E:187:ARG:HA	2.00	0.43
1:B:309:LYS:O	1:B:312:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:MET:HE3	1:D:340:ALA:HB2	2.01	0.43
1:F:153:PRO:HD2	1:F:197:MET:SD	2.59	0.42
1:C:352:GLN:HG2	2:C:501:HEM:CBC	2.44	0.42
1:D:193:TRP:HB2	6:D:505:PEG:H12	2.01	0.42
1:D:391:GLN:CD	1:D:409:VAL:HG22	2.44	0.42
1:F:175:ALA:HB2	1:F:179:ARG:CZ	2.50	0.42
1:B:36:LEU:HA	1:B:48:CYS:O	2.20	0.42
1:D:153:PRO:HD2	1:D:197:MET:SD	2.60	0.42
1:C:70:LEU:HD21	1:C:294:GLY:HA3	2.00	0.42
1:E:24:PHE:CE2	1:E:41:LEU:HD11	2.55	0.42
1:E:78:LEU:HD13	1:E:170:VAL:HA	2.01	0.42
1:E:243:PRO:HB2	2:E:501:HEM:C3C	2.54	0.42
1:E:172:ALA:HB1	1:E:180:HIS:HA	2.02	0.42
1:B:309:LYS:HD3	1:B:309:LYS:HA	1.80	0.41
1:A:36:LEU:HA	1:A:48:CYS:O	2.20	0.41
1:A:128:LYS:HD2	1:F:144:ARG:HG2	2.01	0.41
1:A:293:LEU:HG	1:A:318:LEU:HD11	2.01	0.41
1:B:170:VAL:HG21	1:B:246:ALA:HB2	2.02	0.41
1:D:25:ILE:HG21	1:D:317:ASP:HB2	2.02	0.41
1:B:9:LYS:HB3	1:B:9:LYS:HE2	1.85	0.41
1:C:71:PRO:HB2	1:C:73:ARG:HG2	2.01	0.41
1:C:132:VAL:HG13	1:C:137:GLU:HG3	2.02	0.41
1:E:41:LEU:HD23	1:E:41:LEU:HA	1.97	0.41
1:C:84:ILE:HA	1:C:87:MET:SD	2.61	0.40
1:D:175:ALA:HB2	1:D:179:ARG:CZ	2.51	0.40
1:D:364:PRO:HD2	2:D:501:HEM:C3A	2.56	0.40
1:E:393:LEU:HD23	1:E:393:LEU:HA	1.91	0.40
1:C:105:PRO:O	1:C:109:LYS:HG3	2.21	0.40
1:D:132:VAL:HG13	1:D:137:GLU:HG3	2.02	0.40
1:B:364:PRO:HD2	2:B:501:HEM:C2D	2.56	0.40
1:C:364:PRO:HD2	2:C:501:HEM:C3A	2.57	0.40
1:C:206:LEU:HD13	4:C:504:GOL:H12	2.04	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	413/416 (99%)	403 (98%)	9 (2%)	1 (0%)	43	55
1	B	413/416 (99%)	405 (98%)	7 (2%)	1 (0%)	43	55
1	C	412/416 (99%)	404 (98%)	7 (2%)	1 (0%)	43	55
1	D	414/416 (100%)	406 (98%)	7 (2%)	1 (0%)	43	55
1	E	412/416 (99%)	406 (98%)	5 (1%)	1 (0%)	43	55
1	F	413/416 (99%)	407 (98%)	5 (1%)	1 (0%)	43	55
All	All	2477/2496 (99%)	2431 (98%)	40 (2%)	6 (0%)	43	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	291	PRO
1	A	291	PRO
1	D	291	PRO
1	C	291	PRO
1	F	291	PRO
1	B	291	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/356 (100%)	352 (99%)	3 (1%)	73	86
1	B	355/356 (100%)	354 (100%)	1 (0%)	86	93
1	C	353/356 (99%)	350 (99%)	3 (1%)	73	86
1	D	356/356 (100%)	356 (100%)	0	100	100
1	E	354/356 (99%)	354 (100%)	0	100	100
1	F	355/356 (100%)	351 (99%)	4 (1%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2128/2136 (100%)	2117 (100%)	11 (0%)	81 90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	314	VAL
1	A	341	GLU
1	B	416	LYS
1	C	132	VAL
1	C	272	ASN
1	C	337	GLU
1	F	5	ILE
1	F	132	VAL
1	F	254	SER
1	F	381	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	82	ASN
1	B	222	GLN
1	B	261	HIS
1	B	330	HIS
1	C	272	ASN
1	E	65	GLN
1	E	68	ASN
1	E	261	HIS
1	E	272	ASN
1	F	38	GLN
1	F	68	ASN
1	F	305	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	SO4	D	510	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	D	509	-	4,4,4	0.24	0	6,6,6	0.07	0
3	PLM	D	502	-	17,17,17	0.98	1 (5%)	17,17,17	0.72	2 (11%)
4	GOL	A	509	-	5,5,5	0.90	0	5,5,5	1.08	0
4	GOL	A	504	-	5,5,5	0.94	0	5,5,5	1.07	0
4	GOL	F	508	-	5,5,5	0.93	0	5,5,5	1.08	0
4	GOL	F	510	-	5,5,5	0.95	0	5,5,5	1.06	0
4	GOL	C	509	-	5,5,5	0.98	0	5,5,5	0.95	0
5	SO4	F	513	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	F	511	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	B	507	-	4,4,4	0.23	0	6,6,6	0.08	0
2	HEM	E	501	1	50,50,50	1.42	6 (12%)	67,82,82	0.79	2 (2%)
4	GOL	A	503	-	5,5,5	0.90	0	5,5,5	1.09	0
2	HEM	D	501	1	50,50,50	1.42	6 (12%)	67,82,82	0.79	1 (1%)
6	PEG	B	506	-	6,6,6	0.11	0	5,5,5	0.09	0
4	GOL	B	504	-	5,5,5	0.90	0	5,5,5	1.09	0
3	PLM	C	502	-	17,17,17	0.95	1 (5%)	17,17,17	0.73	2 (11%)
4	GOL	D	506	-	5,5,5	0.99	0	5,5,5	0.99	0
5	SO4	C	508	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	C	506	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	F	514	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	504	-	5,5,5	0.94	0	5,5,5	1.04	0
3	PLM	E	502	-	17,17,17	0.91	1 (5%)	17,17,17	0.73	2 (11%)
4	GOL	C	507	-	5,5,5	0.96	0	5,5,5	1.00	0
4	GOL	D	504	-	5,5,5	0.94	0	5,5,5	1.05	0
4	GOL	D	503	-	5,5,5	0.97	0	5,5,5	1.02	0
6	PEG	C	505	-	6,6,6	0.12	0	5,5,5	0.11	0
4	GOL	E	503	-	5,5,5	0.93	0	5,5,5	1.08	0
3	PLM	F	502	-	17,17,17	1.02	1 (5%)	17,17,17	0.73	2 (11%)
2	HEM	B	501	1	50,50,50	1.42	6 (12%)	67,82,82	0.86	3 (4%)
4	GOL	D	507	-	5,5,5	0.95	0	5,5,5	1.05	0
5	SO4	F	512	-	4,4,4	0.23	0	6,6,6	0.06	0
6	PEG	B	503	-	6,6,6	0.10	0	5,5,5	0.13	0
6	PEG	F	505	-	6,6,6	0.13	0	5,5,5	0.06	0
5	SO4	D	511	-	4,4,4	0.24	0	6,6,6	0.09	0
4	GOL	A	506	-	5,5,5	0.97	0	5,5,5	1.04	0
4	GOL	F	506	-	5,5,5	0.95	0	5,5,5	1.09	0
6	PEG	D	505	-	6,6,6	0.11	0	5,5,5	0.11	0
4	GOL	C	504	-	5,5,5	0.90	0	5,5,5	1.07	0
2	HEM	F	501	7,1	50,50,50	1.43	6 (12%)	67,82,82	0.84	2 (2%)
6	PEG	C	510	-	6,6,6	0.13	0	5,5,5	0.08	0
4	GOL	F	504	-	5,5,5	0.95	0	5,5,5	1.02	0
5	SO4	A	510	-	4,4,4	0.24	0	6,6,6	0.06	0
2	HEM	A	501	1	50,50,50	1.42	5 (10%)	67,82,82	0.80	2 (2%)
4	GOL	A	505	-	5,5,5	0.94	0	5,5,5	1.07	0
3	PLM	A	502	-	17,17,17	0.97	1 (5%)	17,17,17	0.73	2 (11%)
6	PEG	D	508	-	6,6,6	0.12	0	5,5,5	0.10	0
6	PEG	F	509	-	6,6,6	0.12	0	5,5,5	0.07	0
2	HEM	C	501	1	50,50,50	1.42	7 (14%)	67,82,82	0.76	2 (2%)
4	GOL	A	507	-	5,5,5	0.93	0	5,5,5	1.04	0
4	GOL	C	503	-	5,5,5	0.96	0	5,5,5	1.04	0
4	GOL	E	505	-	5,5,5	0.93	0	5,5,5	1.09	0
4	GOL	F	507	-	5,5,5	0.91	0	5,5,5	1.10	0
4	GOL	A	508	-	5,5,5	0.95	0	5,5,5	1.04	0
6	PEG	C	511	-	6,6,6	0.11	0	5,5,5	0.10	0
5	SO4	E	506	-	4,4,4	0.23	0	6,6,6	0.06	0
6	PEG	F	503	-	6,6,6	0.11	0	5,5,5	0.09	0
5	SO4	B	508	-	4,4,4	0.24	0	6,6,6	0.07	0
4	GOL	B	505	-	5,5,5	0.89	0	5,5,5	1.09	0
3	PLM	B	502	-	17,17,17	0.94	1 (5%)	17,17,17	0.73	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	D	502	-	-	9/15/15/15	-
4	GOL	A	509	-	-	2/4/4/4	-
4	GOL	A	504	-	-	4/4/4/4	-
4	GOL	F	508	-	-	1/4/4/4	-
4	GOL	F	510	-	-	2/4/4/4	-
4	GOL	C	509	-	-	2/4/4/4	-
2	HEM	E	501	1	-	3/14/54/54	-
4	GOL	A	503	-	-	0/4/4/4	-
2	HEM	D	501	1	-	4/14/54/54	-
6	PEG	B	506	-	-	0/4/4/4	-
4	GOL	B	504	-	-	4/4/4/4	-
3	PLM	C	502	-	-	11/15/15/15	-
4	GOL	D	506	-	-	4/4/4/4	-
4	GOL	E	504	-	-	2/4/4/4	-
3	PLM	E	502	-	-	11/15/15/15	-
4	GOL	C	507	-	-	4/4/4/4	-
4	GOL	D	504	-	-	2/4/4/4	-
4	GOL	D	503	-	-	4/4/4/4	-
6	PEG	C	505	-	-	3/4/4/4	-
4	GOL	E	503	-	-	4/4/4/4	-
3	PLM	F	502	-	-	9/15/15/15	-
2	HEM	B	501	1	-	2/14/54/54	-
4	GOL	D	507	-	-	4/4/4/4	-
6	PEG	B	503	-	-	3/4/4/4	-
6	PEG	F	505	-	-	2/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	F	506	-	-	2/4/4/4	-
6	PEG	D	505	-	-	2/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
2	HEM	F	501	7,1	-	2/14/54/54	-
6	PEG	C	510	-	-	1/4/4/4	-
4	GOL	F	504	-	-	2/4/4/4	-
2	HEM	A	501	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	505	-	-	2/4/4/4	-
3	PLM	A	502	-	-	6/15/15/15	-
6	PEG	D	508	-	-	1/4/4/4	-
6	PEG	F	509	-	-	1/4/4/4	-
2	HEM	C	501	1	-	5/14/54/54	-
4	GOL	A	507	-	-	4/4/4/4	-
4	GOL	C	503	-	-	3/4/4/4	-
4	GOL	E	505	-	-	1/4/4/4	-
4	GOL	F	507	-	-	0/4/4/4	-
4	GOL	A	508	-	-	2/4/4/4	-
6	PEG	C	511	-	-	2/4/4/4	-
6	PEG	F	503	-	-	2/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
3	PLM	B	502	-	-	8/15/15/15	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	4.40	2.08	1.94
2	F	501	HEM	FE-NB	4.39	2.08	1.94
2	C	501	HEM	FE-NB	4.38	2.08	1.94
2	D	501	HEM	FE-NB	4.36	2.08	1.94
2	E	501	HEM	FE-NB	4.32	2.08	1.94
2	B	501	HEM	FE-NB	4.28	2.08	1.94
2	B	501	HEM	FE-NC	3.45	2.06	1.95
2	C	501	HEM	FE-NC	3.45	2.06	1.95
2	F	501	HEM	FE-NC	3.44	2.06	1.95
2	A	501	HEM	FE-NC	3.44	2.06	1.95
2	E	501	HEM	FE-NC	3.40	2.06	1.95
2	D	501	HEM	FE-NC	3.35	2.06	1.95
3	F	502	PLM	C2-C1	3.27	1.58	1.50
3	D	502	PLM	C2-C1	3.20	1.58	1.50
2	A	501	HEM	C4D-ND	-3.19	1.34	1.40
2	C	501	HEM	C4D-ND	-3.17	1.34	1.40
2	E	501	HEM	C4D-ND	-3.17	1.34	1.40
2	F	501	HEM	C4D-ND	-3.14	1.34	1.40
3	A	502	PLM	C2-C1	3.14	1.57	1.50
2	B	501	HEM	C4D-ND	-3.13	1.34	1.40
2	D	501	HEM	C4D-ND	-3.13	1.34	1.40
3	C	502	PLM	C2-C1	3.08	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	PLM	C2-C1	2.90	1.57	1.50
3	E	502	PLM	C2-C1	2.89	1.57	1.50
2	F	501	HEM	FE-NA	2.86	2.04	1.95
2	B	501	HEM	FE-NA	2.84	2.04	1.95
2	E	501	HEM	FE-NA	2.84	2.04	1.95
2	C	501	HEM	FE-NA	2.81	2.04	1.95
2	D	501	HEM	FE-NA	2.81	2.04	1.95
2	A	501	HEM	FE-NA	2.77	2.04	1.95
2	D	501	HEM	C4C-NC	-2.74	1.34	1.39
2	F	501	HEM	C4C-NC	-2.71	1.34	1.39
2	B	501	HEM	C4C-NC	-2.69	1.34	1.39
2	E	501	HEM	C4C-NC	-2.64	1.34	1.39
2	C	501	HEM	C4C-NC	-2.58	1.34	1.39
2	A	501	HEM	C4C-NC	-2.57	1.34	1.39
2	F	501	HEM	C1C-NC	-2.14	1.35	1.39
2	E	501	HEM	C1C-NC	-2.12	1.35	1.39
2	B	501	HEM	C1C-NC	-2.10	1.35	1.39
2	D	501	HEM	C1C-NC	-2.10	1.35	1.39
2	C	501	HEM	C1C-NC	-2.09	1.35	1.39
2	C	501	HEM	C2A-C3A	-2.01	1.33	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-3.04	104.13	112.53
2	D	501	HEM	CBD-CAD-C3D	-3.00	104.25	112.53
2	C	501	HEM	CBD-CAD-C3D	-2.87	104.60	112.53
2	E	501	HEM	CBD-CAD-C3D	-2.51	105.61	112.53
2	B	501	HEM	CBD-CAD-C3D	-2.50	105.61	112.53
2	F	501	HEM	CBD-CAD-C3D	-2.28	106.22	112.53
2	A	501	HEM	O1A-CGA-CBA	-2.14	116.29	123.09
2	F	501	HEM	C4D-ND-C1D	2.14	107.74	105.21
3	B	502	PLM	O1-C1-O2	2.14	128.84	123.33
3	A	502	PLM	O1-C1-O2	2.12	128.79	123.33
3	E	502	PLM	O1-C1-O2	2.11	128.76	123.33
3	C	502	PLM	O1-C1-O2	2.11	128.75	123.33
2	E	501	HEM	C4D-ND-C1D	2.10	107.70	105.21
2	B	501	HEM	C4D-ND-C1D	2.09	107.68	105.21
3	E	502	PLM	O2-C1-C2	-2.08	116.50	123.09
3	D	502	PLM	O1-C1-O2	2.07	128.66	123.33
3	B	502	PLM	O2-C1-C2	-2.05	116.58	123.09
3	F	502	PLM	O2-C1-C2	-2.05	116.58	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	PLM	O1-C1-O2	2.05	128.60	123.33
2	C	501	HEM	C4D-ND-C1D	2.04	107.62	105.21
3	C	502	PLM	O2-C1-C2	-2.03	116.65	123.09
3	A	502	PLM	O2-C1-C2	-2.03	116.66	123.09
2	B	501	HEM	CAA-CBA-CGA	2.02	119.03	113.67
3	D	502	PLM	O2-C1-C2	-2.01	116.72	123.09

