



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 PM UTC

PDB ID : 6POY / pdb_00006poy
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-propoxyphenyl)-4-methylquinolin-2-amine
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2019-07-05
Resolution : 2.30 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

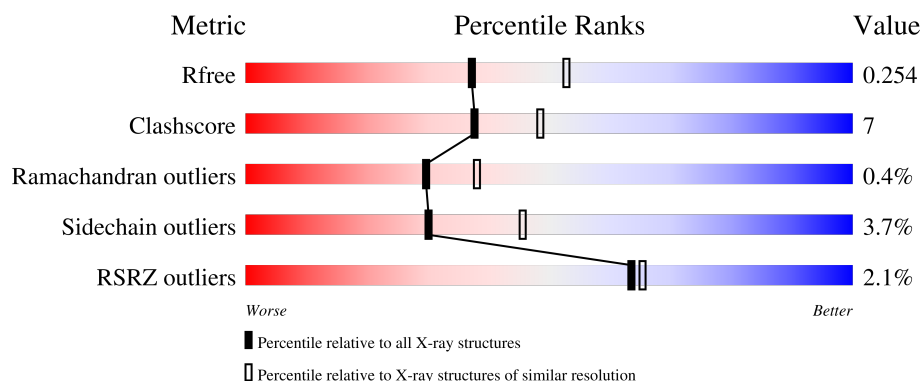
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	440	5% 73% 18% • 8%
1	B	440	79% 11% • 9%
1	C	440	% 76% 14% • 9%
1	D	440	% 75% 16% 8%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13740 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

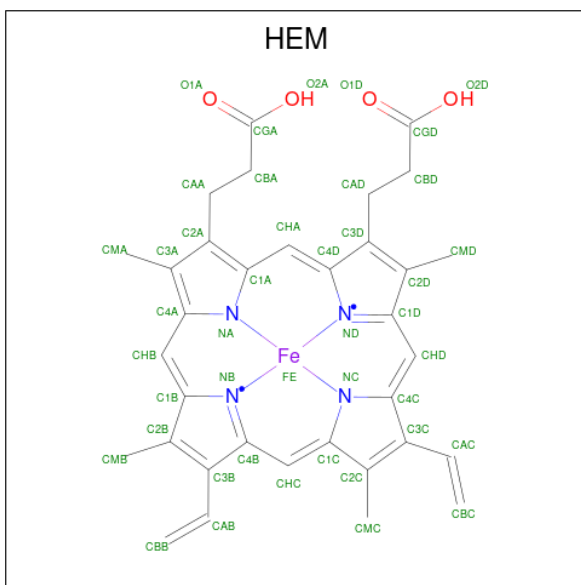
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	404	Total	C	N	O	S	0	3	0
			3241	2063	572	589	17			

There are 4 discrepancies between the modelled and reference sequences:

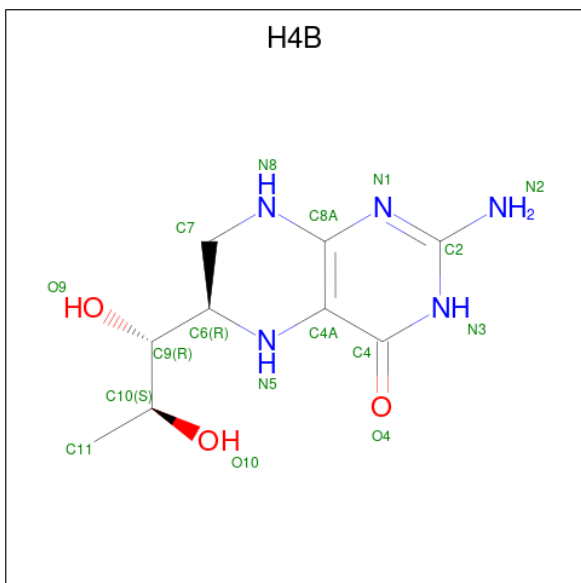
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



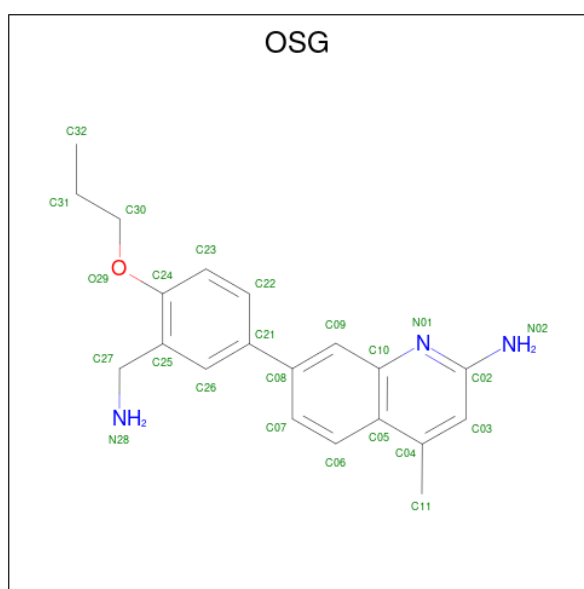
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



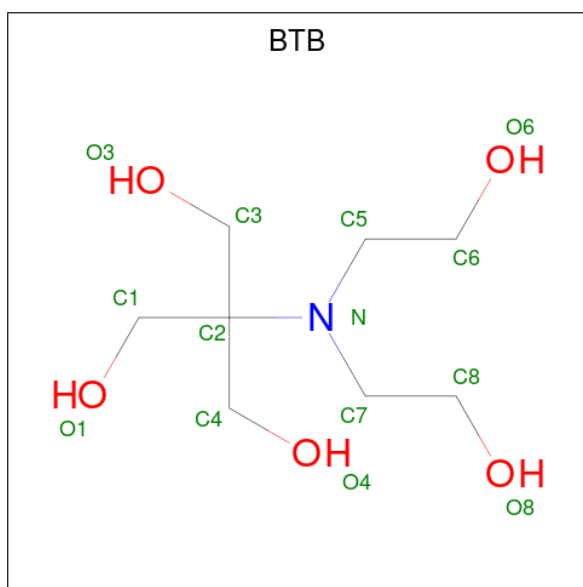
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[3-(aminomethyl)-4-propoxyphenyl]-4-methylquinolin-2-amine (CCD ID: OSG) (formula: $C_{20}H_{23}N_3O$) (labeled as "Ligand of Interest" by depositor).



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	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 7 is GLYCEROL (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	1	Total	Cl	0	0
			1	1		

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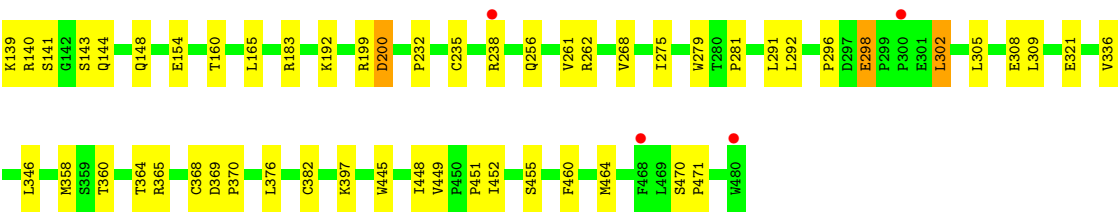
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total 1	Gd 1	0	0

- Molecule 10 is water.

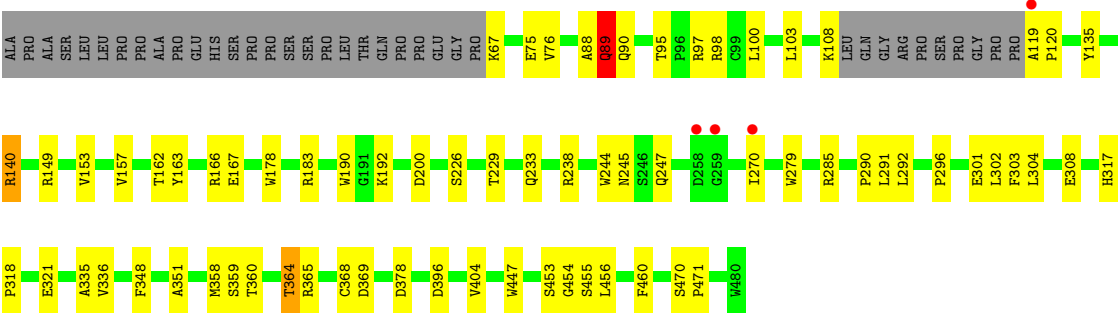
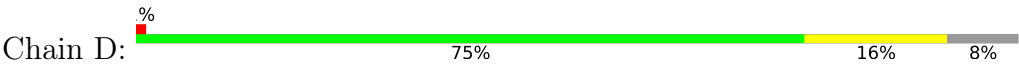
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	63	Total 63	O 63	0	0
10	B	105	Total 105	O 105	0	0
10	C	82	Total 82	O 82	0	0
10	D	98	Total 98	O 98	0	0

- Molecule 1: Nitric oxide synthase, endothelial





● Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.69Å 153.41Å 109.19Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	52.60 – 2.30 52.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (52.60-2.30) 97.3 (52.60-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, R_{free}	0.198 , 0.261 0.189 , 0.254	Depositor DCC
R_{free} test set	4262 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13740	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 3.61% 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: H4B, CL, OSG, GD, BTB, HEM, GOL, ZN

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	0.52	0/4543
1	B	0.36	1/3319 (0.0%)	0.52	0/4523
1	C	0.32	0/3307	0.49	0/4507
1	D	0.38	0/3339	0.56	1/4548 (0.0%)
All	All	0.35	1/13300 (0.0%)	0.52	1/18121 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	ARG	CA-C	-5.22	1.50	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	GLN	N-CA-C	-6.78	99.17	109.95

