



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:49 AM EDT

PDB ID : 1ED4 / pdb_00001ed4
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH IPITU (H4B FREE)
Authors : Raman, C.S.; Li, H.; Martasek, P.; Kral, V.; Masters, B.S.S.; Poulos, T.L.
Deposited on : 2000-01-26
Resolution : 1.86 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

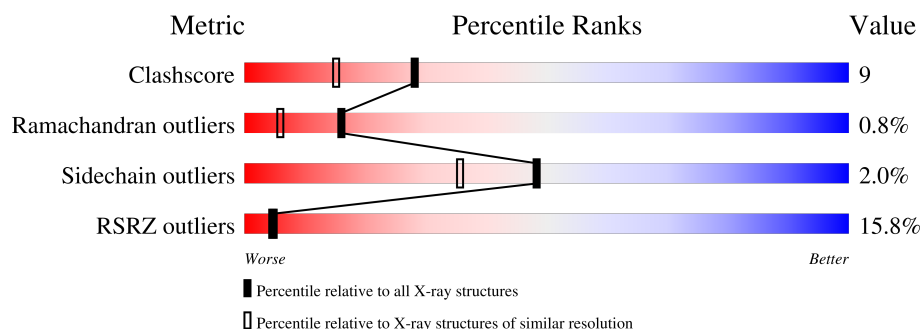
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	444	
1	B	444	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7403 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
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 (CCD ID: ACT) (formula: C₂H₃O₂).



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

Continued on next page...

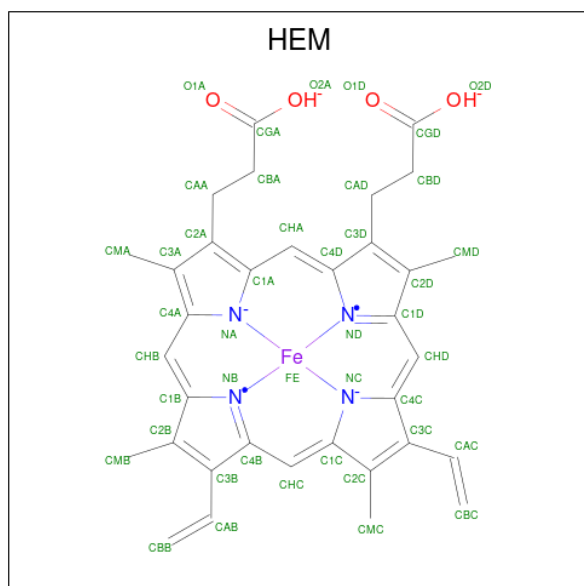
Continued from previous page...

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 ZINC ION (CCD ID: ZN) (formula: Zn).

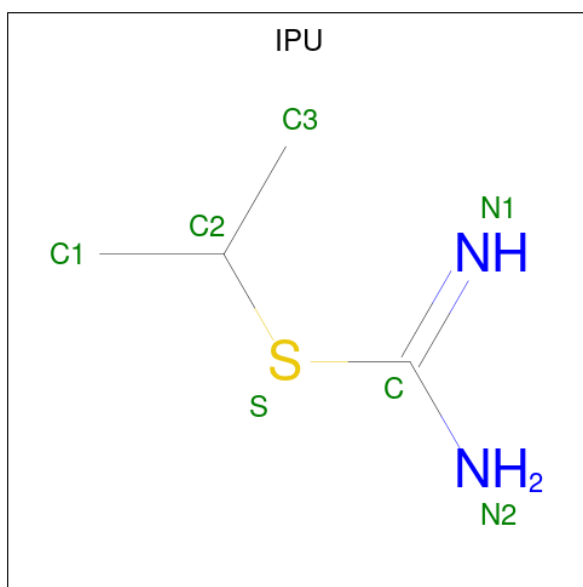
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



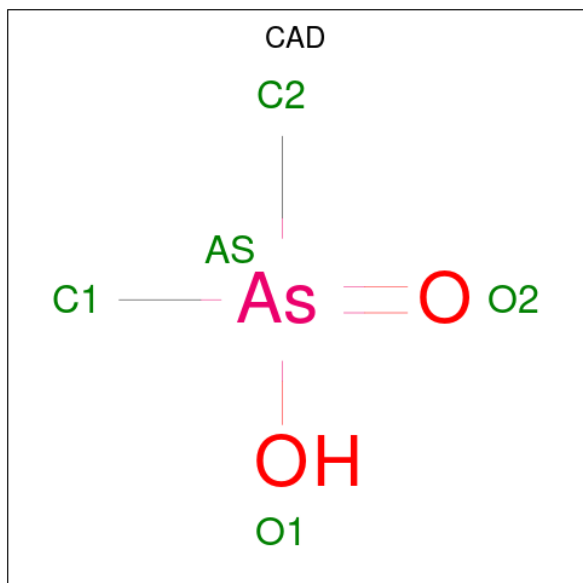
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is S-ISOPROPYL-ISOTHIOUREA (CCD ID: IPU) (formula: $\text{C}_4\text{H}_{10}\text{N}_2\text{S}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			7	4	2	1		
5	A	1	Total	C	N	S	0	0
			7	4	2	1		
5	B	1	Total	C	N	S	0	0
			7	4	2	1		
5	B	1	Total	C	N	S	0	0
			7	4	2	1		

- Molecule 6 is CACODYLIC ACID (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

