Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 10:50 PM EST

PDB ID	:	1DM8
Title	:	BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN COMPLEXED WITH 1,2,4-TRIAZOLE-CARBOXAMIDINE (H4B BOUND)
Authors	:	Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos, T.L.
Deposited on	:	1999-12-13
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

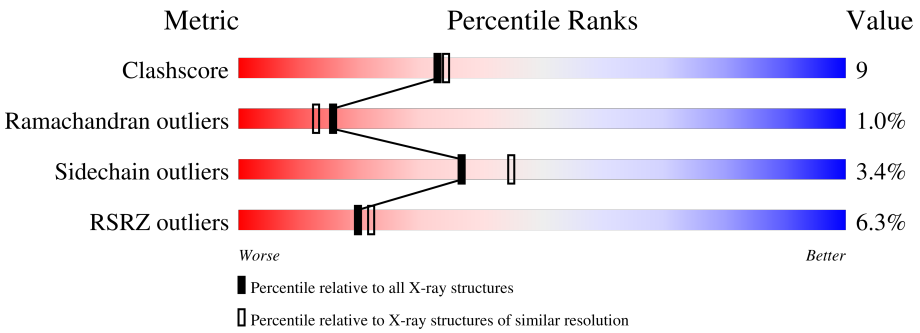
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	5% 76% 16% • 6%
1	B	444	6% 77% 14% • 7%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7024 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.

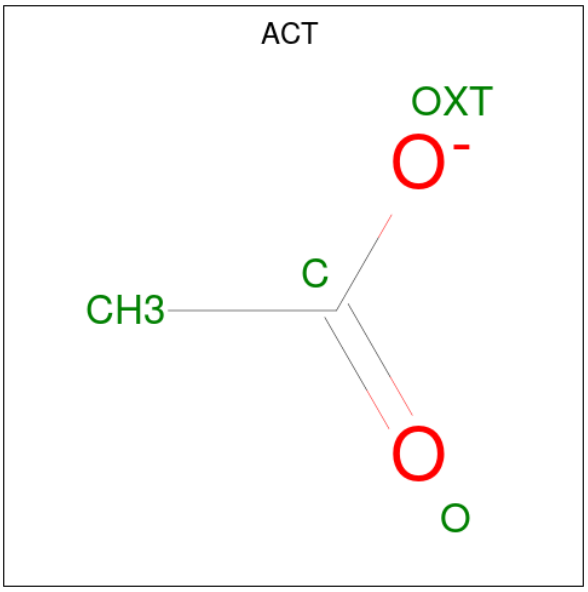
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

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

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: $C_2H_3O_2$).



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

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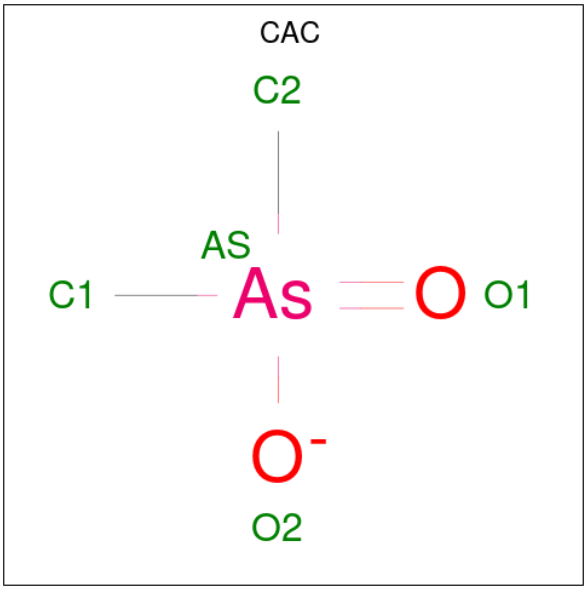
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).

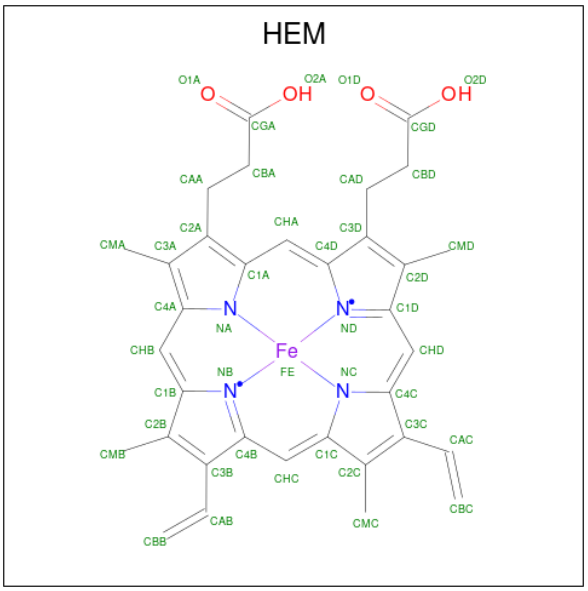


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	C		
3	A	1	3	1	2	0	0
			Total	As	C		
3	B	1	3	1	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

