



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:45 AM UTC

PDB ID : 3VLI / pdb_00003vli
Title : Crystal Structure Analysis of the Cyanide Arg409Leu Variant KatG from HALOARCULA MARISMORTUI
Authors : Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on : 2011-12-01
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

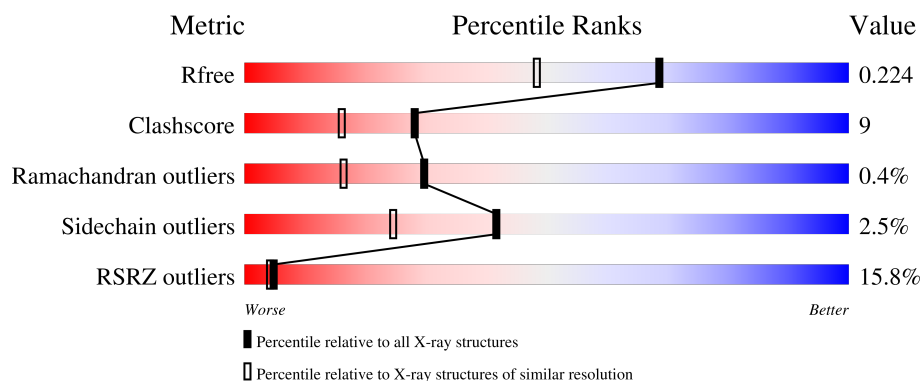
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	737	11% 80% 15% • •
1	B	737	20% 81% 15% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYN	A	802	-	-	X	-
3	CYN	B	802	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11870 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 Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5599	3503	938	1139	19			
1	B	714	Total	C	N	O	S	0	0	0
			5617	3512	942	1144	19			

There are 14 discrepancies between the modelled and reference sequences:

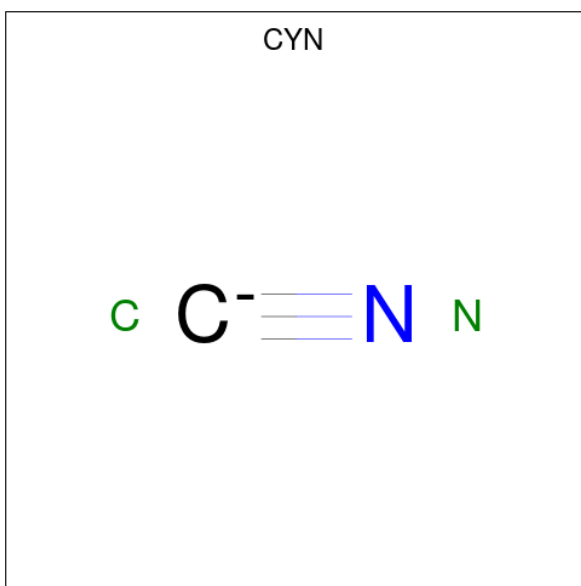
Chain	Residue	Modelled	Actual	Comment	Reference
A	409	LEU	ARG	engineered mutation	UNP O59651
A	732	HIS	-	expression tag	UNP O59651
A	733	HIS	-	expression tag	UNP O59651
A	734	HIS	-	expression tag	UNP O59651
A	735	HIS	-	expression tag	UNP O59651
A	736	HIS	-	expression tag	UNP O59651
A	737	HIS	-	expression tag	UNP O59651
B	409	LEU	ARG	engineered mutation	UNP O59651
B	732	HIS	-	expression tag	UNP O59651
B	733	HIS	-	expression tag	UNP O59651
B	734	HIS	-	expression tag	UNP O59651
B	735	HIS	-	expression tag	UNP O59651
B	736	HIS	-	expression tag	UNP O59651
B	737	HIS	-	expression tag	UNP O59651

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



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

- Molecule 3 is CYANIDE ION (CCD ID: CYN) (formula: CN).



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

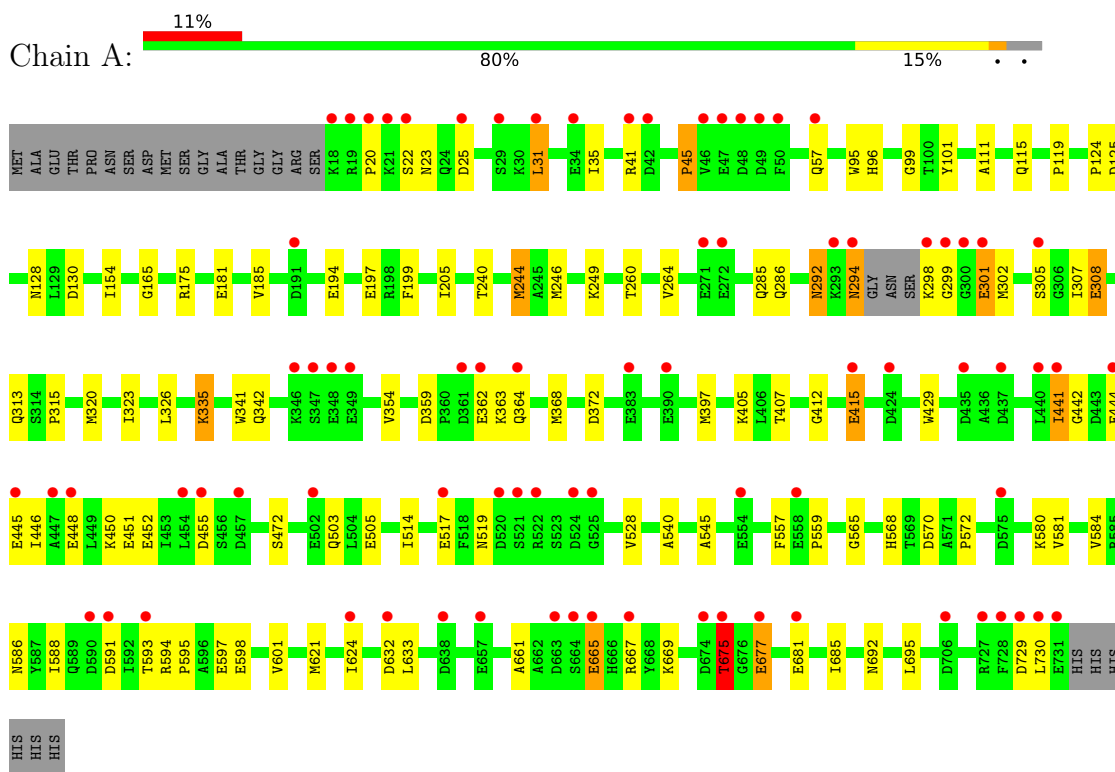
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	352	Total 352	O 352	0	0
4	B	212	Total 212	O 212	0	0

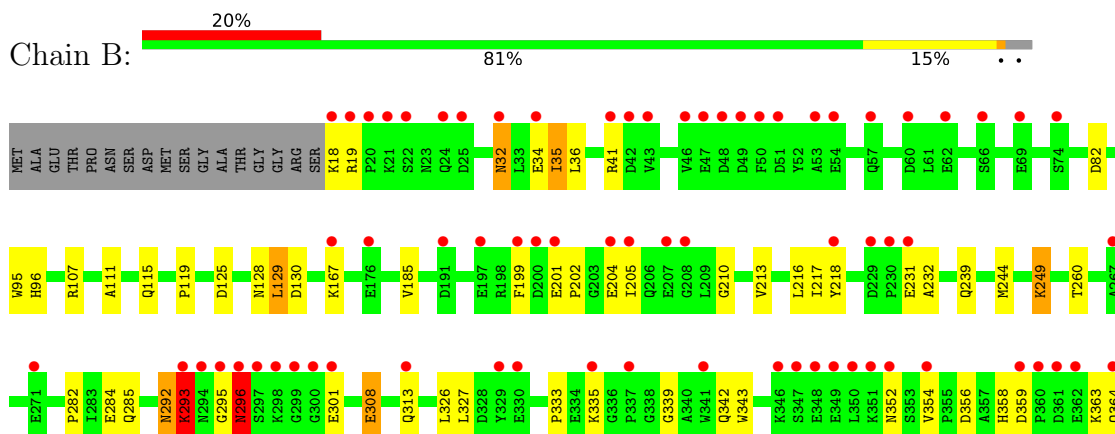
3 Residue-property plots [i](#)

