



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:22 pm BST

PDB ID : 6AV7
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with HW69
Authors : Li, H.; Poulos, T.L.
Deposited on : 2017-09-01
Resolution : 1.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

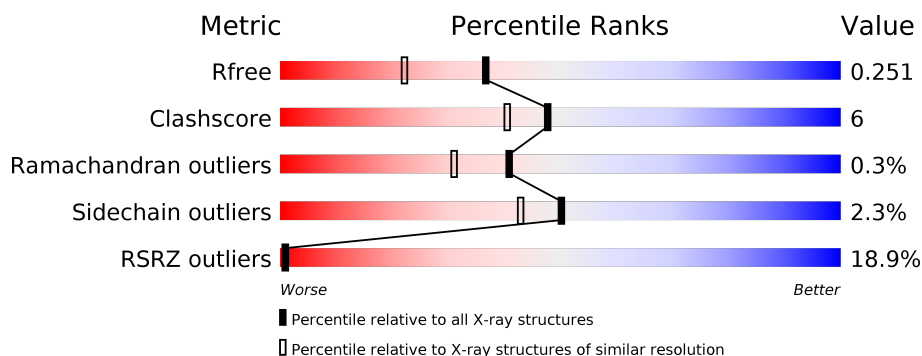
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on 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>29%</div> <div> <div>74%</div> <div>17%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	440	<div> <div>10%</div> <div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
1	C	440	<div> <div>20%</div> <div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	D	440	<div> <div>10%</div> <div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13722 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	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			

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



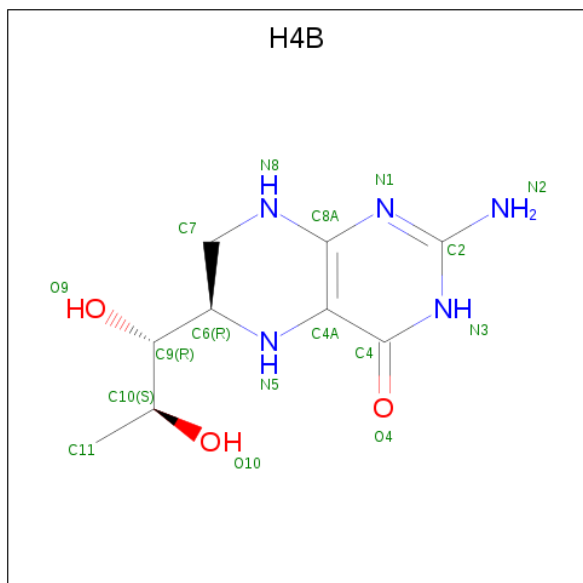
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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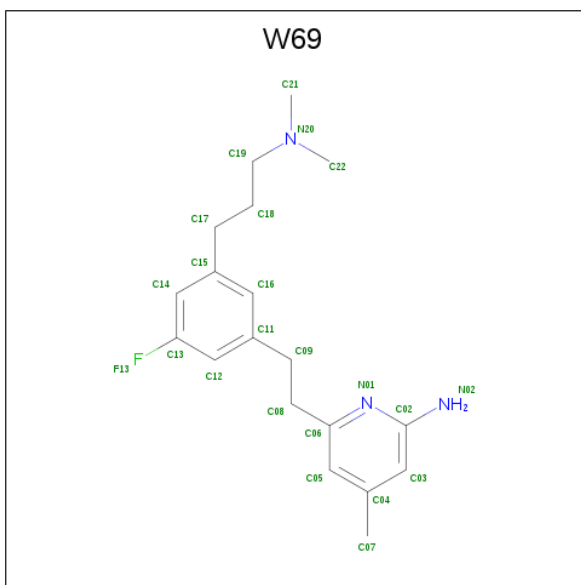
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



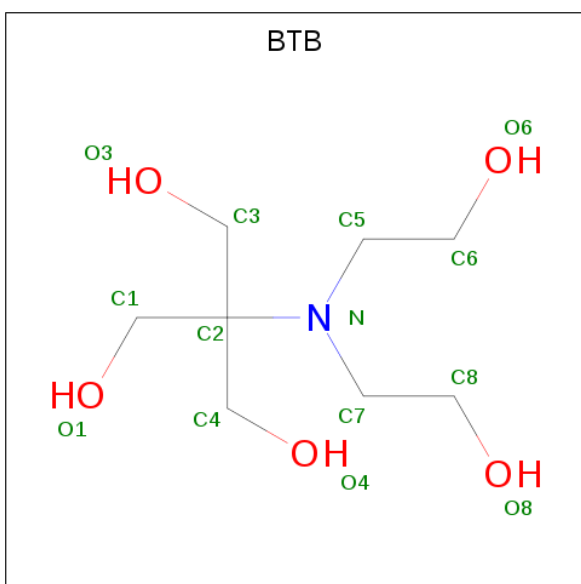
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-(2-{3-[3-(dimethylamino)propyl]-5-fluorophenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: W69) (formula: $C_{19}H_{26}FN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	19	1	3		
4	B	1	Total	C	F	N	0	0
			23	19	1	3		
4	C	1	Total	C	F	N	0	0
			23	19	1	3		
4	D	1	Total	C	F	N	0	0
			23	19	1	3		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).

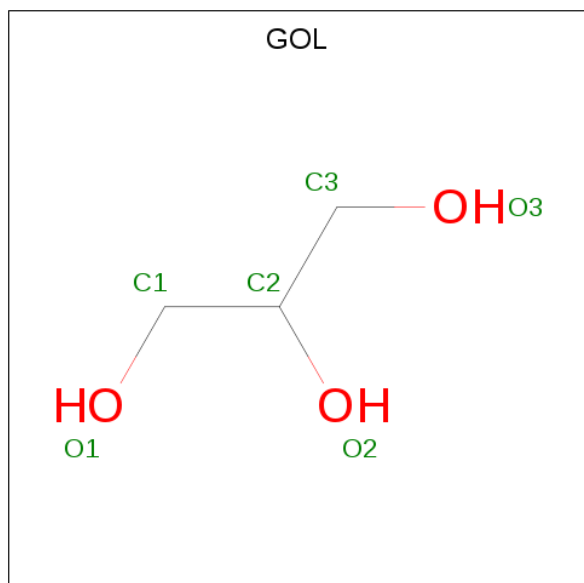


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Gd 1 1	0	0
9	A	1	Total Gd 1 1	0	0
9	D	1	Total Gd 1 1	0	0
9	C	1	Total Gd 1 1	0	0

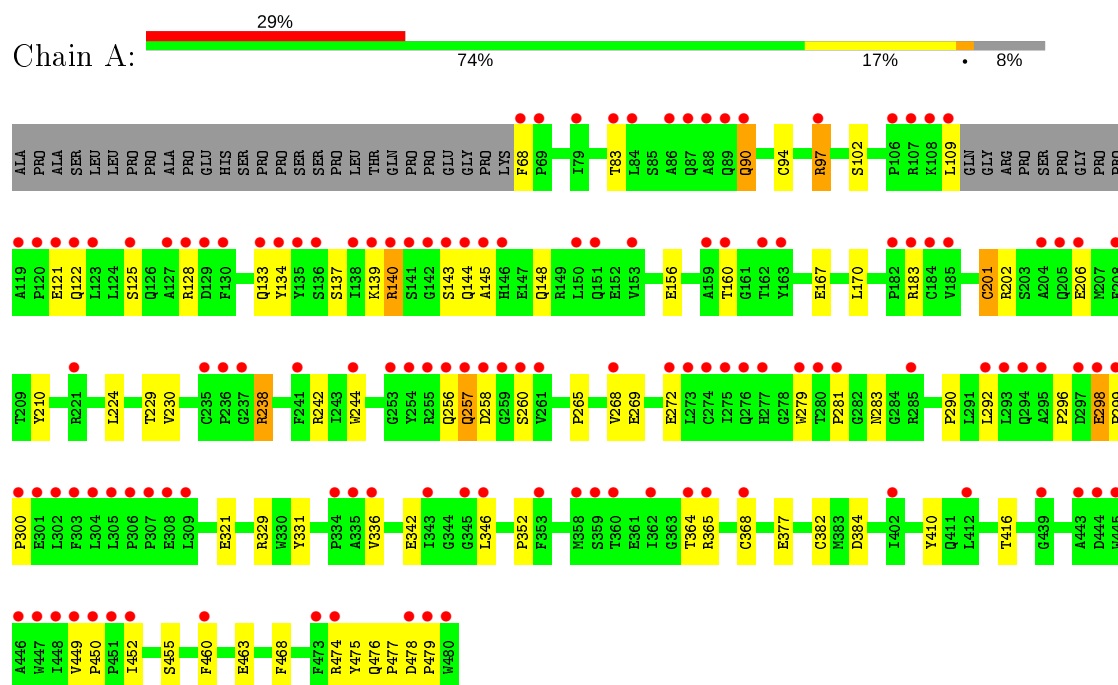
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	34	Total O 34 34	0	0
10	B	117	Total O 117 117	0	0
10	C	73	Total O 73 73	0	0
10	D	130	Total O 130 130	0	0

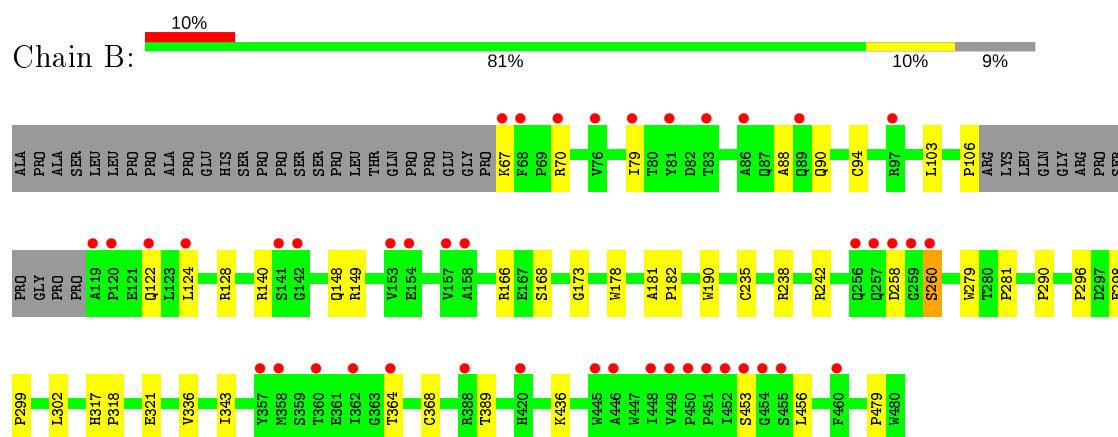
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

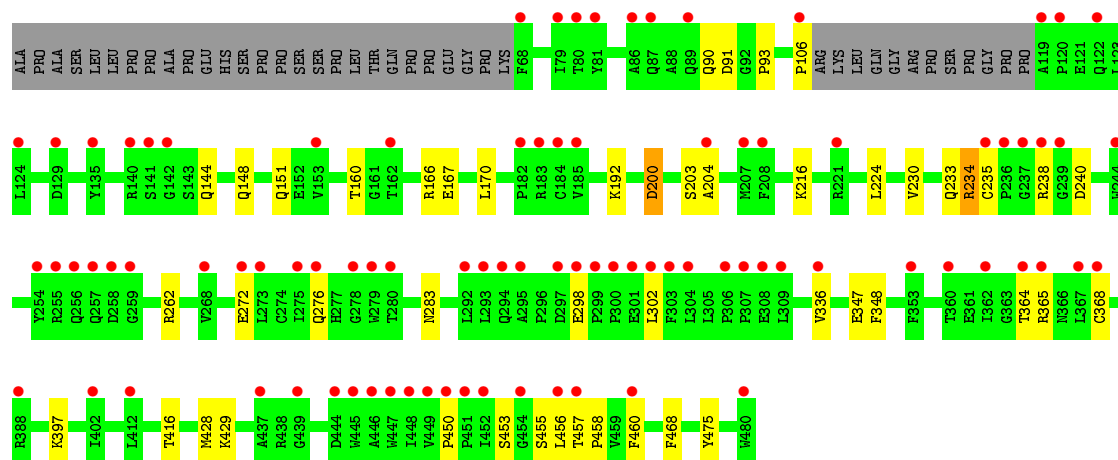
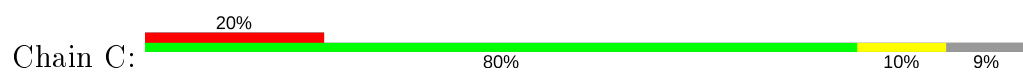
- Molecule 1: Nitric oxide synthase, endothelial



