



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:33 PM EDT

PDB ID : 1D0C / pdb_00001d0c
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH 3-BROMO-7-NITROINDAZOLE (H4B FREE)
Authors : Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos,
T.L.
Deposited on : 1999-09-09
Resolution : 1.65 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

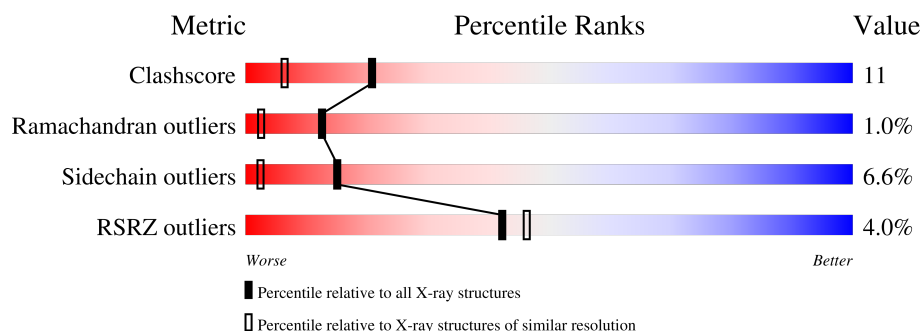
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	3% 73% 16% • 6%
1	B	444	4% 73% 16% • • 7%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7428 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.

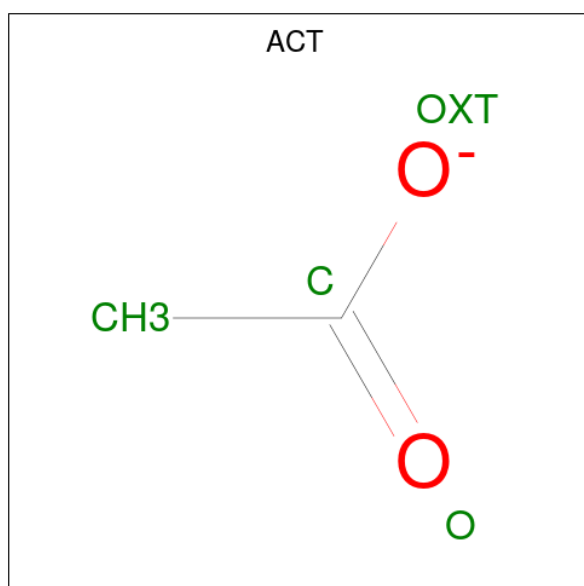
- Molecule 1 is a protein called BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	1	0
			3303	2099	584	604	16			
1	B	414	Total	C	N	O	S	0	1	0
			3292	2092	582	602	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...

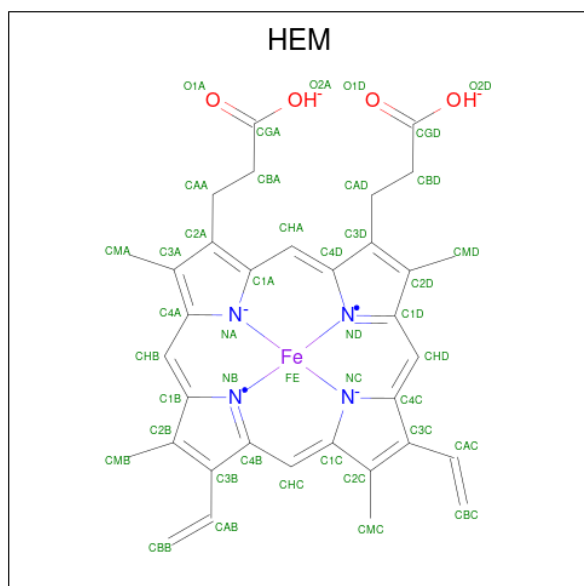
Continued from previous page...

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).

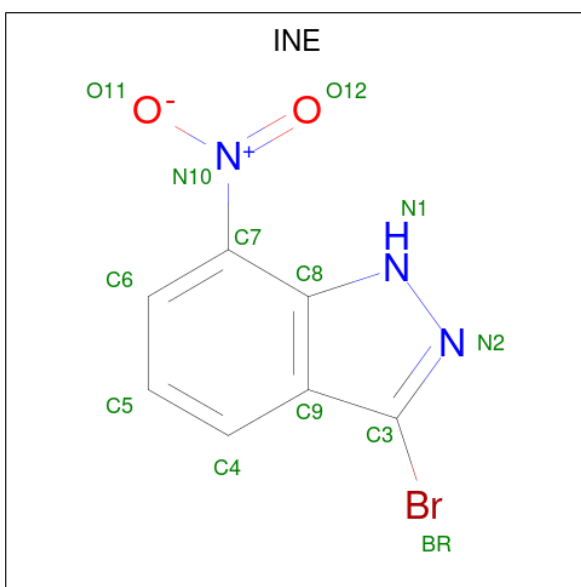
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



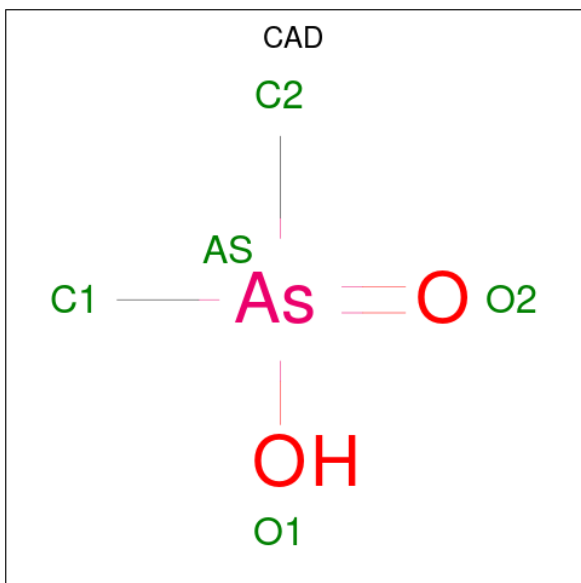
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 48	C 37	Fe 1	N 4	O 6	0	1

- Molecule 5 is 3-BROMO-7-NITROINDAZOLE (CCD ID: INE) (formula: $C_7H_4BrN_3O_2$).



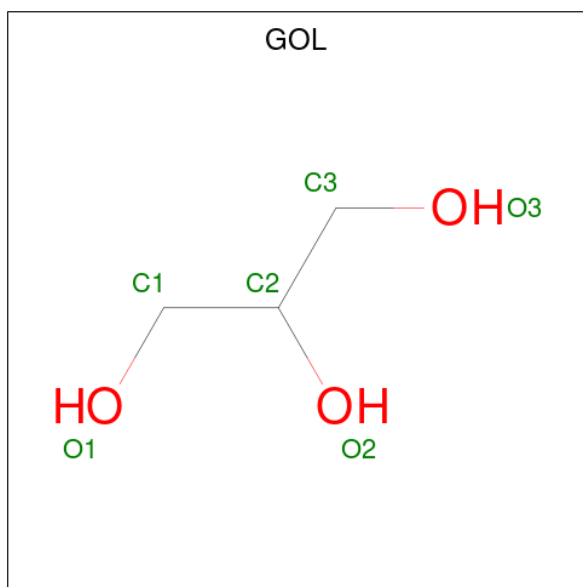
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	A	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	B	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	B	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		

- 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	B	1	Total	C	O	0	0
			6	3	3		