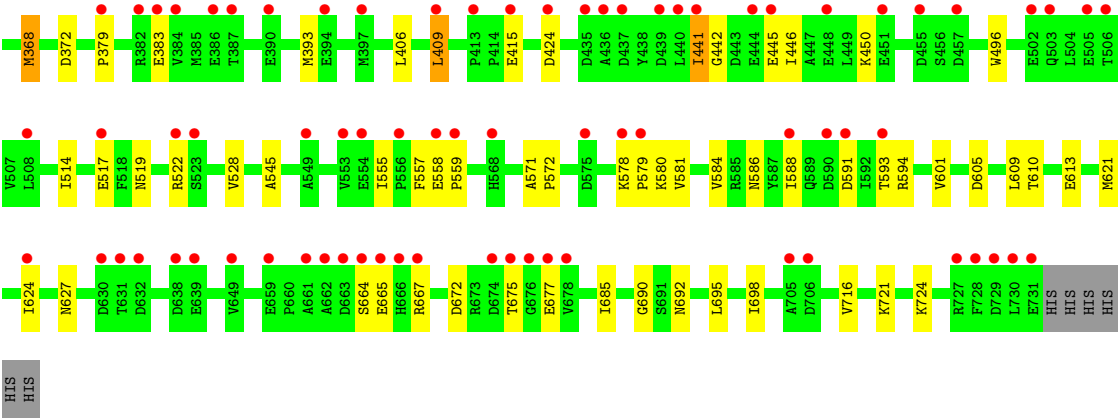
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Catalase-peroxidase 2



• Molecule 1: Catalase-peroxidase 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	315.88Å 81.43Å 75.58Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	39.39 – 1.70 39.39 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.39-1.70) 97.2 (39.39-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.234 0.210 , 0.224	Depositor DCC
R_{free} test set	9892 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11870	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CYN, HEM

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	0.61	0/5734	0.94	17/7790 (0.2%)
1	B	0.50	1/5753 (0.0%)	0.88	9/7817 (0.1%)
All	All	0.56	1/11487 (0.0%)	0.91	26/15607 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	MET	SD-CE	-5.47	1.65	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ALA	N-CA-C	7.32	121.86	112.34
1	B	580	LYS	N-CA-C	-7.00	104.87	113.41
1	A	580	LYS	N-CA-C	-7.00	104.88	113.41
1	A	99	GLY	N-CA-C	6.70	122.04	114.67
1	A	315	PRO	N-CA-C	6.52	122.39	113.98
1	B	260	THR	N-CA-C	-5.99	105.23	112.54
1	A	308	GLU	N-CA-C	5.95	118.82	108.76
1	B	129	LEU	N-CA-C	-5.94	106.00	113.18
1	A	412	GLY	CA-C-N	5.87	126.43	120.38
1	A	412	GLY	C-N-CA	5.87	126.43	120.38
1	A	359	ASP	CA-C-N	5.67	125.34	119.56
1	A	359	ASP	C-N-CA	5.67	125.34	119.56
1	B	111	ALA	N-CA-C	5.56	118.86	111.75
1	B	115	GLN	N-CA-C	-5.48	105.69	112.38
1	B	308	GLU	N-CA-C	5.35	117.62	108.90
1	A	197	GLU	N-CA-C	-5.33	103.95	110.61
1	A	244	MET	CB-CA-C	5.27	119.51	111.02
1	B	627	ASN	N-CA-C	5.25	118.25	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	THR	N-CA-C	-5.19	106.20	112.54
1	A	185	VAL	CB-CA-C	-5.17	105.03	111.08
1	A	472	SER	N-CA-C	5.09	119.12	113.01
1	A	115	GLN	N-CA-C	-5.07	106.19	112.38
1	A	165	GLY	N-CA-C	5.07	122.82	115.32
1	B	296	ASN	N-CA-C	-5.06	105.86	112.23
1	A	667	ARG	N-CA-C	5.04	118.28	110.17
1	B	327	LEU	N-CA-C	5.04	118.58	112.23