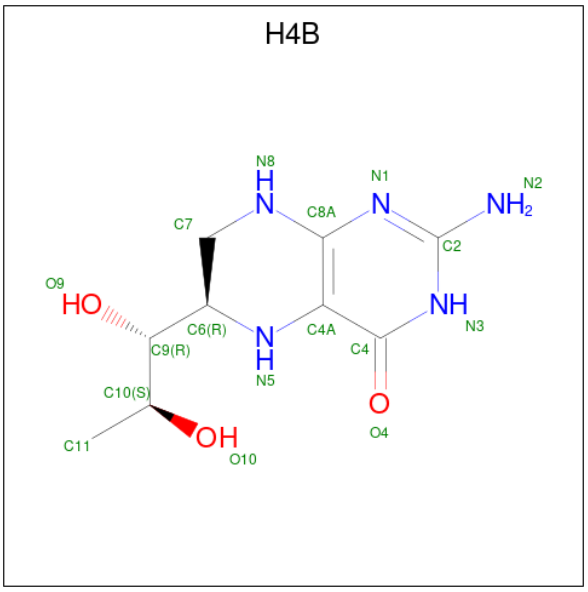
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0

- Molecule 5 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		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

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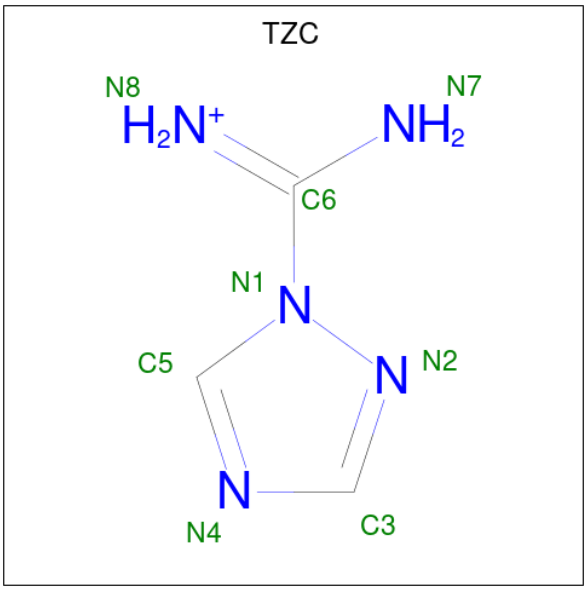
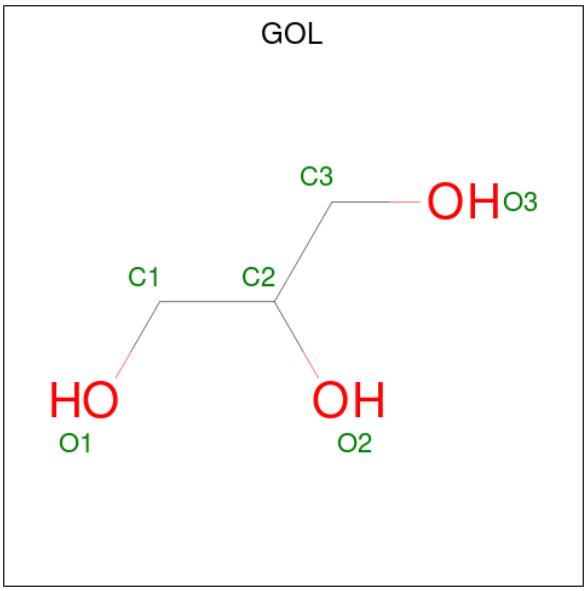
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	17	9	5	3	0	0

- Molecule 7 is 1,2,4-TRIAZOLE-CARBOXAMIDINE (three-letter code: TZC) (formula: $C_3H_6N_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N			
7	A	1	8	3	5		0	0
			Total	C	N			
7	B	1	8	3	5		0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

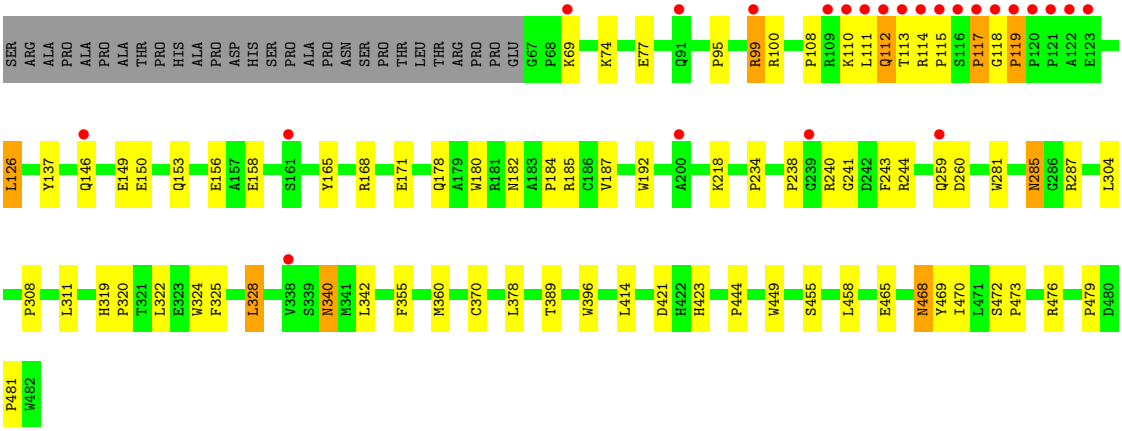
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	136	136	136	0	0
			Total	O		
9	B	124	124	124	0	0

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.