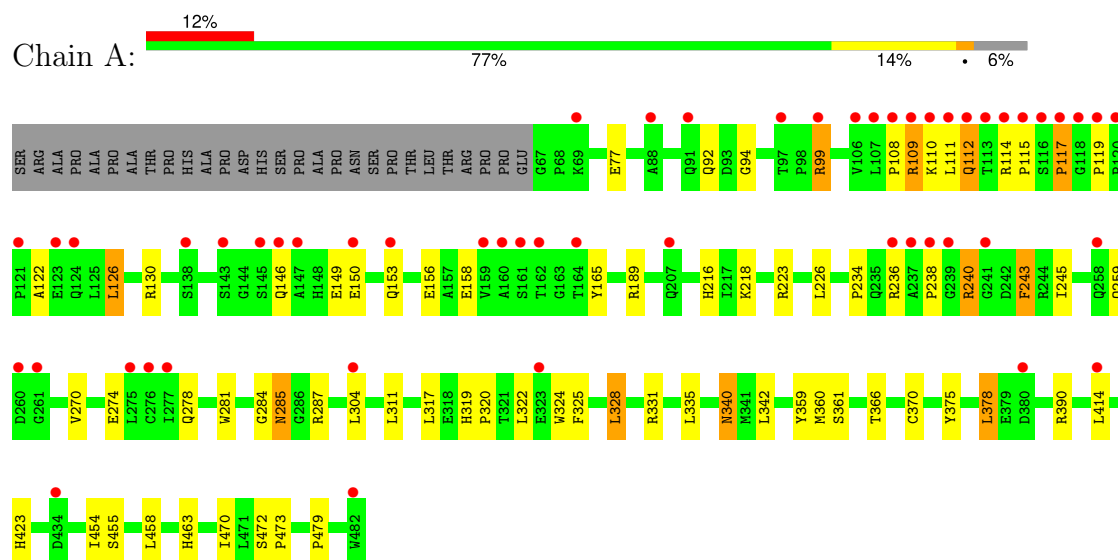
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	329	Total	O	0	0
			329	329		
8	B	320	Total	O	0	0
			320	320		

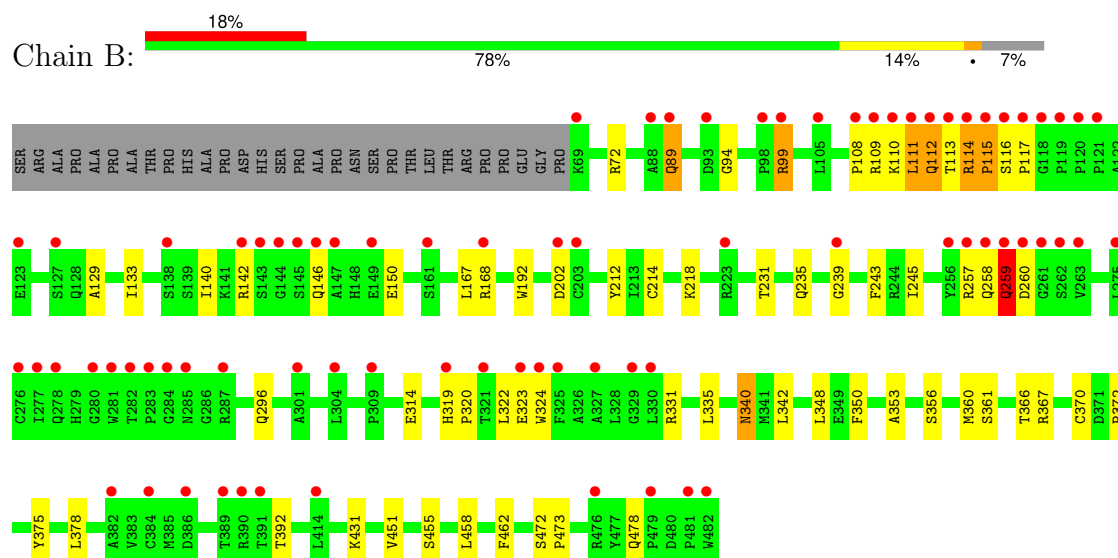
3 Residue-property plots

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



• Molecule 1: NITRIC OXIDE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.03Å 106.79Å 156.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.73 – 1.86 36.73 – 1.86	Depositor EDS
% Data completeness (in resolution range)	94.2 (36.73-1.86) 88.1 (36.73-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.235 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.3	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	7403	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: GOL, IPU, ZN, 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	0.36	0/3397	0.89	9/4631 (0.2%)
1	B	0.36	0/3385	0.91	11/4614 (0.2%)
All	All	0.36	0/6782	0.90	20/9245 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	MET	N-CA-C	-8.86	94.81	109.24
1	B	360	MET	N-CA-C	-8.73	95.02	109.24
1	B	243	PHE	N-CA-C	-8.39	96.94	110.20
1	B	335	LEU	N-CA-C	6.99	121.27	108.69
1	A	335	LEU	N-CA-C	6.49	120.38	108.69
1	A	361	SER	N-CA-C	6.36	119.89	111.75
1	B	245	ILE	N-CA-C	-6.21	98.80	107.80
1	B	361	SER	N-CA-C	6.11	119.57	111.75
1	A	243	PHE	N-CA-C	-6.10	99.33	109.46
1	B	451	VAL	CA-C-N	5.90	123.97	119.66
1	B	451	VAL	C-N-CA	5.90	123.97	119.66
1	B	109	ARG	N-CA-C	-5.63	104.63	112.45
1	A	284	GLY	N-CA-C	-5.61	104.58	112.60
1	A	245	ILE	N-CA-C	-5.58	99.70	107.80
1	A	189	ARG	N-CA-C	5.51	119.48	112.87
1	B	296	GLN	N-CA-C	5.49	117.36	108.41
1	B	192	TRP	N-CA-C	5.44	118.71	111.75
1	A	226	LEU	N-CA-C	5.40	117.85	110.24
1	A	359	TYR	N-CA-C	5.36	118.41	110.48
1	B	367	ARG	N-CA-C	5.13	116.72	111.03