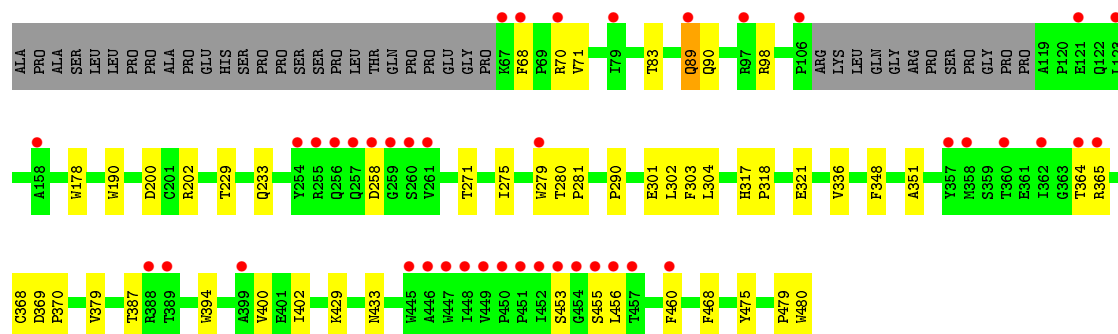
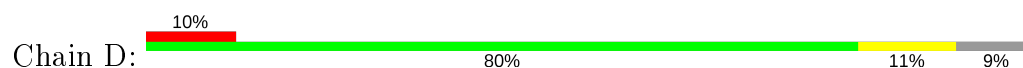
- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



• 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	59.45Å 152.35Å 108.66Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	39.03 – 1.92 39.03 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.5 (39.03-1.92) 95.0 (39.03-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.204 , 0.254 0.206 , 0.251	Depositor DCC
R_{free} test set	7085 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13722	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, ZN, W69, H4B, CL, GD, BTB, HEM

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	0.34	0/3335	0.49	0/4543
1	B	0.39	0/3319	0.52	0/4523
1	C	0.35	0/3307	0.49	0/4507
1	D	0.43	0/3319	0.54	0/4523
All	All	0.38	0/13280	0.51	0/18096

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	89	GLN	Peptide

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	3237	0	3146	56	0
1	B	3221	0	3126	27	0
1	C	3209	0	3109	27	0
1	D	3221	0	3126	28	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	23	0	0	2	0
4	B	23	0	0	3	0
4	C	23	0	0	3	0
4	D	23	0	0	2	0
5	A	28	0	38	6	0
5	B	28	0	36	5	0
5	C	42	0	56	6	0
5	D	28	0	36	5	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	1	0
7	C	6	0	8	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	34	0	0	0	0
10	B	117	0	0	1	0
10	C	73	0	0	3	0
10	D	130	0	0	1	0
All	All	13722	0	12869	161	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 6.

All (161) 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:235:CYS:H	1:C:238:ARG:HD3	1.36	0.88
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.63	0.80
1:A:242:ARG:NH2	1:A:477:PRO:O	2.15	0.79
1:A:125:SER:HA	1:A:128:ARG:HE	1.50	0.76
1:A:382:CYS:HA	5:A:504:BTB:H11	1.70	0.74
1:A:242:ARG:HD3	1:A:479:PRO:HB3	1.69	0.73
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.72	0.72
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.73	0.70
1:A:242:ARG:HE	1:A:479:PRO:HD3	1.56	0.69
1:C:144:GLN:NE2	10:C:603:HOH:O	2.24	0.69
5:D:504:BTB:O6	5:D:504:BTB:H82	1.92	0.69
1:A:145:ALA:HA	1:A:148:GLN:HB3	1.74	0.68
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.74	0.68
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.11	0.68
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.08	0.67
5:A:505:BTB:O1	5:A:505:BTB:O4	2.11	0.65
1:C:347:GLU:OE2	10:C:601:HOH:O	2.15	0.63
1:B:298:GLU:OE2	5:B:505:BTB:N	2.31	0.63
1:A:144:GLN:HG2	1:A:145:ALA:H	1.64	0.63
2:A:501:HEM:HBD2	4:A:503:W69:C13	2.29	0.62
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.81	0.62
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.80	0.62
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.09	0.62
1:B:258:ASP:HB2	1:B:260:SER:HB3	1.82	0.60
1:C:200:ASP:OD1	1:C:200:ASP:N	2.33	0.60
1:A:256:GLN:NE2	1:A:260:SER:OG	2.27	0.60
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.37	0.60
2:B:501:HEM:HBD1	4:B:503:W69:C13	2.32	0.59
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.84	0.59
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.85	0.57
1:A:201:CYS:O	1:A:202:ARG:NH1	2.33	0.56
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.86	0.56
2:D:501:HEM:HBD1	4:D:503:W69:C13	2.35	0.56
1:D:70:ARG:O	10:D:601:HOH:O	2.17	0.56
1:A:167:GLU:OE1	7:A:507:GOL:O3	2.16	0.56
1:A:342:GLU:OE1	1:A:474:ARG:NH1	2.39	0.56
1:D:321:GLU:OE2	5:D:504:BTB:O3	2.25	0.55
2:B:501:HEM:HBD1	4:B:503:W69:F13	1.96	0.55
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.43	0.54
1:A:90:GLN:HG3	1:A:468:PHE:CE2	2.43	0.53
1:C:336:VAL:HG21	4:C:503:W69:C13	2.38	0.53
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:PRO:HG3	1:C:106:PRO:HB3	1.91	0.53
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.90	0.52
1:D:336:VAL:HG21	4:D:503:W69:C13	2.39	0.52
1:A:143:SER:OG	1:A:144:GLN:N	2.42	0.52
1:C:167:GLU:OE1	7:C:508:GOL:O3	2.19	0.51
1:D:429:LYS:NZ	1:D:433:ASN:OD1	2.44	0.51
1:C:170:LEU:HD11	1:C:230:VAL:HG21	1.93	0.51
1:A:139:LYS:HD3	1:A:140:ARG:HG2	1.93	0.50
1:C:262:ARG:NH1	1:C:283:ASN:O	2.43	0.50
2:C:501:HEM:HBD1	4:C:503:W69:C13	2.41	0.50
1:A:242:ARG:HH12	1:A:476:GLN:CD	2.15	0.50
1:B:336:VAL:HG21	4:B:503:W69:C13	2.42	0.50
1:B:321:GLU:OE2	5:B:504:BTB:O3	2.29	0.49
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.27	0.49
1:A:144:GLN:CG	1:A:145:ALA:H	2.24	0.49
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.93	0.49
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.95	0.49
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.48	0.49
1:B:364:THR:O	1:B:368:CYS:HB2	2.13	0.49
1:A:364:THR:O	1:A:368:CYS:HB2	2.13	0.48
1:B:124:LEU:HD13	1:B:128:ARG:HH21	1.78	0.48
2:C:501:HEM:HBD1	4:C:503:W69:F13	2.03	0.48
1:B:290:PRO:HG2	1:B:302:LEU:HD11	1.95	0.48
1:B:173:GLY:HA3	1:B:343:ILE:HD13	1.95	0.48
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.95	0.48
1:C:428:MET:HG3	1:C:458:PRO:HB2	1.94	0.48
1:D:68:PHE:CD2	1:D:83:THR:HA	2.49	0.48
1:C:234:ARG:HB2	1:C:238:ARG:CZ	2.44	0.48
1:C:91:ASP:OD1	10:C:602:HOH:O	2.20	0.48
1:A:242:ARG:NH1	1:A:476:GLN:OE1	2.34	0.47
1:C:224:LEU:HD12	1:C:416:THR:HB	1.95	0.47
1:D:229:THR:O	1:D:351:ALA:HA	2.14	0.47
5:C:505:BTB:H31	5:C:505:BTB:O6	2.14	0.47
1:A:122:GLN:O	1:A:125:SER:OG	2.29	0.47
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.96	0.47
1:D:271:THR:O	1:D:275:ILE:HG12	2.14	0.47
5:D:505:BTB:H42	5:D:505:BTB:H71	1.57	0.47
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.50	0.47
1:C:90:GLN:HB2	1:C:468:PHE:CD2	2.51	0.46
5:C:505:BTB:H72	5:C:505:BTB:H62	1.53	0.46
1:A:257:GLN:H	1:A:257:GLN:CD	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:O	1:A:160:THR:OG1	2.33	0.46
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.98	0.45
1:A:336:VAL:HG21	4:A:503:W69:C13	2.47	0.45
1:A:97:ARG:HG2	1:B:88:ALA:HB3	1.99	0.45
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.98	0.45
1:C:429:LYS:HA	1:C:429:LYS:HD2	1.85	0.45
1:C:397:LYS:HG3	1:D:400:VAL:HG11	1.98	0.45
1:A:269:GLU:O	1:A:272:GLU:HB3	2.17	0.45
1:B:298:GLU:OE1	5:B:505:BTB:H41	2.17	0.45
5:B:505:BTB:O4	5:B:505:BTB:H71	2.16	0.45
1:A:201:CYS:C	1:A:202:ARG:HH11	2.20	0.45
1:A:224:LEU:HB2	1:A:416:THR:HB	1.99	0.45
1:D:280:THR:HA	1:D:281:PRO:HD3	1.85	0.45
1:A:242:ARG:HH21	1:A:478:ASP:HA	1.82	0.44
1:A:455:SER:HA	1:A:460:PHE:CG	2.52	0.44
1:A:244:TRP:CZ2	1:A:300:PRO:HG3	2.52	0.44
1:A:377:GLU:OE1	5:A:505:BTB:O1	2.26	0.44
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.80	0.44
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.99	0.44
1:B:436:LYS:HE2	1:B:436:LYS:HB3	1.77	0.44
5:C:504:BTB:H71	5:C:504:BTB:H42	1.82	0.44
5:D:505:BTB:H61	5:D:505:BTB:H72	1.42	0.44
1:A:298:GLU:HG3	1:A:299:PRO:HD2	2.00	0.43
5:A:504:BTB:H52	5:A:504:BTB:H31	1.73	0.43
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.53	0.43
1:B:140:ARG:HA	1:B:140:ARG:HD3	1.89	0.43
1:A:102:SER:O	3:A:502:H4B:O10	2.27	0.43
1:D:479:PRO:HD2	1:D:480:TRP:CZ3	2.54	0.43
5:D:504:BTB:H71	5:D:504:BTB:H42	1.77	0.43
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.36	0.43
1:A:346:LEU:HA	1:A:346:LEU:HD23	1.89	0.43
1:A:68:PHE:CD2	1:A:83:THR:HA	2.54	0.43
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.54	0.43
2:B:501:HEM:CGA	3:B:502:H4B:HN3	2.32	0.42
1:C:203:SER:OG	1:C:204:ALA:N	2.52	0.42
1:D:364:THR:O	1:D:368:CYS:HB2	2.19	0.42
1:A:90:GLN:H	1:A:90:GLN:HG2	1.55	0.42
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.54	0.42
1:C:148:GLN:OE1	1:C:166:ARG:NH2	2.53	0.42
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.55	0.42
1:A:256:GLN:HB2	1:A:257:GLN:H	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.93	0.42
1:D:369:ASP:HA	1:D:370:PRO:HD3	1.88	0.42
1:D:379:VAL:HG21	1:D:402:ILE:HD11	2.01	0.42
1:A:463:GLU:HB3	1:B:103:LEU:HD12	2.01	0.42
1:D:200:ASP:O	1:D:202:ARG:HG2	2.20	0.42
1:A:183:ARG:HB2	2:A:501:HEM:HAD2	2.02	0.41
1:B:149:ARG:HD3	1:B:166:ARG:CZ	2.50	0.41
1:B:279:TRP:CZ3	1:B:281:PRO:HA	2.55	0.41
5:C:505:BTB:H71	5:C:505:BTB:H12	1.80	0.41
1:C:298:GLU:OE1	5:C:506:BTB:H81	2.19	0.41
1:A:144:GLN:CG	1:A:145:ALA:N	2.84	0.41
1:A:279:TRP:CD1	1:A:290:PRO:HG3	2.55	0.41
1:C:364:THR:O	1:C:368:CYS:HB2	2.19	0.41
1:A:331:TYR:O	1:A:410:TYR:OH	2.36	0.41
1:B:70:ARG:HE	1:B:79:ILE:HD13	1.86	0.41
5:A:504:BTB:O3	5:A:504:BTB:O4	2.18	0.41
5:C:504:BTB:O4	5:C:504:BTB:O8	2.32	0.41
1:B:106:PRO:HB3	10:B:627:HOH:O	2.21	0.41
1:C:272:GLU:O	1:C:276:GLN:HG3	2.20	0.41
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.56	0.41
1:A:201:CYS:HB2	1:A:206:GLU:HG2	2.03	0.41
1:A:229:THR:O	1:A:352:PRO:HD2	2.21	0.41
1:A:384:ASP:OD1	5:A:504:BTB:O4	2.30	0.41
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.89	0.41
1:A:134:TYR:O	1:A:137:SER:OG	2.25	0.41
1:A:201:CYS:HB2	1:A:210:TYR:CE2	2.56	0.41
1:D:387:THR:HA	1:D:394:TRP:CD1	2.56	0.41
1:D:455:SER:HA	1:D:460:PHE:CG	2.56	0.41
1:A:321:GLU:H	1:A:321:GLU:CD	2.25	0.40
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.56	0.40
1:A:296:PRO:O	1:A:298:GLU:N	2.53	0.40
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.96	0.40
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.50	0.40
1:C:455:SER:HA	1:C:460:PHE:CG	2.57	0.40
1:C:453:SER:HB3	1:C:456:LEU:HD12	2.04	0.40
5:B:505:BTB:H52	5:B:505:BTB:H32	1.74	0.40
1:A:94:CYS:HB3	1:B:94:CYS:HB3	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	402/440 (91%)	372 (92%)	26 (6%)	4 (1%)	15	6
1	B	401/440 (91%)	394 (98%)	7 (2%)	0	100	100
1	C	399/440 (91%)	378 (95%)	21 (5%)	0	100	100
1	D	401/440 (91%)	395 (98%)	6 (2%)	0	100	100
All	All	1603/1760 (91%)	1539 (96%)	60 (4%)	4 (0%)	41	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	283	ASN
1	A	238	ARG
1	A	281	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	345/373 (92%)	334 (97%)	11 (3%)	39	29
1	B	344/373 (92%)	334 (97%)	10 (3%)	42	33
1	C	342/373 (92%)	334 (98%)	8 (2%)	50	43
1	D	344/373 (92%)	340 (99%)	4 (1%)	71	69
All	All	1375/1492 (92%)	1342 (98%)	33 (2%)	50	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	109	LEU
1	A	121	GLU
1	A	133	GLN
1	A	140	ARG
1	A	201	CYS
1	A	238	ARG
1	A	257	GLN
1	A	258	ASP
1	A	298	GLU
1	A	329	ARG
1	B	67	LYS
1	B	90	GLN
1	B	122	GLN
1	B	148	GLN
1	B	168[A]	SER
1	B	168[B]	SER
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	260	SER
1	B	389	THR
1	C	151	GLN
1	C	160	THR
1	C	192	LYS
1	C	200	ASP
1	C	216	LYS
1	C	234	ARG
1	C	240	ASP
1	C	302	LEU
1	D	71	VAL
1	D	89	GLN
1	D	98	ARG
1	D	258	ASP