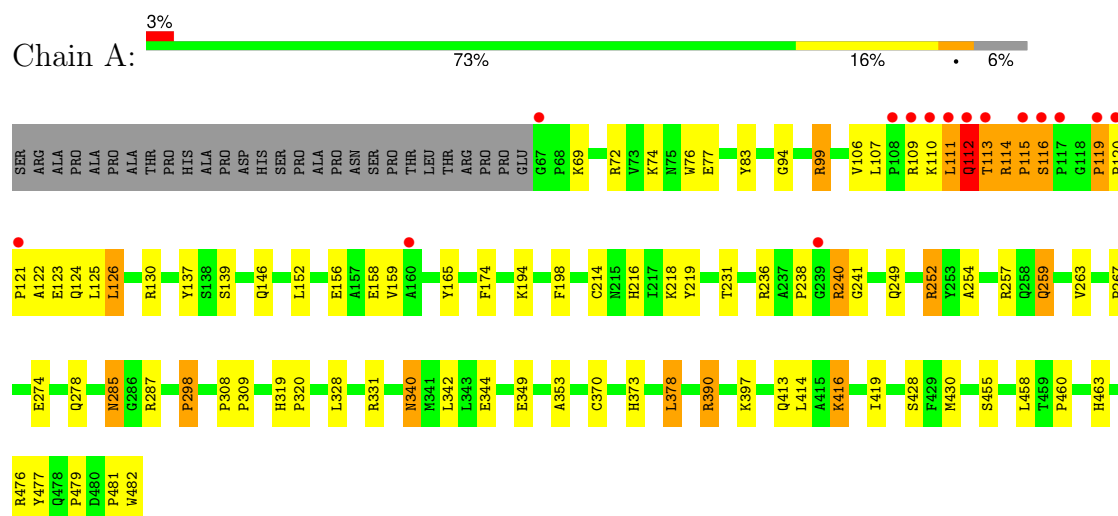
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	348	Total	O	0	0
			348	348		
8	B	307	Total	O	0	0
			307	307		

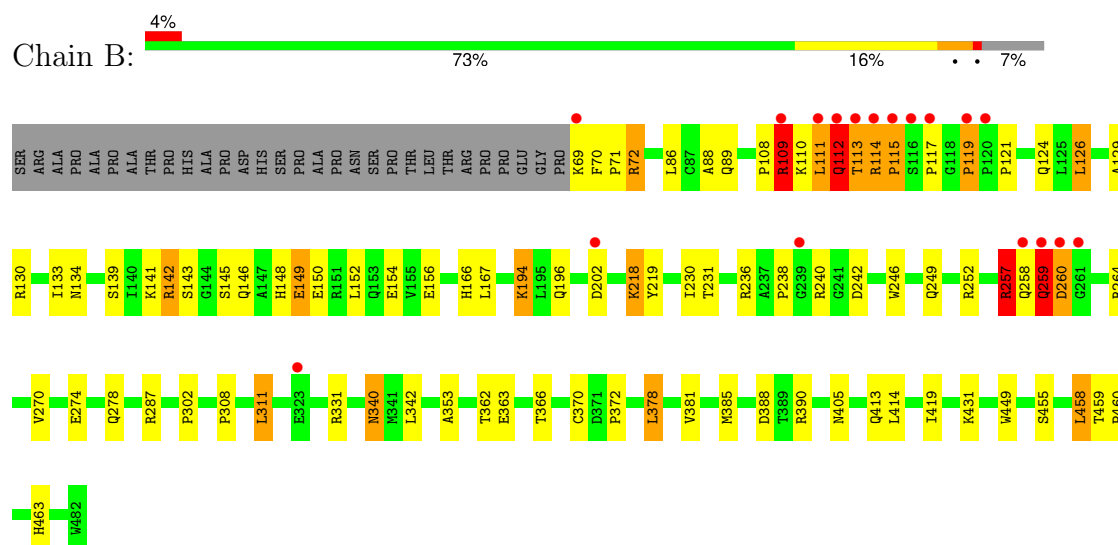
3 Residue-property plots

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: 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	57.44Å 105.98Å 155.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.65 8.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-1.65) 91.7 (8.00-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.65Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.213 , 0.259 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.56 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: CAD, ACT, ZN, INE, HEM, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	2/3403 (0.1%)	1.35	14/4639 (0.3%)
1	B	0.53	0/3391	1.32	11/4622 (0.2%)
All	All	0.55	2/6794 (0.0%)	1.34	25/9261 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428[A]	SER	CB-OG	-6.82	1.28	1.42
1	A	428[B]	SER	CB-OG	-6.82	1.28	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	HIS	CA-CB-CG	-7.34	106.46	113.80
1	A	174	PHE	CA-C-N	6.73	127.60	119.99
1	A	174	PHE	C-N-CA	6.73	127.60	119.99
1	A	298	PRO	CA-C-N	6.11	131.06	122.08
1	A	298	PRO	C-N-CA	6.11	131.06	122.08
1	A	252	ARG	NH1-CZ-NH2	6.02	127.12	119.30
1	B	119	PRO	O-C-N	5.91	124.03	121.31
1	B	240	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	A	254	ALA	O-C-N	5.88	129.79	122.86
1	B	463	HIS	CA-CB-CG	-5.67	108.13	113.80
1	A	137	TYR	CA-CB-CG	-5.50	104.00	113.90
1	B	230	ILE	O-C-N	5.41	129.06	123.05
1	A	216	HIS	CA-CB-CG	5.36	119.16	113.80
1	A	463	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	198	PHE	CA-C-O	5.31	126.38	120.43
1	A	219	TYR	O-C-N	5.25	127.47	122.07
1	A	116	SER	O-C-N	5.25	125.92	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	GLN	CA-C-N	5.17	127.17	120.44
1	B	413	GLN	C-N-CA	5.17	127.17	120.44
1	B	167	LEU	O-C-N	5.17	128.85	123.06
1	B	117	PRO	CA-C-N	5.17	129.99	121.87
1	B	117	PRO	C-N-CA	5.17	129.99	121.87
1	A	139	SER	CA-C-N	-5.16	114.95	122.28
1	A	139	SER	C-N-CA	-5.16	114.95	122.28
1	B	363	GLU	CA-C-O	5.13	125.86	120.42

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	3303	0	3216	73	0
1	B	3292	0	3206	75	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	48	0	8	3	0
5	A	26	0	8	0	0
5	B	26	0	8	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	348	0	0	12	0
8	B	307	0	0	7	0
All	All	7428	0	6504	146	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 11.