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	49	0
1	B	3221	0	3126	35	0
1	C	3209	0	3109	32	0
1	D	3241	0	3152	43	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	24	0	0	2	0
4	B	24	0	0	2	0
4	C	24	0	0	1	0
4	D	24	0	0	2	0
5	A	28	0	38	5	0
5	B	42	0	54	9	0
5	C	28	0	37	6	0
5	D	28	0	36	5	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	1	0
7	C	6	0	8	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	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	63	0	0	4	0
10	B	105	0	0	4	0
10	C	82	0	0	3	0
10	D	98	0	0	2	0
All	All	13740	0	12894	185	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 7.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:HB2	2:C:501:HEM:HBD2	1.60	0.81
1:D:321:GLU:OE1	5:D:504:BTB:O4	2.08	0.72
1:A:139:LYS:HE3	1:A:140:ARG:HG2	1.71	0.72
1:A:183:ARG:HB2	2:A:501:HEM:O1D	1.90	0.71
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.73	0.70
1:D:192:LYS:NZ	1:D:226:SER:H	1.89	0.70
1:C:292:LEU:HD21	1:C:302:LEU:HD12	1.73	0.69
1:B:192:LYS:HZ3	1:B:226:SER:H	1.40	0.68
1:D:100:LEU:HB3	1:D:103:LEU:HD12	1.74	0.68
1:C:70:ARG:NH2	10:C:604:HOH:O	2.28	0.66
1:A:70:ARG:NH1	10:A:607:HOH:O	2.29	0.65
1:A:202:ARG:N	1:A:206:GLU:OE2	2.27	0.65
1:A:298:GLU:OE2	10:A:602:HOH:O	2.14	0.64
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.80	0.64
7:A:507:GOL:O3	7:A:507:GOL:O1	2.11	0.63
1:D:378:ASP:OD1	10:D:601:HOH:O	2.16	0.63
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.80	0.62
1:B:326:LEU:HD12	5:C:504:BTB:H52	1.81	0.62
1:A:382:CYS:HA	5:A:504:BTB:H11	1.83	0.60
1:B:298:GLU:OE2	5:B:505:BTB:N	2.34	0.60
1:B:238:ARG:NH1	10:B:604:HOH:O	2.35	0.60
1:D:95:THR:OG1	1:D:97:ARG:HG2	2.01	0.59
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.83	0.59
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.84	0.59
1:A:144:GLN:HG2	1:A:145:ALA:H	1.67	0.59
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.84	0.58
1:A:432:GLU:HG2	1:A:436:LYS:NZ	2.19	0.58
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.84	0.58
1:B:192:LYS:NZ	1:B:226:SER:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.86	0.57
1:B:183:ARG:HB2	2:B:501:HEM:HBD2	1.86	0.57
1:D:336:VAL:HG21	4:D:503:OSG:C07	2.34	0.57
1:C:91:ASP:OD1	10:C:601:HOH:O	2.17	0.56
1:D:192:LYS:HZ2	1:D:226:SER:H	1.52	0.56
1:C:68:PHE:N	10:C:609:HOH:O	2.39	0.55
1:A:321:GLU:H	1:A:321:GLU:CD	2.13	0.55
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.88	0.55
1:A:145:ALA:HA	1:A:148:GLN:HB3	1.88	0.54
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.89	0.54
1:A:331:TYR:O	1:A:410:TYR:OH	2.24	0.54
1:A:214:HIS:ND1	1:A:229:THR:HG23	2.23	0.53
1:C:336:VAL:HG21	4:C:503:OSG:C07	2.39	0.53
1:A:196:PHE:HD2	1:A:229:THR:HG22	1.73	0.53
1:A:223:ASN:OD1	10:A:603:HOH:O	2.18	0.53
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.42	0.53
5:B:508:BTB:O3	5:B:508:BTB:H71	2.08	0.53
1:D:455:SER:HA	1:D:460:PHE:CG	2.44	0.53
1:A:192:LYS:NZ	1:A:226:SER:H	2.07	0.52
5:B:508:BTB:H41	5:B:508:BTB:O8	2.09	0.52
1:D:153:VAL:O	1:D:157:VAL:HG12	2.09	0.52
1:C:261:VAL:HG11	1:C:268:VAL:HG11	1.92	0.52
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.91	0.52
1:B:292:LEU:HD22	1:B:300:PRO:HB2	1.92	0.52
1:D:135:TYR:HE1	1:D:140:ARG:HH11	1.58	0.52
1:A:361:GLU:OE2	4:A:503:OSG:N02	2.43	0.51
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.26	0.51
1:B:173:GLY:HA3	1:B:343:ILE:HD13	1.93	0.51
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.93	0.51
1:B:124:LEU:O	1:B:128:ARG:HG3	2.09	0.51
1:A:207:MET:HE2	1:A:293:LEU:HB3	1.93	0.50
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.46	0.50
1:B:336:VAL:HG21	4:B:503:OSG:C07	2.42	0.50
1:C:451:PRO:HB2	1:D:455:SER:OG	2.12	0.50
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.93	0.50
5:A:505:BTB:O4	5:A:505:BTB:O3	2.27	0.50
5:B:505:BTB:H32	10:B:689:HOH:O	2.11	0.50
1:C:199:ARG:O	1:C:232:PRO:HG3	2.11	0.50
1:B:364:THR:O	1:B:368:CYS:HB2	2.12	0.49
1:B:358:MET:HE3	1:B:360:THR:OG1	2.13	0.49
1:D:183:ARG:HB2	2:D:501:HEM:HBD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ILE:H	1:D:270:ILE:HD12	1.77	0.49
2:D:501:HEM:O2A	4:D:503:OSG:N28	2.46	0.49
1:A:312:GLU:OE2	1:A:329:ARG:NH1	2.42	0.49
1:A:192:LYS:HZ1	1:A:226:SER:H	1.60	0.49
1:A:139:LYS:HD2	1:A:140:ARG:HE	1.79	0.48
1:A:196:PHE:HB2	1:A:229:THR:HG22	1.95	0.48
1:A:358:MET:HE3	1:A:360:THR:OG1	2.13	0.48
1:D:89:GLN:HA	1:D:89:GLN:OE1	2.13	0.48
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.94	0.48
2:A:501:HEM:HMD1	2:A:501:HEM:HBD2	1.95	0.48
1:C:139:LYS:O	1:C:140:ARG:HD2	2.14	0.48
1:D:229:THR:O	1:D:351:ALA:HA	2.14	0.48
1:C:455:SER:HA	1:C:460:PHE:CG	2.49	0.48
1:C:119:ALA:HB1	1:C:122:GLN:HB2	1.96	0.47
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.27	0.47
1:B:326:LEU:HD11	5:C:504:BTB:H71	1.96	0.47
5:C:504:BTB:H51	5:C:504:BTB:H32	1.61	0.47
1:D:183:ARG:HD3	1:D:447:TRP:CD2	2.49	0.47
1:A:265:PRO:HA	1:A:268:VAL:HG13	1.96	0.47
1:D:245:ASN:HD21	1:D:291:LEU:HA	1.80	0.47
5:D:504:BTB:H32	5:D:504:BTB:H51	1.61	0.47
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.49	0.47
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.55	0.47
2:A:501:HEM:HBD2	2:A:501:HEM:CMD	2.45	0.47
1:B:124:LEU:HD11	1:B:154:GLU:HG2	1.96	0.46
1:C:358:MET:HE3	1:C:360:THR:OG1	2.15	0.46
5:A:505:BTB:H11	5:A:505:BTB:H71	1.41	0.46
1:A:270:ILE:HA	1:A:273:LEU:HD12	1.97	0.46
5:B:505:BTB:H42	5:B:505:BTB:H72	1.81	0.46
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.29	0.46
4:B:503:OSG:O29	4:B:503:OSG:N28	2.50	0.45
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.97	0.45
1:D:97:ARG:HG3	1:D:98:ARG:HD2	1.99	0.45
5:B:508:BTB:H52	5:B:508:BTB:H82	1.42	0.45
1:B:326:LEU:CD1	5:C:504:BTB:H71	2.47	0.45
1:A:336:VAL:HG21	4:A:503:OSG:C07	2.47	0.45
5:A:505:BTB:H52	5:A:505:BTB:H81	1.48	0.45
1:D:454:GLY:O	1:D:460:PHE:HB2	2.17	0.45
1:B:104:VAL:O	1:B:106:PRO:HD3	2.17	0.45
5:B:508:BTB:H11	5:B:508:BTB:H51	1.48	0.45
5:D:505:BTB:H52	5:D:505:BTB:H81	1.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:CD2	1:A:229:THR:HG22	2.51	0.44
1:D:245:ASN:OD1	1:D:245:ASN:N	2.49	0.44
1:D:285:ARG:HD3	10:D:682:HOH:O	2.16	0.44
1:D:302:LEU:HD12	1:D:302:LEU:HA	1.80	0.44
1:B:182:PRO:HD2	2:B:501:HEM:O2D	2.18	0.44
1:C:291:LEU:HG	1:C:305:LEU:HD11	1.99	0.44
5:C:505:BTB:O4	5:C:505:BTB:O1	2.35	0.44
5:B:505:BTB:O3	5:B:505:BTB:H51	2.17	0.44
5:D:505:BTB:H32	5:D:505:BTB:H51	1.42	0.44
1:A:279:TRP:CD1	1:A:290:PRO:HG3	2.53	0.44
1:A:140:ARG:HD3	1:A:144:GLN:CD	2.43	0.43
1:A:144:GLN:CG	1:A:145:ALA:H	2.31	0.43
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.53	0.43
1:A:453:SER:HB3	1:A:456:LEU:HD12	2.00	0.43
1:C:296:PRO:C	1:C:298:GLU:H	2.25	0.43
1:C:448:ILE:HG21	1:C:464:MET:HE1	2.00	0.43
2:D:501:HEM:CGA	3:D:502:H4B:HN22	2.31	0.43
5:D:505:BTB:H11	5:D:505:BTB:H71	1.34	0.43
1:A:263:GLY:HA2	1:A:285:ARG:HA	2.01	0.43
1:C:445:TRP:CE2	1:C:449:VAL:HG21	2.53	0.43
1:B:285:ARG:NH2	10:B:602:HOH:O	2.17	0.43
1:C:397:LYS:HZ1	1:D:404:VAL:HG21	1.84	0.43
1:D:364:THR:O	1:D:368:CYS:HB2	2.18	0.43
1:D:162:THR:OG1	1:D:163:TYR:N	2.52	0.42
1:B:258:ASP:HB2	1:B:260:SER:OG	2.19	0.42
1:B:238:ARG:HG2	1:B:296:PRO:HB3	2.00	0.42
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.60	0.42
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.00	0.42
1:C:124:LEU:O	1:C:128:ARG:HG3	2.19	0.42
1:D:244:TRP:HB2	1:D:292:LEU:HB2	2.01	0.42
1:A:364:THR:O	1:A:368:CYS:HB2	2.19	0.42
1:B:396:ASP:OD1	1:B:396:ASP:N	2.52	0.42
1:C:200:ASP:OD1	1:C:200:ASP:N	2.37	0.42
1:A:90:GLN:H	1:A:90:GLN:HG2	1.67	0.42
1:B:229:THR:O	1:B:351:ALA:HA	2.20	0.42
1:D:470:SER:HA	1:D:471:PRO:C	2.44	0.42
1:B:121:GLU:HB3	1:B:122:GLN:OE1	2.20	0.42
1:A:234:ARG:NH1	1:A:347:GLU:OE2	2.53	0.42
1:A:333:LEU:HD11	1:A:354:SER:HB2	2.01	0.42
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.54	0.42
1:A:166:ARG:NH2	10:A:608:HOH:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLN:HA	1:D:335:ALA:O	2.20	0.42
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.01	0.42
5:B:504:BTB:H61	10:B:654:HOH:O	2.19	0.42
1:D:308:GLU:OE1	1:D:308:GLU:N	2.31	0.42
1:A:144:GLN:CG	1:A:145:ALA:N	2.83	0.41
1:B:89:GLN:H	1:B:89:GLN:HG2	1.74	0.41
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.55	0.41
1:A:455:SER:HA	1:A:460:PHE:CG	2.56	0.41
1:A:202:ARG:HD2	1:A:202:ARG:HA	1.89	0.41
1:C:165:LEU:HG	1:C:346:LEU:HD12	2.02	0.41
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.56	0.41
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.56	0.41
1:B:306:PRO:HA	1:B:307:PRO:HD3	1.97	0.41
1:C:98:ARG:HH11	1:C:98:ARG:HG3	1.85	0.41
1:C:382:CYS:HA	5:C:504:BTB:H42	2.02	0.41
1:D:238:ARG:HG3	1:D:296:PRO:HB3	2.03	0.41
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.53	0.41
1:D:119:ALA:HB3	1:D:120:PRO:HD3	2.02	0.41
1:B:242:ARG:HA	1:B:242:ARG:HD2	1.95	0.41
1:D:88:ALA:O	1:D:89:GLN:HB2	2.19	0.41
1:B:68:PHE:CD2	1:B:83:THR:HG22	2.56	0.41
1:B:128:ARG:NH1	1:B:128:ARG:HB3	2.36	0.41
1:B:269:GLU:H	1:B:269:GLU:CD	2.29	0.41
1:C:141:SER:C	1:C:143:SER:H	2.29	0.41
1:C:470:SER:HA	1:C:471:PRO:C	2.45	0.41
1:A:94:CYS:HB3	1:B:94:CYS:HB3	2.02	0.41
1:A:100:LEU:HB3	1:A:103:LEU:HD13	2.03	0.41
1:A:138:ILE:O	1:A:139:LYS:HB3	2.21	0.41
5:A:505:BTB:H51	5:A:505:BTB:H32	1.54	0.40
1:D:358:MET:HE3	1:D:360:THR:OG1	2.21	0.40
1:B:334:PRO:HB3	1:B:357:TYR:CZ	2.57	0.40
1:C:370:PRO:HG2	1:D:75:GLU:HG3	2.03	0.40
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/440 (91%)	373 (93%)	24 (6%)	5 (1%)	10	12
1	B	401/440 (91%)	391 (98%)	10 (2%)	0	100	100
1	C	399/440 (91%)	385 (96%)	13 (3%)	1 (0%)	36	46
1	D	403/440 (92%)	389 (96%)	13 (3%)	1 (0%)	43	55
All	All	1605/1760 (91%)	1538 (96%)	60 (4%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	90	GLN
1	C	89	GLN
1	A	145	ALA
1	A	281	PRO
1	D	89	GLN
1	A	93	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/373 (92%)	330 (96%)	15 (4%)	26	39
1	B	344/373 (92%)	332 (96%)	12 (4%)	32	48
1	C	342/373 (92%)	325 (95%)	17 (5%)	22	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	346/373 (93%)	337 (97%)	9 (3%)	40 59
All	All	1377/1492 (92%)	1324 (96%)	53 (4%)	30 44

