



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:33 am BST

PDB ID : 1D1Y
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH 1,3-PBITU (H4B FREE)
Authors : Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos,
T.L.
Deposited on : 1999-09-21
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 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

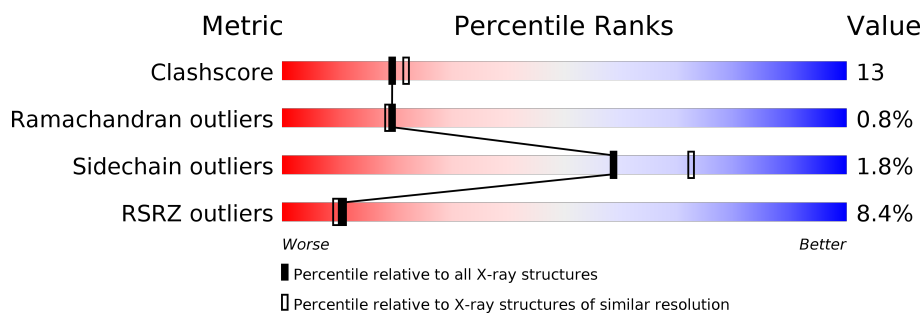
1 Overall quality at a glance

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))
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 on 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	444	<div> <div>8%</div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div>
1	B	444	<div> <div>8%</div> <div>71%</div> <div>21%</div> <div>• 7%</div> </div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7086 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.

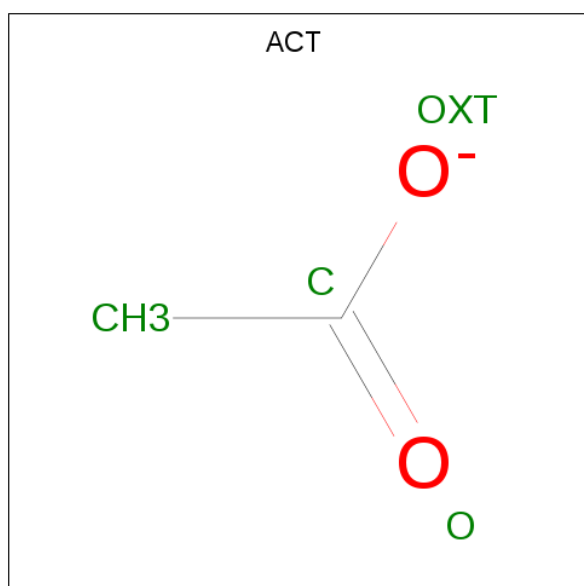
- Molecule 1 is a protein called BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3302	2099	584	603	16			
1	B	414	Total	C	N	O	S	0	0	0
			3291	2092	582	601	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	CONFLICT	UNP P29473
B	100	ARG	CYS	CONFLICT	UNP P29473

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



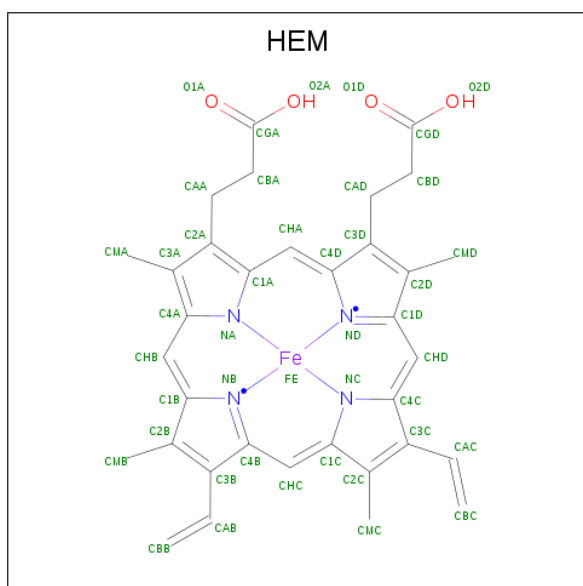
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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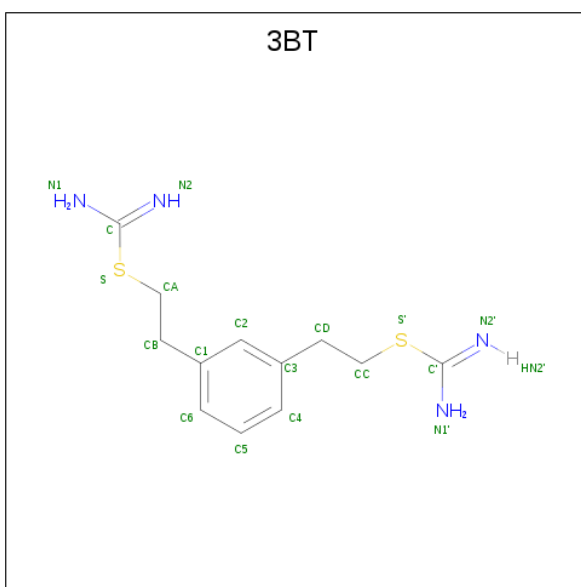
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 2-{2-[3-(2-CARBAMIMIDOYLSULFANYL-ETHYL)-PHENYL]-ETHYL}-IS OTHIOUREA (three-letter code: 3BT) (formula: C₁₂H₁₈N₄S₂).



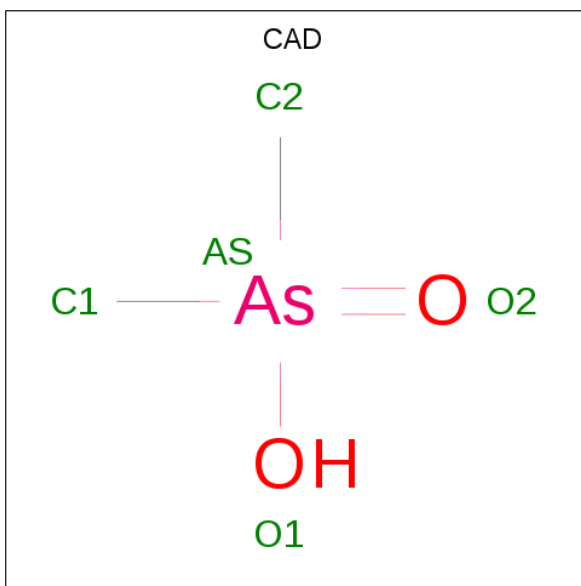
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			18	12	4	2		
4	B	1	Total	C	N	S	0	0
			18	12	4	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



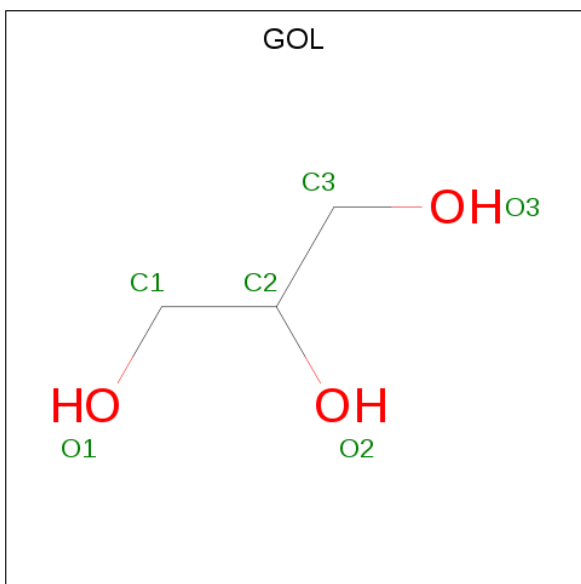
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	As	C	0	0
			3	1	2		
6	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		

