



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:58 AM UTC

PDB ID : 6PP2 / pdb\_00006pp2  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 4-((4-(2-Amino-4-methylquinolin-7-yl)-2-(aminomethyl)phenoxy)methyl)benzotrile  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : 2019-07-05  
Resolution : 2.02 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](mailto: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>.

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

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

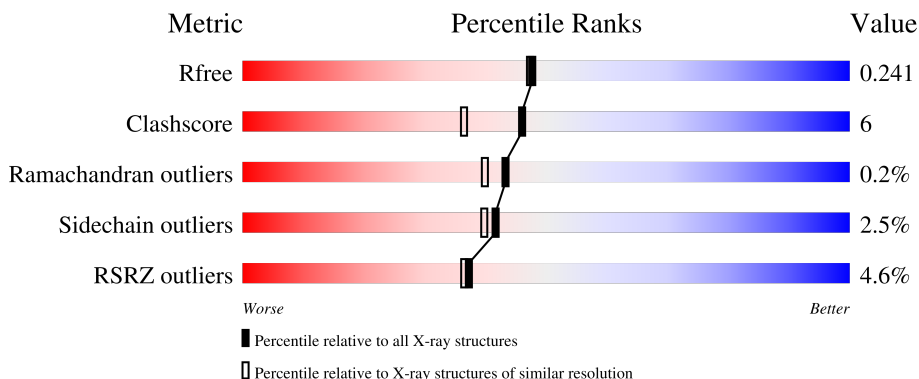
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


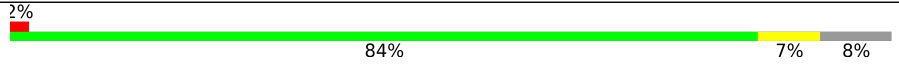
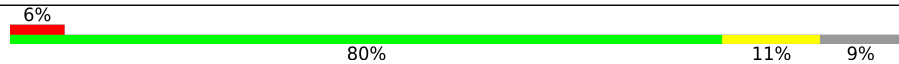

The reported resolution of this entry is 2.02 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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  $\geq 3$ , 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	 7% 79% 12% 8%
1	B	440	 2% 84% 7% 8%
1	C	440	 6% 80% 11% 9%
1	D	440	 2% 82% 9% 9%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	BTB	D	505	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14200 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
			Total	C	N	O	S			
1	A	404	3237	2062	570	589	16	0	2	0
1	B	403	3232	2057	570	588	17	0	3	0
1	C	401	3209	2044	563	586	16	0	2	0
1	D	402	3221	2051	566	587	17	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

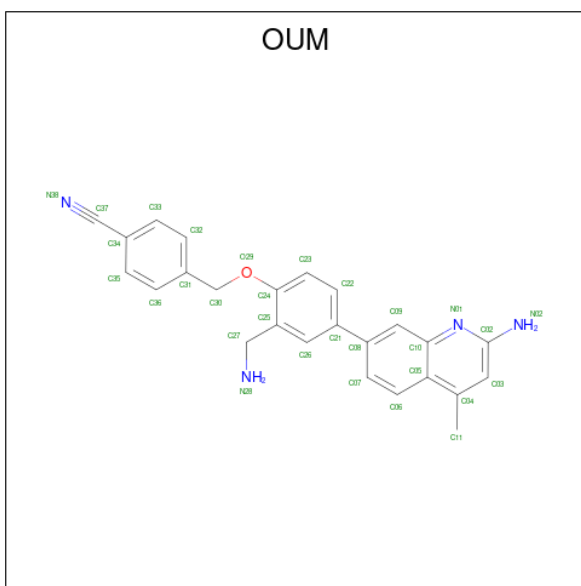
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



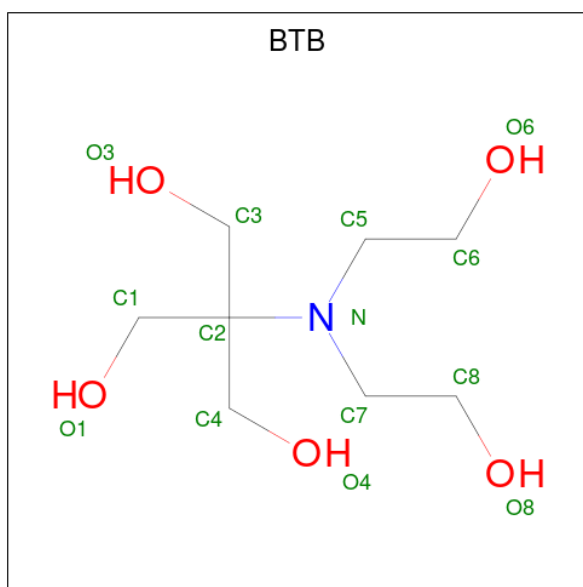
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-{{2-(aminomethyl)-4-(2-amino-4-methylquinolin-7-yl)phenoxy}methyl}benzotrile (CCD ID: OUM) (formula: C<sub>25</sub>H<sub>22</sub>N<sub>4</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	25	4	1		
4	B	1	Total	C	N	O	0	0
			30	25	4	1		
4	C	1	Total	C	N	O	0	0
			30	25	4	1		
4	D	1	Total	C	N	O	0	0
			30	25	4	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

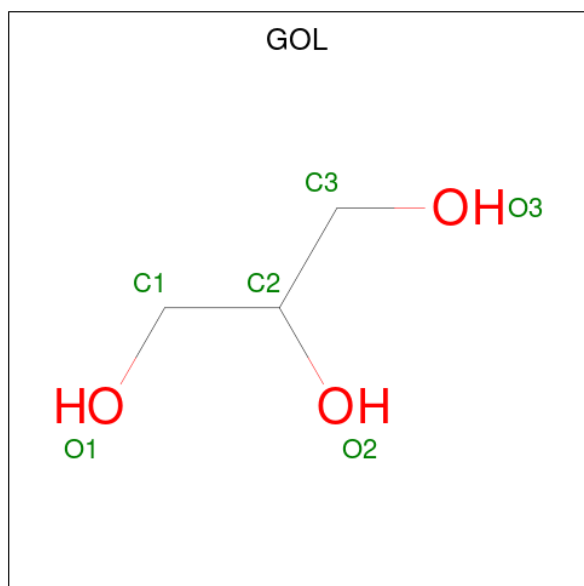
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	Total 1	Zn 1	0	0

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

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

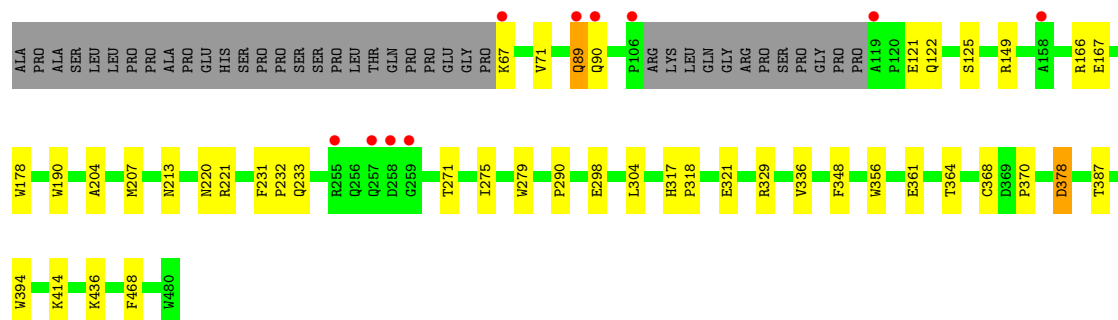
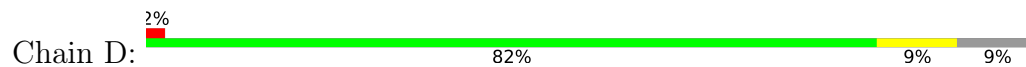
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	143	Total	O	0	0
			143	143		
10	B	239	Total	O	0	0
			239	239		
10	C	148	Total	O	0	0
			148	148		
10	D	237	Total	O	0	0
			237	237		





- Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.54Å 154.89Å 109.18Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	89.23 – 2.02 89.23 – 2.02	Depositor EDS
% Data completeness (in resolution range)	94.5 (89.23-2.02) 98.0 (89.23-2.02)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.02Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.199 , 0.246 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	6515 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtrriage
Anisotropy	0.649	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, CL, H4B, HEM, OUM, GD, ZN, GOL

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	0.32	0/3335	0.50	0/4543
1	B	0.39	0/3330	0.54	0/4537
1	C	0.32	0/3307	0.51	0/4507
1	D	0.41	0/3319	0.53	0/4523
All	All	0.36	0/13291	0.52	0/18110

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	238	ARG	Peptide
1	D	89	GLN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	33	1
1	B	3232	0	3139	22	0
1	C	3209	0	3109	35	0
1	D	3221	0	3126	27	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	9	0
2	D	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
3	C	17	0	15	2	0
3	D	17	0	15	0	0
4	A	30	0	0	4	0
4	B	30	0	0	4	0
4	C	30	0	0	3	0
4	D	30	0	0	3	0
5	A	28	0	38	4	0
5	B	42	0	56	8	0
5	C	42	0	57	3	0
5	D	42	0	56	13	1
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	3	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	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	143	0	0	6	0
10	B	239	0	0	7	1
10	C	148	0	0	6	0
10	D	237	0	0	5	1
All	All	14200	0	12923	153	2