Some 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 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$
5	BTB	B	505	-	13,13,13	0.40	0	7,16,16	0.78	0
5	BTB	B	504	9	13,13,13	0.50	0	7,16,16	0.41	0
3	H4B	A	502	-	16,18,18	0.98	0	11,26,26	2.69	6 (54%)
2	HEM	C	501	1	27,50,50	2.18	6 (22%)	17,82,82	1.60	4 (23%)
4	W69	A	503	-	24,24,24	0.46	0	32,32,32	1.42	4 (12%)
5	BTB	D	505	-	13,13,13	0.48	0	7,16,16	0.74	0
2	HEM	B	501	1	27,50,50	2.12	6 (22%)	17,82,82	1.61	3 (17%)
2	HEM	D	501	1	27,50,50	2.13	6 (22%)	17,82,82	1.94	5 (29%)
5	BTB	C	504	9	13,13,13	0.36	0	7,16,16	0.61	0
5	BTB	C	506	-	13,13,13	0.37	0	7,16,16	0.36	0
5	BTB	D	504	9	13,13,13	0.39	0	7,16,16	0.60	0
5	BTB	C	505	-	13,13,13	0.65	0	7,16,16	1.02	1 (14%)
5	BTB	A	505	-	13,13,13	0.44	0	7,16,16	0.61	0
7	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.39	0
3	H4B	C	502	-	16,18,18	0.89	0	11,26,26	2.67	6 (54%)
4	W69	B	503	-	24,24,24	0.60	0	32,32,32	1.66	6 (18%)
4	W69	C	503	-	24,24,24	0.45	0	32,32,32	1.61	4 (12%)
5	BTB	A	504	9	13,13,13	0.38	0	7,16,16	0.46	0
3	H4B	D	502	-	16,18,18	0.82	0	11,26,26	2.65	6 (54%)
4	W69	D	503	-	24,24,24	0.60	0	32,32,32	1.52	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	B	502	-	16,18,18	0.94	0	11,26,26	2.77	5 (45%)
7	GOL	C	508	-	5,5,5	0.40	0	5,5,5	0.43	0
2	HEM	A	501	1	27,50,50	2.17	6 (22%)	17,82,82	1.34	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
5	BTB	B	505	-	-	2/21/21/21	-
5	BTB	B	504	9	-	1/21/21/21	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	4/6/54/54	-
4	W69	A	503	-	-	3/11/11/11	0/2/2/2
5	BTB	D	505	-	-	8/21/21/21	-
2	HEM	B	501	1	-	2/6/54/54	-
2	HEM	D	501	1	-	3/6/54/54	-
5	BTB	C	504	9	-	1/21/21/21	-
5	BTB	C	506	-	-	8/21/21/21	-
5	BTB	D	504	9	-	5/21/21/21	-
5	BTB	C	505	-	-	5/21/21/21	-
5	BTB	A	505	-	-	7/21/21/21	-
7	GOL	A	507	-	-	4/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	W69	B	503	-	-	3/11/11/11	0/2/2/2
4	W69	C	503	-	-	5/11/11/11	0/2/2/2
5	BTB	A	504	9	-	9/21/21/21	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
4	W69	D	503	-	-	6/11/11/11	0/2/2/2
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
7	GOL	C	508	-	-	4/4/4/4	-
2	HEM	A	501	1	-	5/6/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	5.44	1.53	1.37
2	C	501	HEM	C3D-C2D	5.43	1.53	1.37
2	D	501	HEM	C3D-C2D	5.22	1.53	1.37
2	B	501	HEM	C3D-C2D	5.14	1.52	1.37
2	B	501	HEM	C3B-C2B	-4.69	1.33	1.40
2	C	501	HEM	C3B-C2B	-4.34	1.34	1.40
2	A	501	HEM	C3B-C2B	-4.34	1.34	1.40
2	D	501	HEM	C3B-C2B	-4.15	1.34	1.40
2	C	501	HEM	C3B-CAB	4.04	1.56	1.47
2	B	501	HEM	C3C-CAC	4.00	1.56	1.47
2	D	501	HEM	C3C-C2C	-3.93	1.34	1.40
2	C	501	HEM	C3C-CAC	3.88	1.55	1.47
2	A	501	HEM	C3C-CAC	3.83	1.55	1.47
2	D	501	HEM	C3B-CAB	3.83	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.82	1.35	1.40
2	A	501	HEM	C3B-CAB	3.81	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.78	1.35	1.40
2	B	501	HEM	C3B-CAB	3.69	1.55	1.47
2	D	501	HEM	C3C-CAC	3.66	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.30	1.35	1.40
2	C	501	HEM	CAA-C2A	2.60	1.55	1.52
2	D	501	HEM	CAA-C2A	2.54	1.55	1.52
2	A	501	HEM	CAA-C2A	2.34	1.55	1.52
2	B	501	HEM	CAA-C2A	2.29	1.55	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	W69	C02-N01-C06	5.85	122.54	118.10
3	A	502	H4B	C4-C4A-C8A	5.72	119.65	114.57
3	C	502	H4B	C4-C4A-C8A	5.36	119.33	114.57
3	B	502	H4B	C4-C4A-C8A	5.18	119.17	114.57
4	B	503	W69	C02-N01-C06	5.14	121.99	118.10
3	D	502	H4B	C4-C4A-C8A	5.00	119.01	114.57
4	A	503	W69	C02-N01-C06	4.82	121.76	118.10
4	D	503	W69	C02-N01-C06	4.35	121.40	118.10
2	B	501	HEM	CMA-C3A-C4A	-3.93	122.42	128.46
2	D	501	HEM	CMA-C3A-C4A	-3.80	122.63	128.46
3	B	502	H4B	N3-C2-N1	-3.74	119.56	125.42
3	D	502	H4B	C4-C4A-N5	3.64	122.17	119.12
2	D	501	HEM	C1D-C2D-C3D	-3.53	104.54	107.00
3	B	502	H4B	C4-N3-C2	3.40	121.33	115.93
4	C	503	W69	C05-C06-N01	-3.37	119.33	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	N3-C2-N1	-3.34	120.18	125.42
4	D	503	W69	C08-C09-C11	-3.30	101.69	113.28
3	D	502	H4B	N3-C2-N1	-3.24	120.33	125.42
3	D	502	H4B	C4-N3-C2	3.18	120.98	115.93
3	C	502	H4B	N3-C2-N1	-3.18	120.44	125.42
3	C	502	H4B	C4-N3-C2	3.07	120.80	115.93
3	A	502	H4B	C4-N3-C2	3.02	120.73	115.93
3	B	502	H4B	C4-C4A-N5	2.99	121.63	119.12
2	D	501	HEM	C4A-C3A-C2A	2.99	109.08	107.00
4	B	503	W69	C14-C13-C12	-2.97	119.77	123.52
4	A	503	W69	C05-C06-N01	-2.95	119.77	122.90
3	B	502	H4B	C2-N1-C8A	2.94	121.14	114.54
2	D	501	HEM	CMC-C2C-C3C	2.91	130.13	124.68
2	C	501	HEM	CAD-CBD-CGD	-2.87	107.86	112.67
2	D	501	HEM	CBD-CAD-C3D	-2.87	107.19	112.48
3	C	502	H4B	C4-C4A-N5	2.84	121.50	119.12
3	A	502	H4B	C2-N1-C8A	2.83	120.87	114.54
4	B	503	W69	C08-C06-N01	2.81	120.13	115.95
4	A	503	W69	C14-C13-C12	-2.79	119.99	123.52
4	D	503	W69	C14-C13-C12	-2.75	120.04	123.52
3	C	502	H4B	C2-N1-C8A	2.75	120.70	114.54
2	A	501	HEM	C4A-C3A-C2A	2.73	108.90	107.00
3	D	502	H4B	C2-N1-C8A	2.70	120.60	114.54
4	C	503	W69	C14-C13-C12	-2.70	120.11	123.52
2	B	501	HEM	CMA-C3A-C2A	2.64	129.92	124.94
4	D	503	W69	C09-C08-C06	-2.58	107.21	112.99
4	B	503	W69	C05-C06-N01	-2.52	120.23	122.90
2	C	501	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
3	C	502	H4B	N2-C2-N3	2.52	121.17	117.25
3	A	502	H4B	C4-C4A-N5	2.51	121.23	119.12
4	D	503	W69	C04-C05-C06	-2.51	118.68	120.32
2	C	501	HEM	CMA-C3A-C4A	-2.47	124.67	128.46
4	C	503	W69	C08-C06-N01	2.37	119.49	115.95
4	B	503	W69	C08-C09-C11	-2.36	105.00	113.28
2	C	501	HEM	C4A-C3A-C2A	2.26	108.57	107.00
2	B	501	HEM	CMC-C2C-C3C	2.23	128.85	124.68
3	A	502	H4B	N2-C2-N3	2.20	120.67	117.25
4	D	503	W69	F13-C13-C14	2.18	121.36	118.25
5	C	505	BTB	O1-C1-C2	-2.11	105.66	111.44
4	A	503	W69	C08-C06-N01	2.08	119.05	115.95
2	A	501	HEM	CMA-C3A-C4A	-2.01	125.37	128.46
4	B	503	W69	F13-C13-C14	2.00	121.11	118.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	N2-C2-N3	2.00	120.36	117.25

