



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 04:15 PM EDT

PDB ID : 7UAO
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with (6-(3-(4,4-difluoropiperidin-1-yl)propyl)-4-methylpyridin-2-amine)
Authors : Li, H.; Poulos, T.L.
Deposited on : 2022-03-13
Resolution : 1.90 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

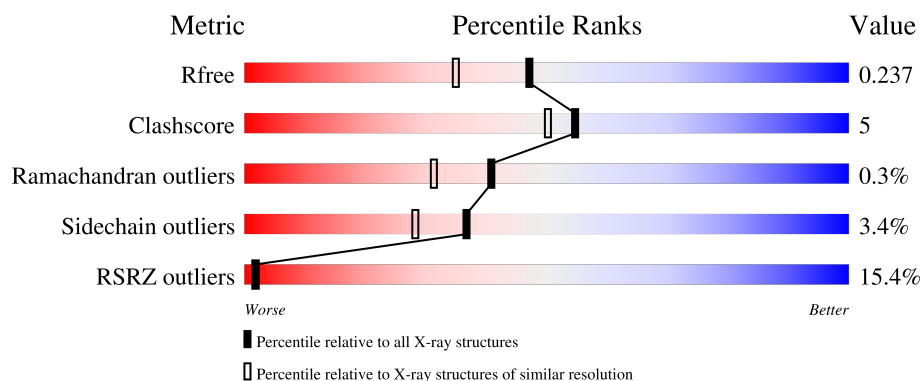
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	440	<div> <div>24%</div> <div>78% 11% 9%</div> </div>
1	B	440	<div> <div>6%</div> <div>82% 9% 9%</div> </div>
1	C	440	<div> <div>19%</div> <div>79% 12% 9%</div> </div>
1	D	440	<div> <div>7%</div> <div>82% 9% 9%</div> </div>

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
6	GOL	A	513	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13979 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.

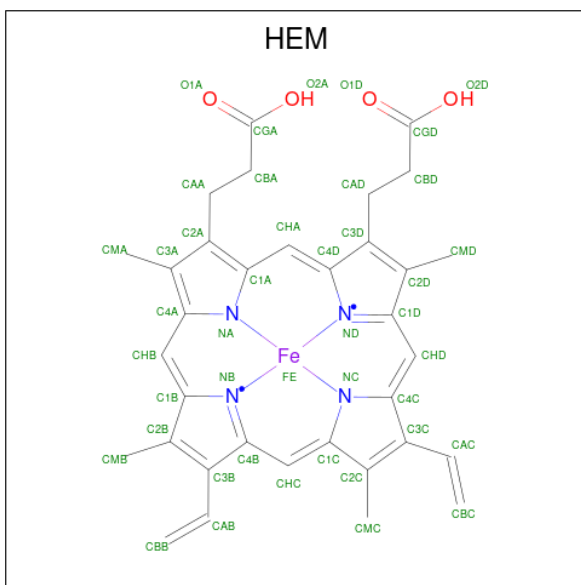
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	B	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	D	402	Total	C	N	O	S	0	1	0
			3214	2046	567	585	16			

There are 4 discrepancies between the modelled and reference sequences:

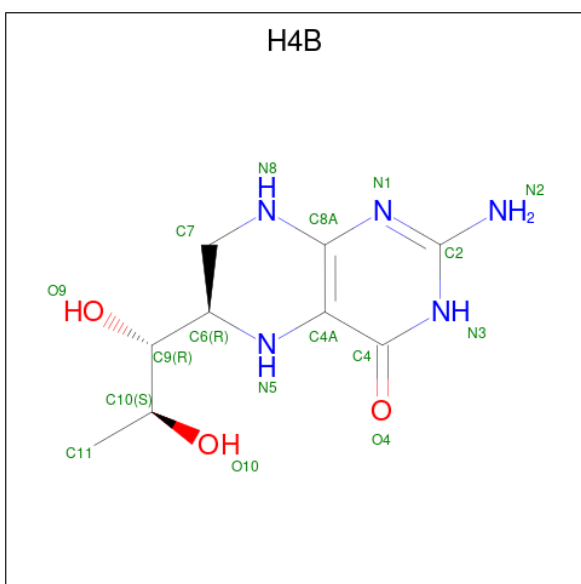
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



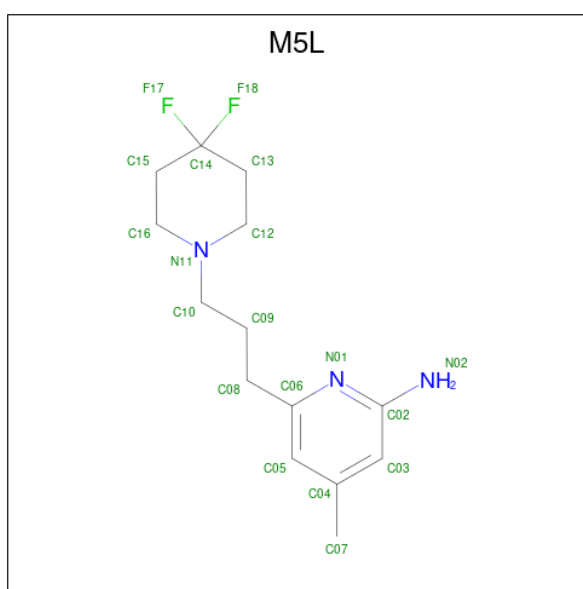
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[3-(4,4-difluoropiperidin-1-yl)propyl]-4-methylpyridin-2-amine (three-letter code: M5L) (formula: C₁₄H₂₁F₂N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			19	14	2	3		
4	B	1	Total	C	F	N	0	0
			19	14	2	3		
4	C	1	Total	C	F	N	0	0
			19	14	2	3		
4	D	1	Total	C	F	N	0	0
			19	14	2	3		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Cl	0	0
			2	2		

- Molecule 8 is GADOLINIUM ATOM (three-letter code: Gd) (formula: Gd).

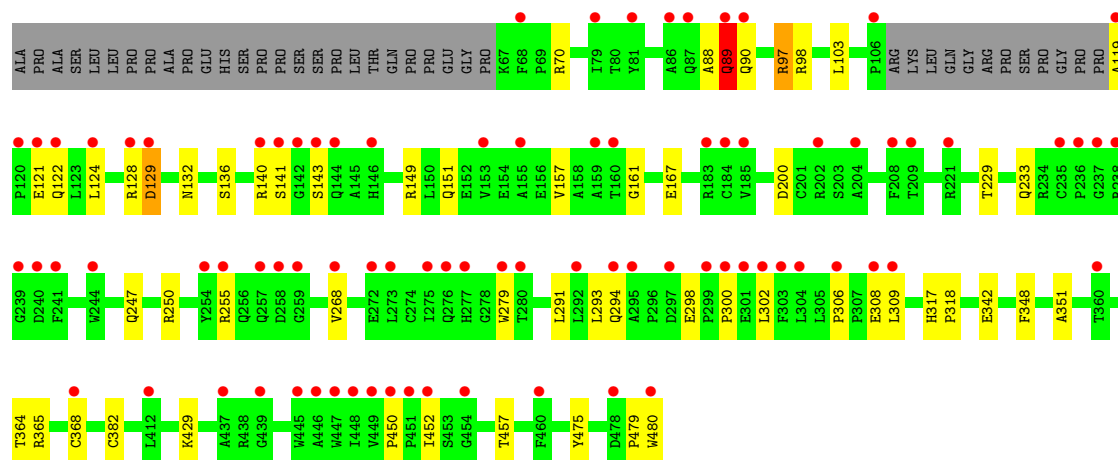
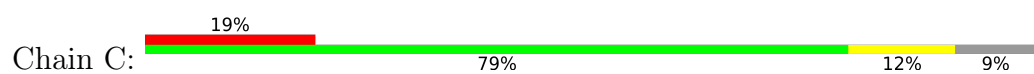
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Gd	0	0
			1	1		
8	B	2	Total	Gd	0	0
			2	2		
8	D	1	Total	Gd	0	0
			1	1		

- Molecule 9 is ZINC ION (three-letter code: Zn) (formula: Zn).

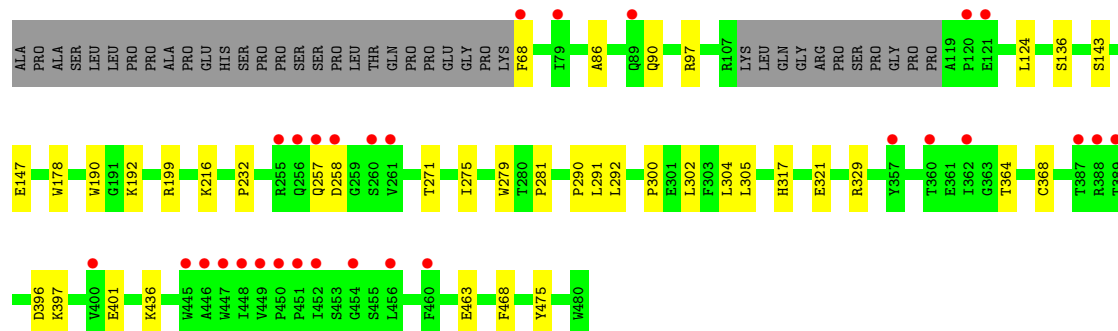
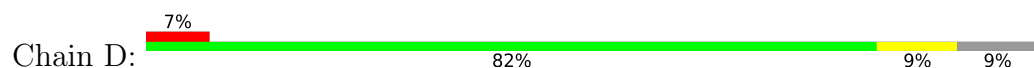
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		
9	C	1	Total	Zn	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	120	Total	O	0	0
			120	120		
10	B	191	Total	O	0	0
			191	191		
10	C	124	Total	O	0	0
			124	124		
10	D	179	Total	O	0	0
			179	179		



- Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.49Å 152.85Å 108.74Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	39.06 – 1.90 39.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.4 (39.06-1.90) 87.7 (39.05-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.201 , 0.245 0.192 , 0.237	Depositor DCC
R_{free} test set	6712 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.094 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13979	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: HEM, H4B, CL, GOL, GD, M5L, ZN, BTB

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	0.35	0/3302	0.52	0/4498
1	B	0.40	0/3312	0.53	0/4514
1	C	0.36	0/3307	0.51	0/4506
1	D	0.43	0/3309	0.56	0/4509
All	All	0.39	0/13230	0.53	0/18027

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	3207	0	3112	38	0
1	B	3211	0	3114	27	0
1	C	3212	0	3116	31	0
1	D	3214	0	3116	21	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	19	0	0	1	0
4	B	19	0	0	0	0
4	C	19	0	0	0	0
4	D	19	0	0	0	0
5	A	42	0	56	9	0
5	B	28	0	35	4	0
5	C	42	0	55	12	0
5	D	28	0	36	4	0
6	A	24	0	32	4	0
6	B	6	0	8	0	0
6	C	18	0	24	1	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	120	0	0	5	0
10	B	191	0	0	1	0
10	C	124	0	0	1	0
10	D	179	0	0	3	1
All	All	13979	0	12892	137	1

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 5.

