



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:49 AM UTC

PDB ID : 5UOA / pdb_00005uoa
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
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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	:	4-5-2 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

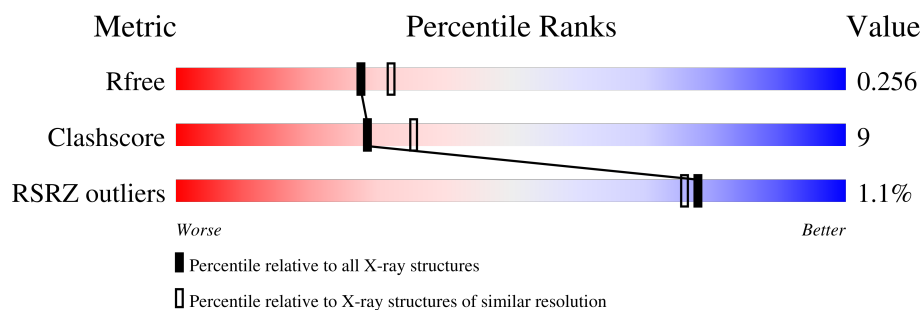
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (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	73% 18% 9%
1	B	440	74% 17% 9%

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.

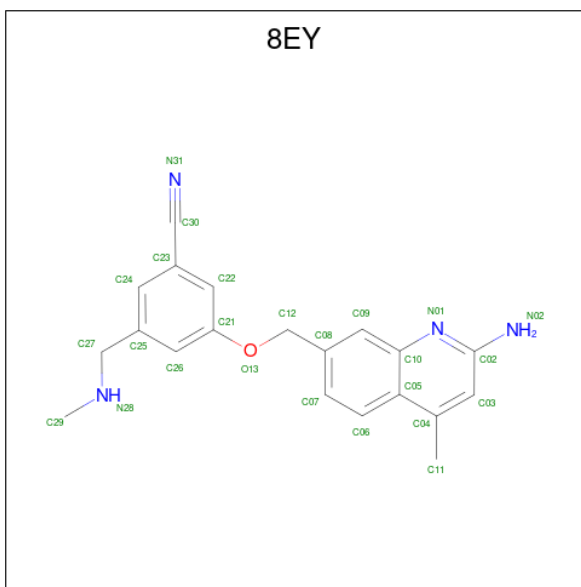
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	3	0
			3212	2046	563	587	16			
1	B	402	Total	C	N	O	S	0	5	0
			3230	2057	566	590	17			

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



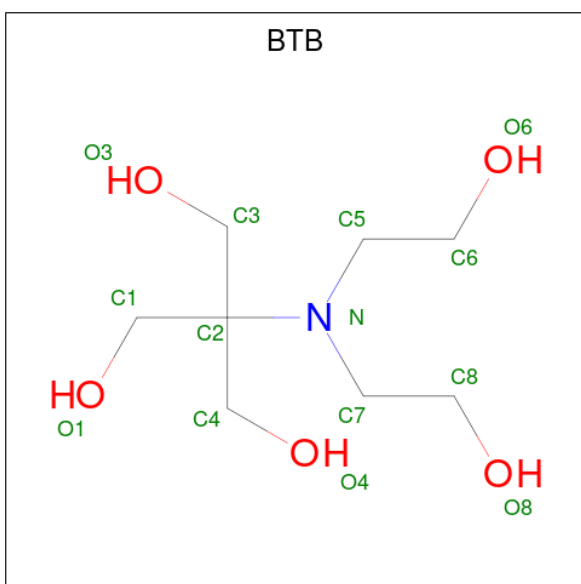
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).

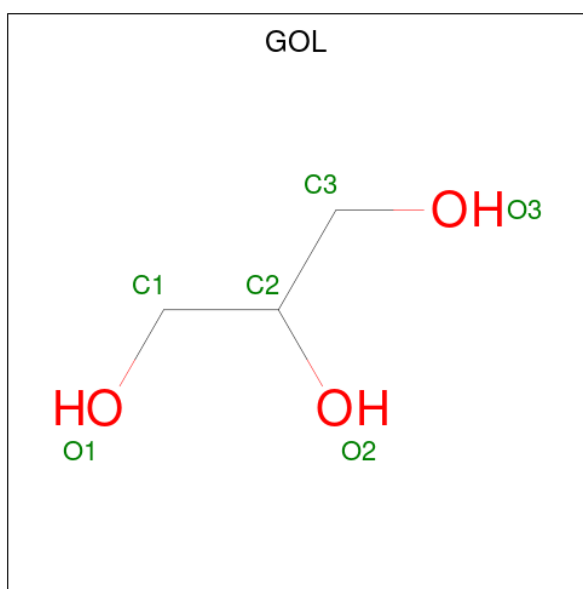


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is GLYCEROL (CCD ID: 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 (CCD ID: GD) (formula: Gd).

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

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

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

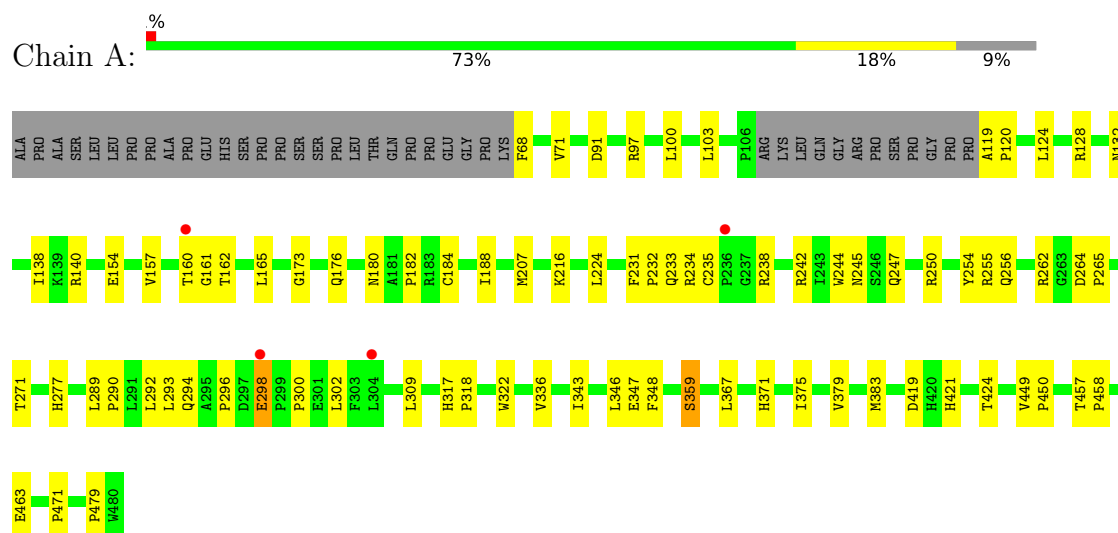
- Molecule 9 is water.