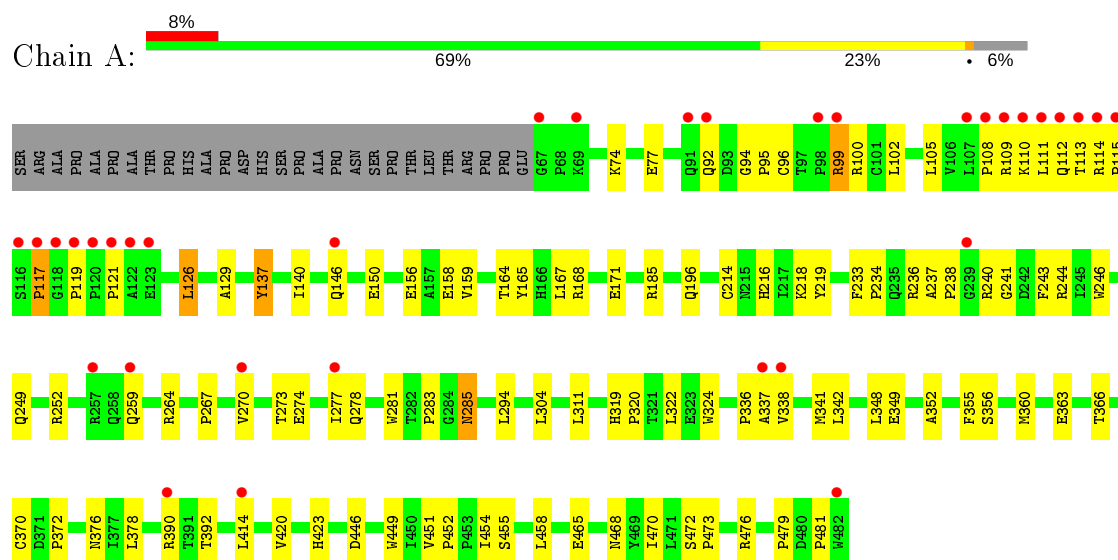
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	170	Total	O	0	0
			170	170		
9	B	152	Total	O	0	0
			152	152		

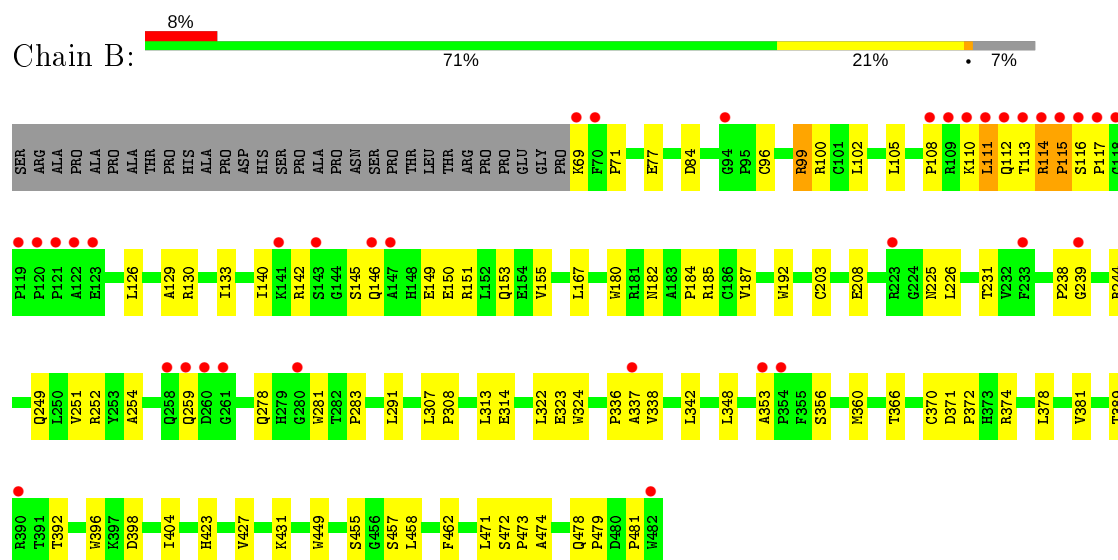
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN



• Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.66Å 106.25Å 156.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.32 – 2.20 30.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	76.4 (30.32-2.20) 82.8 (30.32-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.268 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, ZN, 3BT, EDO, ACT, HEM, CAD

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	0.38	0/3397	0.62	0/4631
1	B	0.39	0/3385	0.63	1/4614 (0.0%)
All	All	0.38	0/6782	0.63	1/9245 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	360	MET	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