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	5599	0	5248	101	0
1	B	5617	0	5263	100	0
2	A	43	0	30	3	0
2	B	43	0	30	0	0
3	A	2	0	0	4	0
3	B	2	0	0	2	0
4	A	352	0	0	6	0
4	B	212	0	0	3	0
All	All	11870	0	10571	195	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 (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.16	1.58
1:B:95:TRP:HH2	1:B:218:TYR:CE1	0.97	1.57
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.86	1.57
1:A:199:PHE:HB3	1:A:205:ILE:HD13	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HD2	1:A:301:GLU:HB3	1.41	0.98
1:A:95:TRP:CD1	3:A:802:CYN:N	2.36	0.94
1:B:95:TRP:HH2	1:B:218:TYR:CD1	1.86	0.93
1:B:326:LEU:HD13	1:B:368:MET:HE2	1.51	0.92
1:A:101:TYR:O	1:A:244:MET:HE2	1.71	0.91
1:A:565:GLY:H	1:A:568:HIS:HD2	1.16	0.91
1:A:632:ASP:HB2	1:A:681:GLU:OE1	1.72	0.89
1:A:95:TRP:HD1	3:A:802:CYN:N	1.69	0.88
1:A:675:THR:HG22	1:A:677:GLU:H	1.39	0.87
1:A:45:PRO:HD3	1:B:698:ILE:HD12	1.56	0.85
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.64	0.83
1:A:588:ILE:HD11	1:A:685:ILE:HD11	1.59	0.83
1:B:32:ASN:ND2	1:B:34:GLU:HG2	1.93	0.82
1:B:95:TRP:CZ3	1:B:218:TYR:HE1	1.96	0.82
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.62	0.82
1:B:692:ASN:HD22	1:B:695:LEU:H	1.28	0.79
1:A:519:ASN:HD21	1:A:528:VAL:H	1.30	0.79
1:A:362:GLU:HG2	1:A:363:LYS:N	1.99	0.77
1:B:35:ILE:HD12	1:B:605:ASP:HB2	1.67	0.77
1:A:692:ASN:HD22	1:A:695:LEU:H	1.34	0.75
1:B:326:LEU:HD13	1:B:368:MET:CE	2.17	0.73
1:B:514:ILE:O	1:B:517:GLU:HG2	1.88	0.73
1:A:154:ILE:HD12	1:A:175:ARG:CZ	2.19	0.72
1:B:368:MET:HE3	1:B:372:ASP:HB3	1.73	0.71
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.71	0.71
1:B:588:ILE:HD11	1:B:685:ILE:HD11	1.72	0.70
1:A:675:THR:HG21	4:A:808:HOH:O	1.91	0.69
1:A:299:GLY:HA2	1:A:302:MET:HE3	1.73	0.69
1:B:441:ILE:HD11	1:B:559:PRO:HB3	1.74	0.69
1:B:19:ARG:HD3	1:B:19:ARG:H	1.58	0.68
1:B:95:TRP:CZ3	1:B:218:TYR:CE1	2.76	0.68
1:A:397:MET:HA	1:A:397:MET:HE2	1.76	0.68
1:A:154:ILE:HD12	1:A:175:ARG:NE	2.10	0.67
1:B:519:ASN:HD21	1:B:528:VAL:H	1.43	0.67
1:B:368:MET:CE	1:B:372:ASP:HB3	2.25	0.66
1:B:581:VAL:HG13	1:B:588:ILE:HD13	1.78	0.66
1:B:199:PHE:HB3	1:B:205:ILE:HD13	1.77	0.66
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.77	0.66
1:A:362:GLU:HG2	1:A:363:LYS:H	1.62	0.65
1:A:354:VAL:HB	1:A:364:GLN:HG3	1.79	0.64
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASN:HD21	1:B:34:GLU:HG2	1.61	0.63
1:A:199:PHE:CB	1:A:205:ILE:HD13	2.23	0.63
1:A:452:GLU:HG3	1:A:514:ILE:HD12	1.81	0.63
1:A:368:MET:HG3	1:A:372:ASP:HB2	1.81	0.63
1:A:565:GLY:H	1:A:568:HIS:CD2	2.07	0.62
1:A:675:THR:HG22	1:A:677:GLU:N	2.13	0.62
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.81	0.62
1:A:441:ILE:HD11	1:A:559:PRO:HB3	1.82	0.62
1:A:22:SER:HB3	1:A:25:ASP:OD1	2.01	0.61
1:A:633:LEU:HD23	1:A:681:GLU:HG3	1.83	0.60
1:A:31:LEU:HD21	1:A:597:GLU:HG3	1.83	0.60
1:B:308:GLU:H	1:B:342:GLN:HE22	1.48	0.60
1:A:308:GLU:H	1:A:342:GLN:HE22	1.50	0.60
1:B:558:GLU:HG2	1:B:724:LYS:HE3	1.85	0.58
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.84	0.58
1:A:364:GLN:NE2	4:A:743:HOH:O	2.36	0.57
1:B:333:PRO:HD3	1:B:343:TRP:CZ3	2.40	0.57
1:B:326:LEU:CD1	1:B:368:MET:HE2	2.32	0.56
1:B:441:ILE:H	1:B:441:ILE:HD13	1.70	0.56
1:B:557:PHE:CE2	1:B:559:PRO:HG3	2.41	0.56
1:A:514:ILE:O	1:A:517:GLU:HG3	2.06	0.55
1:B:249:LYS:HB2	1:B:249:LYS:NZ	2.21	0.55
1:A:181:GLU:H	1:A:181:GLU:CD	2.14	0.55
1:A:444:GLU:O	1:A:448:GLU:HG3	2.07	0.55
1:A:305:SER:HB3	1:A:307:ILE:HD12	1.89	0.54
1:A:299:GLY:O	1:A:302:MET:HG3	2.07	0.54
1:A:441:ILE:H	1:A:441:ILE:HD13	1.73	0.54
1:A:326:LEU:HA	1:A:368:MET:HE3	1.90	0.53
1:B:441:ILE:HD13	1:B:441:ILE:N	2.23	0.53
1:A:292:ASN:HD21	1:A:294:ASN:ND2	2.06	0.53
1:B:301:GLU:HB3	4:B:924:HOH:O	2.08	0.53
1:A:124:PRO:HG3	1:A:194:GLU:HG3	1.91	0.53
1:B:514:ILE:HA	1:B:517:GLU:OE1	2.09	0.53
1:A:441:ILE:HB	1:A:445:GLU:HB2	1.92	0.52
1:B:96:HIS:CD2	1:B:217:ILE:HG13	2.44	0.52
1:A:452:GLU:CG	1:A:514:ILE:HD12	2.39	0.52
1:B:368:MET:HE3	1:B:372:ASP:CB	2.39	0.52
1:A:292:ASN:CG	1:A:298:LYS:HE3	2.34	0.51
1:A:581:VAL:HG13	1:A:588:ILE:HD13	1.92	0.51
1:B:292:ASN:C	1:B:292:ASN:HD22	2.17	0.51
1:B:293:LYS:HB3	1:B:293:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LYS:HD2	1:A:540:ALA:HB2	1.91	0.51
1:A:23:ASN:HD21	1:B:119:PRO:HD3	1.76	0.51
1:B:202:PRO:HG2	1:B:232:ALA:HB1	1.92	0.51
1:A:320:MET:HE1	1:A:323:ILE:HD12	1.92	0.51
1:B:588:ILE:HD11	1:B:685:ILE:CD1	2.41	0.51
1:B:292:ASN:HD22	1:B:293:LYS:N	2.09	0.50
1:B:352:ASN:HD22	1:B:363:LYS:HB2	1.76	0.50
1:A:595:PRO:HD2	1:A:598:GLU:CD	2.36	0.50
1:A:154:ILE:HD13	1:A:407:THR:HB	1.93	0.50
1:A:503:GLN:HG2	4:A:1085:HOH:O	2.12	0.50
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.12	0.50
1:B:95:TRP:CD1	3:B:802:CYN:N	2.79	0.50
1:B:199:PHE:CB	1:B:205:ILE:HD13	2.42	0.50
1:A:415:GLU:CD	1:A:415:GLU:H	2.17	0.50
1:B:35:ILE:CD1	1:B:605:ASP:HB2	2.40	0.50
1:B:356:ASP:HB3	1:B:359:ASP:O	2.12	0.50
1:B:545:ALA:HB1	1:B:624:ILE:HD12	1.93	0.50
1:B:609:LEU:HD23	1:B:721:LYS:HE3	1.92	0.50
1:A:305:SER:OG	2:A:800:HEM:HBA1	2.12	0.49
1:B:96:HIS:CE1	1:B:125:ASP:O	2.64	0.49
1:B:393:MET:HB2	4:B:896:HOH:O	2.12	0.49
1:B:95:TRP:HD1	3:B:802:CYN:N	2.10	0.49
1:B:406:LEU:O	1:B:409:LEU:HD22	2.12	0.49
1:A:505:GLU:HG2	4:A:976:HOH:O	2.12	0.49
1:B:19:ARG:HD3	1:B:19:ARG:N	2.25	0.49
1:B:675:THR:HG23	1:B:677:GLU:H	1.77	0.48
1:A:593:THR:HG23	1:A:594:ARG:N	2.27	0.48
1:A:397:MET:HE2	1:A:397:MET:CA	2.43	0.48
1:A:633:LEU:HA	1:A:681:GLU:HG3	1.95	0.48
1:A:588:ILE:HD11	1:A:685:ILE:CD1	2.39	0.48
1:B:107:ARG:HD3	1:B:185:VAL:HG22	1.96	0.48
1:B:593:THR:HG23	1:B:594:ARG:N	2.28	0.48
1:A:632:ASP:CB	1:A:681:GLU:OE1	2.55	0.48
1:B:35:ILE:HG13	1:B:36:LEU:N	2.28	0.48
1:A:665:GLU:H	1:A:665:GLU:CD	2.22	0.48
1:B:201:GLU:HB2	1:B:204:GLU:HG3	1.96	0.47
1:A:633:LEU:HD23	1:A:681:GLU:CG	2.44	0.47
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.96	0.47
1:A:326:LEU:CA	1:A:368:MET:HE3	2.45	0.47
1:B:41:ARG:NH1	4:B:856:HOH:O	2.47	0.47
1:B:82:ASP:OD2	1:B:358:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:HIS:HE1	1:B:125:ASP:O	1.97	0.47
1:A:661:ALA:HB1	1:A:669:LYS:NZ	2.29	0.47
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.03	0.47
1:A:441:ILE:HD13	1:A:441:ILE:N	2.29	0.46
1:B:496:TRP:CD1	1:B:578:LYS:HE2	2.50	0.46
1:B:354:VAL:HB	1:B:364:GLN:HG3	1.98	0.46
1:A:264:VAL:HG12	2:A:800:HEM:CAA	2.46	0.46
1:A:450:LYS:CD	1:A:540:ALA:HB2	2.45	0.46
1:B:231:GLU:H	1:B:231:GLU:CD	2.23	0.46
1:B:441:ILE:H	1:B:441:ILE:CD1	2.29	0.46
1:A:545:ALA:HB1	1:A:624:ILE:HD12	1.97	0.46
1:B:593:THR:HG23	1:B:594:ARG:H	1.81	0.45
1:B:442:GLY:O	1:B:446:ILE:HG13	2.16	0.45
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.99	0.45
1:A:305:SER:CB	1:A:307:ILE:HD12	2.47	0.45
1:B:35:ILE:CD1	1:B:601:VAL:HG12	2.41	0.45
1:B:205:ILE:HG12	1:B:239:GLN:OE1	2.17	0.45
1:A:96:HIS:CE1	1:A:125:ASP:O	2.70	0.45
1:B:18:LYS:HB3	1:B:19:ARG:HD3	1.99	0.44
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.98	0.44
1:A:570:ASP:OD1	1:A:572:PRO:HD2	2.17	0.44
1:B:664:SER:HG	1:B:667:ARG:H	1.65	0.44
1:A:286:GLN:HE22	1:B:690:GLY:HA3	1.82	0.44
1:B:249:LYS:HB2	1:B:249:LYS:HZ3	1.82	0.44
1:B:32:ASN:HD21	1:B:34:GLU:CG	2.30	0.44
1:A:308:GLU:H	1:A:342:GLN:NE2	2.14	0.43
1:A:335:LYS:HE2	1:A:341:TRP:CE2	2.53	0.43
1:A:364:GLN:NE2	4:A:833:HOH:O	2.48	0.43
1:A:292:ASN:HD21	1:A:294:ASN:HD22	1.66	0.43
1:B:665:GLU:H	1:B:667:ARG:NH2	2.15	0.43
1:B:335:LYS:HE3	1:B:339:GLY:O	2.17	0.43
1:A:730:LEU:C	1:A:730:LEU:HD23	2.43	0.43
1:A:41:ARG:HB3	1:B:41:ARG:HB3	2.00	0.43
1:A:124:PRO:HG3	1:A:194:GLU:CG	2.49	0.43
1:A:441:ILE:H	1:A:441:ILE:CD1	2.32	0.43
1:B:672:ASP:HB3	1:B:675:THR:HG23	2.00	0.43
1:A:95:TRP:HE1	3:A:802:CYN:C	2.32	0.43
1:A:264:VAL:HG12	2:A:800:HEM:HAA1	2.00	0.43
1:B:514:ILE:HA	1:B:517:GLU:CD	2.44	0.43
1:B:445:GLU:HG3	1:B:522:ARG:HH21	1.83	0.42
1:A:249:LYS:NZ	1:A:249:LYS:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ILE:HD13	1:B:517:GLU:OE1	2.19	0.42
1:A:240:THR:O	1:A:244:MET:HG3	2.19	0.42
1:A:294:ASN:ND2	1:A:294:ASN:N	2.67	0.42
1:A:96:HIS:NE2	3:A:802:CYN:C	2.83	0.42
1:B:610:THR:OG1	1:B:613:GLU:HG3	2.20	0.42
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.88	0.42
1:B:578:LYS:HA	1:B:579:PRO:HD3	1.87	0.42
1:A:96:HIS:HE1	1:A:125:ASP:O	2.03	0.41
1:B:282:PRO:HB2	1:B:284:GLU:CD	2.45	0.41
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.19	0.41
1:B:167:LYS:HE3	1:B:167:LYS:HB3	1.95	0.41
1:A:545:ALA:HB1	1:A:624:ILE:CD1	2.50	0.41
1:A:557:PHE:CE2	1:A:559:PRO:HG3	2.56	0.41
1:B:296:ASN:HD22	1:B:296:ASN:HA	1.65	0.41
1:A:451:GLU:HG2	1:A:455:ASP:OD2	2.21	0.41
1:A:20:PRO:HB3	1:B:185:VAL:O	2.21	0.41
1:A:154:ILE:HD12	1:A:175:ARG:NH2	2.34	0.41
1:A:545:ALA:CB	1:A:624:ILE:HD12	2.50	0.41
1:A:581:VAL:HG13	1:A:588:ILE:CD1	2.51	0.41
1:B:210:GLY:O	1:B:244:MET:HE3	2.21	0.41
1:B:379:PRO:O	1:B:383:GLU:HG3	2.21	0.41
1:A:31:LEU:HD21	1:A:597:GLU:CG	2.48	0.40
1:A:249:LYS:HG3	4:A:921:HOH:O	2.19	0.40
1:A:286:GLN:NE2	1:B:690:GLY:HA3	2.37	0.40
1:A:405:LYS:HA	1:A:429:TRP:CZ2	2.57	0.40
1:A:442:GLY:O	1:A:446:ILE:HG13	2.20	0.40
1:B:496:TRP:NE1	1:B:578:LYS:HE2	2.37	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	707/737 (96%)	687 (97%)	17 (2%)	3 (0%)	30	16
1	B	712/737 (97%)	691 (97%)	18 (2%)	3 (0%)	30	16
All	All	1419/1474 (96%)	1378 (97%)	35 (2%)	6 (0%)	30	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	729	ASP
1	B	591	ASP
1	A	591	ASP
1	A	675	THR
1	B	293	LYS
1	B	295	GLY

