



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 09:41 PM EDT

PDB ID : 5UOA
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 3-[(2-Amino-4-methylquinolin-7-yl)methoxy]-5-((methylamino)methyl)benzonitrile
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

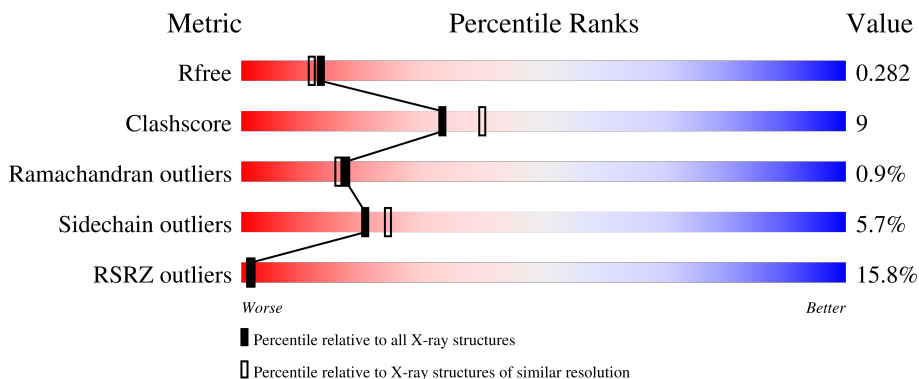
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	8EY	A	502	-	-	-	X

2 Entry composition [i](#)

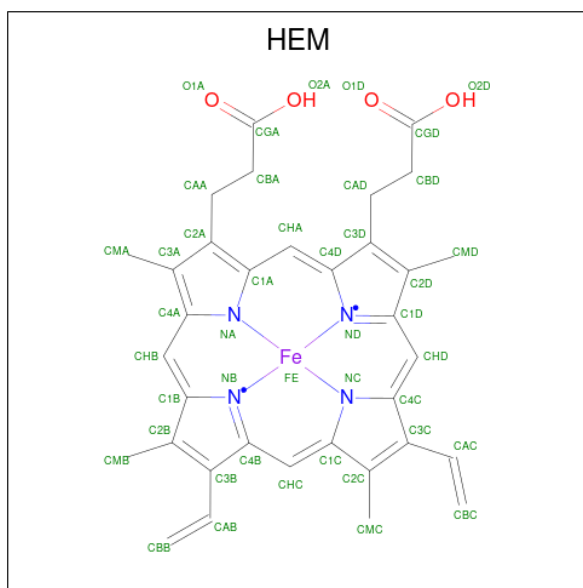
There are 9 unique types of molecules in this entry. The entry contains 6811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

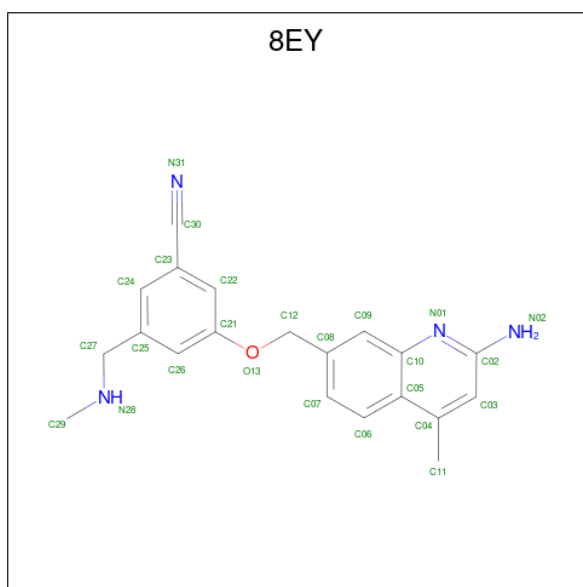
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	Total 3212	C 2046	N 563	O 587	S 16	0	3	0
1	B	402	Total 3230	C 2057	N 566	O 590	S 17	0	5	0

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



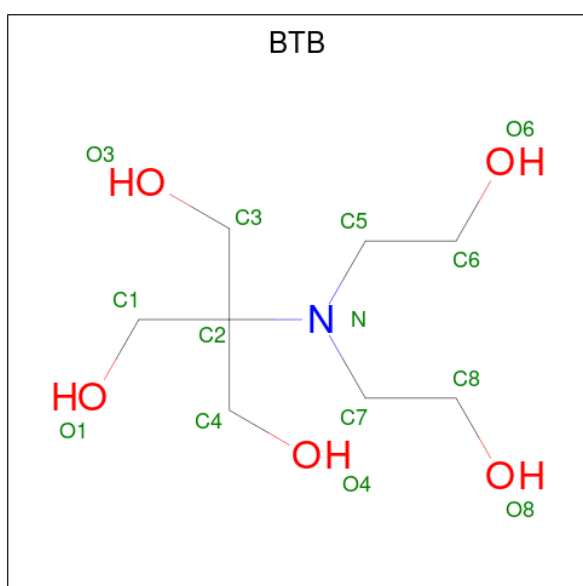
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(methylamino)methyl]benzonitrile (three-letter code: 8EY) (formula: $C_{20}H_{20}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	25	20	4	1	0	0
3	A	1	25	20	4	1	0	0
3	B	1	25	20	4	1	0	0
3	B	1	25	20	4	1	0	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).

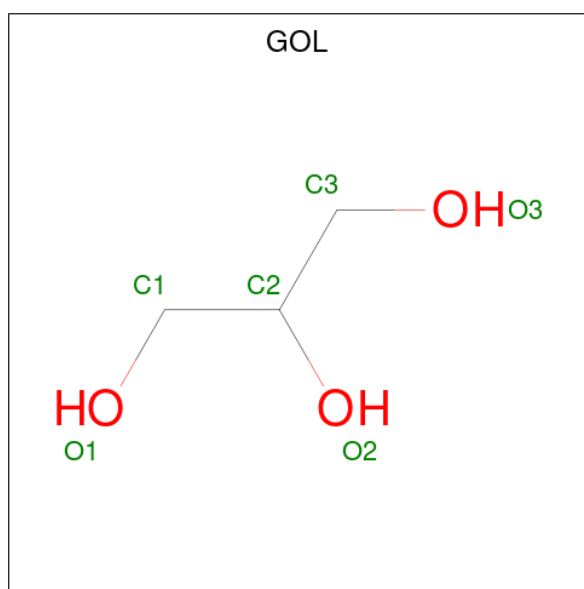


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		

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



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

- Molecule 7 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

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

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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	28	Total O 28 28	0	0
9	B	30	Total O 30 30	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.48Å 109.66Å 154.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.51 – 2.20 38.51 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.51-2.20) 96.5 (38.51-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.281 0.226 , 0.282	Depositor DCC
R_{free} test set	2524 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtrriage
Anisotropy	0.518	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6811	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/3313	0.53	0/4515
1	B	0.45	1/3334 (0.0%)	0.54	0/4543
All	All	0.43	1/6647 (0.0%)	0.53	0/9058

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	CYS	CB-SG	5.87	1.92	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3212	0	3114	54	0
1	B	3230	0	3137	45	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	50	0	0	2	0
3	B	50	0	0	1	0
4	A	28	0	38	6	0
4	B	84	0	111	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	0	0
6	A	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	28	0	0	1	0
9	B	30	0	0	1	0
All	All	6811	0	6468	114	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 9.