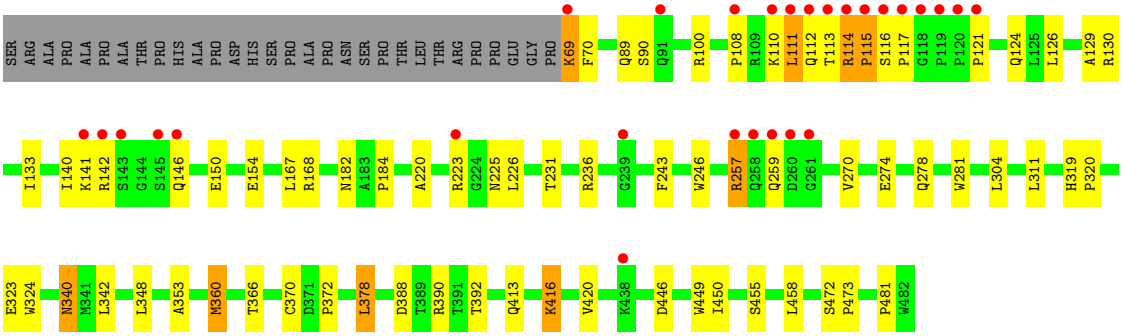
• Molecule 1: NITRIC OXIDE SYNTHASE

Chain A:



• Molecule 1: NITRIC OXIDE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.53Å 106.60Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.65 – 2.25 36.65 – 2.24	Depositor EDS
% Data completeness (in resolution range)	69.0 (36.65-2.25) 69.1 (36.65-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.239 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ACT, CAC, HEM, H4B, ZN, GOL, TZC