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	3302	0	3215	59	0
1	B	3291	0	3205	60	0
2	A	8	0	6	1	0
2	B	8	0	6	0	0
3	A	1	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	0	0
5	A	14	0	15	1	0
5	B	14	0	15	2	0
6	A	3	0	0	0	0
6	B	3	0	0	1	0
7	A	12	0	12	2	0
7	B	12	0	11	1	0
8	A	329	0	0	2	0
8	B	320	0	0	3	0
All	All	7403	0	6545	118	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 (118) 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	1.35	1.04
1:A:287:ARG:HH21	7:A:1885:GOL:H12	1.21	1.03
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.22	1.02
1:B:112:GLN:HG3	1:B:113:THR:H	1.25	1.01
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.27	0.97
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.40	0.85
1:A:115:PRO:O	1:A:117:PRO:HD3	1.78	0.84
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.61	0.82
1:B:114:ARG:HA	1:B:114:ARG:NH1	1.96	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HG3	1:A:238:PRO:HB3	1.61	0.80
1:B:259:GLN:HG2	1:B:260:ASP:H	1.47	0.78
1:A:375:TYR:HA	7:A:1885:GOL:H11	1.64	0.78
1:A:111:LEU:HD12	1:A:111:LEU:H	1.49	0.76
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.16	0.76
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.68	0.76
1:B:375:TYR:HA	7:B:2885:GOL:H11	1.70	0.73
1:A:119:PRO:HG3	1:A:238:PRO:CB	2.20	0.70
1:A:99:ARG:HB2	1:A:99:ARG:NH1	2.04	0.67
1:A:149:GLU:O	1:A:153:GLN:HG2	1.95	0.66
1:B:89:GLN:HE21	1:B:89:GLN:HA	1.60	0.66
1:A:126:LEU:O	1:A:130:ARG:HG3	1.96	0.66
1:B:146:GLN:O	1:B:150:GLU:HG3	1.97	0.64
1:A:146:GLN:O	1:A:150:GLU:HG3	1.98	0.64
1:B:110:LYS:C	1:B:112:GLN:H	2.08	0.62
1:A:259:GLN:CD	1:A:259:GLN:H	2.09	0.61
2:A:1860:ACT:H2	4:A:1500:HEM:HMB3	1.82	0.61
1:A:94:GLY:O	1:A:110:LYS:HE2	2.02	0.60
1:B:94:GLY:HA2	1:B:111:LEU:HD21	1.82	0.60
1:B:112:GLN:HG3	1:B:113:THR:N	2.06	0.60
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.83	0.59
1:B:324:TRP:HB2	6:B:2950:CAD:C1	2.32	0.59
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.85	0.58
1:A:463:HIS:HA	5:A:2840:IPU:H13	1.86	0.57
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.45	0.57
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.70	0.56
1:B:259:GLN:CG	1:B:260:ASP:H	2.16	0.56
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.45	0.56
1:A:99:ARG:HH11	1:A:99:ARG:CB	2.11	0.56
1:A:259:GLN:CD	1:A:259:GLN:N	2.65	0.55
1:A:111:LEU:O	1:A:112:GLN:C	2.48	0.55
1:B:72:ARG:HH11	1:B:72:ARG:HB3	1.71	0.54
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.43	0.53
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.91	0.53
1:B:378:LEU:HB2	8:B:2987:HOH:O	2.08	0.53
1:A:122:ALA:O	1:A:126:LEU:HB2	2.09	0.53
1:A:378:LEU:HB2	8:A:2883:HOH:O	2.09	0.53
1:B:110:LYS:O	1:B:112:GLN:N	2.40	0.52
1:B:259:GLN:HG2	1:B:260:ASP:N	2.23	0.52
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.92	0.52
1:B:340:ASN:HD22	1:B:340:ASN:H	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:O	1:A:110:LYS:N	2.43	0.52
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.40	0.52
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.51
1:B:99:ARG:HH11	1:B:99:ARG:CB	2.18	0.51
1:A:114:ARG:HA	1:A:479:PRO:HG2	1.91	0.51
1:A:270:VAL:O	1:A:274:GLU:HG3	2.10	0.51
1:A:274:GLU:O	1:A:278:GLN:HG3	2.10	0.51
1:B:89:GLN:HE21	1:B:89:GLN:CA	2.22	0.50
1:B:366:THR:O	1:B:370:CYS:HB2	2.11	0.50
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.92	0.50
1:A:285:ASN:HD22	1:A:285:ASN:C	2.19	0.50
1:A:92:GLN:HE22	1:A:472:SER:HB2	1.78	0.49
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.27	0.49
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.26	0.48
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.39	0.48
1:B:314:GLU:CD	1:B:331:ARG:HH21	2.22	0.48
1:A:111:LEU:HG	1:A:470:ILE:HD13	1.96	0.48
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.49	0.48
1:B:146:GLN:HE21	1:B:150:GLU:CG	2.28	0.47
1:B:231:THR:O	1:B:353:ALA:HA	2.15	0.47
1:A:342:LEU:C	1:A:342:LEU:HD23	2.39	0.47
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.95	0.47
1:B:472:SER:HA	1:B:473:PRO:C	2.40	0.46
1:A:94:GLY:C	1:A:110:LYS:HE2	2.39	0.46
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.98	0.46
1:B:392:THR:HG22	8:B:3267:HOH:O	2.16	0.46
1:A:109:ARG:O	1:A:110:LYS:HD2	2.16	0.46
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.98	0.46
1:B:259:GLN:CG	1:B:260:ASP:N	2.80	0.45
1:B:340:ASN:HD22	1:B:340:ASN:N	2.13	0.45
1:B:462:PHE:CE2	5:B:1840:IPU:H11	2.52	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.51	0.45