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	3302	0	3215	88	0
1	B	3291	0	3205	84	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	43	0	30	0	0
3	B	43	0	30	4	0
4	A	18	0	18	2	0
4	B	18	0	18	3	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	3	0	0	0	0
6	B	3	0	0	1	0
7	A	12	0	16	2	0
7	B	6	0	8	1	0
8	B	1	0	0	0	0
9	A	170	0	0	3	0
9	B	152	0	0	6	0
All	All	7086	0	6564	170	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 13.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.25	1.14
1:B:99:ARG:HH11	1:B:99:ARG:HG3	1.15	1.08
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.42	0.99
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.49	0.93
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.53	0.91
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.48	0.78
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.65	0.78
1:A:146:GLN:O	1:A:150:GLU:HG3	1.86	0.76
1:B:112:GLN:HG3	1:B:113:THR:H	1.53	0.73
1:A:277:ILE:HD11	1:A:283:PRO:HB3	1.71	0.71
1:B:99:ARG:NH1	1:B:99:ARG:HG3	1.95	0.71
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.26	0.70
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.07	0.70
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.73	0.69
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:O	1:A:117:PRO:HD3	1.94	0.68
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.76	0.67
1:B:378:LEU:HB2	9:B:958:HOH:O	1.95	0.67
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.76	0.67
1:A:119:PRO:HG3	1:A:238:PRO:HB3	1.76	0.67
1:B:153:GLN:HB2	9:B:1057:HOH:O	1.93	0.67
1:A:102:LEU:HB3	1:A:105:LEU:HD22	1.78	0.66
1:A:378:LEU:HB2	9:A:1088:HOH:O	1.97	0.65
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.81	0.63
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.81	0.63
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.82	0.61
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.82	0.61
1:A:113:THR:HG21	1:A:342:LEU:HD22	1.82	0.61
1:A:94:GLY:O	1:A:110:LYS:HE2	2.00	0.61
1:A:285:ASN:C	1:A:285:ASN:HD22	2.03	0.61
1:B:116:SER:O	1:B:238:PRO:HA	2.01	0.60
1:A:449:TRP:CD2	7:A:890:GOL:H11	2.36	0.59
1:B:69:LYS:HB2	1:B:69:LYS:NZ	2.18	0.59
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.33	0.59
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.84	0.58
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.18	0.58
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.84	0.58
1:A:277:ILE:HD12	1:A:283:PRO:HD3	1.86	0.57
1:B:313:LEU:HD12	1:B:314:GLU:H	1.68	0.57
1:B:102:LEU:HB3	1:B:105:LEU:HD22	1.86	0.57
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.87	0.56
1:A:277:ILE:CD1	1:A:283:PRO:HB3	2.34	0.56
1:A:338:VAL:CG1	1:A:341:MET:HG3	2.35	0.56
1:B:117:PRO:HA	1:B:239:GLY:H	1.69	0.56
1:A:115:PRO:C	1:A:117:PRO:HD3	2.25	0.56
1:A:249:GLN:HB2	1:A:252:ARG:CD	2.31	0.56
1:B:149:GLU:O	1:B:153:GLN:HG3	2.06	0.55
1:A:472:SER:HA	1:A:473:PRO:C	2.26	0.55
1:A:273:THR:O	1:A:277:ILE:HG12	2.07	0.55
1:A:336:PRO:HB2	4:A:820:3BT:H61	1.88	0.55
1:A:126:LEU:HD11	1:A:156:GLU:CG	2.32	0.54
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.90	0.54
1:A:237:ALA:HB3	1:A:240:ARG:HB3	1.89	0.54
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.43	0.54
1:A:294:LEU:HD21	1:A:304:LEU:HD13	1.90	0.54
1:B:112:GLN:HE21	1:B:478:GLN:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:O	1:B:133:ILE:HG12	2.08	0.53
1:A:99:ARG:CG	1:A:99:ARG:HH11	2.19	0.53
1:B:126:LEU:O	1:B:130:ARG:HG3	2.08	0.53
1:B:249:GLN:CB	1:B:252:ARG:HD3	2.18	0.53
1:B:471:LEU:O	1:B:474:ALA:HB2	2.08	0.53
1:A:372:PRO:HB2	1:B:77:GLU:HG3	1.90	0.53
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.48	0.53
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.73	0.53
1:B:113:THR:HG21	1:B:342:LEU:CD1	2.39	0.53
1:B:472:SER:HA	1:B:473:PRO:C	2.29	0.53
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.49	0.52
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.92	0.52
1:B:366:THR:O	1:B:370:CYS:HB2	2.09	0.52
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.45	0.52
1:B:278:GLN:NE2	9:B:1039:HOH:O	2.41	0.52
1:A:111:LEU:H	1:A:111:LEU:HD12	1.74	0.52
1:A:236:ARG:HD3	1:A:349:GLU:HB2	1.90	0.52
1:B:449:TRP:CE2	7:B:891:GOL:H2	2.45	0.52
1:A:214:CYS:O	1:A:218:LYS:HG3	2.10	0.52
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.18	0.51
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.46	0.51
1:B:342:LEU:C	1:B:342:LEU:HD23	2.31	0.51
1:B:203:CYS:SG	1:B:208:GLU:HB3	2.52	0.50
1:A:285:ASN:C	1:A:285:ASN:ND2	2.64	0.50
1:B:108:PRO:HG3	9:B:1064:HOH:O	2.11	0.50
1:B:99:ARG:HH11	1:B:99:ARG:CG	2.04	0.50
1:B:457:SER:HA	1:B:462:PHE:CG	2.46	0.50
1:A:274:GLU:O	1:A:278:GLN:HG3	2.12	0.50
1:A:74:LYS:O	1:A:465:GLU:HG3	2.12	0.50
1:B:110:LYS:C	1:B:112:GLN:H	2.16	0.50
1:A:240:ARG:HG2	1:A:241:GLY:N	2.28	0.49
1:B:187:VAL:O	1:B:187:VAL:HG22	2.12	0.49
1:B:337:ALA:CB	1:B:356:SER:HB3	2.43	0.49
3:B:500:HEM:HBC2	3:B:500:HEM:HMC1	1.95	0.48
1:A:109:ARG:O	1:A:110:LYS:HD2	2.13	0.48
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.29	0.48
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.42	0.48
1:A:446:ASP:HB2	9:A:1075:HOH:O	2.14	0.47
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.78	0.47
1:B:478:GLN:HB2	1:B:479:PRO:HD2	1.97	0.47
1:A:113:THR:CG2	1:A:476:ARG:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.95	0.47
1:A:449:TRP:CE2	7:A:890:GOL:H11	2.49	0.47
1:A:111:LEU:HG	1:A:470:ILE:HD13	1.97	0.47
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.97	0.46
1:A:243:PHE:O	1:A:352:ALA:HB2	2.14	0.46
1:B:251:VAL:O	1:B:252:ARG:HD2	2.15	0.46
1:B:226:LEU:HD12	1:B:226:LEU:N	2.31	0.46
1:B:281:TRP:O	1:B:283:PRO:HD3	2.14	0.46
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.51	0.46
1:A:267:PRO:O	1:A:270:VAL:HG23	2.16	0.46
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.81	0.46
1:B:324:TRP:HB2	6:B:951:CAD:C1	2.46	0.46
1:A:234:PRO:HB2	1:A:243:PHE:CD1	2.51	0.46
1:B:251:VAL:HA	9:B:1009:HOH:O	2.15	0.46
1:A:252:ARG:HD2	1:A:252:ARG:HA	1.75	0.46
3:B:500:HEM:HBC2	3:B:500:HEM:CMC	2.45	0.45
3:B:500:HEM:O2A	4:B:821:3BT:HCD2	2.16	0.45
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.98	0.45
1:B:146:GLN:O	1:B:150:GLU:HG3	2.16	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.51	0.45
1:A:363:GLU:OE2	4:A:820:3BT:N2	2.50	0.45
1:B:151:ARG:O	1:B:155:VAL:HG23	2.16	0.45
1:B:69:LYS:HB2	1:B:69:LYS:HZ1	1.82	0.45
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.47	0.45
1:B:244:ARG:CZ	1:B:481:PRO:HD3	2.46	0.45
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.53	0.44
1:B:182:ASN:O	1:B:184:PRO:HD3	2.16	0.44
1:A:196:GLN:HG2	1:A:219:TYR:CE1	2.53	0.44
1:A:294:LEU:CD2	1:A:304:LEU:HD13	2.48	0.44
1:A:233:PHE:HB3	1:A:234:PRO:HD2	1.99	0.44
1:B:338:VAL:HG23	4:B:821:3BT:C1	2.48	0.43
1:A:92:GLN:HE22	1:A:111:LEU:HA	1.84	0.43
1:B:112:GLN:HG3	1:B:113:THR:N	2.29	0.43
1:A:281:TRP:O	1:A:283:PRO:HD3	2.18	0.43
1:A:159:VAL:HA	1:A:164:THR:O	2.19	0.43
1:A:337:ALA:HB2	1:A:356:SER:HB3	2.00	0.43
1:B:336:PRO:HB2	4:B:821:3BT:H61	1.99	0.43
1:B:140:ILE:O	1:B:142:ARG:HG2	2.18	0.43
1:A:109:ARG:NH1	1:A:109:ARG:HG2	2.34	0.43
1:A:216:HIS:C	1:A:216:HIS:CD2	2.92	0.43
1:B:381:VAL:HG21	1:B:404:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HD3	1:B:449:TRP:CE3	2.54	0.42
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.01	0.42
1:B:431:LYS:HE3	9:B:1069:HOH:O	2.19	0.42
1:B:252:ARG:HB2	1:B:291:LEU:HD12	2.00	0.42
1:A:92:GLN:OE1	1:A:476:ARG:NH1	2.52	0.42
1:A:376:ASN:ND2	9:A:1088:HOH:O	2.42	0.42
1:B:69:LYS:NZ	1:B:69:LYS:CB	2.81	0.42
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.01	0.42
1:A:99:ARG:NH1	1:A:99:ARG:CG	2.81	0.41
1:B:313:LEU:HD12	1:B:314:GLU:N	2.33	0.41
3:B:500:HEM:HMC1	3:B:500:HEM:CB	2.49	0.41
1:A:158:GLU:HG2	1:A:165:TYR:HA	2.02	0.41
1:A:392:THR:HB	1:B:423:HIS:HB2	2.02	0.41
1:A:114:ARG:HA	1:A:479:PRO:HG2	2.02	0.41
1:A:360:MET:HA	1:A:420:VAL:O	2.19	0.41
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.56	0.41
1:B:110:LYS:O	1:B:112:GLN:N	2.53	0.41
1:A:338:VAL:HG11	1:A:341:MET:CG	2.45	0.41
1:B:231:THR:O	1:B:353:ALA:HA	2.21	0.41
1:B:254:ALA:HB2	1:B:291:LEU:CD2	2.50	0.41
1:B:112:GLN:NE2	1:B:478:GLN:HA	2.35	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.91	0.41
1:A:423:HIS:HB2	1:B:392:THR:HB	2.02	0.41
1:A:129:ALA:HB2	1:A:165:TYR:CE2	2.56	0.40
1:A:246:TRP:HB2	1:A:294:LEU:HB2	2.04	0.40
1:B:307:LEU:HA	1:B:308:PRO:HD3	1.96	0.40
1:B:371:ASP:HB2	1:B:374:ARG:HG2	2.02	0.40
1:B:423:HIS:O	1:B:427:VAL:HG23	2.21	0.40
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.96	0.40
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.57	0.40
1:B:117:PRO:HA	1:B:239:GLY:N	2.36	0.40
1:B:389:THR:HA	1:B:396:TRP:CD1	2.57	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	414/444 (93%)	388 (94%)	23 (6%)	3 (1%)	22	22
1	B	412/444 (93%)	379 (92%)	29 (7%)	4 (1%)	15	14
All	All	826/888 (93%)	767 (93%)	52 (6%)	7 (1%)	19	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	A	112	GLN
1	B	111	LEU
1	B	145	SER
1	A	117	PRO
1	B	115	PRO
1	A	121	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	354/377 (94%)	347 (98%)	7 (2%)	55	69
1	B	353/377 (94%)	347 (98%)	6 (2%)	60	74
All	All	707/754 (94%)	694 (98%)	13 (2%)	59	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	126	LEU
1	A	259	GLN
1	A	285	ASN