All (114) 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)
4:B:505:BTB:HO6	4:B:505:BTB:HO4	1.24	0.81
1:B:446:ALA:O	3:B:503:8EY:N02	2.24	0.70
1:A:244:TRP:HB2	1:A:292:LEU:HB3	1.77	0.67
1:A:124:LEU:HG	1:A:157:VAL:HG11	1.79	0.65
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.78	0.64
1:B:298:GLU:OE1	4:B:506:BTB:O6	2.15	0.64
1:A:359:SER:OG	1:A:419:ASP:HA	1.98	0.63
1:A:173:GLY:HA3	1:A:343:ILE:HD13	1.81	0.63
1:B:134:TYR:HH	1:B:168[A]:SER:HB3	1.64	0.61
1:B:138:ILE:O	1:B:140:ARG:N	2.30	0.60
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.84	0.59
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.84	0.59
1:B:321:GLU:OE1	4:B:504:BTB:O6	2.21	0.58
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.85	0.58
1:B:321:GLU:OE2	4:B:504:BTB:O3	2.21	0.58
1:B:238:ARG:NH1	1:B:239:GLY:O	2.37	0.57
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.86	0.57
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.86	0.56
1:A:176:GLN:HB3	1:A:471:PRO:HD2	1.88	0.56
1:A:277:HIS:CD2	1:A:292:LEU:HD21	2.41	0.56
4:A:504:BTB:O4	4:A:504:BTB:O3	2.21	0.55
1:B:342[A]:GLU:OE1	1:B:470:SER:OG	2.24	0.55
4:A:505:BTB:O6	4:A:505:BTB:O4	2.19	0.55
1:A:138:ILE:HG13	1:A:140:ARG:HG2	1.89	0.55
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.89	0.53
1:A:244:TRP:CZ2	1:A:300:PRO:HG3	2.44	0.53
1:A:160:THR:O	1:A:162:THR:N	2.41	0.53
1:B:200:ASP:OD1	4:B:509:BTB:O3	2.22	0.52
1:A:367:LEU:HB3	1:A:375:ILE:HD13	1.92	0.52
1:B:247:GLN:HB2	1:B:250:ARG:HG2	1.92	0.52
1:A:296:PRO:O	1:A:298:GLU:N	2.43	0.51
1:A:165:LEU:HG	1:A:346:LEU:HD12	1.93	0.51
1:B:128:ARG:O	1:B:132:ASN:ND2	2.43	0.51
1:A:294:GLN:HB2	1:A:300:PRO:HB3	1.94	0.50
1:B:145:ALA:HA	1:B:148:GLN:HB3	1.93	0.50
1:A:255:ARG:O	1:A:256:GLN:NE2	2.31	0.50
1:A:216:LYS:HB2	1:A:309:LEU:HD11	1.94	0.49
1:A:207:MET:HE2	1:A:293:LEU:HB3	1.93	0.49
1:A:235:CYS:HB3	1:A:238:ARG:HD2	1.94	0.49
4:A:504:BTB:H72	4:A:504:BTB:H12	1.56	0.49
1:A:247:GLN:HB2	1:A:250:ARG:HG2	1.96	0.48
1:B:157:VAL:HG13	1:B:161:GLY:O	2.14	0.48
1:A:277:HIS:NE2	1:A:300:PRO:HG2	2.28	0.48
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.28	0.47
1:A:128:ARG:O	1:A:132:ASN:ND2	2.47	0.47
1:A:128:ARG:HH21	1:A:154:GLU:CD	2.18	0.47
1:A:336:VAL:HG21	3:A:502:8EY:C07	2.45	0.47
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.50	0.47
1:A:322:TRP:CD1	4:A:504:BTB:H52	2.50	0.47
1:A:424:THR:OG1	1:A:458:PRO:HD2	2.15	0.46
1:A:71:VAL:HG22	1:A:463:GLU:HB3	1.98	0.46
1:B:379:VAL:O	1:B:383:MET:HG3	2.15	0.46
4:B:507:BTB:O4	4:B:507:BTB:O1	2.28	0.46
4:B:508:BTB:H51	4:B:508:BTB:H12	1.55	0.46
1:A:100:LEU:HB3	1:A:103:LEU:HD22	1.98	0.45
1:A:231:PHE:HB3	1:A:232:PRO:HD2	1.97	0.45
1:A:91:ASP:HB3	1:B:96:PRO:HB3	1.98	0.45
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.32	0.45
1:B:233:GLN:O	1:B:238:ARG:NH2	2.46	0.45
1:B:306:PRO:HA	1:B:307:PRO:HD3	1.88	0.45
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.96	0.45
1:B:124:LEU:HD21	1:B:154:GLU:HA	1.98	0.45
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.56	0.45
4:A:504:BTB:H42	4:A:504:BTB:H51	1.39	0.45
1:B:156:GLU:O	1:B:160:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:HIS:HB2	3:A:503:8EY:N31	2.32	0.44
1:A:359:SER:HG	1:A:419:ASP:HA	1.82	0.44
1:A:157:VAL:HG13	1:A:161:GLY:O	2.18	0.44
1:A:254:TYR:HB2	1:A:262:ARG:HB3	2.00	0.44
1:A:421:HIS:HB2	1:B:390:THR:HB	1.99	0.44
1:B:320:LEU:HD13	1:B:322:TRP:CZ2	2.52	0.44
4:B:505:BTB:H32	4:B:505:BTB:H72	1.46	0.44
1:A:245:ASN:HB3	1:A:247:GLN:O	2.18	0.43
1:B:255:ARG:HH12	1:B:259:GLY:HA2	1.83	0.43
1:B:265:PRO:O	1:B:268:VAL:HG23	2.17	0.43
1:A:180:ASN:O	1:A:182:PRO:HD3	2.19	0.43
1:B:428:MET:HG3	1:B:458:PRO:HB2	2.00	0.43
1:B:313:VAL:HA	1:B:314:PRO:HD2	1.93	0.43
4:B:507:BTB:H51	4:B:507:BTB:H11	1.68	0.43
1:A:234:ARG:HA	1:A:238:ARG:NH1	2.34	0.43
1:B:147:GLU:HA	1:B:150:LEU:HD12	2.01	0.43
1:B:347:GLU:O	1:B:349:PRO:HD3	2.19	0.42
1:B:178:TRP:CZ3	1:B:190:TRP:HA	2.53	0.42
4:B:506:BTB:H51	4:B:506:BTB:H42	1.38	0.42
1:B:175:LYS:HB3	1:B:190:TRP:CE3	2.55	0.42
1:B:229:THR:O	1:B:351:ALA:HA	2.19	0.42
1:A:97:ARG:HE	1:A:97:ARG:HB3	1.61	0.42
4:B:509:BTB:H71	4:B:509:BTB:H41	1.79	0.42
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.53	0.41
4:B:509:BTB:H12	4:B:509:BTB:H52	1.66	0.41
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.82	0.41
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.81	0.41
4:B:505:BTB:H11	4:B:505:BTB:H51	1.45	0.41
1:A:119:ALA:N	1:A:120:PRO:HD3	2.35	0.41
1:A:271:THR:OG1	1:A:289:LEU:HD21	2.20	0.41
1:A:290:PRO:HB2	1:A:302:LEU:HD22	2.03	0.41
1:B:357:TYR:CD2	1:B:362:ILE:HD11	2.54	0.41
4:A:505:BTB:H12	4:A:505:BTB:H51	1.88	0.41
1:B:323:PHE:HB3	9:B:609:HOH:O	2.20	0.41
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.97	0.41
1:B:199:ARG:O	1:B:232:PRO:HG3	2.21	0.41
1:B:319:THR:O	1:B:321:GLU:OE1	2.39	0.41
4:B:504:BTB:H42	4:B:504:BTB:H71	1.78	0.41
1:A:379:VAL:O	1:A:383:MET:HG3	2.21	0.41
1:B:244:TRP:CZ2	1:B:300:PRO:HG3	2.56	0.40
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:NE2	1:A:300:PRO:HD3	2.36	0.40
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.56	0.40
1:B:357:TYR:O	1:B:418:VAL:HG12	2.22	0.40
1:A:224:LEU:O	9:A:601:HOH:O	2.21	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.83	0.40
1:A:419:ASP:OD2	1:B:390:THR:OG1	2.32	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	400/440 (91%)	377 (94%)	21 (5%)	2 (0%)	29	31
1	B	403/440 (92%)	378 (94%)	20 (5%)	5 (1%)	13	10
All	All	803/880 (91%)	755 (94%)	41 (5%)	7 (1%)	17	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	GLN
1	B	140	ARG
1	A	161	GLY
1	B	139	LYS
1	B	143	SER
1	A	141	SER
1	B	138	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/373 (92%)	329 (96%)	14 (4%)	30	39
1	B	346/373 (93%)	320 (92%)	26 (8%)	13	14
All	All	689/746 (92%)	649 (94%)	40 (6%)	20	23