All (137) 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:C:233:GLN:NE2	10:C:601:HOH:O	2.17	0.75
5:C:505:BTB:HO1	5:C:505:BTB:HO6	1.34	0.75
5:A:505:BTB:O4	5:A:505:BTB:O3	2.03	0.74
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.69	0.72
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:504:BTB:O3	10:A:601:HOH:O	2.10	0.69
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.68
1:A:237:GLY:HA3	6:A:509:GOL:H12	1.76	0.67
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.76	0.66
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.78	0.65
1:A:147:GLU:O	1:A:151:GLN:NE2	2.28	0.65
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.79	0.63
1:A:70:ARG:NH2	10:A:604:HOH:O	2.31	0.63
1:A:321:GLU:H	1:A:321:GLU:CD	2.01	0.62
5:C:505:BTB:O6	5:C:505:BTB:O1	2.12	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.83	0.61
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.83	0.61
1:C:129:ASP:HA	1:C:132:ASN:HD22	1.67	0.60
1:A:125:SER:HA	1:A:128:ARG:NH1	2.18	0.58
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.68	0.57
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.23	0.56
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.17	0.56
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.18	0.56
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.87	0.56
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.89	0.55
1:B:298:GLU:OE1	5:B:505:BTB:H42	2.07	0.54
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.17	0.54
1:D:68:PHE:N	10:D:603:HOH:O	2.40	0.54
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.89	0.54
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.90	0.54
1:D:271:THR:O	1:D:275:ILE:HG12	2.08	0.53
5:B:505:BTB:H31	10:B:608:HOH:O	2.08	0.53
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.14	0.52
1:C:103:LEU:HA	1:D:463:GLU:HG2	1.90	0.52
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.43	0.52
1:C:167:GLU:OE2	6:C:507:GOL:O2	2.27	0.52
1:A:384:ASP:O	6:A:513:GOL:H12	2.10	0.51
6:A:507:GOL:H12	10:A:642:HOH:O	2.09	0.51
1:C:294:GLN:HB2	1:C:300:PRO:HB3	1.93	0.51
1:A:133:GLN:NE2	10:A:612:HOH:O	2.45	0.50
1:A:347:GLU:OE2	10:A:602:HOH:O	2.19	0.50
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.94	0.50
1:D:143:SER:O	1:D:147:GLU:HG2	2.11	0.49
1:A:256:GLN:C	1:A:258:ASP:H	2.15	0.49
1:C:157:VAL:HG13	1:C:161:GLY:O	2.12	0.49
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:LYS:NZ	10:D:605:HOH:O	2.45	0.49
1:A:147:GLU:OE1	1:A:147:GLU:N	2.42	0.48
1:B:124:LEU:HB3	1:B:128:ARG:HH22	1.77	0.48
5:D:504:BTB:H61	10:D:720:HOH:O	2.12	0.48
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.48	0.48
1:B:149:ARG:NH1	1:B:152:GLU:OE1	2.47	0.48
5:A:504:BTB:H51	5:A:504:BTB:H32	1.58	0.48
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.96	0.47
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.49	0.47
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.78	0.47
1:C:364:THR:O	1:C:368:CYS:HB2	2.14	0.47
5:C:506:BTB:H72	5:C:506:BTB:H31	1.53	0.47
5:D:505:BTB:H11	5:D:505:BTB:H71	1.56	0.47
5:B:505:BTB:H42	5:B:505:BTB:H72	1.61	0.47
1:D:364:THR:O	1:D:368:CYS:HB2	2.14	0.47
1:A:320:LEU:HD13	1:A:322:TRP:CZ2	2.50	0.46
5:A:506:BTB:H11	5:A:506:BTB:H51	1.59	0.46
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.51	0.46
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.39	0.46
1:A:202:ARG:HB2	1:A:202:ARG:NH1	2.30	0.46
1:C:119:ALA:HB1	1:C:122:GLN:HB2	1.98	0.46
1:C:89:GLN:H	1:C:89:GLN:HG2	1.57	0.45
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.51	0.45
5:A:505:BTB:H51	5:A:505:BTB:H11	1.48	0.45
5:B:505:BTB:H11	5:B:505:BTB:H51	1.53	0.45
1:B:326:LEU:HD12	5:C:504:BTB:H72	1.99	0.45
1:A:229:THR:O	1:A:352:PRO:HD2	2.16	0.45
1:C:128:ARG:O	1:C:132:ASN:ND2	2.49	0.45
1:D:291:LEU:HD11	1:D:305:LEU:HD21	1.98	0.45
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.99	0.45
1:A:92:GLY:N	1:B:96:PRO:O	2.49	0.45
1:B:139:LYS:N	1:B:139:LYS:HD2	2.32	0.45
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.52	0.45
1:A:396:ASP:O	1:A:400:VAL:HG23	2.17	0.45
1:C:149:ARG:HD2	1:C:149:ARG:HA	1.74	0.45
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.53	0.44
5:C:505:BTB:H81	5:C:505:BTB:H52	1.66	0.44
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.32	0.44
1:B:93:PRO:HB3	1:B:106:PRO:HB3	1.99	0.44
1:C:97:ARG:NH2	1:D:86:ALA:HA	2.33	0.44
1:A:67:LYS:HB3	1:A:67:LYS:HE2	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:506:BTB:H41	5:A:506:BTB:H72	1.50	0.44
1:A:361:GLU:OE2	4:A:503:M5L:N02	2.51	0.43
1:D:292:LEU:HD22	1:D:300:PRO:HB2	1.99	0.43
1:C:247:GLN:HB2	1:C:250:ARG:HG2	2.00	0.43
1:C:382:CYS:HA	5:C:504:BTB:H12	2.00	0.43
1:A:463:GLU:HB3	1:B:103:LEU:HD12	2.00	0.43
1:B:379:VAL:HG21	1:B:402:ILE:HD11	2.01	0.43
1:C:255:ARG:HB2	1:C:255:ARG:NH1	2.34	0.43
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.54	0.43
1:C:255:ARG:HH12	1:C:268:VAL:HG11	1.83	0.43
1:A:89:GLN:HG3	1:A:90:GLN:N	2.34	0.43
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.37	0.42
1:C:124:LEU:O	1:C:128:ARG:HG3	2.19	0.42
1:C:291:LEU:HB3	1:C:293:LEU:HD21	2.01	0.42
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.85	0.42
1:B:364:THR:O	1:B:368:CYS:HB2	2.20	0.42
1:D:216:LYS:HB3	1:D:216:LYS:HE2	1.84	0.42
1:B:465:VAL:HG12	1:B:467:TYR:HD1	1.84	0.42
5:C:506:BTB:H41	5:C:506:BTB:H51	1.71	0.42
1:A:89:GLN:CG	1:A:90:GLN:N	2.83	0.42
1:B:298:GLU:HG3	1:B:299:PRO:HD2	2.02	0.42
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	2.01	0.42
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.82	0.42
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.83	0.42
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.02	0.42
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.55	0.42
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.01	0.41
1:B:447:TRP:HA	3:B:502:H4B:N1	2.34	0.41
5:C:505:BTB:H72	5:C:505:BTB:H31	1.62	0.41
1:A:298:GLU:OE2	5:A:506:BTB:O8	2.33	0.41
1:A:364:THR:O	1:A:368:CYS:HB2	2.20	0.41
1:C:298:GLU:OE2	5:C:506:BTB:O8	2.37	0.41
1:A:246:SER:HA	1:A:338:ASN:HB3	2.02	0.41
1:C:88:ALA:HB3	1:D:97:ARG:HD2	2.02	0.41
1:C:229:THR:O	1:C:351:ALA:HA	2.21	0.41
1:A:237:GLY:CA	6:A:509:GOL:H12	2.46	0.41
1:B:290:PRO:HG2	1:B:302:LEU:HD11	2.01	0.41
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.61	0.41
1:D:199:ARG:O	1:D:232:PRO:HG3	2.21	0.41
1:A:139:LYS:HE3	1:A:139:LYS:HB2	1.85	0.41
1:B:326:LEU:HD11	5:C:504:BTB:H41	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.03	0.41
5:C:504:BTB:H51	5:C:504:BTB:H32	1.70	0.41
5:C:505:BTB:H51	5:C:505:BTB:H42	1.57	0.41
1:C:306:PRO:O	1:C:309:LEU:HB2	2.21	0.40
1:A:298:GLU:OE1	5:A:506:BTB:H32	2.21	0.40
1:C:88:ALA:HB3	1:D:97:ARG:CD	2.51	0.40
1:A:263:GLY:H	1:A:285:ARG:HG3	1.86	0.40
1:B:173:GLY:HA3	1:B:343:ILE:HD13	2.04	0.40
5:D:505:BTB:O4	5:D:505:BTB:H51	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:778:HOH:O	10:D:779:HOH:O[1_655]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/440 (90%)	377 (95%)	19 (5%)	2 (0%)	29	18
1	B	400/440 (91%)	391 (98%)	9 (2%)	0	100	100
1	C	399/440 (91%)	386 (97%)	11 (3%)	2 (0%)	29	18
1	D	399/440 (91%)	391 (98%)	8 (2%)	0	100	100
All	All	1596/1760 (91%)	1545 (97%)	47 (3%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASP

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Mol	Chain	Res	Type
1	A	257	GLN
1	C	89	GLN
1	C	143	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	342/373 (92%)	325 (95%)	17 (5%)	24	15
1	B	343/373 (92%)	336 (98%)	7 (2%)	55	51
1	C	342/373 (92%)	327 (96%)	15 (4%)	28	19
1	D	342/373 (92%)	334 (98%)	8 (2%)	50	45
All	All	1369/1492 (92%)	1322 (97%)	47 (3%)	37	28

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	97	ARG
1	A	121	GLU
1	A	122	GLN
1	A	124	LEU
1	A	125	SER
1	A	128	ARG
1	A	202	ARG
1	A	216	LYS
1	A	285	ARG
1	A	291	LEU
1	A	309	LEU
1	A	321	GLU
1	A	342	GLU
1	A	389	THR
1	A	470	SER
1	A	474	ARG
1	B	97	ARG

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Mol	Chain	Res	Type
1	B	122	GLN
1	B	128	ARG
1	B	202	ARG
1	B	255	ARG
1	B	257	GLN
1	B	396	ASP
1	C	70	ARG
1	C	89	GLN
1	C	90	GLN
1	C	97	ARG
1	C	98	ARG
1	C	121	GLU
1	C	129	ASP
1	C	136	SER
1	C	140	ARG
1	C	141	SER
1	C	151	GLN
1	C	200	ASP
1	C	308	GLU
1	C	342	GLU
1	C	429	LYS
1	D	124	LEU
1	D	136	SER
1	D	192	LYS
1	D	257	GLN
1	D	258	ASP
1	D	329	ARG
1	D	396	ASP
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 11 are monoatomic - leaving 31 for Mogul analysis.