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Mol	Chain	Res	Type
1	A	414	LEU
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	114	ARG
1	B	225	ASN
1	B	323	GLU
1	B	398	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	153	GLN
1	A	191	GLN
1	A	259	GLN
1	A	278	GLN
1	A	285	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	112	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	405	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is 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	HEM	A	500	1	27,50,50	1.48	5 (18%)	17,82,82	1.16	1 (5%)
3	HEM	B	500	1	27,50,50	1.65	5 (18%)	17,82,82	1.34	3 (17%)
5	EDO	A	870	-	3,3,3	0.44	0	2,2,2	0.26	0
4	3BT	B	821	-	16,18,18	3.39	7 (43%)	20,22,22	1.21	3 (15%)
2	ACT	B	851	-	1,3,3	4.57	1 (100%)	0,3,3	0.00	-
7	GOL	B	891	-	5,5,5	0.28	0	5,5,5	0.15	0
6	CAD	B	951	1	0,2,4	0.00	-	0,1,6	0.00	-
7	GOL	A	890	-	5,5,5	0.29	0	5,5,5	0.34	0
2	ACT	A	850	-	1,3,3	3.03	1 (100%)	0,3,3	0.00	-
2	ACT	B	861	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
6	CAD	A	950	1	0,2,4	0.00	-	0,1,6	0.00	-
7	GOL	A	881	-	5,5,5	0.39	0	5,5,5	0.22	0
4	3BT	A	820	-	16,18,18	3.23	7 (43%)	20,22,22	1.24	3 (15%)
5	EDO	B	871	-	3,3,3	0.53	0	2,2,2	0.24	0
2	ACT	A	860	-	1,3,3	2.50	1 (100%)	0,3,3	0.00	-

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	HEM	A	500	1	-	0/6/54/54	-
3	HEM	B	500	1	-	0/6/54/54	-
5	EDO	A	870	-	-	0/1/1/1	-
4	3BT	B	821	-	-	2/12/12/12	0/1/1/1
7	GOL	B	891	-	-	0/4/4/4	-
7	GOL	A	890	-	-	2/4/4/4	-
7	GOL	A	881	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3BT	A	820	-	-	0/12/12/12	0/1/1/1
5	EDO	B	871	-	-	0/1/1/1	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	821	3BT	C2-C3	9.79	1.56	1.39
4	A	820	3BT	C2-C3	9.37	1.55	1.39
2	B	851	ACT	CH3-C	4.57	1.54	1.48
4	B	821	3BT	C'-N1'	4.41	1.43	1.34
4	A	820	3BT	C'-N2'	4.30	1.43	1.28
3	B	500	HEM	C3C-C2C	-4.27	1.34	1.40
4	B	821	3BT	C'-N2'	4.15	1.43	1.28
3	A	500	HEM	C3B-CAB	-4.05	1.39	1.47
4	B	821	3BT	C-N1	4.02	1.42	1.34
4	A	820	3BT	C'-N1'	4.02	1.42	1.34
3	B	500	HEM	C3B-C2B	-4.00	1.34	1.40
4	A	820	3BT	C-N2	3.79	1.41	1.28
4	A	820	3BT	C-N1	3.76	1.42	1.34
4	B	821	3BT	C-N2	3.52	1.40	1.28
3	B	500	HEM	C3B-CAB	-3.21	1.41	1.47
2	A	850	ACT	CH3-C	3.03	1.52	1.48
3	A	500	HEM	C3C-CAC	-2.89	1.41	1.47
2	A	860	ACT	CH3-C	2.50	1.51	1.48
3	A	500	HEM	C1A-NA	2.38	1.41	1.36
4	A	820	3BT	C6-C1	2.34	1.43	1.38
4	B	821	3BT	C6-C1	2.32	1.43	1.38
3	B	500	HEM	C1A-NA	2.31	1.40	1.36
3	B	500	HEM	C3C-CAC	-2.29	1.43	1.47
3	A	500	HEM	C4A-NA	2.27	1.40	1.36
4	A	820	3BT	C5-C4	2.12	1.43	1.38
4	B	821	3BT	C5-C4	2.03	1.43	1.38
3	A	500	HEM	C4B-NB	2.02	1.40	1.36
2	B	861	ACT	CH3-C	2.01	1.51	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	820	3BT	CA-S-C	3.75	112.35	102.69
3	B	500	HEM	CBA-CAA-C2A	-3.72	105.63	112.49
4	B	821	3BT	CC-S'-C'	2.83	109.97	102.69
4	B	821	3BT	CA-S-C	2.75	109.77	102.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	HEM	C1D-C2D-C3D	-2.58	105.20	107.00
3	B	500	HEM	C4C-C3C-C2C	-2.55	105.12	106.90
4	A	820	3BT	CC-S'-C'	2.34	108.72	102.69
4	A	820	3BT	C1-C2-C3	-2.18	118.55	121.23
3	B	500	HEM	C3B-C4B-NB	2.12	111.95	109.21
4	B	821	3BT	C1-C2-C3	-2.10	118.65	121.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