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C2A-CAA-CBA-CGA
4	A	503	W69	C06-C08-C09-C11
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
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	C6-C5-N-C7
2	B	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C2A-CAA-CBA-CGA
5	C	506	BTB	C4-C2-C3-O3
5	C	506	BTB	C1-C2-C4-O4
5	C	506	BTB	C3-C2-C4-O4
5	C	506	BTB	N-C2-C4-O4
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	N-C7-C8-O8
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	505	BTB	C6-C5-N-C7
5	A	505	BTB	C1-C2-C3-O3
5	A	505	BTB	C4-C2-C3-O3
5	A	505	BTB	N-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
7	A	507	GOL	O1-C1-C2-C3
7	A	507	GOL	C1-C2-C3-O3
4	B	503	W69	C06-C08-C09-C11
4	C	503	W69	C15-C17-C18-C19
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	N-C2-C3-O3
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
4	D	503	W69	C06-C08-C09-C11
7	C	508	GOL	O1-C1-C2-C3
7	C	508	GOL	C1-C2-C3-O3
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C2D-C3D-CAD-CBD
2	A	501	HEM	C4D-C3D-CAD-CBD
5	C	506	BTB	N-C7-C8-O8
4	A	503	W69	C18-C19-N20-C22
4	D	503	W69	C18-C19-N20-C22
4	C	503	W69	C17-C18-C19-N20
7	A	507	GOL	O2-C2-C3-O3
7	C	508	GOL	O1-C1-C2-O2
5	C	505	BTB	N-C5-C6-O6
4	B	503	W69	C15-C17-C18-C19
4	A	503	W69	C18-C19-N20-C21
4	D	503	W69	C18-C19-N20-C21
5	B	505	BTB	N-C5-C6-O6
7	A	507	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C5-C6-O6
4	D	503	W69	C15-C17-C18-C19
5	D	505	BTB	N-C7-C8-O8
4	B	503	W69	C18-C19-N20-C21
4	C	503	W69	C06-C08-C09-C11
4	C	503	W69	C18-C19-N20-C22
7	C	508	GOL	O2-C2-C3-O3
3	A	502	H4B	N5-C6-C9-O9
5	C	506	BTB	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	C4-C2-C3-O3
5	B	504	BTB	O1-C1-C2-N
5	C	506	BTB	N-C2-C3-O3
5	C	506	BTB	N-C5-C6-O6
5	B	505	BTB	N-C7-C8-O8
4	D	503	W69	C14-C15-C17-C18
4	D	503	W69	C16-C15-C17-C18
5	D	504	BTB	N-C5-C6-O6
2	C	501	HEM	C3D-CAD-CBD-CGD
4	C	503	W69	C18-C19-N20-C21
3	D	502	H4B	N5-C6-C9-O9
5	C	504	BTB	O1-C1-C2-C4

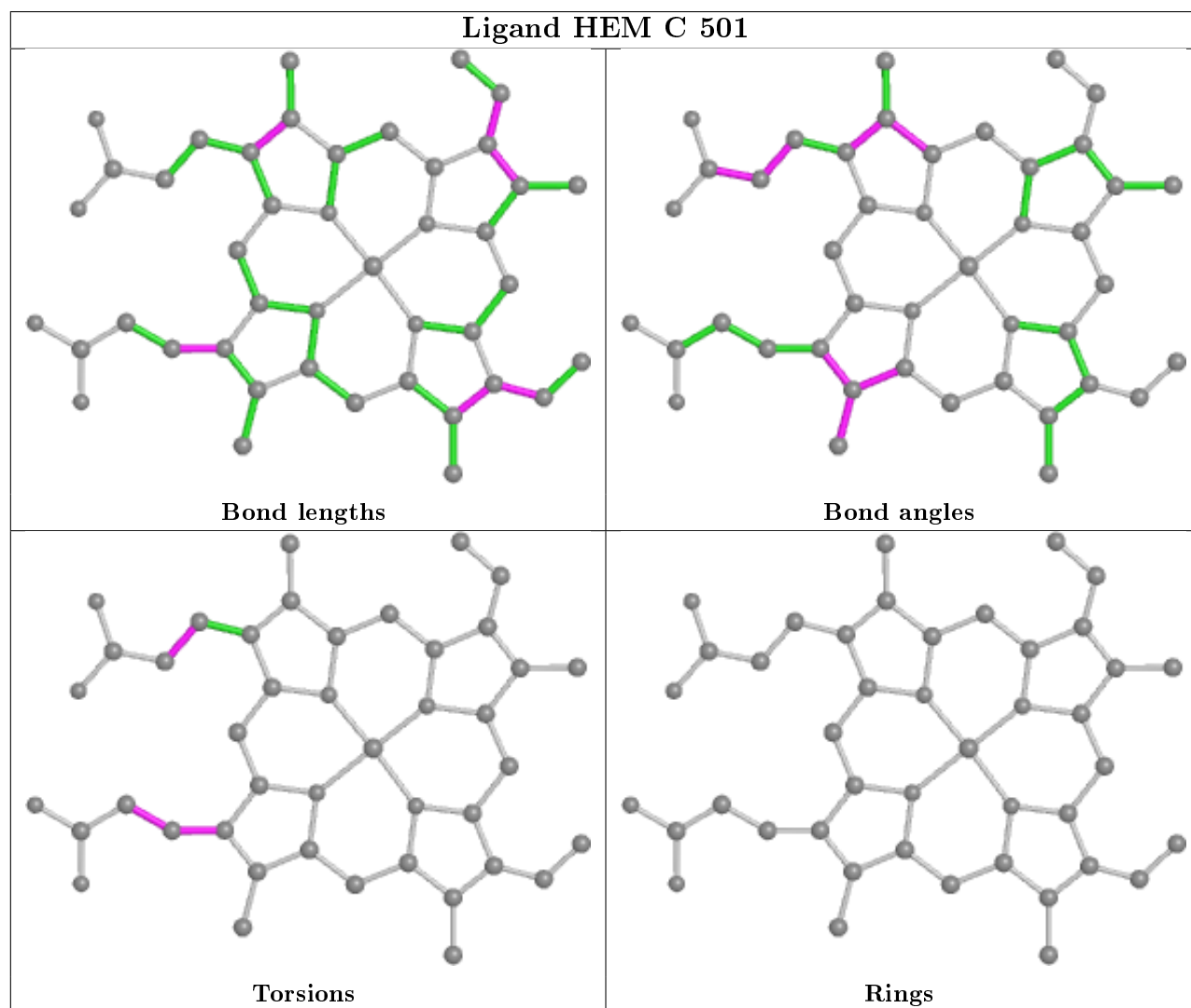
There are no ring outliers.

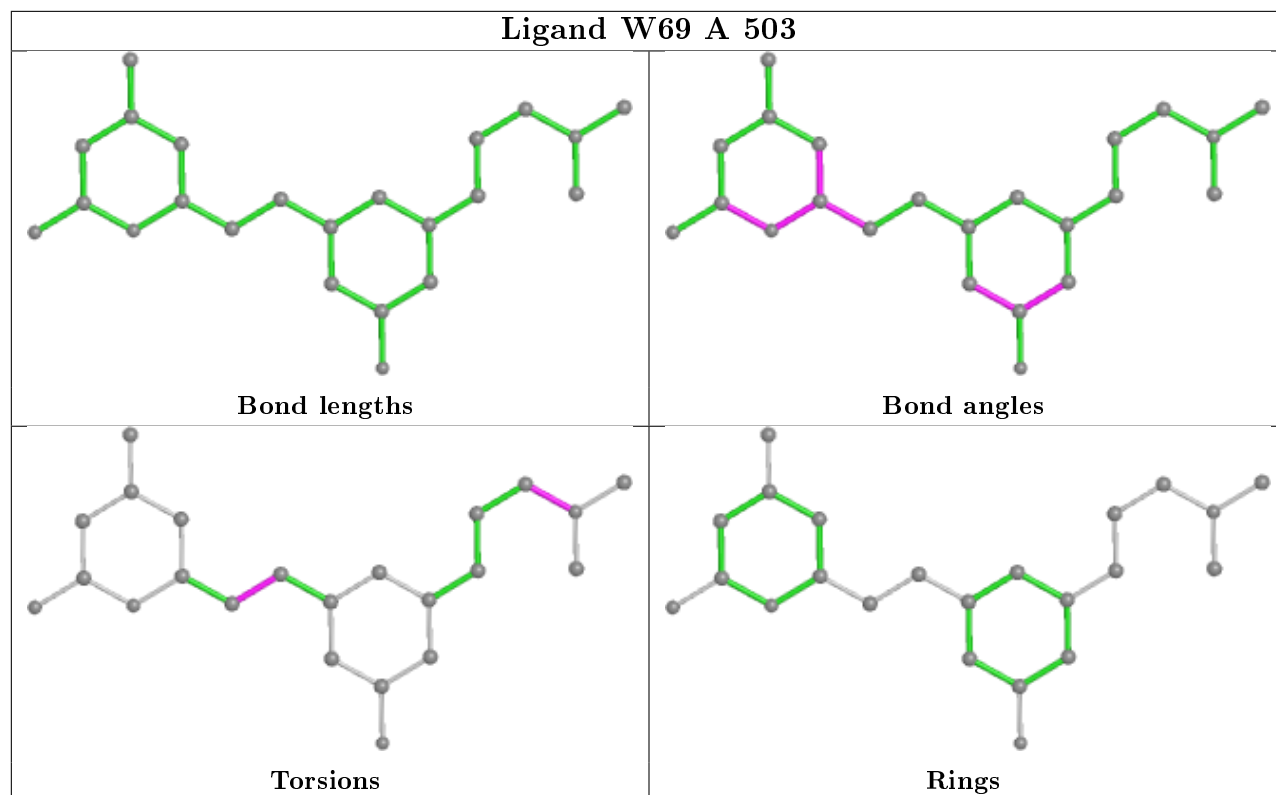
22 monomers are involved in 48 short contacts:

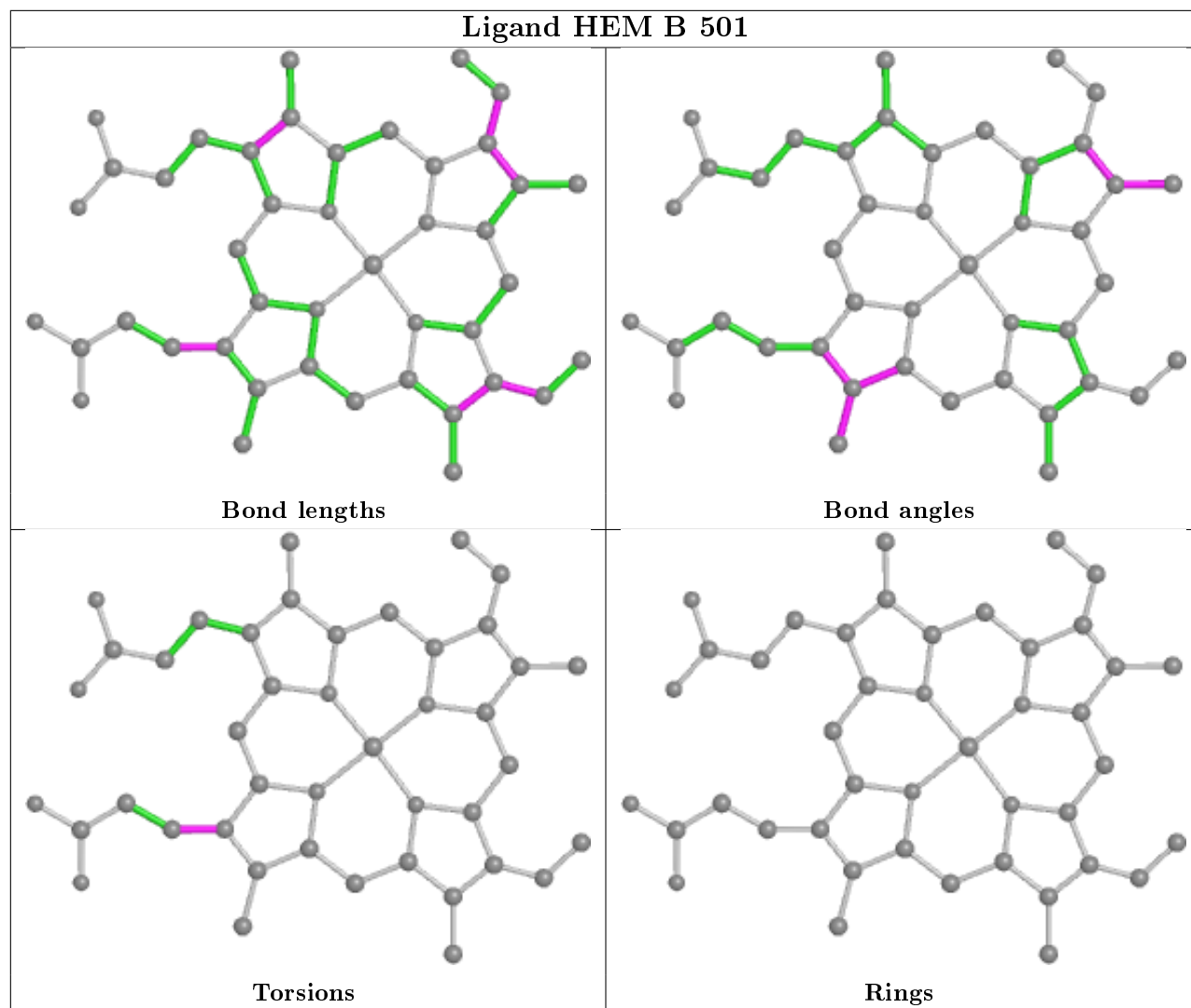
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	BTB	4	0
5	B	504	BTB	1	0
3	A	502	H4B	2	0
2	C	501	HEM	5	0
4	A	503	W69	2	0
5	D	505	BTB	2	0
2	B	501	HEM	4	0
2	D	501	HEM	3	0
5	C	504	BTB	2	0
5	C	506	BTB	1	0
5	D	504	BTB	3	0
5	C	505	BTB	3	0
5	A	505	BTB	2	0
7	A	507	GOL	1	0
3	C	502	H4B	1	0
4	B	503	W69	3	0
4	C	503	W69	3	0
5	A	504	BTB	4	0
4	D	503	W69	2	0
3	B	502	H4B	1	0
7	C	508	GOL	1	0
2	A	501	HEM	5	0

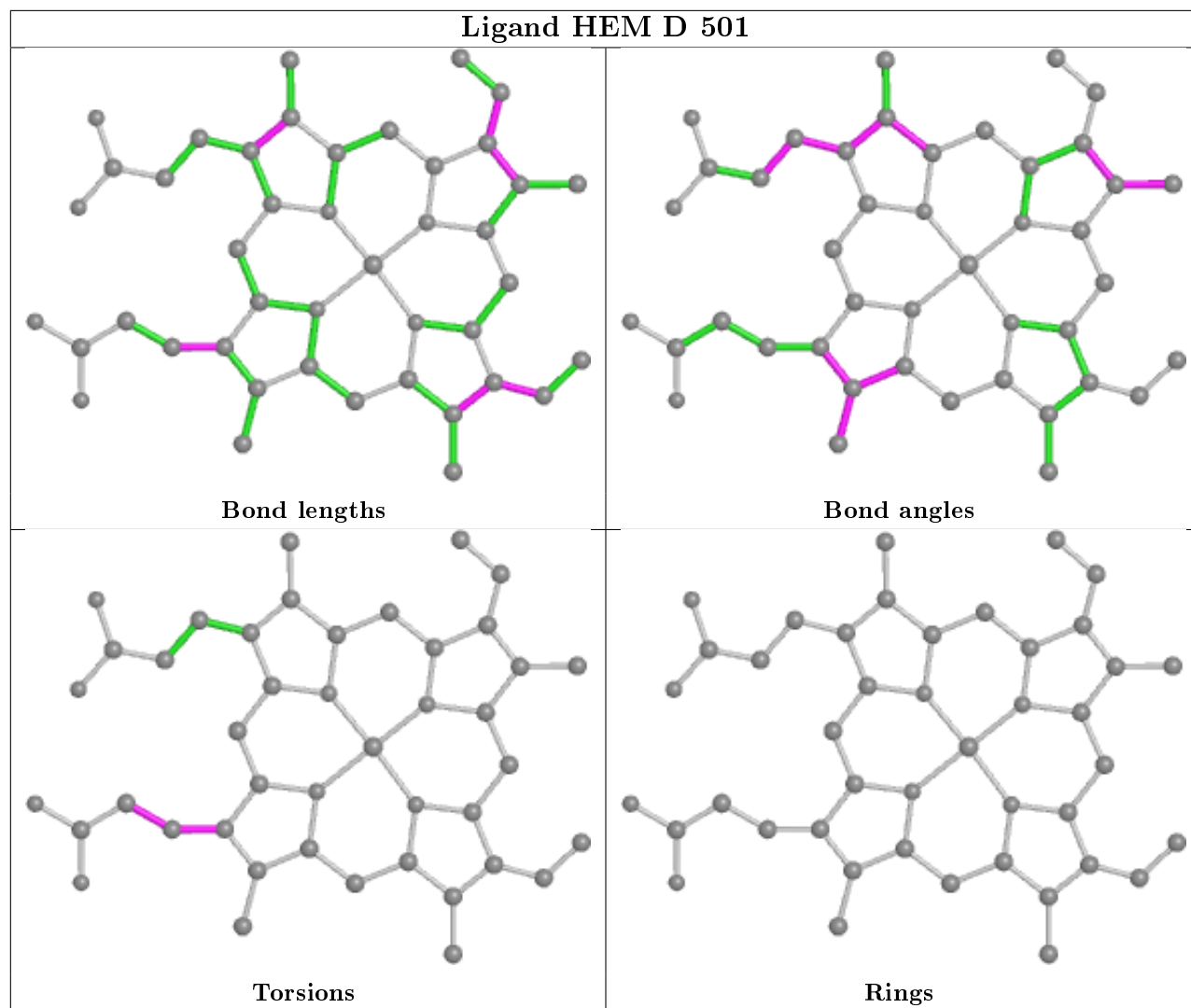
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

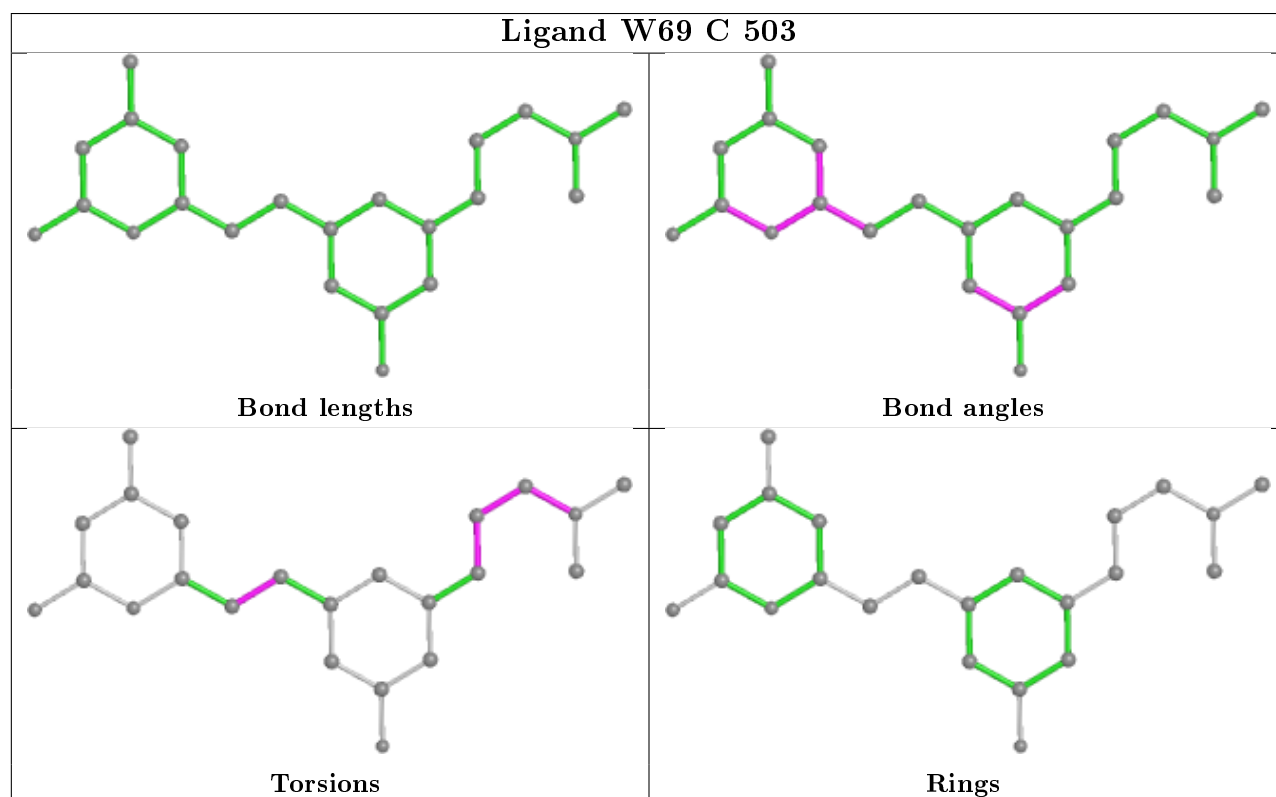
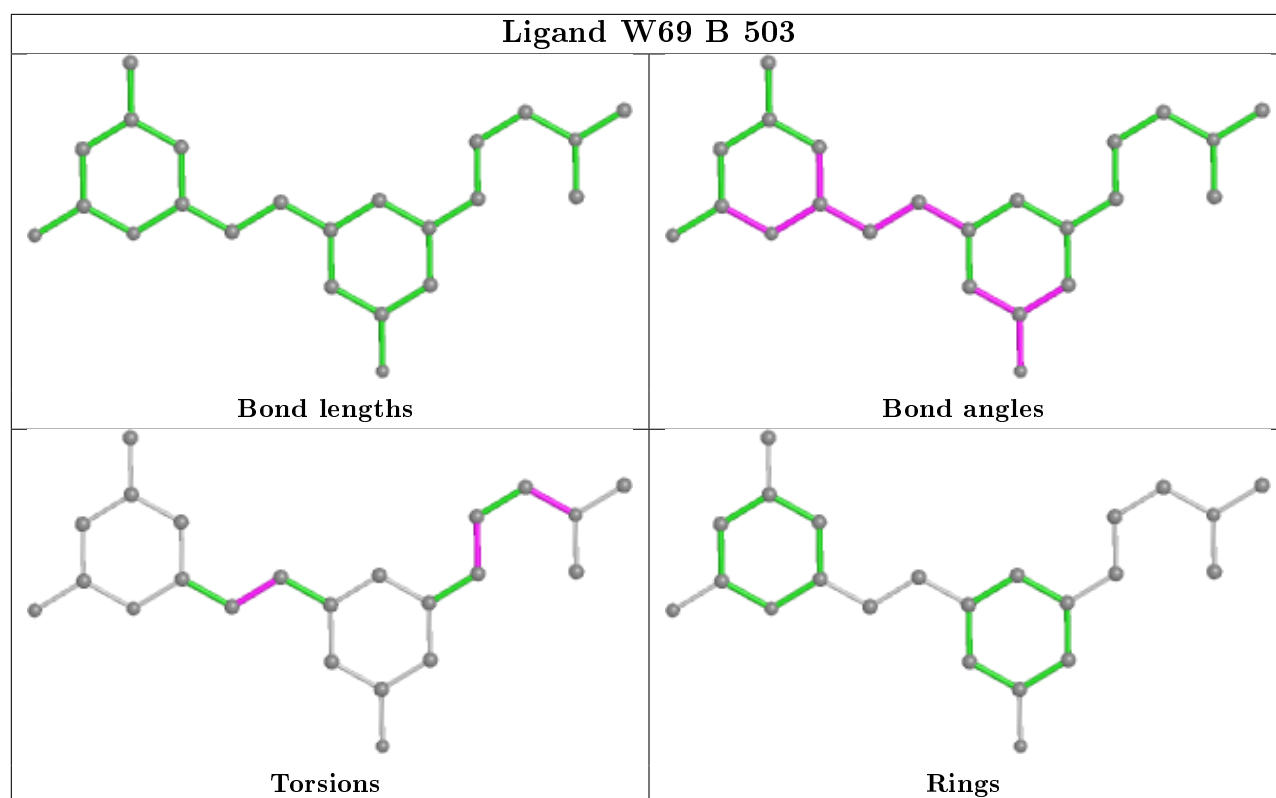
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