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
6	GOL	A	509	-	5,5,5	0.44	0	5,5,5	0.30	0
6	GOL	A	513	-	5,5,5	0.73	0	5,5,5	1.92	2 (40%)
6	GOL	A	508	-	5,5,5	0.45	0	5,5,5	0.46	0
2	HEM	A	501	1	41,50,50	1.49	5 (12%)	45,82,82	1.68	11 (24%)
6	GOL	C	509	-	5,5,5	0.32	0	5,5,5	0.31	0
6	GOL	C	507	-	5,5,5	0.43	0	5,5,5	0.33	0
2	HEM	D	501	1	41,50,50	1.44	3 (7%)	45,82,82	1.97	10 (22%)
5	BTB	C	504	8	13,13,13	0.37	0	7,16,16	1.71	1 (14%)
3	H4B	D	502	-	16,18,18	0.84	0	11,26,26	2.67	5 (45%)
6	GOL	C	508	-	5,5,5	0.33	0	5,5,5	0.35	0
6	GOL	B	506	-	5,5,5	0.37	0	5,5,5	0.30	0
2	HEM	B	501	1	41,50,50	1.44	5 (12%)	45,82,82	1.87	11 (24%)
5	BTB	A	504	8	13,13,13	0.63	0	7,16,16	1.48	1 (14%)
4	M5L	D	503	-	20,20,20	1.47	4 (20%)	26,28,28	1.81	6 (23%)
3	H4B	B	502	-	16,18,18	0.76	0	11,26,26	2.79	5 (45%)
4	M5L	C	503	-	20,20,20	1.34	4 (20%)	26,28,28	1.87	2 (7%)
5	BTB	C	505	-	13,13,13	0.60	0	7,16,16	0.90	0
5	BTB	D	504	8	13,13,13	0.44	0	7,16,16	0.49	0
6	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.36	0
5	BTB	D	505	-	13,13,13	0.58	0	7,16,16	0.89	0
6	GOL	D	506	-	5,5,5	0.37	0	5,5,5	0.26	0
3	H4B	A	502	-	16,18,18	0.84	0	11,26,26	2.64	5 (45%)
2	HEM	C	501	1	41,50,50	1.50	6 (14%)	45,82,82	2.01	11 (24%)
5	BTB	A	506	-	13,13,13	0.37	0	7,16,16	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	C	502	-	16,18,18	0.80	0	11,26,26	2.71	6 (54%)
4	M5L	B	503	-	20,20,20	1.52	4 (20%)	26,28,28	1.94	4 (15%)
5	BTB	B	504	8	13,13,13	0.48	0	7,16,16	0.96	0
5	BTB	C	506	-	13,13,13	0.41	0	7,16,16	0.34	0
5	BTB	B	505	-	13,13,13	0.48	0	7,16,16	0.93	0
4	M5L	A	503	-	20,20,20	1.36	4 (20%)	26,28,28	1.93	2 (7%)
5	BTB	A	505	-	13,13,13	0.54	0	7,16,16	0.66	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
6	GOL	A	509	-	-	4/4/4/4	-
6	GOL	A	513	-	-	4/4/4/4	-
6	GOL	A	508	-	-	3/4/4/4	-
2	HEM	A	501	1	-	2/12/54/54	-
6	GOL	C	509	-	-	2/4/4/4	-
6	GOL	C	507	-	-	2/4/4/4	-
2	HEM	D	501	1	-	2/12/54/54	-
5	BTB	C	504	8	-	3/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
6	GOL	C	508	-	-	2/4/4/4	-
6	GOL	B	506	-	-	2/4/4/4	-
2	HEM	B	501	1	-	0/12/54/54	-
5	BTB	A	504	8	-	5/21/21/21	-
4	M5L	D	503	-	-	2/6/18/18	0/2/2/2
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	M5L	C	503	-	-	2/6/18/18	0/2/2/2
5	BTB	C	505	-	-	17/21/21/21	-
5	BTB	D	504	8	-	6/21/21/21	-
6	GOL	A	507	-	-	0/4/4/4	-
5	BTB	D	505	-	-	7/21/21/21	-
6	GOL	D	506	-	-	2/4/4/4	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
2	HEM	C	501	1	-	1/12/54/54	-
5	BTB	A	506	-	-	4/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	M5L	B	503	-	-	2/6/18/18	0/2/2/2
5	BTB	B	504	8	-	3/21/21/21	-
5	BTB	C	506	-	-	5/21/21/21	-
5	BTB	B	505	-	-	14/21/21/21	-
4	M5L	A	503	-	-	2/6/18/18	0/2/2/2
5	BTB	A	505	-	-	11/21/21/21	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-3.95	1.34	1.40
2	A	501	HEM	C3C-CAC	3.81	1.55	1.47
2	D	501	HEM	C3C-CAC	3.75	1.55	1.47
2	C	501	HEM	C3C-CAC	3.70	1.55	1.47
4	B	503	M5L	C13-C14	3.69	1.53	1.50
4	D	503	M5L	C13-C14	3.54	1.53	1.50
2	A	501	HEM	C3C-C2C	-3.52	1.35	1.40
4	B	503	M5L	C15-C14	3.39	1.53	1.50
2	B	501	HEM	C3C-CAC	3.18	1.54	1.47
2	C	501	HEM	C3C-C2C	-3.17	1.36	1.40
2	A	501	HEM	CAB-C3B	3.14	1.56	1.47
2	B	501	HEM	C3C-C2C	-3.12	1.36	1.40
4	A	503	M5L	F17-C14	-3.07	1.32	1.38
2	C	501	HEM	CAB-C3B	3.05	1.55	1.47
4	C	503	M5L	F17-C14	-3.05	1.32	1.38
4	D	503	M5L	F18-C14	-3.04	1.32	1.38
4	D	503	M5L	F17-C14	-3.04	1.32	1.38
4	C	503	M5L	C13-C14	3.03	1.53	1.50
4	A	503	M5L	F18-C14	-3.01	1.32	1.38
4	C	503	M5L	F18-C14	-3.01	1.32	1.38
2	B	501	HEM	CAB-C3B	2.94	1.55	1.47
4	A	503	M5L	C13-C14	2.94	1.53	1.50
4	A	503	M5L	C15-C14	2.80	1.53	1.50
2	A	501	HEM	FE-NB	2.78	2.10	1.96
2	C	501	HEM	FE-ND	2.75	2.10	1.96
4	B	503	M5L	F17-C14	-2.75	1.33	1.38
2	D	501	HEM	CAB-C3B	2.71	1.54	1.47
4	B	503	M5L	F18-C14	-2.68	1.33	1.38
4	C	503	M5L	C15-C14	2.36	1.52	1.50
2	B	501	HEM	FE-NB	2.28	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	M5L	C15-C14	2.24	1.52	1.50
2	C	501	HEM	FE-NB	2.21	2.07	1.96
2	B	501	HEM	CMB-C2B	2.12	1.55	1.50
2	A	501	HEM	CMD-C2D	2.01	1.55	1.50
2	C	501	HEM	CAA-C2A	2.01	1.55	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	M5L	C02-N01-C06	7.46	123.75	118.10
4	C	503	M5L	C02-N01-C06	7.09	123.47	118.10
4	B	503	M5L	C02-N01-C06	6.60	123.11	118.10
2	D	501	HEM	CBA-CAA-C2A	-6.48	101.57	112.62
4	D	503	M5L	C02-N01-C06	5.96	122.61	118.10
3	A	502	H4B	C8A-C4A-C4	5.77	119.70	114.57
3	C	502	H4B	C8A-C4A-C4	5.46	119.42	114.57
3	B	502	H4B	C8A-C4A-C4	5.43	119.39	114.57
2	C	501	HEM	CBA-CAA-C2A	-5.39	103.43	112.62
2	C	501	HEM	C4B-CHC-C1C	4.61	128.64	122.56
3	D	502	H4B	C8A-C4A-C4	4.52	118.58	114.57
2	B	501	HEM	CBA-CAA-C2A	-4.27	105.34	112.62
2	C	501	HEM	C1B-NB-C4B	4.25	109.47	105.07
2	D	501	HEM	C4C-CHD-C1D	4.21	128.12	122.56
2	C	501	HEM	CBD-CAD-C3D	-4.21	100.92	112.63
4	C	503	M5L	C05-C06-N01	-4.08	118.57	122.90
2	B	501	HEM	C1B-NB-C4B	3.97	109.17	105.07
5	C	504	BTB	O3-C3-C2	3.92	122.17	111.44
4	A	503	M5L	C05-C06-N01	-3.81	118.86	122.90
2	D	501	HEM	CBD-CAD-C3D	-3.80	102.08	112.63
2	A	501	HEM	CBA-CAA-C2A	-3.79	106.14	112.62
4	B	503	M5L	C05-C06-N01	-3.70	118.97	122.90
2	A	501	HEM	C4B-CHC-C1C	3.62	127.33	122.56
2	C	501	HEM	C4D-ND-C1D	3.60	108.80	105.07
3	D	502	H4B	C4-C4A-N5	3.59	122.13	119.12
2	A	501	HEM	CBD-CAD-C3D	-3.56	102.72	112.63
3	D	502	H4B	N1-C2-N3	-3.53	119.88	125.42
6	A	513	GOL	O2-C2-C1	-3.52	93.62	109.12
3	D	502	H4B	C2-N3-C4	3.52	121.52	115.93
2	B	501	HEM	C4D-ND-C1D	3.49	108.67	105.07
3	B	502	H4B	C4-C4A-N5	3.48	122.04	119.12
3	B	502	H4B	N1-C2-N3	-3.47	119.98	125.42
2	D	501	HEM	C4D-ND-C1D	3.46	108.65	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C3B-C2B-C1B	3.45	109.05	106.49
3	B	502	H4B	C2-N3-C4	3.45	121.41	115.93
2	D	501	HEM	C3D-C4D-ND	-3.43	106.35	110.17
3	C	502	H4B	N1-C2-N3	-3.37	120.13	125.42
3	C	502	H4B	C2-N3-C4	3.33	121.22	115.93
2	D	501	HEM	CMC-C2C-C3C	3.28	130.82	124.68
3	A	502	H4B	C2-N3-C4	3.27	121.13	115.93
4	B	503	M5L	C15-C16-N11	3.26	114.45	111.23
4	D	503	M5L	C05-C06-N01	-3.19	119.52	122.90
2	C	501	HEM	C3D-C4D-ND	-3.19	106.62	110.17
2	B	501	HEM	C3B-C2B-C1B	3.19	108.85	106.49
3	A	502	H4B	N1-C2-N3	-3.18	120.43	125.42
2	A	501	HEM	C3B-C2B-C1B	3.17	108.83	106.49
5	A	504	BTB	O3-C3-C2	3.12	119.98	111.44
2	A	501	HEM	C1B-NB-C4B	3.10	108.28	105.07
2	A	501	HEM	C4D-ND-C1D	3.05	108.23	105.07
2	B	501	HEM	CMC-C2C-C3C	3.03	130.35	124.68
2	B	501	HEM	C4B-CHC-C1C	2.94	126.44	122.56
3	B	502	H4B	C2-N1-C8A	2.93	121.11	114.54
3	C	502	H4B	C4-C4A-N5	2.91	121.56	119.12
4	B	503	M5L	C13-C12-N11	2.87	114.07	111.23
2	B	501	HEM	C3D-C4D-ND	-2.85	106.99	110.17
3	D	502	H4B	C2-N1-C8A	2.82	120.86	114.54
3	C	502	H4B	C2-N1-C8A	2.79	120.79	114.54
3	A	502	H4B	C2-N1-C8A	2.77	120.74	114.54
2	B	501	HEM	C2B-C1B-NB	-2.76	106.57	109.84
2	B	501	HEM	CAD-CBD-CGD	-2.67	107.86	113.60
2	D	501	HEM	C4B-CHC-C1C	2.65	126.05	122.56
4	D	503	M5L	C16-C15-C14	-2.65	108.60	111.43
2	C	501	HEM	C2B-C1B-NB	-2.59	106.77	109.84
2	A	501	HEM	CMA-C3A-C4A	-2.53	124.57	128.46
2	C	501	HEM	C4A-C3A-C2A	2.47	108.71	107.00
4	D	503	M5L	C08-C06-C05	2.44	124.44	121.22
2	D	501	HEM	C3B-C2B-C1B	2.43	108.29	106.49
2	D	501	HEM	CHD-C1D-ND	2.38	127.01	124.43
6	A	513	GOL	O1-C1-C2	-2.36	98.87	110.20
4	D	503	M5L	C09-C10-N11	-2.30	108.04	113.84
3	A	502	H4B	C4-C4A-N5	2.21	120.97	119.12
2	C	501	HEM	CHC-C4B-C3B	2.16	127.88	124.57
2	D	501	HEM	CAD-C3D-C2D	-2.16	123.86	127.88
2	A	501	HEM	C3D-C4D-ND	-2.12	107.80	110.17
2	B	501	HEM	C4C-CHD-C1D	2.12	125.35	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-C3B	2.10	127.79	124.57
4	D	503	M5L	F17-C14-C15	-2.09	108.01	109.37
2	C	501	HEM	CMC-C2C-C3C	2.07	128.56	124.68
2	B	501	HEM	C2D-C1D-ND	-2.07	107.41	109.88
2	A	501	HEM	C4A-C3A-C2A	2.05	108.42	107.00
3	C	502	H4B	N2-C2-N1	2.04	120.42	117.25
2	A	501	HEM	CMC-C2C-C3C	2.03	128.48	124.68