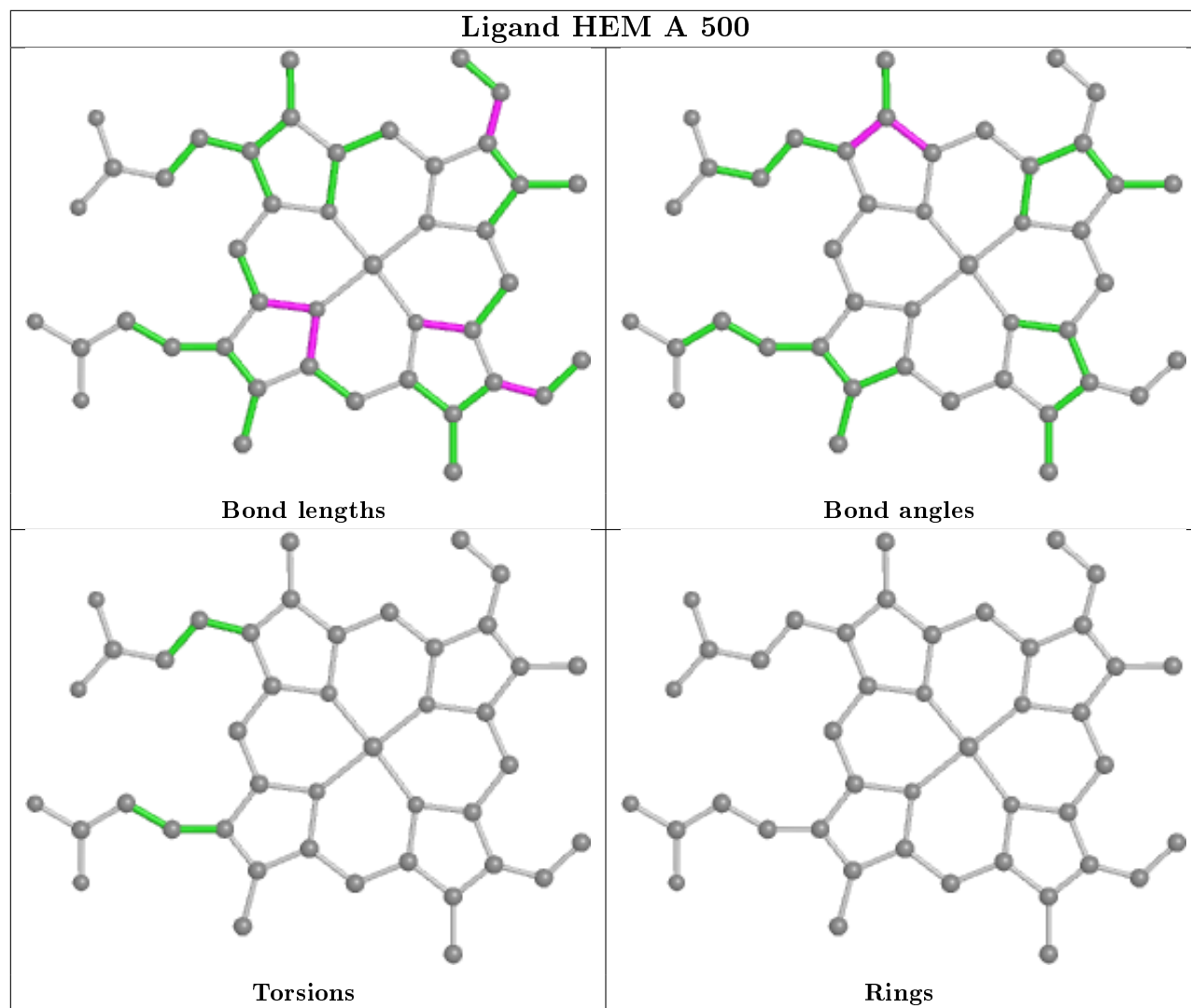
Mol	Chain	Res	Type	Atoms
4	B	821	3BT	S'-CC-CD-C3
7	A	890	GOL	O1-C1-C2-C3
7	A	881	GOL	O1-C1-C2-C3
7	A	890	GOL	O1-C1-C2-O2
7	A	881	GOL	O1-C1-C2-O2
4	B	821	3BT	CD-CC-S'-C'

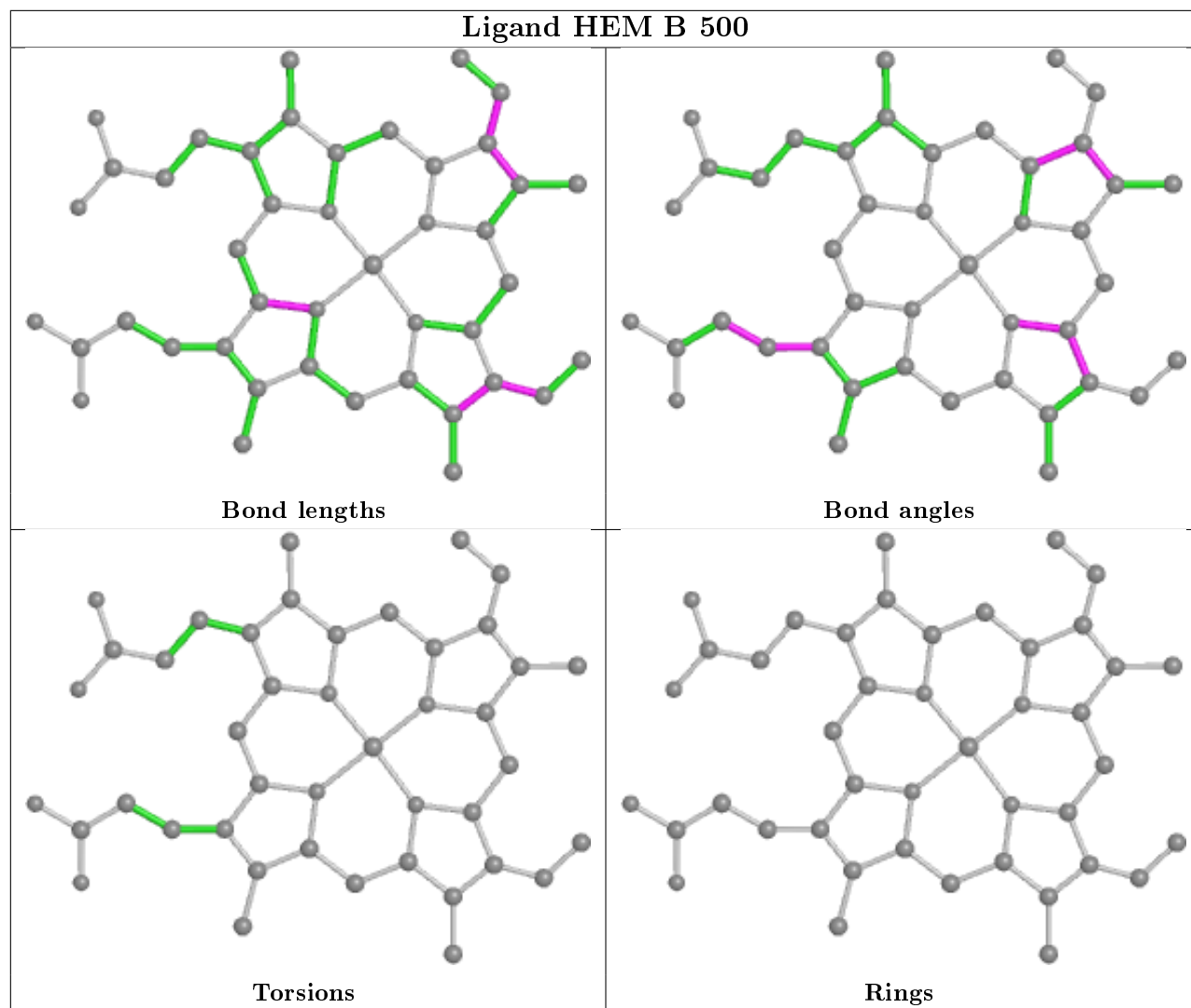
There are no ring outliers.