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	588/608 (97%)	572 (97%)	16 (3%)	39	23
1	B	590/608 (97%)	577 (98%)	13 (2%)	45	29
All	All	1178/1216 (97%)	1149 (98%)	29 (2%)	42	24

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	45	PRO
1	A	57	GLN
1	A	119	PRO
1	A	246	MET
1	A	285	GLN
1	A	292	ASN
1	A	294	ASN
1	A	301	GLU
1	A	335	LYS

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Mol	Chain	Res	Type
1	A	415	GLU
1	A	441	ILE
1	A	586	ASN
1	A	665	GLU
1	A	675	THR
1	A	677	GLU
1	B	32	ASN
1	B	35	ILE
1	B	249	LYS
1	B	285	GLN
1	B	292	ASN
1	B	293	LYS
1	B	296	ASN
1	B	409	LEU
1	B	415	GLU
1	B	424	ASP
1	B	441	ILE
1	B	450	LYS
1	B	586	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	24	GLN
1	A	286	GLN
1	A	291	GLN
1	A	292	ASN
1	A	294	ASN
1	A	342	GLN
1	A	352	ASN
1	A	364	GLN
1	A	493	GLN
1	A	513	ASN
1	A	515	GLN
1	A	519	ASN
1	A	568	HIS
1	A	586	ASN
1	A	608	ASN
1	A	692	ASN
1	B	32	ASN
1	B	286	GLN

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Mol	Chain	Res	Type
1	B	291	GLN
1	B	292	ASN
1	B	294	ASN
1	B	296	ASN
1	B	342	GLN
1	B	358	HIS
1	B	364	GLN
1	B	513	ASN
1	B	515	GLN
1	B	519	ASN
1	B	568	HIS
1	B	586	ASN
1	B	589	GLN
1	B	666	HIS
1	B	692	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYN	B	802	-	1,1,1	0.23	0	-		
2	HEM	A	800	1	50,50,50	1.94	15 (30%)	67,82,82	3.26	36 (53%)
3	CYN	A	802	-	1,1,1	0.21	0	-		
2	HEM	B	800	1	50,50,50	2.16	11 (22%)	67,82,82	5.42	40 (59%)