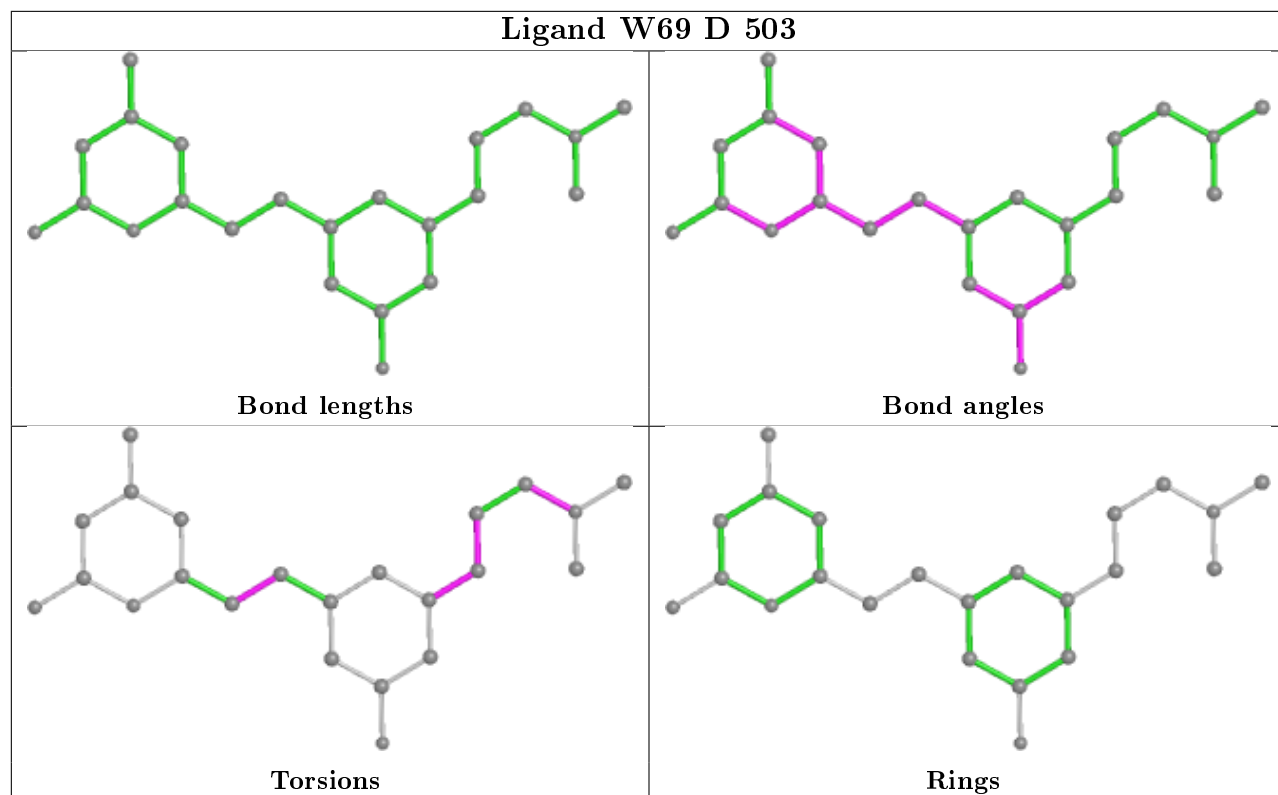


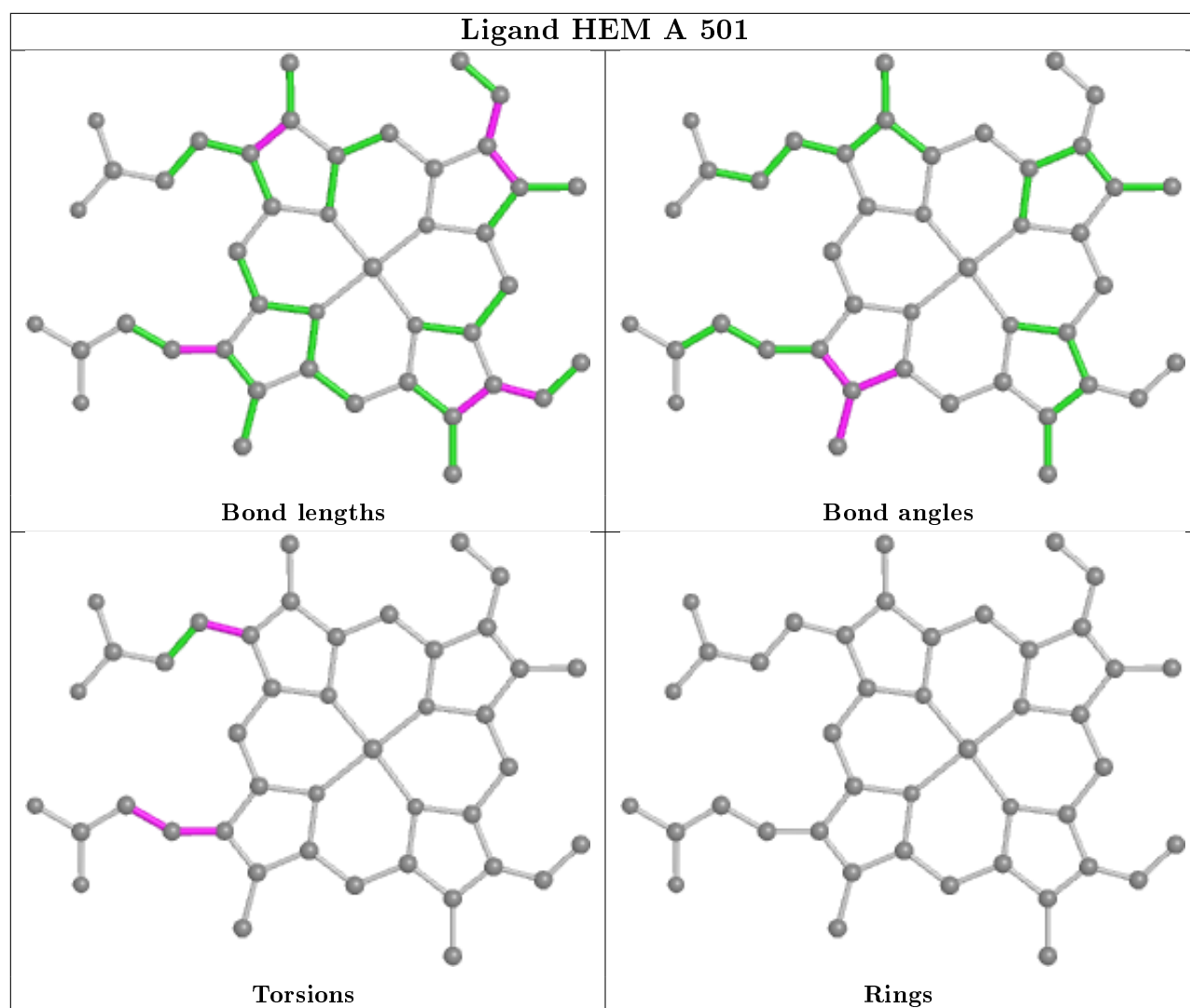












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	1.66	129 (31%) 0 0	37, 75, 139, 169	0
1	B	402/440 (91%)	0.66	43 (10%) 6 7	32, 51, 93, 141	0
1	C	401/440 (91%)	1.17	90 (22%) 0 0	38, 66, 112, 156	0
1	D	402/440 (91%)	0.53	42 (10%) 6 7	31, 51, 85, 138	0
All	All	1609/1760 (91%)	1.00	304 (18%) 1 1	31, 59, 117, 169	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	9.6
1	A	153	VAL	8.3
1	A	107	ARG	7.9
1	A	244	TRP	7.8
1	A	480	TRP	7.4
1	A	119	ALA	7.1
1	A	259	GLY	6.7
1	A	204	ALA	6.2
1	A	447	TRP	6.1
1	A	293	LEU	6.0
1	C	480	TRP	5.9
1	C	275	ILE	5.9
1	A	141	SER	5.9
1	A	144	GLN	5.8
1	A	280	THR	5.7
1	A	279	TRP	5.7
1	A	304	LEU	5.7
1	A	448	ILE	5.7
1	C	448	ILE	5.6
1	B	257	GLN	5.6
1	A	300	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	67	LYS	5.6
1	C	452	ILE	5.5
1	A	235	CYS	5.5
1	A	88	ALA	5.4
1	C	238	ARG	5.4
1	A	86	ALA	5.3
1	C	304	LEU	5.3
1	A	452	ILE	5.3
1	A	108	LYS	5.3
1	A	89	GLN	5.3
1	B	460	PHE	5.2
1	A	303	PHE	5.1
1	D	257	GLN	5.1
1	C	68	PHE	5.1
1	B	452	ILE	5.1
1	A	120	PRO	5.0
1	C	447	TRP	4.9
1	C	299	PRO	4.9
1	A	446	ALA	4.9
1	A	275	ILE	4.8
1	D	255	ARG	4.8
1	C	446	ALA	4.7
1	A	142	GLY	4.7
1	A	122	GLN	4.7
1	A	302	LEU	4.6
1	A	274	CYS	4.6
1	A	129	ASP	4.5
1	B	79	ILE	4.5
1	A	451	PRO	4.5
1	A	301	GLU	4.5
1	C	451	PRO	4.5
1	B	89	GLN	4.4
1	D	89	GLN	4.4
1	A	140	ARG	4.3
1	A	145	ALA	4.3
1	B	259	GLY	4.3
1	A	309	LEU	4.3
1	C	445	TRP	4.2
1	A	184	CYS	4.2
1	C	303	PHE	4.2
1	A	256	GLN	4.2
1	A	257	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	79	ILE	4.2
1	C	89	GLN	4.2
1	A	255	ARG	4.2
1	C	449	VAL	4.1
1	A	445	TRP	4.1
1	A	237	GLY	4.0
1	B	449	VAL	4.0
1	D	449	VAL	4.0
1	B	68	PHE	4.0
1	A	254	TYR	3.9
1	A	281	PRO	3.9
1	A	272	GLU	3.9
1	C	184	CYS	3.9
1	D	452	ILE	3.9
1	D	68	PHE	3.9
1	D	446	ALA	3.9
1	A	236	PRO	3.9
1	B	388	ARG	3.9
1	A	479	PRO	3.9
1	C	86	ALA	3.9
1	A	273	LEU	3.9
1	D	67	LYS	3.9
1	A	450	PRO	3.9
1	A	305	LEU	3.8
1	A	299	PRO	3.8
1	A	346	LEU	3.8
1	C	185	VAL	3.8
1	A	353	PHE	3.8
1	A	136	SER	3.8
1	A	360	THR	3.8
1	B	446	ALA	3.7
1	B	454	GLY	3.7
1	A	449	VAL	3.7
1	A	364	THR	3.7
1	B	157	VAL	3.7
1	B	158	ALA	3.7
1	C	236	PRO	3.7
1	A	162	THR	3.7
1	C	258	ASP	3.7
1	C	292	LEU	3.7
1	A	185	VAL	3.7
1	A	295	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	297	ASP	3.6
1	D	258	ASP	3.6
1	B	124	LEU	3.6
1	C	280	THR	3.6
1	D	259	GLY	3.6
1	C	244	TRP	3.6
1	C	257	GLN	3.6
1	D	460	PHE	3.5
1	A	128	ARG	3.5
1	B	119	ALA	3.5
1	C	301	GLU	3.5
1	D	456	LEU	3.5
1	D	79	ILE	3.4
1	C	360	THR	3.4
1	A	308	GLU	3.4
1	C	122	GLN	3.4
1	A	163	TYR	3.4
1	A	183	ARG	3.3
1	A	150	LEU	3.3
1	A	444	ASP	3.3
1	A	268	VAL	3.3
1	B	97	ARG	3.3
1	C	81	TYR	3.3
1	D	260	SER	3.3
1	C	300	PRO	3.3
1	A	412	LEU	3.3
1	C	119	ALA	3.3
1	B	450	PRO	3.3
1	C	140	ARG	3.2
1	D	454	GLY	3.2
1	C	450	PRO	3.2
1	B	70	ARG	3.2
1	A	146	HIS	3.2
1	A	297	ASP	3.2
1	D	121	GLU	3.2
1	B	260	SER	3.2
1	B	120	PRO	3.1
1	A	365	ARG	3.1
1	A	336	VAL	3.1
1	C	204	ALA	3.1
1	A	258	ASP	3.1
1	C	454	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	PHE	3.1
1	A	130	PHE	3.1
1	C	364	THR	3.1
1	C	293	LEU	3.1
1	A	134	TYR	3.1
1	C	307	PRO	3.0
1	B	76	VAL	3.0
1	C	302	LEU	3.0
1	B	142	GLY	3.0
1	C	142	GLY	3.0
1	C	239	GLY	3.0
1	B	153	VAL	3.0
1	B	453	SER	3.0
1	C	306	PRO	3.0
1	B	445	TRP	3.0
1	C	439	GLY	3.0
1	C	460	PHE	2.9
1	B	451	PRO	2.9
1	D	256	GLN	2.9
1	C	259	GLY	2.9
1	B	258	ASP	2.9
1	C	444	ASP	2.9
1	D	388	ARG	2.9
1	A	83	THR	2.9
1	D	70	ARG	2.9
1	C	273	LEU	2.9
1	C	237	GLY	2.9
1	C	183	ARG	2.9
1	C	80	THR	2.8
1	D	451	PRO	2.8
1	D	445	TRP	2.8
1	A	87	GLN	2.8
1	A	151	GLN	2.8
1	C	294	GLN	2.8
1	A	307	PRO	2.8
1	A	121	GLU	2.8
1	D	448	ILE	2.8
1	C	141	SER	2.8
1	A	276	GLN	2.8
1	A	306	PRO	2.7
1	C	437	ALA	2.7
1	A	292	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	309	LEU	2.7
1	B	141[A]	SER	2.7