All (146) 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:111:LEU:HD23	1:A:476:ARG:HG2	1.35	1.08
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.22	1.04
1:B:115:PRO:HA	1:B:236:ARG:HH12	1.26	0.99
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.46	0.95
1:A:109:ARG:O	1:A:110:LYS:HD2	1.71	0.90
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.45	0.81
1:B:121:PRO:HD2	1:B:124:GLN:OE1	1.81	0.81
1:A:111:LEU:CD2	1:A:476:ARG:HG2	2.12	0.80
1:B:152:LEU:O	1:B:156:GLU:HG3	1.83	0.78
1:B:258:GLN:OE1	1:B:264:ARG:HB2	1.83	0.78
1:A:119:PRO:HG3	1:A:238:PRO:HG3	1.66	0.77
1:A:152:LEU:O	1:A:156:GLU:HG3	1.85	0.77
1:A:106:VAL:HG12	1:A:107:LEU:HD23	1.69	0.73
1:B:126:LEU:O	1:B:130:ARG:HG3	1.93	0.69
1:B:86:LEU:O	1:B:89:GLN:HG2	1.94	0.68
1:A:274:GLU:O	1:A:278:GLN:HG3	1.93	0.68
1:B:119:PRO:HG3	1:B:238:PRO:HG3	1.76	0.67
1:B:257:ARG:HH11	1:B:270:VAL:HG11	1.62	0.64
1:B:150:GLU:O	1:B:154:GLU:HG3	1.98	0.63
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.81	0.62
1:B:113:THR:HG21	1:B:342:LEU:HD22	1.82	0.62
1:B:126:LEU:HD22	1:B:130:ARG:HG3	1.81	0.62
1:B:115:PRO:HA	1:B:236:ARG:NH1	2.07	0.61
1:B:257:ARG:HD3	1:B:270:VAL:HG11	1.84	0.60
1:A:397:LYS:HE3	8:A:1245:HOH:O	2.01	0.59
1:A:413:GLN:O	1:A:416:LYS:HE3	2.01	0.59
1:A:74:LYS:HE2	1:A:76:TRP:CE3	2.37	0.59
1:A:94:GLY:HA3	8:A:1281:HOH:O	2.03	0.59
1:A:113:THR:O	1:A:115:PRO:HD3	2.03	0.59
1:B:126:LEU:HD21	1:B:156:GLU:HG2	1.85	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.43	0.58
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.86	0.57
1:A:126:LEU:O	1:A:130:ARG:HG3	2.04	0.57
1:A:340:ASN:H	1:A:340:ASN:HD22	1.51	0.57
1:A:120:PRO:HB2	1:A:125:LEU:HB2	1.87	0.57
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.85	0.57
1:A:481:PRO:HD2	1:A:482:TRP:CZ3	2.40	0.56
1:A:378:LEU:HB2	8:A:1013:HOH:O	2.06	0.56
1:B:249:GLN:HB2	1:B:252:ARG:HG3	1.87	0.56
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.88	0.56
1:B:114:ARG:HA	1:B:114:ARG:NH1	2.06	0.56
1:B:119:PRO:HG3	1:B:238:PRO:CG	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG12	1:A:107:LEU:CD2	2.35	0.55
1:A:109:ARG:C	1:A:110:LYS:HD2	2.32	0.54
1:B:381:VAL:O	1:B:385:MET:HG3	2.07	0.54
1:B:236:ARG:HD2	1:B:242:ASP:OD2	2.07	0.54
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.38	0.54
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.90	0.54
1:A:285:ASN:HB2	8:A:1190:HOH:O	2.07	0.53
1:A:69:LYS:O	1:A:69:LYS:HG2	2.06	0.53
1:A:99:ARG:HH21	1:B:88:ALA:HA	1.73	0.53
1:A:130:ARG:HD3	8:A:1148:HOH:O	2.08	0.53
1:A:99:ARG:HH11	1:A:99:ARG:CB	2.20	0.53
1:B:111:LEU:O	1:B:112:GLN:O	2.27	0.53
1:B:449:TRP:CZ3	4:B:500[B]:HEM:O1A	2.63	0.52
1:B:449:TRP:CE3	4:B:500[B]:HEM:O1A	2.63	0.52
1:A:390:ARG:N	1:A:390:ARG:HD3	2.24	0.51
1:B:274:GLU:HA	1:B:274:GLU:OE1	2.10	0.51
1:B:114:ARG:O	1:B:115:PRO:O	2.29	0.51
1:B:246:TRP:CZ2	1:B:302:PRO:HG3	2.46	0.51
1:B:388:ASP:OD2	1:B:390:ARG:NH2	2.44	0.51
1:A:72:ARG:HD2	1:A:83:TYR:CE2	2.46	0.51
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.41	0.50
1:A:390:ARG:HD3	1:A:390:ARG:H	1.76	0.50
1:A:112:GLN:NE2	1:A:477:TYR:HB2	2.25	0.50
1:B:149:GLU:O	1:B:149:GLU:OE1	2.30	0.50
1:B:414:LEU:HD23	8:B:1012:HOH:O	2.10	0.50
1:B:287:ARG:HD3	8:B:1060:HOH:O	2.12	0.49
1:A:236:ARG:NH1	1:A:349:GLU:OE2	2.44	0.49
1:B:126:LEU:HD22	1:B:130:ARG:CG	2.42	0.49
1:A:74:LYS:HE2	1:A:76:TRP:CD2	2.48	0.48
1:A:119:PRO:HG3	1:A:238:PRO:CG	2.39	0.48
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.94	0.48
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.54	0.48
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.78	0.48
1:A:106:VAL:C	1:A:107:LEU:HD23	2.39	0.47
1:A:214:CYS:O	1:A:218:LYS:HG3	2.14	0.47
1:B:142:ARG:O	1:B:145:SER:OG	2.30	0.47
1:B:308:PRO:O	1:B:311:LEU:HB2	2.13	0.47
1:A:285:ASN:N	1:A:285:ASN:HD22	2.10	0.47
1:A:373:HIS:H	1:A:373:HIS:HD1	1.62	0.47
1:B:202:ASP:HB3	8:B:1075:HOH:O	2.15	0.47
1:B:146:GLN:NE2	1:B:150:GLU:OE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:HG2	1:B:311:LEU:HD22	1.96	0.47
1:B:388:ASP:OD1	1:B:390:ARG:HG3	2.15	0.47
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.97	0.46
1:A:458:LEU:HD22	1:B:378:LEU:HD21	1.96	0.46
1:B:129:ALA:O	1:B:133:ILE:HG12	2.15	0.46
1:B:108:PRO:CG	1:B:111:LEU:HB2	2.45	0.46
1:B:459:THR:HB	1:B:460:PRO:HD2	1.96	0.46
1:B:258:GLN:O	1:B:260:ASP:N	2.49	0.46
1:A:331:ARG:HD2	8:A:1242:HOH:O	2.15	0.46
1:A:430:MET:HG3	1:A:460:PRO:HB2	1.97	0.46
1:B:257:ARG:NH1	1:B:270:VAL:HG11	2.30	0.46
1:B:340:ASN:HD22	1:B:340:ASN:H	1.64	0.46
1:B:231:THR:O	1:B:353:ALA:HA	2.15	0.46
1:A:259:GLN:O	1:A:259:GLN:NE2	2.50	0.45
1:B:109:ARG:NH2	8:B:1068:HOH:O	2.48	0.45
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.99	0.45
1:A:122:ALA:O	1:A:126:LEU:HB2	2.16	0.45
1:A:107:LEU:HD22	1:A:477:TYR:CE2	2.51	0.45
1:B:112:GLN:CG	1:B:113:THR:H	2.29	0.45
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.98	0.45
1:A:240:ARG:NH2	8:A:1228:HOH:O	2.49	0.45
1:B:259:GLN:HG3	1:B:260:ASP:OD1	2.16	0.45
1:B:431:LYS:NZ	8:B:1108:HOH:O	2.49	0.45
1:A:240:ARG:HD3	1:A:241:GLY:O	2.17	0.45
1:B:126:LEU:HD11	1:B:156:GLU:CG	2.46	0.45
1:A:72:ARG:NH1	8:A:1215:HOH:O	2.49	0.45
1:A:231:THR:O	1:A:353:ALA:HA	2.17	0.45
1:B:72:ARG:NH1	8:B:1125:HOH:O	2.50	0.45
1:A:344:GLU:HG3	8:A:1075:HOH:O	2.17	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.52	0.45
5:B:765:INE:N1	5:B:765:INE:O12	2.50	0.45
1:A:111:LEU:HD21	8:A:994:HOH:O	2.17	0.44
1:A:477:TYR:HD2	8:A:1211:HOH:O	2.00	0.44
1:B:264:ARG:NH1	1:B:287:ARG:HG3	2.32	0.44
1:A:126:LEU:HA	1:A:126:LEU:HD22	1.64	0.44
1:A:112:GLN:NE2	8:A:1211:HOH:O	2.50	0.44
1:B:257:ARG:HD3	1:B:270:VAL:CG1	2.46	0.44
1:A:340:ASN:HD22	1:A:340:ASN:N	2.17	0.43
1:B:70:PHE:HA	1:B:71:PRO:HD3	1.71	0.43
1:A:112:GLN:HE21	1:A:112:GLN:HB2	1.57	0.43
1:A:126:LEU:CD2	1:A:159:VAL:HG21	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TRP:CZ3	4:B:500[A]:HEM:O1A	2.72	0.43
1:A:158:GLU:CD	1:A:165:TYR:HA	2.44	0.42
1:A:121:PRO:HB2	1:A:124:GLN:HB2	2.00	0.42
1:A:113:THR:O	1:A:479:PRO:HD3	2.19	0.42
1:B:196:GLN:HG2	1:B:219:TYR:CE1	2.55	0.42
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.48	0.42
1:A:263:VAL:HG11	1:A:267:PRO:HA	2.01	0.42
1:B:108:PRO:HB3	1:B:111:LEU:HD22	2.00	0.41
1:B:194:LYS:HD3	8:B:1190:HOH:O	2.20	0.41
1:A:114:ARG:HH21	1:A:479:PRO:HB3	1.85	0.41
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.90	0.41
1:A:194:LYS:HG2	1:A:194:LYS:O	2.20	0.41
1:B:218:LYS:HE3	1:B:218:LYS:HB3	1.79	0.41
1:B:246:TRP:CH2	1:B:302:PRO:HG3	2.56	0.41
1:B:258:GLN:CD	1:B:264:ARG:HB2	2.45	0.41
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.91	0.41
1:B:455:SER:O	1:B:458:LEU:HB2	2.21	0.41
1:B:86:LEU:HD12	1:B:89:GLN:HG3	2.03	0.41
1:B:264:ARG:NH1	1:B:264:ARG:HG3	2.36	0.41
1:B:366:THR:O	1:B:370:CYS:HB2	2.21	0.41
1:A:77:GLU:HG3	1:B:372:PRO:HG2	2.03	0.40
1:B:362:THR:HA	1:B:405:ASN:HD21	1.86	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	415/444 (94%)	402 (97%)	10 (2%)	3 (1%)	18	6
1	B	413/444 (93%)	396 (96%)	12 (3%)	5 (1%)	10	2
All	All	828/888 (93%)	798 (96%)	22 (3%)	8 (1%)	12	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	B	115	PRO
1	B	259	GLN
1	A	119	PRO
1	B	257	ARG
1	B	109	ARG
1	A	112	GLN
1	A	115	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	355/377 (94%)	334 (94%)	21 (6%)	18	3
1	B	354/377 (94%)	328 (93%)	26 (7%)	13	2
All	All	709/754 (94%)	662 (93%)	47 (7%)	15	2