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 (153) 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:B:449:VAL:HG11	10:B:832:HOH:O	1.87	0.74
4:A:503:OUM:N28	10:A:601:HOH:O	2.19	0.73
1:C:475:TYR:OH	2:C:501:HEM:O2D	2.07	0.73
3:C:502:H4B:O4	10:C:601:HOH:O	2.10	0.70
2:C:501:HEM:O1A	4:C:503:OUM:N28	2.25	0.70
1:B:336:VAL:HG21	4:B:503:OUM:C07	2.23	0.69
1:D:67:LYS:N	10:D:603:HOH:O	2.25	0.69
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.77	0.66
1:D:336:VAL:HG21	4:D:503:OUM:C07	2.26	0.66
1:A:361:GLU:OE2	4:A:503:OUM:N02	2.28	0.66
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.79	0.65
1:A:151:GLN:OE1	1:A:151:GLN:N	2.29	0.65
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.80	0.64
1:C:294:GLN:NE2	10:C:606:HOH:O	2.31	0.64
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.79	0.64
1:C:475:TYR:CZ	2:C:501:HEM:O1D	2.52	0.61
1:A:207:MET:HE3	1:A:293:LEU:HB3	1.83	0.60
1:A:275:ILE:HG12	1:A:281:PRO:HG3	1.83	0.60
1:A:298:GLU:HG3	1:A:299:PRO:HD2	1.84	0.60
5:A:504:BTB:O1	5:A:504:BTB:O3	2.09	0.60
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.82	0.59
1:C:235:CYS:H	1:C:238:ARG:HD3	1.66	0.59
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.85	0.59
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.83	0.59
1:A:336:VAL:HG21	4:A:503:OUM:C07	2.33	0.59
1:D:213:ASN:ND2	10:D:604:HOH:O	2.28	0.59
1:C:128:ARG:O	1:C:132:ASN:ND2	2.36	0.58
1:C:336:VAL:HG21	4:C:503:OUM:C07	2.33	0.58
1:A:258:ASP:N	1:A:258:ASP:OD1	2.36	0.58
1:A:388:ARG:NH1	10:A:604:HOH:O	2.37	0.57
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.85	0.57
2:C:501:HEM:HMD2	2:C:501:HEM:HBD2	1.86	0.57
5:A:505:BTB:O3	5:A:505:BTB:O1	2.16	0.56
1:C:160:THR:HG23	1:C:162:THR:H	1.70	0.56
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.41	0.56
1:D:378:ASP:OD2	5:D:506:BTB:H51	2.05	0.56
1:C:475:TYR:OH	2:C:501:HEM:CGD	2.54	0.55
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLN:NE2	10:A:606:HOH:O	2.41	0.54
1:B:257:GLN:HG2	1:B:258:ASP:H	1.71	0.54
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.89	0.54
1:C:347:GLU:OE2	10:C:602:HOH:O	2.18	0.54
1:C:257:GLN:NE2	1:C:257:GLN:O	2.41	0.53
1:C:156:GLU:O	1:C:160:THR:HG22	2.08	0.53
1:C:204:ALA:HA	1:C:207:MET:HE2	1.90	0.53
5:C:504:BTB:O8	5:C:504:BTB:H41	2.08	0.53
1:D:271:THR:O	1:D:275:ILE:HG12	2.08	0.52
1:D:329:ARG:NH2	10:D:602:HOH:O	2.23	0.52
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.90	0.52
1:C:200:ASP:OD1	1:C:200:ASP:N	2.43	0.51
1:D:414:LYS:HG3	10:D:612:HOH:O	2.10	0.51
1:B:474:ARG:HD2	10:B:649:HOH:O	2.11	0.51
1:C:238:ARG:HE	1:C:240:ASP:CG	2.19	0.51
5:B:506:BTB:H81	5:B:506:BTB:H42	1.93	0.50
1:C:147:GLU:O	1:C:151:GLN:HG2	2.11	0.50
1:C:219:THR:HA	1:C:224:LEU:HD23	1.93	0.50
1:C:144:GLN:HA	1:C:147:GLU:HG3	1.94	0.50
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.92	0.50
1:A:342:GLU:OE1	1:A:474:ARG:NH1	2.45	0.50
1:B:298:GLU:OE1	5:B:505:BTB:H61	2.12	0.50
3:B:502:H4B:O4	10:B:601:HOH:O	2.19	0.50
1:A:93:PRO:HG3	1:A:106:PRO:HB3	1.93	0.49
1:B:90:GLN:HB2	1:B:468:PHE:CD2	2.47	0.49
2:C:501:HEM:HBD2	2:C:501:HEM:CMD	2.42	0.49
1:A:71:VAL:HG12	10:A:641:HOH:O	2.13	0.49
1:D:298:GLU:CD	5:D:505:BTB:H41	2.38	0.49
1:C:167:GLU:OE2	7:C:508:GOL:O2	2.27	0.49
1:B:150:LEU:O	1:B:154:GLU:HG2	2.13	0.49
2:C:501:HEM:O2D	4:C:503:OUM:C23	2.61	0.49
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.42	0.49
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.49	0.48
1:A:167:GLU:OE2	7:A:507:GOL:O1	2.21	0.48
1:C:364:THR:O	1:C:368:CYS:HB2	2.14	0.48
2:A:501:HEM:HBD1	4:A:503:OUM:C22	2.43	0.48
1:A:166:ARG:HD2	10:A:669:HOH:O	2.14	0.48
1:A:144:GLN:HG2	1:A:145:ALA:H	1.79	0.48
1:C:361:GLU:HG2	10:C:705:HOH:O	2.14	0.48
1:C:144:GLN:NE2	10:C:607:HOH:O	2.33	0.47
1:D:356:TRP:O	4:D:503:OUM:N02	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:PHE:CD2	10:B:832:HOH:O	2.56	0.47
1:C:298:GLU:OE1	5:C:506:BTB:O6	2.32	0.47
5:D:506:BTB:H51	5:D:506:BTB:H32	1.45	0.47
1:D:298:GLU:OE2	5:D:505:BTB:O6	2.25	0.47
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.49	0.47
1:C:75:GLU:HG3	1:D:370:PRO:HG2	1.97	0.47
1:A:152:GLU:O	1:A:156:GLU:HB2	2.15	0.47
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.51	0.46
1:A:90:GLN:HG3	1:A:468:PHE:CE1	2.50	0.46
4:B:503:OUM:N28	10:B:606:HOH:O	2.36	0.46
5:D:505:BTB:H71	5:D:505:BTB:H11	1.49	0.46
1:C:235:CYS:N	1:C:238:ARG:HD3	2.31	0.45
5:A:504:BTB:H11	5:A:504:BTB:H52	1.53	0.45
1:B:68:PHE:HA	10:B:607:HOH:O	2.16	0.45
5:D:505:BTB:O3	5:D:505:BTB:O1	2.35	0.45
1:A:242:ARG:HD3	1:A:479:PRO:HB3	1.98	0.45
5:B:506:BTB:H61	5:B:506:BTB:H72	1.72	0.45
1:D:122:GLN:OE1	10:D:601:HOH:O	2.21	0.45
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.57	0.45
1:B:93:PRO:HG3	1:B:106:PRO:CB	2.47	0.45
1:A:125:SER:HA	1:A:128:ARG:NE	2.32	0.45
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.32	0.44
2:B:501:HEM:HBA2	4:B:503:OUM:C09	2.48	0.44
1:A:167:GLU:OE2	7:A:507:GOL:O2	2.35	0.44
5:A:504:BTB:H82	5:A:504:BTB:H41	2.00	0.44
1:B:93:PRO:HG3	1:B:106:PRO:HB2	2.00	0.44
5:D:505:BTB:H52	5:D:505:BTB:H81	1.41	0.44
1:A:145:ALA:HA	1:A:148:GLN:HB3	1.99	0.44
5:B:504:BTB:H61	10:B:733:HOH:O	2.17	0.44
5:D:505:BTB:H51	5:D:505:BTB:H32	1.36	0.44
5:D:506:BTB:H72	5:D:506:BTB:H12	1.27	0.44
1:D:204:ALA:O	1:D:207:MET:HB2	2.18	0.43
1:A:364:THR:O	1:A:368:CYS:HB2	2.19	0.43
5:B:506:BTB:O4	5:B:506:BTB:O1	2.32	0.43
1:C:238:ARG:NE	1:C:240:ASP:OD1	2.51	0.43
1:A:125:SER:HA	1:A:128:ARG:HE	1.83	0.43
1:B:257:GLN:HG2	1:B:258:ASP:N	2.34	0.43
1:D:364:THR:O	1:D:368:CYS:HB2	2.18	0.43
1:A:450:PRO:HG2	1:A:457:THR:HG21	2.01	0.43
1:B:298:GLU:OE2	5:B:505:BTB:N	2.52	0.42
1:C:103:LEU:O	10:C:603:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HD2	1:A:216:LYS:HA	1.89	0.42
1:D:279:TRP:CD1	1:D:290:PRO:HG3	2.53	0.42
1:C:141:SER:C	1:C:143:SER:H	2.27	0.42
1:D:361:GLU:OE2	4:D:503:OUM:N02	2.53	0.42
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.55	0.42
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.55	0.42
1:D:387:THR:HA	1:D:394:TRP:CD1	2.55	0.42
5:D:504:BTB:H72	5:D:504:BTB:H12	1.64	0.42
1:A:321:GLU:H	1:A:321:GLU:CD	2.28	0.42
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.37	0.42
1:B:378:ASP:OD1	5:B:506:BTB:H51	2.20	0.42
1:B:214:HIS:CD2	1:B:214:HIS:C	2.98	0.41
1:D:290:PRO:HB3	1:D:304:LEU:CD2	2.50	0.41
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.89	0.41
7:A:507:GOL:O2	10:A:602:HOH:O	2.22	0.41
5:C:504:BTB:H41	5:C:504:BTB:C8	2.50	0.41
1:C:262:ARG:HD3	1:C:283:ASN:O	2.21	0.41
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.56	0.41
1:D:220:ASN:O	1:D:221:ARG:HG2	2.20	0.41
2:B:501:HEM:HBD1	4:B:503:OUM:C22	2.50	0.41
1:C:257:GLN:C	1:C:259:GLY:H	2.29	0.41
1:C:449:VAL:HA	1:C:450:PRO:HD3	1.93	0.41
1:D:231:PHE:HB3	1:D:232:PRO:CD	2.51	0.41
1:B:261:VAL:HG11	1:B:265:PRO:HA	2.03	0.41
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.34	0.41
1:A:214:HIS:C	1:A:214:HIS:CD2	2.99	0.41
1:C:358:MET:HE3	1:C:360:THR:OG1	2.21	0.41
5:D:504:BTB:H62	5:D:504:BTB:O8	2.21	0.40
1:A:86:ALA:O	1:B:97:ARG:NH2	2.54	0.40
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.56	0.40
5:D:504:BTB:H51	5:D:504:BTB:H32	1.59	0.40
1:A:144:GLN:HG2	1:A:145:ALA:N	2.36	0.40
1:B:122:GLN:CD	1:B:122:GLN:N	2.80	0.40

All (2) 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:B:620:HOH:O	10:D:661:HOH:O[1_456]	2.17	0.03
1:A:152:GLU:OE2	5:D:505:BTB:O4[2_851]	2.19	0.01

## 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	402/440 (91%)	384 (96%)	16 (4%)	2 (0%)	24	17
1	B	402/440 (91%)	393 (98%)	8 (2%)	1 (0%)	43	40
1	C	399/440 (91%)	385 (96%)	14 (4%)	0	100	100
1	D	401/440 (91%)	392 (98%)	9 (2%)	0	100	100
All	All	1604/1760 (91%)	1554 (97%)	47 (3%)	3 (0%)	43	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ALA
1	A	283	ASN
1	B	258	ASP

### 5.3.2 Protein sidechains [i](#)

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%)	333 (96%)	12 (4%)	32	27
1	B	345/373 (92%)	337 (98%)	8 (2%)	44	43
1	C	342/373 (92%)	335 (98%)	7 (2%)	48	48
1	D	344/373 (92%)	337 (98%)	7 (2%)	48	48
All	All	1376/1492 (92%)	1342 (98%)	34 (2%)	42	40

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	97	ARG
1	A	109	LEU
1	A	121	GLU
1	A	122	GLN
1	A	156	GLU
1	A	256	GLN
1	A	258	ASP
1	A	285	ARG
1	A	301	GLU
1	A	329	ARG
1	A	384	ASP
1	B	71	VAL
1	B	98	ARG
1	B	122	GLN
1	B	148	GLN
1	B	301	GLU
1	B	309	LEU
1	B	326	LEU
1	B	396	ASP
1	C	71	VAL
1	C	90	GLN
1	C	154	GLU
1	C	216	LYS
1	C	342	GLU
1	C	384	ASP
1	C	396	ASP
1	D	71	VAL
1	D	89	GLN
1	D	121	GLU
1	D	125	SER
1	D	167	GLU
1	D	378	ASP
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	277	HIS
1	A	435	GLN
1	B	87	GLN
1	B	194	GLN