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

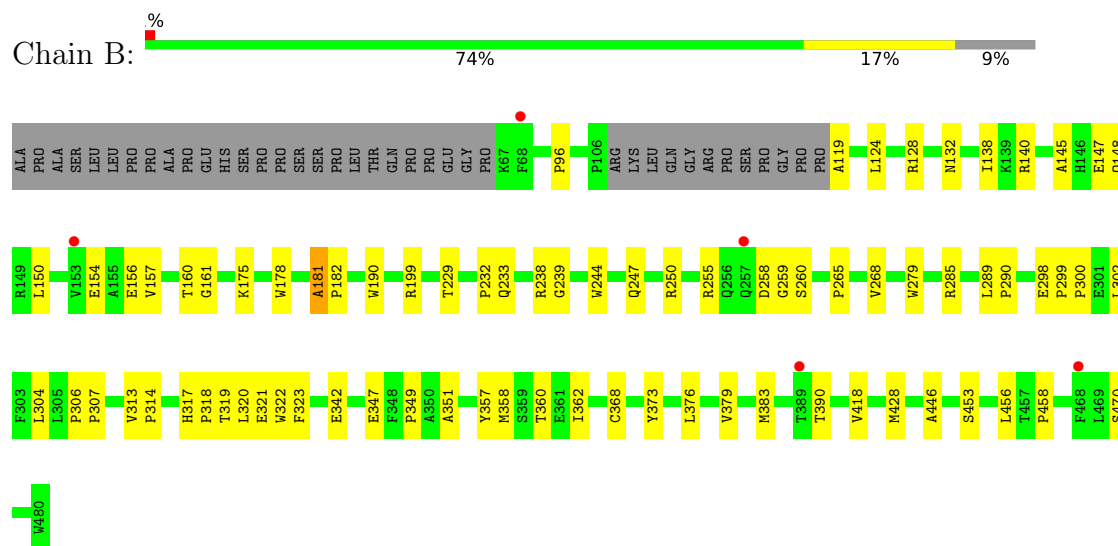
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



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 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.51-2.20) 99.1 (38.51-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.281 (Not available) , 0.256	Depositor DCC
R_{free} test set	2524 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3313	0.88	5/4515 (0.1%)
1	B	0.56	0/3334	0.86	6/4543 (0.1%)
All	All	0.54	0/6647	0.87	11/9058 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLU	CA-C-N	11.83	132.57	120.38
1	A	298	GLU	C-N-CA	11.83	132.57	120.38
1	B	289	LEU	CA-C-N	-6.34	114.20	120.98
1	B	289	LEU	C-N-CA	-6.34	114.20	120.98
1	A	68	PHE	CA-C-N	6.04	126.39	119.93
1	A	68	PHE	C-N-CA	6.04	126.39	119.93
1	B	119	ALA	CA-C-N	5.93	125.32	118.85
1	B	119	ALA	C-N-CA	5.93	125.32	118.85
1	B	181	ALA	CA-C-N	5.52	125.14	119.56
1	B	181	ALA	C-N-CA	5.52	125.14	119.56
1	A	359	SER	N-CA-C	5.45	117.65	111.11

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	3212	0	3114	54	0
1	B	3230	0	3137	47	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	13	0
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	116	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 (116) 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	1.28	0.79
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:128:ARG:HH21	1:A:154:GLU:CD	2.18	0.51
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:358:MET:HE3	1:B:360:THR:OG1	2.17	0.45
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:285:ARG:O	1:B:373:TYR:OH	2.32	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:383:MET:HE2	1:B:383:MET:HB3	1.95	0.42
1:A:207:MET:HE2	1:A:293:LEU:HB3	2.00	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
1:B:258:ASP:OD2	1:B:260:SER:OG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

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
3	8EY	B	503	-	27,27,27	1.70	3 (11%)	35,37,37	0.99	1 (2%)
3	8EY	B	502	-	27,27,27	1.67	1 (3%)	35,37,37	0.88	2 (5%)
4	BTB	A	504	7	13,13,13	0.56	0	7,16,16	1.05	1 (14%)
4	BTB	B	506	-	13,13,13	0.50	0	7,16,16	0.60	0
4	BTB	B	509	-	13,13,13	0.41	0	7,16,16	0.28	0
2	HEM	A	501	1	50,50,50	2.30	9 (18%)	67,82,82	1.54	10 (14%)
3	8EY	A	503	-	27,27,27	1.68	2 (7%)	35,37,37	1.23	6 (17%)
4	BTB	A	505	-	13,13,13	0.45	0	7,16,16	0.90	0
4	BTB	B	504	7	13,13,13	0.78	0	7,16,16	1.21	1 (14%)
2	HEM	B	501	1	50,50,50	2.19	10 (20%)	67,82,82	1.63	12 (17%)
4	BTB	B	507	-	13,13,13	0.60	0	7,16,16	1.20	1 (14%)
4	BTB	B	508	-	13,13,13	0.37	0	7,16,16	0.55	0
3	8EY	A	502	-	27,27,27	1.65	1 (3%)	35,37,37	0.91	2 (5%)
6	GOL	A	507	-	5,5,5	0.29	0	5,5,5	0.42	0
4	BTB	B	505	-	13,13,13	0.36	0	7,16,16	0.86	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
3	8EY	B	503	-	-	2/10/10/10	0/3/3/3
3	8EY	B	502	-	-	2/10/10/10	0/3/3/3
4	BTB	A	504	7	-	9/21/21/21	-
4	BTB	B	506	-	-	12/21/21/21	-
4	BTB	B	509	-	-	4/21/21/21	-
2	HEM	A	501	1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8EY	A	503	-	-	0/10/10/10	0/3/3/3
4	BTB	A	505	-	-	10/21/21/21	-
4	BTB	B	504	7	-	6/21/21/21	-
2	HEM	B	501	1	-	1/14/54/54	-
4	BTB	B	507	-	-	11/21/21/21	-
4	BTB	B	508	-	-	10/21/21/21	-
3	8EY	A	502	-	-	1/10/10/10	0/3/3/3
6	GOL	A	507	-	-	2/4/4/4	-
4	BTB	B	505	-	-	12/21/21/21	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	8.20	2.20	1.94
2	A	501	HEM	C3D-C2D	8.19	1.54	1.36
2	B	501	HEM	C3D-C2D	7.57	1.53	1.36
3	B	502	8EY	C23-C30	-7.25	1.29	1.44
3	A	502	8EY	C23-C30	-7.25	1.29	1.44
3	A	503	8EY	C23-C30	-7.21	1.29	1.44
3	B	503	8EY	C23-C30	-7.04	1.29	1.44
2	A	501	HEM	FE-NA	7.03	2.18	1.95
2	B	501	HEM	FE-NA	6.49	2.16	1.95
2	B	501	HEM	FE-NB	6.39	2.14	1.94
2	B	501	HEM	FE-NC	4.51	2.10	1.95
2	B	501	HEM	FE-ND	4.34	2.08	1.94
2	A	501	HEM	FE-NC	3.55	2.06	1.95
2	B	501	HEM	CAC-C3C	3.25	1.56	1.47
2	A	501	HEM	CAB-C3B	3.17	1.55	1.47
2	B	501	HEM	CAB-C3B	3.05	1.55	1.47
2	A	501	HEM	CAC-C3C	2.94	1.55	1.47
2	A	501	HEM	CMC-C2C	2.84	1.56	1.50
2	A	501	HEM	FE-ND	2.44	2.02	1.94
2	B	501	HEM	CMC-C2C	2.40	1.55	1.50
3	B	503	8EY	C03-C04	2.31	1.41	1.37
3	B	503	8EY	C09-C10	-2.23	1.38	1.41
3	A	503	8EY	C05-C10	-2.10	1.39	1.42
2	B	501	HEM	CMA-C3A	2.08	1.55	1.50
2	B	501	HEM	CMB-C2B	2.06	1.55	1.50
2	A	501	HEM	CMB-C2B	2.00	1.54	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4D-ND-C1D	6.68	113.12	105.21
2	B	501	HEM	C4D-ND-C1D	6.18	112.52	105.21
2	B	501	HEM	C3B-C2B-C1B	3.70	109.19	106.41
2	B	501	HEM	C3B-C4B-NB	-3.37	107.05	109.47
2	B	501	HEM	C1B-NB-C4B	3.26	109.07	105.21
2	A	501	HEM	C3B-C2B-C1B	3.10	108.73	106.41
2	B	501	HEM	C2B-C1B-NB	-2.80	106.63	109.84
2	A	501	HEM	C2A-C1A-NA	-2.75	107.10	110.15
3	A	503	8EY	N02-C02-N01	2.69	120.46	118.24
3	A	502	8EY	C04-C05-C10	2.68	119.63	118.00
3	A	503	8EY	C05-C10-N01	-2.67	119.97	122.80
3	A	502	8EY	C05-C10-N01	-2.66	119.98	122.80
4	B	504	BTB	O3-C3-C2	2.64	117.61	111.40
2	B	501	HEM	C2A-C1A-NA	-2.62	107.25	110.15
3	B	503	8EY	C12-C08-C09	-2.59	115.47	121.23
2	A	501	HEM	C3D-C4D-ND	-2.57	107.36	110.17
3	A	503	8EY	C04-C05-C10	2.52	119.53	118.00
2	A	501	HEM	C1B-NB-C4B	2.51	108.18	105.21
3	A	503	8EY	C12-O13-C21	2.44	123.43	117.62
2	B	501	HEM	C3D-C4D-ND	-2.31	107.63	110.17
2	B	501	HEM	CHB-C1B-NB	2.31	127.23	124.37
2	B	501	HEM	CBA-CAA-C2A	-2.27	106.26	112.53
2	B	501	HEM	CAD-C3D-C4D	2.26	128.63	124.70
2	A	501	HEM	CBD-CAD-C3D	-2.24	106.34	112.53
4	A	504	BTB	O4-C4-C2	2.22	116.63	111.40
3	A	503	8EY	C24-C23-C30	2.21	122.53	119.55
4	B	507	BTB	O4-C4-C2	-2.20	106.22	111.40
2	A	501	HEM	CBA-CAA-C2A	-2.20	106.44	112.53
2	B	501	HEM	CBD-CAD-C3D	-2.16	106.56	112.53
2	A	501	HEM	CHA-C4D-ND	2.12	126.99	124.37
2	A	501	HEM	C2B-C1B-NB	-2.10	107.43	109.84
2	A	501	HEM	C3B-C4B-NB	-2.09	107.96	109.47
3	B	502	8EY	C12-O13-C21	2.09	122.59	117.62
3	A	503	8EY	C25-C27-N28	-2.05	107.75	112.67
3	B	502	8EY	C04-C05-C10	2.05	119.25	118.00
2	B	501	HEM	CHD-C1D-ND	2.03	126.60	124.42