1:B:258:GLN:O	1:B:259:GLN:C	2.60	0.45
1:A:236:ARG:CB	1:A:236:ARG:HH11	2.30	0.44
1:A:111:LEU:H	1:A:111:LEU:CD1	2.26	0.44
1:A:325:PHE:O	1:A:328:LEU:HB2	2.17	0.44
1:A:317:LEU:HG	1:A:331:ARG:HA	1.99	0.44
1:B:214:CYS:O	1:B:218:LYS:HG3	2.17	0.44
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.52	0.44
1:B:202:ASP:OD1	1:B:212:TYR:OH	2.34	0.44
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:C	1:A:240:ARG:H	2.26	0.44
1:B:72:ARG:HB3	1:B:72:ARG:NH1	2.32	0.44
1:B:146:GLN:HE21	1:B:150:GLU:CD	2.26	0.44
1:B:168:ARG:HD3	1:B:168:ARG:HA	1.80	0.44
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.52	0.44
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.99	0.44
1:A:115:PRO:C	1:A:117:PRO:HD3	2.42	0.43
1:A:423:HIS:HB2	1:B:392:THR:HB	2.00	0.43
1:A:366:THR:O	1:A:370:CYS:HB2	2.19	0.43
1:A:340:ASN:H	1:A:340:ASN:HD22	1.66	0.43
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.83	0.42
1:A:285:ASN:C	1:A:285:ASN:ND2	2.75	0.42
1:B:323:GLU:HG2	1:B:324:TRP:N	2.35	0.42
1:B:129:ALA:O	1:B:133:ILE:HG12	2.19	0.42
1:B:112:GLN:CG	1:B:113:THR:N	2.75	0.42
1:B:431:LYS:HG3	8:B:3022:HOH:O	2.20	0.42
1:B:116:SER:N	1:B:117:PRO:CD	2.82	0.42
1:B:117:PRO:HA	1:B:239:GLY:H	1.85	0.41
1:A:114:ARG:NH2	8:A:3067:HOH:O	2.53	0.41
1:B:356:SER:HA	5:B:2830:IPU:H11	2.02	0.41
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.66	0.41
1:B:235:GLN:HB3	1:B:350:PHE:CE1	2.56	0.40
1:B:112:GLN:NE2	1:B:478:GLN:HA	2.35	0.40
1:A:158:GLU:HG2	1:A:165:TYR:HA	2.04	0.40
1:A:340:ASN:HD22	1:A:340:ASN:N	2.19	0.40
1:A:216:HIS:C	1:A:216:HIS:CD2	2.99	0.40
1:B:340:ASN:H	1:B:340:ASN:ND2	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/444 (93%)	395 (95%)	16 (4%)	3 (1%)	18	8
1	B	412/444 (93%)	391 (95%)	17 (4%)	4 (1%)	12	4
All	All	826/888 (93%)	786 (95%)	33 (4%)	7 (1%)	16	6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	LEU
1	B	259	GLN
1	A	109	ARG
1	A	112	GLN
1	A	117	PRO
1	B	112	GLN
1	B	115	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%)	346 (98%)	8 (2%)	44	30
1	B	353/377 (94%)	347 (98%)	6 (2%)	53	42
All	All	707/754 (94%)	693 (98%)	14 (2%)	48	36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	126	LEU
1	A	240	ARG
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	414	LEU
1	B	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	99	ARG
1	B	114	ARG
1	B	257	ARG
1	B	259	GLN
1	B	340	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	128	GLN
1	A	191	GLN
1	A	278	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	437	GLN
1	A	468	ASN
1	A	478	GLN
1	B	89	GLN
1	B	112	GLN
1	B	146	GLN
1	B	153	GLN
1	B	191	GLN
1	B	196	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	278	GLN
1	B	279	HIS
1	B	340	ASN
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 [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 [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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
7	GOL	A	1885	-	5,5,5	0.27	0	5,5,5	0.29	0
2	ACT	B	2850	-	3,3,3	0.98	0	3,3,3	0.78	0
5	IPU	A	2840	7	5,6,6	1.57	1 (20%)	4,7,7	0.77	0
7	GOL	B	1880	5	5,5,5	0.27	0	5,5,5	0.28	0
5	IPU	A	1830	-	5,6,6	1.74	1 (20%)	4,7,7	0.52	0
2	ACT	A	1850	-	3,3,3	0.97	0	3,3,3	0.79	0
6	CAD	A	1950	1	0,2,4	-	-	0,1,6	-	-
4	HEM	A	1500	1	50,50,50	1.13	4 (8%)	67,82,82	0.97	1 (1%)
7	GOL	A	2880	5	5,5,5	0.30	0	5,5,5	0.29	0
7	GOL	B	2885	-	5,5,5	0.23	0	5,5,5	0.25	0
6	CAD	B	2950	1	0,2,4	-	-	0,1,6	-	-
4	HEM	B	2500	1	50,50,50	1.11	4 (8%)	67,82,82	1.00	1 (1%)
5	IPU	B	2830	-	5,6,6	1.80	1 (20%)	4,7,7	0.50	0
5	IPU	B	1840	7	5,6,6	2.02	1 (20%)	4,7,7	0.63	0
2	ACT	B	2860	-	3,3,3	0.96	0	3,3,3	0.79	0
2	ACT	A	1860	-	3,3,3	0.92	0	3,3,3	0.79	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
5	IPU	A	2840	7	-	2/2/4/4	-
7	GOL	B	1880	5	-	2/4/4/4	-
5	IPU	A	1830	-	-	0/2/4/4	-
4	HEM	A	1500	1	-	2/14/54/54	-
7	GOL	A	2880	5	-	1/4/4/4	-
7	GOL	B	2885	-	-	0/4/4/4	-
4	HEM	B	2500	1	-	2/14/54/54	-
5	IPU	B	2830	-	-	0/2/4/4	-
7	GOL	A	1885	-	-	0/4/4/4	-
5	IPU	B	1840	7	-	2/2/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1840	IPU	C-N2	4.27	1.43	1.34
5	B	2830	IPU	C-N2	3.55	1.41	1.34
5	A	1830	IPU	C-N2	3.52	1.41	1.34
5	A	2840	IPU	C-N2	3.31	1.41	1.34
4	B	2500	HEM	FE-NA	2.65	2.03	1.95
4	A	1500	HEM	FE-NC	2.53	2.03	1.95
4	A	1500	HEM	CAB-C3B	-2.48	1.40	1.47
4	A	1500	HEM	CAC-C3C	-2.22	1.41	1.47
4	B	2500	HEM	FE-NB	2.17	2.01	1.94
4	B	2500	HEM	FE-NC	2.13	2.02	1.95
4	B	2500	HEM	CAB-C3B	-2.06	1.41	1.47
4	A	1500	HEM	FE-NB	2.06	2.01	1.94

