



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:11 AM EDT

PDB ID : 5UO9 / pdb_00005uo9
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-[(3-Ethyl-5-((methylamino)methyl)phenoxy)methyl]quinolin-2-amine
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

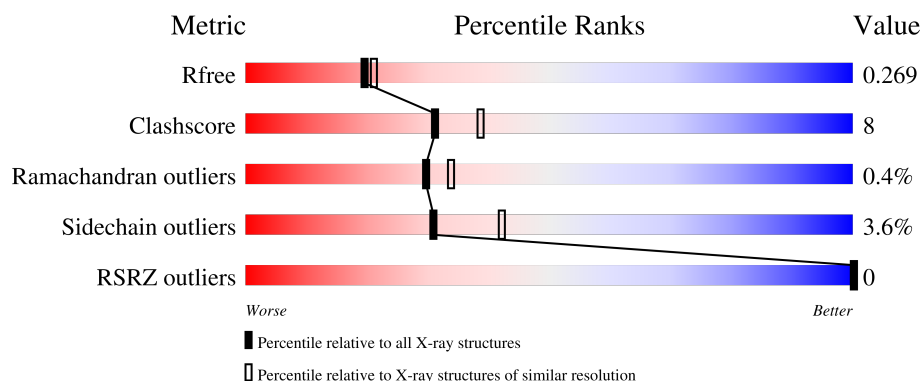
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

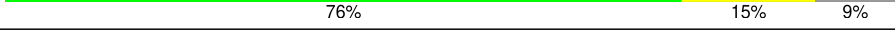
The reported resolution of this entry is 2.19 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

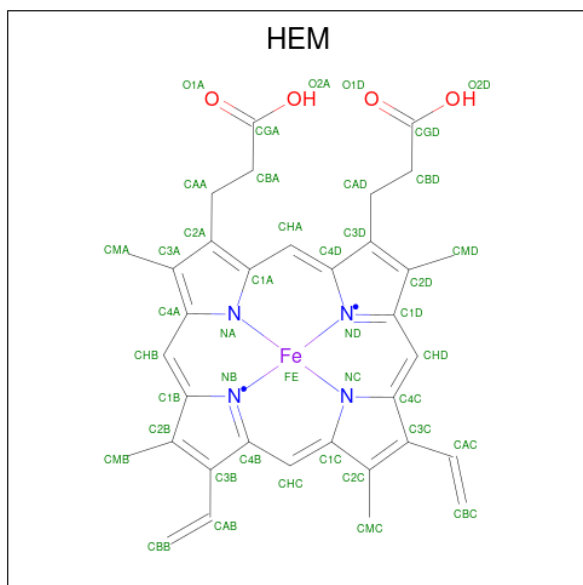
Mol	Chain	Length	Quality of chain
1	A	440	
1	B	440	
1	C	440	
1	D	440	

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 3237	C 2062	N 570	O 589	S 16	0	2	0
1	B	402	Total 3221	C 2051	N 566	O 587	S 17	0	3	0
1	C	401	Total 3209	C 2044	N 563	O 586	S 16	0	2	0
1	D	402	Total 3221	C 2051	N 566	O 587	S 17	0	3	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



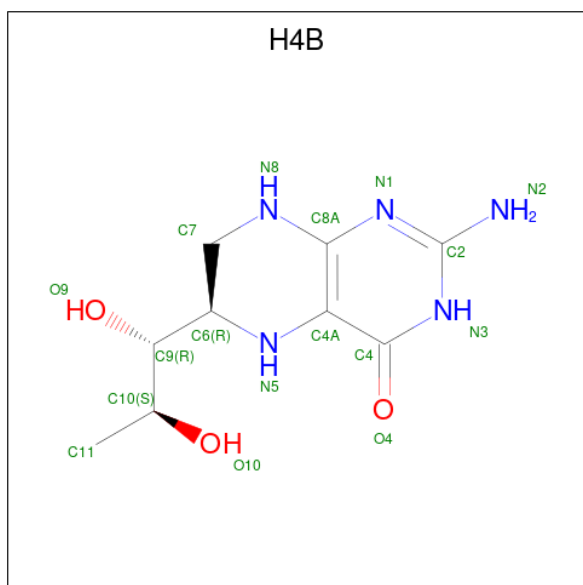
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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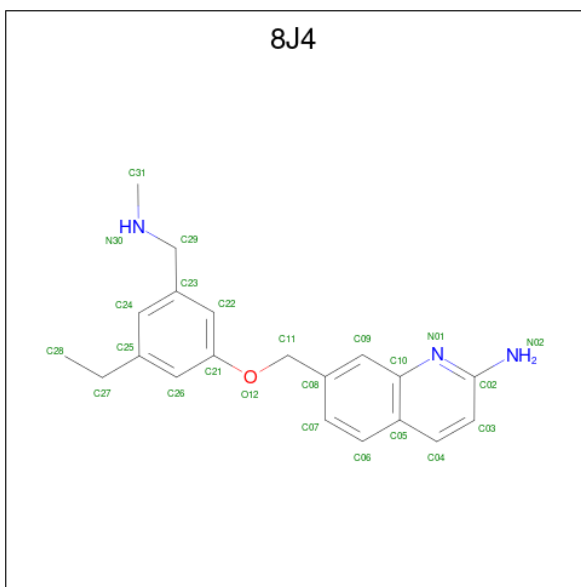
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



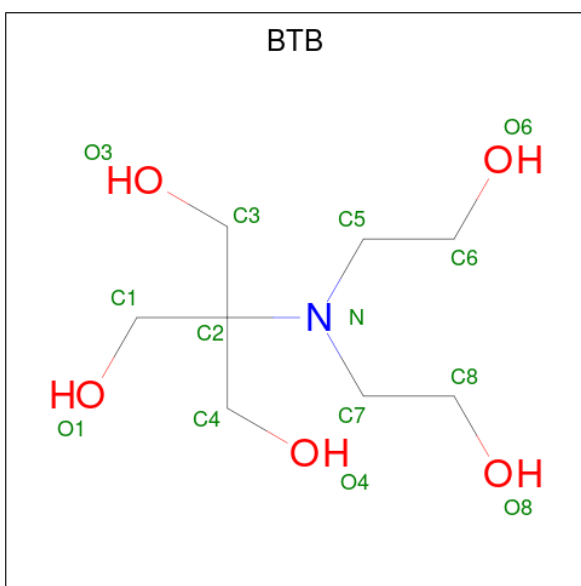
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-({3-ethyl-5-[(methylamino)methyl]phenoxy}methyl)quinolin-2-amine (CCD ID: 8J4) (formula: $C_{20}H_{23}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	20	3	1		
4	B	1	Total	C	N	O	0	0
			24	20	3	1		
4	C	1	Total	C	N	O	0	0
			24	20	3	1		
4	D	1	Total	C	N	O	0	0
			24	20	3	1		

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



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

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

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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	2	Total	Cl	0	0
			2	2		

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

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

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

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

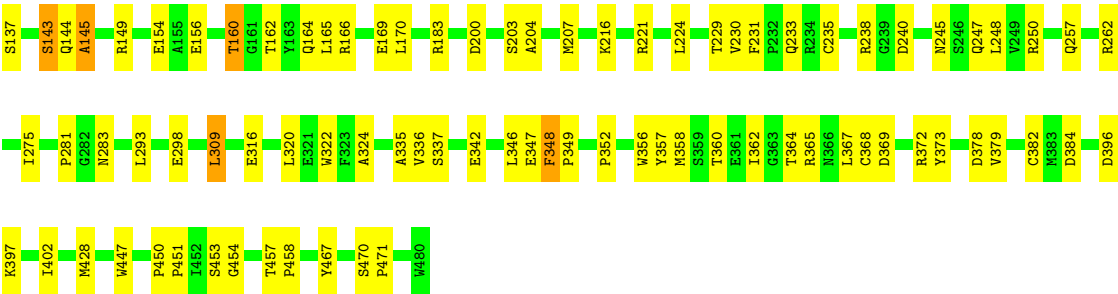
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Ca	0	0
			1	1		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

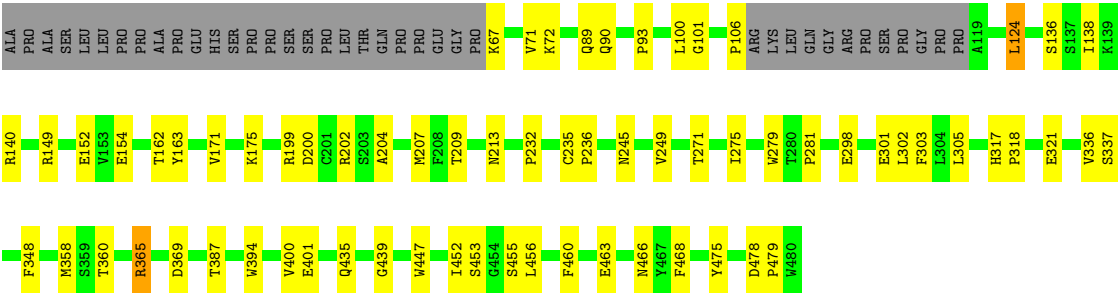
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	118	Total	O	0	0
			118	118		
12	C	76	Total	O	0	0
			76	76		
12	D	114	Total	O	0	0
			114	114		



● 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	59.38Å 152.09Å 108.22Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	38.87 – 2.19 38.87 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.0 (38.87-2.19) 92.3 (38.87-2.19)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.212 , 0.276 0.208 , 0.269	Depositor DCC
R_{free} test set	4651 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13803	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, HEM, GD, 8J4, H4B, ZN, MG, CL, GOL, CA

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	0.48	0/3335	0.83	2/4543 (0.0%)
1	B	0.54	0/3319	0.87	3/4523 (0.1%)
1	C	0.48	0/3307	0.84	3/4507 (0.1%)
1	D	0.56	0/3319	0.87	5/4523 (0.1%)
All	All	0.52	0/13280	0.85	13/18096 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ALA	CA-C-N	6.54	126.48	119.28
1	B	181	ALA	C-N-CA	6.54	126.48	119.28
1	C	348	PHE	CA-C-N	6.09	125.98	119.28
1	C	348	PHE	C-N-CA	6.09	125.98	119.28
1	B	256	GLN	N-CA-C	5.83	115.97	108.34
1	A	366	ASN	N-CA-C	5.66	117.45	111.28
1	C	145	ALA	N-CA-C	-5.28	105.70	111.82
1	D	305	LEU	CA-C-N	5.11	125.65	120.38
1	D	305	LEU	C-N-CA	5.11	125.65	120.38
1	D	365	ARG	N-CA-C	5.10	116.53	110.97
1	A	359	SER	N-CA-C	5.04	116.77	111.28
1	D	348	PHE	CA-C-N	5.01	124.80	119.28
1	D	348	PHE	C-N-CA	5.01	124.80	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	62	0
1	B	3221	0	3126	38	0
1	C	3209	0	3109	55	0
1	D	3221	0	3126	42	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	24	0	0	1	0
4	B	24	0	0	1	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
5	A	28	0	38	5	0
5	B	84	0	111	12	0
5	C	14	0	19	4	0
5	D	42	0	54	10	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	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	2	0	0	1	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	1	0	0	0	0
11	D	1	0	0	0	0
12	A	78	0	0	11	0
12	B	118	0	0	7	0
12	C	76	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	114	0	0	4	0
All	All	13803	0	12925	217	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 8.