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	8EY	C25-C27-N28-C29
3	B	502	8EY	C25-C27-N28-C29

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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	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
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	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	N-C2-C4-O4
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
3	B	503	8EY	C26-C21-O13-C12

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Mol	Chain	Res	Type	Atoms
4	A	505	BTB	N-C5-C6-O6
3	B	503	8EY	C22-C21-O13-C12
4	B	506	BTB	N-C5-C6-O6
4	B	508	BTB	N-C7-C8-O8
6	A	507	GOL	O1-C1-C2-O2
4	B	507	BTB	N-C5-C6-O6
4	A	504	BTB	C3-C2-C4-O4
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	A	504	BTB	N-C2-C4-O4
4	A	504	BTB	C4-C2-N-C5
4	B	504	BTB	N-C2-C4-O4
4	B	505	BTB	N-C2-C3-O3
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	504	BTB	C3-C2-C4-O4
4	B	507	BTB	N-C7-C8-O8
4	B	505	BTB	C4-C2-C3-O3
4	B	506	BTB	C1-C2-C4-O4
4	B	508	BTB	C8-C7-N-C5
4	A	504	BTB	C1-C2-N-C5
4	B	506	BTB	C1-C2-N-C5
4	B	507	BTB	C1-C2-N-C7
4	B	508	BTB	C3-C2-N-C5
4	B	508	BTB	C4-C2-N-C5
4	B	508	BTB	C4-C2-N-C7
3	B	502	8EY	C22-C23-C30-N31

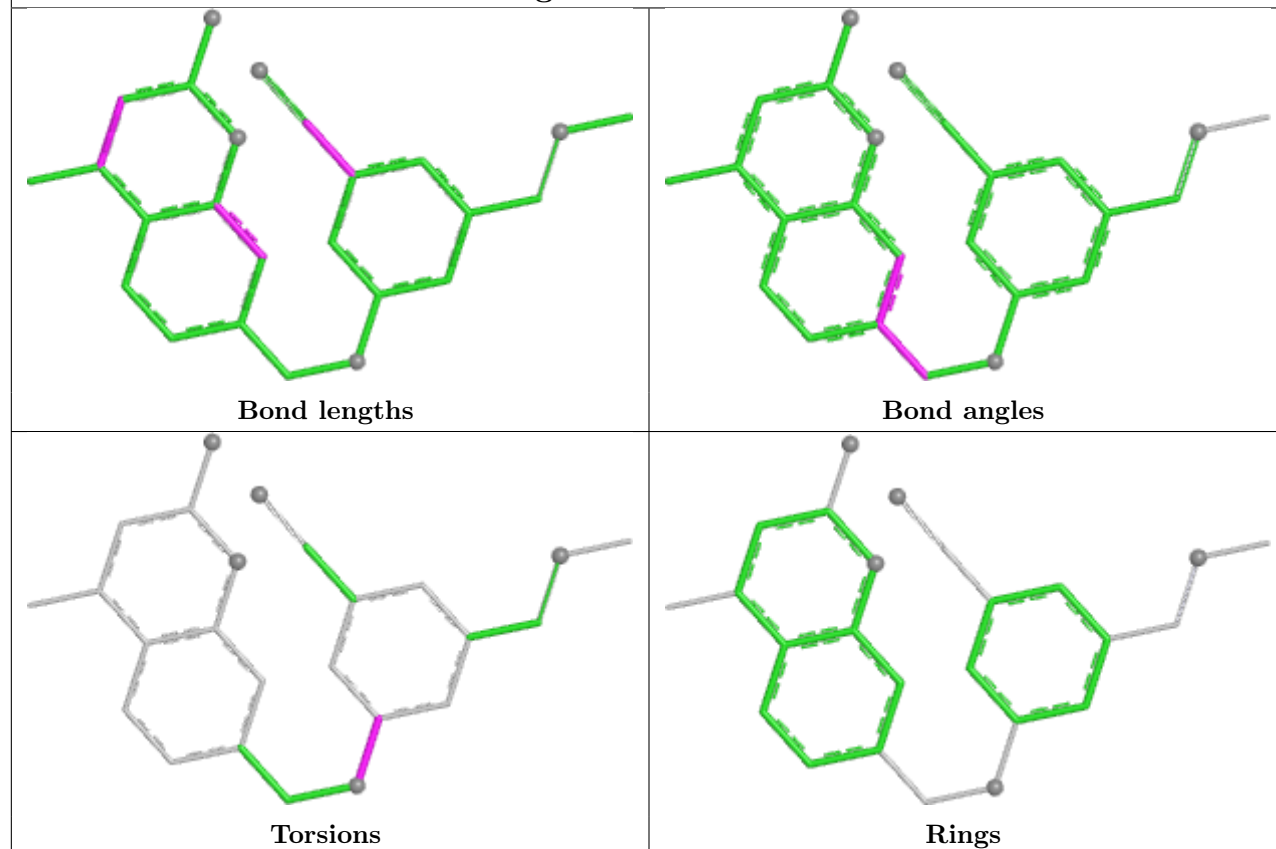
There are no ring outliers.