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	97	ARG
1	A	98	ARG
1	A	152	GLU
1	A	202	ARG
1	A	238	ARG
1	A	262	ARG
1	A	277	HIS
1	A	304	LEU
1	A	359	SER
1	A	391	SER
1	A	411	GLN
1	A	455	SER
1	A	470	SER
1	B	67	LYS
1	B	68	PHE
1	B	89	GLN
1	B	90	GLN
1	B	97	ARG
1	B	98	ARG
1	B	103	LEU
1	B	137	SER
1	B	138	ILE
1	B	147	GLU
1	B	162	THR
1	B	168[A]	SER
1	B	168[B]	SER

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Mol	Chain	Res	Type
1	B	224	LEU
1	B	226	SER
1	B	255	ARG
1	B	257	GLN
1	B	258	ASP
1	B	298	GLU
1	B	326	LEU
1	B	329	ARG
1	B	359	SER
1	B	384	ASP
1	B	396	ASP
1	B	468	PHE
1	B	470	SER

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	BTB	B	505	-	13,13,13	0.36	0	7,16,16	0.82	0
4	BTB	B	509	-	13,13,13	0.39	0	7,16,16	0.26	0
4	BTB	B	507	-	13,13,13	0.58	0	7,16,16	1.09	0
6	GOL	A	507	-	5,5,5	0.29	0	5,5,5	0.38	0
4	BTB	B	506	-	13,13,13	0.48	0	7,16,16	0.53	0
2	HEM	B	501	1	41,50,50	1.96	7 (17%)	45,82,82	2.20	15 (33%)
4	BTB	B	504	7	13,13,13	0.72	0	7,16,16	1.09	1 (14%)
2	HEM	A	501	1	41,50,50	2.04	6 (14%)	45,82,82	2.05	12 (26%)
3	8EY	B	502	-	27,27,27	1.61	1 (3%)	35,37,37	0.88	3 (8%)
4	BTB	A	504	7	13,13,13	0.52	0	7,16,16	0.92	0
3	8EY	A	503	-	27,27,27	1.62	2 (7%)	35,37,37	1.24	5 (14%)
4	BTB	A	505	-	13,13,13	0.44	0	7,16,16	0.83	0
3	8EY	B	503	-	27,27,27	1.64	4 (14%)	35,37,37	0.98	1 (2%)
3	8EY	A	502	-	27,27,27	1.59	1 (3%)	35,37,37	0.94	2 (5%)
4	BTB	B	508	-	13,13,13	0.37	0	7,16,16	0.51	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
4	BTB	B	505	-	-	13/21/21/21	-
4	BTB	B	509	-	-	4/21/21/21	-
4	BTB	B	507	-	-	10/21/21/21	-
6	GOL	A	507	-	-	2/4/4/4	-
4	BTB	B	506	-	-	10/21/21/21	-
2	HEM	B	501	1	-	1/12/54/54	-
4	BTB	B	504	7	-	6/21/21/21	-
2	HEM	A	501	1	-	1/12/54/54	-
3	8EY	B	502	-	-	1/9/10/10	0/3/3/3
4	BTB	A	504	7	-	8/21/21/21	-
3	8EY	A	503	-	-	0/9/10/10	0/3/3/3
4	BTB	A	505	-	-	10/21/21/21	-
3	8EY	B	503	-	-	2/9/10/10	0/3/3/3
3	8EY	A	502	-	-	0/9/10/10	0/3/3/3
4	BTB	B	508	-	-	7/21/21/21	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	8.32	1.54	1.36
2	B	501	HEM	C3D-C2D	7.69	1.53	1.36
3	B	502	8EY	C23-C30	-6.89	1.29	1.44
3	A	502	8EY	C23-C30	-6.89	1.29	1.44
3	A	503	8EY	C23-C30	-6.86	1.29	1.44
3	B	503	8EY	C23-C30	-6.69	1.29	1.44
2	A	501	HEM	FE-NB	4.71	2.20	1.96
2	B	501	HEM	C3C-CAC	4.03	1.56	1.47
2	A	501	HEM	C3C-CAC	3.62	1.55	1.47
2	B	501	HEM	FE-NB	3.58	2.14	1.96
2	B	501	HEM	C3C-C2C	-3.56	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.15	1.36	1.40
2	A	501	HEM	CAB-C3B	3.08	1.55	1.47
2	B	501	HEM	CAB-C3B	2.97	1.55	1.47
2	B	501	HEM	FE-ND	2.30	2.08	1.96
3	B	503	8EY	C03-C04	2.29	1.41	1.37
3	B	503	8EY	C09-C10	-2.17	1.38	1.41
2	A	501	HEM	CMC-C2C	2.11	1.56	1.51
2	B	501	HEM	CHA-C4D	2.04	1.40	1.35
3	B	503	8EY	C06-C07	2.02	1.40	1.36
3	A	503	8EY	C05-C10	-2.01	1.39	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4D-ND-C1D	7.79	113.12	105.07
2	B	501	HEM	C4D-ND-C1D	7.21	112.52	105.07
2	B	501	HEM	C4C-CHD-C1D	5.54	129.87	122.56
2	B	501	HEM	C1B-NB-C4B	3.87	109.07	105.07
2	B	501	HEM	CBA-CAA-C2A	-3.72	106.26	112.62
2	B	501	HEM	C3B-C2B-C1B	3.64	109.19	106.49
2	A	501	HEM	CBA-CAA-C2A	-3.62	106.44	112.62
2	A	501	HEM	C4B-CHC-C1C	3.35	126.98	122.56
2	A	501	HEM	C3B-C2B-C1B	3.03	108.73	106.49
2	A	501	HEM	C4C-CHD-C1D	3.02	126.55	122.56
2	A	501	HEM	C1B-NB-C4B	3.01	108.18	105.07
3	A	502	8EY	C04-C05-C10	3.00	119.63	118.01
3	A	503	8EY	C04-C05-C10	2.82	119.53	118.01
2	B	501	HEM	C4B-CHC-C1C	2.77	126.21	122.56
2	B	501	HEM	C2B-C1B-NB	-2.71	106.63	109.84
3	A	503	8EY	C05-C10-N01	-2.68	119.97	122.81
3	A	502	8EY	C05-C10-N01	-2.66	119.98	122.81
3	A	503	8EY	N02-C02-N01	2.66	120.46	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	8EY	C12-C08-C09	-2.63	115.47	121.22
2	A	501	HEM	CMC-C2C-C3C	2.60	129.54	124.68
2	A	501	HEM	C4A-C3A-C2A	2.58	108.79	107.00
2	A	501	HEM	C3D-C4D-ND	-2.52	107.36	110.17
3	A	503	8EY	C12-O13-C21	2.34	123.43	117.65
2	B	501	HEM	CHB-C1B-NB	2.30	127.23	124.38
2	B	501	HEM	CHC-C4B-C3B	2.30	128.09	124.57
3	B	502	8EY	C04-C05-C10	2.29	119.25	118.01
2	B	501	HEM	CAD-C3D-C4D	2.28	128.63	124.66
2	B	501	HEM	C3D-C4D-ND	-2.28	107.63	110.17
2	A	501	HEM	CBD-CAD-C3D	-2.26	106.34	112.63
4	B	504	BTB	O3-C3-C2	2.26	117.61	111.44
3	A	503	8EY	C24-C23-C30	2.25	122.53	119.54
2	B	501	HEM	CBD-CAD-C3D	-2.18	106.56	112.63
2	B	501	HEM	CMC-C2C-C3C	2.16	128.72	124.68
2	A	501	HEM	CHA-C4D-ND	2.11	126.99	124.38
2	A	501	HEM	C2B-C1B-NB	-2.03	107.43	109.84
2	B	501	HEM	CAD-CBD-CGD	-2.01	109.28	113.60
3	B	502	8EY	C05-C10-N01	-2.00	120.69	122.81
3	B	502	8EY	C12-O13-C21	2.00	122.59	117.65
2	B	501	HEM	CHD-C1D-ND	2.00	126.60	124.43

There are no chirality outliers.