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	111	LEU
1	A	112	GLN
1	A	113	THR
1	A	114	ARG
1	A	116	SER
1	A	123	GLU
1	A	126	LEU
1	A	146	GLN
1	A	240	ARG
1	A	257	ARG
1	A	259	GLN
1	A	285	ASN
1	A	287	ARG
1	A	328	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	414	LEU
1	A	416	LYS
1	A	419	ILE
1	B	69	LYS
1	B	72	ARG
1	B	109	ARG
1	B	110	LYS
1	B	111	LEU
1	B	112	GLN
1	B	113	THR
1	B	114	ARG
1	B	126	LEU
1	B	139	SER
1	B	141	LYS
1	B	142	ARG
1	B	143	SER
1	B	149	GLU
1	B	194	LYS
1	B	218	LYS
1	B	257	ARG
1	B	259	GLN
1	B	260	ASP
1	B	278	GLN
1	B	311	LEU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	419	ILE
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	191	GLN
1	A	259	GLN
1	A	278	GLN
1	A	285	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	128	GLN
1	B	146	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
1	B	478	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	HEM	B	500[A]	-	50,50,50	1.70	7 (14%)	67,82,82	1.46	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	500	1	50,50,50	1.08	2 (4%)	67,82,82	1.50	14 (20%)
6	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-
4	HEM	B	500[B]	-	50,50,50	1.72	8 (16%)	67,82,82	1.42	12 (17%)
2	ACT	A	860	-	3,3,3	0.90	0	3,3,3	1.06	0
2	ACT	A	850	-	3,3,3	0.95	0	3,3,3	0.61	0
2	ACT	B	861	-	3,3,3	0.97	0	3,3,3	0.95	0
5	INE	A	766	-	14,14,14	3.79	7 (50%)	11,20,20	2.98	3 (27%)
7	GOL	A	880	-	5,5,5	0.31	0	5,5,5	0.34	0
2	ACT	B	851	-	3,3,3	0.96	0	3,3,3	0.76	0
7	GOL	B	881	-	5,5,5	0.75	0	5,5,5	0.99	0
6	CAD	B	951	1	0,2,4	-	-	0,1,6	-	-
5	INE	B	765	-	14,14,14	3.80	7 (50%)	11,20,20	3.29	3 (27%)
5	INE	B	761	-	14,14,14	3.54	7 (50%)	11,20,20	2.86	4 (36%)
5	INE	A	760	-	14,14,14	3.85	7 (50%)	11,20,20	3.36	4 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	500[A]	-	-	0/14/54/54	-
4	HEM	A	500	1	-	1/14/54/54	-
4	HEM	B	500[B]	-	-	0/14/54/54	-
5	INE	A	766	-	-	0/2/4/4	0/2/2/2
7	GOL	A	880	-	-	1/4/4/4	-
7	GOL	B	881	-	-	4/4/4/4	-
5	INE	B	765	-	-	0/2/4/4	0/2/2/2
5	INE	B	761	-	-	0/2/4/4	0/2/2/2
5	INE	A	760	-	-	0/2/4/4	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	INE	BR-C3	-7.95	1.76	1.87
5	A	766	INE	BR-C3	-7.54	1.77	1.87
5	A	760	INE	C7-N10	-7.25	1.32	1.45
5	B	765	INE	BR-C3	-7.20	1.77	1.87
4	B	500[B]	HEM	CAA-C2A	7.03	1.69	1.51
4	B	500[A]	HEM	CAA-C2A	6.97	1.69	1.51
5	B	761	INE	C7-N10	-6.81	1.33	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	765	INE	C7-N10	-6.44	1.34	1.45
5	A	766	INE	C7-N10	-6.31	1.34	1.45
5	B	765	INE	C3-N2	6.22	1.45	1.32
5	A	766	INE	C3-N2	6.12	1.45	1.32
5	B	761	INE	BR-C3	-6.10	1.79	1.87
5	B	761	INE	C8-N1	-6.00	1.31	1.36
5	B	765	INE	C8-N1	-5.97	1.31	1.36
5	A	766	INE	C8-N1	-5.62	1.31	1.36
5	A	760	INE	C8-N1	-5.58	1.31	1.36
5	A	760	INE	C3-N2	5.07	1.43	1.32
5	B	761	INE	C3-N2	4.91	1.42	1.32
4	B	500[A]	HEM	CAD-C3D	4.55	1.63	1.51
4	B	500[B]	HEM	CAD-C3D	4.55	1.63	1.51
5	A	766	INE	C9-C3	-4.13	1.38	1.45
5	B	765	INE	C9-C3	-3.71	1.39	1.45
5	A	760	INE	C9-C3	-3.63	1.39	1.45
5	B	761	INE	C9-C3	-3.56	1.39	1.45
5	A	760	INE	C9-C8	-3.48	1.37	1.41
5	B	765	INE	C9-C8	-3.32	1.37	1.41
4	B	500[A]	HEM	CMA-C3A	3.27	1.57	1.50
4	B	500[B]	HEM	CMA-C3A	3.27	1.57	1.50
5	A	766	INE	C9-C8	-3.23	1.37	1.41
5	B	761	INE	C9-C8	-3.17	1.37	1.41
4	B	500[A]	HEM	CMC-C2C	3.03	1.57	1.50
4	B	500[B]	HEM	CMC-C2C	3.03	1.57	1.50
4	A	500	HEM	CAC-C3C	-2.80	1.39	1.47
4	B	500[A]	HEM	CAB-C3B	-2.77	1.40	1.47
4	B	500[B]	HEM	CAB-C3B	-2.77	1.40	1.47
4	B	500[A]	HEM	CMD-C2D	2.55	1.56	1.50
4	B	500[B]	HEM	CMD-C2D	2.55	1.56	1.50
5	B	761	INE	O11-N10	-2.49	1.18	1.35
4	A	500	HEM	CAB-C3B	-2.47	1.40	1.47
4	B	500[A]	HEM	CAC-C3C	-2.46	1.40	1.47
4	B	500[B]	HEM	CAC-C3C	-2.46	1.40	1.47
5	B	765	INE	O11-N10	-2.43	1.19	1.35
4	B	500[B]	HEM	CBA-CAA	2.31	1.60	1.51
5	A	766	INE	O11-N10	-2.31	1.19	1.35
5	A	760	INE	O11-N10	-2.01	1.21	1.35