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Mol	Chain	Res	Type
1	B	213	ASN
1	C	126	GLN
1	C	220	ASN
1	C	466	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 8 are monoatomic - leaving 25 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	0.59	0	7,16,16	0.74	0
4	OUM	B	503	-	33,33,33	1.79	4 (12%)	45,46,46	1.88	13 (28%)
5	BTB	B	506	-	13,13,13	0.66	0	7,16,16	1.29	1 (14%)
5	BTB	D	506	-	13,13,13	0.42	0	7,16,16	0.51	0
5	BTB	A	505	-	13,13,13	0.55	0	7,16,16	0.81	0
5	BTB	D	504	9	13,13,13	0.38	0	7,16,16	1.06	1 (14%)
3	H4B	C	502	-	17,18,18	0.86	0	14,26,26	1.88	4 (28%)
7	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.30	0
2	HEM	C	501	1	50,50,50	1.68	9 (18%)	67,82,82	1.40	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	D	501	1	50,50,50	1.74	9 (18%)	67,82,82	1.54	14 (20%)
3	H4B	D	502	-	17,18,18	0.80	0	14,26,26	1.94	4 (28%)
5	BTB	C	505	-	13,13,13	1.10	2 (15%)	7,16,16	1.41	2 (28%)
5	BTB	B	504	9	13,13,13	0.57	0	7,16,16	0.98	0
7	GOL	C	508	-	5,5,5	0.52	0	5,5,5	0.83	0
4	OUM	C	503	-	33,33,33	1.70	5 (15%)	45,46,46	1.85	8 (17%)
4	OUM	D	503	-	33,33,33	1.80	6 (18%)	45,46,46	2.04	13 (28%)
5	BTB	C	506	-	13,13,13	0.35	0	7,16,16	0.54	0
4	OUM	A	503	-	33,33,33	1.79	5 (15%)	45,46,46	2.16	12 (26%)
5	BTB	D	505	-	13,13,13	0.89	1 (7%)	7,16,16	1.79	3 (42%)
3	H4B	A	502	-	17,18,18	0.76	0	14,26,26	1.93	4 (28%)
3	H4B	B	502	-	17,18,18	0.82	0	14,26,26	1.94	4 (28%)
5	BTB	A	504	-	13,13,13	5.16	3 (23%)	7,16,16	2.52	2 (28%)
5	BTB	C	504	-	13,13,13	2.98	1 (7%)	7,16,16	1.47	2 (28%)
2	HEM	B	501	1	50,50,50	1.80	8 (16%)	67,82,82	1.35	9 (13%)
2	HEM	A	501	1	50,50,50	1.58	10 (20%)	67,82,82	1.38	7 (10%)

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	-	-	5/21/21/21	-
4	OUM	B	503	-	-	2/13/13/13	0/4/4/4
5	BTB	B	506	-	-	8/21/21/21	-
5	BTB	D	506	-	-	14/21/21/21	-
5	BTB	A	505	-	-	5/21/21/21	-
5	BTB	D	504	9	-	3/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
7	GOL	A	507	-	-	4/4/4/4	-
2	HEM	C	501	1	-	4/14/54/54	-
2	HEM	D	501	1	-	2/14/54/54	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
5	BTB	C	505	-	-	5/21/21/21	-
5	BTB	B	504	9	-	2/21/21/21	-
7	GOL	C	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OUM	C	503	-	-	5/13/13/13	0/4/4/4
4	OUM	D	503	-	-	2/13/13/13	0/4/4/4
5	BTB	C	506	-	-	3/21/21/21	-
4	OUM	A	503	-	-	1/13/13/13	0/4/4/4
5	BTB	D	505	-	-	14/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	504	-	-	14/21/21/21	-
5	BTB	C	504	-	-	7/21/21/21	-
2	HEM	B	501	1	-	2/14/54/54	-
2	HEM	A	501	1	-	2/14/54/54	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	BTB	C1-C2	-18.05	1.32	1.53
5	C	504	BTB	C5-N	-10.49	1.33	1.48
4	B	503	OUM	C34-C37	-8.10	1.27	1.44
4	A	503	OUM	C34-C37	-7.79	1.28	1.44
4	D	503	OUM	C34-C37	-7.74	1.28	1.44
4	C	503	OUM	C34-C37	-7.65	1.28	1.44
2	B	501	HEM	FE-NB	6.71	2.15	1.94
2	C	501	HEM	FE-NB	6.01	2.13	1.94
2	D	501	HEM	FE-NC	5.71	2.14	1.95
2	B	501	HEM	FE-NC	5.69	2.13	1.95
2	D	501	HEM	FE-ND	4.75	2.09	1.94
2	C	501	HEM	FE-NC	4.73	2.10	1.95
2	A	501	HEM	FE-NC	4.30	2.09	1.95
2	A	501	HEM	FE-NB	4.26	2.08	1.94
2	A	501	HEM	FE-NA	4.08	2.08	1.95
2	D	501	HEM	FE-NB	4.04	2.07	1.94
2	D	501	HEM	FE-NA	3.87	2.07	1.95
2	C	501	HEM	FE-NA	3.74	2.07	1.95
2	B	501	HEM	CMB-C2B	3.41	1.57	1.50
2	B	501	HEM	CAC-C3C	3.18	1.55	1.47
2	B	501	HEM	CAB-C3B	3.10	1.55	1.47
2	A	501	HEM	CAB-C3B	3.09	1.55	1.47
2	A	501	HEM	CAC-C3C	3.09	1.55	1.47
2	C	501	HEM	CAB-C3B	3.08	1.55	1.47
2	C	501	HEM	CAC-C3C	2.98	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	BTB	C3-C2	-2.96	1.49	1.53
2	D	501	HEM	CAB-C3B	2.88	1.55	1.47
4	B	503	OUM	C05-C10	-2.82	1.38	1.42
2	B	501	HEM	CMA-C3A	2.70	1.56	1.50
4	A	503	OUM	C26-C25	-2.68	1.35	1.39
5	C	505	BTB	C4-C2	-2.68	1.50	1.53
5	A	504	BTB	C4-C2	-2.61	1.50	1.53
4	D	503	OUM	C05-C10	-2.61	1.38	1.42
2	A	501	HEM	CMC-C2C	2.59	1.56	1.50
2	D	501	HEM	CAC-C3C	2.59	1.54	1.47
4	D	503	OUM	C09-C10	-2.55	1.38	1.41
2	C	501	HEM	CMA-C3A	2.55	1.56	1.50
2	A	501	HEM	CMD-C2D	2.41	1.55	1.50
4	D	503	OUM	C26-C21	-2.40	1.35	1.39
5	C	505	BTB	C1-C2	-2.39	1.50	1.53
2	D	501	HEM	CMD-C2D	2.35	1.55	1.50
4	C	503	OUM	C02-N01	2.33	1.36	1.33
4	A	503	OUM	C05-C10	-2.29	1.38	1.42
4	B	503	OUM	C04-C05	-2.24	1.38	1.42
2	A	501	HEM	FE-ND	2.24	2.01	1.94
2	C	501	HEM	FE-ND	2.23	2.01	1.94
2	D	501	HEM	CMC-C2C	2.23	1.55	1.50
4	C	503	OUM	C26-C21	-2.22	1.35	1.39
2	B	501	HEM	FE-NA	2.18	2.02	1.95
2	A	501	HEM	CMA-C3A	2.13	1.55	1.50
4	B	503	OUM	C02-N01	2.13	1.36	1.33
2	C	501	HEM	CMB-C2B	2.13	1.55	1.50
4	A	503	OUM	C26-C21	-2.10	1.36	1.39
4	D	503	OUM	C04-C05	-2.09	1.38	1.42
4	D	503	OUM	C23-C22	-2.05	1.35	1.38
5	D	505	BTB	C4-C2	-2.04	1.50	1.53
2	A	501	HEM	CMB-C2B	2.03	1.54	1.50
2	D	501	HEM	CMA-C3A	2.03	1.54	1.50
4	C	503	OUM	C22-C21	-2.03	1.35	1.39
2	C	501	HEM	CMD-C2D	2.03	1.54	1.50
4	A	503	OUM	C09-C10	-2.03	1.38	1.41
4	C	503	OUM	C05-C10	-2.00	1.39	1.42
2	B	501	HEM	CMD-C2D	2.00	1.54	1.50