6 monomers are involved in 12 short contacts:

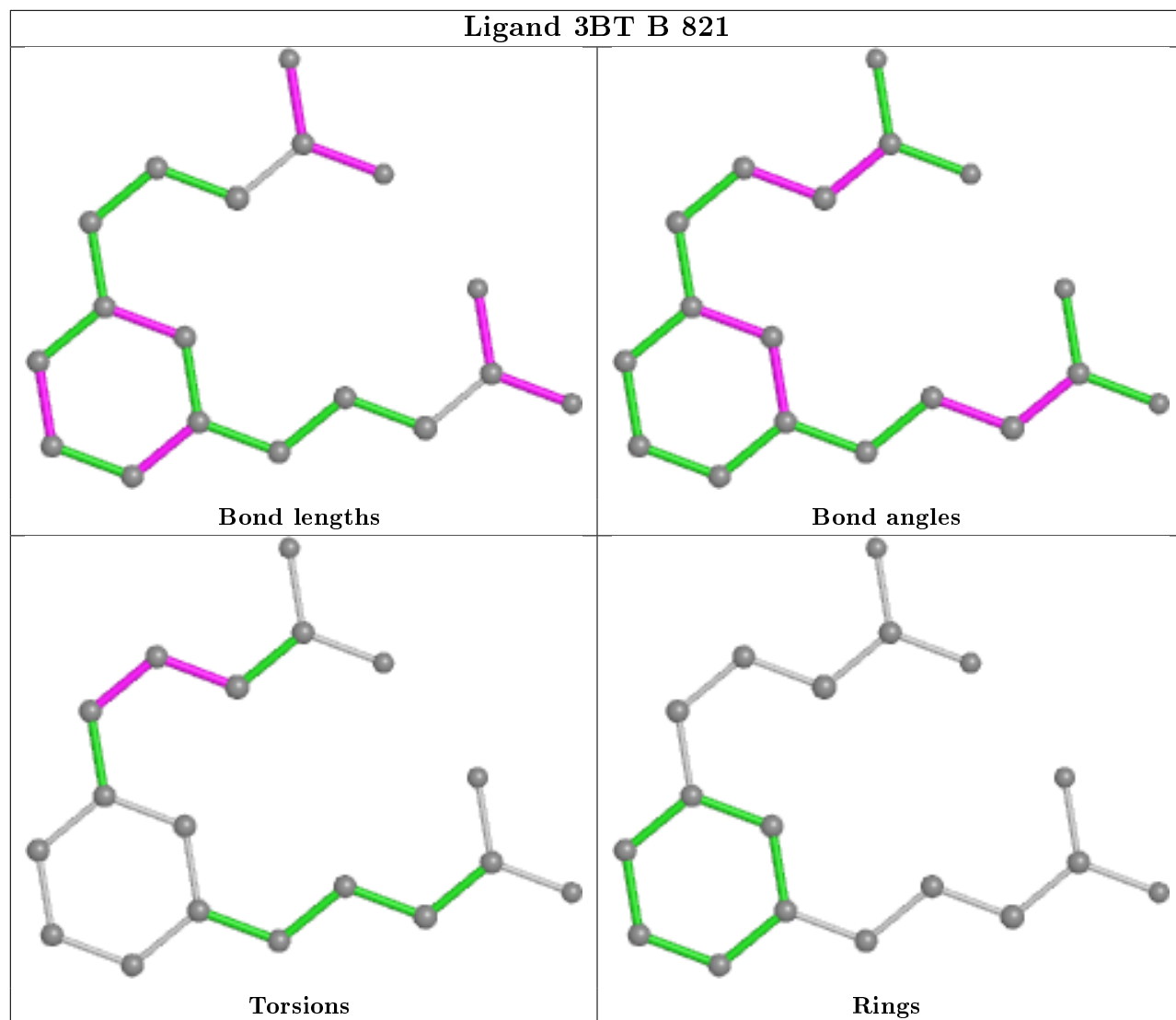
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	HEM	4	0
4	B	821	3BT	3	0
7	B	891	GOL	1	0
6	B	951	CAD	1	0
7	A	890	GOL	2	0
4	A	820	3BT	2	0

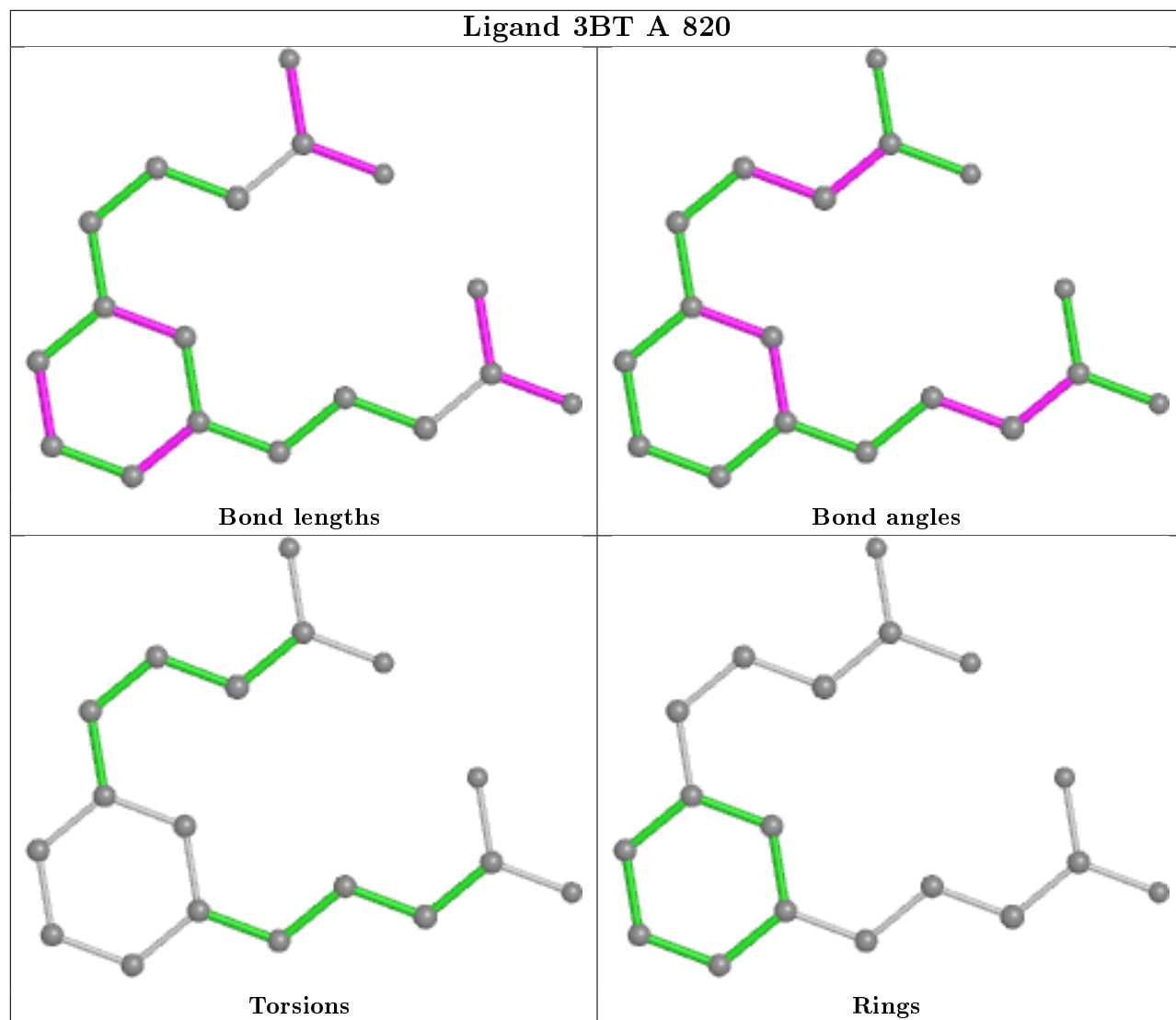
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand 3BT B 821