All (217) 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)
5:C:504:BTB:HO8	5:C:504:BTB:HO6	1.23	0.82
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.66	0.77
1:C:347:GLU:OE2	12:C:601:HOH:O	2.03	0.76
1:A:144:GLN:O	12:A:601:HOH:O	2.03	0.75
1:C:235:CYS:H	1:C:238:ARG:HD3	1.51	0.75
1:D:93:PRO:HG3	1:D:106:PRO:HB3	1.67	0.74
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.70	0.72
1:A:201:CYS:SG	12:A:639:HOH:O	2.47	0.72
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.70	0.71
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.74	0.70
5:A:505:BTB:O1	5:A:505:BTB:O4	2.04	0.69
1:C:378:ASP:OD1	12:C:602:HOH:O	2.09	0.69
1:B:408:HIS:ND1	12:B:604:HOH:O	2.26	0.69
1:A:298:GLU:HG3	1:A:299:PRO:HD2	1.75	0.69
1:B:70:ARG:HE	1:B:79:ILE:HD13	1.58	0.68
1:B:149:ARG:NH1	1:B:152:GLU:OE1	2.26	0.68
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.13	0.67
1:B:326:LEU:HD12	5:B:510:BTB:H72	1.77	0.67
1:A:201:CYS:O	1:A:202:ARG:NH1	2.24	0.67
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.75	0.67
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.77	0.67
1:A:432:GLU:HG2	1:A:436:LYS:HE3	1.78	0.66
1:A:70:ARG:NH1	12:A:609:HOH:O	2.27	0.66
1:A:125:SER:HA	1:A:128:ARG:HE	1.60	0.66
1:D:209:THR:O	1:D:213:ASN:ND2	2.28	0.66
1:A:331:TYR:O	1:A:410:TYR:OH	2.14	0.65
1:A:89:GLN:O	12:A:602:HOH:O	2.15	0.65
1:C:262:ARG:NH1	1:C:283:ASN:O	2.31	0.64
1:A:167:GLU:OE2	7:A:507:GOL:O1	2.15	0.63
1:A:256:GLN:O	12:A:603:HOH:O	2.15	0.63
1:A:87:GLN:O	1:A:89:GLN:NE2	2.31	0.63
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:GLY:N	12:D:604:HOH:O	2.30	0.62
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.82	0.62
1:D:321:GLU:OE2	5:D:504:BTB:O3	2.17	0.62
5:B:510:BTB:O3	1:C:384:ASP:OD2	2.18	0.62
5:B:511:BTB:HO1	5:B:511:BTB:HO3	1.37	0.62
1:D:336:VAL:HG21	4:D:503:8J4:C07	2.31	0.60
1:A:476:GLN:OE1	12:A:604:HOH:O	2.16	0.59
1:A:119:ALA:N	12:A:611:HOH:O	2.34	0.58
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.85	0.57
1:C:336:VAL:HG21	4:C:503:8J4:C07	2.35	0.57
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.20	0.56
1:A:86:ALA:O	1:B:97:ARG:NH2	2.39	0.55
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.33	0.55
1:C:200:ASP:OD1	1:C:200:ASP:N	2.37	0.55
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.41	0.55
1:D:149:ARG:NH1	1:D:152:GLU:OE1	2.39	0.55
1:C:128:ARG:O	1:C:132:ASN:ND2	2.40	0.55
1:C:143:SER:O	1:C:145:ALA:N	2.40	0.55
1:C:170:LEU:HD11	1:C:230:VAL:HG21	1.88	0.55
1:D:124:LEU:HD21	1:D:154:GLU:HG2	1.87	0.55
1:D:447:TRP:HA	3:D:502:H4B:N1	2.22	0.54
1:D:67:LYS:O	12:D:601:HOH:O	2.18	0.54
1:C:379:VAL:HG21	1:C:402:ILE:HD11	1.89	0.54
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.90	0.54
1:C:149:ARG:NE	1:C:169:GLU:OE2	2.38	0.53
5:A:504:BTB:O8	5:A:504:BTB:H42	2.09	0.53
1:C:364:THR:O	1:C:368:CYS:HB2	2.09	0.53
1:A:171:VAL:HA	1:A:195:VAL:HG21	1.91	0.53
1:C:320:LEU:HD13	1:C:322:TRP:CZ2	2.44	0.53
1:C:451:PRO:HB2	1:D:455:SER:OG	2.09	0.52
5:D:504:BTB:O3	5:D:504:BTB:O4	2.28	0.52
1:C:78:SER:OG	12:C:603:HOH:O	2.19	0.52
1:B:414:LYS:NZ	12:B:605:HOH:O	2.30	0.52
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.45	0.52
1:A:263:GLY:HA2	1:A:285:ARG:HA	1.92	0.52
1:A:455:SER:HA	1:A:460:PHE:CG	2.45	0.52
1:A:450:PRO:HG3	1:A:457:THR:HG21	1.90	0.52
5:A:505:BTB:O4	12:A:605:HOH:O	2.19	0.52
1:A:143:SER:OG	1:A:144:GLN:N	2.44	0.51
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.91	0.51
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:N	1:C:169:GLU:OE1	2.44	0.51
1:D:358:MET:HE3	1:D:360:THR:OG1	2.10	0.51
1:C:238:ARG:HE	1:C:240:ASP:CG	2.18	0.51
5:D:504:BTB:O8	8:D:510:CL:CL	2.64	0.51
1:D:100:LEU:N	12:D:604:HOH:O	2.43	0.51
1:D:455:SER:HA	1:D:460:PHE:CG	2.46	0.51
1:A:448:ILE:HG21	1:A:464:MET:HE1	1.91	0.50
1:A:387:THR:O	5:A:505:BTB:H61	2.10	0.50
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.46	0.50
1:C:450:PRO:HG3	1:C:457:THR:HG21	1.93	0.50
1:C:156:GLU:OE2	1:C:164:GLN:N	2.43	0.50
1:A:367:LEU:HA	1:A:373:TYR:HB2	1.94	0.50
1:B:378:ASP:OD1	5:B:507:BTB:H71	2.12	0.50
1:B:106:PRO:HB3	12:B:668:HOH:O	2.11	0.49
1:C:453:SER:HA	1:D:452:ILE:HG22	1.94	0.49
1:A:341:LEU:HB3	1:A:348:PHE:HB2	1.95	0.49
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.94	0.49
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.39	0.49
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.94	0.48
1:D:271:THR:O	1:D:275:ILE:HG12	2.12	0.48
1:B:336:VAL:HG21	4:B:503:8J4:C07	2.44	0.48
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.47	0.48
1:C:240:ASP:OD1	1:C:349:PRO:HG2	2.14	0.48
1:C:229:THR:O	1:C:352:PRO:HD2	2.14	0.48
1:A:250:ARG:NH1	1:A:267:ASN:OD1	2.46	0.48
1:B:68:PHE:CD2	1:B:83:THR:HG22	2.49	0.47
1:C:367:LEU:HA	1:C:373:TYR:HB2	1.95	0.47
1:D:138:ILE:HD12	1:D:140:ARG:HD3	1.95	0.47
1:A:347:GLU:O	1:A:349:PRO:HD3	2.15	0.47
1:B:243:ILE:HG21	1:B:337:SER:HB2	1.97	0.47
1:C:119:ALA:N	12:C:611:HOH:O	2.47	0.47
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.44	0.47
1:C:247:GLN:HB2	1:C:250:ARG:HG2	1.97	0.47
5:B:511:BTB:H32	5:B:511:BTB:H71	1.50	0.47
1:C:316[B]:GLU:OE1	12:C:605:HOH:O	2.20	0.47
1:C:428:MET:HG3	1:C:458:PRO:HB2	1.95	0.47
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.50	0.47
1:B:90:GLN:HB2	1:B:468:PHE:CD1	2.50	0.46
5:D:505:BTB:H42	5:D:505:BTB:H71	1.51	0.46
1:B:447:TRP:HA	3:B:502:H4B:N1	2.30	0.46
1:C:160:THR:HG23	1:C:162:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:504:BTB:H42	5:C:504:BTB:H52	1.59	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.46
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.81	0.46
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	1.97	0.46
1:D:171:VAL:HG12	1:D:175:LYS:HE3	1.98	0.46
5:B:505:BTB:H72	12:B:602:HOH:O	2.16	0.45
1:C:203:SER:OG	1:C:204:ALA:N	2.47	0.45
1:A:99:CYS:HB3	1:B:466:ASN:HB3	1.98	0.45
1:A:207:MET:HE3	1:A:293:LEU:HB3	1.98	0.45
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.97	0.45
1:C:248:LEU:HD12	1:C:335:ALA:HB1	1.99	0.45
5:B:506:BTB:H52	5:B:506:BTB:H32	1.51	0.45
1:C:85:SER:HB3	1:C:467:TYR:CE2	2.52	0.45
1:C:309:LEU:HA	1:C:309:LEU:HD12	1.72	0.45
1:C:298:GLU:OE1	5:C:504:BTB:N	2.50	0.45
1:D:298:GLU:OE1	5:D:505:BTB:N	2.50	0.45
1:B:312:GLU:CD	1:B:329:ARG:HH21	2.25	0.45
1:B:448:ILE:HG21	1:B:464:MET:HE1	1.99	0.45
1:C:358:MET:HE3	1:C:360:THR:OG1	2.17	0.45
5:D:505:BTB:H11	5:D:505:BTB:H51	1.30	0.45
5:D:505:BTB:H72	5:D:505:BTB:H61	1.46	0.45
1:C:91:ASP:OD1	12:C:604:HOH:O	2.20	0.44
5:B:507:BTB:O8	12:B:602:HOH:O	2.21	0.44
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.57	0.44
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.98	0.44
1:A:275:ILE:HG12	1:A:281:PRO:HG3	1.98	0.44
5:D:504:BTB:H71	5:D:504:BTB:H42	1.53	0.44
1:A:339:MET:HE2	1:A:473:PHE:HB3	2.00	0.44
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.99	0.44
1:A:336:VAL:HG21	4:A:503:8J4:C07	2.47	0.44
1:A:396:ASP:OD1	1:A:396:ASP:N	2.49	0.44
1:B:247:GLN:HB2	1:B:250:ARG:HG2	2.00	0.44
1:D:200:ASP:O	1:D:202:ARG:HG2	2.17	0.44
1:A:144:GLN:CG	1:A:145:ALA:H	2.30	0.43
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.00	0.43
1:A:70:ARG:NH2	12:A:614:HOH:O	2.43	0.43
1:B:106:PRO:O	12:B:603:HOH:O	2.21	0.43
1:A:334:PRO:HB3	1:A:357:TYR:CZ	2.53	0.43
1:A:90:GLN:HB2	1:A:468:PHE:CD1	2.53	0.43
1:A:127:ALA:O	1:A:131:ILE:HG12	2.19	0.43
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ARG:HD3	1:B:166:ARG:CZ	2.48	0.43
1:B:71:VAL:HG13	1:B:463:GLU:HB2	2.00	0.43
1:B:321:GLU:OE1	5:B:504:BTB:H62	2.18	0.43
1:B:388:ARG:HE	1:B:388:ARG:HB2	1.44	0.43
1:A:94:CYS:SG	1:A:100:LEU:N	2.70	0.43
5:B:505:BTB:H52	5:B:505:BTB:H32	1.50	0.43
5:D:506:BTB:H11	5:D:506:BTB:H71	1.76	0.43
1:A:269:GLU:O	1:A:272:GLU:HB3	2.19	0.43
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.54	0.43
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.53	0.43
1:B:67:LYS:N	12:B:622:HOH:O	2.52	0.43
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.00	0.43
1:A:242:ARG:NE	1:A:479:PRO:HD3	2.33	0.42
5:B:507:BTB:H11	5:B:507:BTB:H52	1.50	0.42
1:C:396:ASP:OD2	1:D:453:SER:OG	2.18	0.42
1:A:246:SER:OG	1:A:250:ARG:HD2	2.19	0.42
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.54	0.42
1:C:245:ASN:O	1:C:337:SER:OG	2.37	0.42
1:C:397:LYS:HG3	1:D:400:VAL:HG11	2.02	0.42
1:D:199:ARG:O	1:D:232:PRO:HG3	2.19	0.42
1:B:249:VAL:O	1:B:250:ARG:HG2	2.18	0.42
1:C:470:SER:HA	1:C:471:PRO:C	2.45	0.42
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.55	0.42
1:D:204:ALA:O	1:D:207:MET:HB2	2.20	0.42
1:D:478:ASP:HA	1:D:479:PRO:HD3	1.81	0.42
1:A:228:ILE:HG13	1:A:353:PHE:HB3	2.00	0.42
1:A:359:SER:OG	1:A:419:ASP:HA	2.20	0.42
1:C:369:ASP:HB2	1:C:372:ARG:HG2	2.02	0.42
1:A:144:GLN:CD	1:A:145:ALA:H	2.29	0.41
1:A:298:GLU:OE2	12:A:606:HOH:O	2.22	0.41
1:A:382:CYS:HA	5:A:504:BTB:H11	2.02	0.41
1:C:224:LEU:HD12	1:C:356:TRP:HB3	2.02	0.41
1:D:72:LYS:H	1:D:463:GLU:HB2	1.86	0.41
5:D:506:BTB:H32	5:D:506:BTB:H52	1.59	0.41
1:B:301:GLU:HB3	1:B:303:PHE:HE1	1.85	0.41
1:B:396:ASP:OD1	1:B:396:ASP:N	2.47	0.41
1:D:213:ASN:N	1:D:213:ASN:HD22	2.19	0.41
5:C:504:BTB:H71	5:C:504:BTB:H32	1.77	0.41
1:D:249:VAL:HA	12:D:611:HOH:O	2.21	0.41
1:D:301:GLU:HB3	1:D:303:PHE:HE1	1.86	0.41
1:A:128:ARG:O	1:A:132:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.03	0.41
5:B:510:BTB:H32	1:C:382:CYS:HA	2.01	0.41
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.33	0.41
1:A:370:PRO:HB2	1:B:75:GLU:HG3	2.03	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.48	0.41
1:D:235[B]:CYS:HA	1:D:236:PRO:HD3	1.93	0.41
1:D:245:ASN:O	1:D:337:SER:OG	2.37	0.41
1:A:384:ASP:HB3	12:A:656:HOH:O	2.21	0.41
1:D:435:GLN:O	1:D:439:GLY:HA2	2.21	0.41
1:A:393:LEU:HD12	1:B:404:VAL:HG23	2.03	0.40
1:A:104:VAL:O	1:A:106:PRO:HD3	2.21	0.40
1:A:288:VAL:HG12	1:A:289:LEU:O	2.21	0.40
1:C:238:ARG:NH2	1:C:240:ASP:OD2	2.50	0.40
1:D:387:THR:HA	1:D:394:TRP:CD1	2.56	0.40
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.35	0.40
1:A:466:ASN:HB3	1:B:99:CYS:HB3	2.03	0.40
1:B:429:LYS:HA	1:B:429:LYS:HD2	1.89	0.40
1:D:162:THR:OG1	1:D:163:TYR:N	2.54	0.40
1:C:165:LEU:HG	1:C:346:LEU:HD12	2.04	0.40
1:C:453:SER:O	1:C:454:GLY:C	2.65	0.40
1:B:364:THR:HG21	1:B:452:ILE:HG23	2.02	0.40