All (112) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	OUM	C26-C21-C08	-7.66	108.00	120.84
4	C	503	OUM	O29-C24-C25	7.37	125.41	115.89
4	A	503	OUM	C22-C21-C08	6.78	132.96	121.25
5	A	504	BTB	O1-C1-C2	-6.07	97.14	111.40
4	A	503	OUM	C30-O29-C24	5.46	128.57	117.76
4	D	503	OUM	C26-C21-C08	-5.29	111.97	120.84
4	D	503	OUM	O29-C24-C25	5.08	122.45	115.89
2	A	501	HEM	CBD-CAD-C3D	-4.86	99.09	112.53
4	B	503	OUM	C26-C21-C08	-4.86	112.70	120.84
3	B	502	H4B	C2-N1-C8A	4.49	121.28	113.36
4	D	503	OUM	C22-C21-C08	4.48	128.99	121.25
4	B	503	OUM	O29-C24-C25	4.42	121.60	115.89
3	A	502	H4B	C2-N1-C8A	4.25	120.86	113.36
3	C	502	H4B	C2-N1-C8A	4.16	120.70	113.36
3	D	502	H4B	C2-N1-C8A	4.06	120.53	113.36
2	B	501	HEM	CBA-CAA-C2A	-3.87	101.84	112.53
4	C	503	OUM	C27-C25-C26	-3.86	113.53	120.37
4	B	503	OUM	C22-C21-C08	3.81	127.83	121.25
4	D	503	OUM	C27-C25-C26	-3.80	113.63	120.37
2	D	501	HEM	CBD-CAD-C3D	-3.61	102.55	112.53
2	B	501	HEM	CAD-CBD-CGD	-3.57	104.21	113.67
2	D	501	HEM	CBA-CAA-C2A	-3.50	102.85	112.53
2	C	501	HEM	C3B-C4B-NB	-3.48	106.97	109.47
4	C	503	OUM	O29-C24-C23	-3.48	116.36	123.95
2	A	501	HEM	C3B-C4B-NB	-3.37	107.05	109.47
2	C	501	HEM	C1B-NB-C4B	3.31	109.12	105.21
4	B	503	OUM	C27-C25-C26	-3.26	114.59	120.37
4	B	503	OUM	C35-C34-C37	-3.26	114.67	119.97
2	C	501	HEM	CBA-CAA-C2A	-3.25	103.55	112.53
4	D	503	OUM	C27-C25-C24	3.24	126.44	120.15
2	D	501	HEM	C3D-C4D-ND	-3.21	106.66	110.17
4	A	503	OUM	C09-C08-C21	-3.20	113.88	121.05
4	D	503	OUM	O29-C30-C31	-3.19	99.80	109.16
4	C	503	OUM	C27-C25-C24	3.18	126.33	120.15
2	D	501	HEM	C2A-C1A-NA	-3.13	106.68	110.15
4	A	503	OUM	C07-C08-C21	3.09	126.59	121.25
3	A	502	H4B	O4-C4-C4A	-3.09	119.82	127.26
4	D	503	OUM	C09-C08-C21	-3.07	114.17	121.05
2	A	501	HEM	C3D-C4D-ND	-3.07	106.80	110.17
4	D	503	OUM	C07-C08-C21	3.05	126.52	121.25
2	A	501	HEM	C4D-ND-C1D	3.01	108.77	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	505	BTB	O3-C3-C2	-3.00	104.34	111.40
4	A	503	OUM	C27-C25-C26	-2.97	115.11	120.37
3	D	502	H4B	O4-C4-C4A	-2.92	120.22	127.26
5	C	505	BTB	O1-C1-C2	-2.89	104.61	111.40
2	D	501	HEM	CMC-C2C-C1C	-2.86	119.69	124.73
3	A	502	H4B	C4A-C4-N3	2.85	119.95	112.13
3	C	502	H4B	O4-C4-C4A	-2.83	120.43	127.26
2	A	501	HEM	C1B-NB-C4B	2.81	108.53	105.21
5	C	504	BTB	C8-C7-N	2.80	122.50	111.59
3	B	502	H4B	O4-C4-C4A	-2.79	120.54	127.26
4	A	503	OUM	C03-C04-C05	2.77	120.64	117.84
4	B	503	OUM	C27-C25-C24	2.75	125.49	120.15
3	B	502	H4B	C4A-C4-N3	2.73	119.62	112.13
3	D	502	H4B	C4A-C4-N3	2.71	119.57	112.13
4	C	503	OUM	C05-C10-N01	-2.69	119.95	122.80
4	B	503	OUM	C03-C04-C05	2.66	120.53	117.84
3	C	502	H4B	C2-N3-C4	-2.62	120.36	125.11
2	C	501	HEM	C3B-C2B-C1B	2.60	108.36	106.41
3	C	502	H4B	C4A-C4-N3	2.57	119.19	112.13
2	A	501	HEM	CHA-C4D-ND	2.57	127.54	124.37
5	D	505	BTB	O4-C4-C2	-2.55	105.41	111.40
3	A	502	H4B	C2-N3-C4	-2.54	120.50	125.11
2	D	501	HEM	C4D-ND-C1D	2.53	108.20	105.21
2	C	501	HEM	C4D-ND-C1D	2.52	108.20	105.21
2	D	501	HEM	CHC-C1C-NC	2.50	127.18	124.45
4	D	503	OUM	O29-C24-C23	-2.50	118.49	123.95
3	D	502	H4B	C2-N3-C4	-2.48	120.61	125.11
5	C	504	BTB	O3-C3-C2	2.48	117.23	111.40
3	B	502	H4B	C2-N3-C4	-2.48	120.62	125.11
5	D	505	BTB	O1-C1-C2	-2.46	105.61	111.40
4	D	503	OUM	C30-O29-C24	2.46	122.62	117.76
2	C	501	HEM	C3D-C4D-ND	-2.41	107.53	110.17
2	A	501	HEM	C3B-C2B-C1B	2.41	108.22	106.41
4	C	503	OUM	C30-O29-C24	2.41	122.53	117.76
4	B	503	OUM	O29-C30-C31	-2.40	102.11	109.16
4	D	503	OUM	C33-C34-C37	-2.38	116.10	119.97
2	D	501	HEM	C4C-NC-C1C	2.37	109.68	105.82
2	B	501	HEM	C3B-C4B-NB	-2.36	107.78	109.47
2	D	501	HEM	C4A-NA-C1A	2.34	109.63	105.82
4	C	503	OUM	C04-C05-C10	2.31	119.41	118.00
5	B	506	BTB	C8-C7-N	2.30	120.58	111.59
2	B	501	HEM	CBD-CAD-C3D	-2.30	106.17	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	OUM	C25-C27-N28	-2.29	102.89	114.98
4	C	503	OUM	C03-C04-C05	2.28	120.14	117.84
4	B	503	OUM	C33-C34-C37	2.27	123.67	119.97
2	C	501	HEM	CAD-CBD-CGD	-2.26	107.67	113.67
4	A	503	OUM	C26-C25-C24	2.25	120.73	118.26
2	D	501	HEM	C3B-C2B-C1B	2.23	108.08	106.41
4	A	503	OUM	N02-C02-N01	2.23	120.08	118.24
4	B	503	OUM	C09-C08-C21	-2.22	116.09	121.05
2	D	501	HEM	C1B-NB-C4B	2.21	107.82	105.21
4	B	503	OUM	C30-C31-C36	-2.21	115.56	120.64
4	B	503	OUM	O29-C24-C23	-2.19	119.17	123.95
2	C	501	HEM	C2B-C1B-NB	-2.18	107.34	109.84
5	D	504	BTB	O4-C4-C2	-2.17	106.29	111.40
5	C	505	BTB	O4-C4-C2	-2.14	106.36	111.40
2	B	501	HEM	C3D-C4D-ND	-2.14	107.82	110.17
2	C	501	HEM	C2A-C1A-NA	-2.13	107.79	110.15
5	A	504	BTB	C8-C7-N	2.11	119.82	111.59
4	B	503	OUM	C30-O29-C24	2.11	121.93	117.76
2	B	501	HEM	C2A-C1A-NA	-2.10	107.83	110.15
2	D	501	HEM	O1A-CGA-CBA	-2.09	116.47	123.09
4	D	503	OUM	C03-C04-C05	2.08	119.94	117.84
2	D	501	HEM	CHB-C1B-NB	2.06	126.92	124.37
4	A	503	OUM	C27-C25-C24	2.06	124.14	120.15
4	A	503	OUM	O29-C30-C31	-2.05	103.13	109.16
2	B	501	HEM	C4C-NC-C1C	2.05	109.16	105.82
4	D	503	OUM	C35-C34-C37	2.04	123.30	119.97
2	B	501	HEM	C4D-ND-C1D	2.02	107.60	105.21
2	B	501	HEM	CHA-C1A-NA	2.02	127.52	123.86
2	D	501	HEM	O2A-CGA-CBA	2.01	120.36	114.00

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2D-C3D-CAD-CBD
2	C	501	HEM	C4D-C3D-CAD-CBD
4	B	503	OUM	C24-C25-C27-N28
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	N-C2-C3-O3
5	A	504	BTB	C1-C2-N-C5
5	A	504	BTB	C1-C2-N-C7
5	A	504	BTB	C3-C2-N-C7

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C4-C2-N-C7
5	A	504	BTB	C6-C5-N-C7
5	A	504	BTB	C8-C7-N-C2
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	B	504	BTB	C3-C2-C4-O4
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	506	BTB	O1-C1-C2-C3
5	B	506	BTB	O1-C1-C2-C4
5	B	506	BTB	O1-C1-C2-N
5	B	506	BTB	N-C2-C3-O3
5	B	506	BTB	C8-C7-N-C2
5	C	504	BTB	O1-C1-C2-C4
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	C6-C5-N-C7
5	C	504	BTB	C8-C7-N-C2
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	C8-C7-N-C5
5	C	506	BTB	C1-C2-C3-O3
5	C	506	BTB	C4-C2-C3-O3
5	C	506	BTB	N-C2-C3-O3
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
5	D	505	BTB	C4-C2-N-C7
5	D	505	BTB	C8-C7-N-C5
5	D	506	BTB	O1-C1-C2-C3
5	D	506	BTB	O1-C1-C2-N
5	D	506	BTB	C1-C2-C3-O3
5	D	506	BTB	C4-C2-C3-O3
5	D	506	BTB	N-C2-C3-O3
5	D	506	BTB	C1-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	D	506	BTB	C1-C2-N-C7
5	D	506	BTB	C3-C2-N-C5
5	D	506	BTB	C3-C2-N-C7
5	D	506	BTB	C4-C2-N-C5
5	D	506	BTB	C4-C2-N-C7
7	A	507	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-C3
7	C	508	GOL	O1-C1-C2-C3
5	B	506	BTB	N-C5-C6-O6
5	C	504	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
5	A	504	BTB	N-C7-C8-O8
5	D	504	BTB	N-C5-C6-O6
5	D	505	BTB	N-C7-C8-O8
4	C	503	OUM	C25-C24-O29-C30
4	C	503	OUM	C24-C25-C27-N28
5	A	505	BTB	N-C5-C6-O6
7	A	507	GOL	C1-C2-C3-O3
5	D	505	BTB	N-C5-C6-O6
5	D	506	BTB	N-C7-C8-O8
7	A	507	GOL	O2-C2-C3-O3
7	C	508	GOL	O1-C1-C2-O2
4	C	503	OUM	C31-C30-O29-C24
5	D	506	BTB	N-C5-C6-O6
4	A	503	OUM	C24-C25-C27-N28
5	A	504	BTB	N-C5-C6-O6
5	A	504	BTB	O1-C1-C2-C3
5	B	506	BTB	C4-C2-C3-O3
5	C	504	BTB	O1-C1-C2-C3
5	B	505	BTB	N-C7-C8-O8
4	C	503	OUM	C23-C24-O29-C30
4	D	503	OUM	C24-C25-C27-N28
5	A	505	BTB	C3-C2-C4-O4
5	D	505	BTB	O1-C1-C2-C4
5	A	504	BTB	C3-C2-N-C5
5	A	504	BTB	C4-C2-N-C5
5	B	506	BTB	C1-C2-N-C7
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
5	A	504	BTB	C4-C2-C3-O3
5	D	504	BTB	C3-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	506	BTB	C1-C2-C4-O4
5	C	504	BTB	N-C7-C8-O8
2	B	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAD-CBD-CGD-O2D
5	B	505	BTB	N-C5-C6-O6
2	A	501	HEM	C4B-C3B-CAB-CBB
5	D	505	BTB	O1-C1-C2-C3
4	B	503	OUM	C35-C34-C37-N38
4	C	503	OUM	C35-C34-C37-N38
3	D	502	H4B	N5-C6-C9-O9
5	B	504	BTB	N-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
4	D	503	OUM	C35-C34-C37-N38

There are no ring outliers.