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	0.40	0/3397	0.66	1/4631 (0.0%)
1	B	0.37	0/3385	0.66	2/4614 (0.0%)
All	All	0.38	0/6782	0.66	3/9245 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	MET	N-CA-C	-5.70	95.62	111.00
1	A	360	MET	N-CA-C	-5.67	95.68	111.00
1	B	243	PHE	N-CA-C	-5.11	97.21	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	63	0
1	B	3291	0	3205	58	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
4	A	1	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	0	0
6	A	17	0	15	0	0
6	B	17	0	15	1	0
7	A	8	0	6	1	0
7	B	8	0	6	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	136	0	0	2	0
9	B	124	0	0	1	0
All	All	7024	0	6550	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)
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.45	0.98
1:A:113:THR:HG21	1:A:342:LEU:HD22	1.51	0.93
1:B:112:GLN:HG3	1:B:113:THR:H	1.35	0.91
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.46	0.81
1:B:89:GLN:HE21	1:B:89:GLN:HA	1.47	0.79
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.68	0.74
1:B:69:LYS:HE2	1:B:69:LYS:N	2.05	0.71
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.73	0.71
1:A:308:PRO:HD2	1:A:311:LEU:HD12	1.71	0.70
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:O	1:A:117:PRO:HD3	1.91	0.69
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.76	0.68
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.77	0.67
1:B:89:GLN:HA	1:B:89:GLN:NE2	2.14	0.63
1:B:129:ALA:O	1:B:133:ILE:HG12	1.98	0.62
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.39	0.62
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.64	0.61
1:B:112:GLN:HG3	1:B:113:THR:N	2.13	0.60
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.83	0.60
1:A:114:ARG:HA	1:A:479:PRO:HG2	1.84	0.58
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.38	0.58
1:A:111:LEU:HD23	1:A:476:ARG:NH1	2.20	0.57
1:A:468:ASN:HD22	1:A:469:TYR:H	1.53	0.56
1:A:468:ASN:HD22	1:A:469:TYR:N	2.04	0.56
1:A:178:GLN:HG2	9:A:1982:HOH:O	2.05	0.56
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.22	0.54
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.41	0.54
1:A:378:LEU:HB2	9:A:2001:HOH:O	2.07	0.54
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.89	0.54
1:A:240:ARG:HG2	1:A:241:GLY:N	2.23	0.54
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.91	0.53
1:A:472:SER:HA	1:A:473:PRO:C	2.29	0.53
1:A:114:ARG:HD2	1:A:479:PRO:HG3	1.90	0.53
1:B:257:ARG:HE	1:B:270:VAL:HG11	1.74	0.53
1:B:110:LYS:C	1:B:112:GLN:H	2.12	0.52
1:B:113:THR:HG21	1:B:342:LEU:CD1	2.37	0.52
1:A:146:GLN:O	1:A:150:GLU:HG3	2.10	0.52
1:A:259:GLN:HG2	1:A:260:ASP:N	2.25	0.51
1:B:472:SER:HA	1:B:473:PRO:C	2.31	0.51
1:B:449:TRP:HA	6:B:2600:H4B:N1	2.26	0.51
1:A:114:ARG:HA	1:A:479:PRO:CG	2.40	0.50
1:A:126:LEU:CD1	1:A:156:GLU:HG2	2.41	0.50
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.93	0.50
1:A:340:ASN:H	1:A:340:ASN:HD22	1.60	0.50
1:B:146:GLN:O	1:B:150:GLU:HG3	2.11	0.50
1:B:366:THR:O	1:B:370:CYS:HB2	2.12	0.50
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.25	0.50
1:A:325:PHE:O	1:A:328:LEU:HB2	2.11	0.49
1:A:355:PHE:CD1	7:A:1790:TZC:H3	2.46	0.49
1:B:270:VAL:O	1:B:274:GLU:HG3	2.12	0.49
1:A:111:LEU:HG	1:A:470:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:HD22	1:A:285:ASN:C	2.14	0.49
1:A:182:ASN:O	1:A:184:PRO:HD3	2.12	0.49
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.94	0.49
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.53	0.49
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.42	0.48
1:B:114:ARG:HA	1:B:114:ARG:NH1	2.21	0.48
1:A:69:LYS:O	1:A:69:LYS:HG2	2.14	0.48
1:A:95:PRO:HD3	1:A:110:LYS:HG3	1.94	0.48
1:A:111:LEU:O	1:A:112:GLN:C	2.52	0.48
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.43	0.48
1:B:388:ASP:OD1	1:B:390:ARG:HG3	2.14	0.47
1:A:149:GLU:O	1:A:153:GLN:HG3	2.14	0.47
1:B:342:LEU:C	1:B:342:LEU:HD23	2.35	0.47
1:B:413:GLN:O	1:B:416:LYS:HE3	2.14	0.47
1:A:110:LYS:HE3	1:A:110:LYS:HA	1.97	0.47
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.50	0.47
1:B:340:ASN:HD22	1:B:340:ASN:H	1.62	0.47
1:B:69:LYS:HE3	1:B:70:PHE:CD1	2.50	0.47
1:B:110:LYS:O	1:B:112:GLN:N	2.48	0.46
1:B:111:LEU:HD12	1:B:111:LEU:N	2.31	0.46
1:A:115:PRO:C	1:A:117:PRO:HD3	2.35	0.46
1:B:246:TRP:CD1	1:B:481:PRO:HG3	2.51	0.46
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.45	0.46
1:B:150:GLU:O	1:B:154:GLU:HG3	2.17	0.45
1:A:421:ASP:OD2	1:A:423:HIS:HB2	2.16	0.45
1:A:99:ARG:HG3	1:A:99:ARG:NH1	2.33	0.44
1:B:140:ILE:O	1:B:142:ARG:HG2	2.17	0.44
1:B:142:ARG:HA	1:B:142:ARG:HD3	1.85	0.44
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.33	0.44
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.52	0.44
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.99	0.44
1:B:378:LEU:HB2	9:B:2896:HOH:O	2.17	0.44
1:A:95:PRO:HG3	1:A:108:PRO:HG3	2.00	0.43
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.99	0.43
1:A:99:ARG:HH11	1:A:99:ARG:HB2	1.83	0.43
1:B:69:LYS:HE3	1:B:70:PHE:CE1	2.53	0.43
1:B:446:ASP:O	1:B:450:ILE:HG12	2.18	0.43
1:A:389:THR:HA	1:A:396:TRP:CD1	2.53	0.43
1:A:423:HIS:HB2	1:B:392:THR:HB	1.99	0.43
1:A:74:LYS:O	1:A:465:GLU:HG3	2.18	0.43
1:B:126:LEU:O	1:B:130:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:NH2	1:B:90:SER:O	2.51	0.43
1:B:116:SER:N	1:B:117:PRO:CD	2.81	0.43
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.54	0.42
1:B:223:ARG:HA	1:B:223:ARG:CZ	2.49	0.42
1:B:182:ASN:O	1:B:184:PRO:HD3	2.19	0.42
1:A:99:ARG:CG	1:A:99:ARG:NH1	2.82	0.42
1:B:116:SER:HB2	1:B:236:ARG:CZ	2.50	0.42
1:B:220:ALA:O	1:B:226:LEU:HA	2.20	0.42
1:B:324:TRP:HB2	3:B:950:CAC:C1	2.49	0.42
1:A:117:PRO:O	1:A:118:GLY:C	2.59	0.42
1:A:126:LEU:HD22	1:A:126:LEU:HA	1.82	0.41
1:B:231:THR:O	1:B:353:ALA:HA	2.21	0.41
1:B:111:LEU:HD12	1:B:111:LEU:H	1.84	0.41
1:B:360:MET:HA	1:B:420:VAL:O	2.20	0.41
1:A:458:LEU:HD22	1:B:378:LEU:HD21	2.02	0.41
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.55	0.41
1:A:187:VAL:HG22	1:A:187:VAL:O	2.21	0.41
1:A:285:ASN:C	1:A:285:ASN:ND2	2.74	0.41
1:A:308:PRO:CD	1:A:311:LEU:HD12	2.47	0.41
1:A:259:GLN:HG2	1:A:260:ASP:H	1.85	0.40
1:B:89:GLN:HE21	1:B:89:GLN:CA	2.17	0.40
1:A:218:LYS:CG	1:A:311:LEU:HD22	2.52	0.40
1:A:340:ASN:HD22	1:A:340:ASN:N	2.18	0.40
1:A:444:PRO:HB3	1:A:469:TYR:CE1	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%)	390 (94%)	20 (5%)	4 (1%)	15 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/444 (93%)	390 (95%)	18 (4%)	4 (1%)	15	13
All	All	826/888 (93%)	780 (94%)	38 (5%)	8 (1%)	15	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	B	259	GLN
1	A	112	GLN
1	B	111	LEU
1	A	119	PRO
1	B	115	PRO
1	A	238	PRO
1	B	121	PRO

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	354/377 (94%)	344 (97%)	10 (3%)	43	52
1	B	353/377 (94%)	339 (96%)	14 (4%)	31	37
All	All	707/754 (94%)	683 (97%)	24 (3%)	37	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	119	PRO
1	A	126	LEU
1	A	285	ASN
1	A	287	ARG
1	A	328	LEU
1	A	340	ASN