There are no symmetry-related clashes.

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%)	369 (92%)	29 (7%)	4 (1%)	12	11
1	B	401/440 (91%)	387 (96%)	14 (4%)	0	100	100
1	C	399/440 (91%)	380 (95%)	16 (4%)	3 (1%)	16	16
1	D	401/440 (91%)	388 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1603/1760 (91%)	1524 (95%)	72 (4%)	7 (0%)	30	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	A	90	GLN
1	C	89	GLN
1	C	143	SER
1	A	297	ASP
1	A	107	ARG
1	A	181	ALA

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%)	322 (93%)	23 (7%)	15	17
1	B	344/373 (92%)	331 (96%)	13 (4%)	29	40
1	C	342/373 (92%)	332 (97%)	10 (3%)	37	51
1	D	344/373 (92%)	340 (99%)	4 (1%)	63	78
All	All	1375/1492 (92%)	1325 (96%)	50 (4%)	31	42

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	76	VAL
1	A	109	LEU
1	A	121	GLU
1	A	124	LEU
1	A	133	GLN
1	A	140	ARG
1	A	152	GLU

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Mol	Chain	Res	Type
1	A	226	SER
1	A	228	ILE
1	A	238	ARG
1	A	242	ARG
1	A	256	GLN
1	A	257	GLN
1	A	285	ARG
1	A	298	GLU
1	A	301	GLU
1	A	309	LEU
1	A	329	ARG
1	A	342	GLU
1	A	396	ASP
1	A	403	ASN
1	A	470	SER
1	B	90	GLN
1	B	148	GLN
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	238	ARG
1	B	246	SER
1	B	298	GLU
1	B	326	LEU
1	B	342	GLU
1	B	343	ILE
1	B	364	THR
1	B	389	THR
1	B	396	ASP
1	C	71	VAL
1	C	90	GLN
1	C	137	SER
1	C	154	GLU
1	C	160	THR
1	C	216	LYS
1	C	221	ARG
1	C	257	GLN
1	C	309	LEU
1	C	342	GLU
1	D	71	VAL
1	D	89	GLN
1	D	124	LEU
1	D	136	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	220	ASN
1	A	403	ASN
1	A	466	ASN
1	B	213	ASN
1	B	403	ASN
1	B	476	GLN
1	C	122	GLN
1	C	126	GLN
1	C	164	GLN
1	C	233	GLN
1	C	256	GLN
1	C	430	HIS
1	C	476	GLN
1	D	213	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 39 ligands modelled in this entry, 13 are monoatomic - leaving 26 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
2	HEM	C	501	1	50,50,50	2.05	9 (18%)	67,82,82	1.36	7 (10%)
5	BTB	B	506	-	13,13,13	0.72	0	7,16,16	0.80	0
4	8J4	A	503	-	26,26,26	0.89	0	33,35,35	0.94	0
3	H4B	B	502	-	17,18,18	0.80	0	14,26,26	2.00	6 (42%)
5	BTB	C	504	-	13,13,13	0.34	0	7,16,16	0.40	0
5	BTB	B	510	9	13,13,13	0.48	0	7,16,16	0.64	0
5	BTB	D	505	-	13,13,13	0.43	0	7,16,16	0.84	0
5	BTB	B	504	9	13,13,13	0.42	0	7,16,16	0.41	0
5	BTB	B	507	-	13,13,13	0.39	0	7,16,16	0.77	0
4	8J4	D	503	-	26,26,26	0.83	0	33,35,35	1.03	1 (3%)
3	H4B	A	502	-	17,18,18	0.74	0	14,26,26	1.90	6 (42%)
5	BTB	B	511	-	13,13,13	0.65	0	7,16,16	1.08	1 (14%)
3	H4B	D	502	-	17,18,18	0.87	0	14,26,26	1.90	5 (35%)
7	GOL	C	506	-	5,5,5	0.43	0	5,5,5	0.55	0
2	HEM	D	501	1	50,50,50	1.99	8 (16%)	67,82,82	1.56	13 (19%)
2	HEM	A	501	1	50,50,50	1.99	9 (18%)	67,82,82	1.35	9 (13%)
5	BTB	D	504	9	13,13,13	0.49	0	7,16,16	0.45	0
2	HEM	B	501	1	50,50,50	1.99	10 (20%)	67,82,82	1.57	10 (14%)
5	BTB	B	505	-	13,13,13	0.36	0	7,16,16	0.45	0
5	BTB	A	505	-	13,13,13	0.37	0	7,16,16	0.59	0
3	H4B	C	502	-	17,18,18	0.76	0	14,26,26	2.00	5 (35%)
4	8J4	C	503	-	26,26,26	0.92	0	33,35,35	1.12	3 (9%)
5	BTB	D	506	-	13,13,13	0.43	0	7,16,16	0.85	0
4	8J4	B	503	-	26,26,26	0.96	2 (7%)	33,35,35	1.12	2 (6%)
5	BTB	A	504	9	13,13,13	0.38	0	7,16,16	0.46	0
7	GOL	A	507	-	5,5,5	0.46	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	7/14/54/54	-
5	BTB	B	506	-	-	3/21/21/21	-
4	8J4	A	503	-	-	2/10/19/19	0/3/3/3
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
5	BTB	C	504	-	-	2/21/21/21	-
5	BTB	B	510	9	-	5/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	D	505	-	-	14/21/21/21	-
5	BTB	B	504	9	-	2/21/21/21	-
5	BTB	B	507	-	-	3/21/21/21	-
4	8J4	D	503	-	-	2/10/19/19	0/3/3/3
3	H4B	A	502	-	-	1/8/17/17	0/2/2/2
5	BTB	B	511	-	-	7/21/21/21	-
3	H4B	D	502	-	-	1/8/17/17	0/2/2/2
7	GOL	C	506	-	-	4/4/4/4	-
2	HEM	D	501	1	-	2/14/54/54	-
2	HEM	A	501	1	-	4/14/54/54	-
5	BTB	D	504	9	-	8/21/21/21	-
2	HEM	B	501	1	-	2/14/54/54	-
5	BTB	B	505	-	-	8/21/21/21	-
5	BTB	A	505	-	-	6/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	8J4	C	503	-	-	3/10/19/19	0/3/3/3
5	BTB	D	506	-	-	5/21/21/21	-
4	8J4	B	503	-	-	0/10/19/19	0/3/3/3
5	BTB	A	504	9	-	8/21/21/21	-
7	GOL	A	507	-	-	3/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3D-C2D	7.97	1.54	1.36
2	B	501	HEM	C3D-C2D	7.40	1.52	1.36
2	D	501	HEM	C3D-C2D	7.37	1.52	1.36
2	A	501	HEM	C3D-C2D	7.20	1.52	1.36
2	D	501	HEM	FE-NB	6.48	2.14	1.94
2	A	501	HEM	FE-NA	5.87	2.14	1.95
2	C	501	HEM	FE-NB	5.56	2.12	1.94
2	B	501	HEM	FE-NB	5.41	2.11	1.94
2	A	501	HEM	FE-ND	5.40	2.11	1.94
2	C	501	HEM	FE-ND	5.16	2.10	1.94
2	B	501	HEM	FE-NC	5.16	2.12	1.95
2	D	501	HEM	FE-NC	4.63	2.10	1.95
2	C	501	HEM	FE-NA	4.02	2.08	1.95
2	B	501	HEM	FE-ND	3.96	2.07	1.94
2	A	501	HEM	FE-NB	3.76	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NA	3.52	2.06	1.95
2	B	501	HEM	FE-NA	3.49	2.06	1.95
2	C	501	HEM	FE-NC	3.40	2.06	1.95
2	B	501	HEM	CAB-C3B	3.35	1.56	1.47
2	C	501	HEM	CAB-C3B	3.07	1.55	1.47
2	A	501	HEM	CAC-C3C	3.06	1.55	1.47
2	D	501	HEM	CAC-C3C	3.04	1.55	1.47
2	C	501	HEM	CAC-C3C	3.04	1.55	1.47
2	D	501	HEM	CAB-C3B	3.01	1.55	1.47