22 monomers are involved in 62 short contacts:

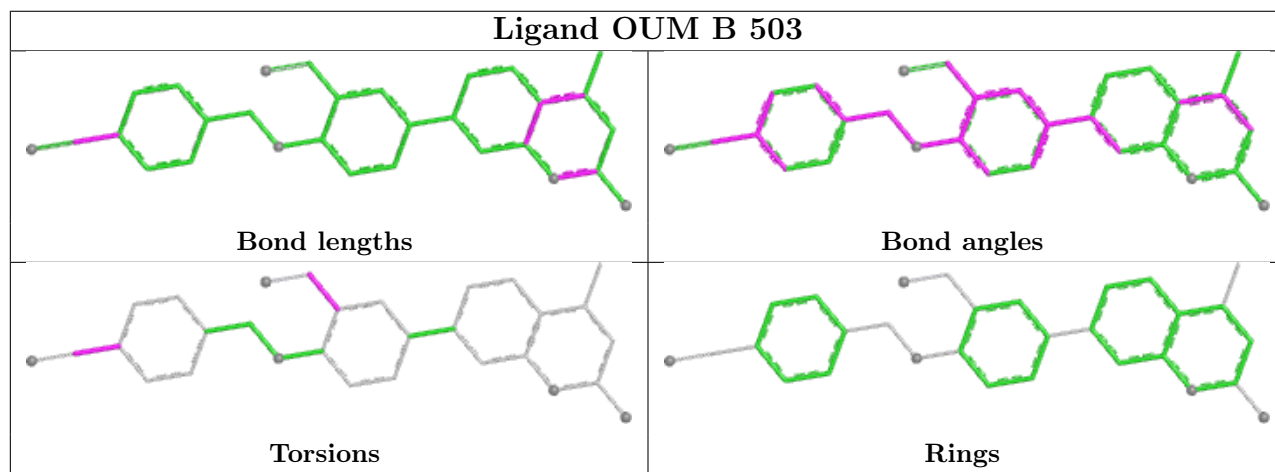
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	BTB	2	0
4	B	503	OUM	4	0
5	B	506	BTB	4	0
5	D	506	BTB	3	0
5	A	505	BTB	1	0
5	D	504	BTB	4	0
3	C	502	H4B	2	0
7	A	507	GOL	3	0
2	C	501	HEM	9	0
2	D	501	HEM	2	0
5	B	504	BTB	2	0
7	C	508	GOL	1	0
4	C	503	OUM	3	0
4	D	503	OUM	3	0
5	C	506	BTB	1	0
4	A	503	OUM	4	0
5	D	505	BTB	6	1
3	B	502	H4B	1	0
5	A	504	BTB	3	0
5	C	504	BTB	2	0

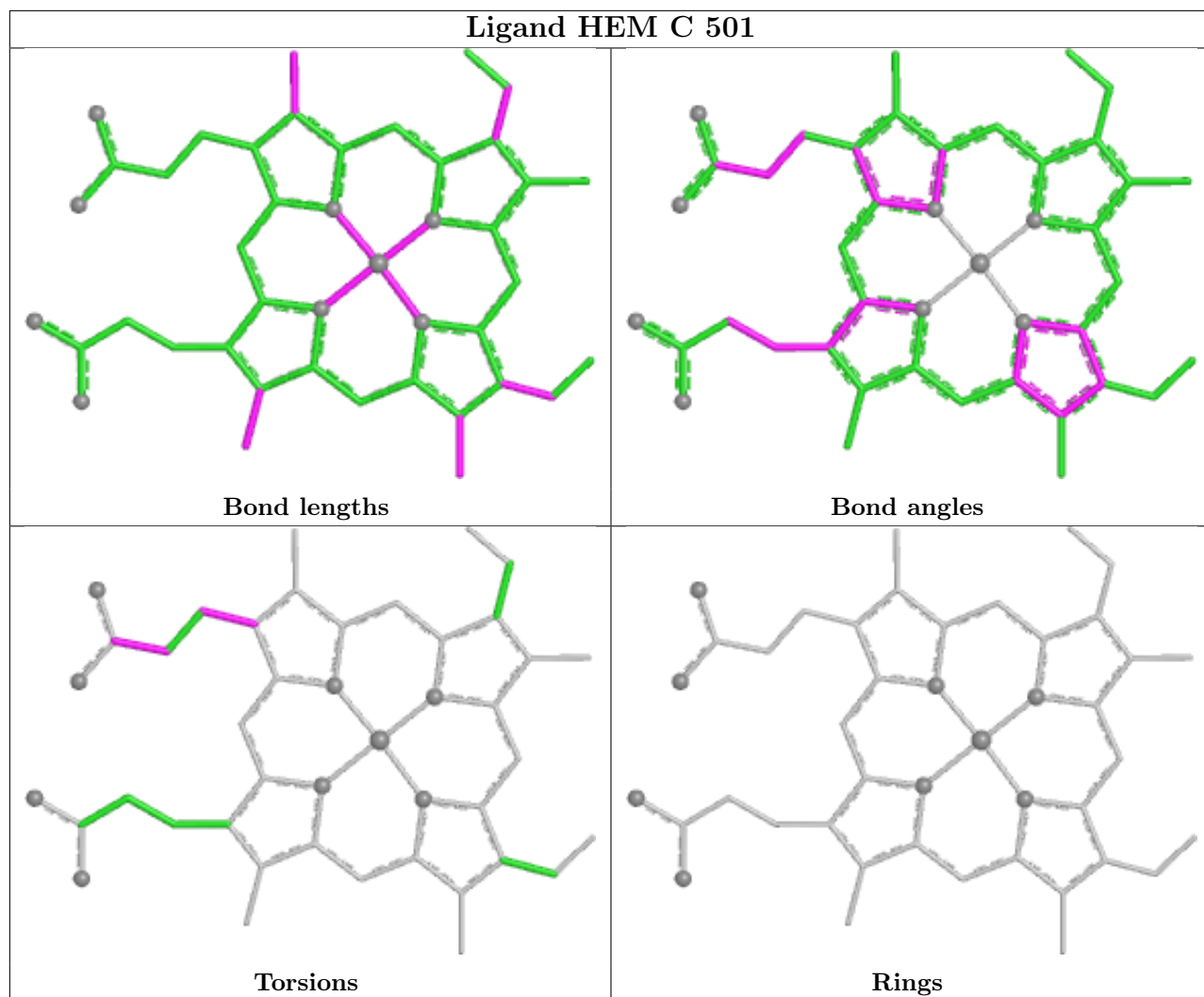
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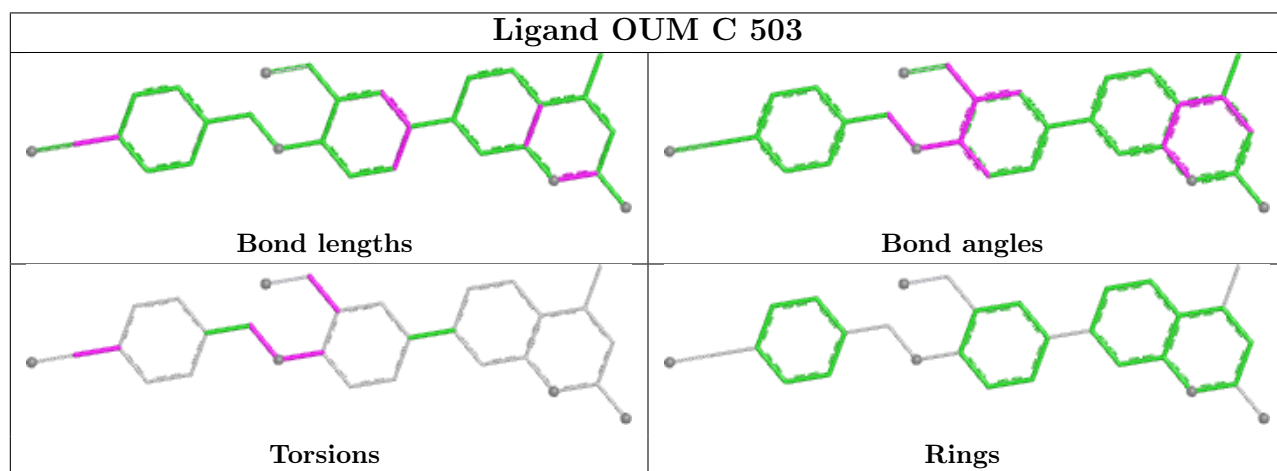
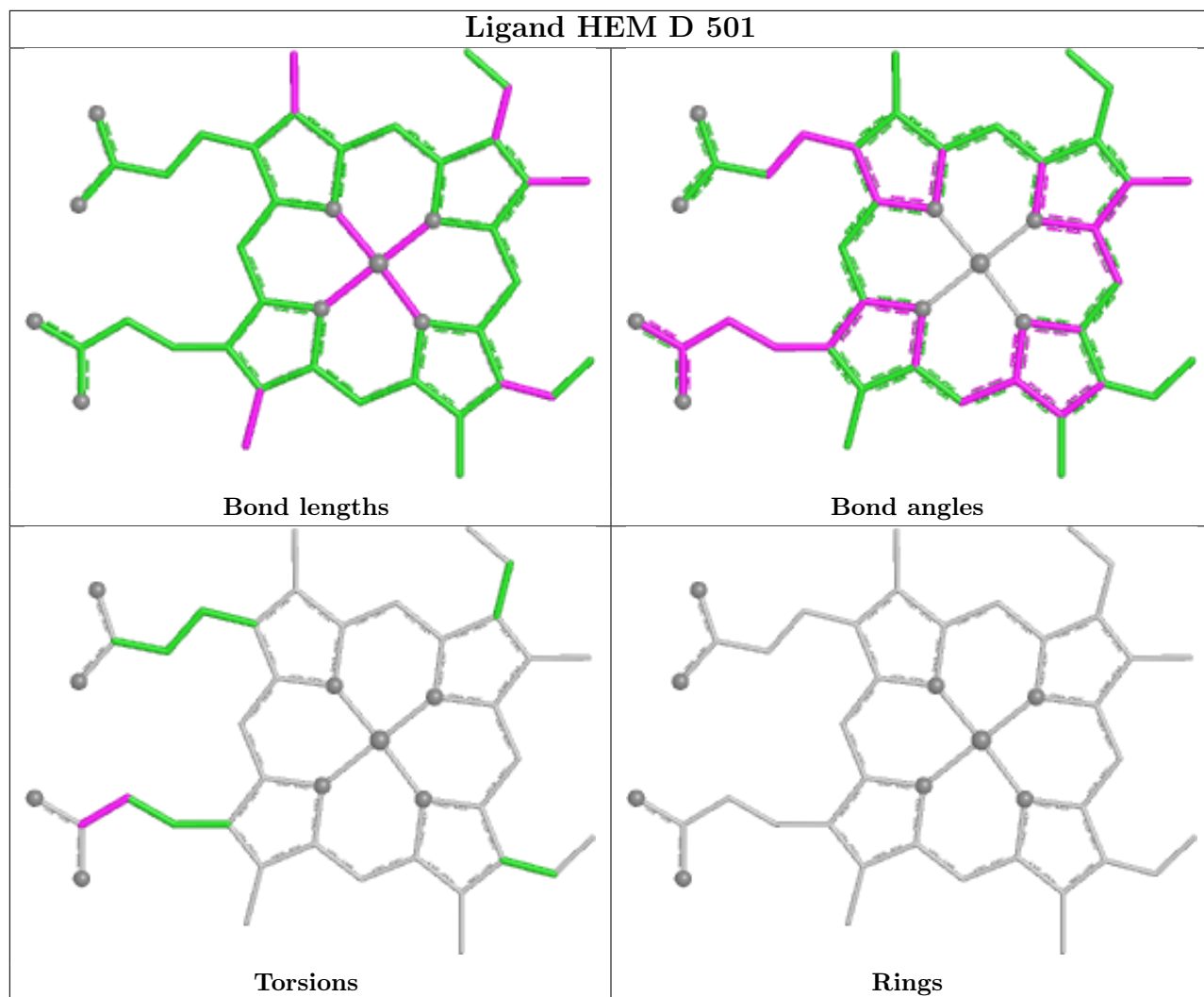
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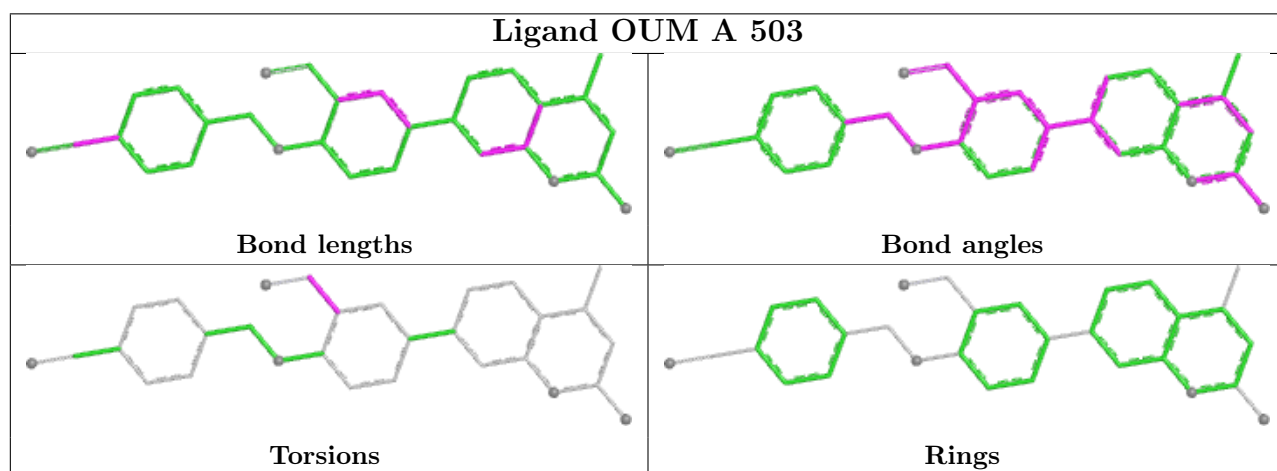
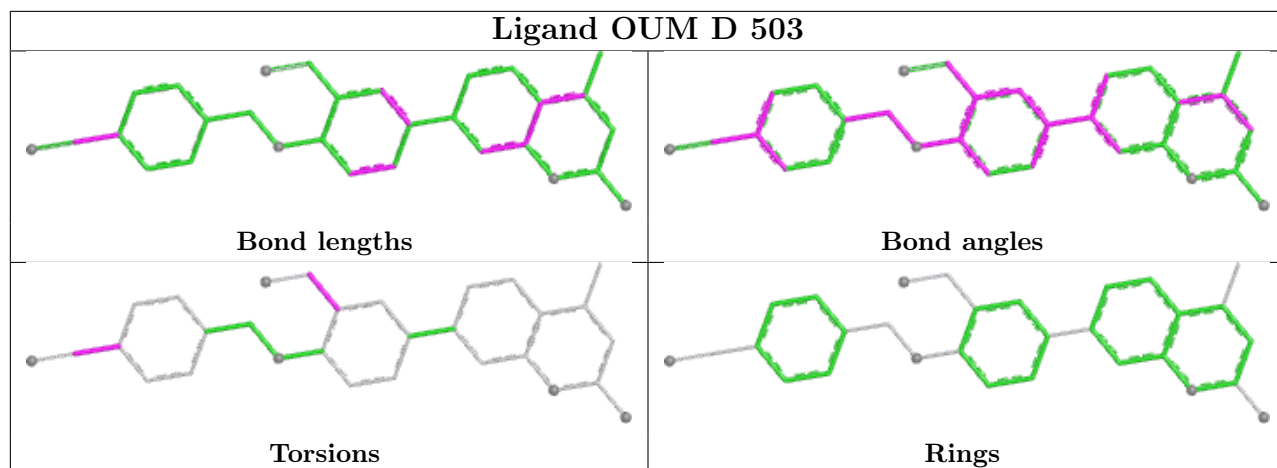
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	4	0
2	A	501	HEM	2	0