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	89	GLN
1	A	121	GLU
1	A	124	LEU
1	A	125	SER
1	A	128	ARG
1	A	129	ASP
1	A	139	LYS
1	A	151	GLN
1	A	203	SER
1	A	221	ARG
1	A	256	GLN
1	A	257	GLN
1	A	285	ARG
1	A	308	GLU
1	B	97	ARG
1	B	124	LEU
1	B	125	SER
1	B	168[A]	SER
1	B	168[B]	SER
1	B	213	ASN
1	B	235[A]	CYS
1	B	235[B]	CYS
1	B	269	GLU
1	B	326	LEU
1	B	389	THR
1	B	396	ASP
1	C	71	VAL
1	C	98	ARG
1	C	125	SER
1	C	144	GLN
1	C	148	GLN
1	C	154	GLU
1	C	160	THR
1	C	192	LYS
1	C	200	ASP

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Mol	Chain	Res	Type
1	C	235	CYS
1	C	256	GLN
1	C	262	ARG
1	C	298	GLU
1	C	302	LEU
1	C	308	GLU
1	C	309	LEU
1	C	321	GLU
1	D	67	LYS
1	D	76	VAL
1	D	108	LYS
1	D	140	ARG
1	D	167	GLU
1	D	200	ASP
1	D	359	SER
1	D	364	THR
1	D	396	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	233	GLN
1	A	476	GLN
1	B	256	GLN
1	C	133	GLN
1	C	151	GLN
1	D	205	GLN
1	D	247	GLN
1	D	256	GLN
1	D	408	HIS
1	D	421	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OSG	D	503	-	26,26,26	0.84	0	35,36,36	1.19	3 (8%)
3	H4B	C	502	-	17,18,18	0.75	0	14,26,26	2.07	6 (42%)
4	OSG	C	503	-	26,26,26	0.86	1 (3%)	35,36,36	1.38	4 (11%)
5	BTB	B	505	-	13,13,13	0.55	0	7,16,16	1.13	1 (14%)
5	BTB	B	504	9	13,13,13	0.47	0	7,16,16	0.27	0
2	HEM	D	501	1	50,50,50	2.01	6 (12%)	67,82,82	1.61	15 (22%)
5	BTB	B	508	-	13,13,13	0.84	1 (7%)	7,16,16	1.63	2 (28%)
5	BTB	C	505	-	13,13,13	0.61	0	7,16,16	0.43	0
3	H4B	B	502	-	17,18,18	0.83	0	14,26,26	2.09	6 (42%)
4	OSG	B	503	-	26,26,26	0.90	1 (3%)	35,36,36	1.27	3 (8%)
7	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.34	0
5	BTB	D	504	9	13,13,13	0.59	0	7,16,16	0.47	0
3	H4B	D	502	-	17,18,18	0.83	0	14,26,26	1.81	4 (28%)
5	BTB	C	504	9	13,13,13	0.68	0	7,16,16	1.12	1 (14%)
5	BTB	D	505	-	13,13,13	0.53	0	7,16,16	0.84	0
2	HEM	C	501	1	50,50,50	1.68	8 (16%)	67,82,82	1.48	9 (13%)
7	GOL	C	507	-	5,5,5	0.50	0	5,5,5	0.40	0
5	BTB	A	505	-	13,13,13	0.39	0	7,16,16	0.80	0
5	BTB	A	504	9	13,13,13	0.42	0	7,16,16	0.67	0
3	H4B	A	502	-	17,18,18	0.80	0	14,26,26	1.97	5 (35%)
2	HEM	A	501	1	50,50,50	1.76	10 (20%)	67,82,82	1.43	10 (14%)
4	OSG	A	503	-	26,26,26	0.80	0	35,36,36	1.31	5 (14%)
2	HEM	B	501	1	50,50,50	1.94	8 (16%)	67,82,82	1.59	15 (22%)