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Mol	Chain	Res	Type
1	A	414	LEU
1	A	468	ASN
1	B	69	LYS
1	B	100	ARG
1	B	114	ARG
1	B	124	GLN
1	B	141	LYS
1	B	168	ARG
1	B	225	ASN
1	B	257	ARG
1	B	278	GLN
1	B	311	LEU
1	B	323	GLU
1	B	340	ASN
1	B	378	LEU
1	B	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	146	GLN
1	A	153	GLN
1	A	191	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	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	340	ASN
1	B	405	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	B	2850	-	3,3,3	0.79	0	3,3,3	0.94	0
6	H4B	A	1600	-	16,18,18	2.02	3 (18%)	11,26,26	4.13	9 (81%)
2	ACT	B	2860	-	3,3,3	0.85	0	3,3,3	0.76	0
8	GOL	A	1880	-	5,5,5	0.13	0	5,5,5	0.34	0
6	H4B	B	2600	-	16,18,18	2.05	3 (18%)	11,26,26	4.33	9 (81%)
8	GOL	B	2880	-	5,5,5	0.28	0	5,5,5	0.36	0
7	TZC	A	1790	-	4,8,8	1.29	1 (25%)	5,10,10	5.82	4 (80%)
5	HEM	A	1500	1	41,50,50	1.24	6 (14%)	45,82,82	1.40	5 (11%)
2	ACT	A	1850	-	3,3,3	0.78	0	3,3,3	0.89	0
2	ACT	A	1860	-	3,3,3	1.04	0	3,3,3	0.80	0
7	TZC	B	2790	-	4,8,8	1.37	0	5,10,10	5.85	4 (80%)
3	CAC	A	950	1	0,2,4	-	-	0,1,6	-	-
3	CAC	B	950	1	0,2,4	-	-	0,1,6	-	-
5	HEM	B	2500	1	41,50,50	1.41	6 (14%)	45,82,82	1.57	7 (15%)

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
6	H4B	A	1600	-	-	0/8/17/17	0/2/2/2
8	GOL	A	1880	-	-	0/4/4/4	-
6	H4B	B	2600	-	-	0/8/17/17	0/2/2/2
8	GOL	B	2880	-	-	2/4/4/4	-
7	TZC	A	1790	-	-	0/0/4/4	0/1/1/1
5	HEM	A	1500	1	-	0/12/54/54	-
7	TZC	B	2790	-	-	0/0/4/4	0/1/1/1
5	HEM	B	2500	1	-	0/12/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2600	H4B	C4-N3	5.06	1.41	1.33
6	A	1600	H4B	C4-N3	4.69	1.41	1.33
6	B	2600	H4B	C4A-N5	4.39	1.47	1.38
6	A	1600	H4B	C4A-N5	4.14	1.46	1.38
6	B	2600	H4B	C6-N5	3.65	1.53	1.45
5	B	2500	HEM	C3C-CAC	-3.64	1.40	1.47
6	A	1600	H4B	C6-N5	3.63	1.53	1.45
5	A	1500	HEM	C3C-CAC	-3.43	1.40	1.47
5	B	2500	HEM	CHB-C1B	2.94	1.42	1.35
5	B	2500	HEM	CAB-C3B	-2.87	1.39	1.47
5	B	2500	HEM	C3C-C2C	-2.71	1.36	1.40
5	A	1500	HEM	C4A-NA	2.53	1.41	1.36
5	A	1500	HEM	CAB-C3B	-2.41	1.40	1.47
5	B	2500	HEM	CHA-C4D	2.24	1.40	1.35
5	A	1500	HEM	C3C-C2C	-2.07	1.37	1.40
7	A	1790	TZC	C5-N4	2.06	1.39	1.34
5	B	2500	HEM	C3B-C2B	-2.05	1.33	1.37
5	A	1500	HEM	CHA-C4D	2.04	1.40	1.35
5	A	1500	HEM	C3B-C4B	2.01	1.48	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1790	TZC	C3-N2-N1	9.91	110.70	102.85
6	B	2600	H4B	C8A-C4A-C4	9.47	122.98	114.57
7	B	2790	TZC	C3-N2-N1	9.38	110.28	102.85
6	A	1600	H4B	C8A-C4A-C4	8.85	122.43	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2790	TZC	N7-C6-N1	7.48	122.37	115.34
7	A	1790	TZC	N7-C6-N1	6.57	121.52	115.34
6	A	1600	H4B	C2-N3-C4	5.59	124.82	115.93
6	B	2600	H4B	C2-N3-C4	5.59	124.82	115.93
5	B	2500	HEM	CBA-CAA-C2A	-4.96	104.16	112.62
5	B	2500	HEM	C3B-C2B-C1B	4.88	110.10	106.49
7	A	1790	TZC	C5-N4-C3	4.79	107.74	102.34
6	B	2600	H4B	N1-C2-N3	-4.69	118.06	125.42
6	A	1600	H4B	N1-C2-N3	-4.66	118.12	125.42
7	B	2790	TZC	C5-N4-C3	4.63	107.56	102.34
5	A	1500	HEM	CBA-CAA-C2A	-3.88	105.99	112.62
6	B	2600	H4B	C4A-C4-N3	-3.68	113.55	124.01
6	A	1600	H4B	N2-C2-N1	3.60	122.84	117.25
6	A	1600	H4B	C2-N1-C8A	3.59	122.59	114.54
6	A	1600	H4B	C4A-C4-N3	-3.57	113.87	124.01
5	A	1500	HEM	CMD-C2D-C1D	3.39	130.21	125.04
6	B	2600	H4B	C2-N1-C8A	3.38	122.12	114.54
6	B	2600	H4B	C4-C4A-N5	-3.29	116.36	119.12
6	B	2600	H4B	N2-C2-N1	3.29	122.37	117.25
5	B	2500	HEM	C4B-C3B-C2B	-3.27	104.52	107.11
5	A	1500	HEM	C4A-C3A-C2A	-2.80	105.05	107.00
6	B	2600	H4B	C4A-N5-C6	-2.76	113.64	121.16
5	B	2500	HEM	C4B-CHC-C1C	2.75	126.18	122.56
6	B	2600	H4B	O9-C9-C6	2.54	115.05	108.98
6	A	1600	H4B	C4A-N5-C6	-2.52	114.31	121.16
5	B	2500	HEM	CHC-C4B-NB	-2.32	121.91	124.43
6	A	1600	H4B	O9-C9-C6	2.30	114.47	108.98
5	A	1500	HEM	C2B-C1B-NB	2.22	112.47	109.84
7	A	1790	TZC	N4-C5-N1	-2.17	110.48	113.30
6	A	1600	H4B	C4-C4A-N5	-2.16	117.31	119.12
5	B	2500	HEM	CAB-C3B-C2B	-2.07	121.78	128.60
5	A	1500	HEM	C1B-NB-C4B	-2.07	102.94	105.07
5	B	2500	HEM	CBD-CAD-C3D	-2.01	107.04	112.63
7	B	2790	TZC	N4-C5-N1	-2.01	110.69	113.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	2880	GOL	O1-C1-C2-C3
8	B	2880	GOL	O1-C1-C2-O2