1	C	221	ARG	2.7
1	A	79	ILE	2.7
1	A	294	GLN	2.7
1	A	241	PHE	2.7
1	A	478	ASP	2.6
1	A	84	LEU	2.6
1	C	106	PRO	2.6
1	A	359	SER	2.6
1	C	336	VAL	2.6
1	B	360	THR	2.6
1	C	276	GLN	2.6
1	B	154	GLU	2.6
1	C	368	CYS	2.6
1	D	362	ILE	2.6
1	D	455	SER	2.6
1	C	272	GLU	2.6
1	D	453	SER	2.6
1	A	106	PRO	2.6
1	D	106	PRO	2.6
1	B	362	ILE	2.6
1	C	162	THR	2.6
1	C	412	LEU	2.5
1	A	160	THR	2.5
1	C	153	VAL	2.5
1	C	208	PHE	2.5
1	B	81	TYR	2.5
1	A	343	ILE	2.5
1	D	450	PRO	2.5
1	D	360	THR	2.5
1	D	389	THR	2.5
1	A	260	SER	2.5
1	A	133	GLN	2.5
1	D	357	TYR	2.5
1	A	368	CYS	2.5
1	C	365	ARG	2.5
1	A	205	GLN	2.4
1	A	139	LYS	2.4
1	D	447	TRP	2.4
1	C	388	ARG	2.4
1	D	123	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	122	GLN	2.4
1	A	345	GLY	2.4
1	C	362	ILE	2.4
1	A	90	GLN	2.4
1	B	357	TYR	2.4
1	A	439	GLY	2.4
1	C	295	ALA	2.4
1	A	125	SER	2.4
1	A	143	SER	2.4
1	D	457	THR	2.4
1	A	123	LEU	2.4
1	B	86	ALA	2.4
1	A	221	ARG	2.4
1	A	285	ARG	2.4
1	D	364	THR	2.4
1	D	261	VAL	2.4
1	A	127	ALA	2.3
1	D	358	MET	2.3
1	C	124	LEU	2.3
1	A	182	PRO	2.3
1	A	298	GLU	2.3
1	C	87	GLN	2.3
1	A	253	GLY	2.3
1	B	358	MET	2.3
1	C	298	GLU	2.3
1	A	443	ALA	2.3
1	B	256	GLN	2.3
1	B	364	THR	2.3
1	C	367	LEU	2.3
1	A	460	PHE	2.2
1	B	83	THR	2.2
1	C	308	GLU	2.2
1	B	448	ILE	2.2
1	D	279	TRP	2.2
1	C	456	LEU	2.2
1	A	135	TYR	2.2
1	A	334	PRO	2.2
1	A	358	MET	2.2
1	C	182	PRO	2.2
1	A	277	HIS	2.2
1	A	402	ILE	2.2
1	A	206	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	120	PRO	2.2
1	A	97	ARG	2.2
1	A	474	ARG	2.2
1	C	135	TYR	2.2
1	D	365	ARG	2.2
1	C	256	GLN	2.2
1	C	268	VAL	2.2
1	A	362	ILE	2.1
1	C	353	PHE	2.1
1	C	279	TRP	2.1
1	D	97	ARG	2.1
1	A	138	ILE	2.1
1	D	158	ALA	2.1
1	B	420	HIS	2.1
1	A	208	PHE	2.1
1	A	473	PHE	2.1
1	A	261	VAL	2.1
1	A	159	ALA	2.1
1	C	254	TYR	2.1
1	D	254	TYR	2.1
1	C	207	MET	2.1
1	C	402	ILE	2.1
1	C	457	THR	2.0
1	C	129	ASP	2.0
1	C	255	ARG	2.0
1	C	278	GLY	2.0
1	B	455	SER	2.0
1	A	69	PRO	2.0
1	A	335	ALA	2.0
1	D	399	ALA	2.0
1	C	235	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

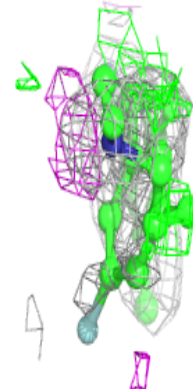
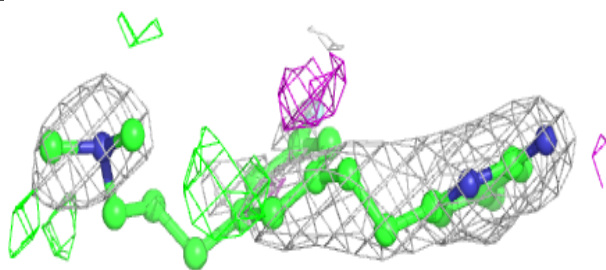
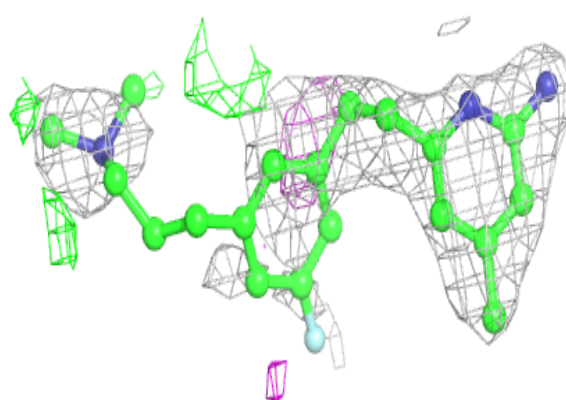
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	H4B	C	502	17/17	0.74	0.32	73,86,103,104	0
3	H4B	A	502	17/17	0.75	0.35	74,86,103,103	0
5	BTB	C	506	14/14	0.78	0.13	88,97,103,109	0
5	BTB	D	504	14/14	0.82	0.17	54,74,87,88	0
5	BTB	B	504	14/14	0.82	0.17	44,68,90,98	0
3	H4B	D	502	17/17	0.82	0.27	59,76,91,91	0
3	H4B	B	502	17/17	0.82	0.25	51,78,100,102	0
4	W69	C	503	23/23	0.84	0.41	47,91,126,128	0
5	BTB	C	505	14/14	0.85	0.18	59,76,90,99	0
4	W69	A	503	23/23	0.88	0.45	56,104,133,134	0
5	BTB	D	505	14/14	0.89	0.20	70,85,93,100	0
5	BTB	B	505	14/14	0.91	0.23	42,74,89,95	0
9	GD	A	509	1/1	0.91	0.05	131,131,131,131	0
7	GOL	A	507	6/6	0.92	0.23	59,83,102,111	0
5	BTB	A	505	14/14	0.92	0.12	64,80,89,91	0
4	W69	D	503	23/23	0.92	0.23	30,78,111,112	0
4	W69	B	503	23/23	0.92	0.22	33,71,101,101	0
5	BTB	C	504	14/14	0.93	0.25	35,85,109,114	0
7	GOL	C	508	6/6	0.93	0.21	50,77,81,86	0
9	GD	C	510	1/1	0.93	0.05	106,106,106,106	0
2	HEM	A	501	43/43	0.94	0.25	53,70,98,110	0
2	HEM	C	501	43/43	0.95	0.21	37,55,86,110	0
2	HEM	D	501	43/43	0.95	0.14	30,41,85,102	0
8	CL	A	508	1/1	0.95	0.22	63,63,63,63	0
5	BTB	A	504	14/14	0.95	0.28	52,91,102,115	0
8	CL	C	509	1/1	0.95	0.20	56,56,56,56	0
2	HEM	B	501	43/43	0.96	0.15	33,41,94,97	0
8	CL	D	507	1/1	0.97	0.10	45,45,45,45	0
6	ZN	A	506	1/1	0.98	0.08	53,53,53,53	0
9	GD	D	506	1/1	0.98	0.12	54,54,54,54	0
9	GD	B	507	1/1	0.98	0.14	54,54,54,54	0
8	CL	B	506	1/1	0.99	0.14	44,44,44,44	0
6	ZN	C	507	1/1	1.00	0.10	46,46,46,46	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.

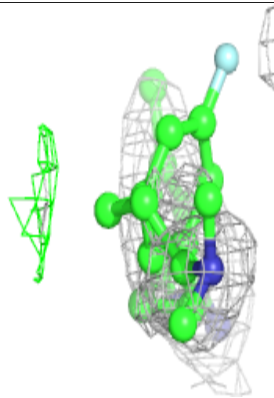
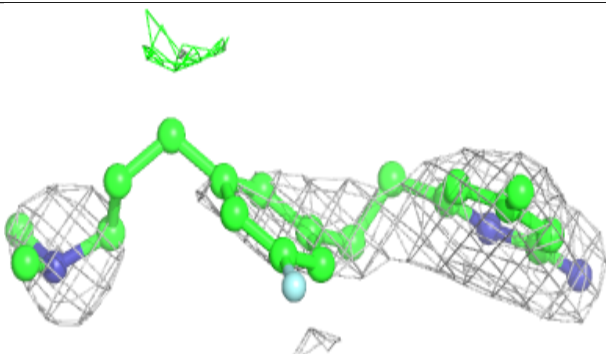
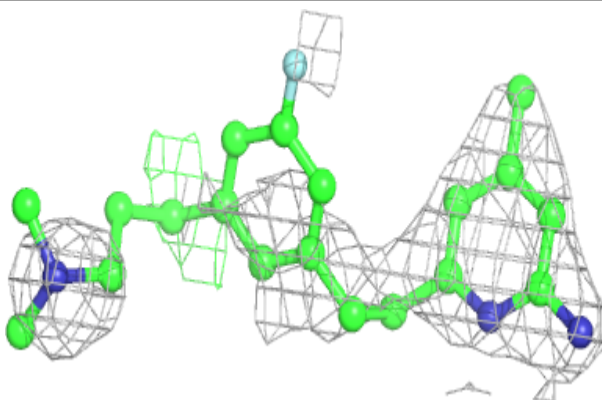
Electron density around W69 C 503:

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



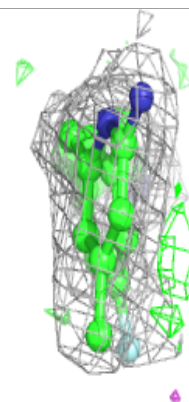
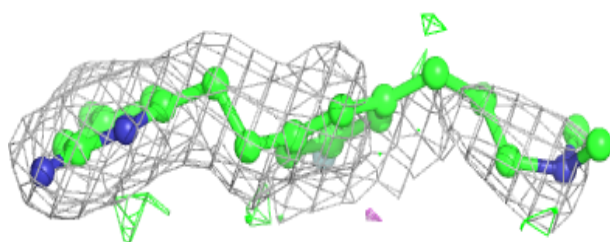
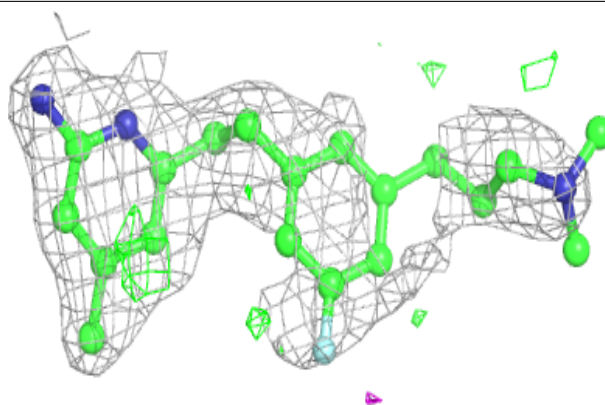
Electron density around W69 A 503:

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

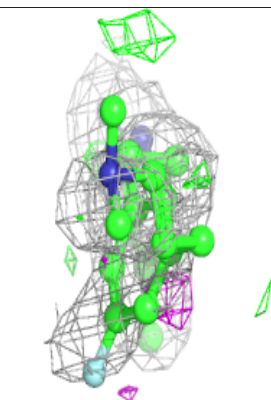
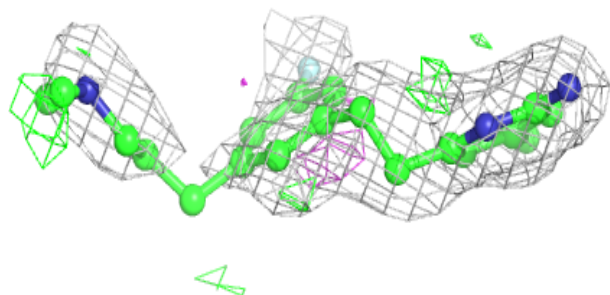
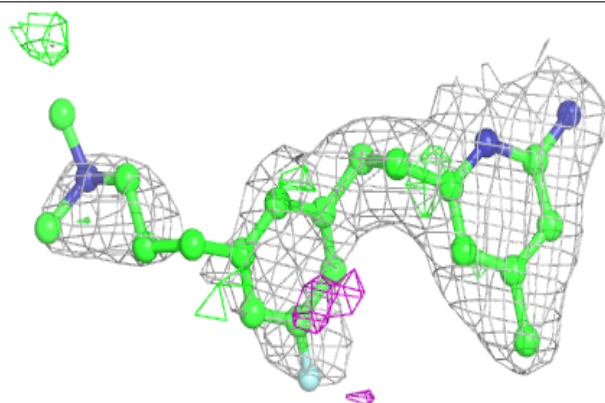


Electron density around W69 D 503:

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

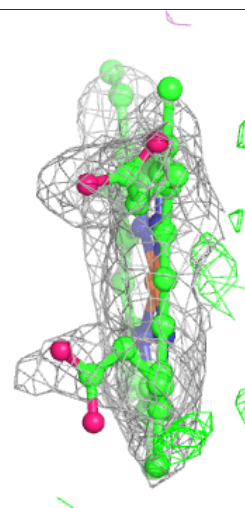
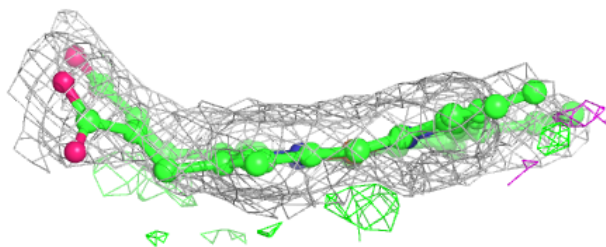
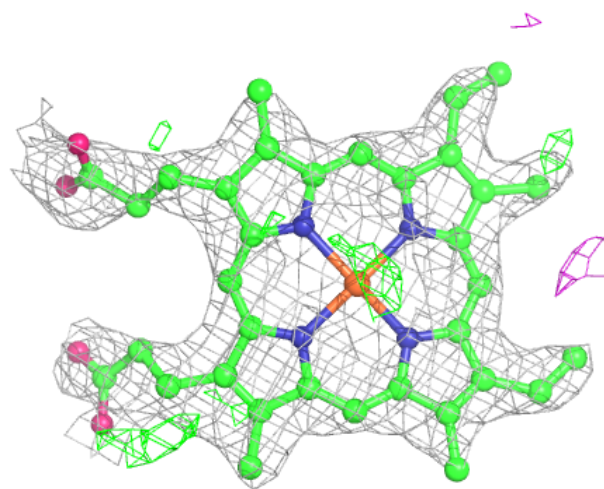
**Electron density around W69 B 503:**

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



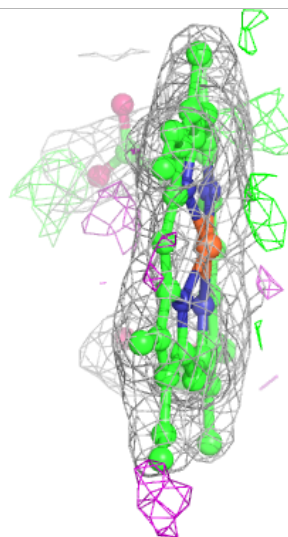
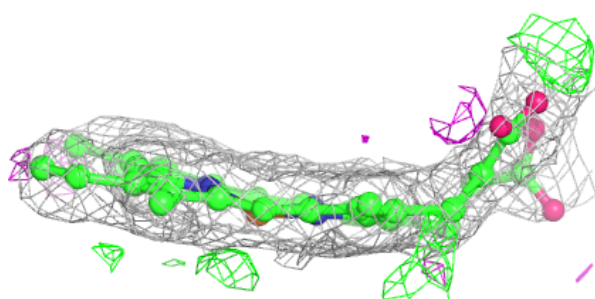
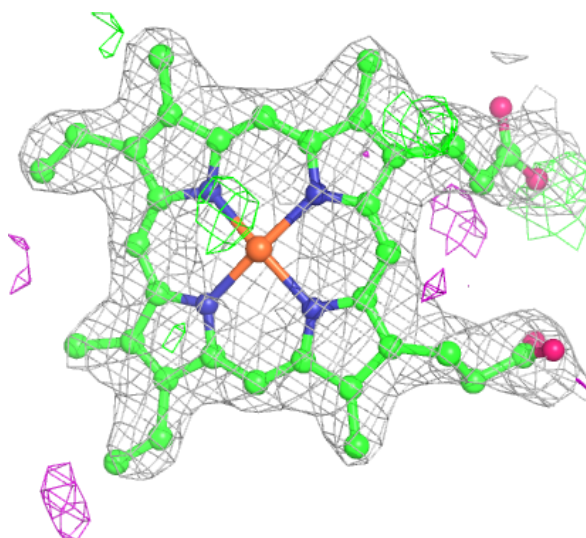
Electron density around HEM A 501:

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



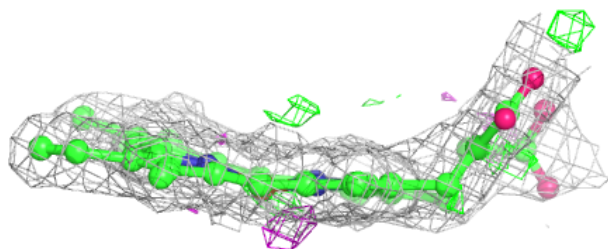
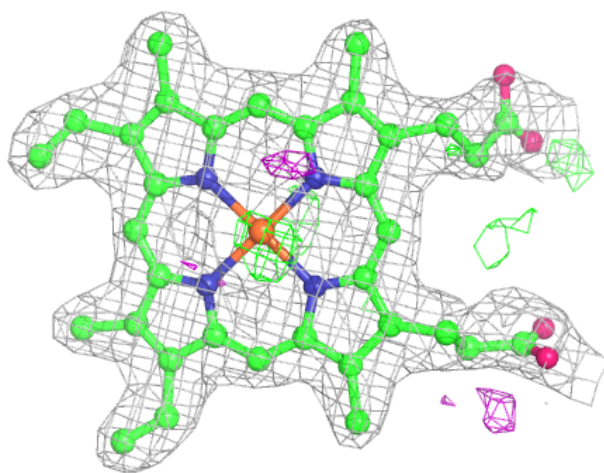
Electron density around HEM C 501:

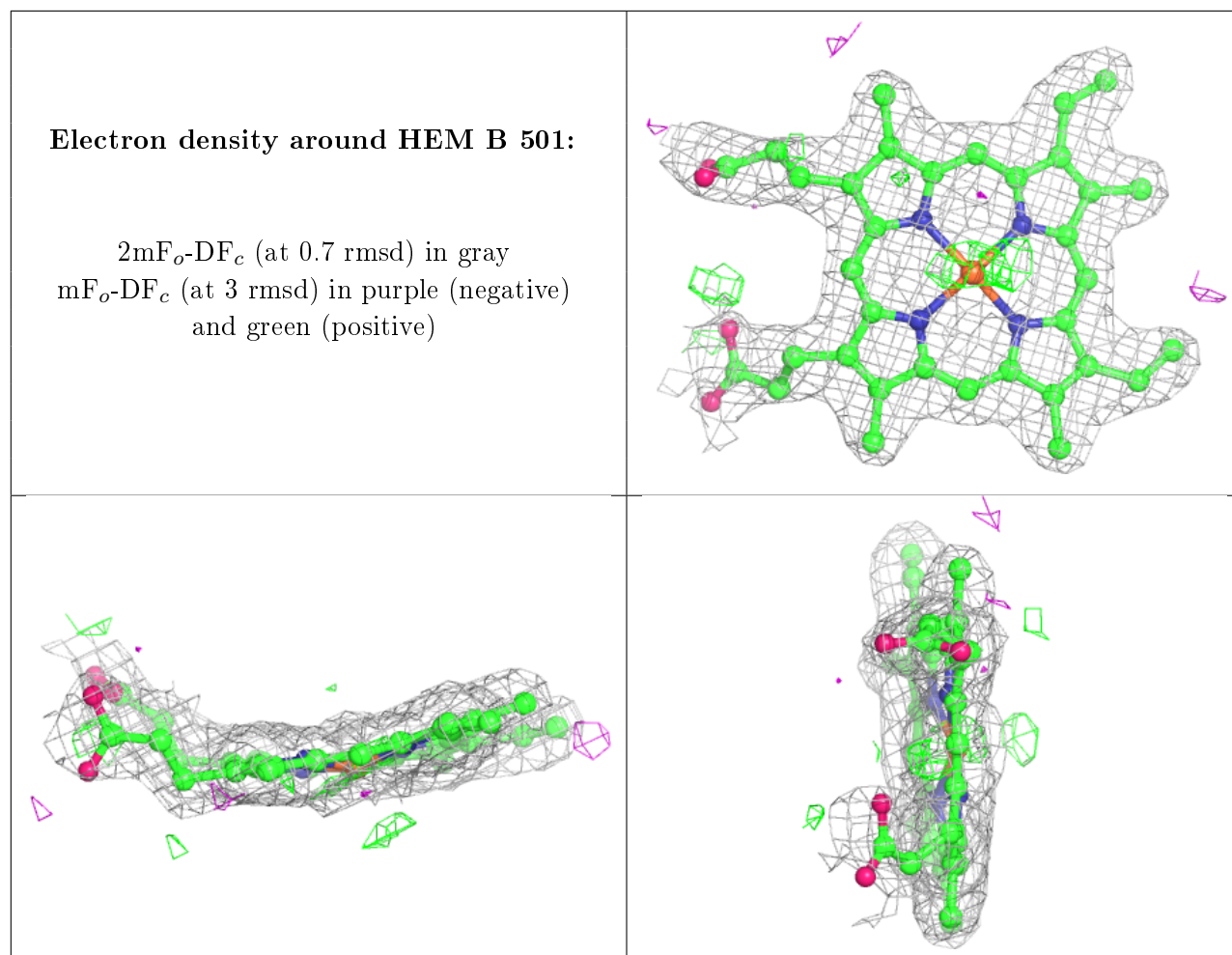
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.