2	D	501	HEM	FE-ND	3.01	2.04	1.94
2	A	501	HEM	CAB-C3B	2.96	1.55	1.47
2	B	501	HEM	CAC-C3C	2.87	1.55	1.47
2	A	501	HEM	CMC-C2C	2.62	1.56	1.50
2	A	501	HEM	FE-NC	2.47	2.03	1.95
2	C	501	HEM	CMB-C2B	2.42	1.55	1.50
2	A	501	HEM	C2A-C3A	-2.40	1.32	1.38
2	C	501	HEM	CMC-C2C	2.25	1.55	1.50
2	B	501	HEM	CMC-C2C	2.23	1.55	1.50
2	B	501	HEM	C2A-C3A	-2.18	1.33	1.38
2	D	501	HEM	CMB-C2B	2.04	1.55	1.50
2	B	501	HEM	CMB-C2B	2.01	1.54	1.50
4	B	503	8J4	C05-C10	-2.01	1.39	1.42
4	B	503	8J4	C09-C10	-2.00	1.38	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	5.72	111.98	105.21
2	D	501	HEM	C4D-ND-C1D	5.40	111.60	105.21
2	C	501	HEM	C4D-ND-C1D	5.39	111.59	105.21
3	B	502	H4B	C2-N1-C8A	4.62	121.51	113.36
3	C	502	H4B	C2-N1-C8A	4.37	121.08	113.36
2	D	501	HEM	CBD-CAD-C3D	-4.31	100.61	112.53
3	D	502	H4B	C2-N1-C8A	4.29	120.93	113.36
3	A	502	H4B	C2-N1-C8A	4.22	120.81	113.36
2	A	501	HEM	C4D-ND-C1D	4.11	110.08	105.21
2	B	501	HEM	C3B-C2B-C1B	3.69	109.18	106.41
2	B	501	HEM	CBA-CAA-C2A	-3.59	102.61	112.53
2	D	501	HEM	C3B-C2B-C1B	3.55	109.08	106.41
2	B	501	HEM	CBD-CAD-C3D	-3.35	103.27	112.53
4	C	503	8J4	C23-C29-N30	-3.22	104.94	112.67
2	A	501	HEM	C3B-C2B-C1B	3.17	108.79	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CHA-C4D-ND	3.00	128.07	124.37
2	A	501	HEM	C3B-C4B-NB	-2.99	107.32	109.47
2	A	501	HEM	C1B-NB-C4B	2.89	108.63	105.21
3	C	502	H4B	O4-C4-C4A	-2.88	120.32	127.26
3	B	502	H4B	C4A-C4-N3	2.82	119.89	112.13
3	A	502	H4B	O4-C4-C4A	-2.79	120.54	127.26
4	B	503	8J4	O12-C11-C08	2.72	117.15	109.16
2	B	501	HEM	C1B-NB-C4B	2.70	108.40	105.21
3	C	502	H4B	C4A-C4-N3	2.63	119.36	112.13
2	D	501	HEM	C1B-NB-C4B	2.62	108.30	105.21
3	B	502	H4B	O4-C4-C4A	-2.61	120.96	127.26
2	D	501	HEM	CAD-C3D-C4D	2.57	129.18	124.70
2	C	501	HEM	C1B-NB-C4B	2.56	108.23	105.21
2	B	501	HEM	C3B-C4B-NB	-2.55	107.63	109.47
2	D	501	HEM	C2B-C1B-NB	-2.53	106.94	109.84
2	D	501	HEM	CMD-C2D-C1D	2.52	128.97	125.03
4	B	503	8J4	C03-C02-N01	-2.52	119.08	122.09
2	C	501	HEM	C3B-C4B-NB	-2.49	107.68	109.47
3	C	502	H4B	C2-N3-C4	-2.49	120.60	125.11
3	D	502	H4B	O4-C4-C4A	-2.48	121.28	127.26
3	A	502	H4B	C4A-C4-N3	2.48	118.94	112.13
2	A	501	HEM	CBD-CAD-C3D	-2.47	105.71	112.53
3	D	502	H4B	C4A-C4-N3	2.46	118.88	112.13
2	B	501	HEM	CAD-CBD-CGD	-2.43	107.22	113.67
3	D	502	H4B	C2-N3-C4	-2.33	120.88	125.11
2	C	501	HEM	C2A-C1A-NA	-2.33	107.57	110.15
2	D	501	HEM	C2A-C1A-NA	-2.30	107.60	110.15
3	A	502	H4B	C2-N3-C4	-2.29	120.95	125.11
4	C	503	8J4	O12-C11-C08	2.28	115.85	109.16
2	C	501	HEM	C3B-C2B-C1B	2.23	108.08	106.41
3	B	502	H4B	C2-N3-C4	-2.23	121.07	125.11
5	B	511	BTB	O1-C1-C2	-2.22	106.19	111.40
2	C	501	HEM	CHC-C1C-NC	2.21	126.86	124.45
3	B	502	H4B	C4-C4A-N5	2.17	122.18	116.27
3	C	502	H4B	N2-C2-N3	2.17	121.33	116.76
2	B	501	HEM	CMD-C2D-C1D	2.16	128.42	125.03
2	C	501	HEM	CHA-C4D-ND	2.16	127.04	124.37
2	D	501	HEM	C3A-C4A-NA	-2.16	106.67	110.14
2	A	501	HEM	CMD-C2D-C1D	2.16	128.41	125.03
2	B	501	HEM	C2B-C1B-NB	-2.11	107.41	109.84
2	D	501	HEM	CBA-CAA-C2A	-2.10	106.72	112.53
2	A	501	HEM	C2B-C1B-NB	-2.09	107.44	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHD-C1D-ND	2.09	126.67	124.42
4	C	503	8J4	C29-C23-C24	-2.06	116.23	120.63
2	D	501	HEM	C1D-C2D-C3D	-2.06	104.82	106.98
3	A	502	H4B	N2-C2-N3	2.05	121.09	116.76
3	A	502	H4B	C4-C4A-N5	2.04	121.83	116.27
2	A	501	HEM	CHA-C4D-ND	2.04	126.89	124.37
3	D	502	H4B	O9-C9-C6	-2.03	104.41	109.28
4	D	503	8J4	C03-C02-N01	-2.03	119.66	122.09
3	B	502	H4B	N3-C2-N1	-2.03	119.61	123.32
2	A	501	HEM	CAD-C3D-C4D	2.01	128.20	124.70
2	D	501	HEM	C4A-NA-C1A	2.01	109.09	105.82

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	8J4	C23-C29-N30-C31
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	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	O1-C1-C2-C3
5	B	505	BTB	O1-C1-C2-C4
5	B	505	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	506	BTB	O1-C1-C2-C3
5	B	506	BTB	O1-C1-C2-N
5	B	507	BTB	C3-C2-C4-O4
5	B	507	BTB	N-C2-C4-O4
5	B	510	BTB	O1-C1-C2-C3
5	B	510	BTB	O1-C1-C2-C4
5	B	510	BTB	O1-C1-C2-N
5	B	511	BTB	C3-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	B	511	BTB	C3-C2-N-C7
5	B	511	BTB	C4-C2-N-C5
5	B	511	BTB	C6-C5-N-C7
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C6-C5-N-C7
5	D	506	BTB	C1-C2-C4-O4
5	D	506	BTB	C3-C2-C4-O4
5	D	506	BTB	N-C2-C4-O4
7	A	507	GOL	O1-C1-C2-C3
7	C	506	GOL	O1-C1-C2-C3
7	C	506	GOL	C1-C2-C3-O3
5	B	505	BTB	N-C5-C6-O6
5	B	505	BTB	N-C7-C8-O8
5	B	506	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C3D-CAD-CBD-CGD
4	C	503	8J4	C26-C21-O12-C11
4	C	503	8J4	C22-C21-O12-C11
5	D	504	BTB	N-C5-C6-O6
3	B	502	H4B	C7-C6-C9-O9
5	B	510	BTB	N-C5-C6-O6
5	D	505	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
7	A	507	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-O2
5	B	507	BTB	N-C7-C8-O8
5	A	504	BTB	C6-C5-N-C7
4	D	503	8J4	C26-C21-O12-C11
2	A	501	HEM	C1A-C2A-CAA-CBA
7	C	506	GOL	O2-C2-C3-O3
4	D	503	8J4	C22-C21-O12-C11
3	B	502	H4B	C7-C6-C9-C10
5	D	504	BTB	N-C7-C8-O8
5	B	510	BTB	C4-C2-C3-O3