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1500	HEM	C3B-C4B-NB	3.15	111.73	109.47
4	B	2500	HEM	C3B-C4B-NB	2.76	111.45	109.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2840	IPU	C1-C2-S-C
5	B	1840	IPU	C1-C2-S-C
5	B	1840	IPU	C3-C2-S-C
7	B	1880	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	1880	GOL	O1-C1-C2-O2
5	A	2840	IPU	C3-C2-S-C
4	B	2500	HEM	CAA-CBA-CGA-O2A
7	A	2880	GOL	O1-C1-C2-O2
4	B	2500	HEM	CAA-CBA-CGA-O1A
4	A	1500	HEM	CAA-CBA-CGA-O2A
4	A	1500	HEM	CAA-CBA-CGA-O1A

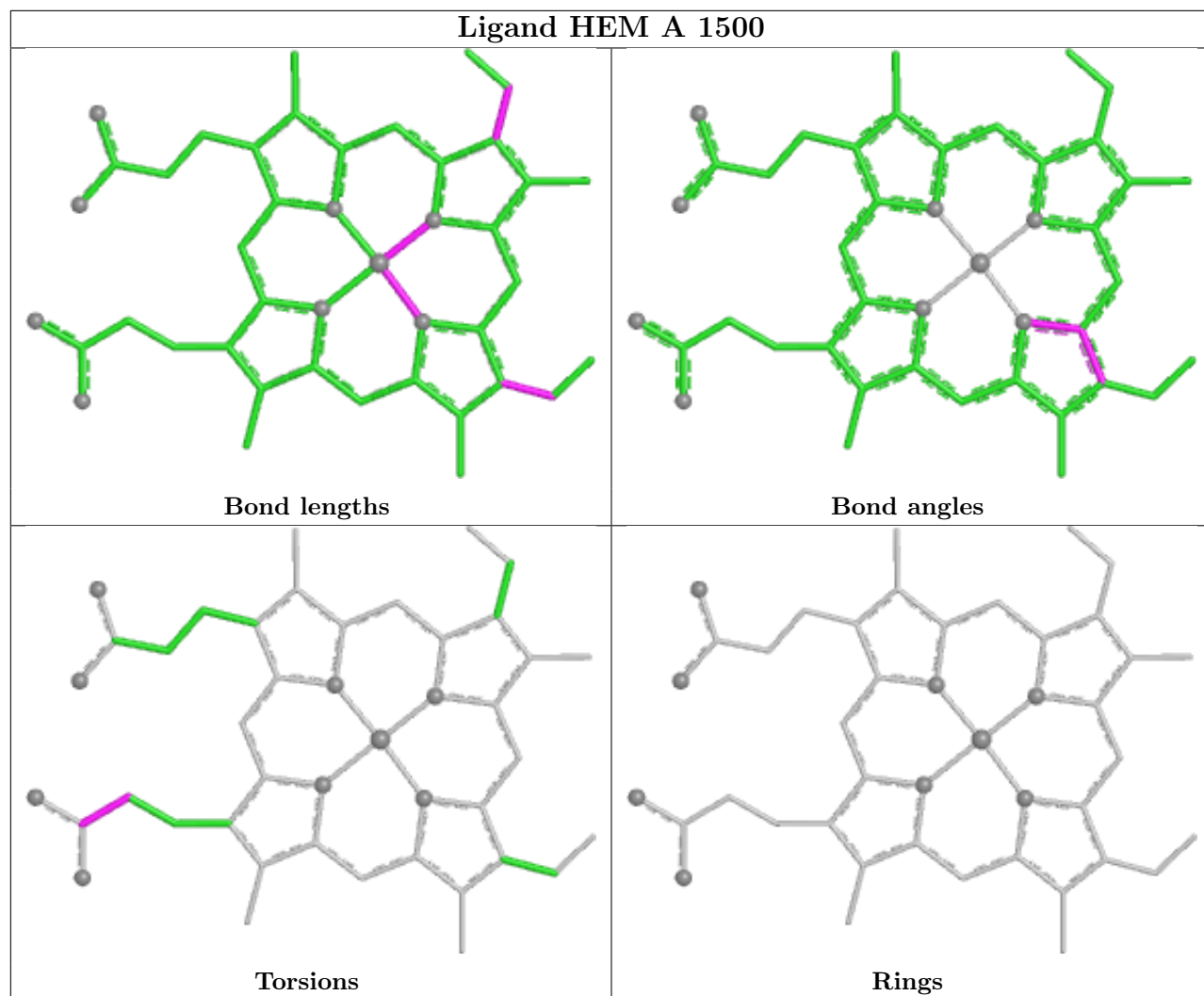
There are no ring outliers.