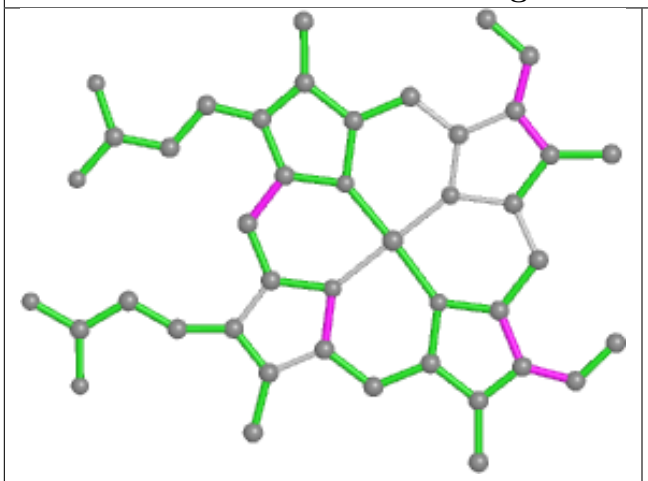
There are no ring outliers.

3 monomers are involved in 3 short contacts:

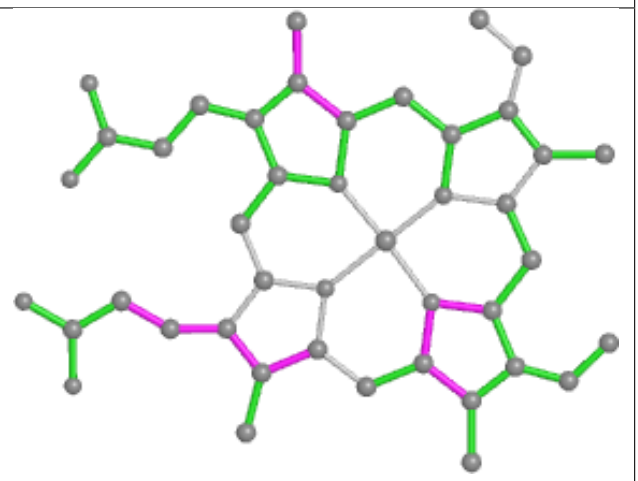
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2600	H4B	1	0
7	A	1790	TZC	1	0
3	B	950	CAC	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