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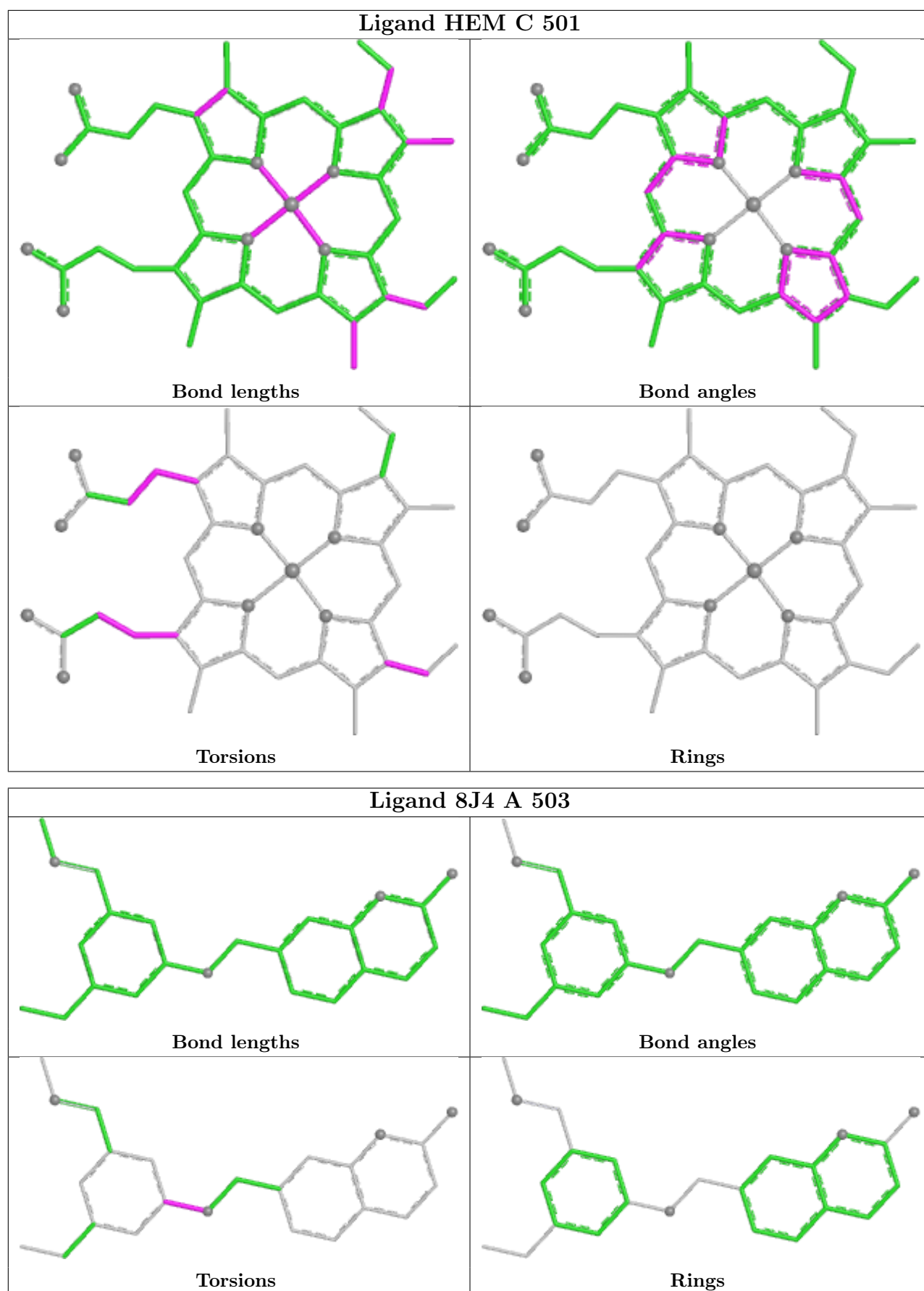
Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
5	A	504	BTB	C4-C2-C3-O3
5	D	506	BTB	N-C5-C6-O6
2	C	501	HEM	C2D-C3D-CAD-CBD
5	B	511	BTB	C1-C2-N-C5
5	B	511	BTB	C1-C2-N-C7
5	C	504	BTB	N-C2-C4-O4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5
4	A	503	8J4	C26-C21-O12-C11
5	A	505	BTB	N-C5-C6-O6
2	C	501	HEM	C4D-C3D-CAD-CBD
5	D	505	BTB	C3-C2-C4-O4
5	D	506	BTB	N-C7-C8-O8
4	A	503	8J4	C22-C21-O12-C11
2	D	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	B	501	HEM	C2A-CAA-CBA-CGA
7	A	507	GOL	O2-C2-C3-O3
5	A	505	BTB	C4-C2-C3-O3
5	C	504	BTB	C1-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
2	C	501	HEM	C3A-C2A-CAA-CBA
3	A	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
3	D	502	H4B	N5-C6-C9-O9
5	A	505	BTB	O1-C1-C2-N
5	B	511	BTB	C4-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

There are no ring outliers.

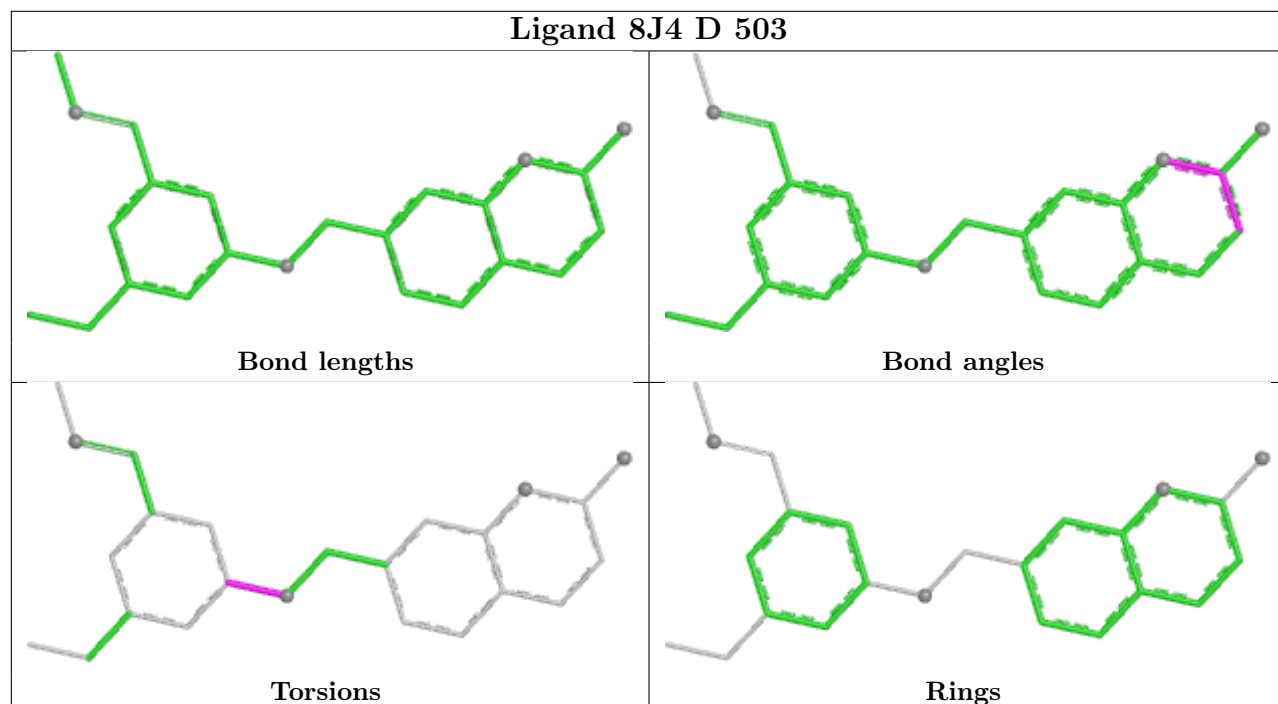
25 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	2	0
5	B	506	BTB	1	0
4	A	503	8J4	1	0
3	B	502	H4B	1	0
5	C	504	BTB	4	0
5	B	510	BTB	3	0
5	D	505	BTB	4	0
5	B	504	BTB	1	0
5	B	507	BTB	3	0
4	D	503	8J4	1	0
3	A	502	H4B	1	0
5	B	511	BTB	2	0
3	D	502	H4B	1	0
2	D	501	HEM	3	0
2	A	501	HEM	4	0
5	D	504	BTB	4	0
2	B	501	HEM	2	0
5	B	505	BTB	2	0
5	A	505	BTB	3	0
3	C	502	H4B	1	0
4	C	503	8J4	1	0
5	D	506	BTB	2	0
4	B	503	8J4	1	0
5	A	504	BTB	2	0
7	A	507	GOL	1	0

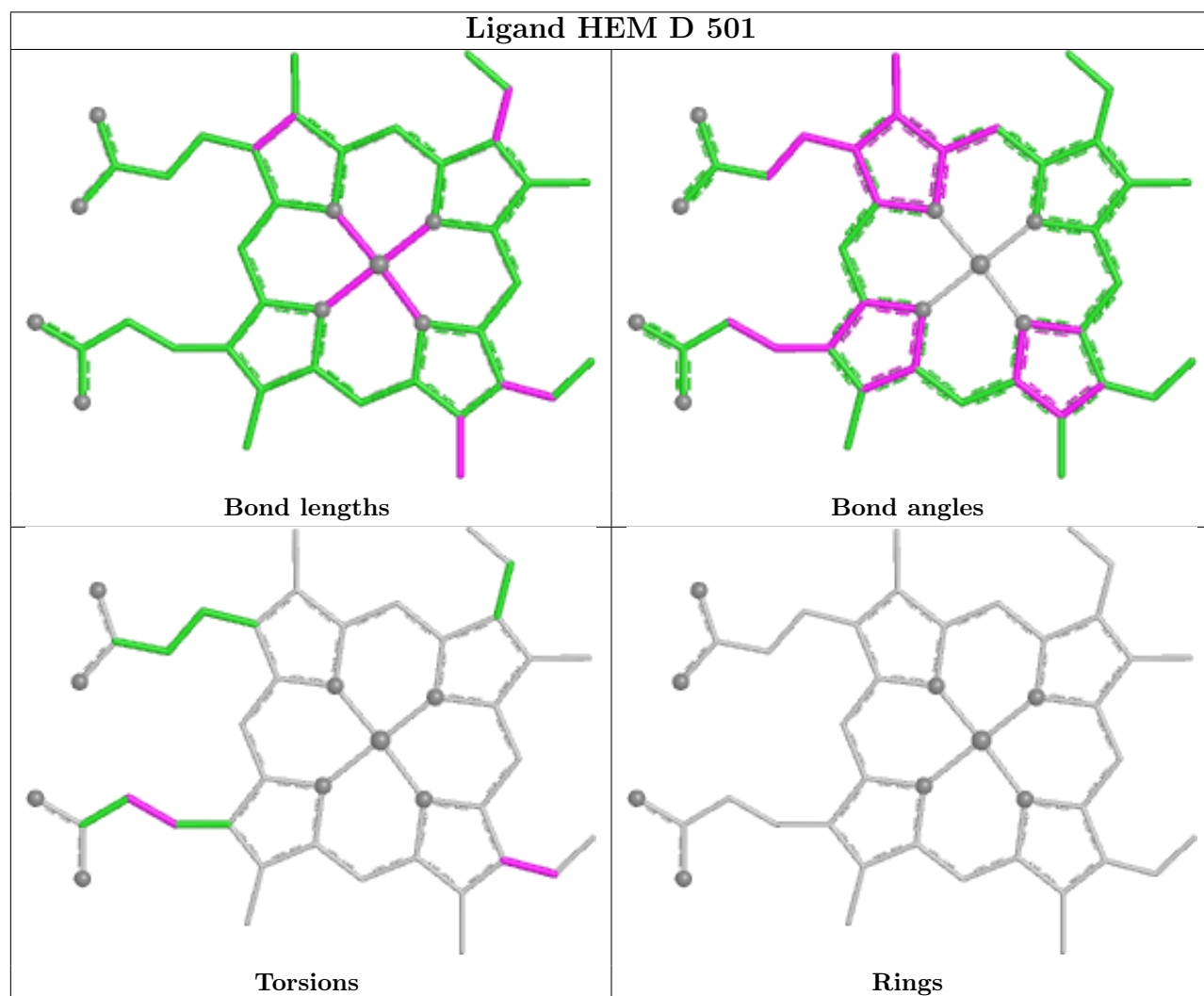
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