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C4-C2-N-C7
5	C	504	BTB	C3-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-C3-O3
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	C	505	BTB	C8-C7-N-C5
5	C	506	BTB	O1-C1-C2-C3
5	C	506	BTB	O1-C1-C2-C4
5	C	506	BTB	O1-C1-C2-N
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C8-C7-N-C5
5	D	505	BTB	N-C7-C8-O8
6	A	513	GOL	O1-C1-C2-C3
6	B	506	GOL	C1-C2-C3-O3
6	C	507	GOL	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-C3
6	C	509	GOL	O1-C1-C2-C3
5	C	505	BTB	N-C5-C6-O6
5	B	505	BTB	N-C5-C6-O6
6	C	507	GOL	O1-C1-C2-O2
6	C	509	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C7-C8-O8
5	A	505	BTB	N-C7-C8-O8
6	A	508	GOL	O1-C1-C2-C3
6	A	509	GOL	O1-C1-C2-C3
6	A	513	GOL	C1-C2-C3-O3
6	C	508	GOL	O1-C1-C2-O2
4	A	503	M5L	C05-C06-C08-C09
5	C	506	BTB	N-C7-C8-O8
4	A	503	M5L	N01-C06-C08-C09
4	C	503	M5L	N01-C06-C08-C09

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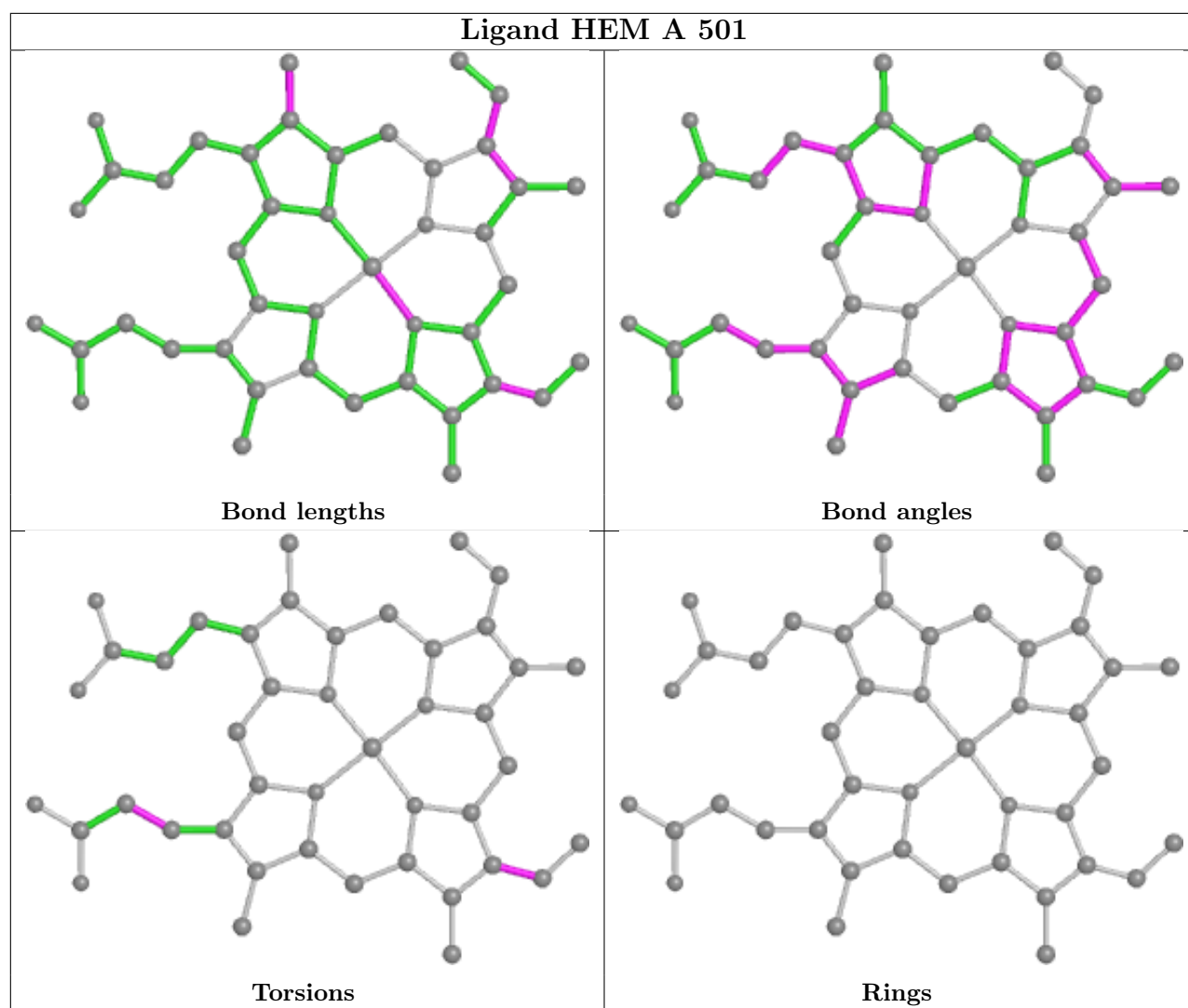
Mol	Chain	Res	Type	Atoms
6	A	508	GOL	O1-C1-C2-O2
6	A	513	GOL	O1-C1-C2-O2
6	B	506	GOL	O2-C2-C3-O3
4	C	503	M5L	C05-C06-C08-C09
5	C	506	BTB	N-C5-C6-O6
5	A	504	BTB	N-C7-C8-O8
4	B	503	M5L	N01-C06-C08-C09
4	D	503	M5L	N01-C06-C08-C09
6	A	509	GOL	O2-C2-C3-O3
4	B	503	M5L	C05-C06-C08-C09
4	D	503	M5L	C05-C06-C08-C09
5	A	505	BTB	N-C5-C6-O6
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
6	A	508	GOL	O2-C2-C3-O3
6	A	513	GOL	O2-C2-C3-O3
6	D	506	GOL	O2-C2-C3-O3
5	A	506	BTB	O1-C1-C2-C4
5	C	504	BTB	C1-C2-C4-O4
2	A	501	HEM	C2A-CAA-CBA-CGA
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C7
5	A	506	BTB	O1-C1-C2-N
5	A	506	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C5
5	A	504	BTB	N-C5-C6-O6
6	A	509	GOL	O1-C1-C2-O2
2	D	501	HEM	C3D-CAD-CBD-CGD
5	D	505	BTB	N-C5-C6-O6
6	A	509	GOL	C1-C2-C3-O3
6	D	506	GOL	C1-C2-C3-O3
5	A	506	BTB	O1-C1-C2-C3
5	D	505	BTB	C3-C2-C4-O4
2	D	501	HEM	CAD-CBD-CGD-O2D

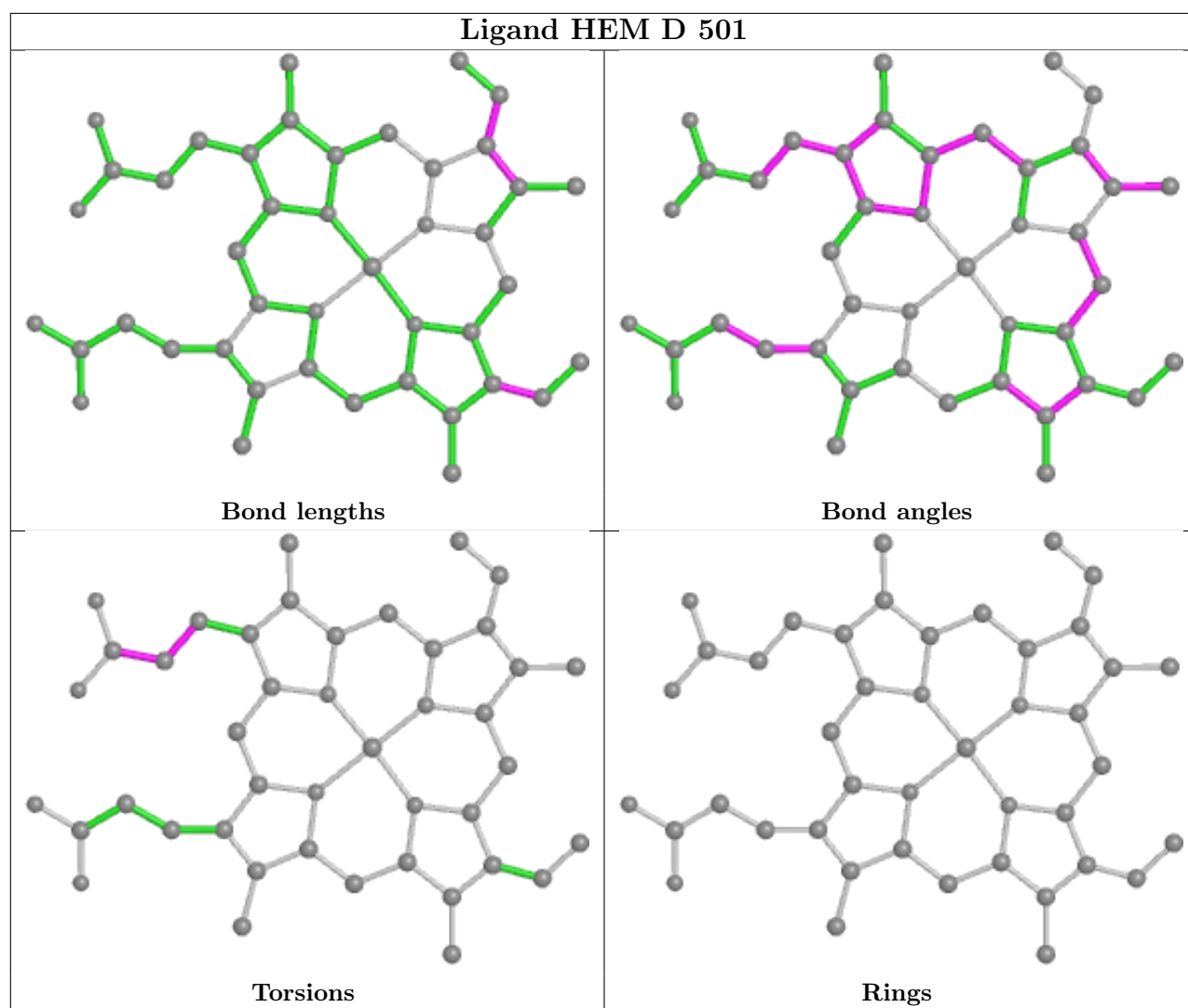
There are no ring outliers.