All (75) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	B	504	BTB	C4-C2-C3-O3
4	B	504	BTB	N-C2-C3-O3
4	B	504	BTB	C1-C2-C4-O4
4	B	504	BTB	C3-C2-C4-O4
4	B	504	BTB	N-C2-C4-O4
4	B	505	BTB	O1-C1-C2-C3
4	B	505	BTB	O1-C1-C2-C4
4	B	505	BTB	O1-C1-C2-N
4	B	505	BTB	C1-C2-N-C5
4	B	505	BTB	C1-C2-N-C7
4	B	505	BTB	C3-C2-N-C5
4	B	505	BTB	C3-C2-N-C7
4	B	505	BTB	C4-C2-N-C5
4	B	505	BTB	C4-C2-N-C7
4	B	506	BTB	C1-C2-C3-O3
4	B	506	BTB	C4-C2-C3-O3
4	B	506	BTB	N-C2-C3-O3
4	B	506	BTB	C1-C2-N-C7
4	B	507	BTB	O1-C1-C2-C3
4	B	507	BTB	O1-C1-C2-C4
4	B	507	BTB	O1-C1-C2-N
4	B	508	BTB	O1-C1-C2-C3
4	B	508	BTB	O1-C1-C2-C4
4	B	508	BTB	O1-C1-C2-N
4	B	509	BTB	C1-C2-C3-O3
4	B	509	BTB	C4-C2-C3-O3
4	B	509	BTB	N-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
4	A	505	BTB	N-C5-C6-O6
4	B	506	BTB	N-C5-C6-O6
3	B	503	8EY	C26-C21-O13-C12
3	B	503	8EY	C22-C21-O13-C12
4	B	508	BTB	N-C7-C8-O8
4	B	507	BTB	N-C5-C6-O6
6	A	507	GOL	O1-C1-C2-O2
4	A	504	BTB	N-C7-C8-O8
4	B	505	BTB	N-C7-C8-O8
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
4	B	505	BTB	C4-C2-C3-O3
4	A	504	BTB	C4-C2-N-C5
4	B	505	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	506	BTB	N-C2-C4-O4
4	B	506	BTB	C3-C2-N-C5
4	B	506	BTB	C3-C2-N-C7
4	B	506	BTB	C4-C2-N-C5
4	B	506	BTB	C4-C2-N-C7
4	B	507	BTB	C1-C2-N-C5
4	B	507	BTB	C3-C2-N-C5
4	B	507	BTB	C3-C2-N-C7
4	B	507	BTB	C4-C2-N-C5
4	B	507	BTB	C4-C2-N-C7
4	B	508	BTB	C1-C2-N-C5
4	B	508	BTB	C3-C2-N-C7
4	B	509	BTB	N-C5-C6-O6
4	B	507	BTB	N-C7-C8-O8
4	B	508	BTB	C8-C7-N-C5
3	B	502	8EY	C22-C23-C30-N31
4	B	505	BTB	C1-C2-C3-O3

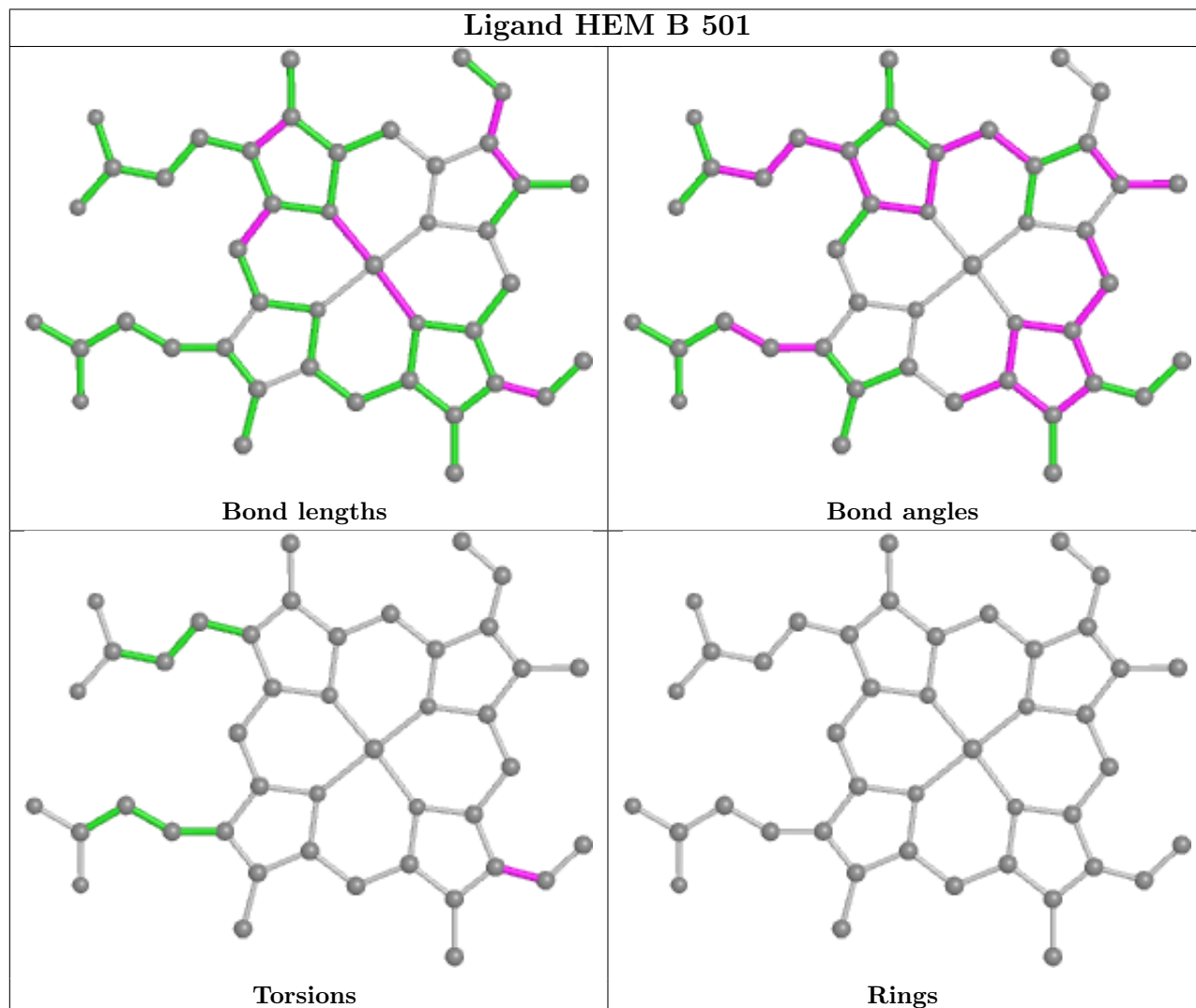
There are no ring outliers.