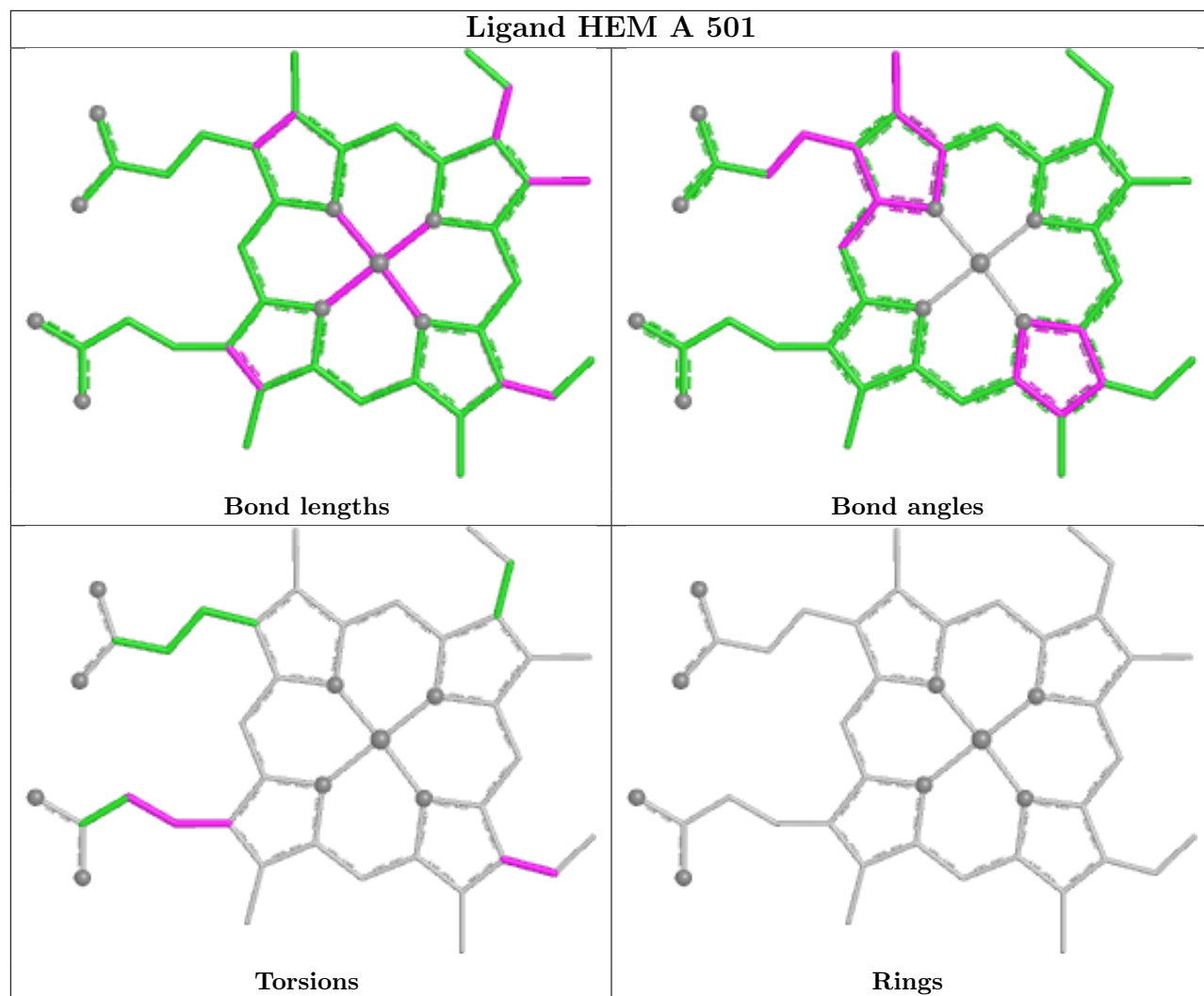


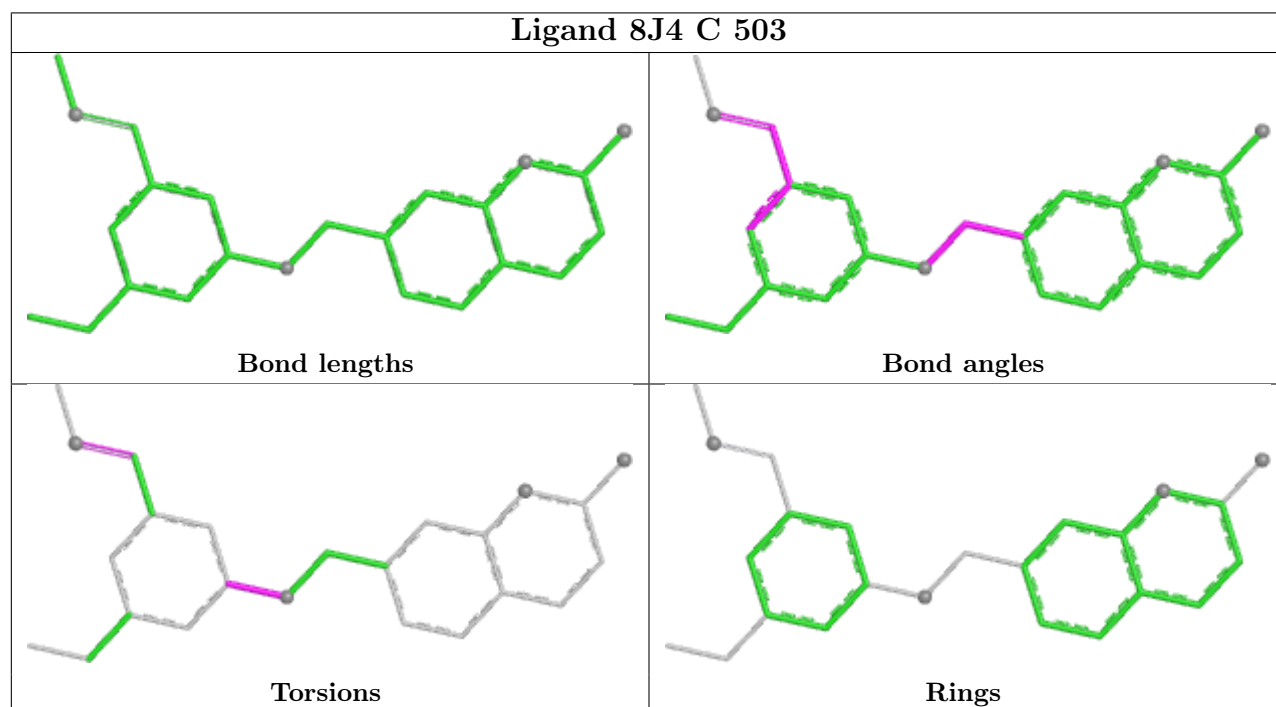
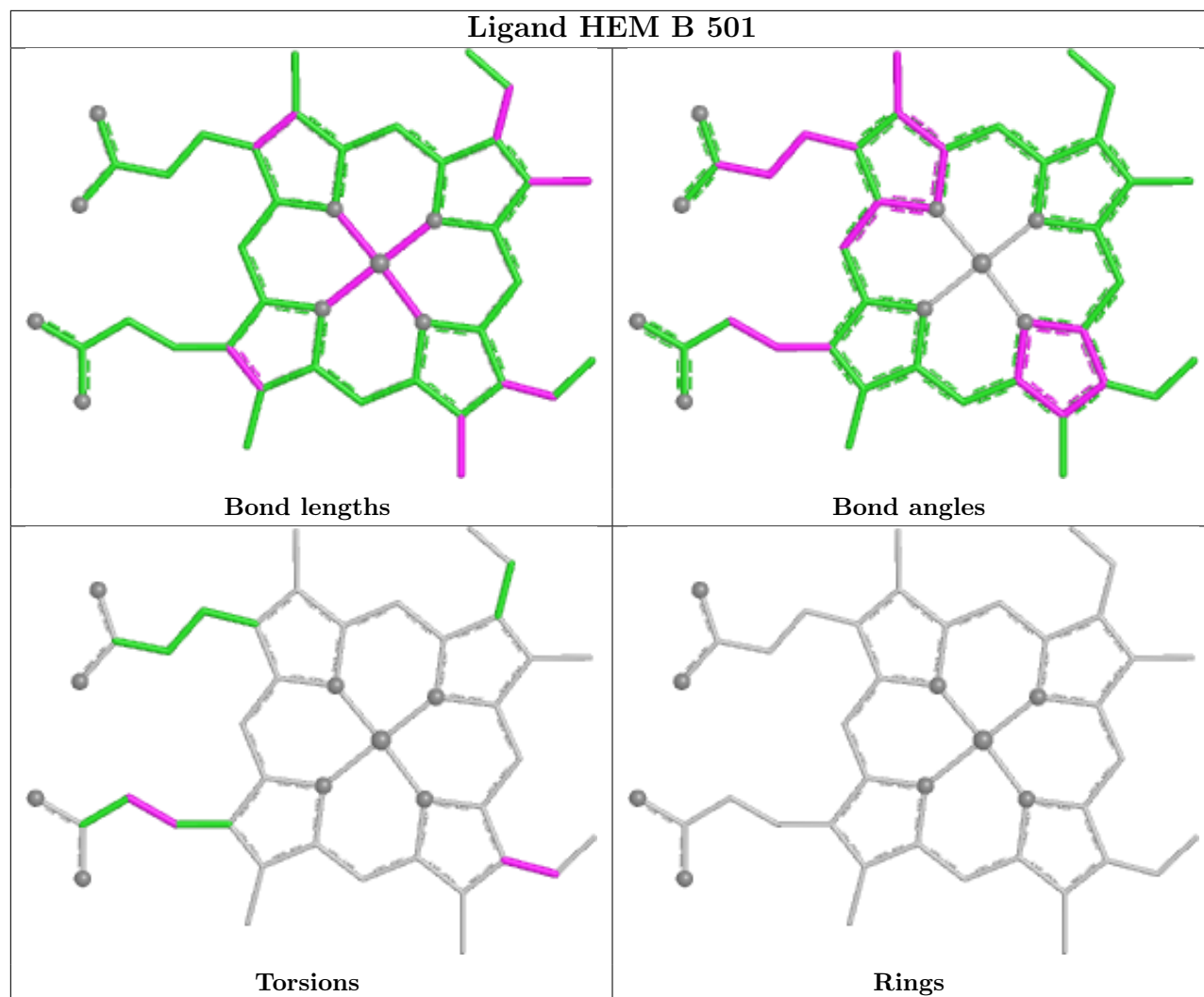
Ligand 8J4 D 503