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2B-C3B-CAB-CBB
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C2B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
2	E	501	HEM	C2B-C3B-CAB-CBB
2	E	501	HEM	C4B-C3B-CAB-CBB
2	F	501	HEM	C2B-C3B-CAB-CBB
2	F	501	HEM	C4B-C3B-CAB-CBB
4	A	504	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
4	A	507	GOL	O1-C1-C2-C3
4	A	509	GOL	O1-C1-C2-C3
4	B	504	GOL	O1-C1-C2-C3
4	B	504	GOL	C1-C2-C3-O3
4	B	505	GOL	O1-C1-C2-C3
4	C	504	GOL	C1-C2-C3-O3
4	C	509	GOL	O1-C1-C2-C3
4	D	503	GOL	C1-C2-C3-O3
4	D	507	GOL	O1-C1-C2-C3
4	E	503	GOL	O1-C1-C2-C3
4	E	503	GOL	C1-C2-C3-O3
4	F	510	GOL	C1-C2-C3-O3
6	C	511	PEG	O2-C3-C4-O4
3	C	502	PLM	C1-C2-C3-C4
4	A	509	GOL	O1-C1-C2-O2
4	C	504	GOL	O2-C2-C3-O3
3	D	502	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
6	F	505	PEG	O2-C3-C4-O4
4	A	504	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	A	507	GOL	C1-C2-C3-O3
4	A	508	GOL	C1-C2-C3-O3
4	C	503	GOL	C1-C2-C3-O3
4	C	507	GOL	O1-C1-C2-C3
4	D	503	GOL	O1-C1-C2-C3
4	D	504	GOL	O1-C1-C2-C3
4	D	506	GOL	O1-C1-C2-C3
4	D	506	GOL	C1-C2-C3-O3
4	D	507	GOL	C1-C2-C3-O3
4	E	504	GOL	O1-C1-C2-C3
4	F	504	GOL	C1-C2-C3-O3
4	F	506	GOL	C1-C2-C3-O3
6	F	503	PEG	O2-C3-C4-O4
3	D	502	PLM	C6-C7-C8-C9
4	A	504	GOL	O1-C1-C2-O2
4	A	504	GOL	O2-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	A	506	GOL	O1-C1-C2-O2
4	A	507	GOL	O2-C2-C3-O3
4	A	508	GOL	O2-C2-C3-O3
4	B	504	GOL	O1-C1-C2-O2
4	B	504	GOL	O2-C2-C3-O3
4	B	505	GOL	O1-C1-C2-O2
4	C	509	GOL	O1-C1-C2-O2
4	D	503	GOL	O1-C1-C2-O2
4	D	507	GOL	O1-C1-C2-O2
4	E	503	GOL	O1-C1-C2-O2
4	F	510	GOL	O2-C2-C3-O3
3	E	502	PLM	CC-CD-CE-CF
3	E	502	PLM	C3-C4-C5-C6
3	B	502	PLM	C4-C5-C6-C7
3	C	502	PLM	C3-C4-C5-C6
3	D	502	PLM	CC-CD-CE-CF
3	A	502	PLM	C9-CA-CB-CC
3	B	502	PLM	CC-CD-CE-CF
3	F	502	PLM	C8-C9-CA-CB
6	B	503	PEG	O2-C3-C4-O4
2	A	501	HEM	C2C-C3C-CAC-CBC
2	C	501	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	A	502	PLM	C4-C5-C6-C7
3	F	502	PLM	CC-CD-CE-CF
3	D	502	PLM	C4-C5-C6-C7
3	E	502	PLM	CB-CC-CD-CE
6	D	505	PEG	O1-C1-C2-O2
3	C	502	PLM	C7-C8-C9-CA
3	E	502	PLM	C6-C7-C8-C9
4	A	507	GOL	O1-C1-C2-O2
4	D	503	GOL	O2-C2-C3-O3
4	D	506	GOL	O2-C2-C3-O3
4	E	503	GOL	O2-C2-C3-O3
3	C	502	PLM	CC-CD-CE-CF
6	B	503	PEG	O1-C1-C2-O2
3	C	502	PLM	CB-CC-CD-CE
3	A	502	PLM	C3-C4-C5-C6
3	B	502	PLM	C3-C4-C5-C6
3	C	502	PLM	CA-CB-CC-CD
3	D	502	PLM	CD-CE-CF-CG
4	C	507	GOL	O1-C1-C2-O2
4	C	507	GOL	O2-C2-C3-O3
4	D	506	GOL	O1-C1-C2-O2
3	F	502	PLM	CD-CE-CF-CG
3	E	502	PLM	CD-CE-CF-CG
3	B	502	PLM	CD-CE-CF-CG
3	B	502	PLM	C7-C8-C9-CA
3	B	502	PLM	C8-C9-CA-CB
4	C	503	GOL	O1-C1-C2-O2
4	F	508	GOL	O2-C2-C3-O3
6	C	505	PEG	O2-C3-C4-O4
6	B	503	PEG	C1-C2-O2-C3
2	D	501	HEM	C2C-C3C-CAC-CBC
6	F	503	PEG	C1-C2-O2-C3
6	D	505	PEG	O2-C3-C4-O4
6	C	510	PEG	C1-C2-O2-C3
2	C	501	HEM	C4C-C3C-CAC-CBC
2	D	501	HEM	C4C-C3C-CAC-CBC
3	E	502	PLM	CA-CB-CC-CD
3	F	502	PLM	C2-C3-C4-C5
4	C	503	GOL	O2-C2-C3-O3
4	D	507	GOL	O2-C2-C3-O3
4	F	504	GOL	O2-C2-C3-O3
4	F	506	GOL	O2-C2-C3-O3