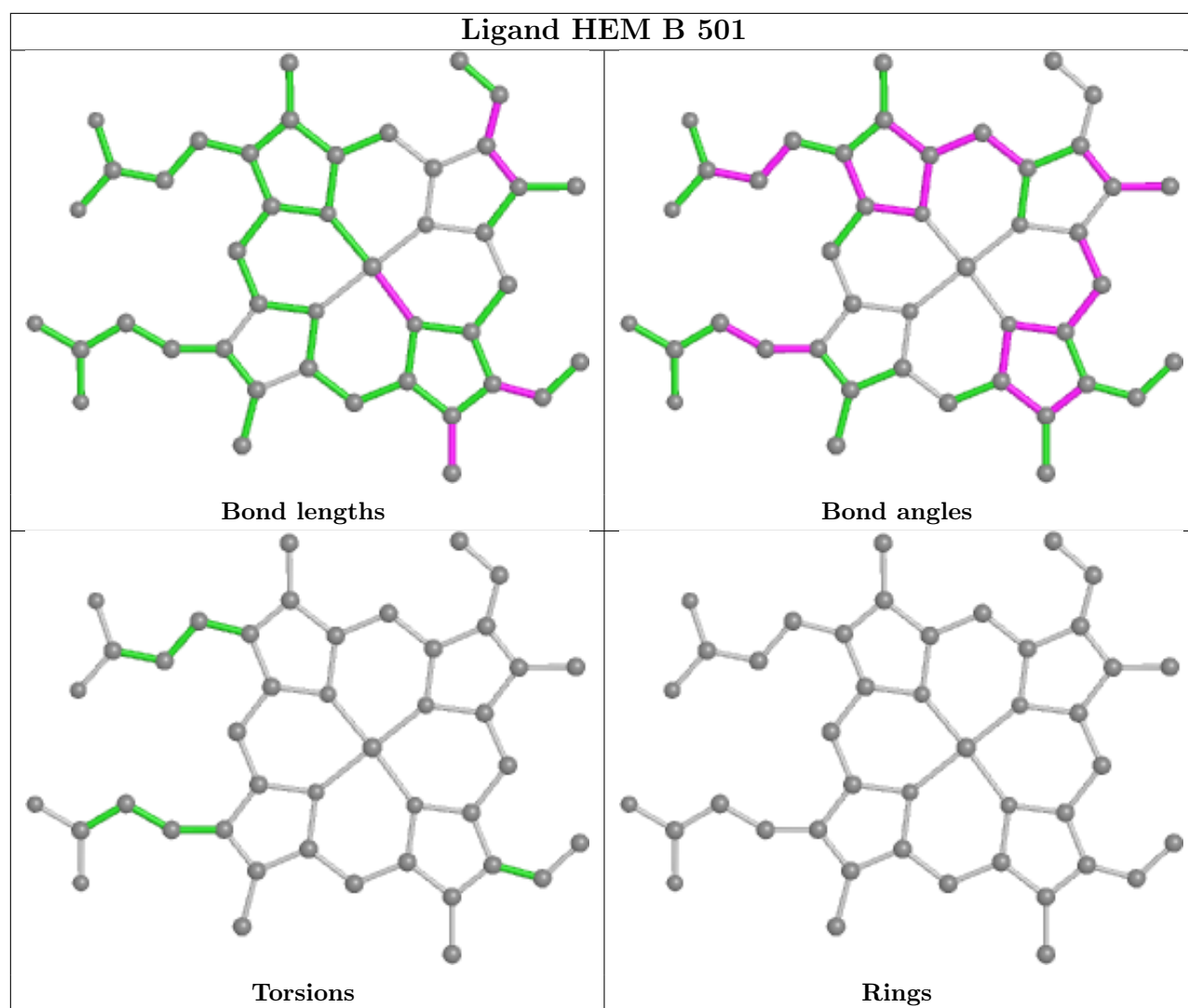
20 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	509	GOL	2	0
6	A	513	GOL	1	0
2	A	501	HEM	3	0
6	C	507	GOL	1	0
2	D	501	HEM	2	0
5	C	504	BTB	4	0
2	B	501	HEM	1	0
5	A	504	BTB	3	0
3	B	502	H4B	1	0
5	C	505	BTB	5	0
5	D	504	BTB	2	0
6	A	507	GOL	1	0
5	D	505	BTB	2	0
2	C	501	HEM	3	0
5	A	506	BTB	4	0
3	C	502	H4B	1	0
5	C	506	BTB	3	0
5	B	505	BTB	4	0
4	A	503	M5L	1	0
5	A	505	BTB	2	0

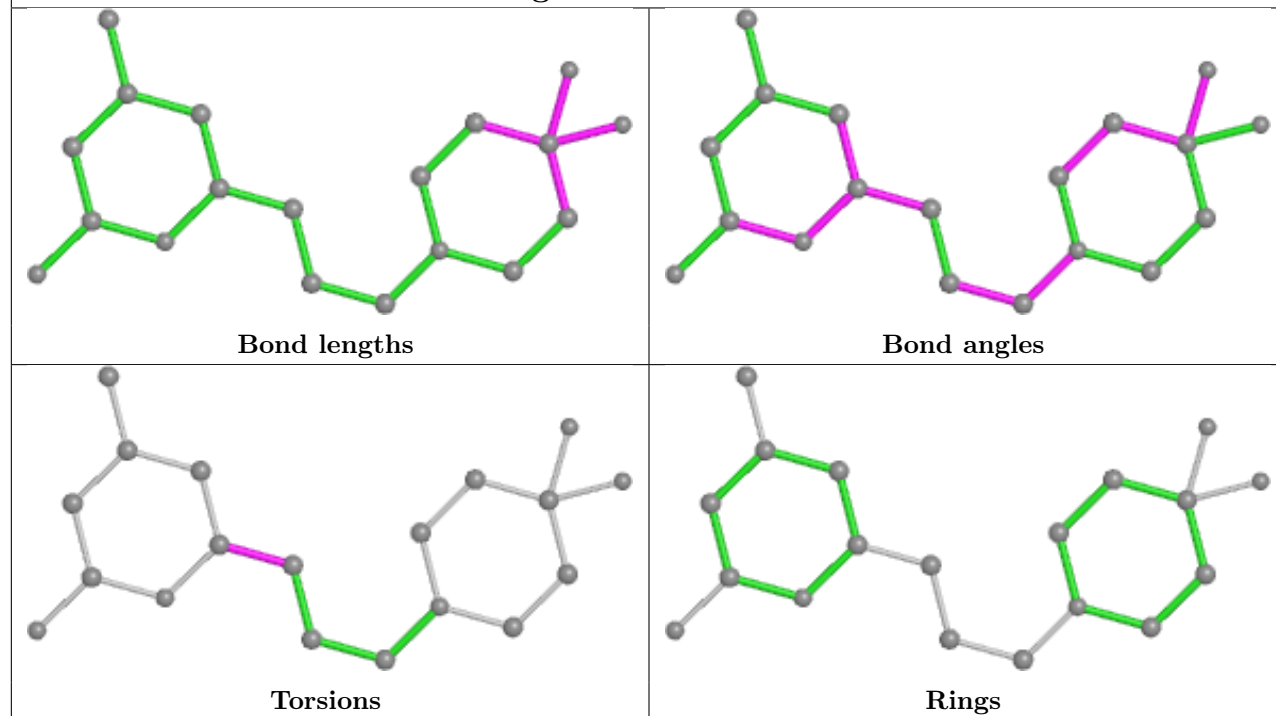
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