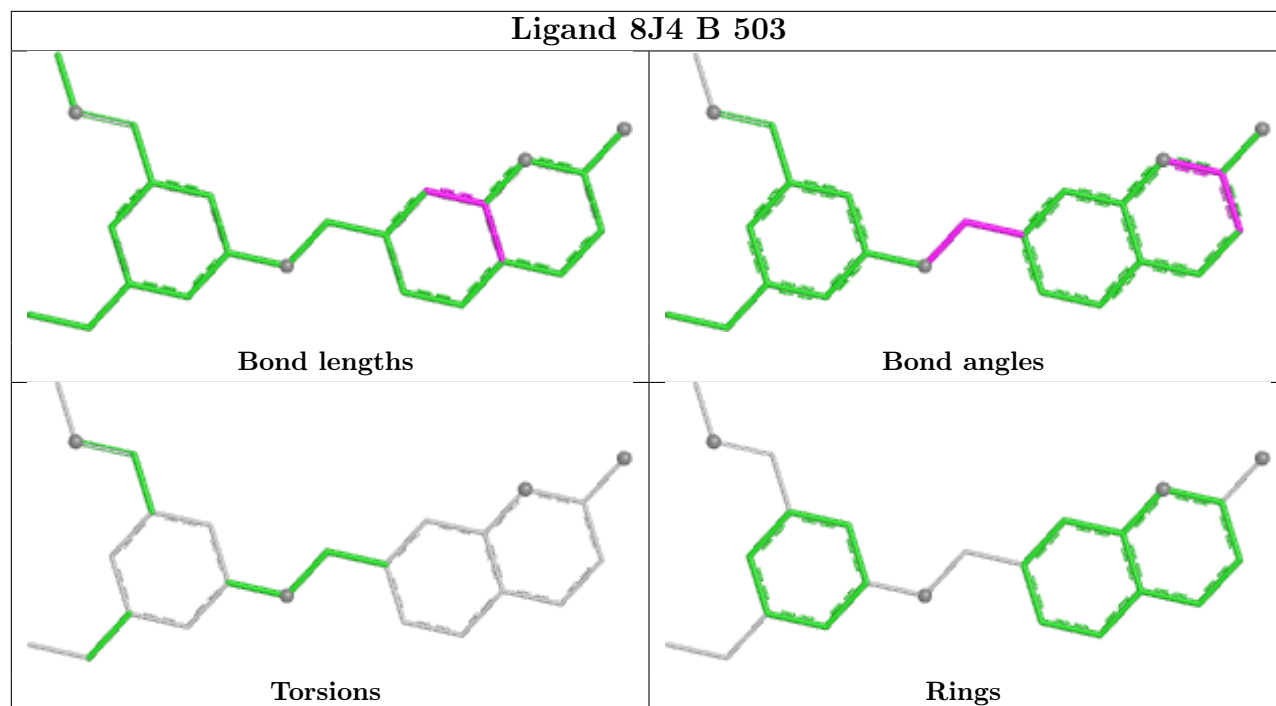


Ligand HEM D 501









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.08	0 100 100	27, 60, 107, 126	2 (0%)
1	B	402/440 (91%)	-1.29	0 100 100	27, 44, 77, 108	3 (0%)
1	C	401/440 (91%)	-1.19	0 100 100	27, 55, 95, 118	2 (0%)
1	D	402/440 (91%)	-1.29	0 100 100	26, 43, 69, 117	3 (0%)
All	All	1609/1760 (91%)	-1.21	0 100 100	26, 50, 93, 126	10 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BTB	B	505	14/14	0.94	0.06	82,95,103,105	0
5	BTB	D	506	14/14	0.95	0.06	95,101,106,106	0
5	BTB	A	505	14/14	0.96	0.05	72,84,90,90	0
5	BTB	B	507	14/14	0.97	0.04	77,82,89,90	0

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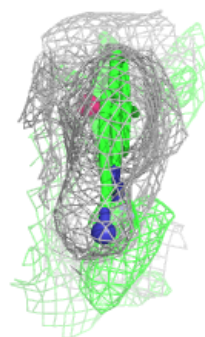
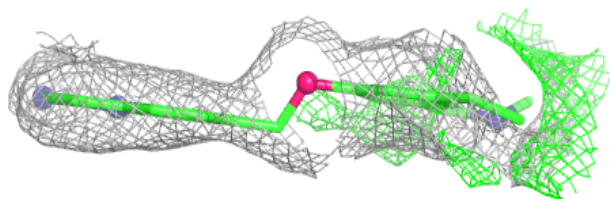
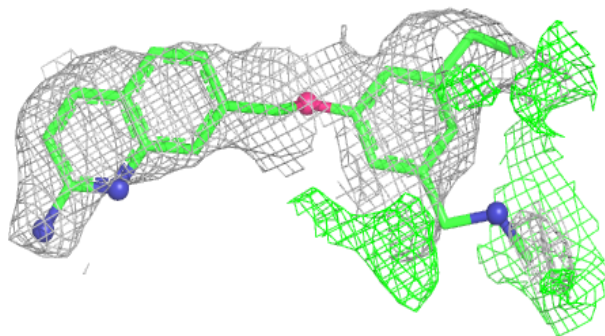
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	C	504	14/14	0.97	0.04	75,87,92,94	0
4	8J4	C	503	24/24	0.97	0.08	67,76,92,96	0
4	8J4	A	503	24/24	0.98	0.08	79,97,117,122	0
3	H4B	A	502	17/17	0.98	0.04	48,60,66,69	0
5	BTB	D	505	14/14	0.98	0.03	65,74,78,79	0
5	BTB	B	506	14/14	0.98	0.04	74,83,88,90	0
3	H4B	C	502	17/17	0.99	0.05	55,66,78,80	0
5	BTB	B	504	14/14	0.99	0.03	35,55,72,73	0
3	H4B	D	502	17/17	0.99	0.04	27,46,52,52	0
2	HEM	C	501	43/43	0.99	0.04	35,54,73,86	0
4	8J4	B	503	24/24	0.99	0.06	50,66,103,106	0
5	BTB	B	510	14/14	0.99	0.04	39,68,83,83	0
5	BTB	B	511	14/14	0.99	0.04	59,63,87,90	0
3	H4B	B	502	17/17	0.99	0.04	34,46,54,61	0
5	BTB	D	504	14/14	0.99	0.04	46,65,77,81	0
4	8J4	D	503	24/24	0.99	0.05	48,61,96,108	0
5	BTB	A	504	14/14	0.99	0.04	75,85,93,96	0
7	GOL	A	507	6/6	0.99	0.03	64,72,77,80	0
7	GOL	C	506	6/6	0.99	0.03	57,65,71,71	0
8	CL	A	508	1/1	0.99	0.03	67,67,67,67	0
8	CL	C	507	1/1	0.99	0.04	71,71,71,71	0
8	CL	D	508	1/1	0.99	0.04	47,47,47,47	0
8	CL	D	510	1/1	0.99	0.03	79,79,79,79	0
9	GD	A	509	1/1	0.99	0.02	129,129,129,129	1
2	HEM	A	501	43/43	1.00	0.04	39,50,73,80	0
8	CL	B	508	1/1	1.00	0.04	50,50,50,50	0
6	ZN	A	506	1/1	1.00	0.01	46,46,46,46	0
6	ZN	C	505	1/1	1.00	0.01	45,45,45,45	0
2	HEM	D	501	43/43	1.00	0.03	31,41,68,71	0
2	HEM	B	501	43/43	1.00	0.03	30,38,61,67	0
9	GD	B	509	1/1	1.00	0.01	52,52,52,52	0
9	GD	C	508	1/1	1.00	0.02	111,111,111,111	1
9	GD	D	507	1/1	1.00	0.00	51,51,51,51	0
10	CA	A	510	1/1	1.00	0.03	37,37,37,37	0
11	MG	D	509	1/1	1.00	0.02	35,35,35,35	0

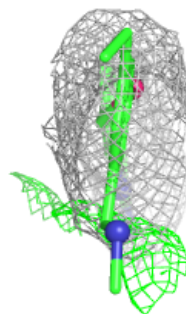
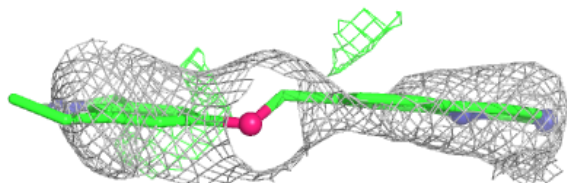
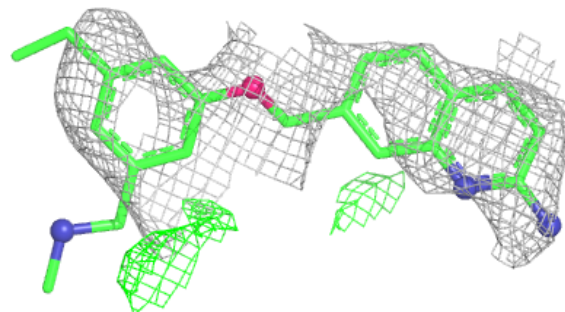
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8J4 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)

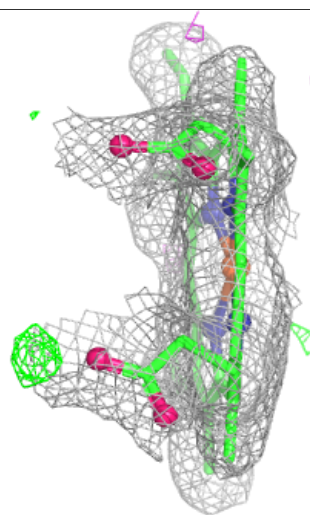
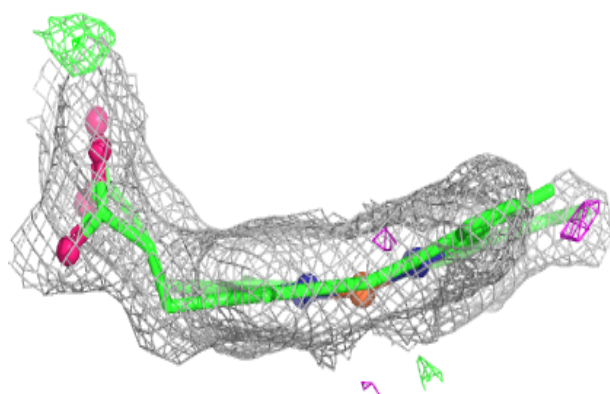
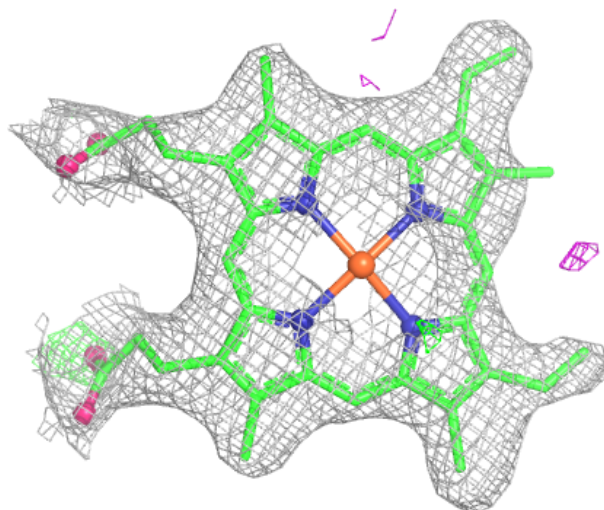
**Electron density around 8J4 A 503:**