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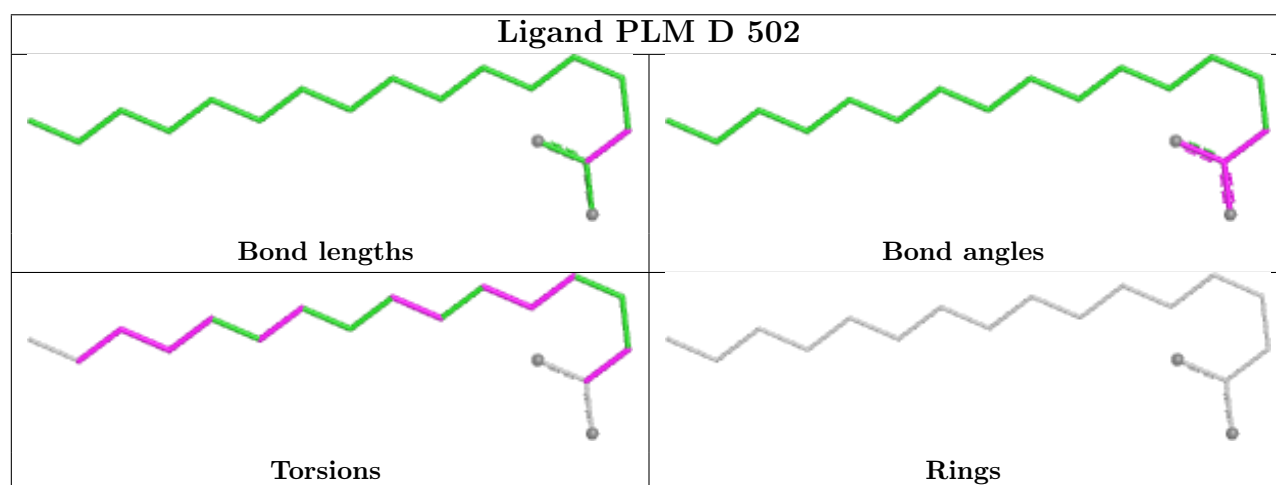
Mol	Chain	Res	Type	Atoms
3	E	502	PLM	C4-C5-C6-C7
3	D	502	PLM	C3-C4-C5-C6
3	E	502	PLM	C9-CA-CB-CC
3	D	502	PLM	CB-CC-CD-CE
3	F	502	PLM	C6-C7-C8-C9
6	F	505	PEG	C4-C3-O2-C2
3	C	502	PLM	C4-C5-C6-C7
6	C	505	PEG	C1-C2-O2-C3
3	F	502	PLM	C3-C4-C5-C6
2	A	501	HEM	C4C-C3C-CAC-CBC
3	A	502	PLM	C7-C8-C9-CA
4	C	507	GOL	C1-C2-C3-O3
3	B	502	PLM	C9-CA-CB-CC
3	C	502	PLM	O2-C1-C2-C3
4	E	504	GOL	O1-C1-C2-O2
3	F	502	PLM	O1-C1-C2-C3
3	E	502	PLM	O1-C1-C2-C3
3	E	502	PLM	O2-C1-C2-C3
3	A	502	PLM	C8-C9-CA-CB
3	D	502	PLM	O1-C1-C2-C3
3	D	502	PLM	O2-C1-C2-C3
3	C	502	PLM	O1-C1-C2-C3
3	F	502	PLM	O2-C1-C2-C3
4	D	504	GOL	O1-C1-C2-O2
3	F	502	PLM	CA-CB-CC-CD
3	C	502	PLM	CD-CE-CF-CG
6	C	505	PEG	O1-C1-C2-O2
4	E	505	GOL	O2-C2-C3-O3
6	C	511	PEG	C1-C2-O2-C3
3	E	502	PLM	C2-C3-C4-C5
6	F	509	PEG	C4-C3-O2-C2
2	C	501	HEM	CAA-CBA-CGA-O1A
3	B	502	PLM	O1-C1-C2-C3
3	A	502	PLM	CB-CC-CD-CE
3	C	502	PLM	C2-C3-C4-C5
2	E	501	HEM	CAD-CBD-CGD-O2D
6	D	508	PEG	O2-C3-C4-O4

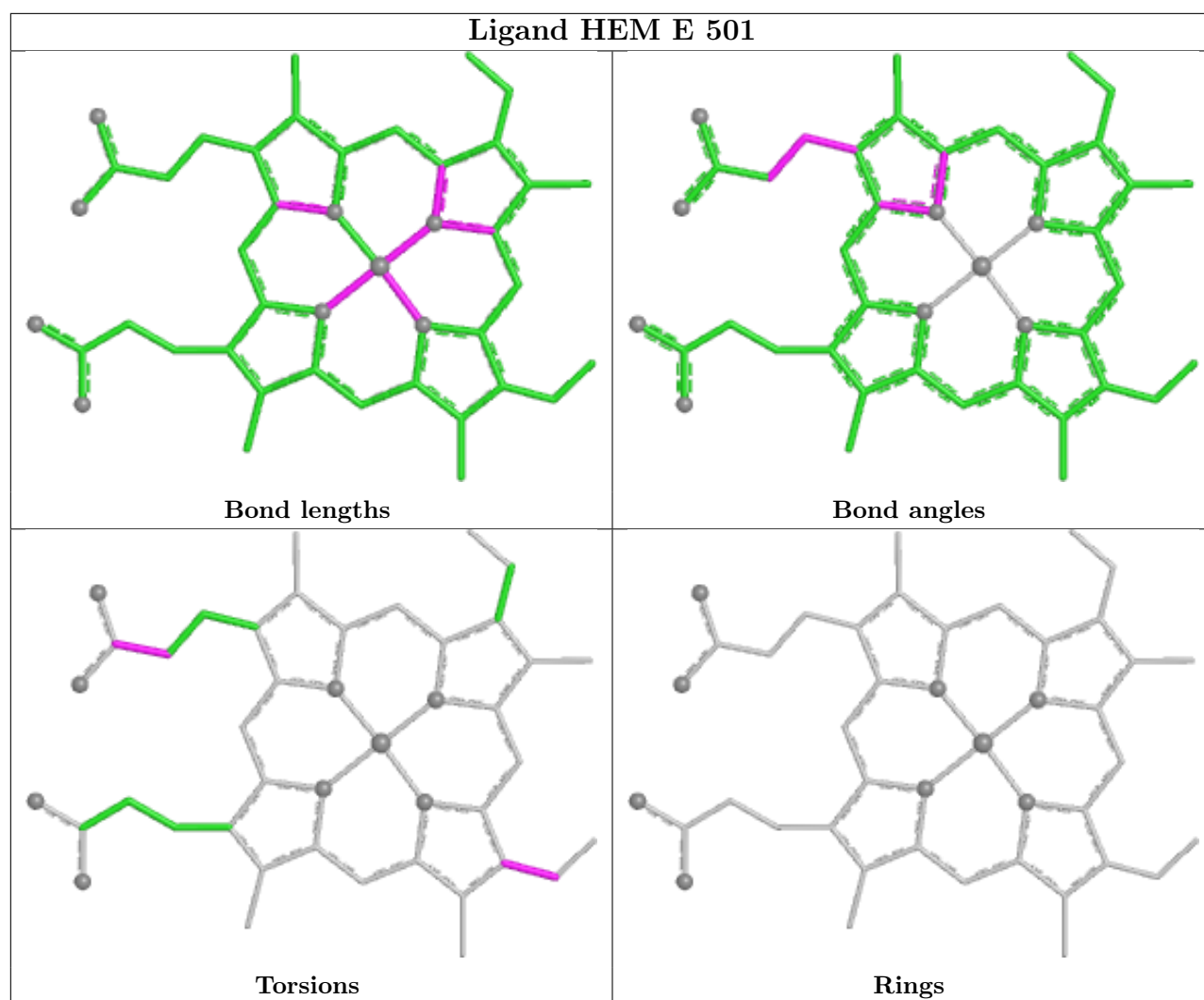
There are no ring outliers.