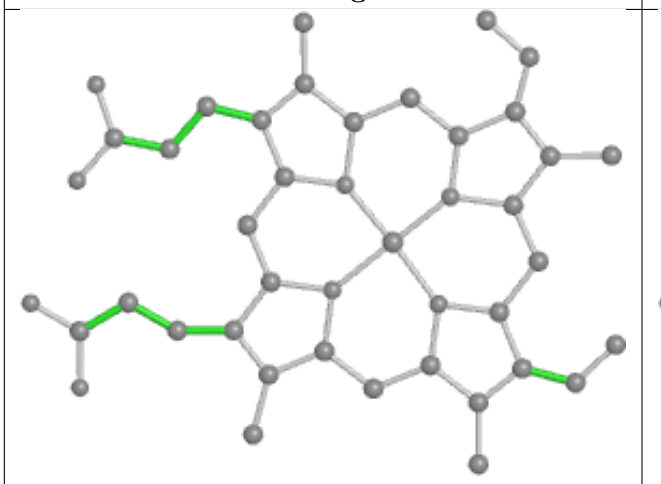
Ligand HEM A 1500



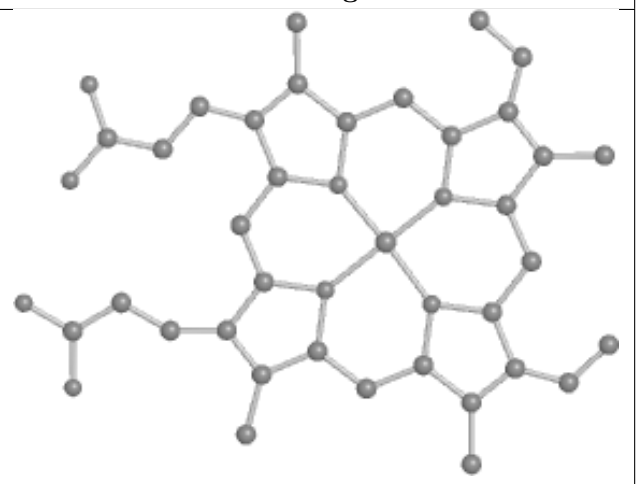
Bond lengths



Bond angles

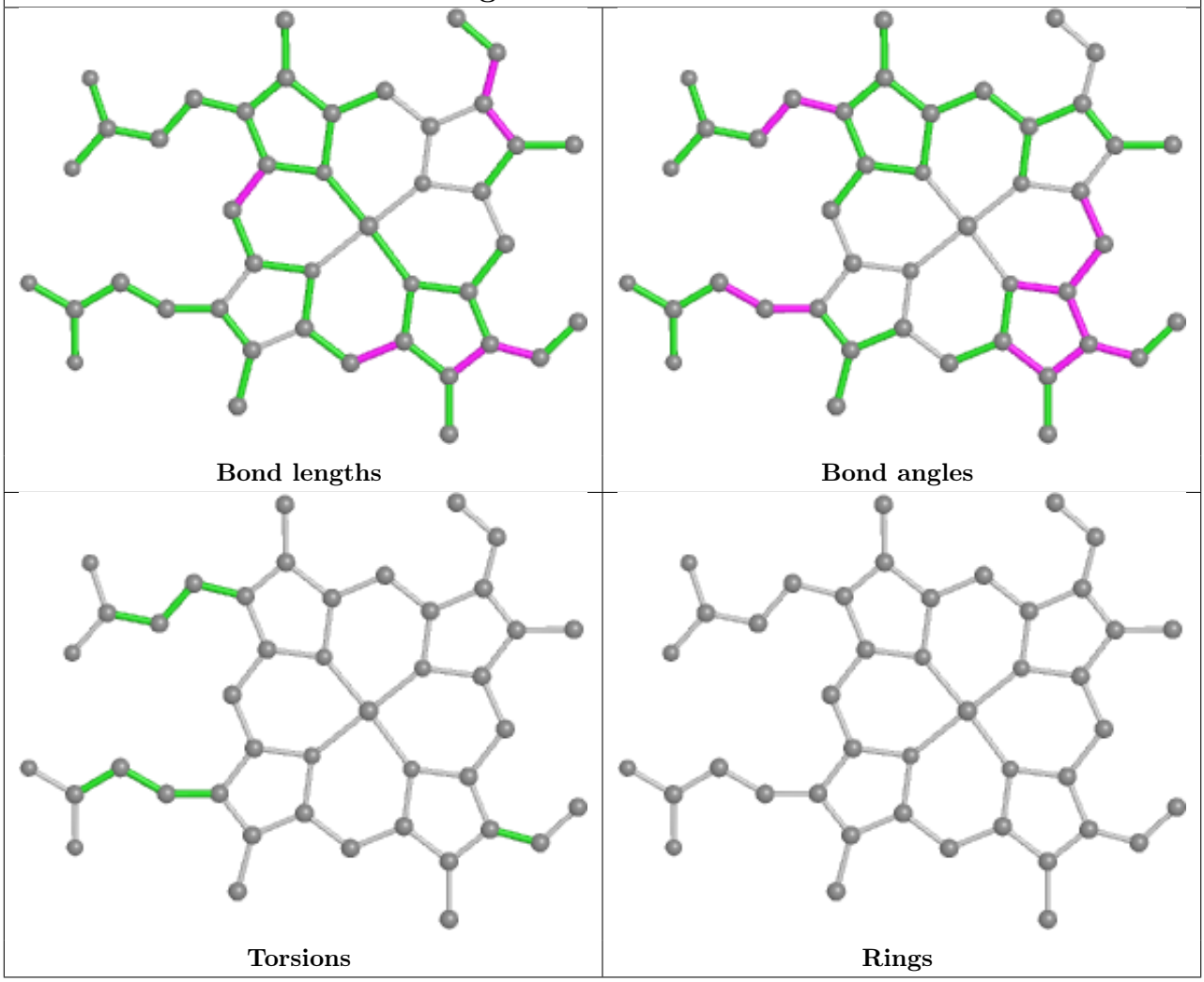


Torsions



Rings

Ligand HEM B 2500



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	416/444 (93%)	0.17	24 (5%)	23	25	28, 42, 75, 99	0
1	B	414/444 (93%)	0.23	28 (6%)	17	18	29, 45, 78, 99	0
All	All	830/888 (93%)	0.20	52 (6%)	20	22	28, 43, 78, 99	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	13.2
1	B	115	PRO	11.2
1	A	117	PRO	11.2
1	B	111	LEU	11.2
1	A	119	PRO	10.7
1	A	113	THR	10.5
1	B	118	GLY	10.1
1	B	110	LYS	9.9
1	B	113	THR	9.2
1	A	118	GLY	9.1
1	A	115	PRO	8.2
1	A	114	ARG	7.6
1	A	111	LEU	7.6
1	B	116	SER	7.2
1	B	119	PRO	7.2
1	A	110	LYS	6.5
1	A	112	GLN	6.3
1	B	114	ARG	5.6
1	B	260	ASP	5.4
1	B	112	GLN	5.2
1	B	121	PRO	5.1
1	A	239	GLY	5.0
1	A	116	SER	5.0
1	B	120	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	109	ARG	4.6
1	A	120	PRO	4.1
1	B	261	GLY	3.9
1	B	146	GLN	3.7
1	A	69	LYS	3.6
1	A	121	PRO	3.6
1	B	142	ARG	3.2
1	B	223	ARG	3.2
1	A	123	GLU	3.1
1	A	91	GLN	3.0
1	B	259	GLN	3.0
1	B	69	LYS	2.9
1	B	108	PRO	2.9
1	B	145	SER	2.7
1	B	143	SER	2.7
1	A	338	VAL	2.5
1	B	91	GLN	2.5
1	B	257	ARG	2.4
1	B	141	LYS	2.4
1	A	200	ALA	2.3
1	A	122	ALA	2.3
1	A	99	ARG	2.2
1	A	146	GLN	2.2
1	B	239	GLY	2.2
1	A	161	SER	2.2
1	B	258	GLN	2.2
1	B	438	LYS	2.1
1	A	259	GLN	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,