All (51) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	765	INE	C6-C7-N10	6.66	123.59	116.47
5	A	760	INE	C6-C7-N10	6.15	123.04	116.47
5	B	765	INE	C9-C8-N1	6.13	109.92	106.95
5	A	766	INE	C9-C8-N1	5.85	109.79	106.95
5	A	760	INE	C9-C8-N1	5.78	109.75	106.95
5	B	765	INE	BR-C3-N2	5.63	127.84	119.74
5	B	761	INE	BR-C3-N2	5.58	127.77	119.74
5	A	766	INE	BR-C3-N2	5.32	127.41	119.74
5	A	766	INE	C6-C7-N10	5.32	122.16	116.47
5	B	761	INE	C6-C7-N10	5.16	121.98	116.47
5	A	760	INE	O12-N10-C7	4.99	127.56	119.03
5	B	761	INE	C9-C8-N1	4.72	109.24	106.95
4	B	500[A]	HEM	CBA-CAA-C2A	-4.54	99.99	112.53
5	A	760	INE	BR-C3-N2	4.43	126.12	119.74
4	A	500	HEM	C3B-C4B-NB	3.97	112.32	109.47
4	A	500	HEM	C1B-NB-C4B	-3.30	101.30	105.21
4	B	500[A]	HEM	CMB-C2B-C1B	3.04	129.79	125.03
4	B	500[B]	HEM	CMB-C2B-C1B	3.04	129.79	125.03
4	B	500[A]	HEM	CAD-C3D-C4D	3.02	129.96	124.70
4	B	500[B]	HEM	CAD-C3D-C4D	3.02	129.96	124.70
4	A	500	HEM	C4D-ND-C1D	-2.89	101.78	105.21
4	A	500	HEM	C2D-C1D-ND	2.85	113.20	109.90
4	B	500[A]	HEM	C3B-C4B-NB	2.81	111.49	109.47
4	B	500[B]	HEM	C3B-C4B-NB	2.81	111.49	109.47
4	B	500[A]	HEM	CMD-C2D-C1D	2.80	129.41	125.03
4	B	500[B]	HEM	CMD-C2D-C1D	2.80	129.41	125.03
4	B	500[A]	HEM	C4D-ND-C1D	-2.77	101.93	105.21
4	B	500[B]	HEM	C4D-ND-C1D	-2.77	101.93	105.21
4	A	500	HEM	CAD-C3D-C4D	2.66	129.33	124.70
4	B	500[A]	HEM	C3D-C4D-ND	2.59	113.01	110.17
4	B	500[B]	HEM	C3D-C4D-ND	2.59	113.01	110.17
4	B	500[B]	HEM	CBA-CAA-C2A	-2.59	105.37	112.53
5	B	761	INE	O12-N10-C7	2.54	123.38	119.03
4	A	500	HEM	C2B-C1B-NB	2.44	112.64	109.84
4	A	500	HEM	CMB-C2B-C1B	2.40	128.78	125.03
4	B	500[A]	HEM	C1B-NB-C4B	-2.35	102.42	105.21
4	B	500[B]	HEM	C1B-NB-C4B	-2.35	102.42	105.21
4	B	500[A]	HEM	CHD-C4C-NC	2.35	127.01	124.45
4	B	500[B]	HEM	CHD-C4C-NC	2.35	127.01	124.45
4	B	500[A]	HEM	C2D-C1D-ND	2.31	112.58	109.90
4	B	500[B]	HEM	C2D-C1D-ND	2.31	112.58	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	HEM	CMD-C2D-C1D	2.28	128.59	125.03
4	A	500	HEM	CMA-C3A-C2A	2.27	130.44	125.62
4	A	500	HEM	CHB-C4A-C3A	-2.24	120.93	127.43
4	B	500[B]	HEM	O2A-CGA-CBA	2.23	121.04	114.00
4	A	500	HEM	C4C-CHD-C1D	-2.19	121.36	126.02
4	A	500	HEM	CHD-C1D-ND	-2.10	122.17	124.42
4	A	500	HEM	CHA-C4D-C3D	-2.08	121.38	125.23
4	A	500	HEM	C3D-C4D-ND	2.07	112.44	110.17
4	B	500[A]	HEM	C4C-CHD-C1D	-2.03	121.71	126.02
4	B	500[B]	HEM	C4C-CHD-C1D	-2.03	121.71	126.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	881	GOL	O1-C1-C2-C3
7	B	881	GOL	C1-C2-C3-O3
7	B	881	GOL	O1-C1-C2-O2
7	B	881	GOL	O2-C2-C3-O3
7	A	880	GOL	O1-C1-C2-C3
4	A	500	HEM	C2A-CAA-CBA-CGA