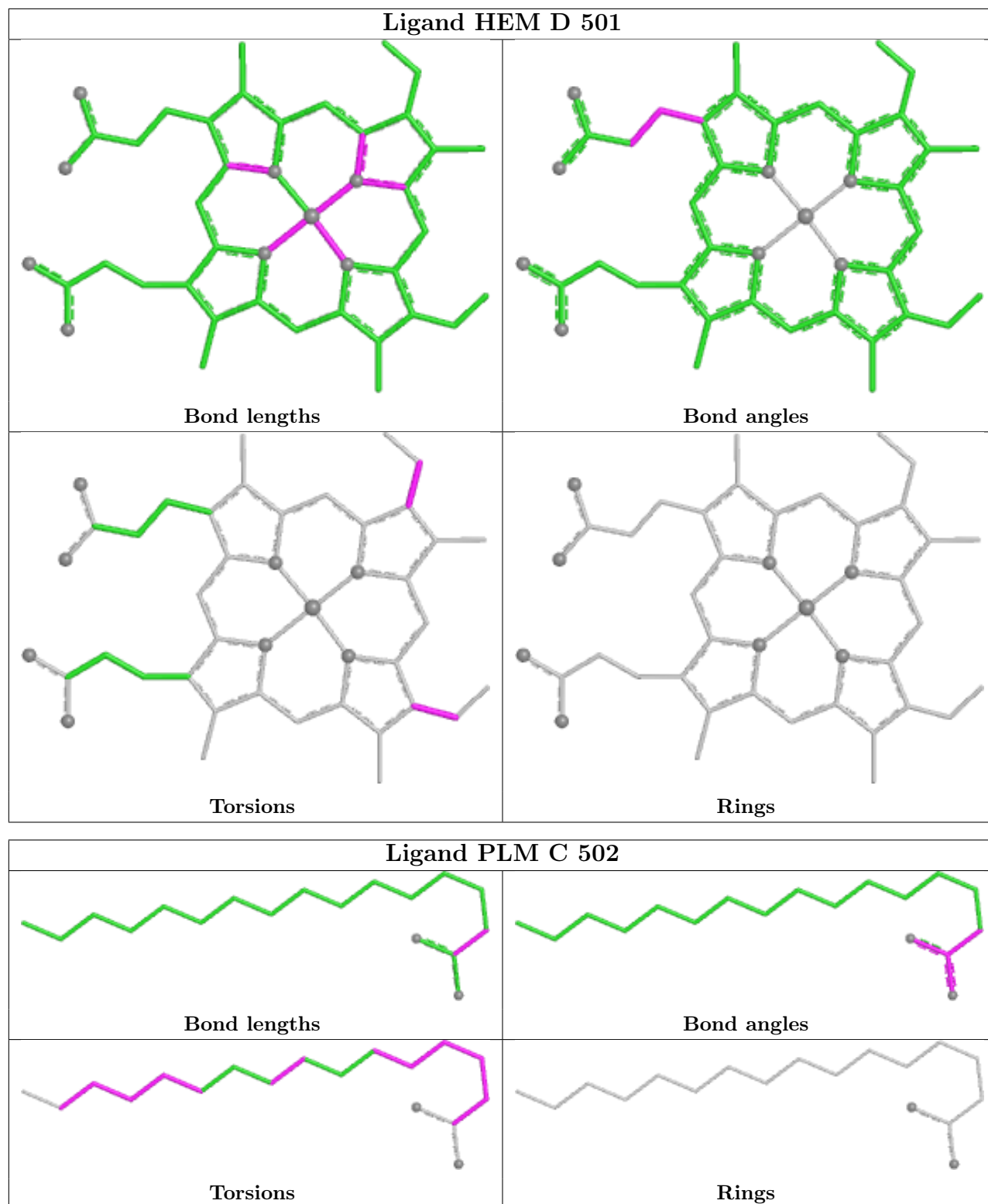
14 monomers are involved in 40 short contacts:

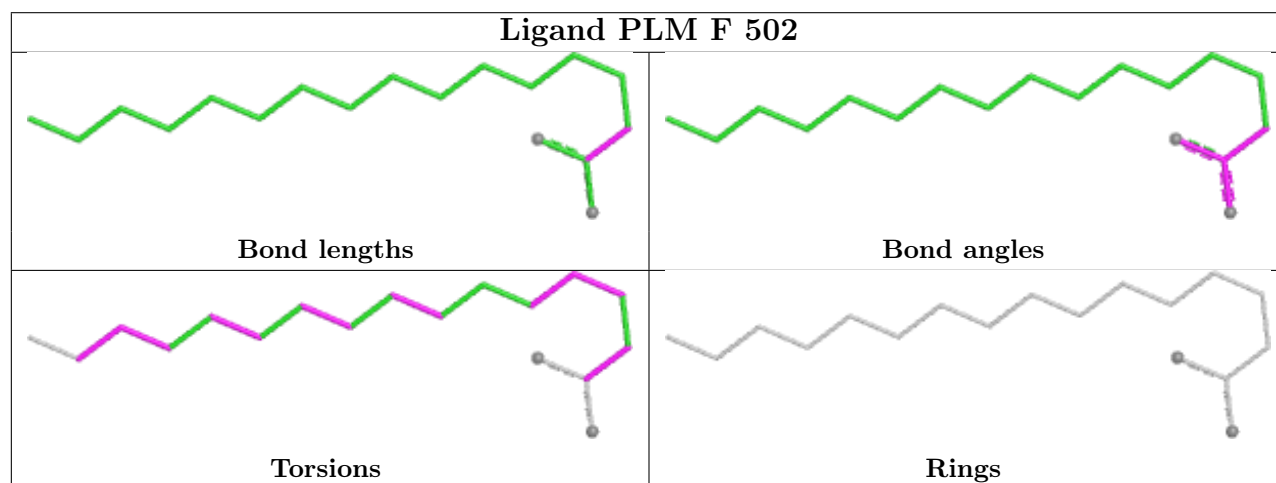
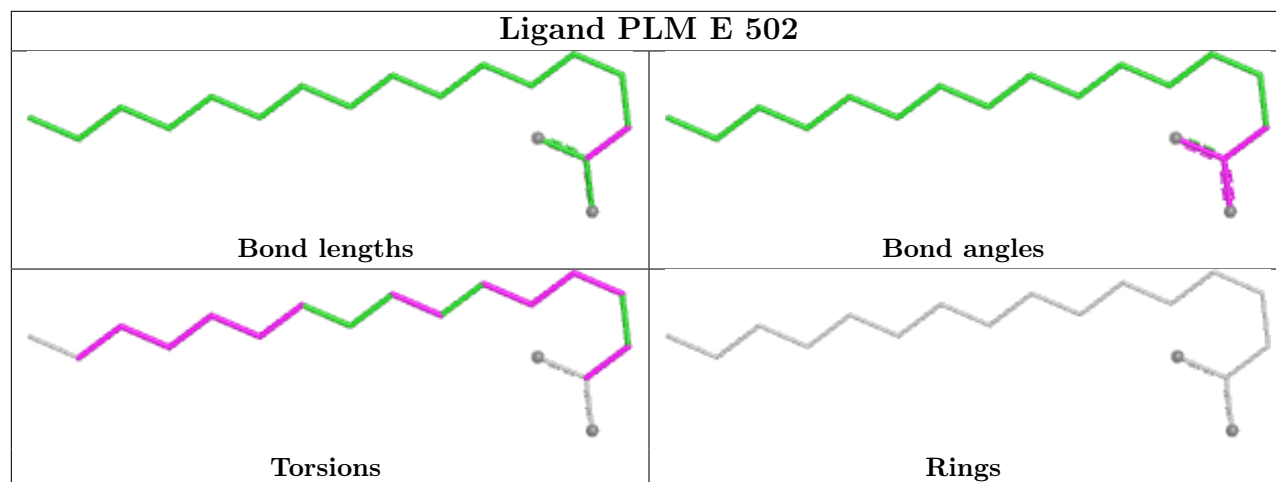
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	HEM	3	0
2	D	501	HEM	6	0
4	E	504	GOL	1	0
4	C	507	GOL	1	0
2	B	501	HEM	5	0
6	B	503	PEG	2	0
6	D	505	PEG	2	0
4	C	504	GOL	1	0
2	F	501	HEM	3	0
6	C	510	PEG	2	0
2	A	501	HEM	5	0
2	C	501	HEM	7	0
4	A	508	GOL	1	0
3	B	502	PLM	1	0