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
4	OSG	D	503	-	-	3/10/19/19	0/3/3/3
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
4	OSG	C	503	-	-	0/10/19/19	0/3/3/3
5	BTB	B	505	-	-	9/21/21/21	-
5	BTB	B	504	9	-	3/21/21/21	-
2	HEM	D	501	1	-	4/14/54/54	-
5	BTB	B	508	-	-	5/21/21/21	-
5	BTB	C	505	-	-	7/21/21/21	-
3	H4B	B	502	-	-	4/8/17/17	0/2/2/2
4	OSG	B	503	-	-	1/10/19/19	0/3/3/3
7	GOL	A	507	-	-	4/4/4/4	-
5	BTB	D	504	9	-	5/21/21/21	-
3	H4B	D	502	-	-	4/8/17/17	0/2/2/2
5	BTB	C	504	9	-	2/21/21/21	-
5	BTB	D	505	-	-	16/21/21/21	-
2	HEM	C	501	1	-	5/14/54/54	-
7	GOL	C	507	-	-	2/4/4/4	-
5	BTB	A	505	-	-	5/21/21/21	-
5	BTB	A	504	9	-	6/21/21/21	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
2	HEM	A	501	1	-	6/14/54/54	-
4	OSG	A	503	-	-	1/10/19/19	0/3/3/3
2	HEM	B	501	1	-	3/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NB	7.46	2.17	1.94
2	D	501	HEM	FE-NC	7.12	2.18	1.95
2	B	501	HEM	FE-NC	6.80	2.17	1.95
2	B	501	HEM	FE-ND	6.70	2.15	1.94
2	A	501	HEM	FE-ND	6.04	2.13	1.94
2	D	501	HEM	FE-ND	5.52	2.11	1.94
2	C	501	HEM	FE-NC	5.34	2.12	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-NB	5.31	2.11	1.94
2	B	501	HEM	FE-NB	5.00	2.10	1.94
2	A	501	HEM	FE-NA	4.28	2.09	1.95
2	A	501	HEM	FE-NC	4.14	2.08	1.95
2	A	501	HEM	FE-NB	3.99	2.07	1.94
2	C	501	HEM	FE-NA	3.75	2.07	1.95
2	B	501	HEM	CAC-C3C	3.39	1.56	1.47
2	D	501	HEM	CAC-C3C	3.28	1.56	1.47
2	A	501	HEM	CAC-C3C	3.21	1.56	1.47
2	C	501	HEM	FE-ND	3.18	2.04	1.94
2	A	501	HEM	CAB-C3B	3.17	1.55	1.47
2	C	501	HEM	CAB-C3B	3.08	1.55	1.47
2	B	501	HEM	CAB-C3B	3.01	1.55	1.47
2	D	501	HEM	CAB-C3B	2.95	1.55	1.47
2	C	501	HEM	CAC-C3C	2.92	1.55	1.47
2	B	501	HEM	FE-NA	2.82	2.04	1.95
2	A	501	HEM	CMD-C2D	2.29	1.55	1.50
2	C	501	HEM	CMB-C2B	2.27	1.55	1.50
2	A	501	HEM	CMC-C2C	2.27	1.55	1.50
2	A	501	HEM	CAD-C3D	2.27	1.57	1.51
2	B	501	HEM	CMC-C2C	2.24	1.55	1.50
2	B	501	HEM	CMB-C2B	2.21	1.55	1.50
2	D	501	HEM	CMD-C2D	2.17	1.55	1.50
4	C	503	OSG	C05-C10	-2.10	1.39	1.42
4	B	503	OSG	C04-C05	-2.08	1.38	1.42
2	A	501	HEM	C2A-C3A	-2.08	1.33	1.38
5	B	508	BTB	C4-C2	-2.04	1.50	1.53
2	C	501	HEM	CMD-C2D	2.03	1.54	1.50

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	OSG	O29-C24-C25	4.54	121.75	115.89
3	B	502	H4B	C2-N1-C8A	4.43	121.19	113.36
3	C	502	H4B	C2-N1-C8A	4.23	120.83	113.36
3	A	502	H4B	C2-N1-C8A	4.13	120.64	113.36
2	B	501	HEM	C3B-C4B-NB	-3.93	106.64	109.47
3	D	502	H4B	C2-N1-C8A	3.93	120.30	113.36
2	C	501	HEM	CBD-CAD-C3D	-3.90	101.75	112.53
2	D	501	HEM	CBD-CAD-C3D	-3.87	101.83	112.53
4	B	503	OSG	C04-C05-C10	3.70	120.26	118.00
2	D	501	HEM	C1B-NB-C4B	3.70	109.58	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C2B-C1B	3.55	109.08	106.41
4	A	503	OSG	O29-C24-C25	3.47	120.37	115.89
2	B	501	HEM	C1B-NB-C4B	3.43	109.27	105.21
4	D	503	OSG	C04-C05-C10	3.36	120.05	118.00
2	B	501	HEM	CBD-CAD-C3D	-3.36	103.25	112.53
2	B	501	HEM	C4D-ND-C1D	3.35	109.17	105.21
2	D	501	HEM	C2A-C1A-NA	-3.26	106.54	110.15
2	A	501	HEM	C3B-C2B-C1B	3.21	108.82	106.41
2	A	501	HEM	C2A-C1A-NA	-3.20	106.60	110.15
2	B	501	HEM	C3D-C4D-ND	-3.17	106.70	110.17
3	A	502	H4B	O4-C4-C4A	-3.11	119.76	127.26
2	D	501	HEM	C2B-C1B-NB	-3.08	106.30	109.84
4	D	503	OSG	C05-C10-N01	-3.07	119.55	122.80
2	C	501	HEM	C3B-C4B-NB	-3.07	107.27	109.47
4	B	503	OSG	O29-C24-C25	3.04	119.81	115.89
2	C	501	HEM	C2A-C1A-NA	-3.03	106.79	110.15
5	B	508	BTB	O4-C4-C2	-3.02	104.30	111.40
2	C	501	HEM	C1B-NB-C4B	2.97	108.73	105.21
2	D	501	HEM	CBA-CAA-C2A	-2.91	104.48	112.53
2	C	501	HEM	C3D-C4D-ND	-2.89	107.00	110.17
3	B	502	H4B	O4-C4-C4A	-2.89	120.29	127.26
2	B	501	HEM	C2D-C1D-ND	-2.81	106.66	109.90
5	C	504	BTB	O4-C4-C2	2.78	117.93	111.40
3	B	502	H4B	C4A-C4-N3	2.76	119.70	112.13
2	A	501	HEM	O2D-CGD-CBD	2.75	122.68	114.00
2	C	501	HEM	C3B-C2B-C1B	2.73	108.46	106.41
3	C	502	H4B	O4-C4-C4A	-2.72	120.71	127.26
4	C	503	OSG	N02-C02-N01	2.66	120.44	118.24
2	D	501	HEM	C4D-ND-C1D	2.64	108.33	105.21
2	B	501	HEM	C2A-C1A-NA	-2.62	107.24	110.15
4	D	503	OSG	C26-C25-C24	2.56	121.07	118.26
2	A	501	HEM	O1D-CGD-CBD	-2.53	115.07	123.09
2	D	501	HEM	C4A-NA-C1A	2.52	109.93	105.82
3	A	502	H4B	C4A-C4-N3	2.51	119.03	112.13
3	B	502	H4B	O10-C10-C9	2.51	113.92	109.77
4	A	503	OSG	C05-C10-N01	-2.50	120.15	122.80
2	B	501	HEM	C3B-C2B-C1B	2.48	108.27	106.41
3	D	502	H4B	C4A-C4-N3	2.47	118.90	112.13
4	C	503	OSG	O29-C24-C23	-2.44	118.62	123.95
2	D	501	HEM	C3A-C4A-NA	-2.44	106.23	110.14
2	A	501	HEM	C4D-ND-C1D	2.44	108.09	105.21
5	B	508	BTB	O1-C1-C2	-2.41	105.73	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C4B-NB	-2.40	107.74	109.47
2	B	501	HEM	CBA-CAA-C2A	-2.40	105.91	112.53
2	C	501	HEM	C4D-ND-C1D	2.39	108.04	105.21
3	C	502	H4B	C4A-C4-N3	2.39	118.70	112.13
3	C	502	H4B	C11-C10-C9	-2.39	109.19	112.11
3	B	502	H4B	C2-N3-C4	-2.39	120.78	125.11
4	A	503	OSG	N02-C02-N01	2.38	120.21	118.24
3	C	502	H4B	N2-C2-N3	2.37	121.76	116.76
2	A	501	HEM	CBD-CAD-C3D	2.35	119.04	112.53
3	D	502	H4B	O4-C4-C4A	-2.31	121.68	127.26
4	A	503	OSG	C04-C05-C10	2.30	119.41	118.00
4	C	503	OSG	C05-C10-N01	-2.27	120.39	122.80
3	A	502	H4B	C2-N3-C4	-2.25	121.02	125.11
2	D	501	HEM	CHA-C1A-NA	2.24	127.92	123.86
2	A	501	HEM	C1B-NB-C4B	2.23	107.85	105.21
2	D	501	HEM	C2D-C1D-ND	-2.22	107.34	109.90
3	D	502	H4B	O10-C10-C9	2.22	113.45	109.77
2	A	501	HEM	C3B-C4B-NB	-2.21	107.88	109.47
5	B	505	BTB	O3-C3-C2	2.20	116.58	111.40
2	B	501	HEM	CHD-C1D-ND	2.19	126.78	124.42
2	B	501	HEM	C4C-NC-C1C	2.19	109.40	105.82
2	A	501	HEM	CMD-C2D-C1D	-2.17	121.64	125.03
2	D	501	HEM	CHB-C4A-NA	2.16	127.78	123.86
2	B	501	HEM	C3A-C4A-NA	-2.16	106.68	110.14
3	B	502	H4B	C4-C4A-N5	2.15	122.14	116.27
3	C	502	H4B	C2-N3-C4	-2.15	121.22	125.11
2	A	501	HEM	CHB-C4A-NA	2.14	127.75	123.86
2	D	501	HEM	C3D-C4D-ND	-2.14	107.83	110.17
2	B	501	HEM	C4A-NA-C1A	2.13	109.30	105.82
2	D	501	HEM	C4C-NC-C1C	2.09	109.24	105.82
4	A	503	OSG	O29-C24-C23	-2.07	119.43	123.95
3	A	502	H4B	N2-C2-N3	2.07	121.13	116.76
2	C	501	HEM	CAD-C3D-C2D	-2.06	124.01	127.87
2	C	501	HEM	CHA-C4D-ND	2.06	126.91	124.37
4	B	503	OSG	C06-C05-C04	-2.06	119.62	123.61
2	B	501	HEM	C2B-C1B-NB	-2.02	107.52	109.84
2	B	501	HEM	CHC-C4B-C3B	2.01	129.07	125.07

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2D-C3D-CAD-CBD
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	B	502	H4B	N5-C6-C9-O9
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	C	502	H4B	C7-C6-C9-O9
3	C	502	H4B	C7-C6-C9-C10
3	D	502	H4B	N5-C6-C9-O9
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
4	B	503	OSG	C24-C25-C27-N28
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-C3-O3
5	A	504	BTB	C4-C2-C3-O3
5	A	504	BTB	N-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C8-C7-N-C5
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	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-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	508	BTB	C1-C2-C4-O4
5	B	508	BTB	C3-C2-C4-O4
5	B	508	BTB	N-C2-C4-O4
5	B	508	BTB	C8-C7-N-C5
5	C	504	BTB	C3-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
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	505	BTB	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C8-C7-N-C5
7	A	507	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-C3
2	A	501	HEM	C4D-C3D-CAD-CBD
5	D	504	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C2A-CAA-CBA-CGA
2	D	501	HEM	C2A-CAA-CBA-CGA
5	A	505	BTB	N-C5-C6-O6
4	A	503	OSG	O29-C30-C31-C32
4	D	503	OSG	O29-C30-C31-C32
5	D	505	BTB	N-C7-C8-O8
2	C	501	HEM	C3D-CAD-CBD-CGD
7	A	507	GOL	C1-C2-C3-O3
7	C	507	GOL	O1-C1-C2-C3
7	C	507	GOL	O1-C1-C2-O2
5	D	504	BTB	N-C7-C8-O8
2	A	501	HEM	C3D-CAD-CBD-CGD
5	B	508	BTB	N-C7-C8-O8
5	B	505	BTB	C4-C2-C3-O3
5	D	505	BTB	C1-C2-C3-O3
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
3	B	502	H4B	N5-C6-C9-C10
3	D	502	H4B	N5-C6-C9-C10
3	A	502	H4B	N5-C6-C9-O9
2	A	501	HEM	C1A-C2A-CAA-CBA
5	C	505	BTB	N-C2-C3-O3
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	D	505	BTB	C1-C2-N-C7