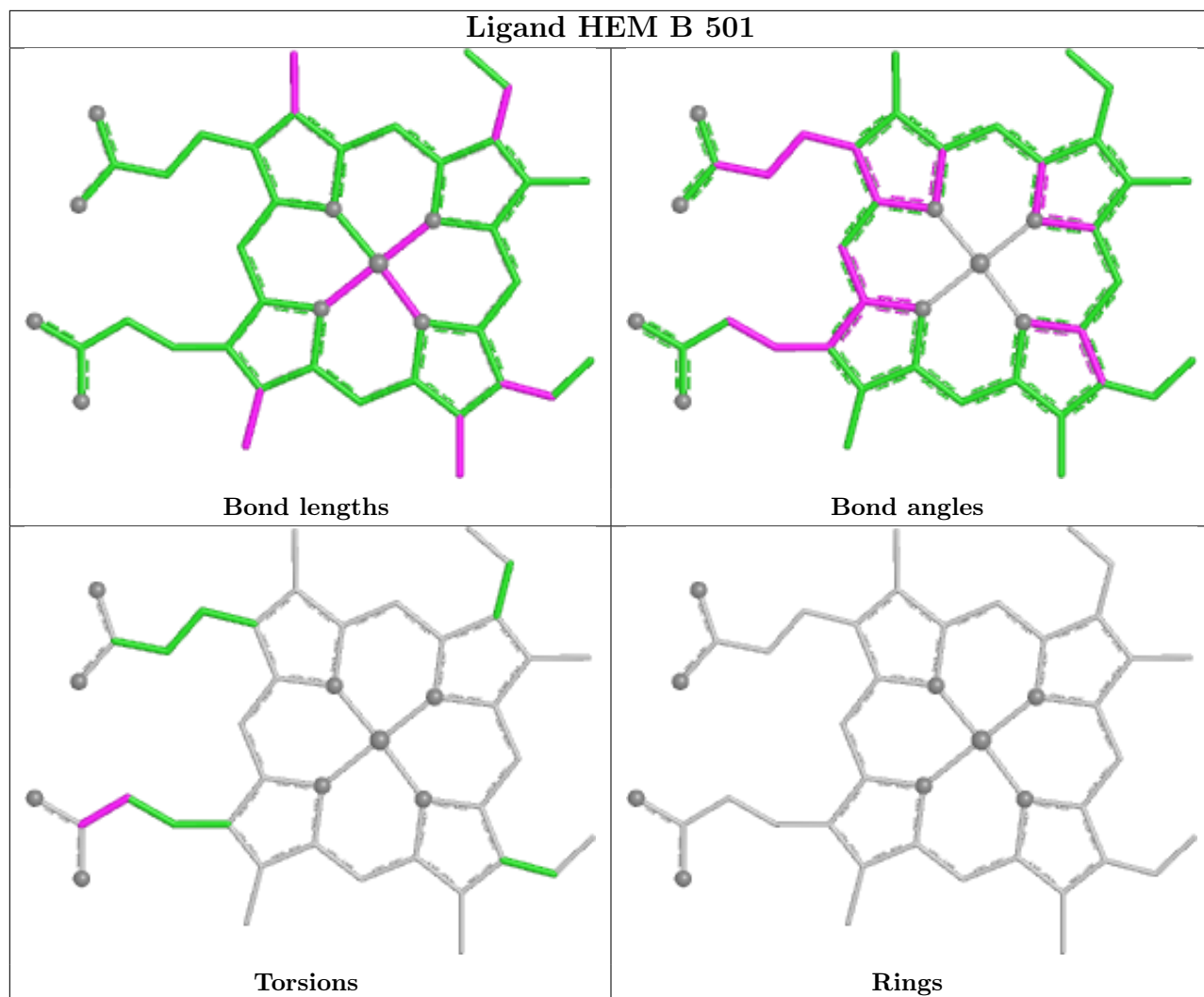
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