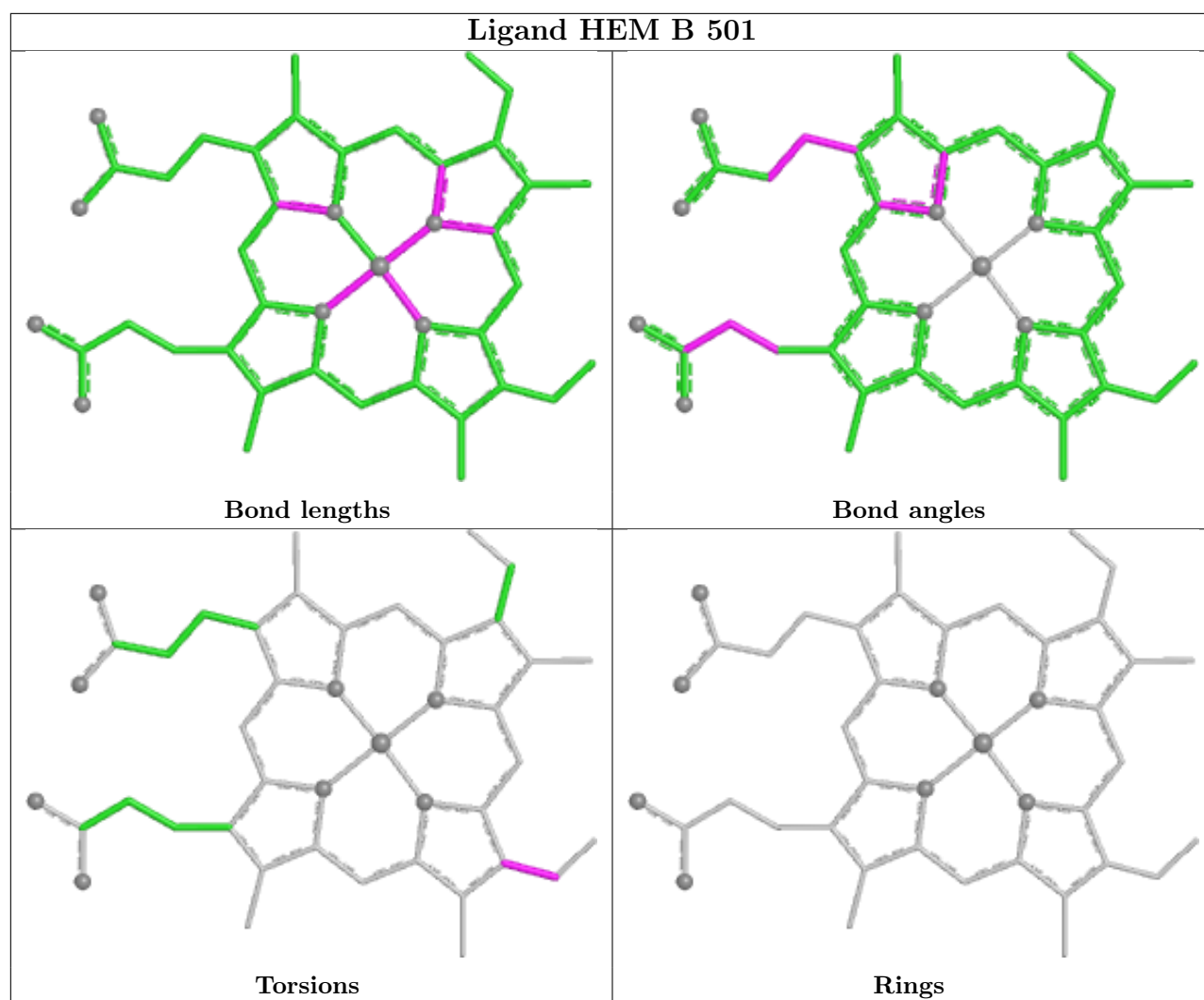
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