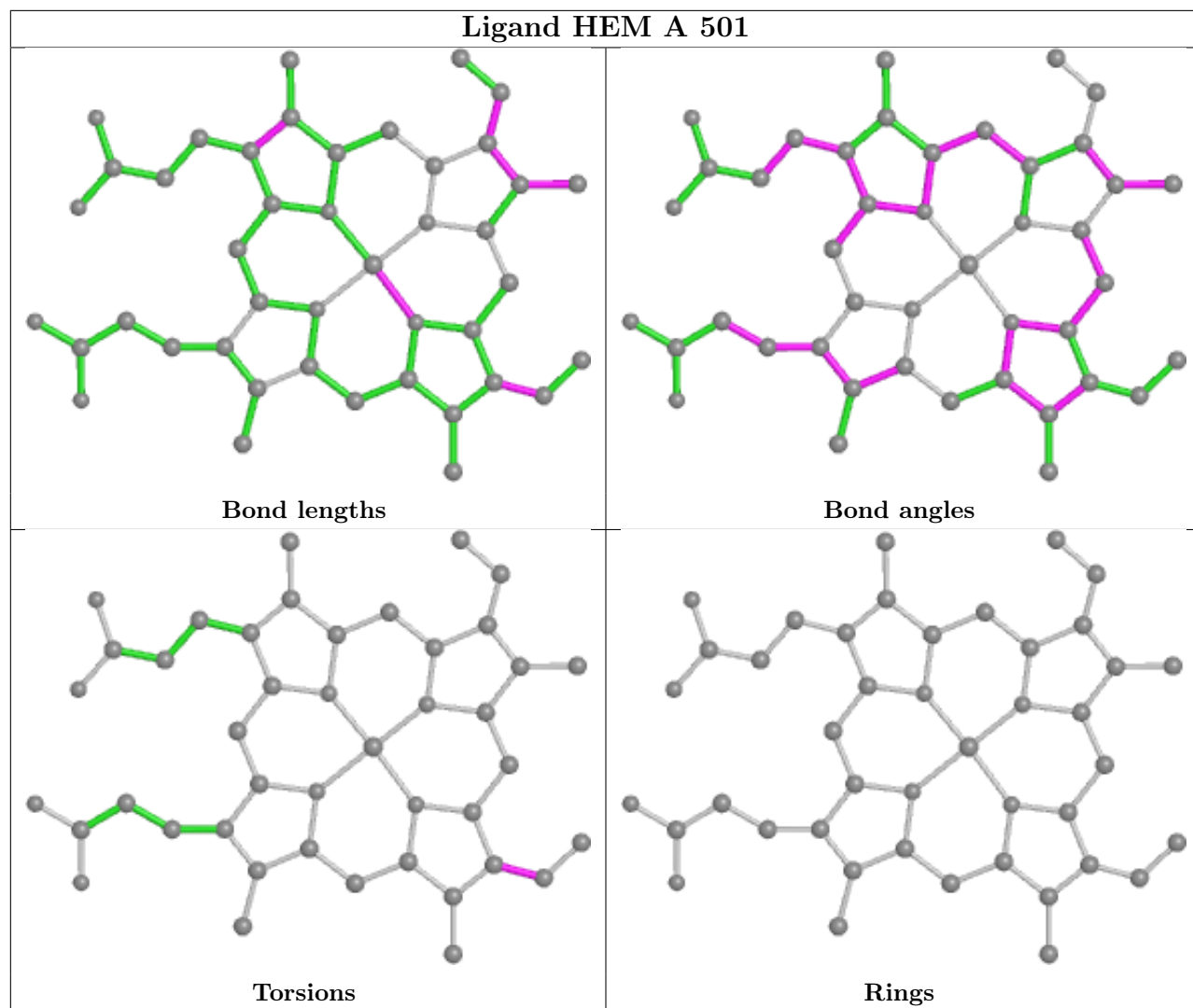
13 monomers are involved in 27 short contacts:

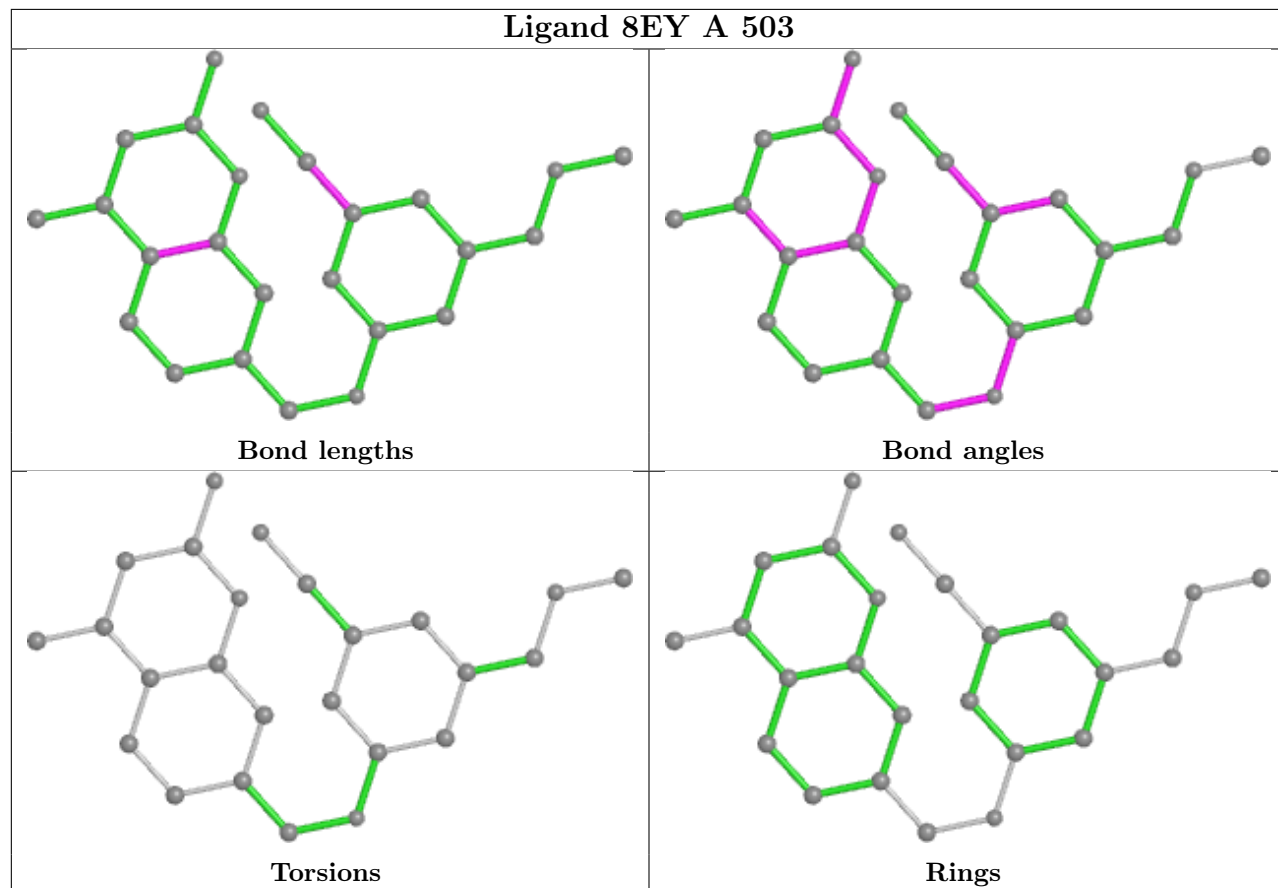
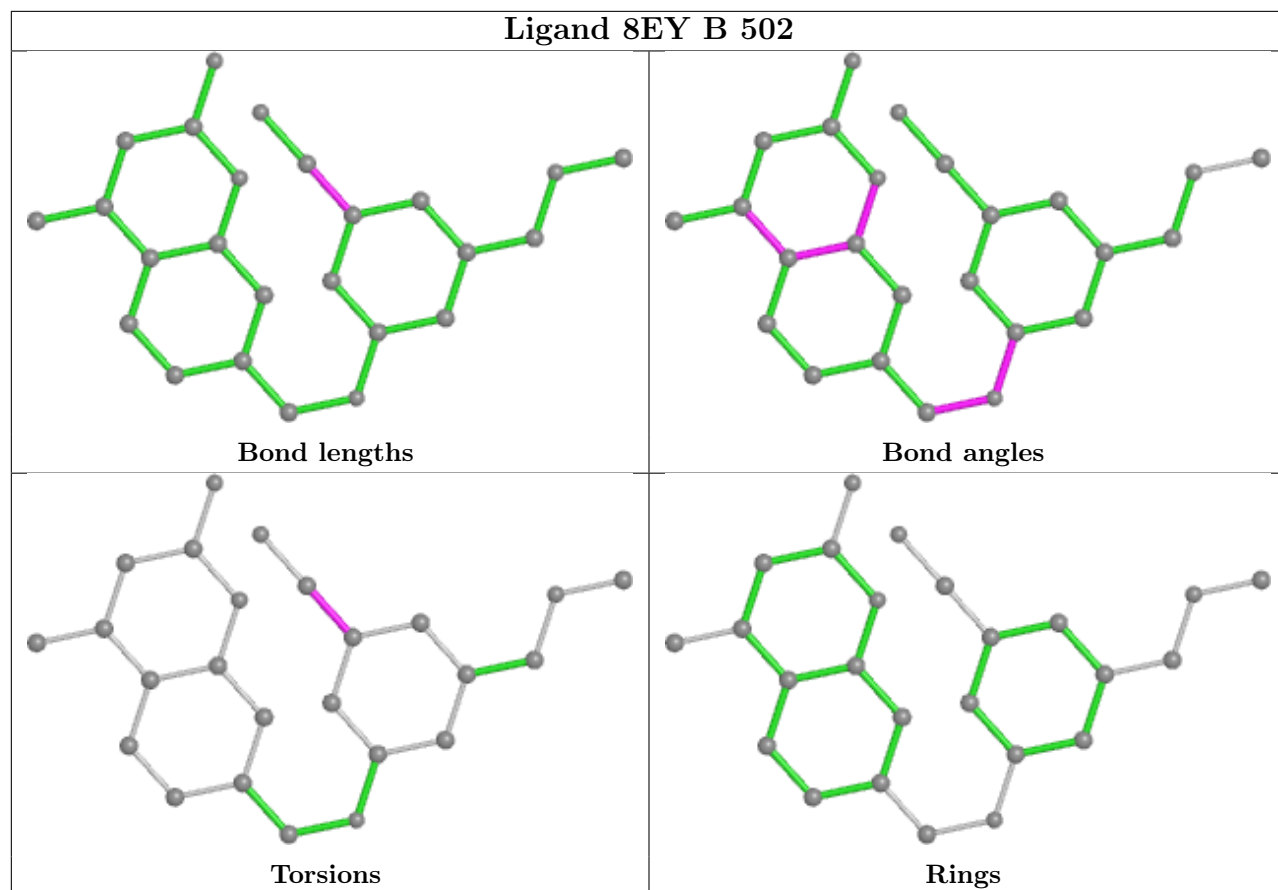
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	BTB	3	0
4	B	509	BTB	3	0
4	B	507	BTB	2	0
4	B	506	BTB	2	0
2	B	501	HEM	2	0
4	B	504	BTB	3	0
2	A	501	HEM	2	0
4	A	504	BTB	4	0
3	A	503	8EY	1	0
4	A	505	BTB	2	0
3	B	503	8EY	1	0
3	A	502	8EY	1	0
4	B	508	BTB	1	0