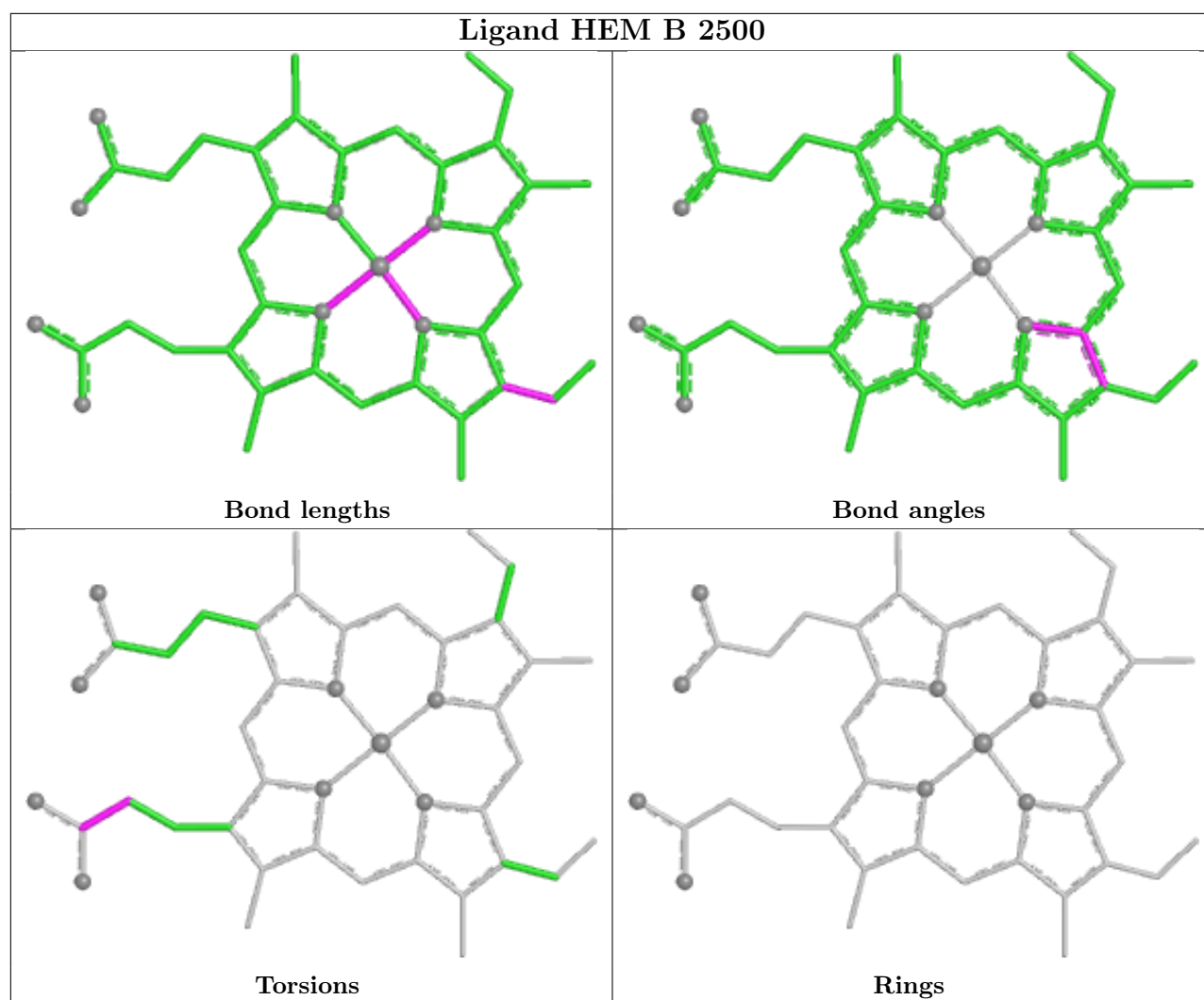
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1885	GOL	2	0
5	A	2840	IPU	1	0
4	A	1500	HEM	1	0
7	B	2885	GOL	1	0
6	B	2950	CAD	1	0
5	B	2830	IPU	1	0
5	B	1840	IPU	1	0
2	A	1860	ACT	1	0