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
2	HEM	A	800	1	-	2/14/54/54	-
2	HEM	B	800	1	-	2/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	FE-NA	7.32	2.19	1.95
2	B	800	HEM	CBC-CAC	5.26	1.55	1.30
2	B	800	HEM	CBB-CAB	5.15	1.55	1.30
2	A	800	HEM	CBB-CAB	5.01	1.54	1.30
2	A	800	HEM	CBC-CAC	4.70	1.53	1.30
2	B	800	HEM	CBA-CGA	-4.64	1.39	1.50
2	B	800	HEM	FE-NC	4.41	2.09	1.95
2	A	800	HEM	FE-NA	4.31	2.09	1.95
2	B	800	HEM	CBD-CGD	-4.09	1.41	1.50
2	A	800	HEM	FE-NC	3.50	2.06	1.95
2	A	800	HEM	O1A-CGA	3.50	1.33	1.22
2	A	800	HEM	FE-ND	3.35	2.05	1.94
2	B	800	HEM	FE-NB	3.11	2.04	1.94
2	B	800	HEM	O1A-CGA	2.93	1.31	1.22
2	A	800	HEM	CAC-C3C	2.73	1.54	1.47
2	A	800	HEM	CBD-CAD	2.61	1.61	1.51
2	A	800	HEM	CBA-CGA	-2.58	1.44	1.50
2	B	800	HEM	CAC-C3C	2.55	1.54	1.47
2	A	800	HEM	O2A-CGA	-2.33	1.23	1.30
2	B	800	HEM	CBD-CAD	2.30	1.59	1.51
2	A	800	HEM	CMC-C2C	2.21	1.55	1.50
2	A	800	HEM	O1D-CGD	2.16	1.29	1.22
2	A	800	HEM	CBD-CGD	-2.12	1.45	1.50
2	A	800	HEM	FE-NB	2.11	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	O1D-CGD	2.09	1.28	1.22
2	A	800	HEM	CAB-C3B	2.05	1.52	1.47

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C2D-C1D-ND	13.32	125.31	109.90
2	B	800	HEM	C3B-C4B-NB	12.88	118.72	109.47
2	B	800	HEM	CHD-C1D-ND	-12.66	110.79	124.42
2	B	800	HEM	C4D-ND-C1D	-12.01	90.98	105.21
2	B	800	HEM	C4A-CHB-C1B	10.80	151.65	126.25
2	B	800	HEM	CHB-C1B-NB	-10.67	111.17	124.37
2	B	800	HEM	CHC-C4B-NB	-10.31	113.33	124.42
2	B	800	HEM	C1D-C2D-C3D	-9.01	97.51	106.98
2	B	800	HEM	CHB-C4A-NA	-8.45	108.54	123.86
2	A	800	HEM	CHC-C1C-NC	8.23	133.41	124.45
2	B	800	HEM	C1B-NB-C4B	-8.15	95.56	105.21
2	B	800	HEM	C3D-C4D-ND	8.07	119.02	110.17
2	B	800	HEM	O2A-CGA-O1A	-7.61	103.75	123.33
2	B	800	HEM	C2A-C1A-NA	-7.60	101.72	110.15
2	A	800	HEM	C4C-C3C-C2C	7.45	113.27	106.81
2	B	800	HEM	C2B-C1B-NB	6.85	117.72	109.84
2	A	800	HEM	C4A-C3A-C2A	-6.83	98.99	106.82
2	A	800	HEM	C2A-C1A-NA	-6.72	102.69	110.15
2	A	800	HEM	C1A-C2A-C3A	6.59	117.07	106.87
2	B	800	HEM	O2A-CGA-CBA	6.51	134.58	114.00
2	B	800	HEM	CHA-C4D-ND	-6.36	116.50	124.37
2	A	800	HEM	CMA-C3A-C2A	6.26	138.89	125.62
2	B	800	HEM	C4C-CHD-C1D	6.19	139.17	126.02
2	B	800	HEM	C1A-C2A-C3A	6.04	116.22	106.87
2	B	800	HEM	CAA-C2A-C1A	-5.61	113.97	124.94
2	A	800	HEM	CHD-C4C-C3C	5.60	134.65	125.21
2	A	800	HEM	CHB-C1B-NB	-5.55	117.50	124.37
2	B	800	HEM	C4A-C3A-C2A	-5.31	100.74	106.82
2	A	800	HEM	C3B-C2B-C1B	-5.25	102.47	106.41
2	B	800	HEM	CHD-C4C-NC	-5.22	118.77	124.45
2	A	800	HEM	CHA-C1A-NA	5.17	133.24	123.86
2	A	800	HEM	CAC-C3C-C4C	-5.16	112.51	124.82
2	B	800	HEM	O2D-CGD-O1D	-4.82	110.93	123.33
2	B	800	HEM	CMD-C2D-C1D	4.79	132.52	125.03
2	A	800	HEM	C2B-C1B-NB	4.75	115.30	109.84
2	B	800	HEM	CHD-C4C-C3C	4.64	133.03	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CHB-C4A-C3A	4.57	140.69	127.43
2	B	800	HEM	C1C-CHC-C4B	4.48	135.54	126.02
2	B	800	HEM	CAA-CBA-CGA	-4.46	101.83	113.67
2	B	800	HEM	CHA-C1A-C2A	4.45	135.05	125.30
2	B	800	HEM	C4B-C3B-C2B	-4.24	103.38	107.28
2	A	800	HEM	C4C-NC-C1C	4.24	112.73	105.82
2	A	800	HEM	C1D-C2D-C3D	-4.24	102.52	106.98
2	B	800	HEM	CHC-C1C-C2C	3.81	133.41	125.49
2	A	800	HEM	C4A-CHB-C1B	3.77	135.11	126.25
2	B	800	HEM	CMC-C2C-C1C	-3.71	118.19	124.73
2	B	800	HEM	CMA-C3A-C2A	3.69	133.45	125.62
2	A	800	HEM	CHB-C4A-NA	-3.64	117.27	123.86
2	B	800	HEM	CHC-C1C-NC	-3.63	120.50	124.45
2	A	800	HEM	CMB-C2B-C3B	3.36	136.55	128.43
2	A	800	HEM	C2D-C1D-ND	3.21	113.61	109.90
2	A	800	HEM	O2A-CGA-CBA	3.12	123.86	114.00
2	A	800	HEM	C1A-CHA-C4D	-3.00	119.19	126.25
2	B	800	HEM	C4A-NA-C1A	2.92	110.58	105.82
2	B	800	HEM	C1A-CHA-C4D	2.83	132.90	126.25
2	A	800	HEM	CBA-CAA-C2A	2.81	120.31	112.53
2	A	800	HEM	CHD-C4C-NC	-2.73	121.48	124.45
2	A	800	HEM	CAA-C2A-C3A	-2.67	121.08	127.07
2	A	800	HEM	CMB-C2B-C1B	-2.61	120.95	125.03
2	A	800	HEM	C1B-NB-C4B	-2.61	102.12	105.21
2	A	800	HEM	CHA-C4D-ND	2.60	127.58	124.37
2	A	800	HEM	C2C-C1C-NC	-2.60	104.83	109.64
2	A	800	HEM	C4B-C3B-C2B	2.58	109.65	107.28
2	A	800	HEM	CMA-C3A-C4A	-2.50	121.62	125.42
2	A	800	HEM	C4D-C3D-C2D	2.44	110.44	106.89
2	A	800	HEM	CAD-CBD-CGD	2.40	120.03	113.67
2	A	800	HEM	CAB-C3B-C2B	-2.38	120.69	128.43
2	B	800	HEM	C3B-C2B-C1B	-2.38	104.62	106.41
2	B	800	HEM	O1D-CGD-CBD	2.27	130.30	123.09
2	B	800	HEM	C3C-C2C-C1C	2.24	109.16	107.05
2	A	800	HEM	CMD-C2D-C3D	2.18	132.04	126.15
2	A	800	HEM	C1C-CHC-C4B	-2.13	121.49	126.02
2	B	800	HEM	CMB-C2B-C1B	2.10	128.32	125.03
2	A	800	HEM	O1D-CGD-CBD	-2.05	116.58	123.09
2	A	800	HEM	CAA-CBA-CGA	-2.05	108.23	113.67
2	B	800	HEM	C2C-C1C-NC	-2.02	105.89	109.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