13 monomers are involved in 26 short contacts:

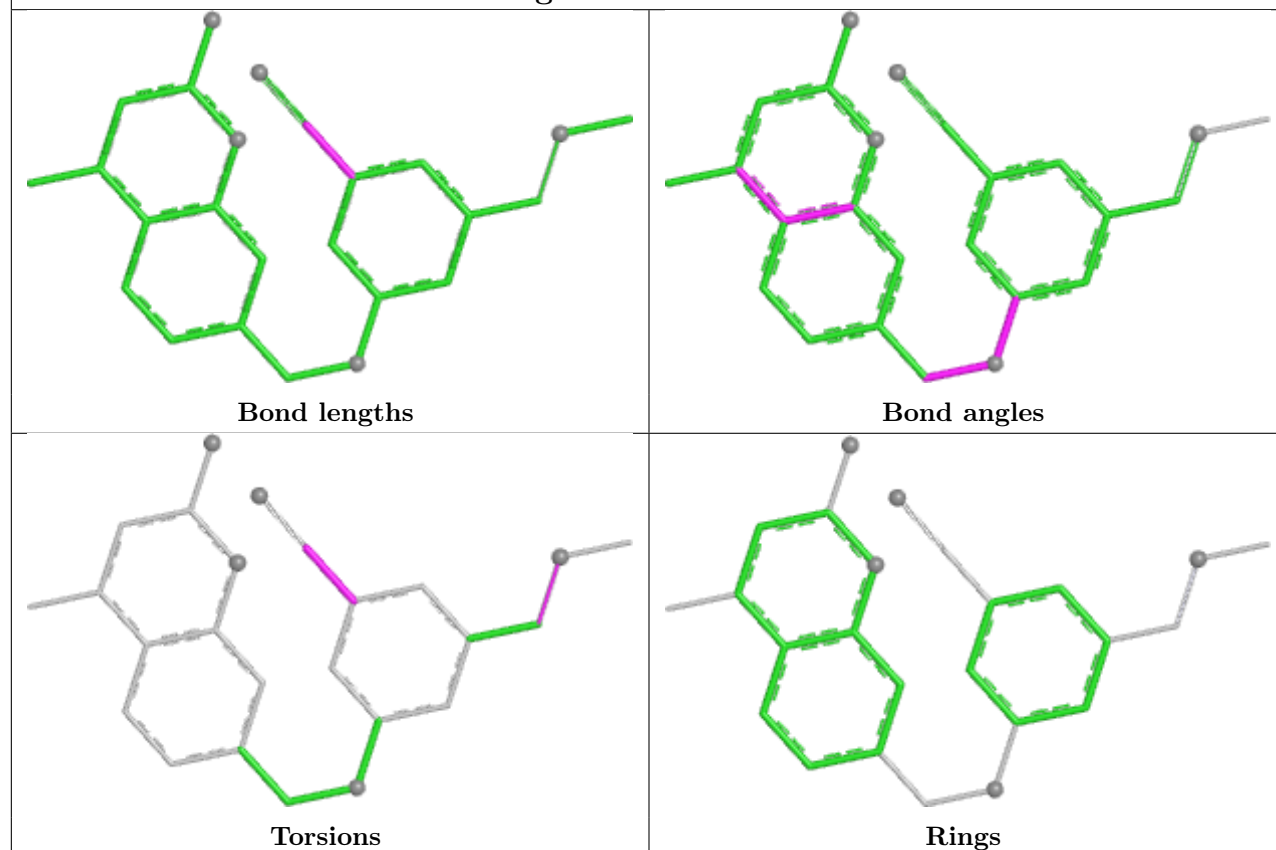
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	8EY	1	0
4	A	504	BTB	4	0
4	B	506	BTB	2	0
4	B	509	BTB	2	0
2	A	501	HEM	2	0
3	A	503	8EY	1	0
4	A	505	BTB	2	0
4	B	504	BTB	3	0
2	B	501	HEM	2	0
4	B	507	BTB	2	0
4	B	508	BTB	1	0
3	A	502	8EY	1	0
4	B	505	BTB	3	0

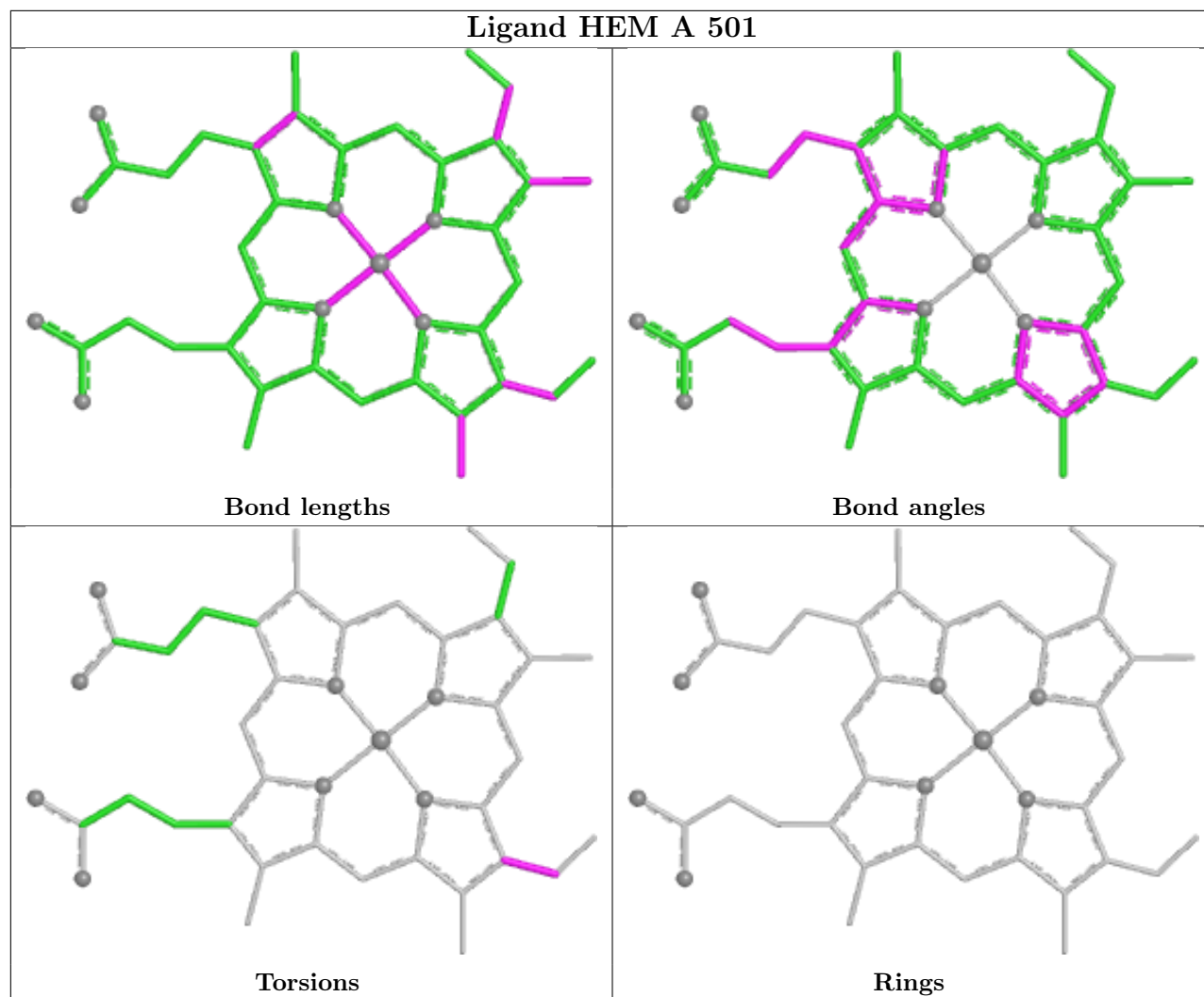
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