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

Ligand HEM A 1500





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%)	0.94	53 (12%) 8 7	20, 30, 49, 68	0
1	B	414/444 (93%)	1.10	78 (18%) 3 3	21, 32, 51, 67	0
All	All	830/888 (93%)	1.02	131 (15%) 5 4	20, 31, 51, 68	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	PRO	8.1
1	A	119	PRO	7.7
1	B	118	GLY	6.2
1	A	239	GLY	6.2
1	A	113	THR	6.1
1	A	118	GLY	5.9
1	A	238	PRO	5.6
1	A	117	PRO	5.6
1	B	113	THR	5.4
1	B	117	PRO	5.3
1	B	261	GLY	5.1
1	A	115	PRO	4.7
1	A	123	GLU	4.4
1	A	120	PRO	4.3
1	B	144	GLY	4.3
1	A	114	ARG	4.0
1	B	120	PRO	3.9
1	A	109	ARG	3.9
1	B	115	PRO	3.9
1	A	112	GLN	3.8
1	B	116	SER	3.8
1	A	110	LYS	3.7
1	B	111	LEU	3.6
1	A	108	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	3.5
1	B	382	ALA	3.4
1	A	164	THR	3.4
1	A	116	SER	3.4
1	B	145	SER	3.4
1	B	121	PRO	3.2
1	B	259	GLN	3.2
1	B	277	ILE	3.1
1	A	107	LEU	3.1
1	B	127	SER	3.1
1	A	69	LYS	3.1
1	A	121	PRO	3.1
1	B	284	GLY	3.1
1	B	258	GLN	3.1
1	B	278	GLN	3.0
1	B	260	ASP	3.0
1	B	281	TRP	3.0
1	A	147	ALA	3.0
1	B	282	THR	2.9
1	B	168	ARG	2.9
1	A	482	TRP	2.8
1	B	123	GLU	2.8
1	B	391	THR	2.8
1	B	324	TRP	2.8
1	A	106	VAL	2.8
1	A	207	GLN	2.7
1	B	69	LYS	2.7
1	B	329	GLY	2.7
1	A	145	SER	2.7
1	B	112	GLN	2.7
1	B	262	SER	2.7
1	B	110	LYS	2.7
1	B	414	LEU	2.6
1	A	91	GLN	2.6
1	A	241	GLY	2.6
1	B	280	GLY	2.6
1	A	275	LEU	2.6
1	B	114	ARG	2.5
1	A	323	GLU	2.5
1	B	149	GLU	2.5
1	A	160	ALA	2.5
1	B	390	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	304	LEU	2.5
1	A	88	ALA	2.5
1	A	159	VAL	2.5
1	A	99	ARG	2.4
1	A	150	GLU	2.4
1	B	323	GLU	2.4
1	B	321	THR	2.4
1	A	434	ASP	2.4
1	B	108	PRO	2.4
1	A	162	THR	2.4
1	A	236	ARG	2.4
1	B	146	GLN	2.4
1	B	93	ASP	2.4
1	B	88	ALA	2.4
1	A	153	GLN	2.4
1	B	301	ALA	2.3
1	B	143	SER	2.3
1	A	260	ASP	2.3
1	B	203	CYS	2.3
1	A	258	GLN	2.3
1	B	89	GLN	2.3
1	B	105	LEU	2.3
1	B	319	HIS	2.3
1	B	147	ALA	2.3
1	B	98	PRO	2.3
1	B	99	ARG	2.3
1	B	275	LEU	2.3
1	B	285	ASN	2.3
1	B	309	PRO	2.3
1	B	327	ALA	2.3
1	B	476	ARG	2.3
1	A	161	SER	2.3
1	B	138	SER	2.3
1	A	124	GLN	2.3
1	A	414	LEU	2.3
1	B	257	ARG	2.2
1	B	389	THR	2.2
1	B	330	LEU	2.2
1	B	239	GLY	2.2
1	B	276	CYS	2.2
1	A	143	SER	2.2
1	B	161	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	202	ASP	2.2
1	B	481	PRO	2.2
1	B	325	PHE	2.2
1	B	223	ARG	2.2
1	B	386	ASP	2.2
1	B	142	ARG	2.1
1	B	283	PRO	2.1
1	B	256	TYR	2.1
1	B	482	TRP	2.1
1	B	263	VAL	2.1
1	A	276	CYS	2.1
1	A	237	ALA	2.1
1	A	277	ILE	2.1
1	A	380	ASP	2.1
1	A	138	SER	2.1
1	A	261	GLY	2.1
1	B	384	CYS	2.1
1	B	109	ARG	2.1
1	B	287	ARG	2.1
1	A	97	THR	2.0
1	A	146	GLN	2.0
1	B	304	LEU	2.0
1	B	479	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Continued on next page...