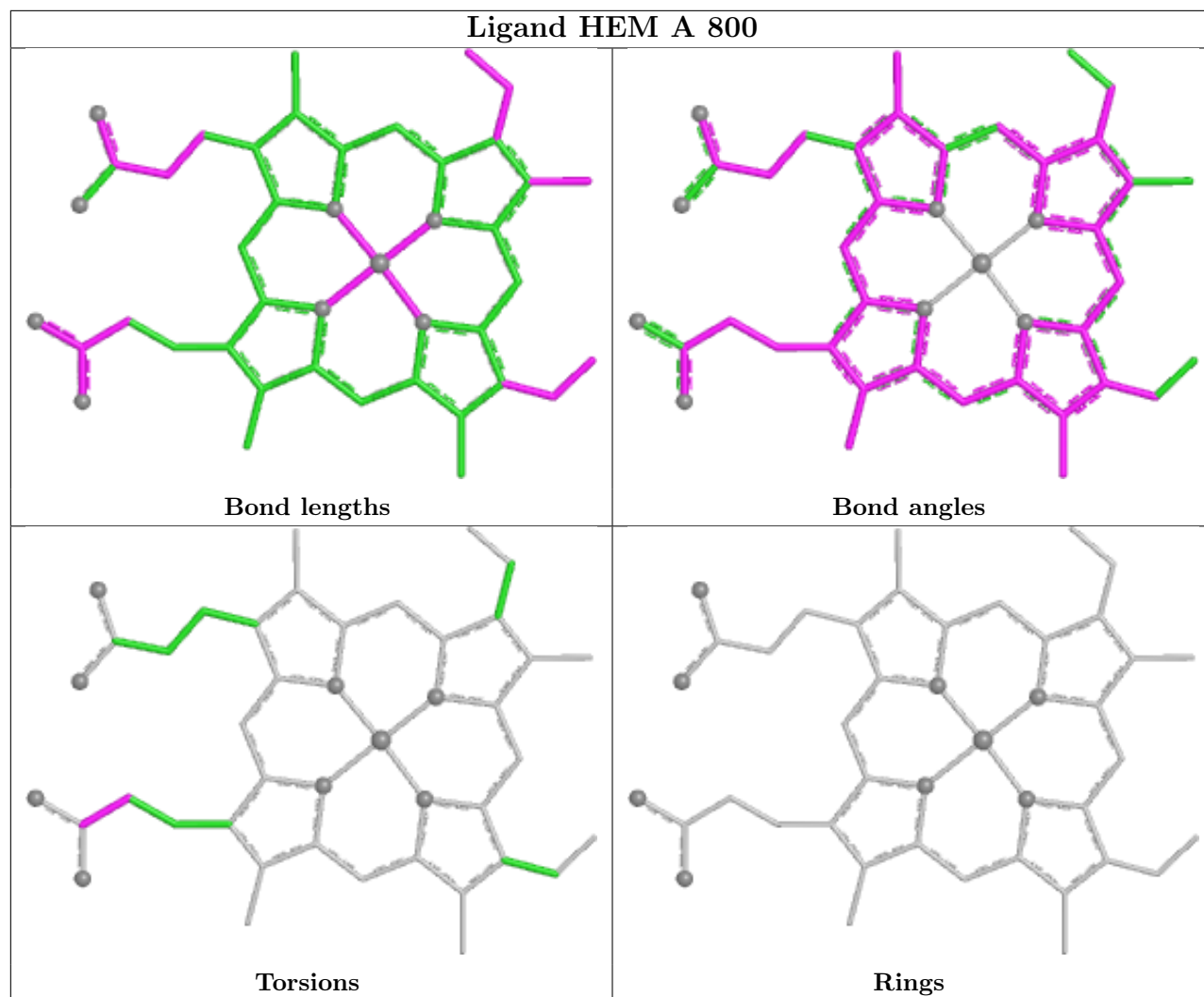
Mol	Chain	Res	Type	Atoms
2	A	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A

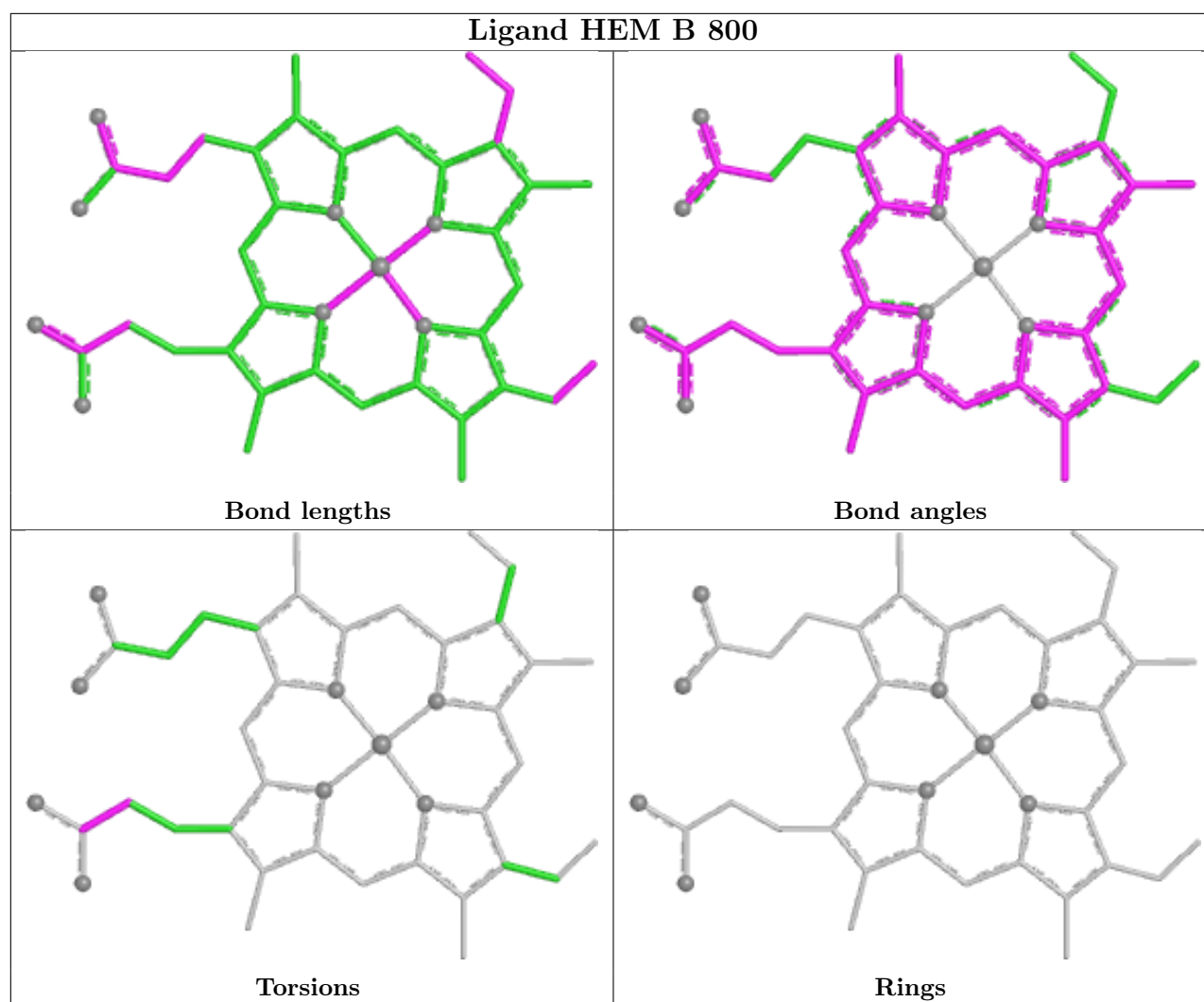
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	CYN	2	0
2	A	800	HEM	3	0
3	A	802	CYN	4	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.