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



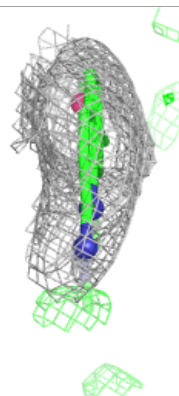
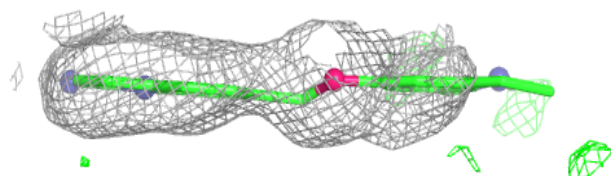
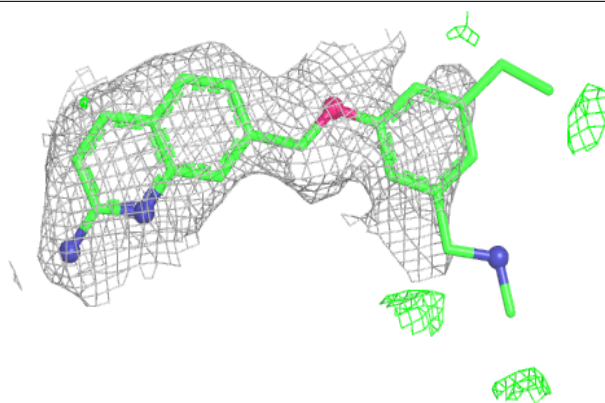
Electron density around HEM C 501:

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

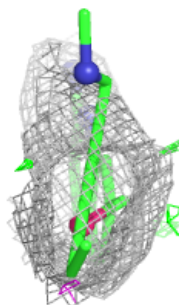
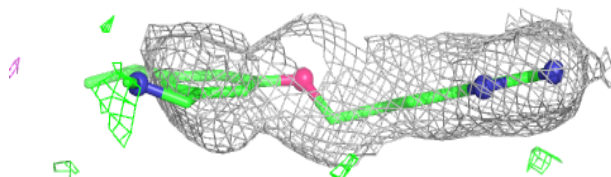
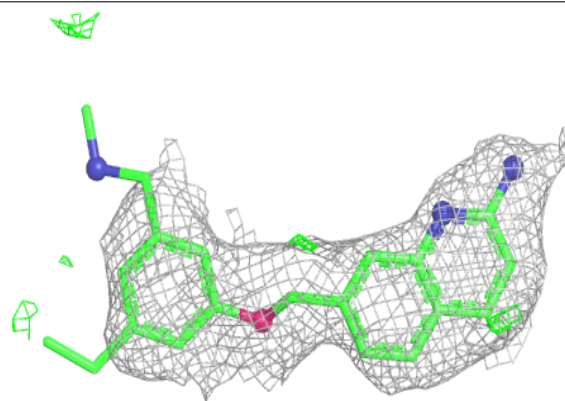


Electron density around 8J4 B 503:

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

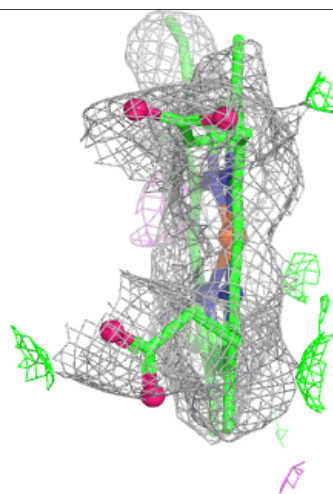
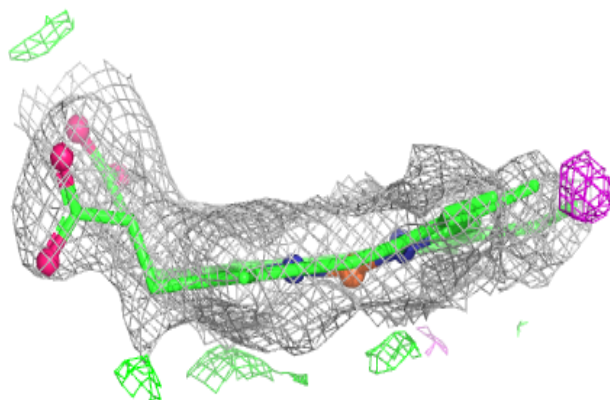
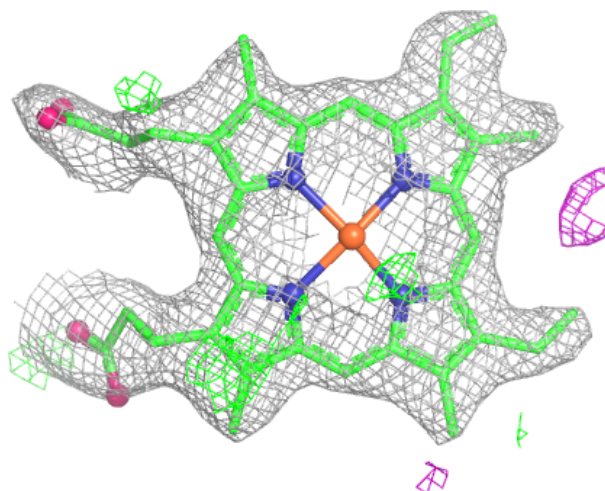
**Electron density around 8J4 D 503:**

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



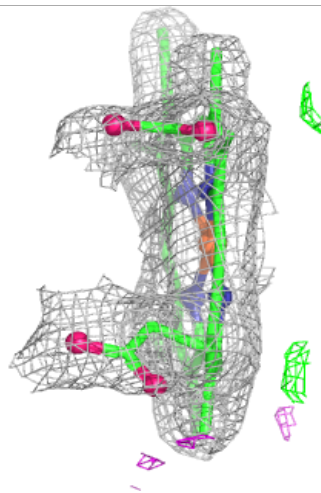
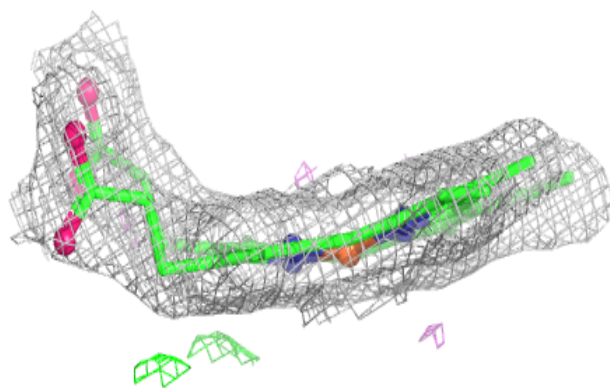
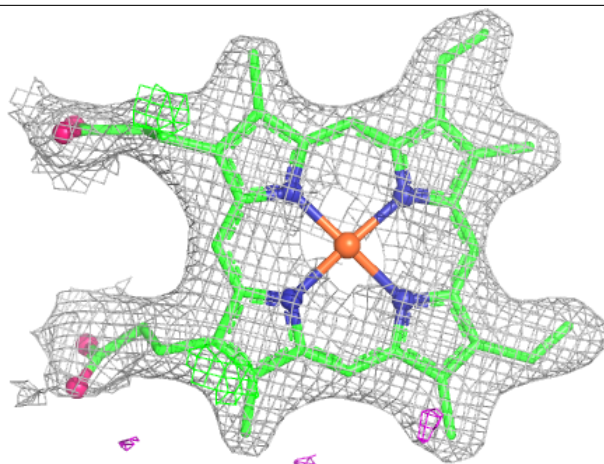
Electron density around HEM A 501:

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



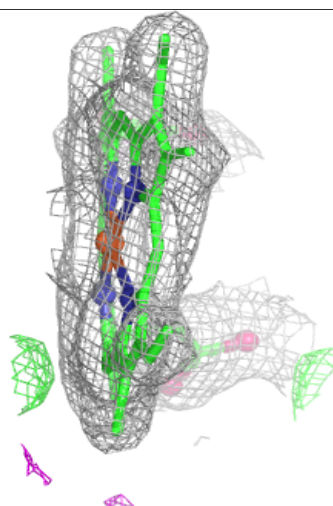
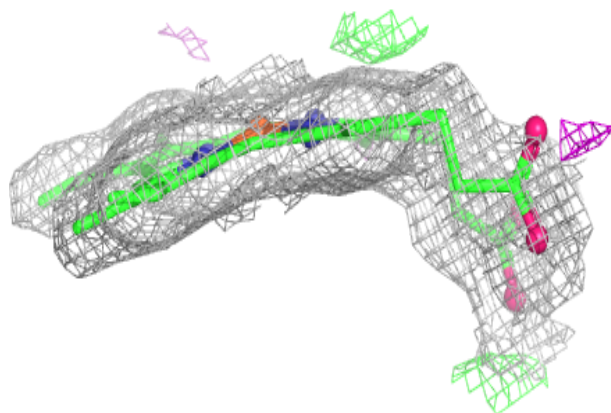
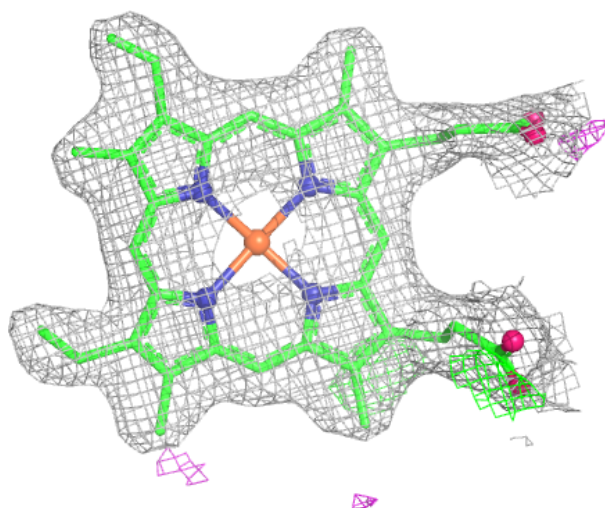
Electron density around HEM D 501:

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



Electron density around HEM 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 ⓘ

There are no such residues in this entry.