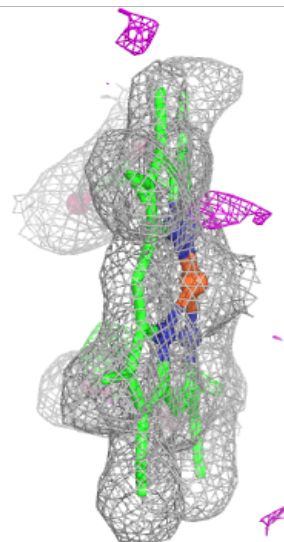
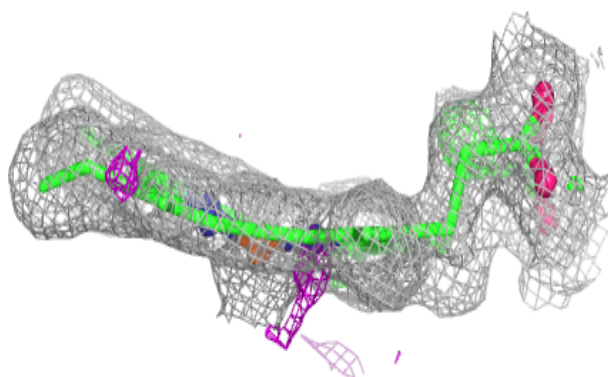
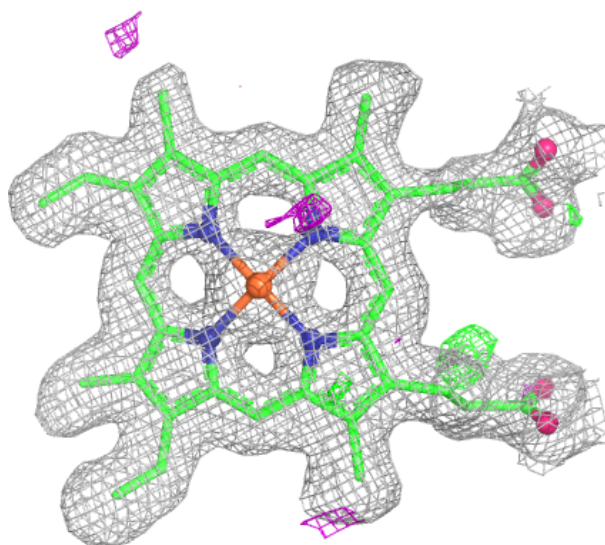
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	B	2885	6/6	0.76	0.20	58,59,59,59	0
7	GOL	A	1885	6/6	0.78	0.22	58,58,58,58	0
7	GOL	A	2880	6/6	0.79	0.20	53,53,53,53	6
7	GOL	B	1880	6/6	0.82	0.18	47,47,47,48	6
5	IPU	B	1840	7/7	0.84	0.14	35,35,35,36	7
5	IPU	A	2840	7/7	0.86	0.16	35,35,36,36	7
6	CAD	A	1950	3/5	0.88	0.23	42,42,43,49	0
2	ACT	B	2860	4/4	0.92	0.11	33,34,34,35	0
2	ACT	B	2850	4/4	0.93	0.07	30,30,30,30	0
2	ACT	A	1860	4/4	0.94	0.07	35,37,37,38	0
2	ACT	A	1850	4/4	0.96	0.09	28,29,29,29	0
6	CAD	B	2950	3/5	0.97	0.10	42,42,43,44	0
4	HEM	A	1500	43/43	0.97	0.08	21,23,28,31	0
4	HEM	B	2500	43/43	0.97	0.08	21,23,31,33	0
5	IPU	B	2830	7/7	0.97	0.10	23,23,24,24	0
5	IPU	A	1830	7/7	0.97	0.07	22,22,23,24	0
3	ZN	A	900	1/1	1.00	0.03	29,29,29,29	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.

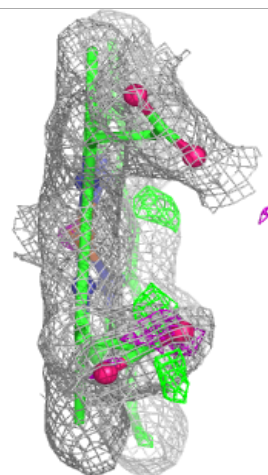
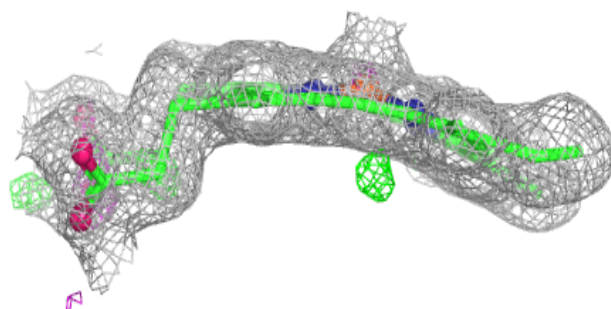
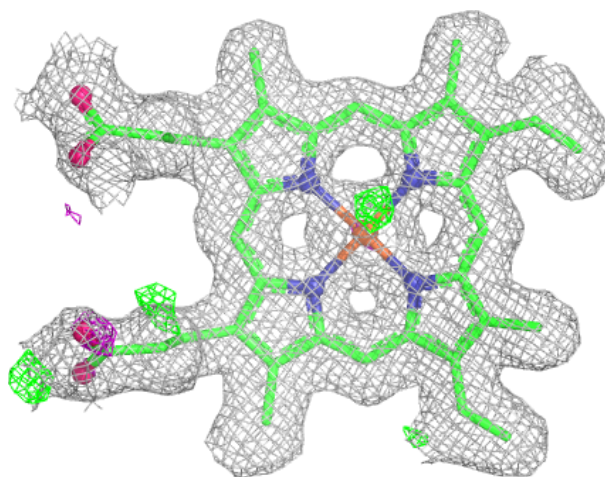
Electron density around HEM A 1500:

$2mF_o-DF_c$ (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.