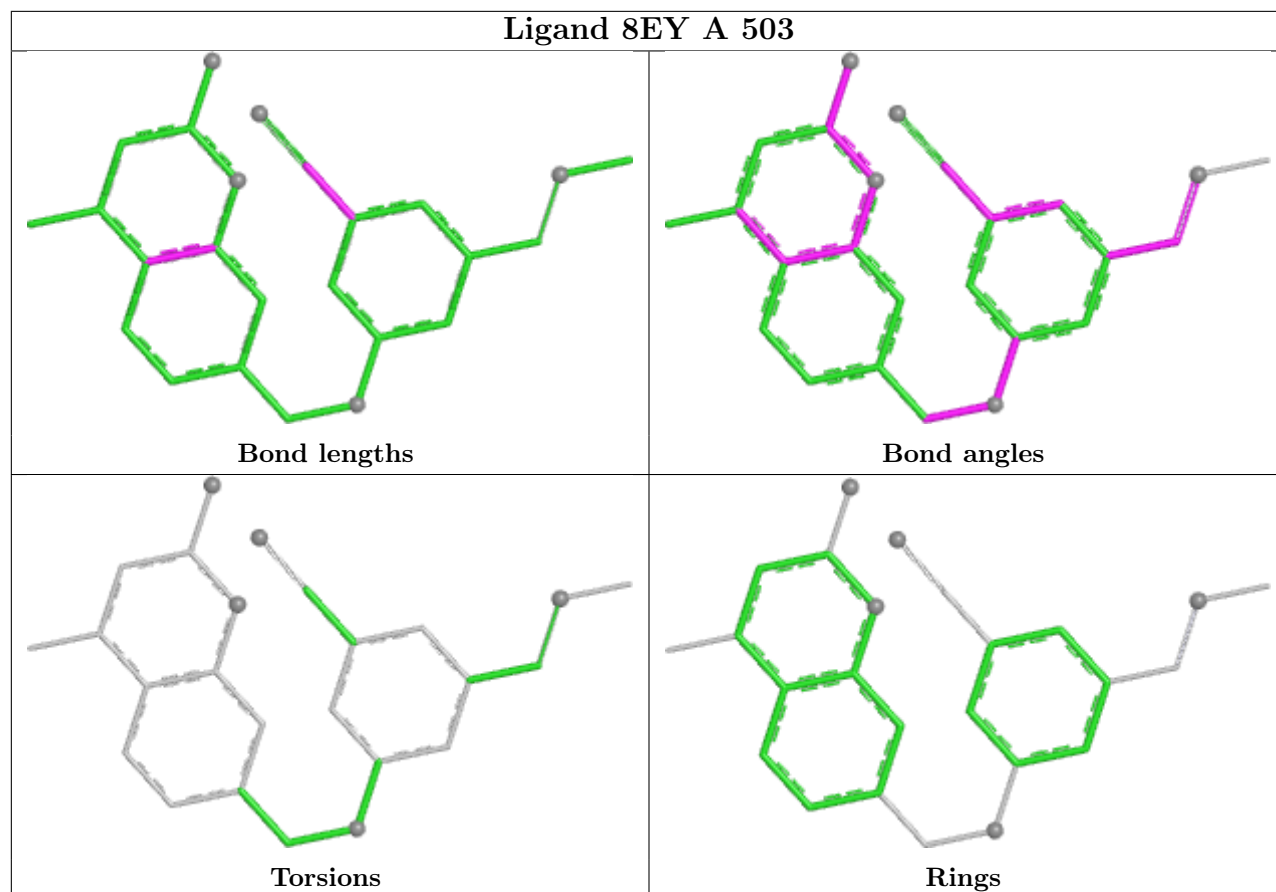
Ligand 8EY B 503

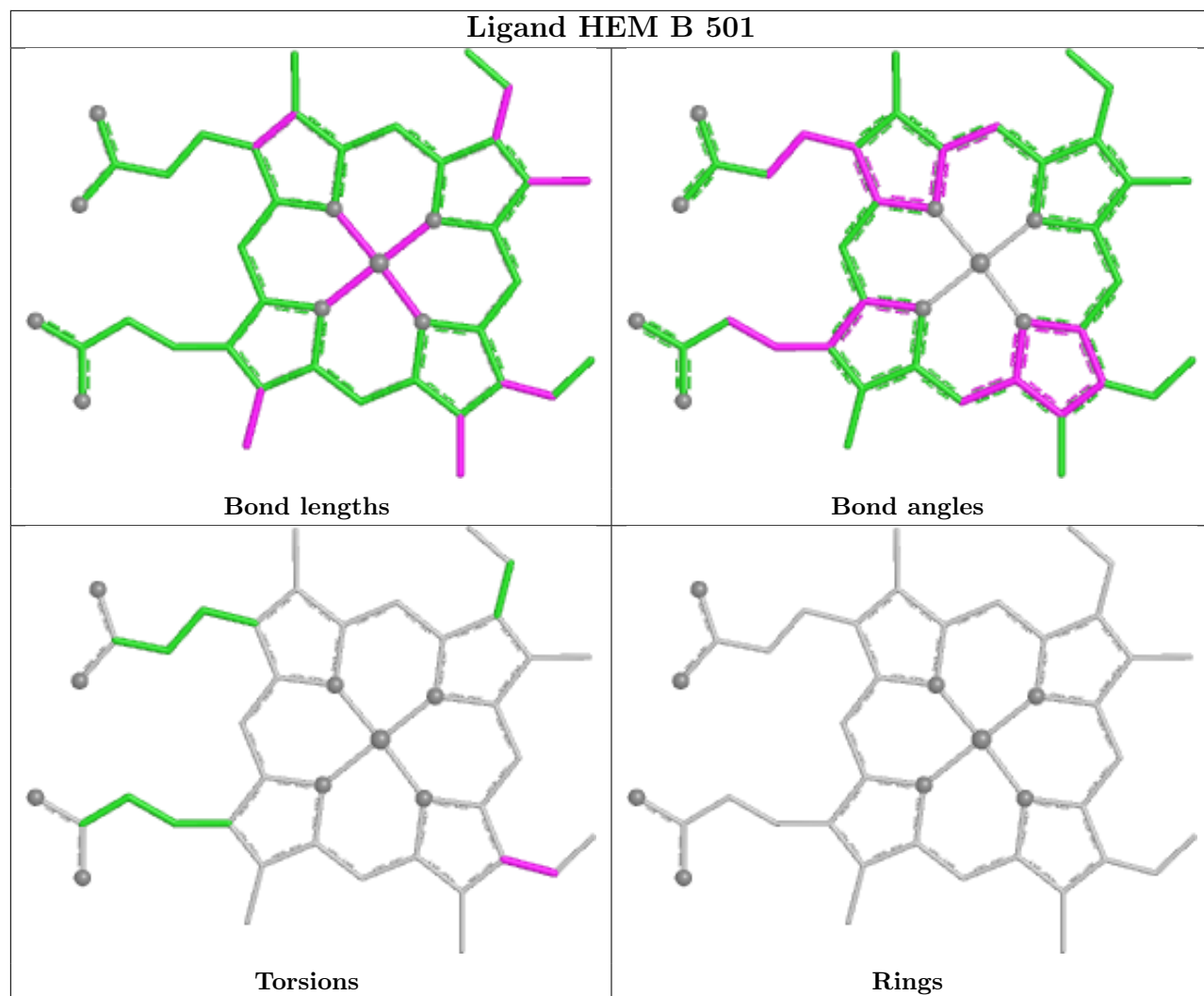


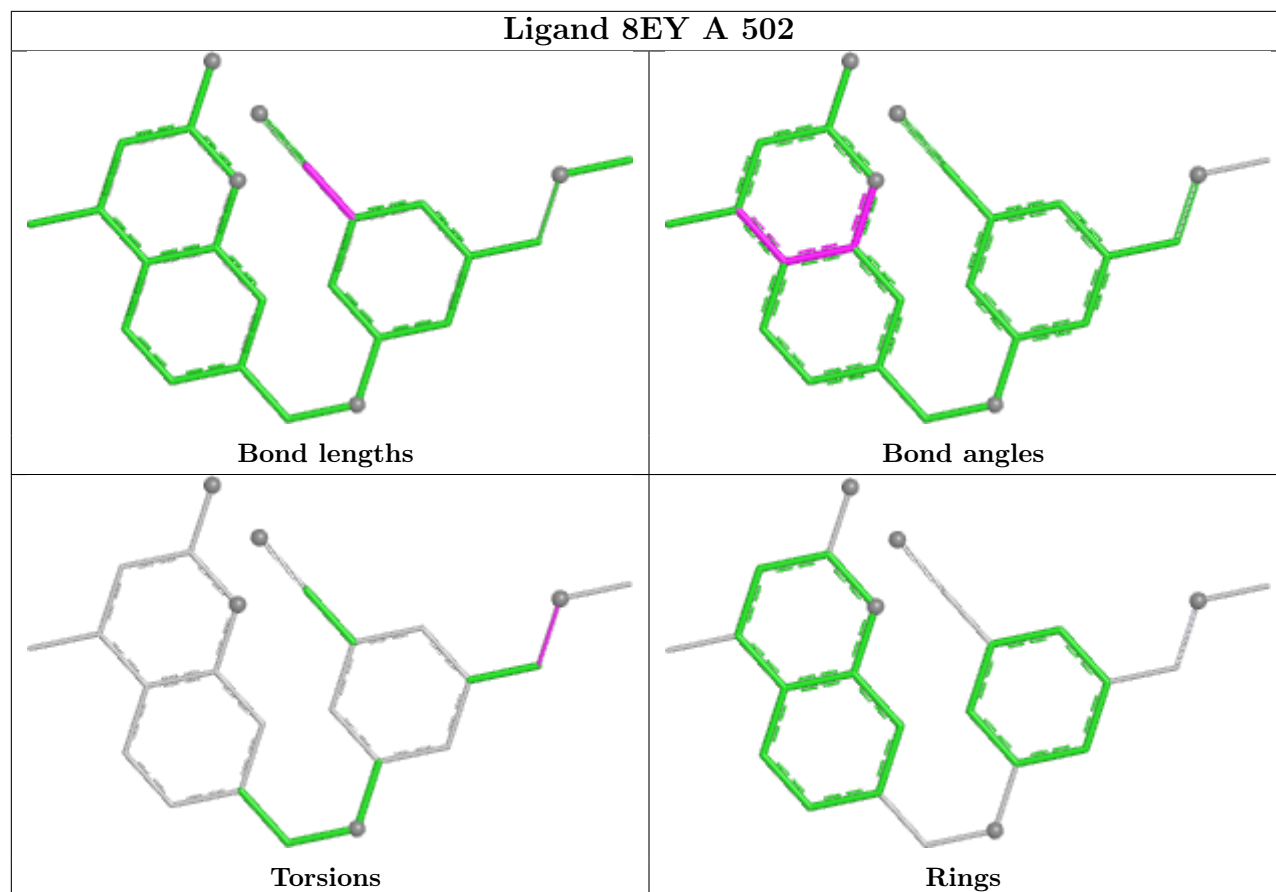
Ligand 8EY B 502











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%)	0.24	4 (0%) 79 77	36, 81, 133, 183	3 (0%)
1	B	402/440 (91%)	0.19	5 (1%) 76 74	44, 73, 122, 185	5 (1%)
All	All	803/880 (91%)	0.22	9 (1%) 78 76	36, 77, 129, 185	8 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	GLU	4.4
1	B	468	PHE	3.9
1	B	68	PHE	2.9
1	A	160	THR	2.6
1	A	236	PRO	2.5
1	A	304	LEU	2.3
1	B	389	THR	2.2
1	B	257	GLN	2.2
1	B	153	VAL	2.1