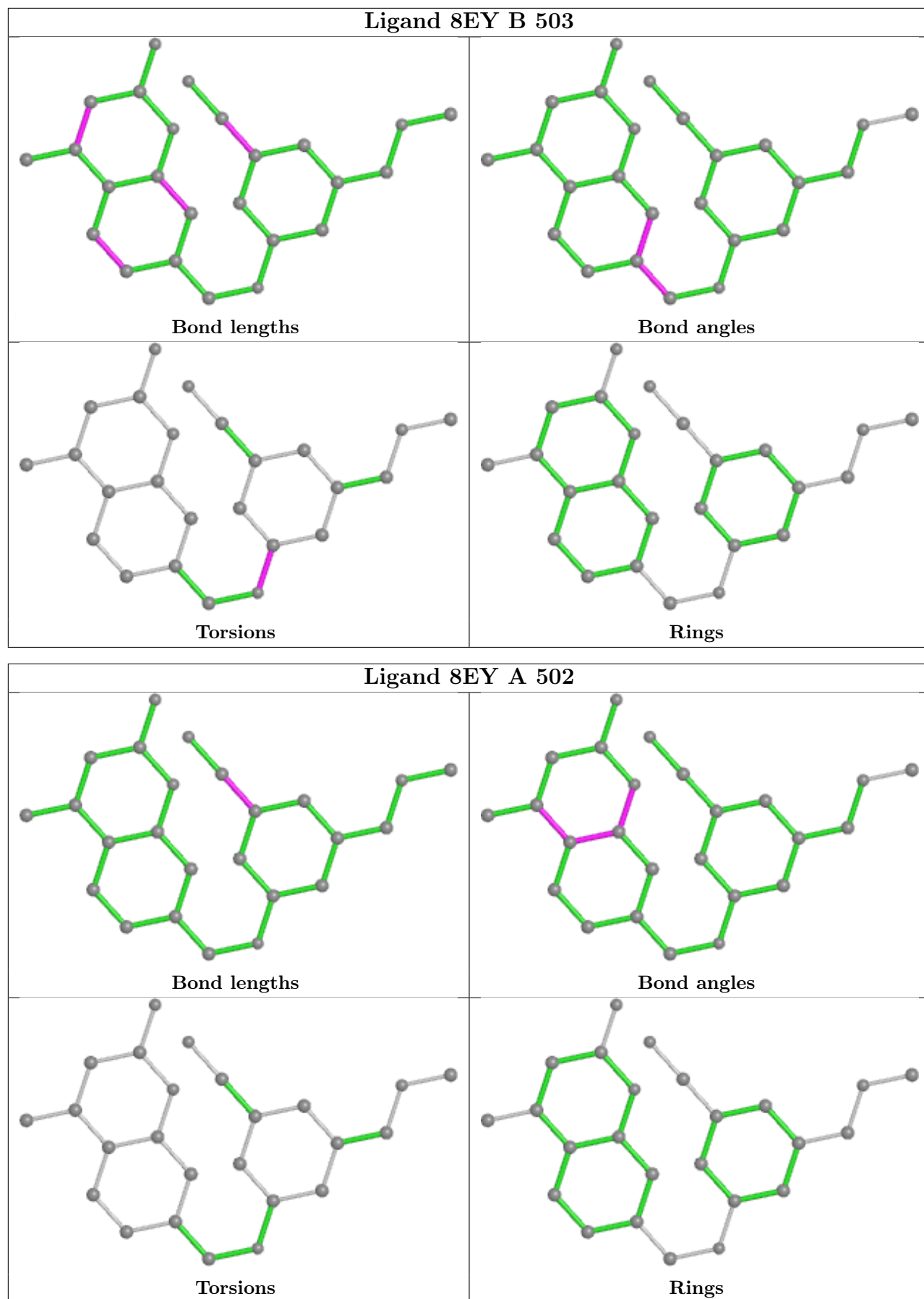
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	401/440 (91%)	1.09	85 (21%) 0 0	42, 81, 133, 183	0
1	B	402/440 (91%)	0.62	42 (10%) 6 5	44, 74, 122, 185	0
All	All	803/880 (91%)	0.86	127 (15%) 2 1	42, 78, 130, 185	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	ARG	8.1
1	A	303	PHE	6.7
1	A	451	PRO	6.0
1	B	68	PHE	5.8
1	B	141[A]	SER	5.7
1	A	275	ILE	5.6
1	A	89	GLN	5.5
1	B	89	GLN	5.5
1	A	141	SER	5.5
1	A	447	TRP	5.5
1	A	280	THR	5.1
1	B	79	ILE	4.8
1	B	161	GLY	4.6
1	A	450	PRO	4.6
1	A	257	GLN	4.6
1	A	259	GLY	4.5
1	A	277	HIS	4.5
1	B	120	PRO	4.3
1	B	452	ILE	4.3
1	A	278	GLY	4.3
1	B	454	GLY	4.1
1	A	86	ALA	4.1
1	B	157	VAL	4.0
1	A	448	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	293	LEU	4.0
1	A	388	ARG	4.0
1	A	452	ILE	3.9
1	B	142	GLY	3.9
1	A	90	GLN	3.9
1	A	302	LEU	3.8
1	A	294	GLN	3.8
1	A	134	TYR	3.8
1	B	124	LEU	3.8
1	A	185	VAL	3.7
1	B	153	VAL	3.7
1	A	449	VAL	3.7
1	A	276	GLN	3.7
1	A	279	TRP	3.7
1	B	119	ALA	3.7
1	B	158	ALA	3.7
1	A	304	LEU	3.7
1	A	140	ARG	3.7
1	A	446	ALA	3.6
1	A	241	PHE	3.5
1	A	68	PHE	3.5
1	A	273	LEU	3.4
1	A	184	CYS	3.4
1	A	479	PRO	3.4
1	A	480	TRP	3.4
1	A	360	THR	3.3
1	A	142	GLY	3.3
1	A	81	TYR	3.3
1	B	67	LYS	3.2
1	A	255	ARG	3.2
1	A	365	ARG	3.1
1	A	70	ARG	3.1
1	B	303	PHE	3.0
1	A	281	PRO	3.0
1	B	450	PRO	3.0
1	A	236	PRO	2.9
1	A	412	LEU	2.9
1	A	272	GLU	2.9
1	A	445	TRP	2.8
1	A	300	PRO	2.8
1	B	255	ARG	2.8
1	A	76	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	298	GLU	2.7
1	A	439	GLY	2.7
1	A	157	VAL	2.7
1	B	455	SER	2.7
1	B	160	THR	2.7
1	A	454	GLY	2.7
1	B	453	SER	2.7
1	A	216	LYS	2.7
1	A	301	GLU	2.7
1	B	150	LEU	2.7
1	A	368	CYS	2.6
1	A	83	THR	2.6
1	B	388	ARG	2.6
1	B	90	GLN	2.6
1	A	436	LYS	2.6
1	A	364	THR	2.5
1	A	239	GLY	2.5
1	A	221	ARG	2.5
1	A	183	ARG	2.5
1	A	363	GLY	2.5
1	A	274	CYS	2.5
1	A	271	THR	2.5
1	A	295	ALA	2.5
1	B	257	GLN	2.4
1	B	446	ALA	2.4
1	A	161	GLY	2.4
1	A	359	SER	2.4
1	B	159	ALA	2.4
1	A	153	VAL	2.4
1	A	150	LEU	2.4
1	A	207	MET	2.4
1	A	254	TYR	2.4
1	B	439	GLY	2.4
1	B	86	ALA	2.3
1	A	244	TRP	2.3
1	B	140	ARG	2.3
1	B	196	PHE	2.3
1	B	468	PHE	2.3
1	A	292	LEU	2.3
1	A	78	SER	2.3
1	B	80	THR	2.3
1	B	260	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	389	THR	2.2
1	A	165	LEU	2.2
1	B	81	TYR	2.2
1	A	435	GLN	2.2
1	A	148	GLN	2.2
1	B	122	GLN	2.2
1	B	460	PHE	2.2
1	A	182	PRO	2.2
1	A	146	HIS	2.1
1	A	353	PHE	2.1
1	B	365	ARG	2.1
1	A	145	ALA	2.1
1	A	162	THR	2.1
1	B	275	ILE	2.1
1	A	163	TYR	2.1
1	B	70	ARG	2.1
1	B	360	THR	2.0
1	A	444	ASP	2.0
1	A	79	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8EY	B	502	25/25	0.79	0.28	63,91,123,130	0
3	8EY	A	502	25/25	0.80	0.49	71,92,125,129	0
4	BTB	B	509	14/14	0.80	0.20	94,103,114,114	0
4	BTB	A	505	14/14	0.84	0.15	82,100,114,117	0