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	416/444 (93%)	0.37	34 (8%) 11 10	30, 45, 78, 100	0
1	B	414/444 (93%)	0.49	36 (8%) 10 8	31, 50, 79, 100	0
All	All	830/888 (93%)	0.43	70 (8%) 11 9	30, 47, 79, 100	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	12.8
1	B	115	PRO	11.1
1	B	118	GLY	10.5
1	B	111	LEU	10.1
1	A	113	THR	10.1
1	B	119	PRO	10.0
1	B	120	PRO	9.9
1	A	119	PRO	9.8
1	B	116	SER	9.6
1	A	117	PRO	9.2
1	B	113	THR	8.9
1	A	115	PRO	8.6
1	A	111	LEU	7.6
1	B	110	LYS	7.6
1	B	112	GLN	7.3
1	A	114	ARG	7.1
1	B	114	ARG	6.8
1	A	118	GLY	6.7
1	A	110	LYS	6.6
1	A	109	ARG	6.5
1	B	121	PRO	5.6
1	A	116	SER	5.6
1	A	112	GLN	5.0
1	B	122	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	99	ARG	4.4
1	A	108	PRO	4.4
1	B	260	ASP	4.3
1	B	259	GLN	4.0
1	A	120	PRO	3.9
1	A	259	GLN	3.8
1	B	94	GLY	3.5
1	B	146	GLN	3.4
1	A	239	GLY	3.4
1	A	107	LEU	3.4
1	A	69	LYS	3.1
1	B	108	PRO	3.1
1	A	390	ARG	3.0
1	A	146	GLN	2.8
1	B	141	LYS	2.8
1	A	121	PRO	2.7
1	A	123	GLU	2.7
1	A	337	ALA	2.6
1	B	147	ALA	2.6
1	A	67	GLY	2.6
1	A	91	GLN	2.6
1	B	337	ALA	2.5
1	B	143	SER	2.5
1	A	257	ARG	2.5
1	B	109	ARG	2.4
1	A	338	VAL	2.4
1	B	123	GLU	2.4
1	B	261	GLY	2.3
1	A	270	VAL	2.3
1	B	239	GLY	2.3
1	A	277	ILE	2.3
1	B	353	ALA	2.3
1	B	258	GLN	2.2
1	B	354	PRO	2.2
1	A	482	TRP	2.2
1	A	98	PRO	2.2
1	B	390	ARG	2.2
1	B	69	LYS	2.1
1	B	233	PHE	2.1
1	B	223	ARG	2.1
1	A	414	LEU	2.1
1	B	482	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLN	2.1
1	B	70	PHE	2.0
1	B	280	GLY	2.0
1	A	122	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

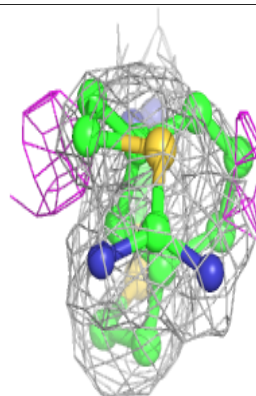
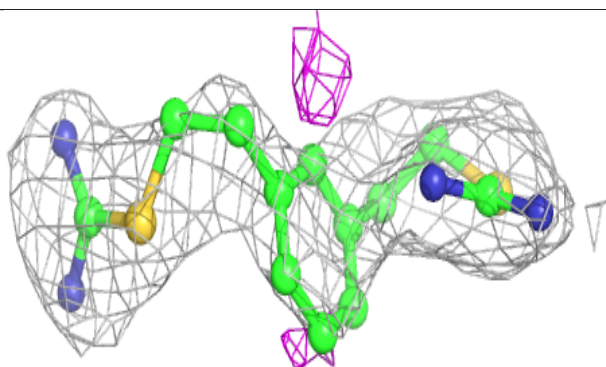
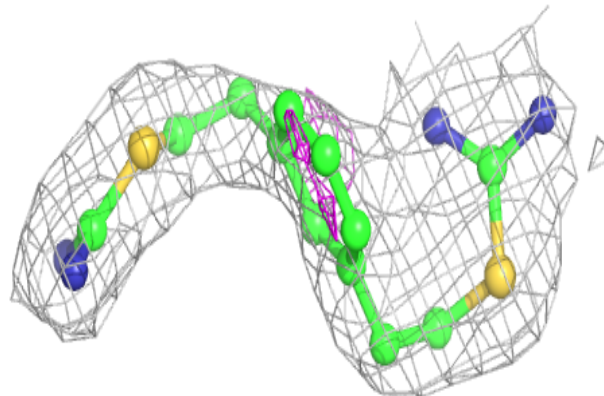
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	871	4/4	0.83	0.16	55,56,57,59	0
5	EDO	A	870	4/4	0.86	0.16	52,54,55,55	0
4	3BT	A	820	18/18	0.90	0.24	44,55,58,60	0
7	GOL	B	891	6/6	0.90	0.26	56,56,57,58	0
4	3BT	B	821	18/18	0.91	0.24	49,60,63,63	0
7	GOL	A	881	6/6	0.91	0.17	53,55,56,56	0
2	ACT	B	861	4/4	0.94	0.12	50,51,52,54	0
7	GOL	A	890	6/6	0.94	0.24	55,55,57,59	0
2	ACT	A	850	4/4	0.95	0.13	53,55,56,56	0
2	ACT	A	860	4/4	0.95	0.11	45,46,46,47	0
2	ACT	B	851	4/4	0.96	0.11	48,49,50,51	0
3	HEM	B	500	43/43	0.97	0.15	29,32,45,46	0
3	HEM	A	500	43/43	0.97	0.17	28,34,48,54	0
6	CAD	B	951	3/5	0.98	0.15	83,83,83,88	0
6	CAD	A	950	3/5	0.98	0.10	53,53,54,59	0
8	ZN	B	900	1/1	0.98	0.03	56,56,56,56	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.