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	711/737 (96%)	0.59	80 (11%)	10 10	13, 21, 41, 60	0
1	B	714/737 (96%)	1.15	145 (20%)	3 2	18, 29, 44, 60	0
All	All	1425/1474 (96%)	0.87	225 (15%)	5 4	13, 26, 43, 60	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLY	16.2
1	A	730	LEU	12.3
1	A	299	GLY	11.6
1	A	50	PHE	11.2
1	B	730	LEU	10.6
1	B	50	PHE	10.0
1	A	298	LYS	8.5
1	B	729	ASP	7.1
1	B	49	ASP	6.8
1	A	590	ASP	6.4
1	B	675	THR	6.2
1	B	590	ASP	6.1
1	B	19	ARG	6.1
1	A	18	LYS	5.9
1	B	296	ASN	5.8
1	B	517	GLU	5.7
1	A	729	ASP	5.6
1	B	20	PRO	5.6
1	B	46	VAL	5.5
1	A	591	ASP	5.4
1	B	455	ASP	5.3
1	A	361	ASP	5.2
1	B	457	ASP	5.1
1	B	21	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	294	ASN	5.1
1	A	19	ARG	5.0
1	B	591	ASP	5.0
1	A	21	LYS	4.9
1	B	299	GLY	4.8
1	B	293	LYS	4.8
1	B	731	GLU	4.8
1	B	295	GLY	4.7
1	A	665	GLU	4.5
1	A	48	ASP	4.5
1	B	48	ASP	4.5
1	A	294	ASN	4.5
1	A	727	ARG	4.4
1	B	437	ASP	4.4
1	B	41	ARG	4.4
1	A	347	SER	4.4
1	A	593	THR	4.3
1	B	663	ASP	4.3
1	A	22	SER	4.2
1	B	298	LYS	4.2
1	A	517	GLU	4.1
1	A	31	LEU	4.1
1	B	727	ARG	4.0
1	A	362	GLU	4.0
1	B	444	GLU	4.0
1	A	674	ASP	4.0
1	A	272	GLU	4.0
1	B	18	LYS	4.0
1	A	455	ASP	3.9
1	B	664	SER	3.9
1	A	554	GLU	3.9
1	A	20	PRO	3.9
1	B	362	GLU	3.8
1	A	445	GLU	3.7
1	B	346	LYS	3.7
1	B	364	GLN	3.7
1	A	49	ASP	3.7
1	B	451	GLU	3.7
1	A	364	GLN	3.7
1	A	191	ASP	3.7
1	A	47	GLU	3.6
1	A	731	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	351	LYS	3.6
1	B	440	LEU	3.6
1	B	674	ASP	3.6
1	A	415	GLU	3.5
1	B	271	GLU	3.5
1	B	409	LEU	3.5
1	B	347	SER	3.4
1	B	25	ASP	3.4
1	A	348	GLU	3.4
1	B	639	GLU	3.4
1	B	677	GLU	3.4
1	B	523	SER	3.4
1	A	301	GLU	3.4
1	A	728	PHE	3.4
1	A	632	ASP	3.3
1	A	663	ASP	3.3
1	B	54	GLU	3.3
1	B	200	ASP	3.3
1	B	706	ASP	3.3
1	B	359	ASP	3.3
1	B	588	ILE	3.3
1	B	42	ASP	3.3
1	A	706	ASP	3.2
1	B	349	GLU	3.2
1	B	593	THR	3.2
1	A	440	LEU	3.2
1	B	505	GLU	3.2
1	B	554	GLU	3.2
1	A	305	SER	3.2
1	A	522	ARG	3.2
1	B	300	GLY	3.2
1	B	191	ASP	3.2
1	B	24	GLN	3.1
1	B	208	GLY	3.1
1	B	229	ASP	3.1
1	B	436	ALA	3.1
1	B	394	GLU	3.1
1	A	271	GLU	3.1
1	B	57	GLN	3.0
1	A	390	GLU	3.0
1	B	667	ARG	3.0
1	B	348	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	25	ASP	3.0
1	B	728	PHE	3.0
1	B	354	VAL	2.9
1	A	349	GLU	2.9
1	B	502	GLU	2.9
1	A	34	GLU	2.9
1	B	665	GLU	2.9
1	B	329	TYR	2.9
1	B	503	GLN	2.9
1	A	293	LYS	2.9
1	B	301	GLU	2.9
1	B	578	LYS	2.9
1	B	361	ASP	2.8
1	B	676	GLY	2.8
1	B	624	ILE	2.8
1	A	675	THR	2.8
1	A	681	GLU	2.8
1	B	662	ALA	2.8
1	B	678	VAL	2.8
1	A	502	GLU	2.8
1	A	457	ASP	2.8
1	A	46	VAL	2.8
1	B	201	GLU	2.8
1	B	558	GLU	2.8
1	B	205	ILE	2.8
1	B	397	MET	2.8
1	A	424	ASP	2.8
1	A	638	ASP	2.7
1	A	441	ILE	2.7
1	B	330	GLU	2.7
1	B	32	ASN	2.7
1	A	437	ASP	2.7
1	A	42	ASP	2.6
1	A	435	ASP	2.6
1	A	448	GLU	2.6
1	A	677	GLU	2.6
1	B	638	ASP	2.6
1	A	664	SER	2.6
1	A	447	ALA	2.6
1	B	360	PRO	2.6
1	B	379	PRO	2.6
1	B	386	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	390	GLU	2.6
1	B	632	ASP	2.5
1	B	508	LEU	2.5
1	B	47	GLU	2.5
1	A	524	ASP	2.5
1	B	297	SER	2.5
1	B	575	ASP	2.5
1	B	579	PRO	2.5
1	B	69	GLU	2.5
1	B	62	GLU	2.4
1	B	384	VAL	2.4
1	B	341	TRP	2.4
1	B	34	GLU	2.4
1	B	335	LYS	2.4
1	A	521	SER	2.4
1	A	520	ASP	2.4
1	B	630	ASP	2.4
1	B	197	GLU	2.4
1	B	666	HIS	2.4
1	B	313	GLN	2.3
1	B	74	SER	2.3
1	A	657	GLU	2.3
1	B	553	VAL	2.3
1	A	444	GLU	2.3
1	A	558	GLU	2.3
1	A	624	ILE	2.3
1	B	441	ILE	2.3
1	A	346	LYS	2.3
1	B	522	ARG	2.3
1	B	43	VAL	2.3
1	B	267	ALA	2.2
1	B	549	ALA	2.2
1	B	382	ARG	2.2
1	A	454	LEU	2.2
1	B	51	ASP	2.2
1	B	439	ASP	2.2
1	B	445	GLU	2.2
1	A	667	ARG	2.2
1	B	176	GLU	2.2
1	B	649	VAL	2.2
1	A	29	SER	2.2
1	B	53	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	352	ASN	2.2
1	B	506	THR	2.2
1	B	559	PRO	2.2
1	B	66	SER	2.2
1	B	448	GLU	2.1
1	B	661	ALA	2.1
1	A	525	GLY	2.1
1	B	22	SER	2.1
1	B	218	TYR	2.1
1	B	231	GLU	2.1
1	B	337	PRO	2.1
1	B	568	HIS	2.1
1	A	575	ASP	2.1
1	B	60	ASP	2.1
1	B	204	GLU	2.1
1	B	383	GLU	2.1
1	A	57	GLN	2.1
1	B	424	ASP	2.1
1	A	41	ARG	2.1
1	B	387	THR	2.1
1	B	413	PRO	2.1
1	A	383	GLU	2.1
1	B	659	GLU	2.1
1	B	556	PRO	2.1
1	B	705	ALA	2.0
1	B	435	ASP	2.0
1	B	350	LEU	2.0
1	B	631	THR	2.0
1	B	230	PRO	2.0
1	B	207	GLU	2.0
1	B	415	GLU	2.0
1	B	199	PHE	2.0
1	B	167	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](#)