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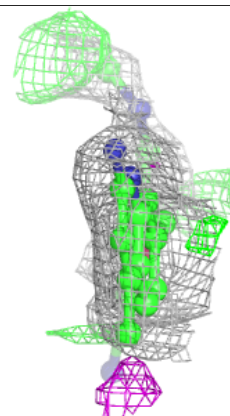
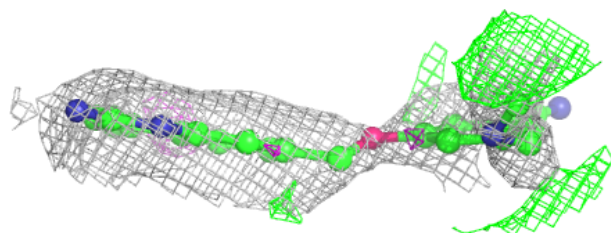
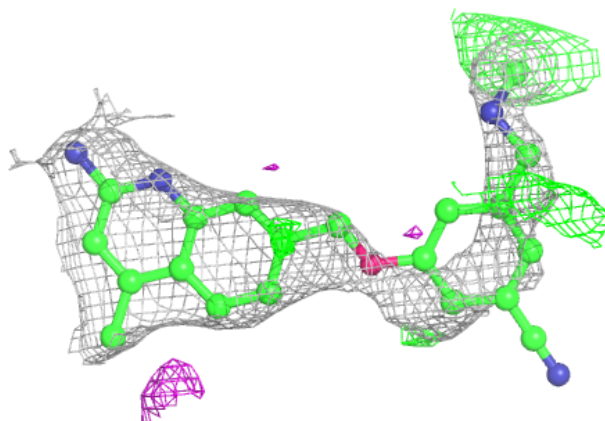
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	507	6/6	0.87	0.29	64,72,72,73	0
4	BTB	B	506	14/14	0.89	0.26	71,89,97,103	0
4	BTB	B	504	14/14	0.89	0.21	48,75,100,107	0
5	ZN	A	509	1/1	0.89	0.14	70,70,70,70	1
4	BTB	B	505	14/14	0.89	0.12	98,107,113,113	0
4	BTB	B	508	14/14	0.90	0.12	86,100,106,110	0
5	ZN	A	510	1/1	0.90	0.15	72,72,72,72	1
4	BTB	B	507	14/14	0.90	0.17	78,89,95,97	0
3	8EY	B	503	25/25	0.91	0.23	35,60,110,111	0
2	HEM	B	501	43/43	0.92	0.20	50,78,91,99	0
4	BTB	A	504	14/14	0.93	0.24	53,85,108,110	0
2	HEM	A	501	43/43	0.94	0.31	40,76,99,119	0
3	8EY	A	503	25/25	0.95	0.18	40,64,93,95	0
8	CL	B	511	1/1	0.96	0.15	61,61,61,61	0
8	CL	A	511	1/1	0.97	0.28	67,67,67,67	0
7	GD	B	510	1/1	0.98	0.14	63,63,63,63	0
7	GD	A	508	1/1	0.99	0.08	99,99,99,99	0
5	ZN	A	506	1/1	0.99	0.10	67,67,67,67	0

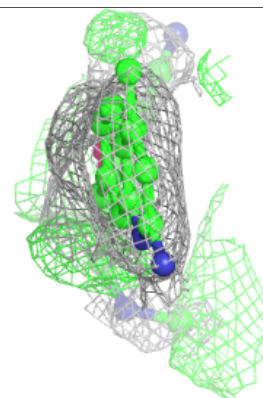
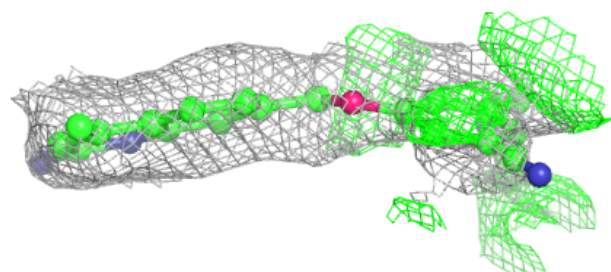
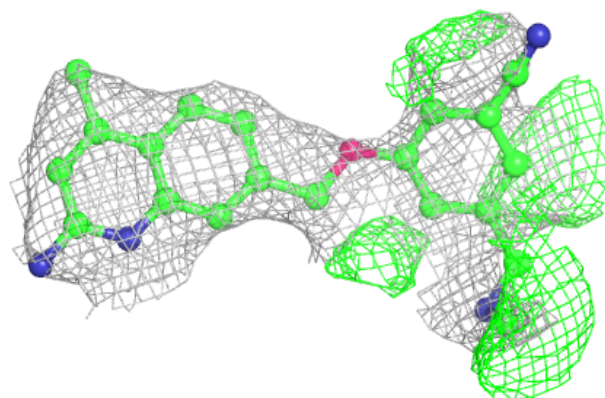
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8EY B 502:

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

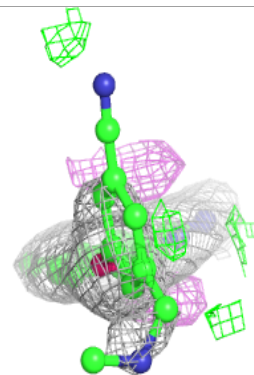
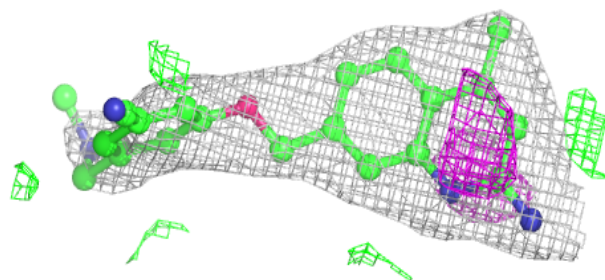
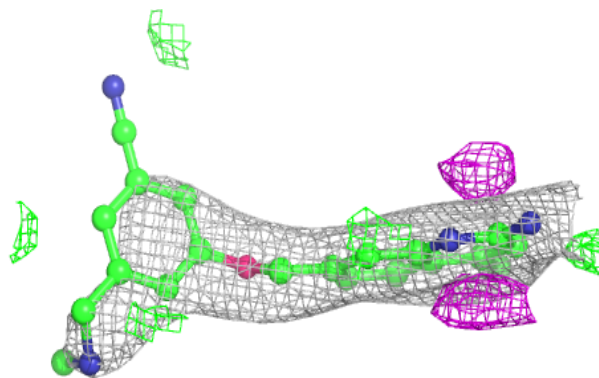
**Electron density around 8EY A 502:**

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



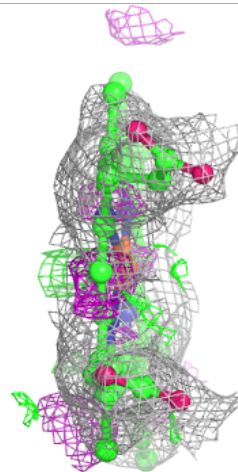
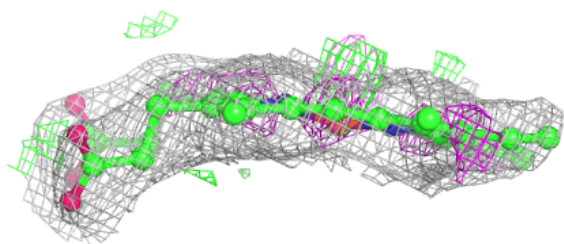
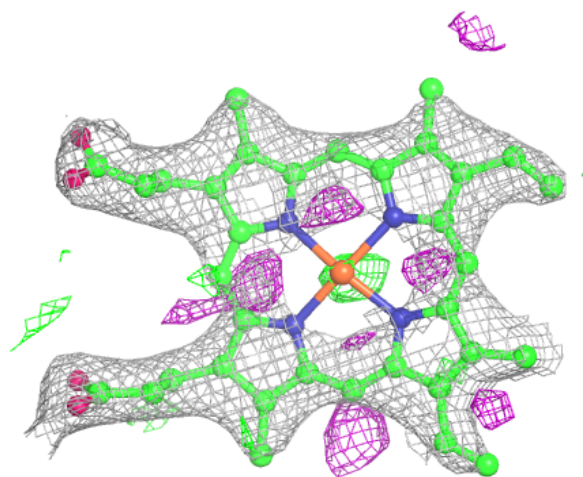
Electron density around 8EY B 503:

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



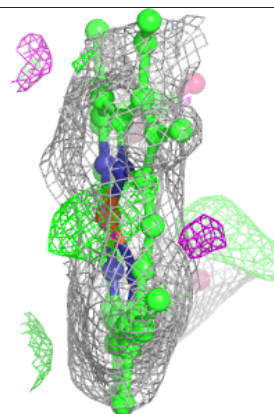
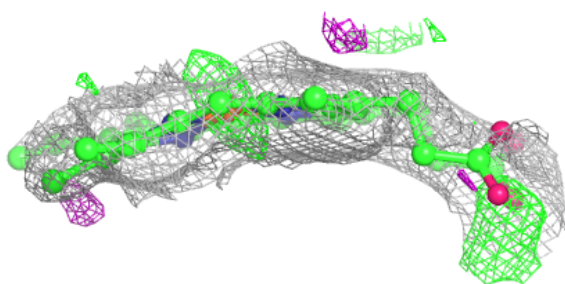
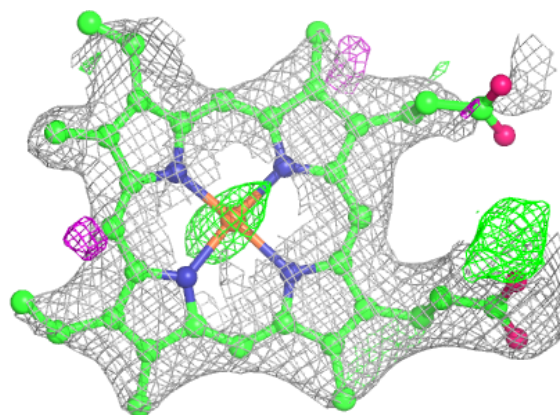
Electron density around HEM B 501:

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

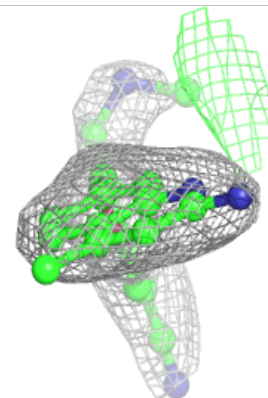
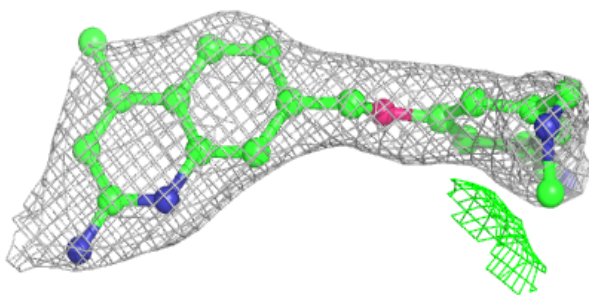
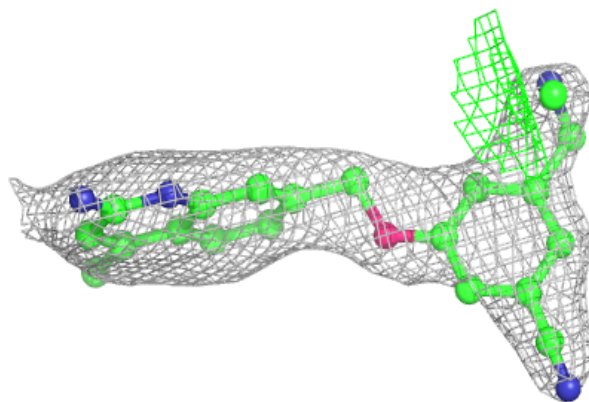


Electron density around HEM A 501:

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

**Electron density around 8EY 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.