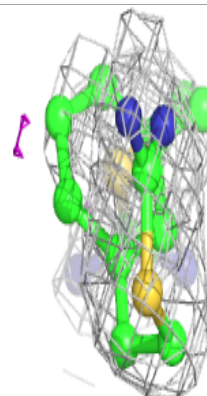
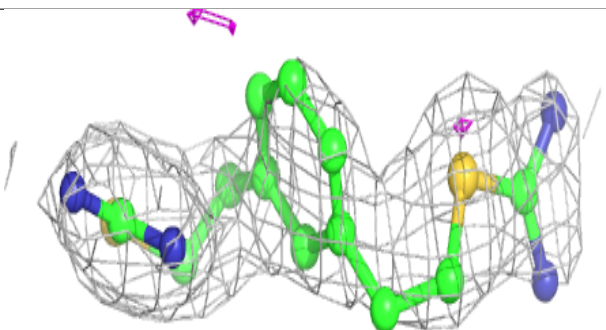
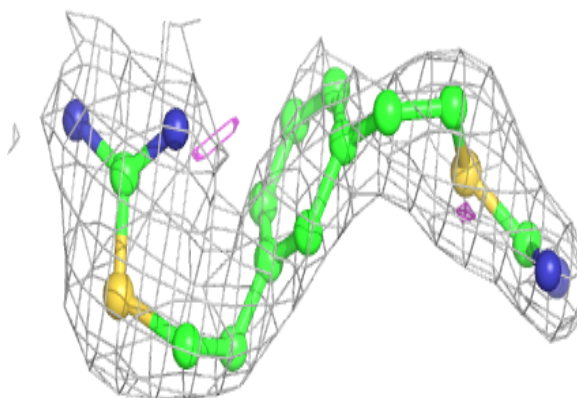
Electron density around 3BT A 820:

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



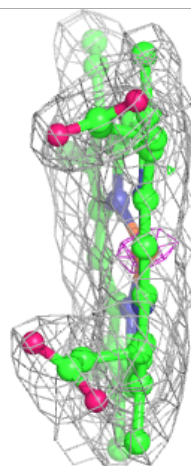
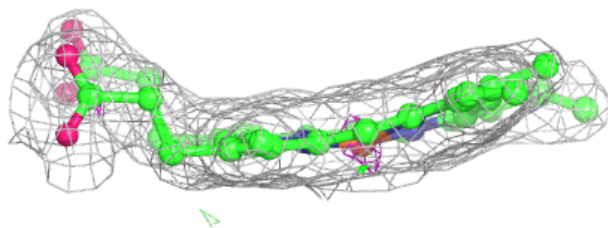
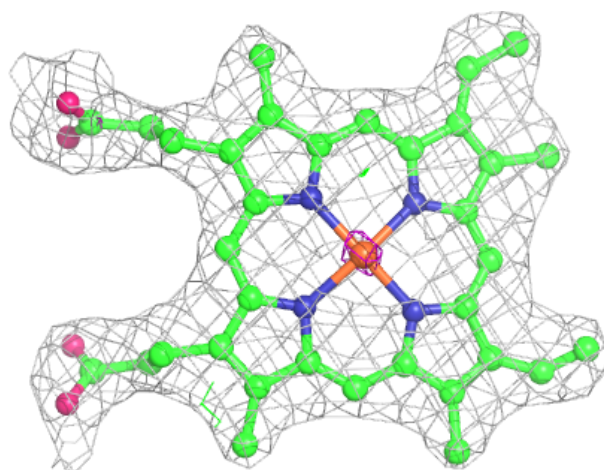
Electron density around 3BT B 821:

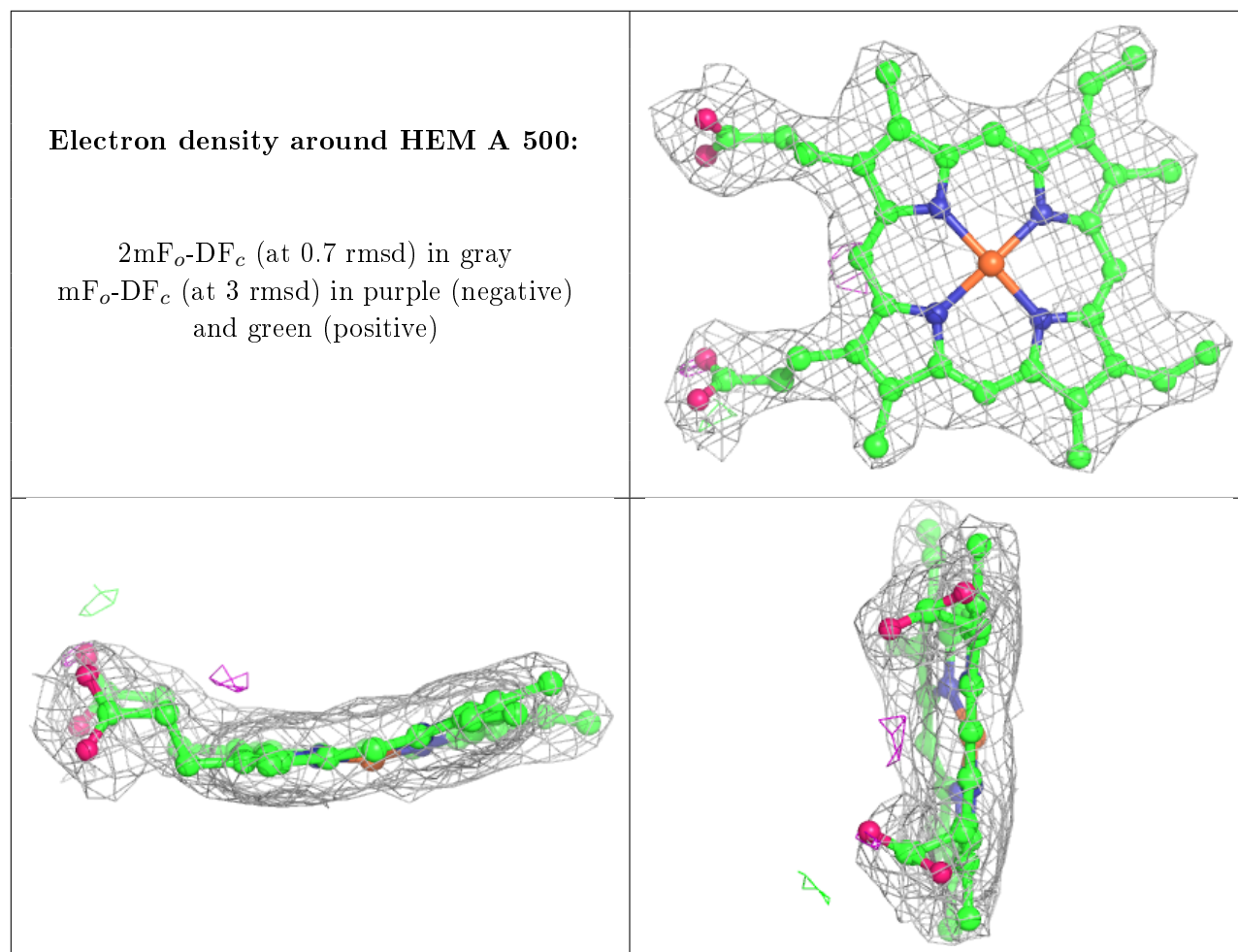
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 500:

$2mF_o-DF_c$ (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.