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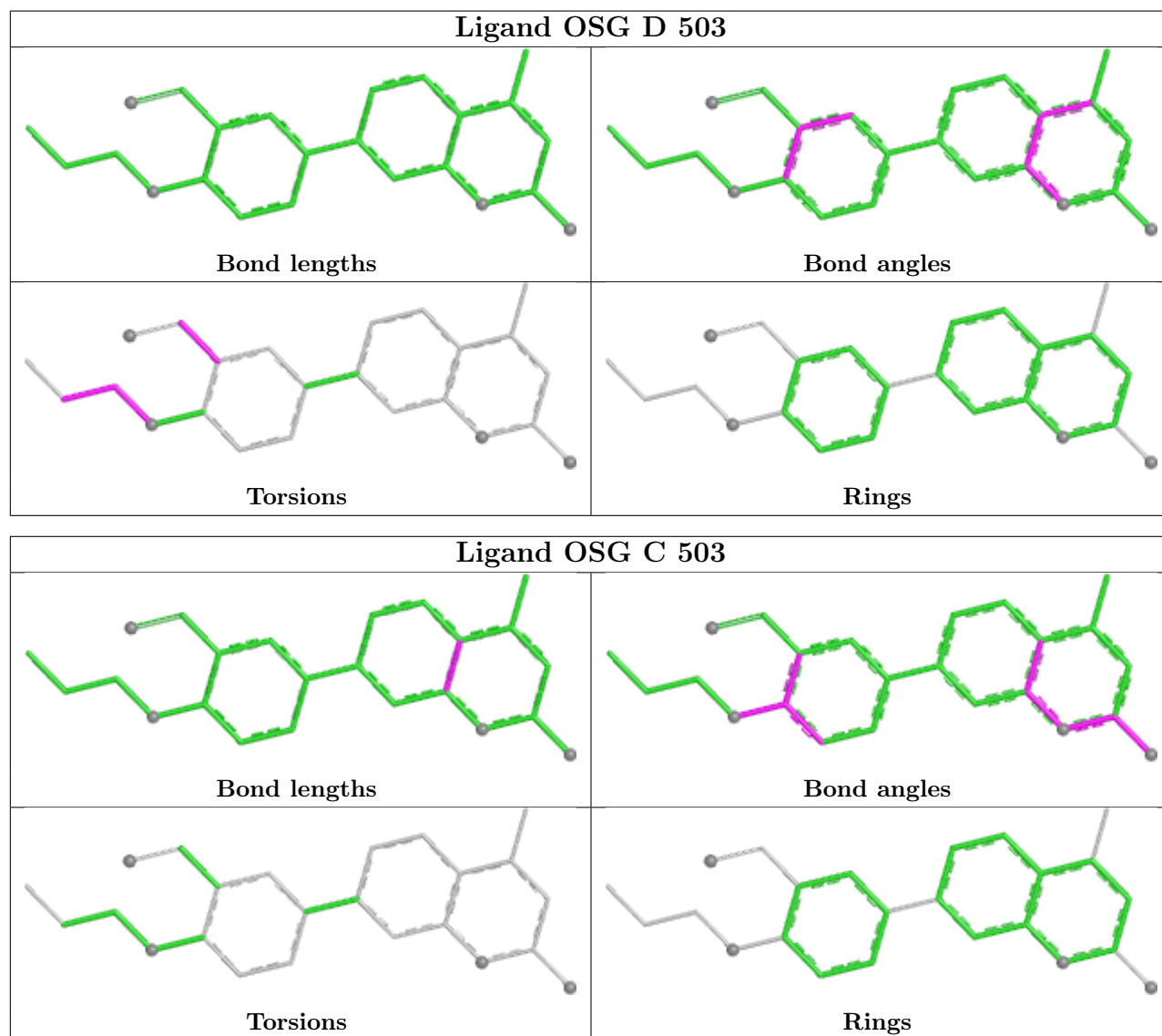
Mol	Chain	Res	Type	Atoms
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
7	A	507	GOL	O2-C2-C3-O3
4	D	503	OSG	C31-C30-O29-C24
2	D	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
4	D	503	OSG	C24-C25-C27-N28
2	D	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	C3A-C2A-CAA-CBA
3	C	502	H4B	N5-C6-C9-O9
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	C1-C2-N-C7
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C4-C2-N-C7

There are no ring outliers.

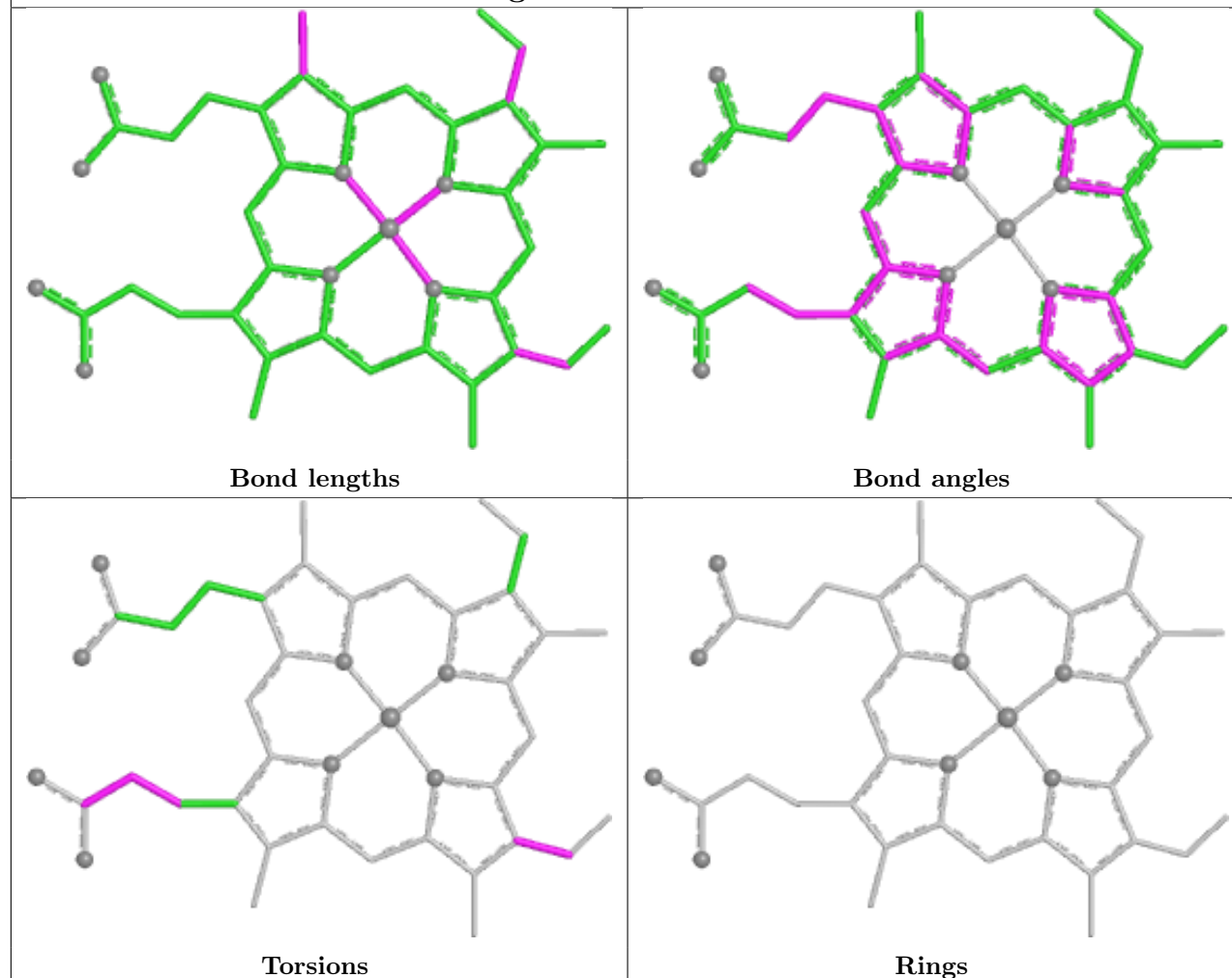
21 monomers are involved in 49 short contacts:

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

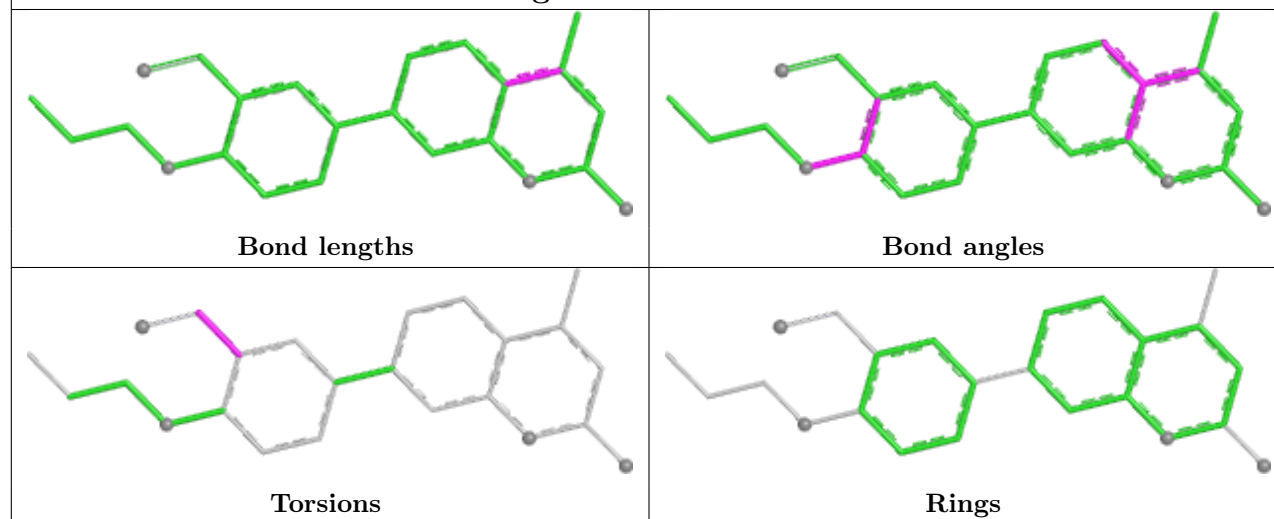
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