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,

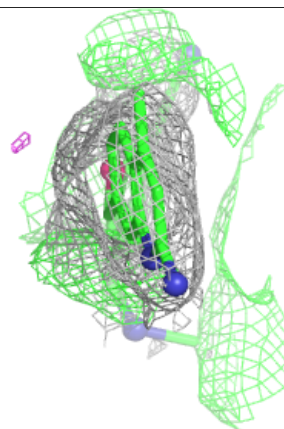
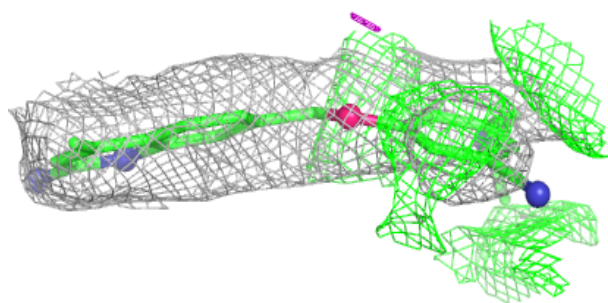
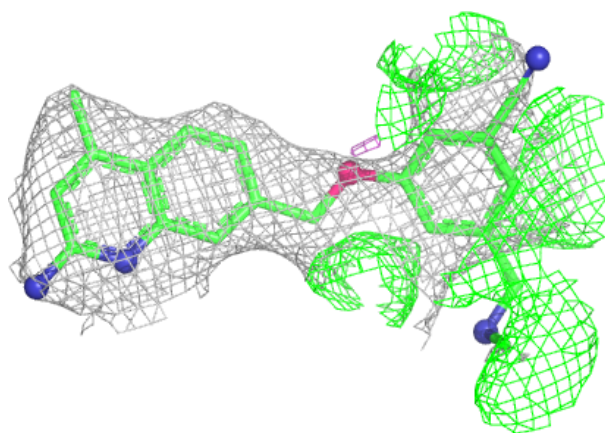
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BTB	B	509	14/14	0.66	0.13	94,103,114,114	0
3	8EY	A	502	25/25	0.73	0.21	71,92,125,129	0
3	8EY	B	502	25/25	0.75	0.19	63,91,123,130	0
4	BTB	B	508	14/14	0.79	0.12	86,100,106,110	0
4	BTB	A	505	14/14	0.79	0.13	82,100,114,117	0
4	BTB	B	505	14/14	0.84	0.10	98,107,113,113	0
4	BTB	B	507	14/14	0.85	0.11	78,89,95,97	0
4	BTB	B	506	14/14	0.87	0.10	71,89,97,103	0
3	8EY	B	503	25/25	0.88	0.14	35,60,110,111	0
6	GOL	A	507	6/6	0.88	0.09	64,72,72,73	0
4	BTB	A	504	14/14	0.89	0.12	53,85,108,110	0
4	BTB	B	504	14/14	0.89	0.13	48,75,100,107	0
3	8EY	A	503	25/25	0.90	0.12	40,64,93,95	0
8	CL	B	511	1/1	0.92	0.09	61,61,61,61	0
2	HEM	B	501	43/43	0.93	0.12	50,78,91,99	0
8	CL	A	511	1/1	0.95	0.07	67,67,67,67	0
2	HEM	A	501	43/43	0.95	0.11	40,76,99,119	0
5	ZN	A	509	1/1	0.97	0.05	70,70,70,70	1
5	ZN	A	510	1/1	0.98	0.04	72,72,72,72	1
7	GD	A	508	1/1	0.98	0.04	99,99,99,99	0
5	ZN	A	506	1/1	0.99	0.02	67,67,67,67	0
7	GD	B	510	1/1	0.99	0.04	63,63,63,63	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.

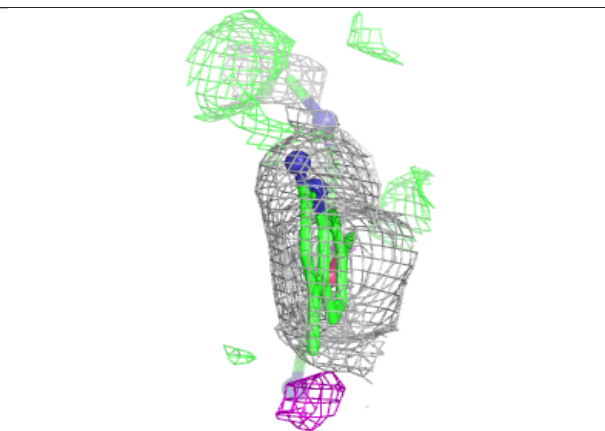
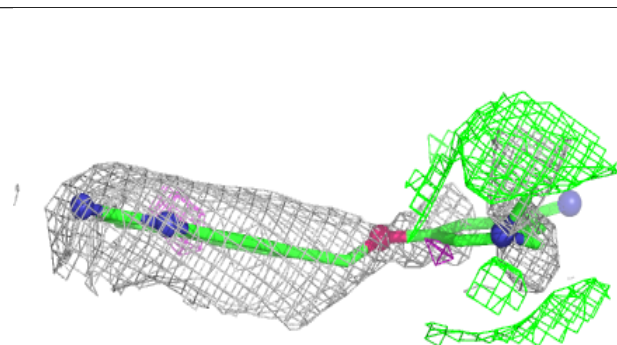
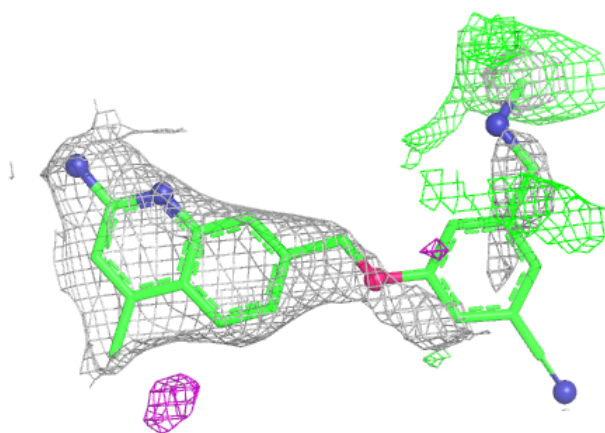
Electron density around 8EY A 502:

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

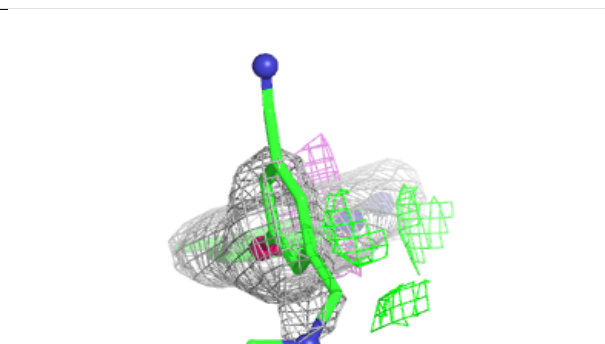
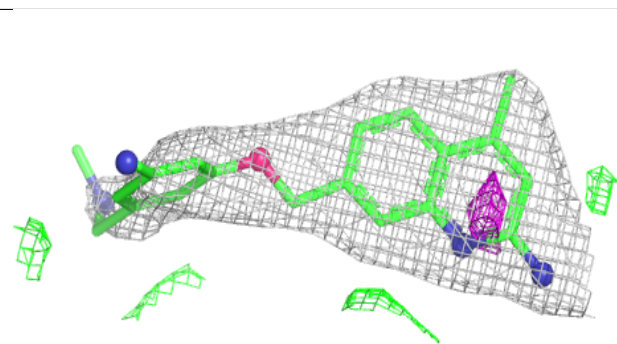
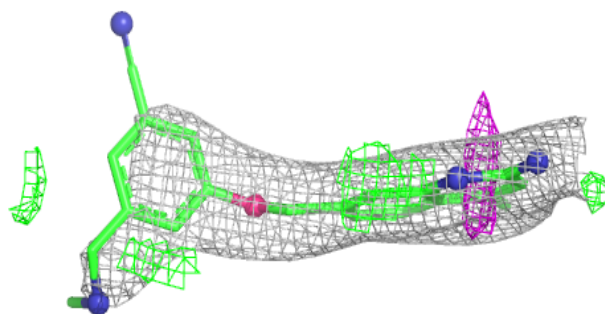


Electron density around 8EY B 502:

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

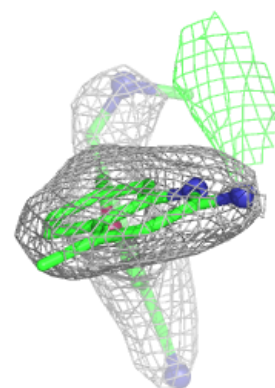
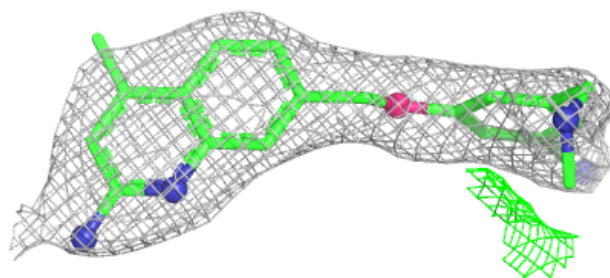
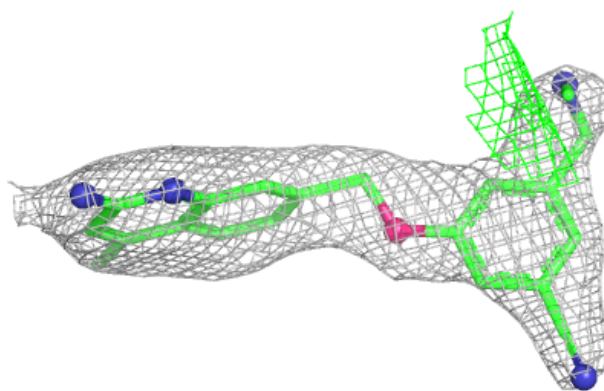
**Electron density around 8EY B 503:**

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



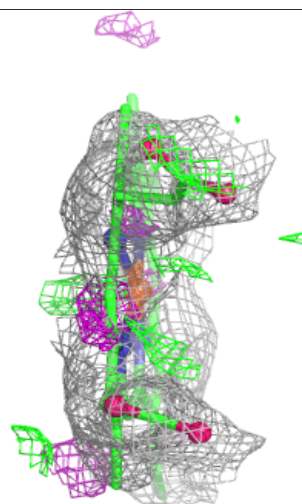
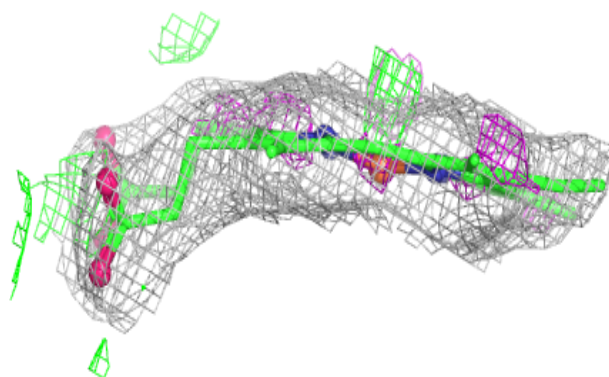
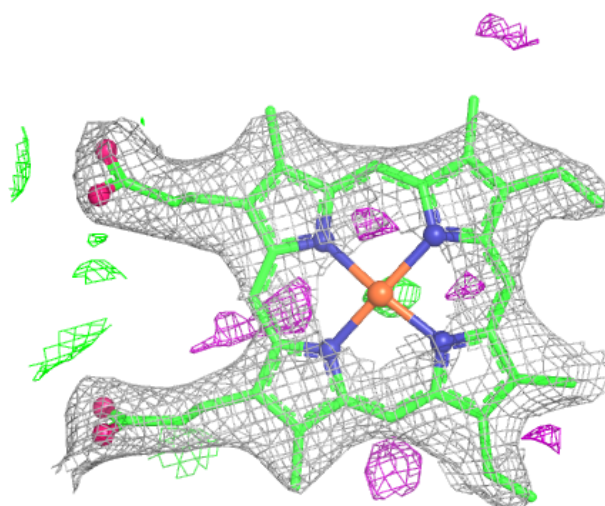
Electron density around 8EY A 503:

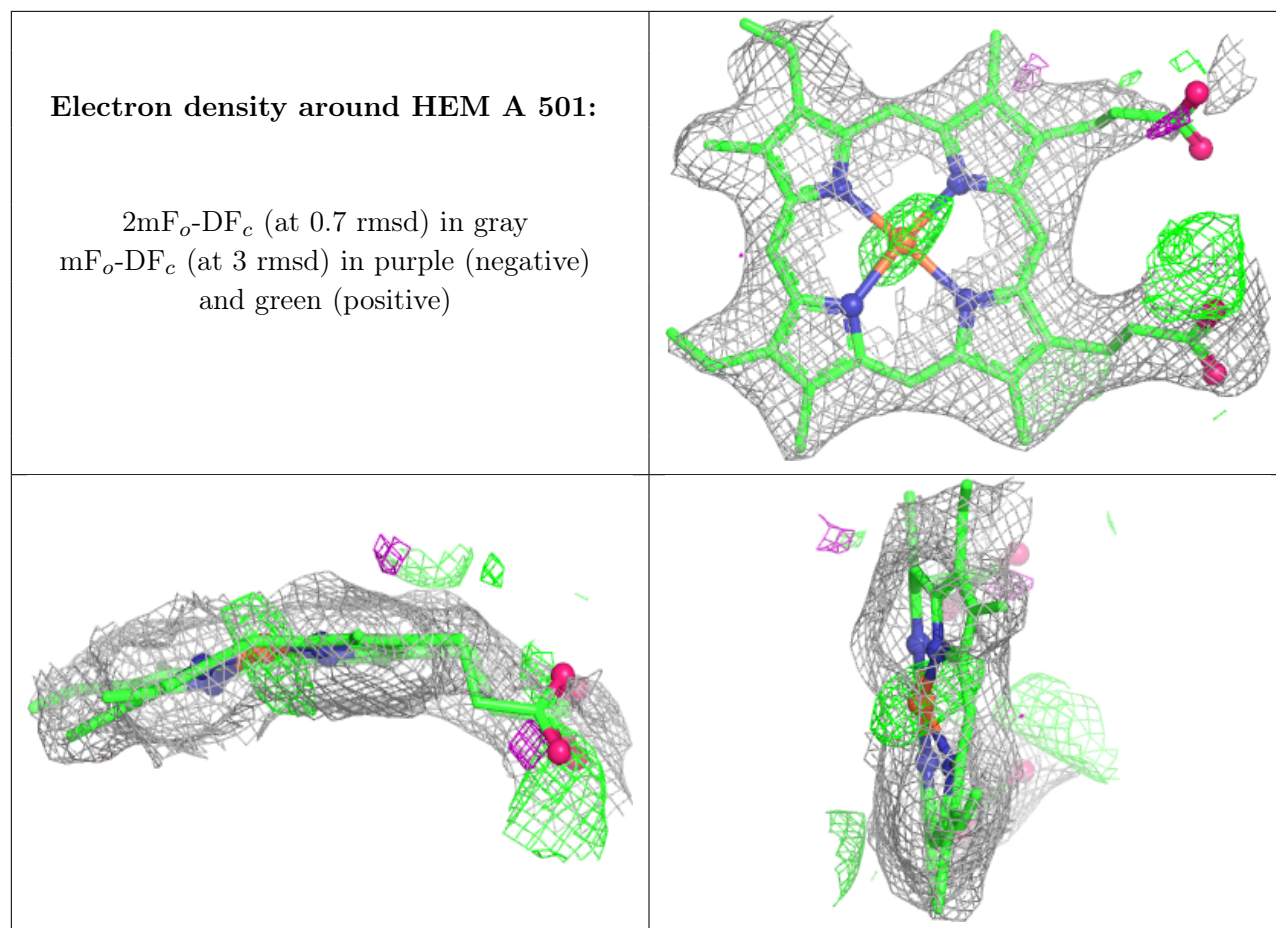
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.