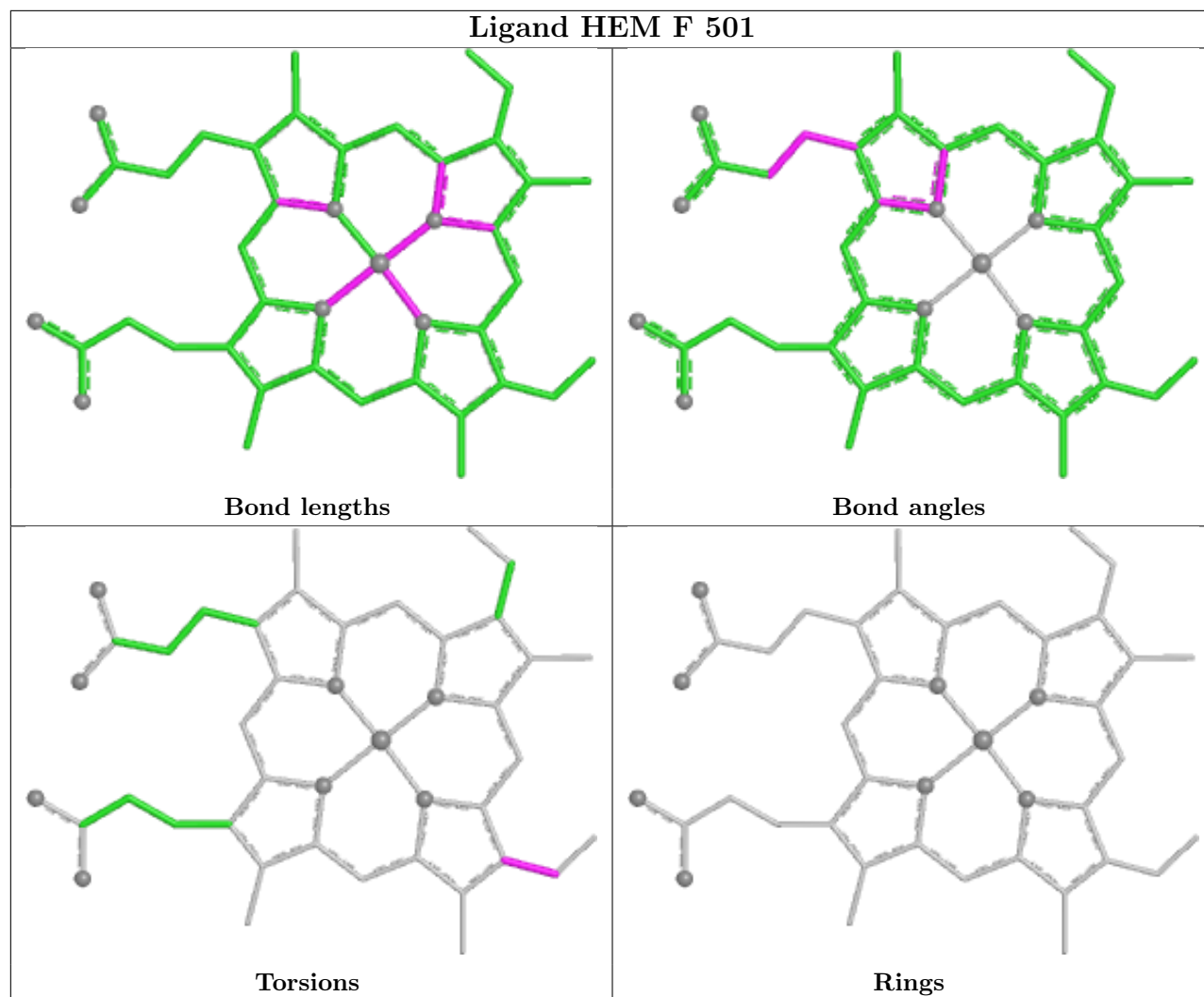


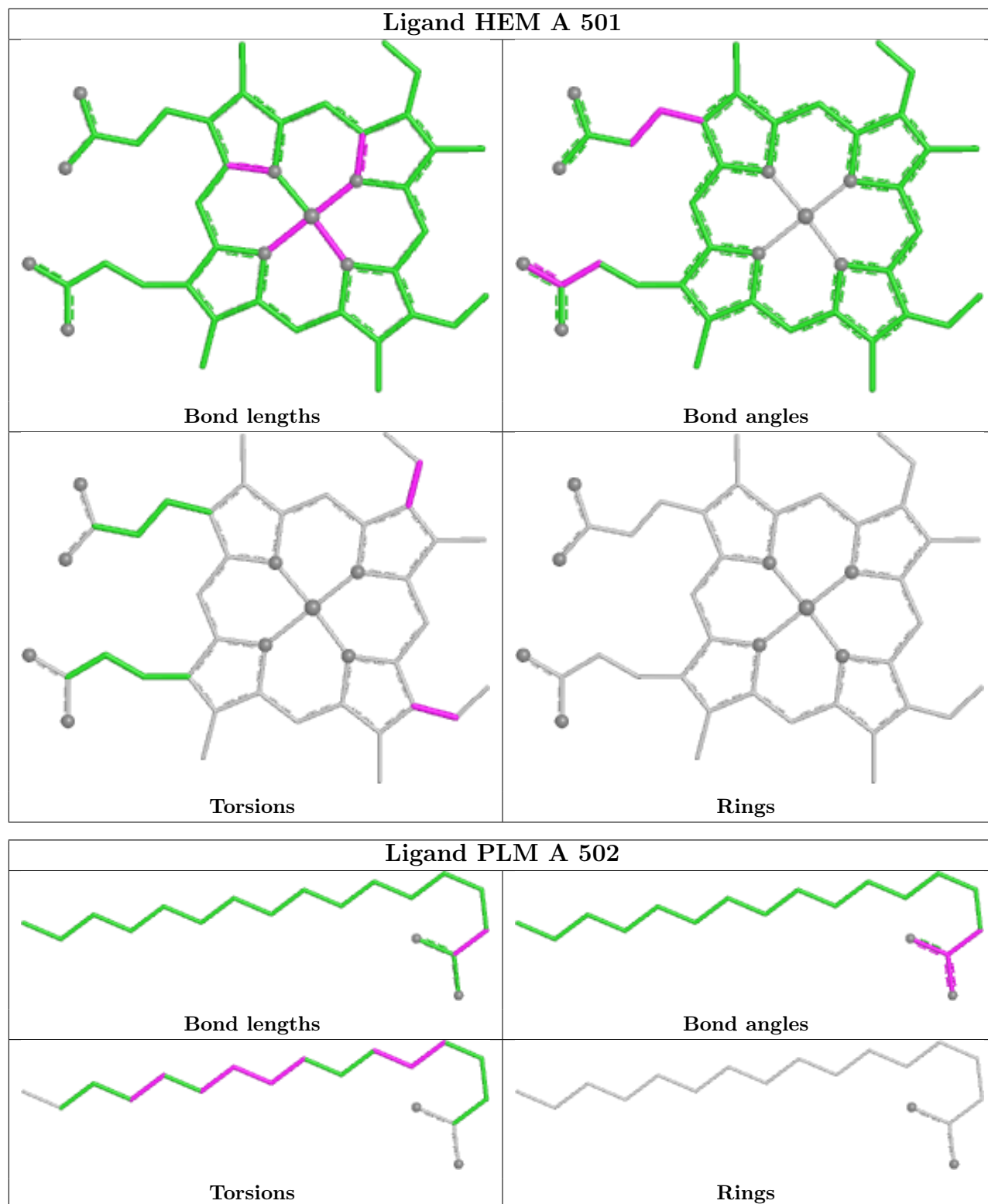


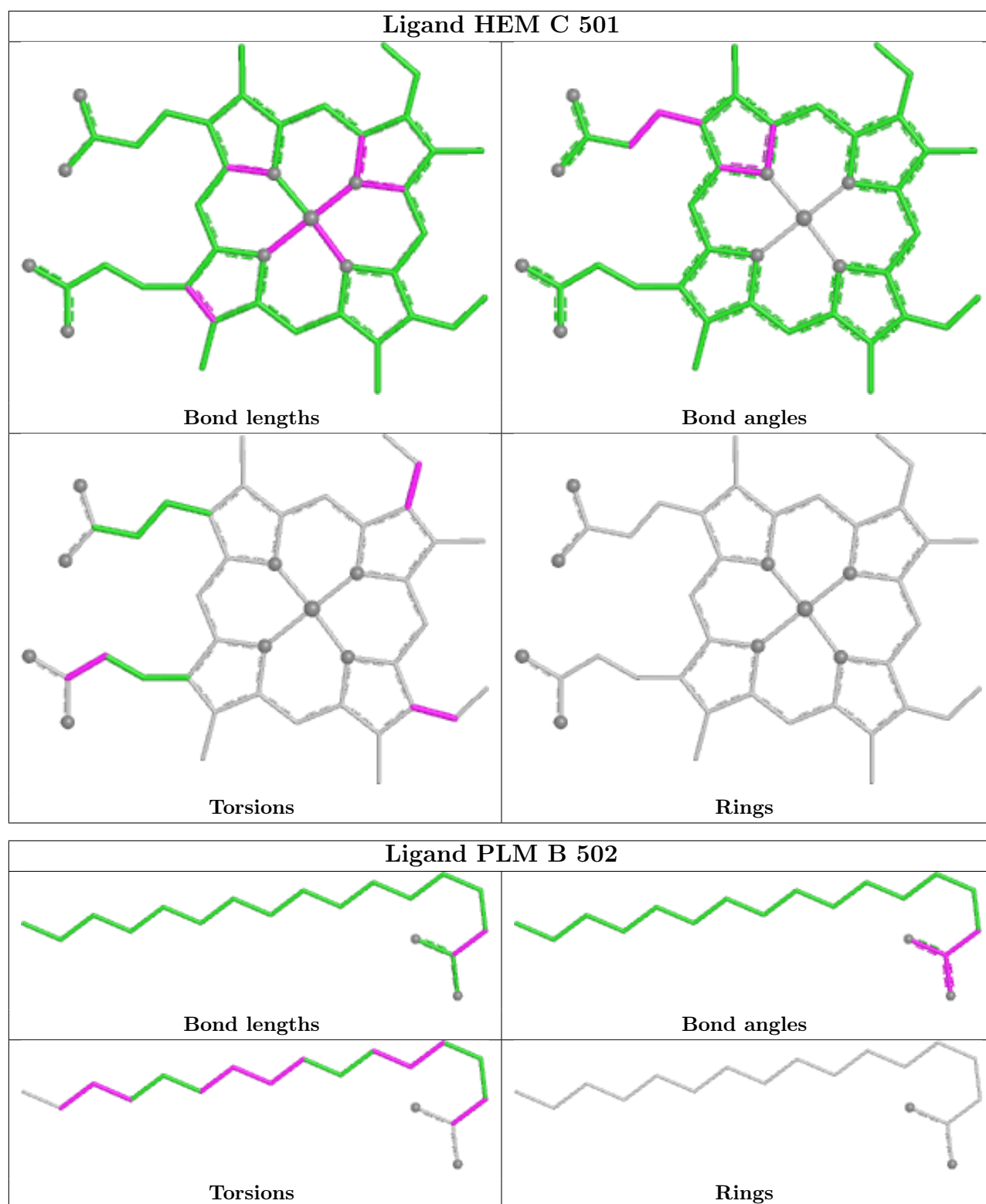












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	415/416 (99%)	0.06	12 (2%) 53 56	20, 31, 48, 81	0
1	B	415/416 (99%)	-0.03	11 (2%) 56 58	19, 28, 46, 91	0
1	C	414/416 (99%)	-0.10	8 (1%) 66 68	19, 27, 43, 69	0
1	D	416/416 (100%)	0.03	12 (2%) 53 56	22, 30, 49, 78	0
1	E	414/416 (99%)	0.02	10 (2%) 59 62	21, 30, 49, 80	0
1	F	415/416 (99%)	-0.10	9 (2%) 62 64	18, 28, 47, 84	0
All	All	2489/2496 (99%)	-0.02	62 (2%) 58 60	18, 29, 48, 91	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	PHE	4.9
1	A	341	GLU	4.5
1	D	11	LEU	4.4
1	D	1	MET	4.3
1	F	4	GLN	4.2
1	C	407	GLY	4.2
1	F	342	ARG	4.0
1	E	272	ASN	3.9
1	B	2	ASN	3.8
1	A	407	GLY	3.8
1	E	3	GLU	3.8
1	A	342	ARG	3.6
1	A	343	GLU	3.6
1	F	2	ASN	3.5
1	C	4	GLN	3.4
1	F	407	GLY	3.3
1	A	340	ALA	3.2
1	E	341	GLU	3.2
1	D	341	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	10	SER	3.1
1	A	11	LEU	3.1
1	E	4	GLN	3.1
1	B	3	GLU	3.0
1	A	12	ASP	3.0
1	B	4	GLN	2.9
1	D	4	GLN	2.8
1	D	343	GLU	2.8
1	D	408	PHE	2.8
1	C	408	PHE	2.7
1	B	397	LEU	2.7
1	E	343	GLU	2.6
1	D	407	GLY	2.6
1	B	406	SER	2.6
1	C	11	LEU	2.5
1	B	341	GLU	2.5
1	E	409	VAL	2.5
1	F	270	SER	2.5
1	B	11	LEU	2.4
1	F	408	PHE	2.4
1	C	79	PHE	2.4
1	C	344	GLU	2.4
1	E	408	PHE	2.3
1	A	4	GLN	2.3
1	B	407	GLY	2.3
1	D	342	ARG	2.3
1	B	343	GLU	2.2
1	D	3	GLU	2.2
1	D	340	ALA	2.2
1	F	409	VAL	2.2
1	E	407	GLY	2.2
1	B	344	GLU	2.2
1	C	3	GLU	2.2
1	A	3	GLU	2.2
1	C	185	ARG	2.1
1	A	70	LEU	2.1
1	D	12	ASP	2.1
1	D	344	GLU	2.1
1	B	342	ARG	2.1
1	E	342	ARG	2.1
1	E	415	ARG	2.0
1	F	414	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	343	GLU	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
4	GOL	E	503	6/6	0.64	0.23	50,57,60,64	0
5	SO4	F	512	5/5	0.64	0.18	49,63,80,91	0
6	PEG	F	505	7/7	0.65	0.23	38,43,48,50	0
4	GOL	A	503	6/6	0.68	0.19	52,58,62,69	0
4	GOL	F	510	6/6	0.72	0.25	46,55,62,64	0
4	GOL	A	508	6/6	0.74	0.21	51,52,58,60	0
4	GOL	D	506	6/6	0.74	0.23	48,50,54,54	0
6	PEG	C	510	7/7	0.75	0.24	32,38,42,49	0
6	PEG	C	505	7/7	0.75	0.17	45,46,58,63	0
4	GOL	A	509	6/6	0.76	0.22	51,53,59,72	0
5	SO4	D	510	5/5	0.76	0.13	73,74,82,95	0
4	GOL	A	505	6/6	0.78	0.18	42,44,49,53	0
5	SO4	E	506	5/5	0.78	0.12	57,64,80,88	0
5	SO4	C	508	5/5	0.78	0.20	61,62,70,82	0
4	GOL	B	505	6/6	0.79	0.22	36,42,45,50	0
4	GOL	E	504	6/6	0.80	0.16	47,55,61,61	0
4	GOL	F	507	6/6	0.80	0.21	45,48,63,66	0
4	GOL	F	506	6/6	0.81	0.15	46,48,51,52	0
4	GOL	A	507	6/6	0.81	0.20	39,42,53,56	0
4	GOL	A	504	6/6	0.81	0.15	40,45,51,55	0
4	GOL	A	506	6/6	0.81	0.21	42,44,47,56	0
6	PEG	F	503	7/7	0.81	0.16	42,48,55,56	0