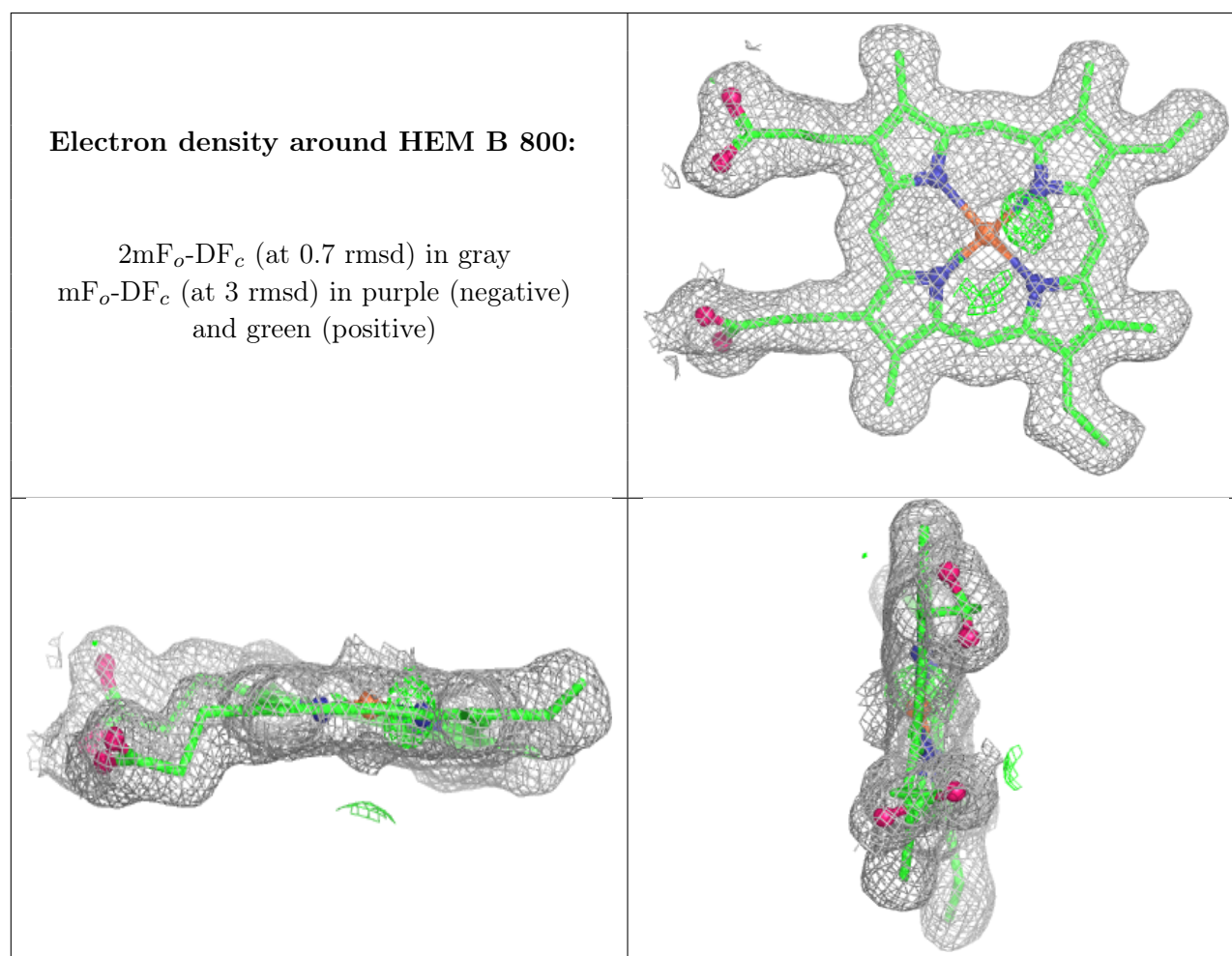
There are no oligosaccharides in this entry.

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.

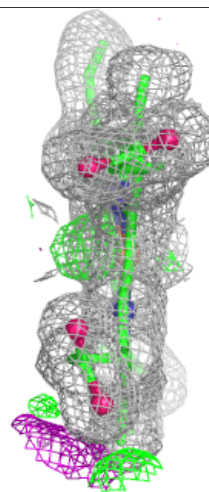
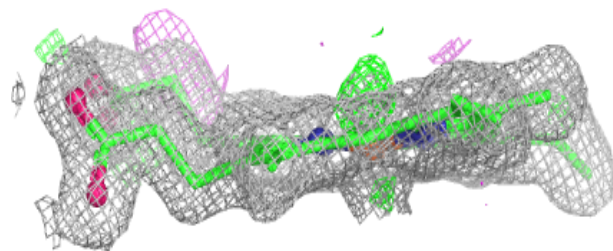
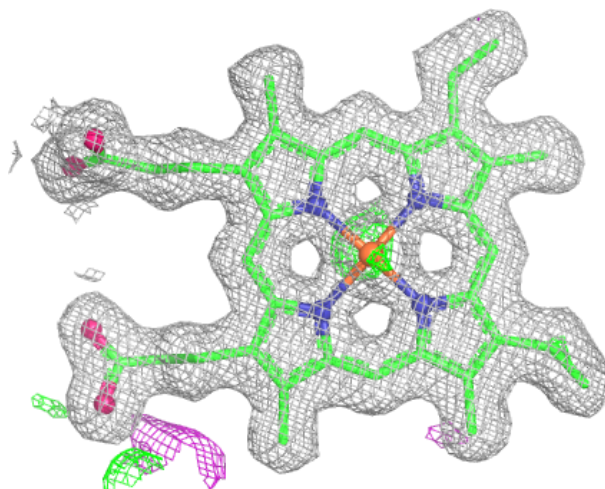
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CYN	B	802	2/2	0.38	0.56	47,47,47,48	0
3	CYN	A	802	2/2	0.68	0.34	34,34,34,36	0
2	HEM	B	800	43/43	0.98	0.07	19,22,25,28	0
2	HEM	A	800	43/43	0.99	0.05	12,14,17,22	0

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 800:

$2mF_o-DF_c$ (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.