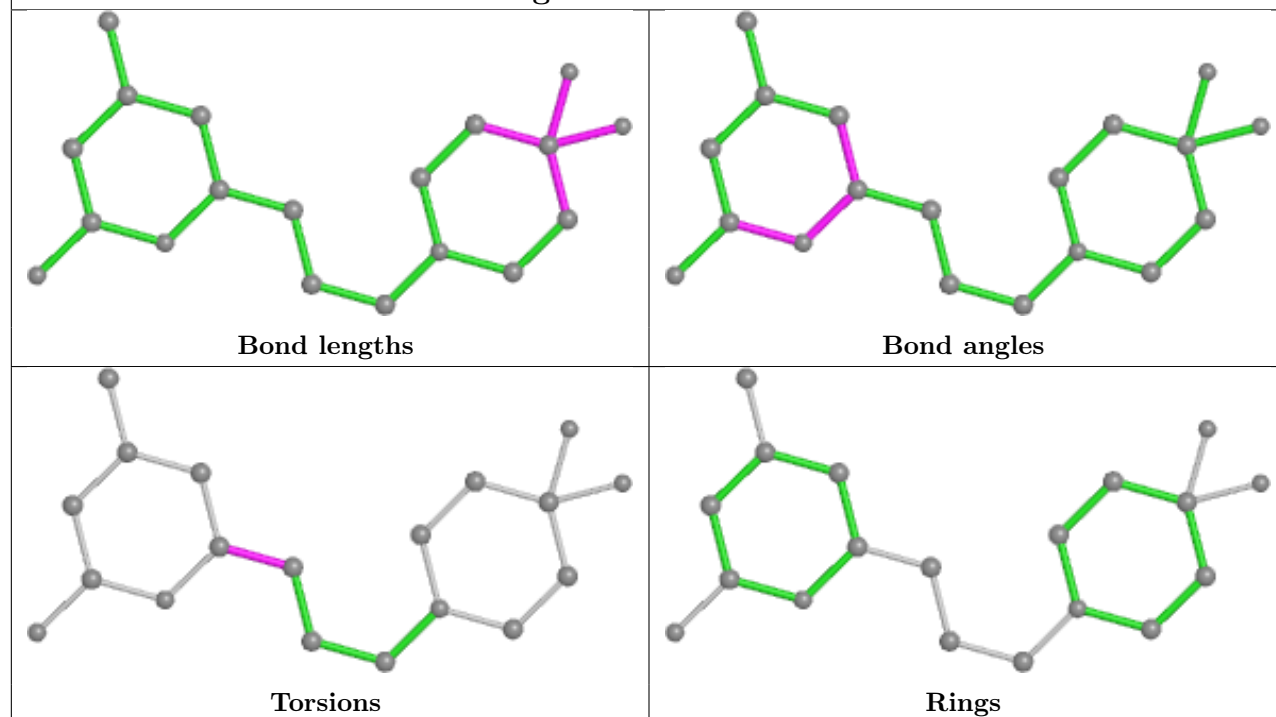


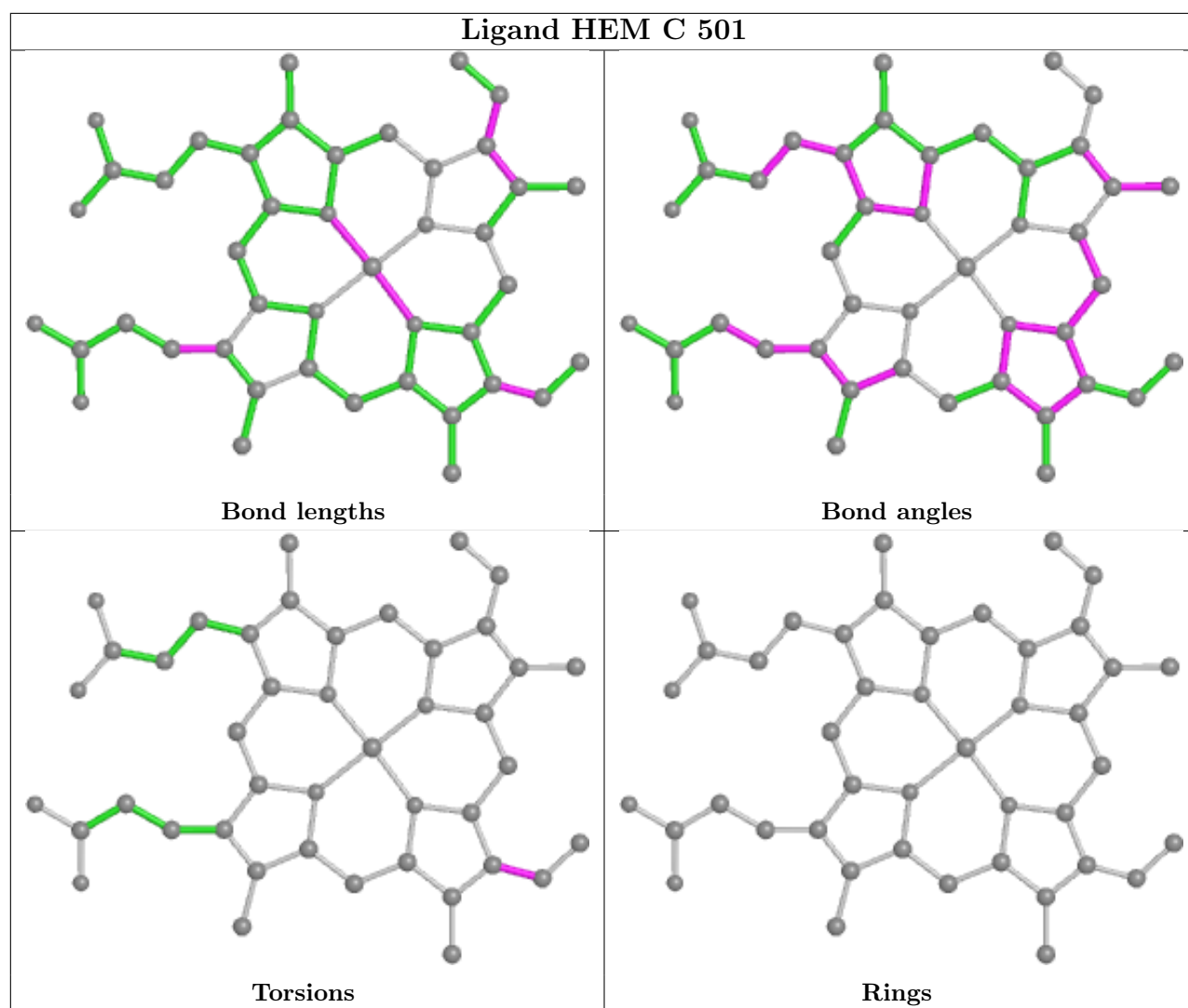


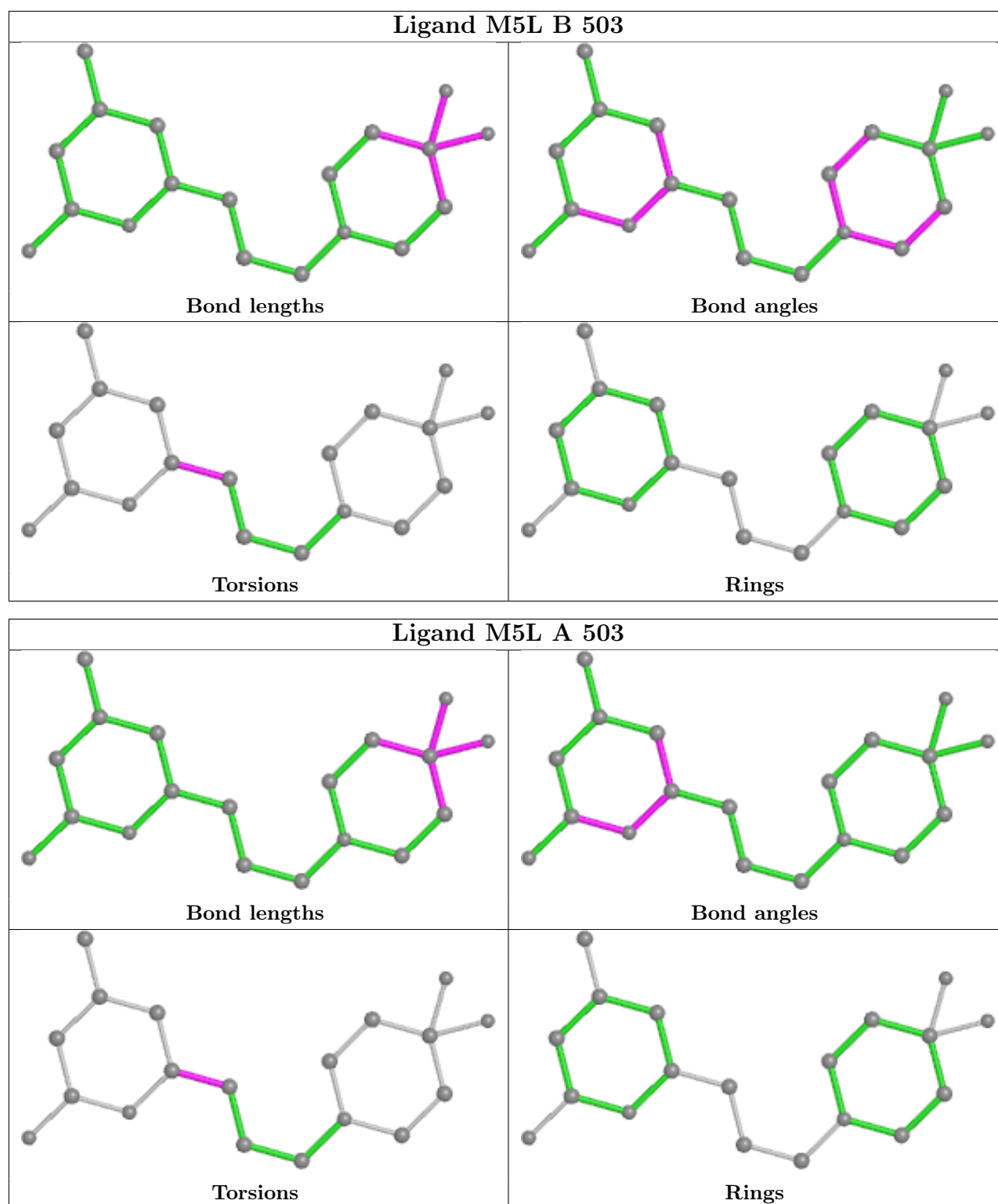
Ligand M5L D 503



Ligand M5L C 503







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/440 (91%)	1.33	106 (26%) 0 0	29, 58, 112, 144	0
1	B	401/440 (91%)	0.43	28 (6%) 16 18	26, 40, 77, 121	0
1	C	402/440 (91%)	1.08	84 (20%) 1 1	28, 54, 103, 140	0
1	D	402/440 (91%)	0.31	29 (7%) 15 17	24, 39, 68, 133	0
All	All	1606/1760 (91%)	0.79	247 (15%) 2 2	24, 47, 99, 144	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	8.7
1	A	480	TRP	8.4
1	A	259	GLY	7.1
1	A	153	VAL	6.6
1	A	295	ALA	6.3
1	A	302	LEU	6.2
1	C	142	GLY	6.2
1	A	141	SER	6.1
1	C	480	TRP	6.0
1	A	447	TRP	5.9
1	C	302	LEU	5.6
1	A	237	GLY	5.6
1	A	275	ILE	5.5
1	A	452	ILE	5.4
1	C	204	ALA	5.3
1	D	89	GLN	5.3
1	A	303	PHE	5.3
1	D	257	GLN	5.3
1	C	275	ILE	5.2
1	C	238	ARG	5.2
1	A	142	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	259	GLY	5.2
1	A	412	LEU	5.1
1	A	448	ILE	5.0
1	C	448	ILE	5.0
1	B	257	GLN	4.9
1	C	68	PHE	4.8
1	B	452	ILE	4.7
1	C	447	TRP	4.6
1	C	141	SER	4.6
1	A	304	LEU	4.6
1	A	449	VAL	4.6
1	A	279	TRP	4.5
1	A	479	PRO	4.5
1	A	238	ARG	4.4
1	A	122	GLN	4.4
1	C	236	PRO	4.3
1	C	153	VAL	4.3
1	A	244	TRP	4.3
1	C	295	ALA	4.2
1	A	254	TYR	4.2
1	A	281	PRO	4.2
1	B	460	PHE	4.2
1	C	449	VAL	4.2
1	D	452	ILE	4.1
1	A	185	VAL	4.0
1	C	452	ILE	4.0
1	A	280	THR	4.0
1	A	451	PRO	4.0
1	C	237	GLY	4.0
1	A	293	LEU	4.0
1	C	292	LEU	4.0
1	C	277	HIS	4.0
1	B	89	GLN	3.9
1	A	273	LEU	3.9
1	C	202	ARG	3.9
1	A	257	GLN	3.9
1	C	280	THR	3.8
1	D	255	ARG	3.8
1	A	184	CYS	3.8
1	C	258	ASP	3.8
1	C	119	ALA	3.8
1	B	122	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	304	LEU	3.8
1	C	268	VAL	3.7
1	A	239	GLY	3.7
1	C	299	PRO	3.7
1	C	450	PRO	3.7
1	A	124	LEU	3.7
1	A	450	PRO	3.7
1	C	445	TRP	3.7
1	A	256	GLN	3.7
1	C	272	GLU	3.6
1	A	278	GLY	3.6
1	C	301	GLU	3.6
1	C	184	CYS	3.6
1	A	127	ALA	3.6
1	C	439	GLY	3.6
1	A	202	ARG	3.6
1	A	128	ARG	3.6
1	A	360	THR	3.6
1	C	303	PHE	3.5
1	A	146	HIS	3.5
1	C	124	LEU	3.5
1	A	446	ALA	3.5
1	A	68	PHE	3.5
1	A	90	GLN	3.5
1	B	454	GLY	3.5
1	A	300	PRO	3.5
1	A	445	TRP	3.5
1	B	449	VAL	3.5
1	C	129	ASP	3.5
1	A	268	VAL	3.4
1	C	255	ARG	3.4
1	A	138	ILE	3.4
1	B	97	ARG	3.4
1	B	388	ARG	3.4
1	D	451	PRO	3.4
1	C	257	GLN	3.3
1	C	79	ILE	3.3
1	D	449	VAL	3.3
1	C	451	PRO	3.3
1	A	272	GLU	3.3
1	B	451	PRO	3.3
1	A	162	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	445	TRP	3.3
1	A	89	GLN	3.3
1	A	144	GLN	3.3
1	C	89	GLN	3.3
1	C	120	PRO	3.3
1	A	145	ALA	3.2
1	A	88	ALA	3.2
1	B	258	ASP	3.2
1	C	221	ARG	3.2
1	C	122	GLN	3.2
1	C	306	PRO	3.2
1	C	259	GLY	3.1
1	D	456	LEU	3.1
1	A	183	ARG	3.1
1	A	439	GLY	3.1
1	A	346	LEU	3.1
1	B	445	TRP	3.1
1	B	260	SER	3.1
1	A	258	ASP	3.0
1	C	254	TYR	3.0
1	A	276	GLN	3.0
1	D	258	ASP	3.0
1	B	157	VAL	3.0
1	C	140	ARG	3.0
1	C	446	ALA	3.0
1	A	478	ASP	3.0
1	C	155	ALA	3.0
1	B	450	PRO	3.0
1	C	297	ASP	3.0
1	C	279	TRP	3.0
1	C	360	THR	3.0
1	B	68	PHE	2.9
1	B	453	SER	2.9
1	C	87	GLN	2.9
1	C	412	LEU	2.9
1	A	79	ILE	2.9
1	C	308	GLU	2.9
1	B	119	ALA	2.9
1	C	276	GLN	2.9
1	A	221	ARG	2.8
1	A	155	ALA	2.8
1	D	79	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	301	GLU	2.8
1	A	151	GLN	2.8
1	D	446	ALA	2.8
1	A	123	LEU	2.8
1	C	90	GLN	2.8
1	D	388	ARG	2.8
1	A	336	VAL	2.8
1	C	160	THR	2.7
1	A	299	PRO	2.7
1	B	158	ALA	2.7
1	C	309	LEU	2.7
1	A	129	ASP	2.7
1	C	235	CYS	2.7
1	A	297	ASP	2.6
1	D	460	PHE	2.6
1	A	307	PRO	2.6
1	C	240	ASP	2.6
1	D	256	GLN	2.6
1	C	185	VAL	2.6
1	C	86	ALA	2.6
1	C	454	GLY	2.6
1	B	90	GLN	2.6
1	A	121	GLU	2.6
1	D	454	GLY	2.6
1	D	121	GLU	2.5
1	C	437	ALA	2.5
1	A	67	LYS	2.5
1	A	368	CYS	2.5