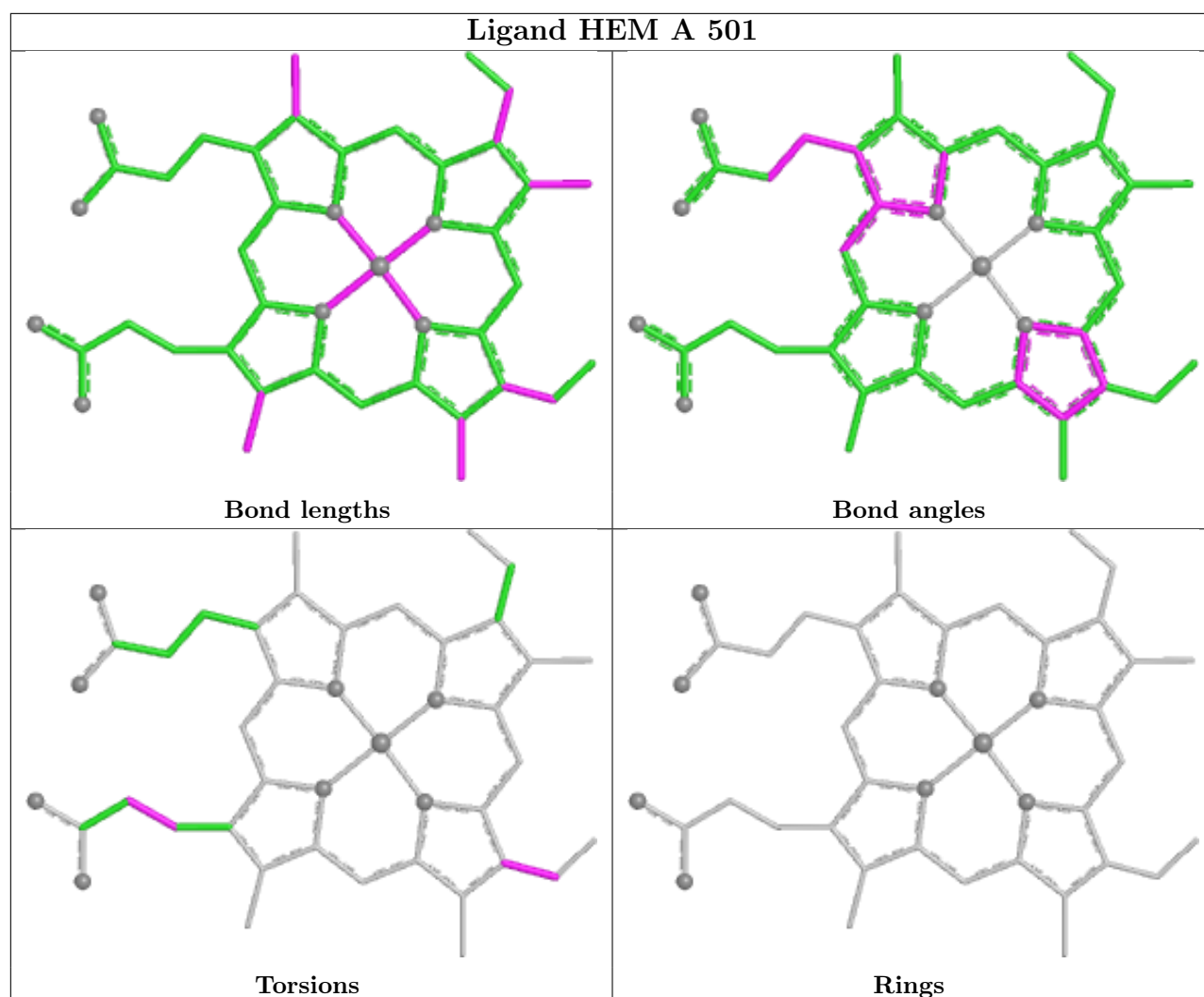












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/440 (91%)	0.63	29 (7%) 21 20	20, 47, 94, 135	2 (0%)
1	B	403/440 (91%)	0.03	9 (2%) 62 62	21, 33, 71, 133	3 (0%)
1	C	401/440 (91%)	0.54	26 (6%) 25 24	19, 46, 89, 122	2 (0%)
1	D	402/440 (91%)	-0.05	10 (2%) 58 58	18, 32, 59, 110	3 (0%)
All	All	1610/1760 (91%)	0.29	74 (4%) 37 36	18, 39, 84, 135	10 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PRO	5.2
1	A	144	GLN	5.1
1	D	119	ALA	4.7
1	A	109	LEU	4.6
1	A	257	GLN	4.5
1	A	120	PRO	4.5
1	A	106	PRO	4.1
1	A	119	ALA	3.9
1	B	119	ALA	3.6
1	C	239	GLY	3.6
1	D	106	PRO	3.6
1	D	259	GLY	3.4
1	A	238	ARG	3.4
1	B	257	GLN	3.2
1	A	298	GLU	3.1
1	C	89	GLN	3.1
1	A	480	TRP	3.1
1	C	105	PHE	3.1
1	C	257	GLN	3.1
1	C	238	ARG	3.0
1	A	89	GLN	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	142	GLY	2.9
1	B	259	GLY	2.9
1	D	67	LYS	2.9
1	D	89	GLN	2.9
1	B	258	ASP	2.9
1	A	468	PHE	2.9
1	C	235	CYS	2.8
1	A	90	GLN	2.8
1	C	153	VAL	2.8
1	B	89	GLN	2.8
1	C	142	GLY	2.8
1	C	237	GLY	2.8
1	C	145	ALA	2.8
1	A	108	LYS	2.7
1	C	159	ALA	2.7
1	B	106	PRO	2.7
1	D	258	ASP	2.7
1	A	107	ARG	2.7
1	A	145	ALA	2.6
1	A	256	GLN	2.5
1	C	236	PRO	2.5
1	A	207	MET	2.5
1	C	119	ALA	2.4
1	D	255	ARG	2.4
1	A	283	ASN	2.4
1	D	90	GLN	2.4
1	B	67	LYS	2.4
1	D	257	GLN	2.3
1	C	480	TRP	2.3
1	A	280	THR	2.2
1	A	148	GLN	2.2
1	C	309	LEU	2.2
1	A	237	GLY	2.2
1	A	301	GLU	2.2
1	A	208	PHE	2.1
1	D	158	ALA	2.1
1	B	144	GLN	2.1
1	C	298	GLU	2.1
1	C	297	ASP	2.1
1	C	148	GLN	2.1
1	A	161	GLY	2.1
1	A	124	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	SER	2.1
1	C	136	SER	2.1
1	C	292	LEU	2.1
1	C	90	GLN	2.1
1	A	299	PRO	2.1
1	B	468	PHE	2.1
1	C	141	SER	2.1
1	C	258	ASP	2.0
1	A	329	ARG	2.0
1	C	97	ARG	2.0
1	C	144	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	BTB	C	506	14/14	0.47	0.20	77,98,115,116	0
5	BTB	B	506	14/14	0.70	0.17	55,70,81,87	0
5	BTB	B	505	14/14	0.70	0.19	57,70,78,84	0
4	OUM	C	503	30/30	0.76	0.27	56,82,93,97	0
5	BTB	D	505	14/14	0.77	0.22	50,63,84,86	0
5	BTB	D	506	14/14	0.78	0.19	38,74,90,94	0
5	BTB	A	505	14/14	0.79	0.17	51,75,79,79	0
4	OUM	D	503	30/30	0.80	0.21	24,62,79,85	0
5	BTB	C	505	14/14	0.81	0.18	22,56,74,75	0
4	OUM	A	503	30/30	0.81	0.23	50,72,85,87	0
4	OUM	B	503	30/30	0.83	0.21	12,64,90,93	0
3	H4B	C	502	17/17	0.83	0.20	67,78,91,91	0

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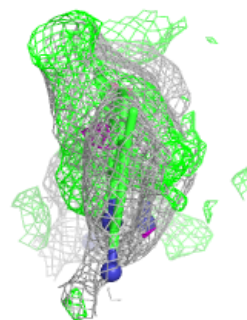
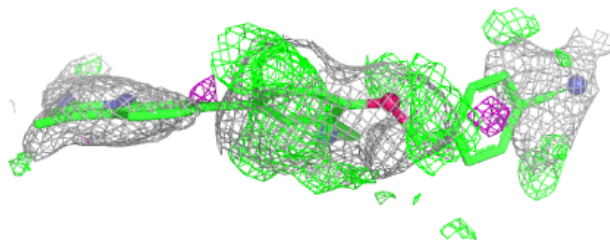
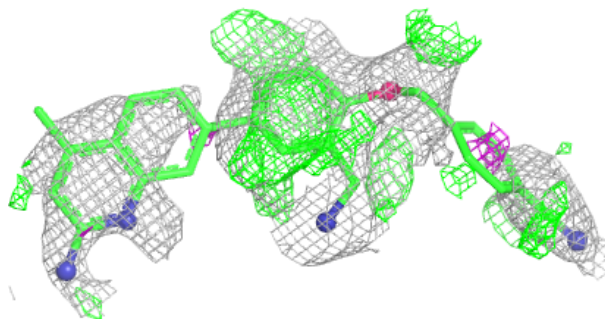
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	A	507	6/6	0.83	0.14	45,68,77,78	0
7	GOL	C	508	6/6	0.84	0.14	45,59,64,67	0
5	BTB	D	504	14/14	0.85	0.18	47,70,80,83	0
3	H4B	B	502	17/17	0.87	0.14	54,62,72,73	0
3	H4B	A	502	17/17	0.87	0.15	58,75,89,90	0
3	H4B	D	502	17/17	0.89	0.14	52,64,78,79	0
5	BTB	B	504	14/14	0.90	0.13	28,55,69,69	0
8	CL	A	508	1/1	0.90	0.15	71,71,71,71	0
5	BTB	A	504	14/14	0.91	0.23	3,49,66,68	0
5	BTB	C	504	14/14	0.91	0.21	3,57,75,77	0
2	HEM	A	501	43/43	0.95	0.12	34,45,79,98	0
2	HEM	C	501	43/43	0.96	0.12	24,39,84,87	0
8	CL	B	507	1/1	0.96	0.07	47,47,47,47	0
2	HEM	B	501	43/43	0.97	0.09	14,24,77,89	0
2	HEM	D	501	43/43	0.98	0.07	15,23,65,75	0
8	CL	D	508	1/1	0.98	0.07	42,42,42,42	0
9	GD	D	507	1/1	0.98	0.03	39,39,39,39	0
6	ZN	A	506	1/1	0.99	0.02	38,38,38,38	0
9	GD	B	508	1/1	0.99	0.03	37,37,37,37	0
8	CL	C	509	1/1	0.99	0.06	54,54,54,54	0
6	ZN	C	507	1/1	1.00	0.04	31,31,31,31	0

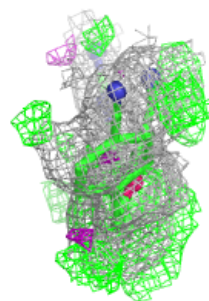
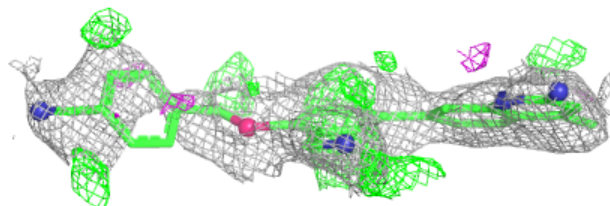
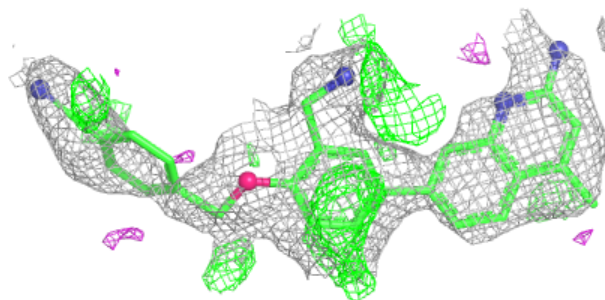
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OUM 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)

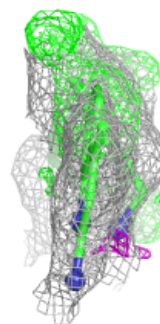
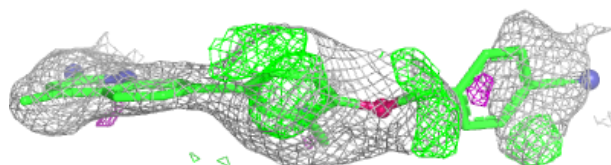
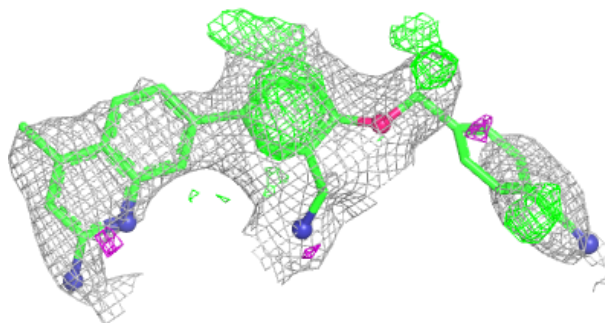
**Electron density around OUM D 503:**

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

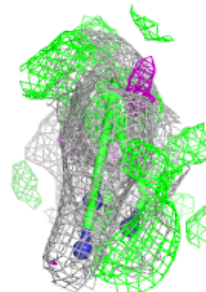
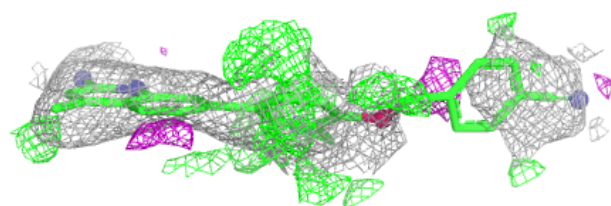
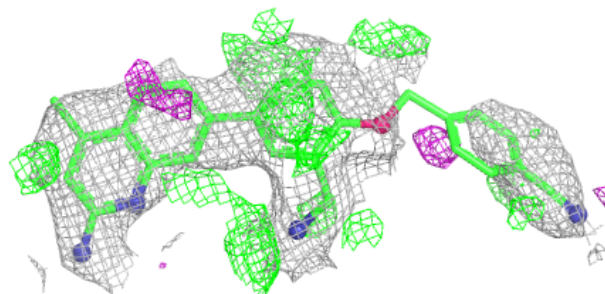