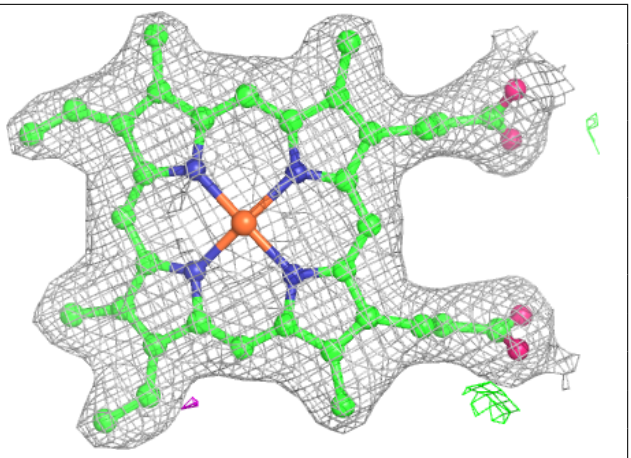
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

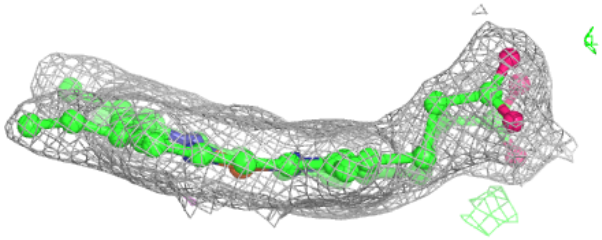
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	B	2860	4/4	0.77	0.22	50,51,52,58	0
8	GOL	B	2880	6/6	0.88	0.17	46,52,54,58	0
8	GOL	A	1880	6/6	0.91	0.26	53,55,58,62	0
2	ACT	A	1860	4/4	0.93	0.12	40,45,46,47	0
2	ACT	A	1850	4/4	0.94	0.22	42,42,42,43	0
2	ACT	B	2850	4/4	0.95	0.13	42,43,46,46	0
7	TZC	B	2790	8/8	0.97	0.24	30,34,36,36	0
6	H4B	B	2600	17/17	0.98	0.16	29,33,38,41	0
7	TZC	A	1790	8/8	0.98	0.20	31,33,33,34	0
3	CAC	A	950	3/5	0.98	0.09	57,57,60,69	0
5	HEM	A	1500	43/43	0.98	0.18	24,30,41,44	0
6	H4B	A	1600	17/17	0.98	0.16	27,31,35,40	0
4	ZN	A	900	1/1	0.99	0.03	47,47,47,47	0
3	CAC	B	950	3/5	0.99	0.06	75,75,76,79	0
5	HEM	B	2500	43/43	0.99	0.15	26,31,36,47	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 HEM A 1500:

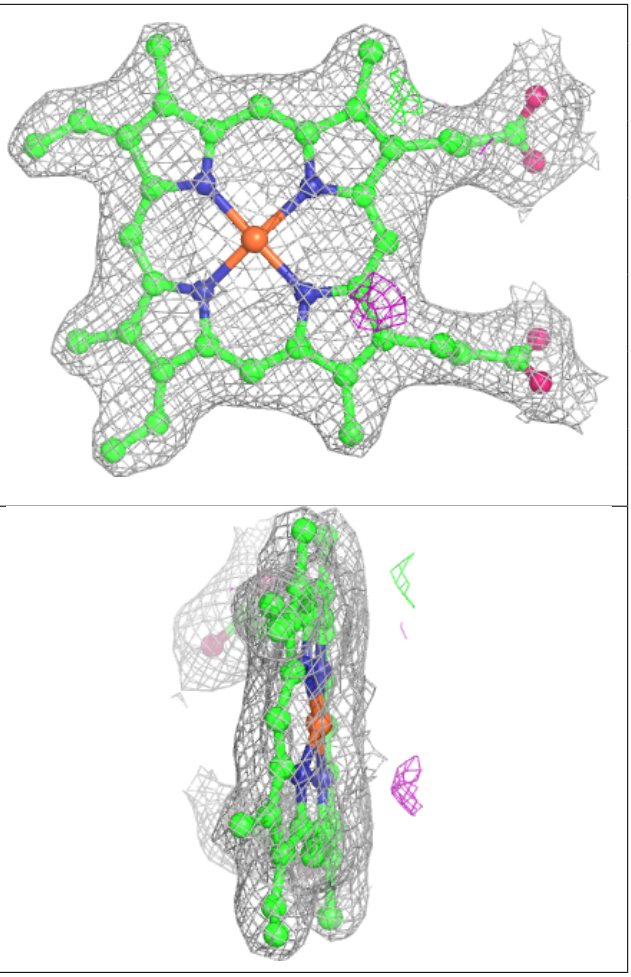
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEM B 2500:

$2mF_o$-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.