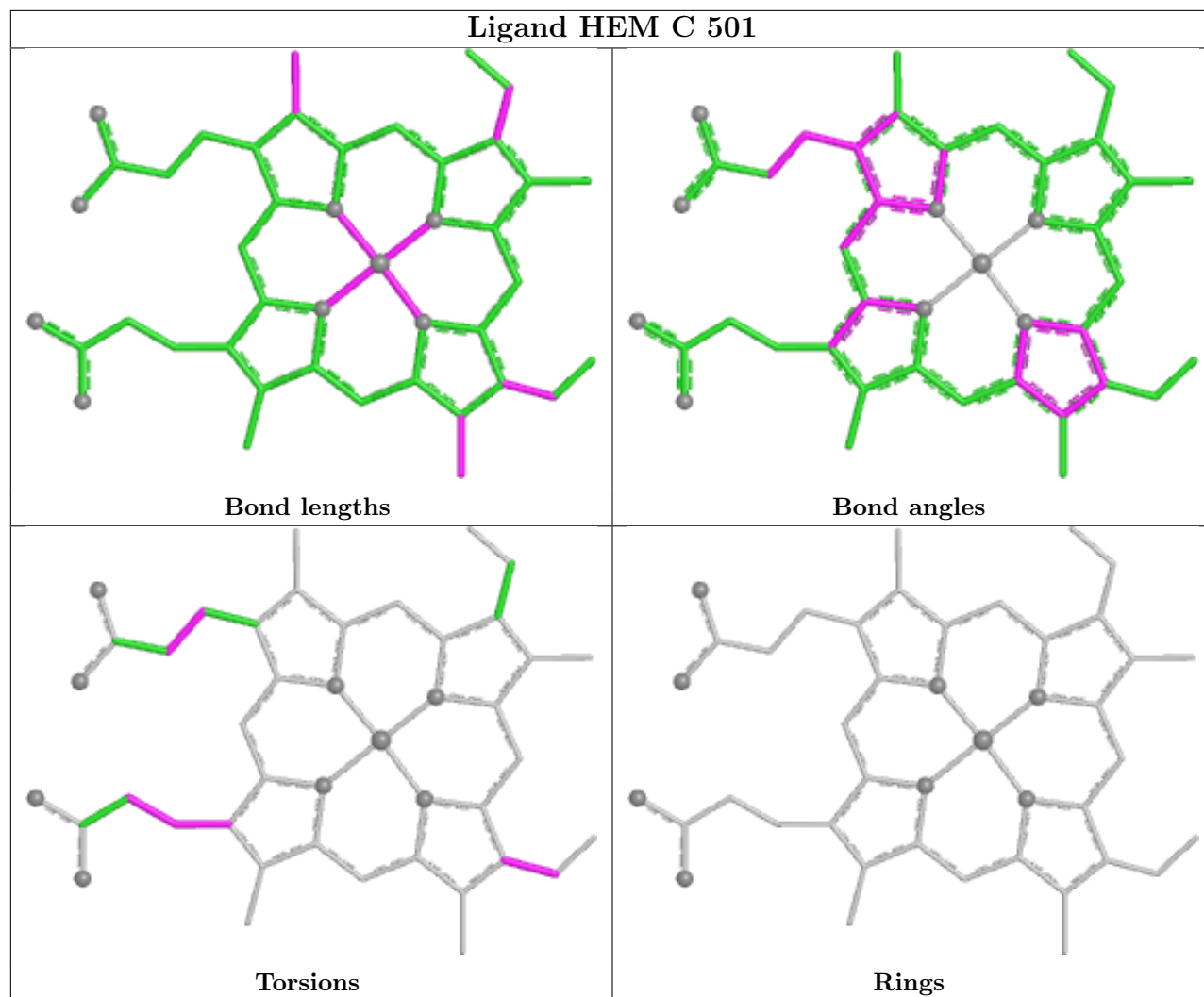


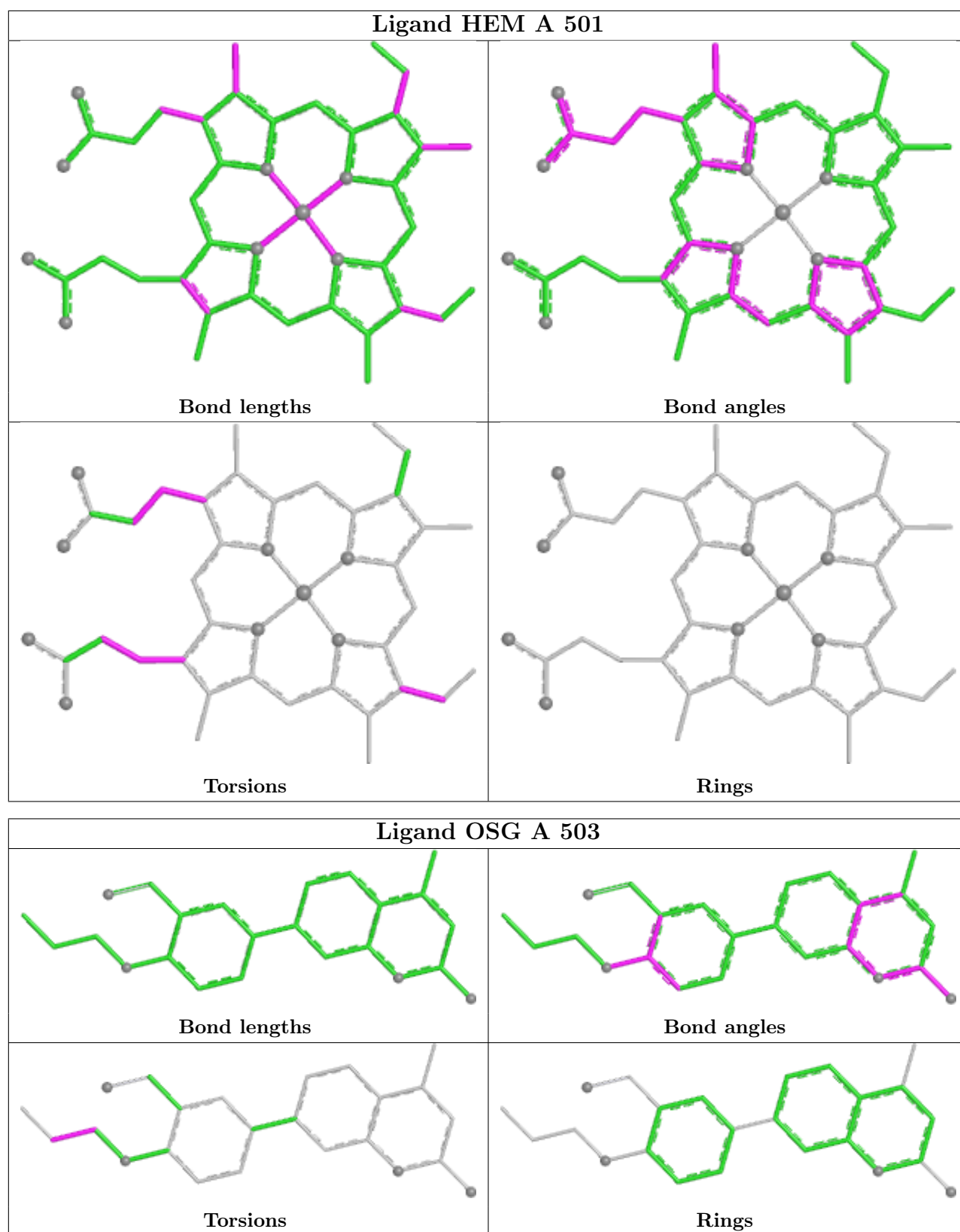
Ligand HEM D 501

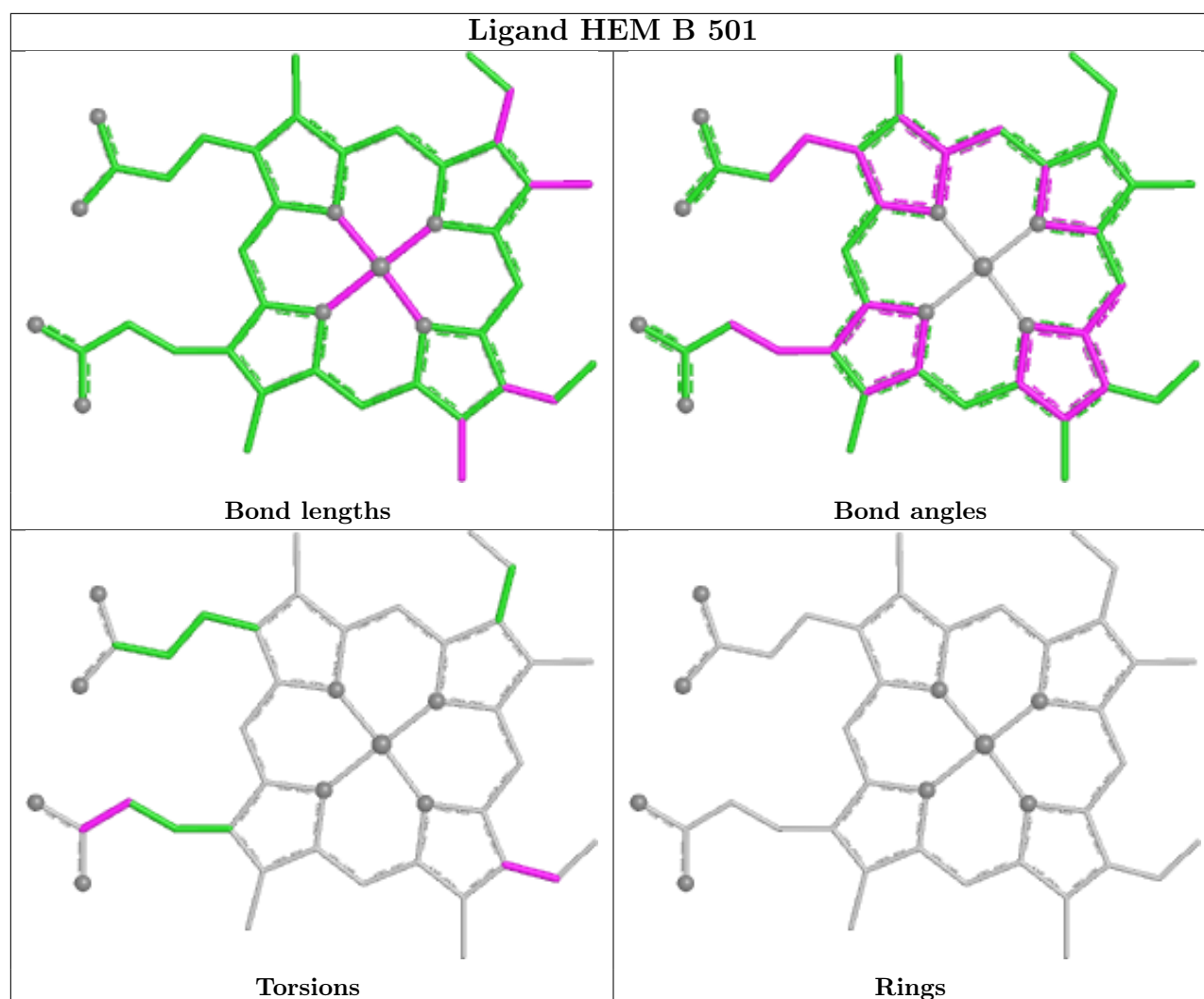


Ligand OSG B 503









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	0.51	23 (5%)	29 31	26, 62, 115, 147	2 (0%)
1	B	402/440 (91%)	-0.02	2 (0%)	87 87	26, 44, 81, 125	3 (0%)
1	C	401/440 (91%)	0.16	5 (1%)	76 77	26, 52, 90, 116	2 (0%)
1	D	404/440 (91%)	-0.06	4 (0%)	79 80	23, 43, 74, 128	3 (0%)
All	All	1611/1760 (91%)	0.15	34 (2%)	63 65	23, 49, 98, 147	10 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	GLN	4.2
1	D	270	ILE	4.1
1	A	480	TRP	3.4
1	A	299	PRO	3.3
1	D	119	ALA	3.3
1	A	120	PRO	3.3
1	A	162	THR	3.2
1	D	258	ASP	2.9
1	A	305	LEU	2.8
1	A	468	PHE	2.8
1	B	119	ALA	2.7
1	C	106	PRO	2.7
1	A	106	PRO	2.7
1	C	300	PRO	2.7
1	A	238	ARG	2.6
1	A	204	ALA	2.5
1	B	257	GLN	2.5
1	A	124	LEU	2.4
1	A	304	LEU	2.4
1	A	236	PRO	2.3
1	A	350	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	259	GLY	2.3
1	A	145	ALA	2.3
1	A	309	LEU	2.2
1	A	298	GLU	2.2
1	A	343	ILE	2.2
1	A	283	ASN	2.2
1	A	207	MET	2.2
1	C	468	PHE	2.2
1	A	396	ASP	2.1
1	C	238	ARG	2.1
1	A	139	LYS	2.1
1	A	142	GLY	2.1
1	C	480	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	C	505	14/14	0.70	0.16	56,88,93,94	0
5	BTB	B	505	14/14	0.77	0.15	43,63,73,75	0
5	BTB	D	505	14/14	0.77	0.14	62,71,84,91	0
5	BTB	A	505	14/14	0.81	0.15	77,87,91,92	0
5	BTB	D	504	14/14	0.82	0.15	40,66,78,78	0
7	GOL	C	507	6/6	0.83	0.20	43,55,64,69	0
3	H4B	B	502	17/17	0.85	0.15	48,58,68,81	0
3	H4B	C	502	17/17	0.85	0.14	42,59,73,80	0
7	GOL	A	507	6/6	0.86	0.10	56,60,69,74	0
3	H4B	D	502	17/17	0.86	0.13	29,54,63,75	0