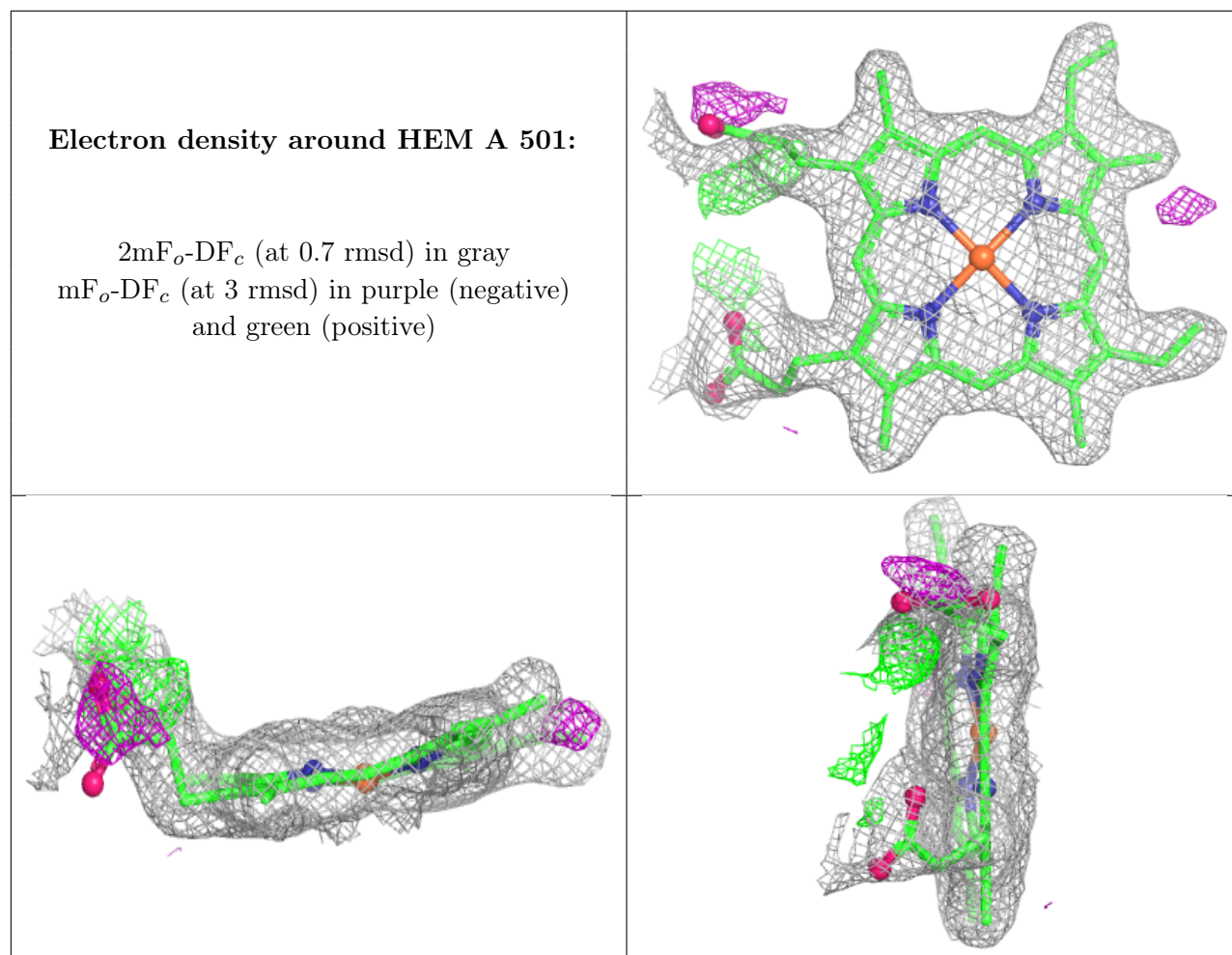
**Electron density around OUM A 503:**

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

**Electron density around OUM B 503:**

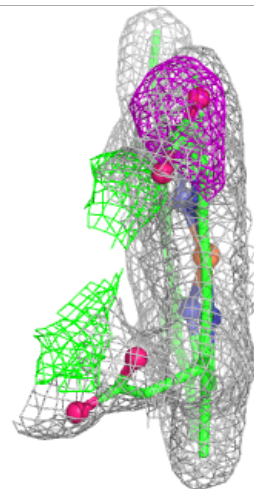
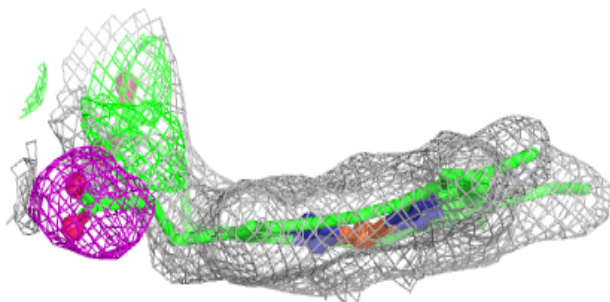
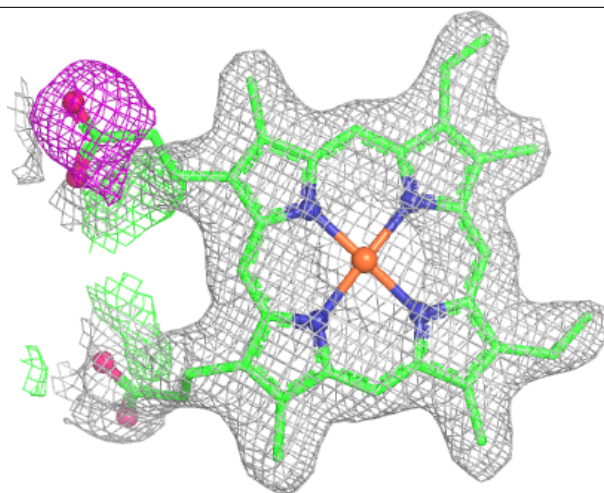
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





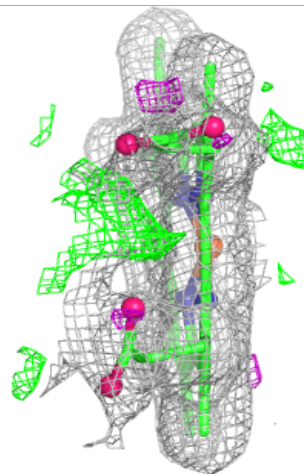
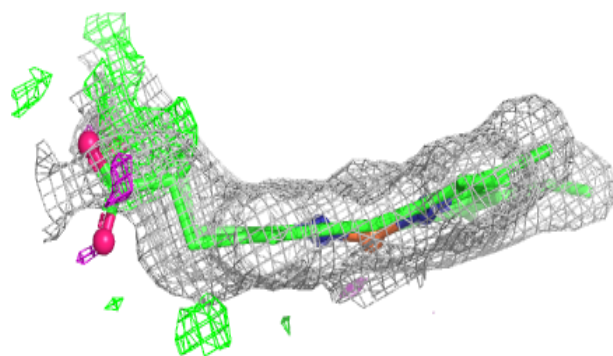
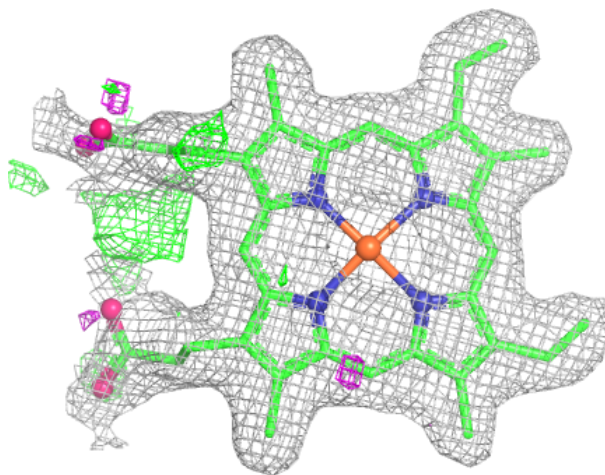
**Electron density around HEM C 501:**

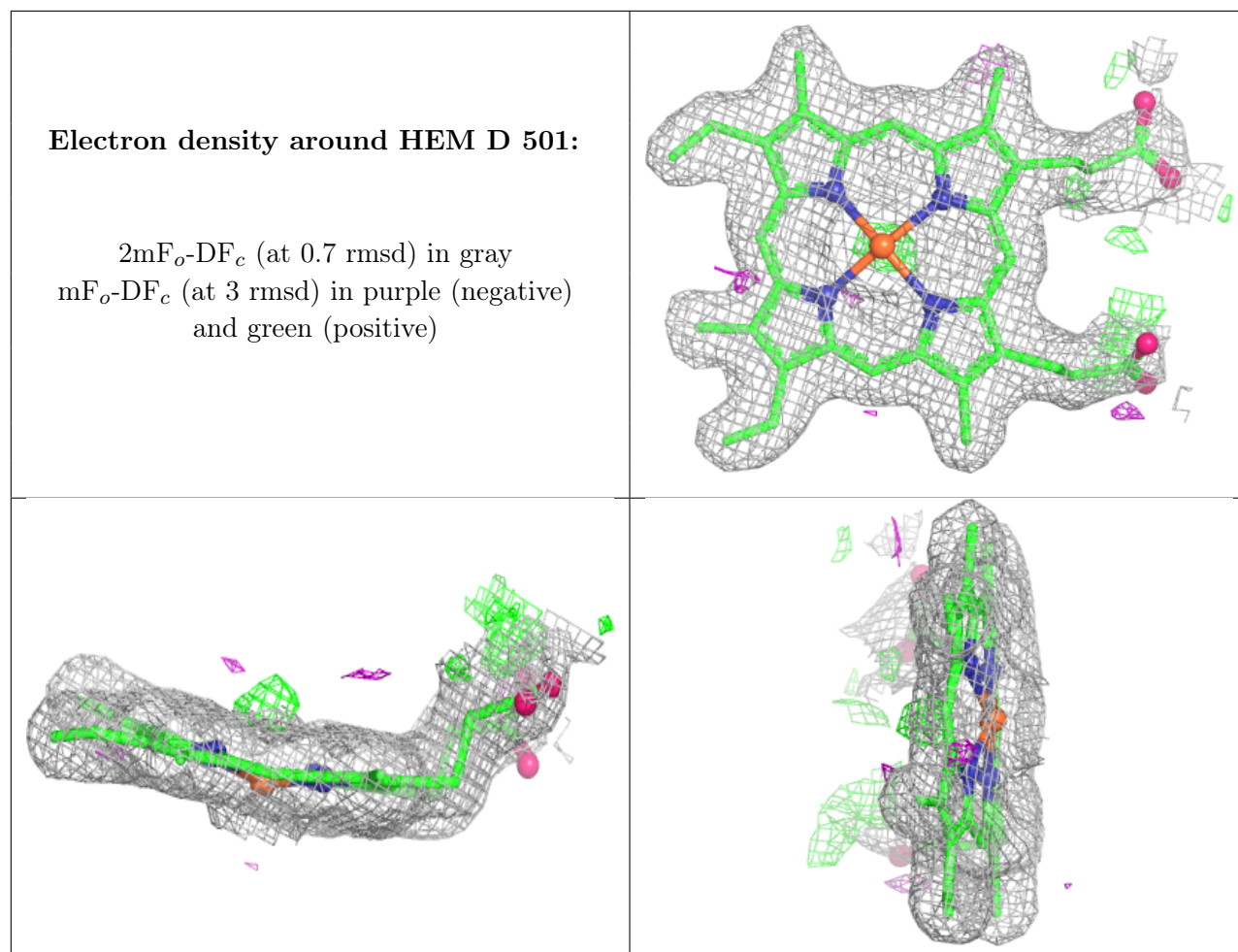
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.