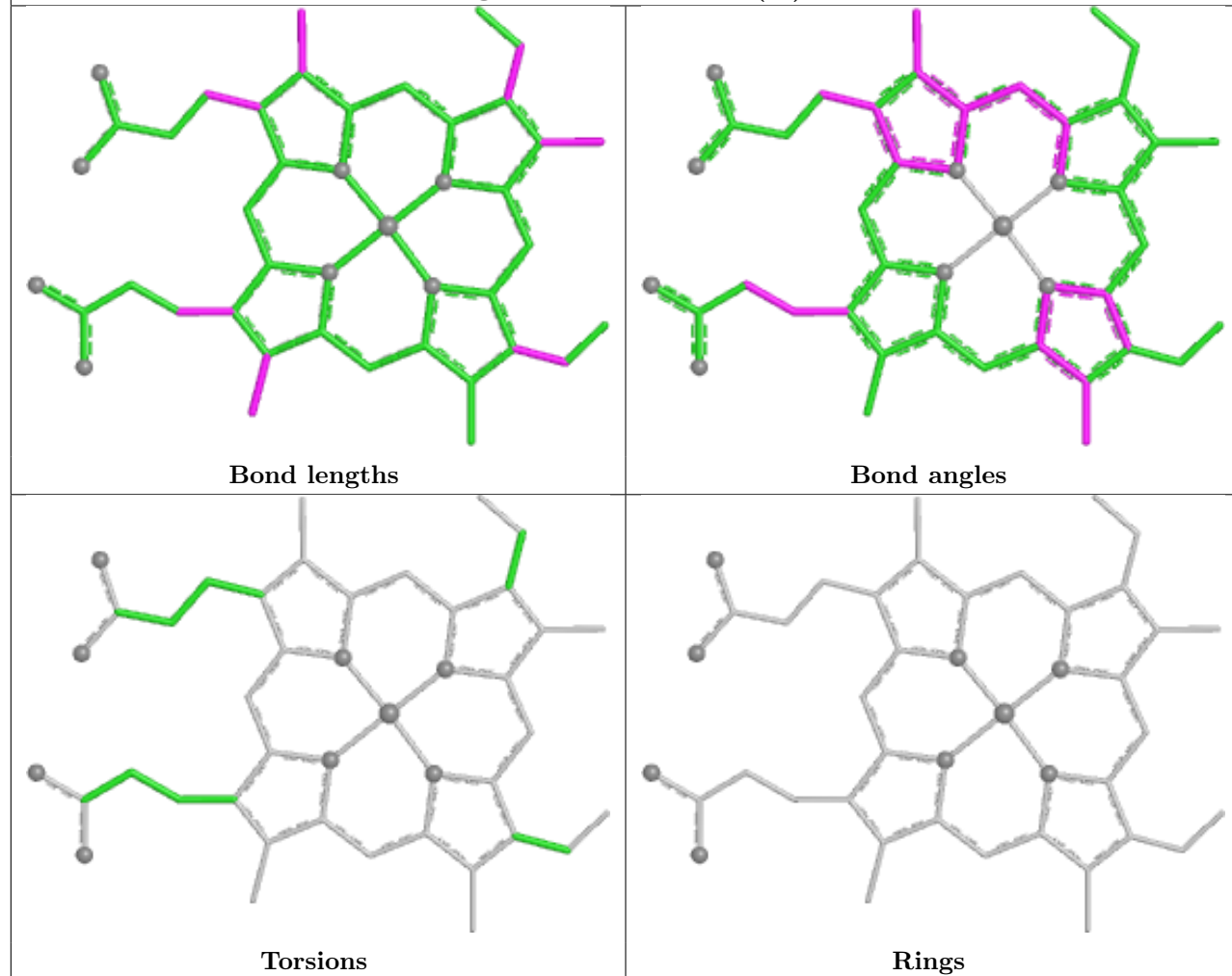
There are no ring outliers.

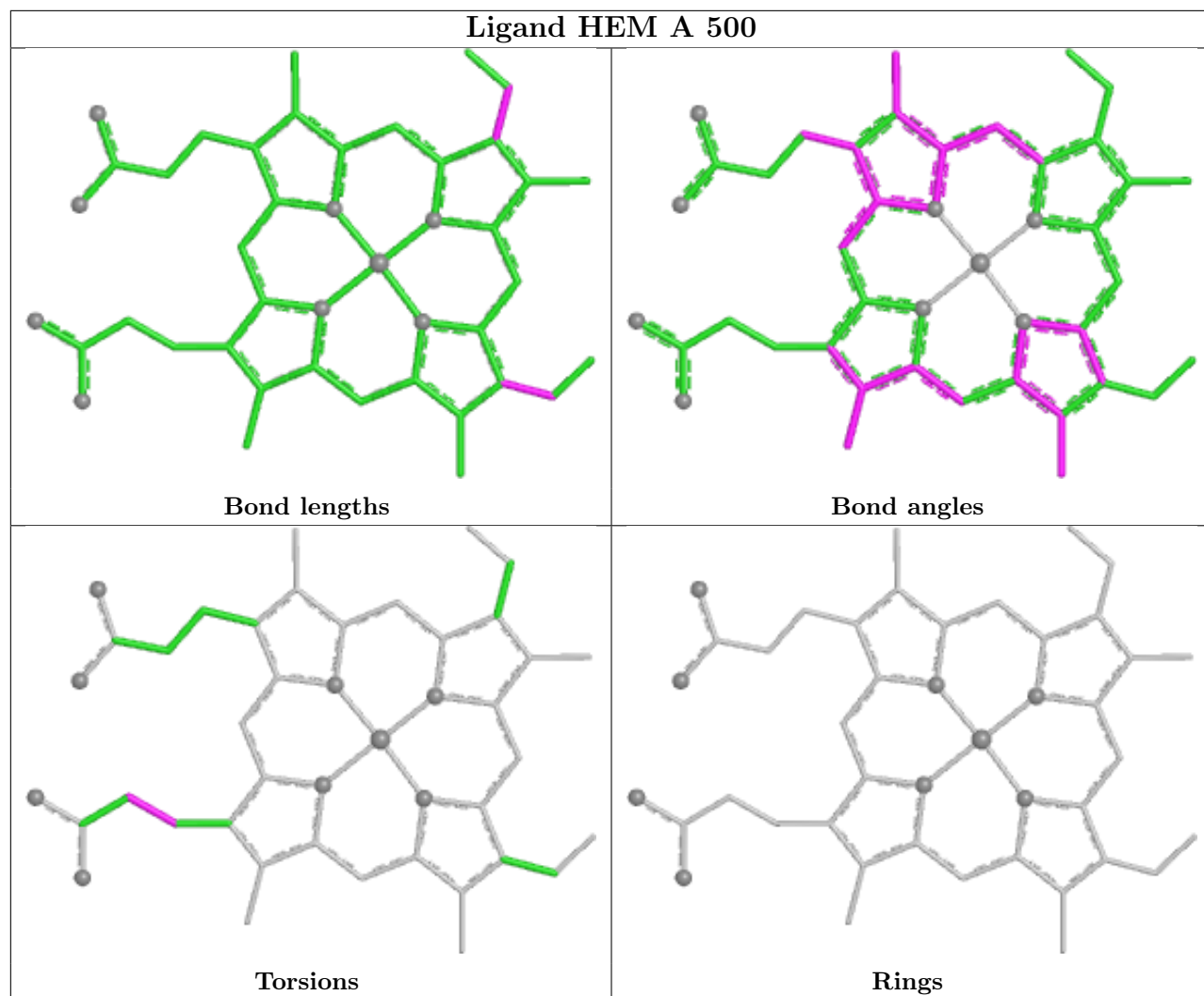
3 monomers are involved in 4 short contacts:

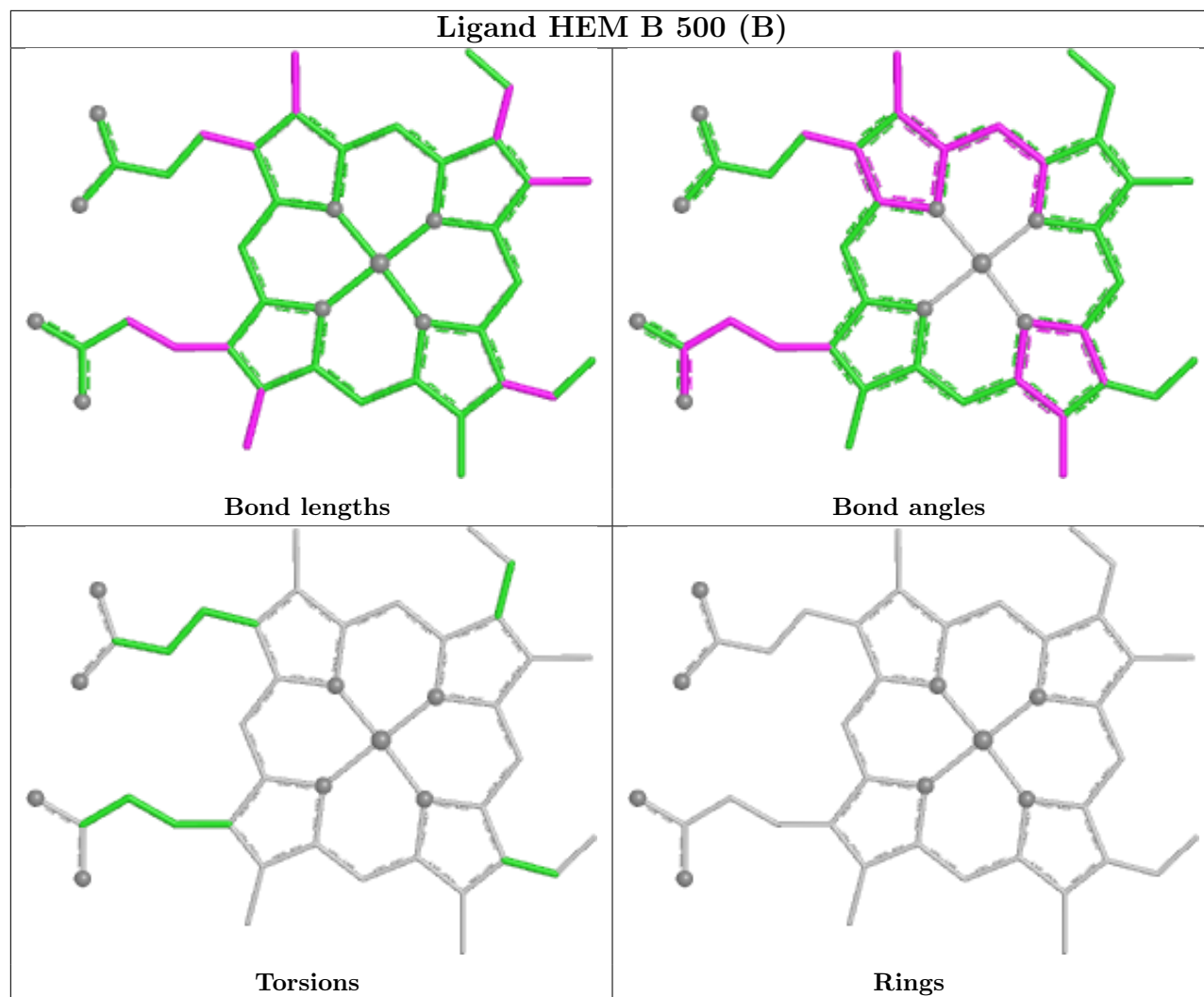
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500[A]	HEM	1	0
4	B	500[B]	HEM	2	0
5	B	765	INE	1	0

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 B 500 (A)







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%)	-0.19	15 (3%) 46 50	17, 27, 63, 123	1 (0%)
1	B	414/444 (93%)	-0.07	18 (4%) 40 43	19, 29, 65, 137	1 (0%)
All	All	830/888 (93%)	-0.13	33 (3%) 42 46	17, 28, 65, 137	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	5.7
1	B	261	GLY	5.1
1	B	113	THR	4.8
1	A	113	THR	4.4
1	B	260	ASP	4.1
1	A	117	PRO	3.5
1	B	119	PRO	3.5
1	A	116	SER	3.4
1	B	120	PRO	3.3
1	A	111	LEU	3.3
1	B	111	LEU	3.2
1	A	119	PRO	3.1
1	B	112	GLN	3.1
1	B	115	PRO	3.0
1	A	239	GLY	3.0
1	A	115	PRO	2.7
1	B	258	GLN	2.7
1	B	114	ARG	2.6
1	A	110	LYS	2.5
1	B	239	GLY	2.4
1	B	323	GLU	2.4
1	A	108	PRO	2.4
1	A	120	PRO	2.4
1	B	259	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	2.3
1	A	112	GLN	2.2
1	A	160	ALA	2.2
1	A	67	GLY	2.2
1	A	109	ARG	2.2
1	B	109	ARG	2.1
1	B	202	ASP	2.1
1	B	116	SER	2.1
1	B	69	LYS	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	B	881	6/6	0.63	0.13	44,54,59,62	0
7	GOL	A	880	6/6	0.85	0.09	34,45,53,61	0
2	ACT	B	861	4/4	0.85	0.08	24,26,31,32	0
6	CAD	A	950	3/5	0.88	0.47	24,24,47,53	0
5	INE	B	765	13/13	0.90	0.09	36,44,56,57	0
5	INE	A	766	13/13	0.91	0.11	36,42,59,59	0
6	CAD	B	951	3/5	0.92	0.38	19,19,38,50	0
2	ACT	B	851	4/4	0.94	0.06	25,32,34,35	0
2	ACT	A	860	4/4	0.96	0.04	28,34,36,39	0
2	ACT	A	850	4/4	0.97	0.03	22,27,31,34	0
4	HEM	A	500	43/43	0.97	0.06	15,19,42,53	0
4	HEM	B	500[A]	43/43	0.98	0.06	16,21,38,49	5
4	HEM	B	500[B]	43/43	0.98	0.06	16,22,32,41	5
5	INE	A	760	13/13	0.99	0.04	17,21,25,32	0

Continued on next page...

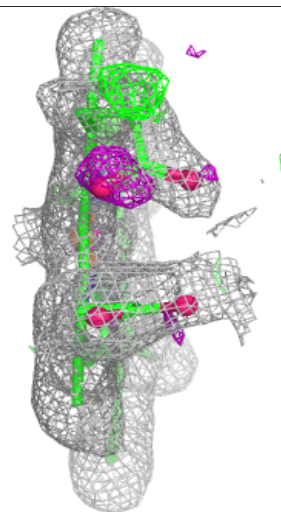
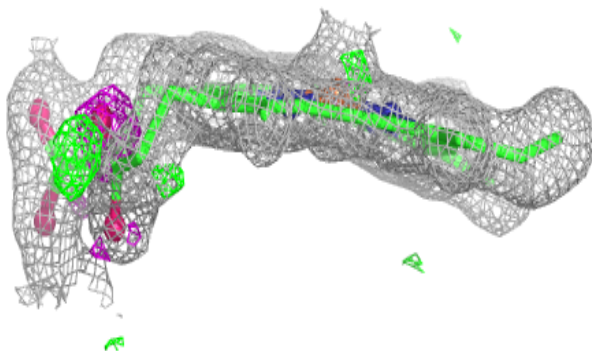
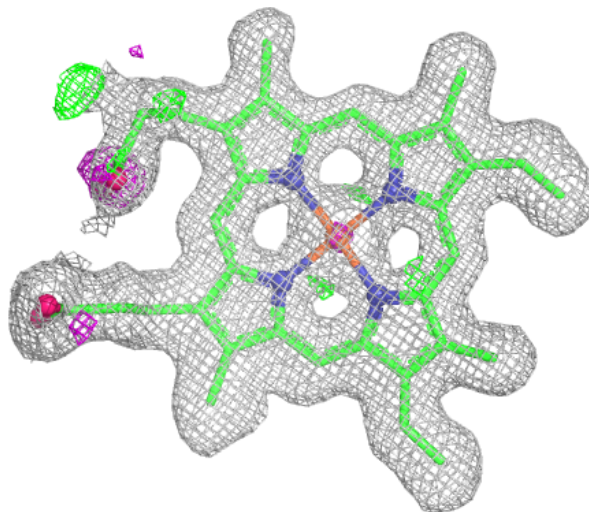
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	INE	B	761	13/13	0.99	0.04	19,24,29,36	0
3	ZN	A	900	1/1	1.00	0.07	26,26,26,26	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.