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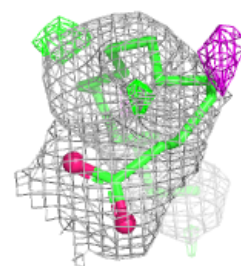
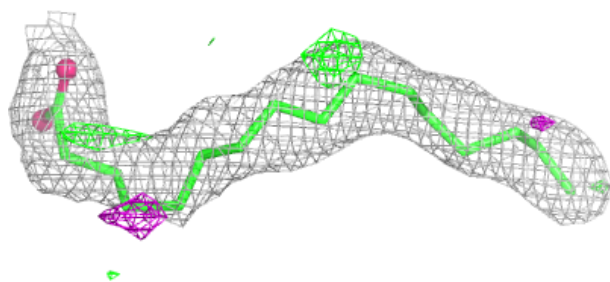
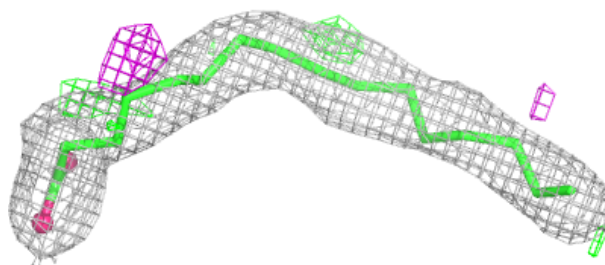
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	504	6/6	0.81	0.18	42,44,54,56	0
5	SO4	D	511	5/5	0.82	0.11	62,71,84,89	0
6	PEG	B	506	7/7	0.82	0.18	37,47,53,54	0
4	GOL	D	504	6/6	0.82	0.16	47,53,57,60	0
6	PEG	C	511	7/7	0.83	0.17	52,57,62,67	0
6	PEG	D	508	7/7	0.83	0.23	40,46,50,52	0
4	GOL	C	509	6/6	0.83	0.19	39,44,53,65	0
4	GOL	C	503	6/6	0.83	0.18	49,53,56,66	0
6	PEG	D	505	7/7	0.84	0.19	34,48,49,50	0
4	GOL	D	507	6/6	0.84	0.17	45,46,50,60	0
5	SO4	F	514	5/5	0.84	0.14	60,61,72,86	0
5	SO4	B	508	5/5	0.84	0.11	55,70,81,89	0
5	SO4	F	513	5/5	0.85	0.11	66,67,76,84	0
4	GOL	E	505	6/6	0.86	0.16	34,46,50,60	0
4	GOL	D	503	6/6	0.86	0.14	36,39,45,46	0
3	PLM	E	502	18/18	0.86	0.16	29,37,45,45	0
6	PEG	B	503	7/7	0.86	0.13	33,38,43,43	0
6	PEG	F	509	7/7	0.86	0.15	39,42,45,45	0
4	GOL	F	508	6/6	0.87	0.19	30,40,48,51	0
4	GOL	F	504	6/6	0.87	0.13	42,47,49,52	0
3	PLM	B	502	18/18	0.87	0.14	25,35,42,48	0
4	GOL	C	507	6/6	0.87	0.13	43,47,50,57	0
3	PLM	A	502	18/18	0.89	0.12	29,33,37,44	0
5	SO4	B	507	5/5	0.89	0.18	55,58,64,65	0
4	GOL	C	504	6/6	0.89	0.13	37,44,47,51	0
3	PLM	D	502	18/18	0.89	0.13	30,39,44,46	0
3	PLM	C	502	18/18	0.90	0.12	23,34,41,41	0
5	SO4	A	510	5/5	0.90	0.13	41,49,55,60	0
5	SO4	F	511	5/5	0.90	0.14	46,54,66,74	0
3	PLM	F	502	18/18	0.90	0.12	26,34,44,45	0
5	SO4	C	506	5/5	0.93	0.12	47,56,59,61	0
5	SO4	D	509	5/5	0.94	0.14	54,55,59,67	0
2	HEM	E	501	43/43	0.94	0.11	19,26,31,33	0
2	HEM	F	501	43/43	0.95	0.10	16,22,31,33	0
2	HEM	B	501	43/43	0.95	0.10	16,23,30,33	0
2	HEM	C	501	43/43	0.95	0.10	16,22,29,36	0
2	HEM	D	501	43/43	0.95	0.11	19,26,32,35	0
2	HEM	A	501	43/43	0.95	0.11	20,27,31,41	0

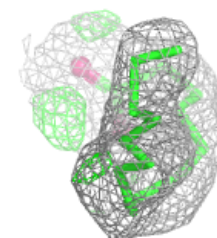
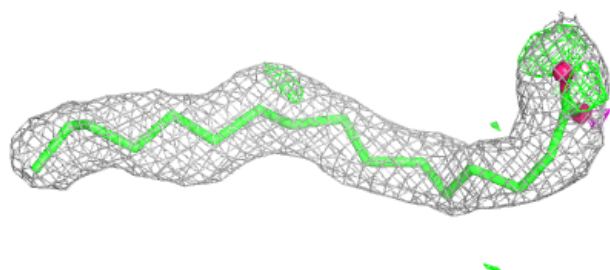
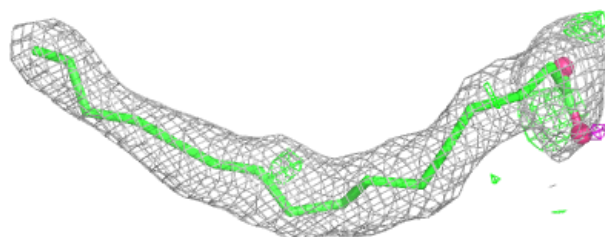
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM E 502:

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

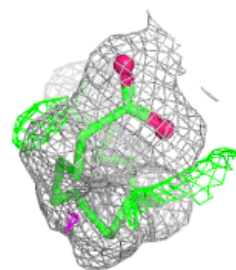
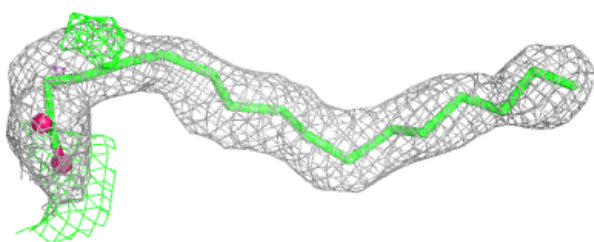
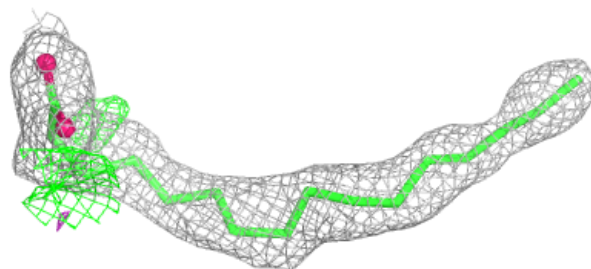
**Electron density around PLM B 502:**

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

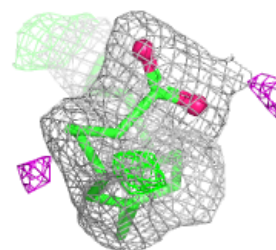
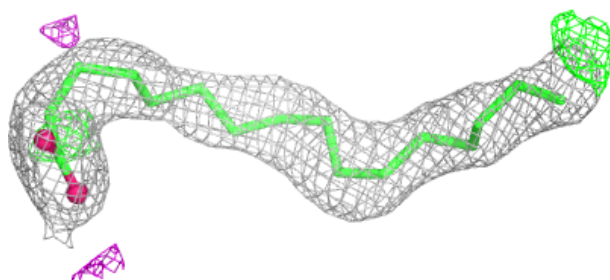
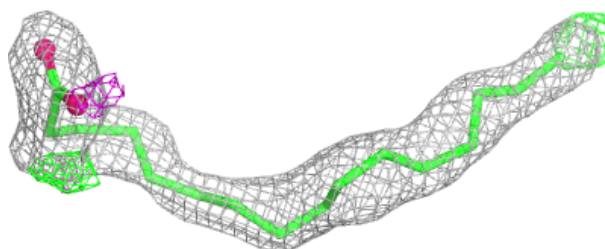


Electron density around PLM A 502:

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

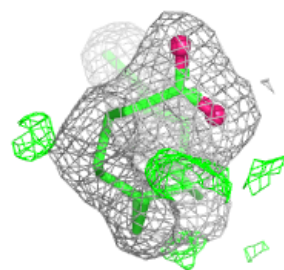
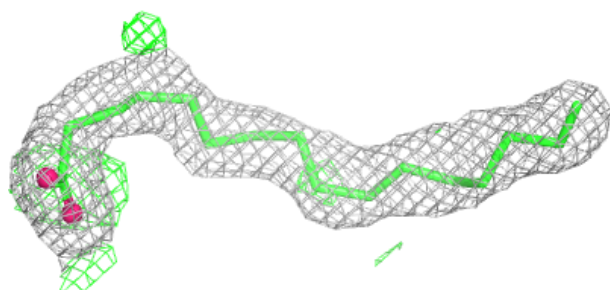
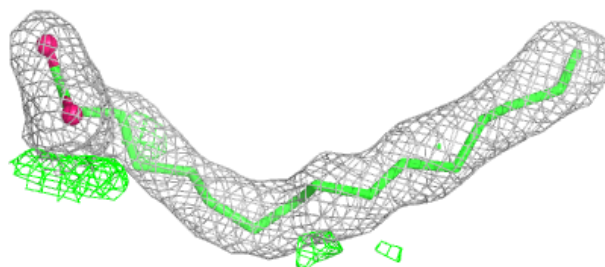
**Electron density around PLM D 502:**

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

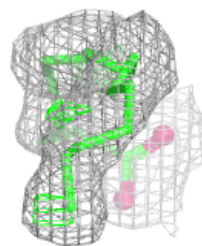
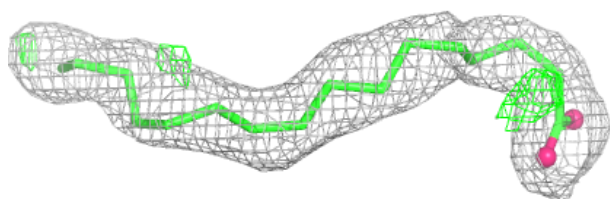
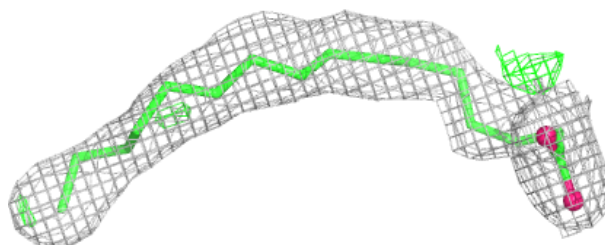


Electron density around PLM C 502:

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

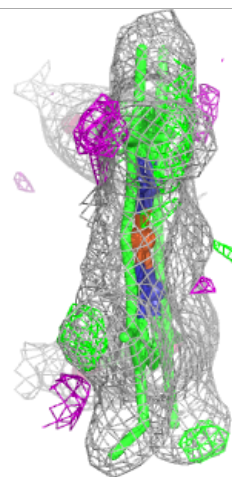
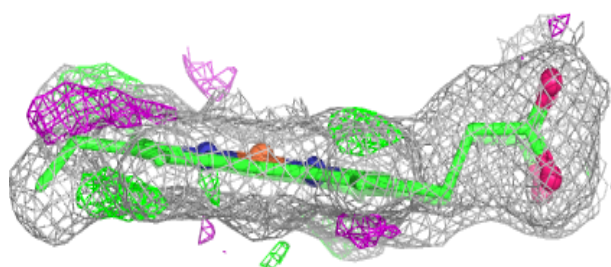
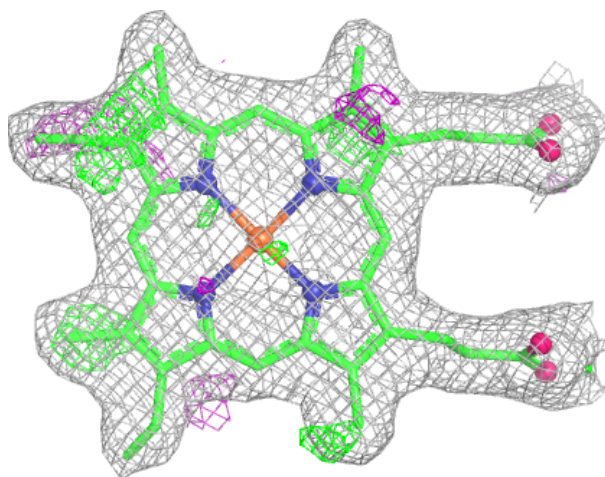
**Electron density around PLM F 502:**