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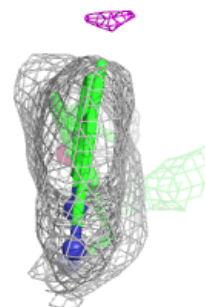
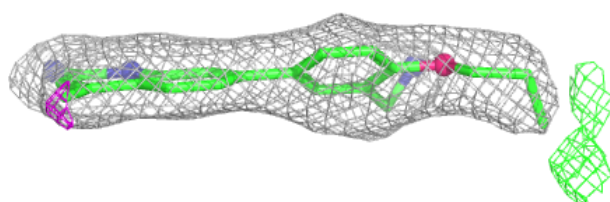
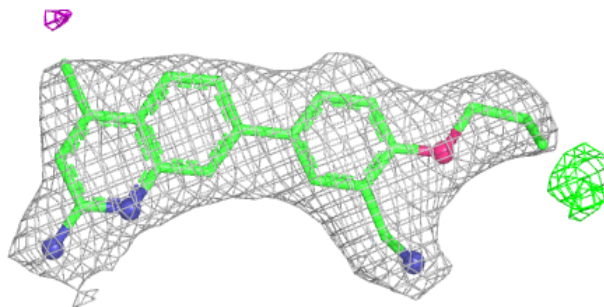
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	B	508	14/14	0.88	0.15	43,66,74,74	0
5	BTB	B	504	14/14	0.88	0.13	33,55,78,84	0
3	H4B	A	502	17/17	0.88	0.12	60,75,85,86	0
5	BTB	A	504	14/14	0.90	0.12	76,85,91,92	0
4	OSG	C	503	24/24	0.90	0.12	36,50,59,61	0
5	BTB	C	504	14/14	0.91	0.13	29,72,93,98	0
4	OSG	A	503	24/24	0.91	0.11	38,59,70,70	0
4	OSG	D	503	24/24	0.93	0.10	17,38,57,61	0
4	OSG	B	503	24/24	0.94	0.10	19,35,63,66	0
2	HEM	A	501	43/43	0.96	0.10	43,56,81,95	0
8	CL	B	506	1/1	0.96	0.08	47,47,47,47	0
8	CL	C	508	1/1	0.96	0.07	55,55,55,55	0
9	GD	A	509	1/1	0.96	0.06	119,119,119,119	0
8	CL	D	507	1/1	0.97	0.06	47,47,47,47	0
2	HEM	C	501	43/43	0.98	0.08	27,42,70,90	0
2	HEM	D	501	43/43	0.98	0.07	17,34,46,65	0
2	HEM	B	501	43/43	0.98	0.07	18,36,60,79	0
8	CL	A	508	1/1	0.98	0.05	55,55,55,55	0
9	GD	B	507	1/1	0.98	0.07	53,53,53,53	0
9	GD	C	509	1/1	0.98	0.04	99,99,99,99	0
9	GD	D	506	1/1	0.98	0.06	54,54,54,54	0
6	ZN	A	506	1/1	0.99	0.02	49,49,49,49	0
6	ZN	C	506	1/1	0.99	0.03	35,35,35,35	0

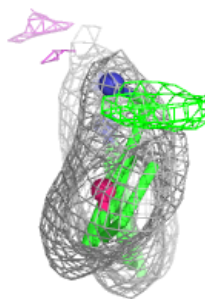
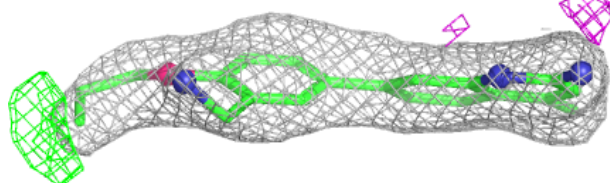
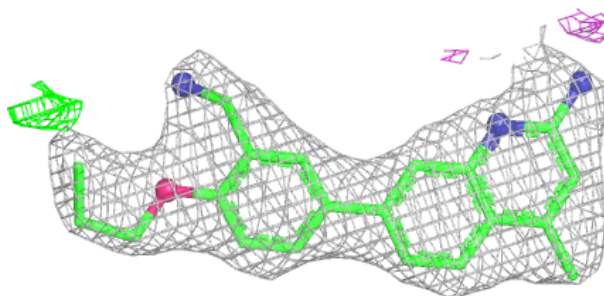
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OSG 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)

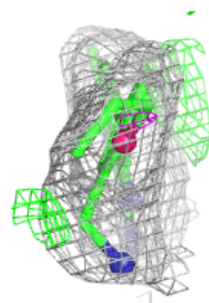
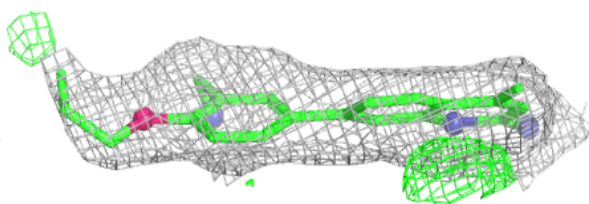
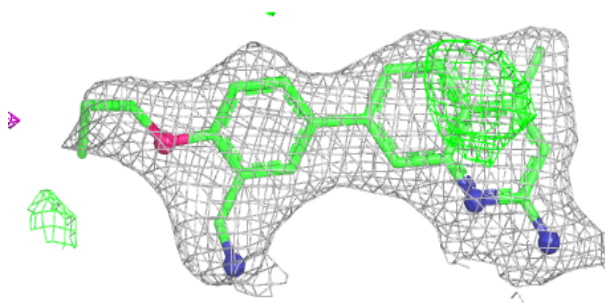
**Electron density around OSG A 503:**