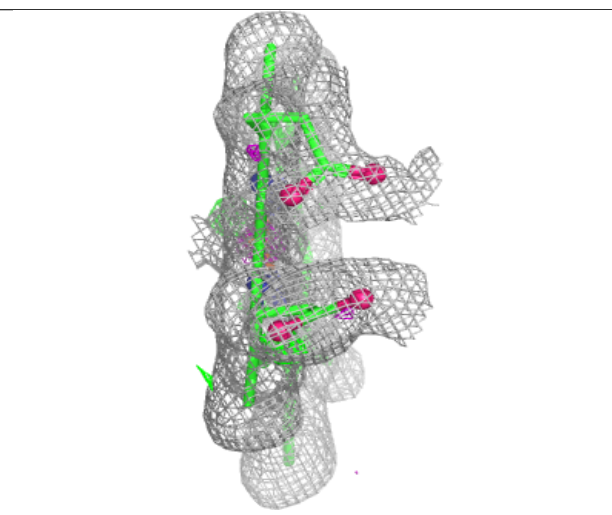
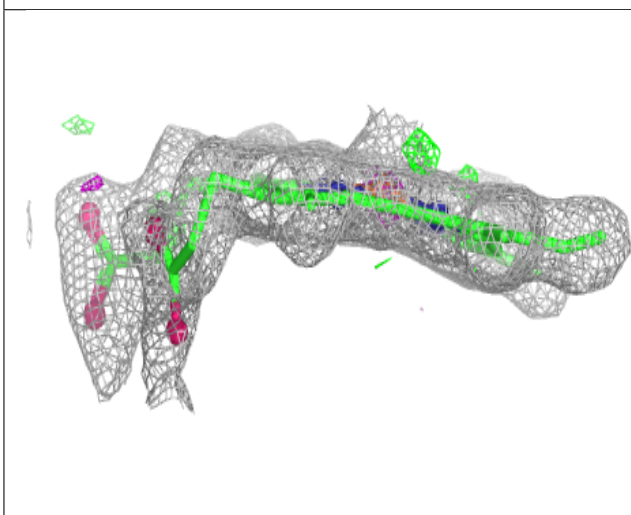
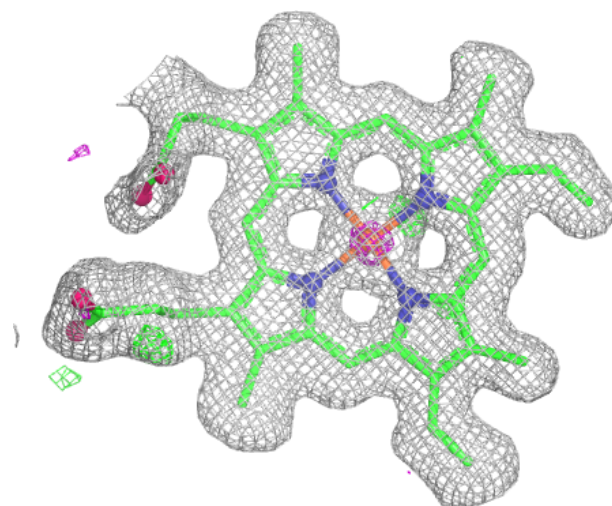
Electron density around HEM A 500:

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



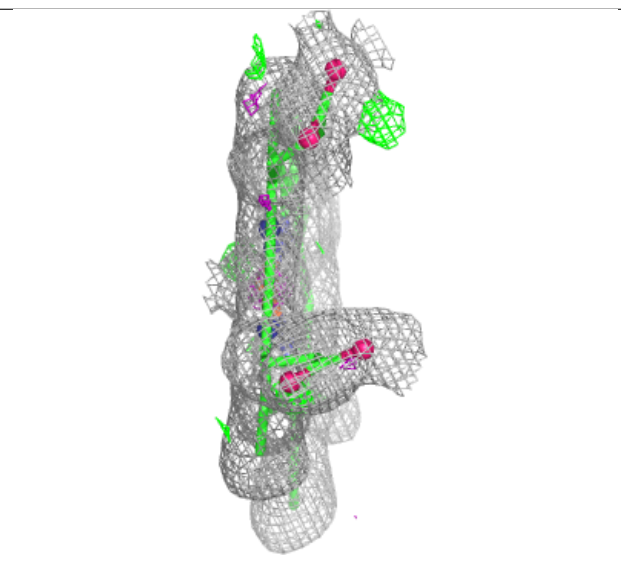
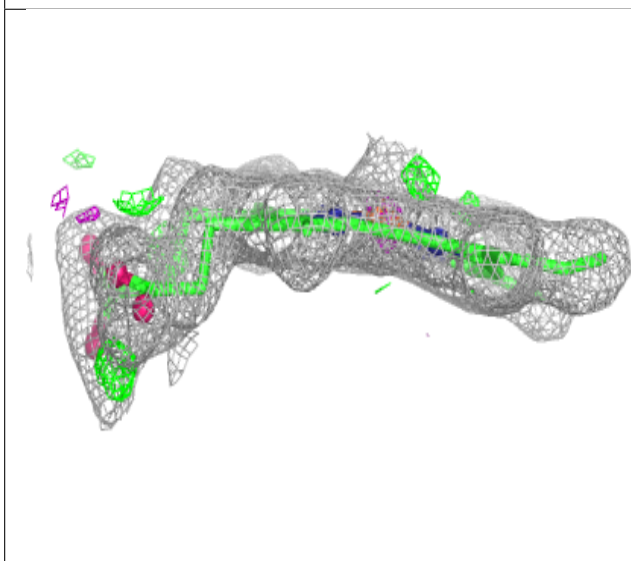
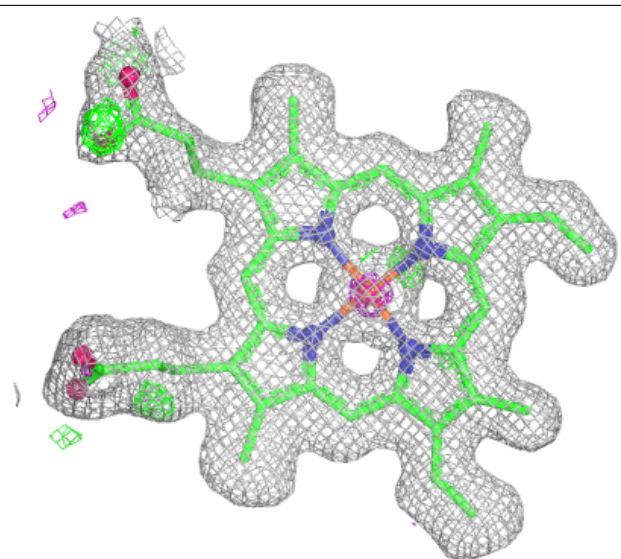
Electron density around HEM B 500 (A):

$2mF_o-DF_c$ (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 (B):

$2mF_o-DF_c$ (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.