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



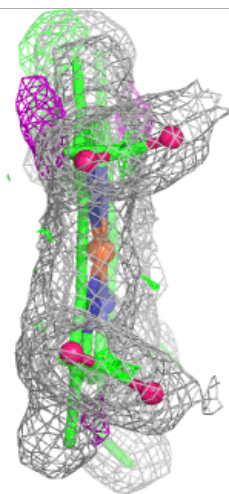
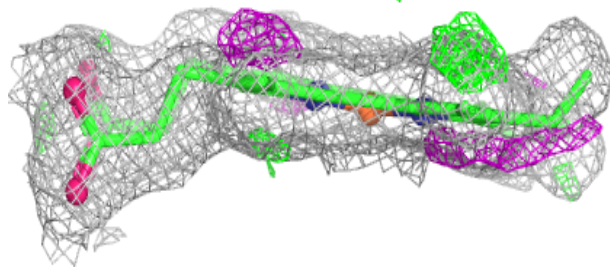
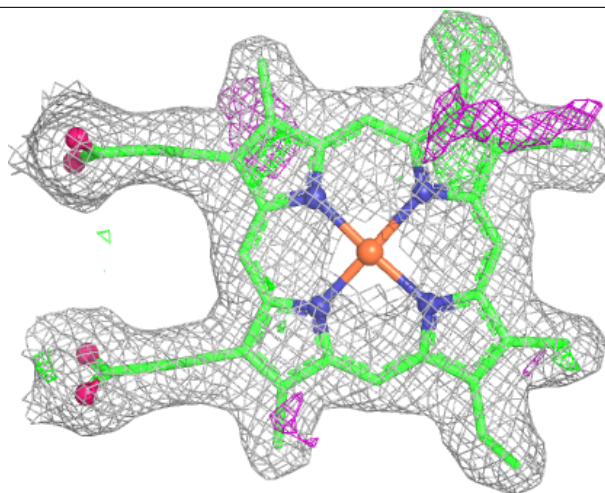
Electron density around HEM E 501:

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



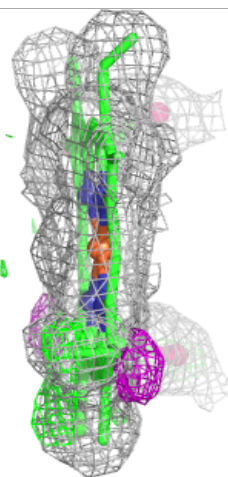
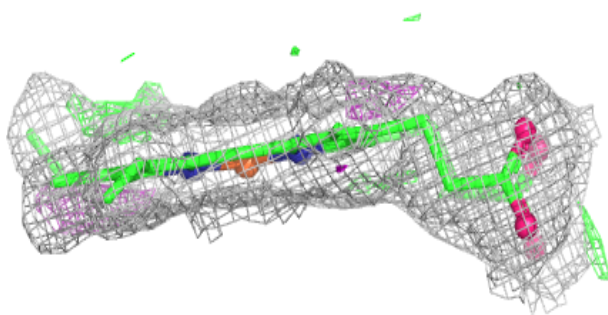
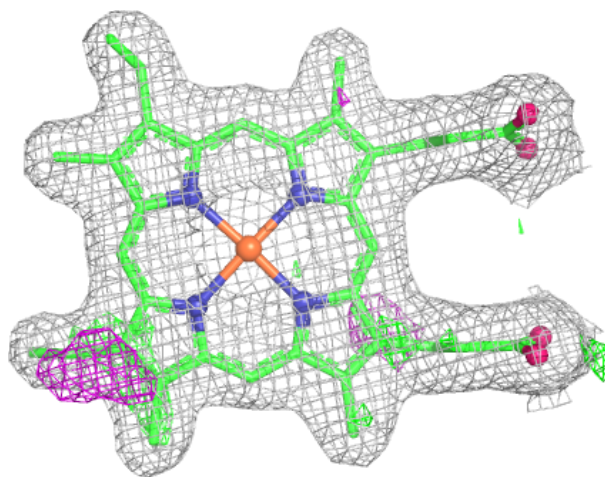
Electron density around HEM F 501:

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



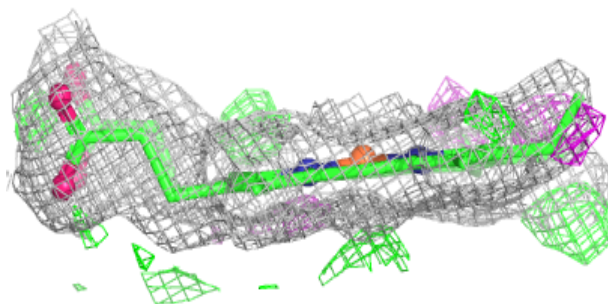
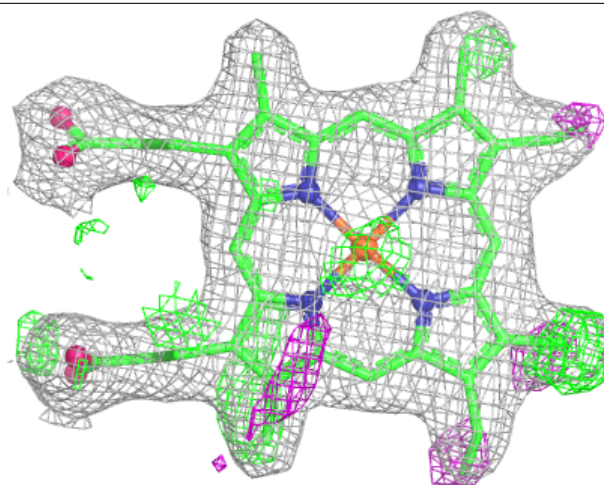
Electron density around HEM B 501:

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



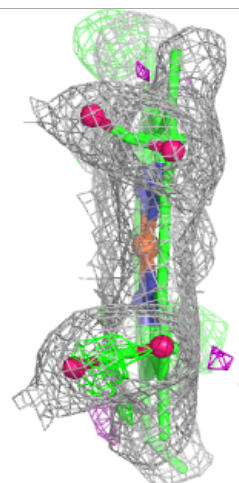
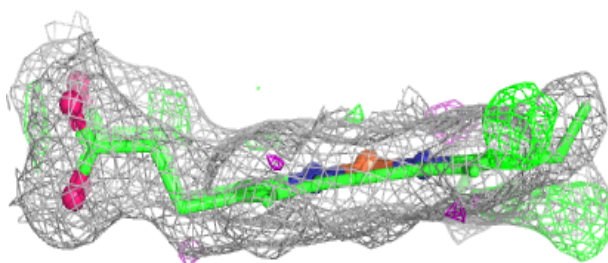
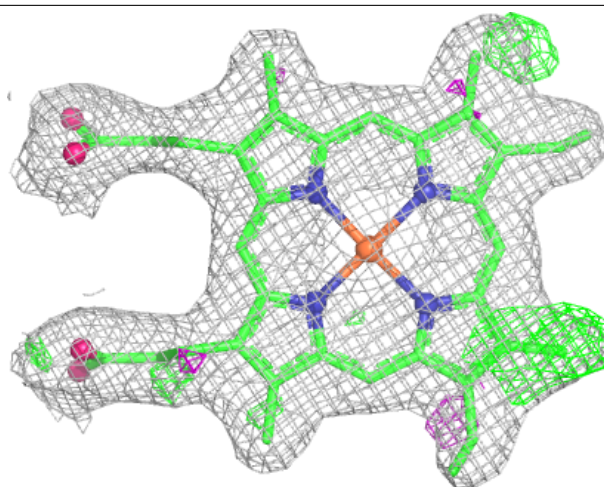
Electron density around HEM C 501:

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



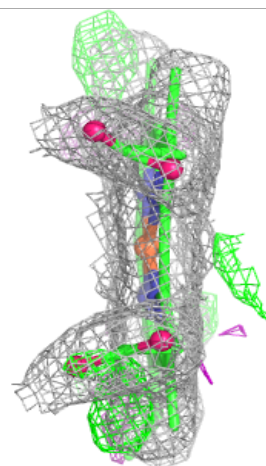
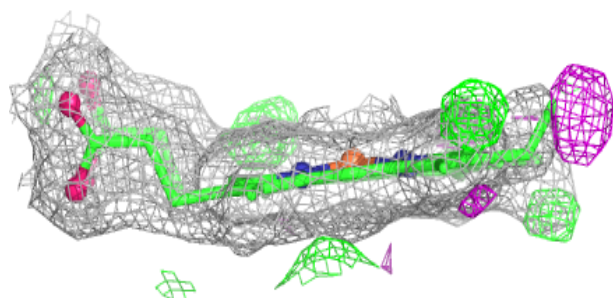
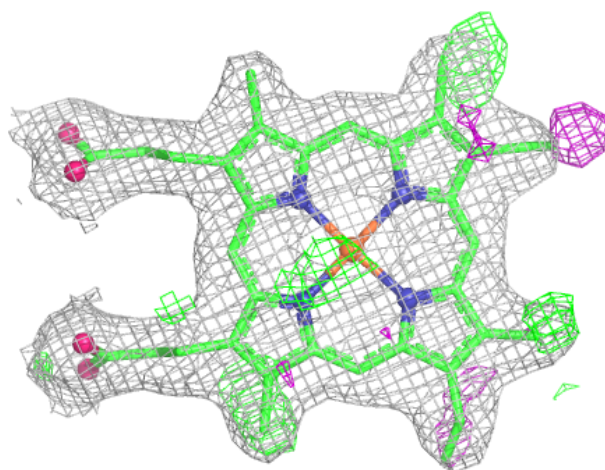
Electron density around HEM D 501:

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

There are no such residues in this entry.