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

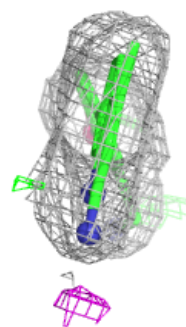
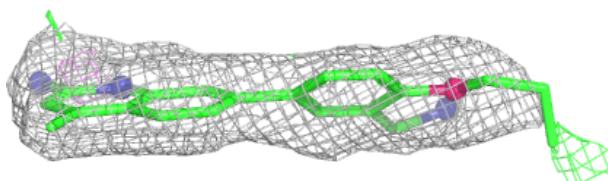
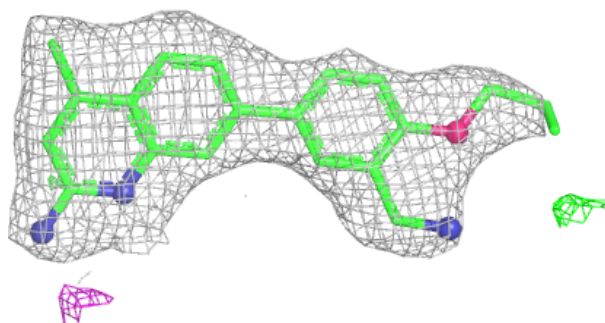


Electron density around OSG D 503:

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

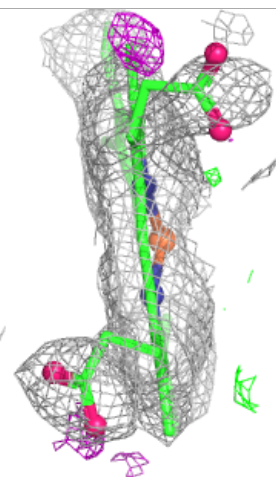
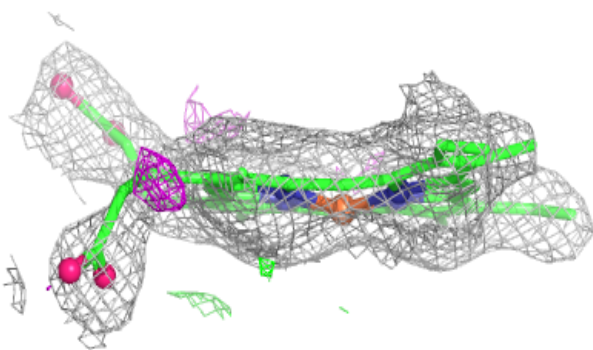
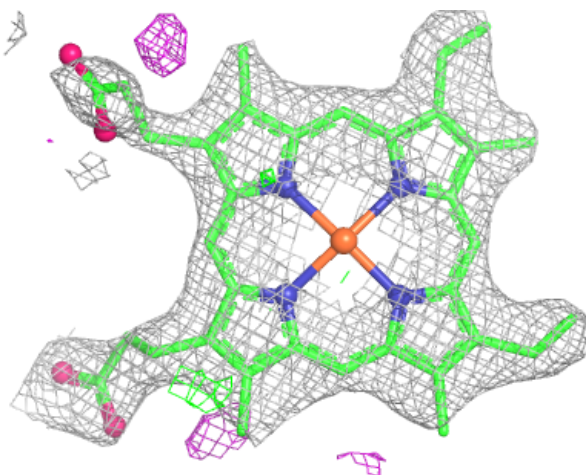
**Electron density around OSG B 503:**

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



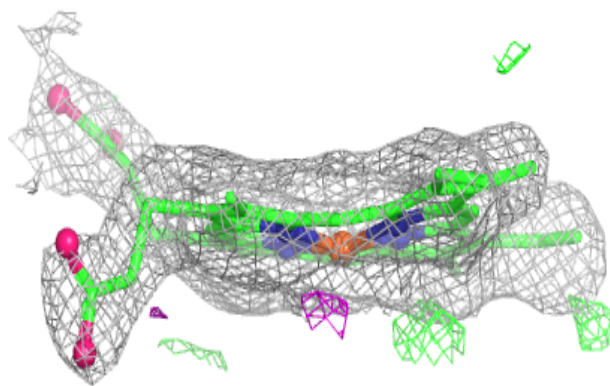
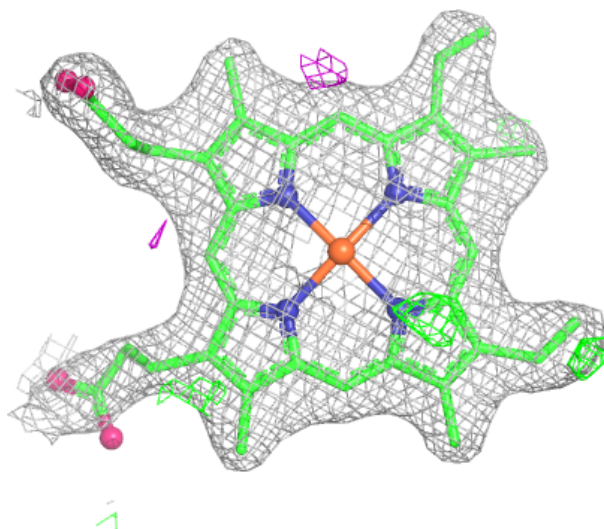
Electron density around HEM A 501:

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



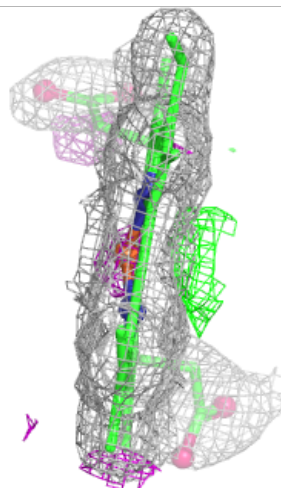
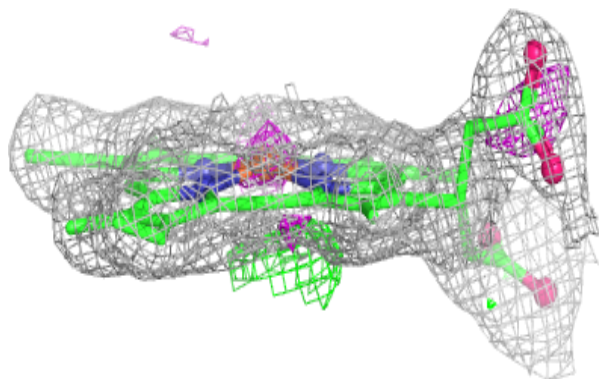
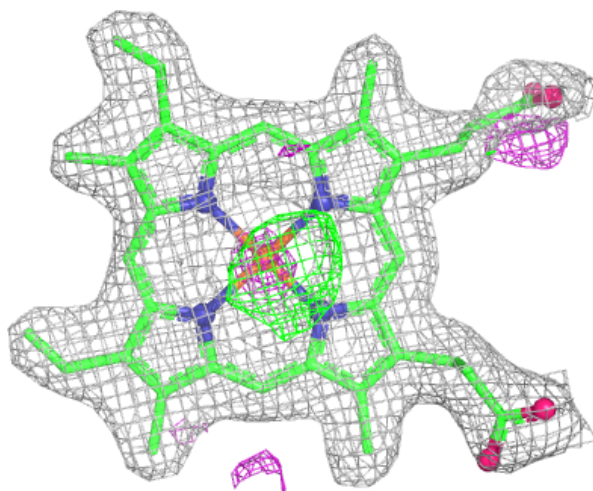
Electron density around HEM C 501:

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



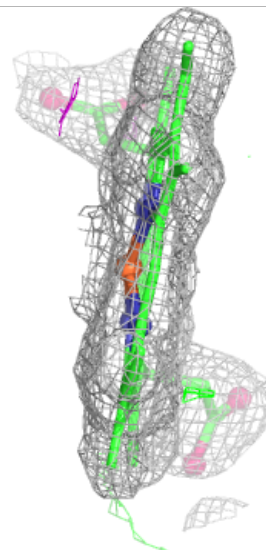
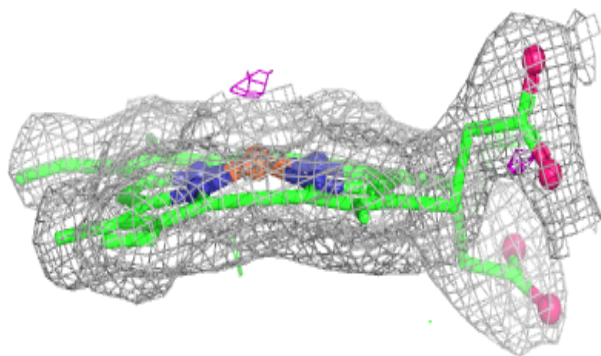
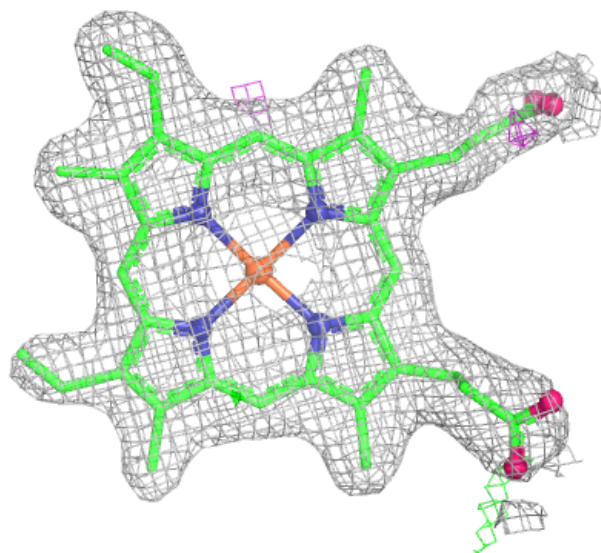
Electron density around HEM D 501:

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



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.