1	C	241	PHE	2.5
1	C	300	PRO	2.5
1	A	357	TYR	2.5
1	A	308	GLU	2.5
1	A	235	CYS	2.5
1	A	277	HIS	2.5
1	D	450	PRO	2.5
1	C	239	GLY	2.5
1	D	68	PHE	2.5
1	A	140	ARG	2.5
1	D	261	VAL	2.4
1	C	294	GLN	2.4
1	A	159	ALA	2.4
1	C	460	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	478	ASP	2.4
1	B	142	GLY	2.4
1	D	360	THR	2.4
1	B	79	ILE	2.4
1	A	345	GLY	2.4
1	A	139	LYS	2.3
1	A	120	PRO	2.3
1	A	444	ASP	2.3
1	D	389	THR	2.3
1	A	205	GLN	2.3
1	A	365	ARG	2.3
1	C	128	ARG	2.3
1	A	364	THR	2.3
1	C	144	GLN	2.3
1	C	368	CYS	2.3
1	C	106	PRO	2.2
1	C	183	ARG	2.2
1	D	357	TYR	2.2
1	B	141[A]	SER	2.2
1	C	209	THR	2.2
1	A	241	PHE	2.2
1	B	446	ALA	2.2
1	C	208	PHE	2.2
1	B	455	SER	2.2
1	A	148	GLN	2.2
1	B	360	THR	2.1
1	C	273	LEU	2.1
1	D	387	THR	2.1
1	C	159	ALA	2.1
1	A	203	SER	2.1
1	A	358	MET	2.1
1	C	81	TYR	2.1
1	A	182	PRO	2.1
1	A	454	GLY	2.1
1	C	121	GLU	2.1
1	A	309	LEU	2.1
1	A	255	ARG	2.1
1	A	86	ALA	2.1
1	A	260	SER	2.1
1	C	146	HIS	2.1
1	A	294	GLN	2.1
1	D	120	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	134	TYR	2.1
1	D	260	SER	2.1
1	A	242	ARG	2.0
1	A	136	SER	2.0
1	A	359	SER	2.0
1	A	236	PRO	2.0
1	D	362	ILE	2.0
1	D	448	ILE	2.0
1	A	274	CYS	2.0
1	A	453	SER	2.0
1	C	143	SER	2.0
1	A	459	VAL	2.0
1	D	400	VAL	2.0
1	C	244	TRP	2.0
1	D	447	TRP	2.0
1	B	362	ILE	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 monosaccharides 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
6	GOL	A	509	6/6	0.64	0.16	71,81,84,85	0
6	GOL	C	508	6/6	0.71	0.16	60,71,75,80	0
5	BTB	D	504	14/14	0.74	0.22	35,66,85,89	0
6	GOL	C	509	6/6	0.75	0.13	69,79,81,85	0
5	BTB	A	506	14/14	0.77	0.22	85,97,102,103	0
5	BTB	B	504	14/14	0.80	0.19	39,50,81,86	0
5	BTB	C	506	14/14	0.80	0.16	76,89,105,108	0

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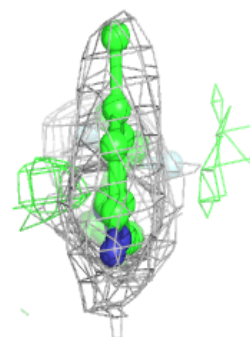
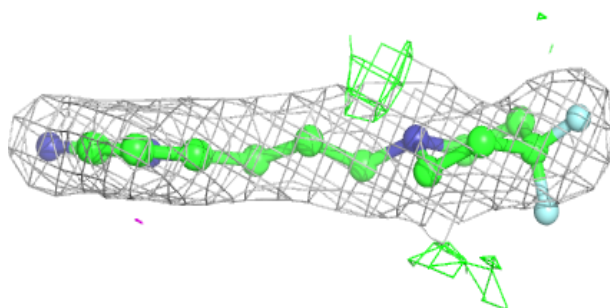
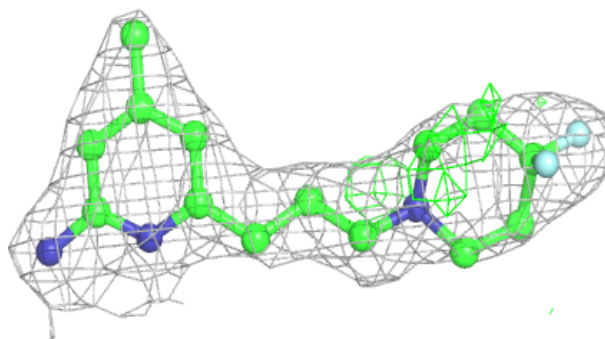
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	D	506	6/6	0.82	0.31	60,71,78,80	0
5	BTB	A	505	14/14	0.85	0.16	59,79,86,90	0
5	BTB	B	505	14/14	0.86	0.18	54,67,76,78	0
6	GOL	A	508	6/6	0.86	0.19	60,71,77,78	0
4	M5L	A	503	19/19	0.89	0.34	37,59,107,108	0
6	GOL	A	513	6/6	0.90	0.14	26,37,55,57	0
4	M5L	B	503	19/19	0.90	0.17	24,37,73,74	0
3	H4B	C	502	17/17	0.91	0.23	37,43,47,51	0
4	M5L	C	503	19/19	0.91	0.26	40,53,91,92	0
5	BTB	A	504	14/14	0.91	0.27	27,74,83,93	0
5	BTB	C	505	14/14	0.92	0.15	25,61,76,80	0
3	H4B	A	502	17/17	0.92	0.25	37,46,55,63	0
6	GOL	B	506	6/6	0.92	0.26	68,76,77,81	0
5	BTB	D	505	14/14	0.93	0.17	57,70,84,94	0
6	GOL	C	507	6/6	0.94	0.22	48,56,60,60	0
2	HEM	A	501	43/43	0.94	0.23	26,53,62,67	0
4	M5L	D	503	19/19	0.94	0.16	24,35,88,91	0
2	HEM	C	501	43/43	0.94	0.22	28,45,64,78	0
3	H4B	B	502	17/17	0.95	0.17	26,39,45,46	0
2	HEM	B	501	43/43	0.95	0.13	18,30,49,56	0
3	H4B	D	502	17/17	0.95	0.19	31,41,48,52	0
5	BTB	C	504	14/14	0.95	0.20	16,63,74,81	0
2	HEM	D	501	43/43	0.96	0.14	20,29,53,73	0
6	GOL	A	507	6/6	0.96	0.24	48,58,68,72	0
7	CL	A	510	1/1	0.97	0.20	60,60,60,60	0
7	CL	D	508	1/1	0.97	0.25	38,38,38,38	0
8	GD	A	511	1/1	0.98	0.07	73,73,73,73	1
8	GD	D	509	1/1	0.98	0.12	47,47,47,47	0
9	ZN	A	512	1/1	0.98	0.09	44,44,44,44	0
7	CL	C	510	1/1	0.99	0.20	48,48,48,48	0
8	GD	B	508	1/1	0.99	0.10	42,42,42,42	0
7	CL	D	507	1/1	0.99	0.07	42,42,42,42	0
7	CL	B	507	1/1	0.99	0.12	48,48,48,48	0
8	GD	B	509	1/1	1.00	0.07	56,56,56,56	1
9	ZN	C	511	1/1	1.00	0.10	36,36,36,36	0

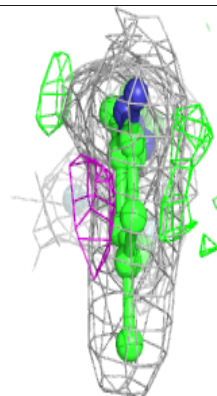
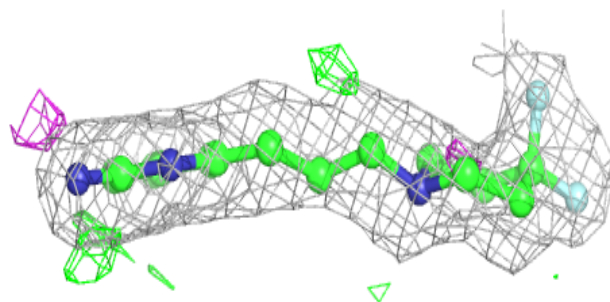
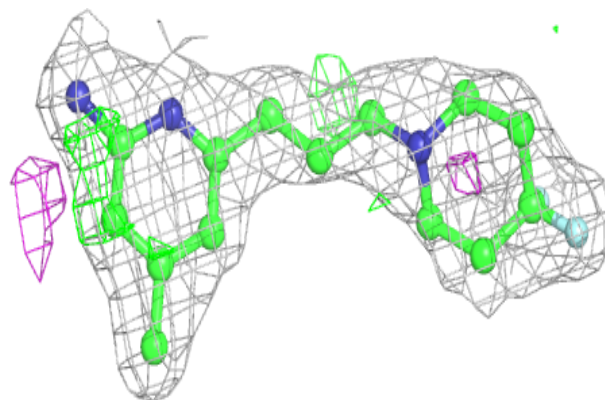
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M5L A 503:

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

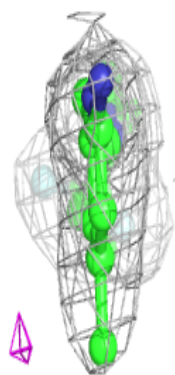
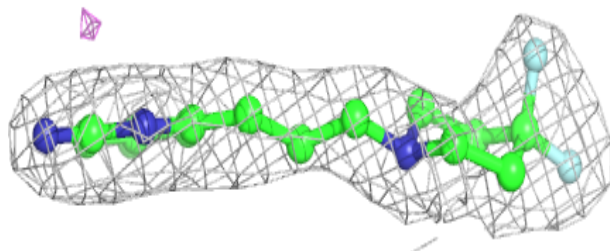
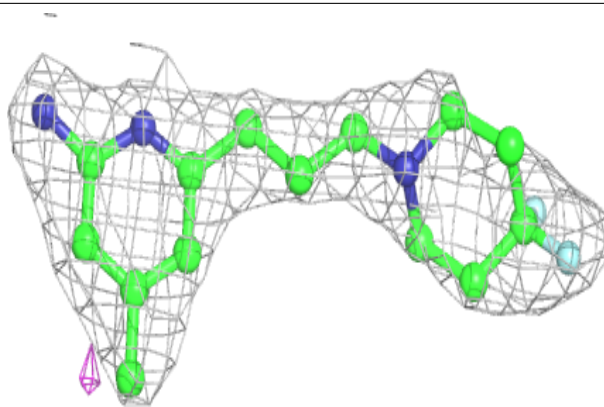
**Electron density around M5L B 503:**

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



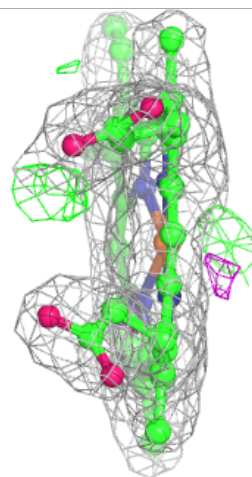
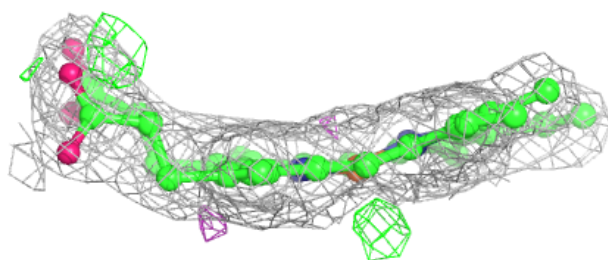
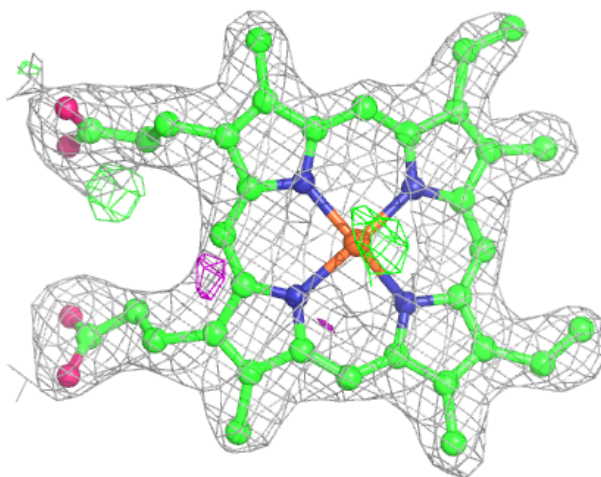
Electron density around M5L C 503:

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



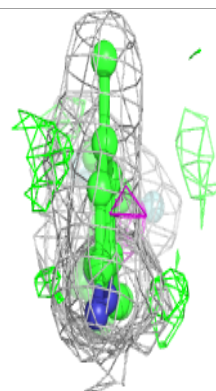
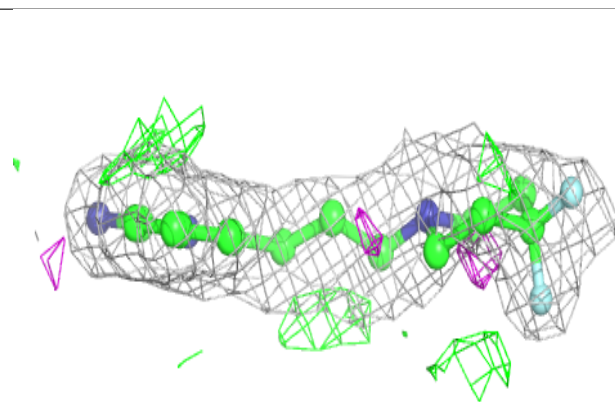
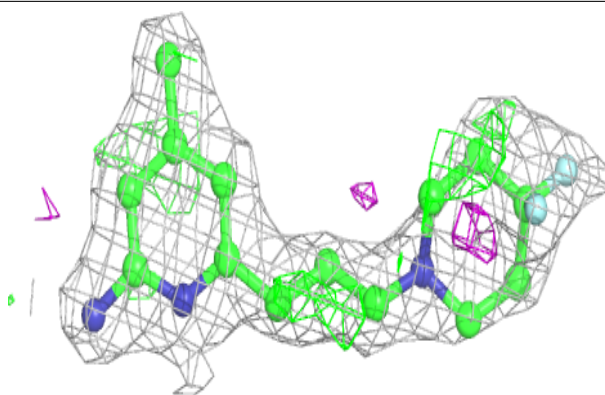
Electron density around HEM A 501:

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



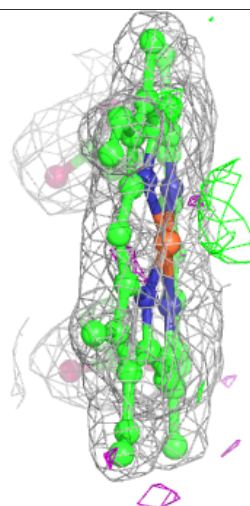
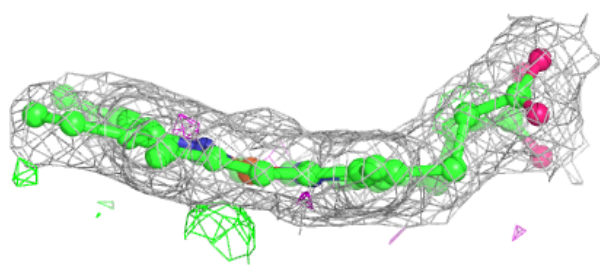
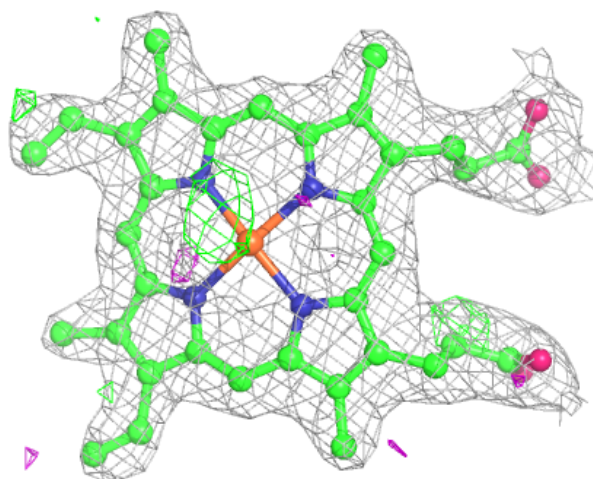
Electron density around M5L D 503:

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



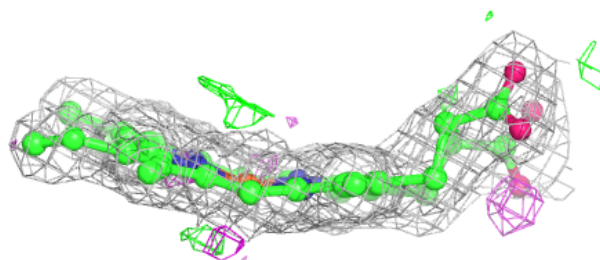
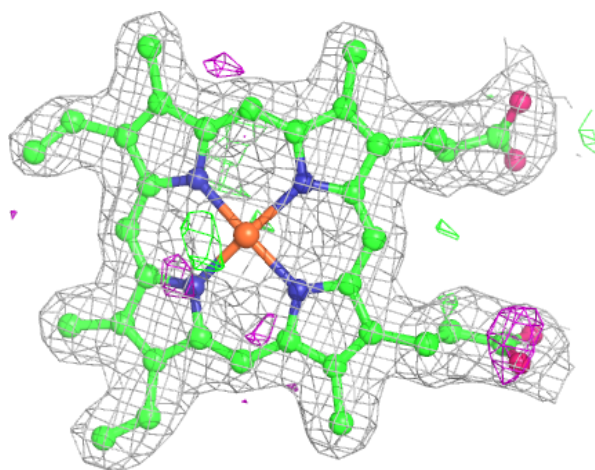
Electron density around HEM C 501:

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



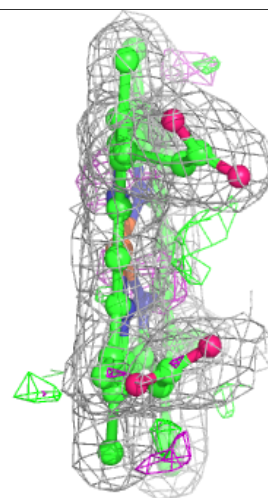
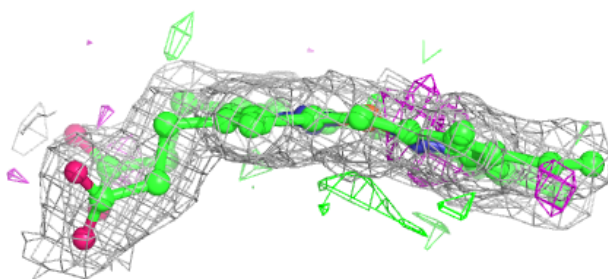
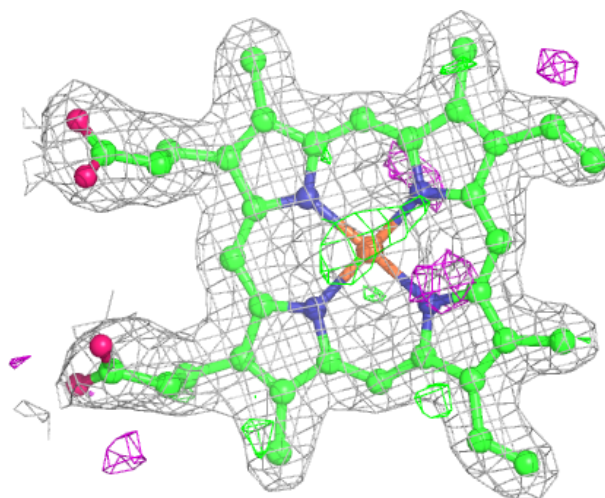
Electron density around HEM B 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.