



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 06:17 PM EST

PDB ID : 3UW8
Title : Crystal Structure Analysis of the Ser305Thr Variants of KatG from *Haloarcula marismortui*
Authors : Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on : 2011-12-01
Resolution : 2.35 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

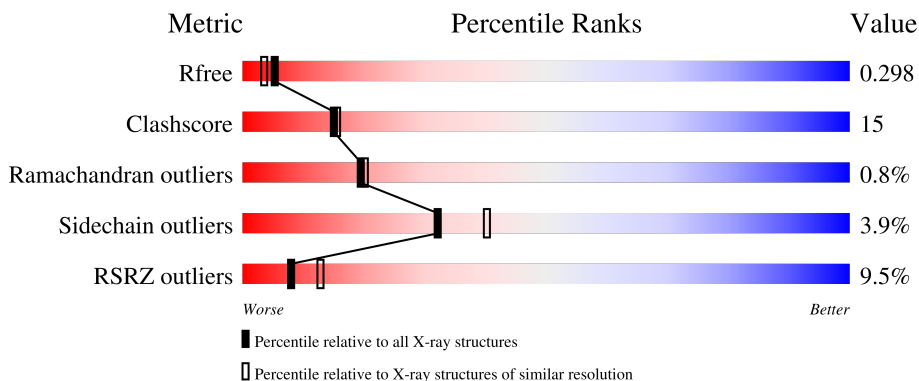
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

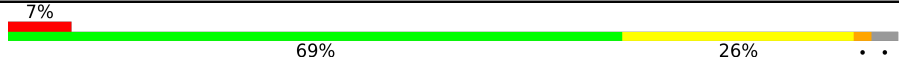
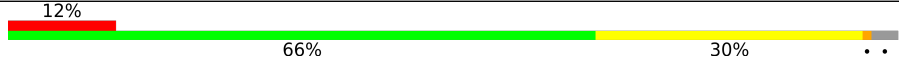
The reported resolution of this entry is 2.35 Å.

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	
1	B	737	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11563 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.

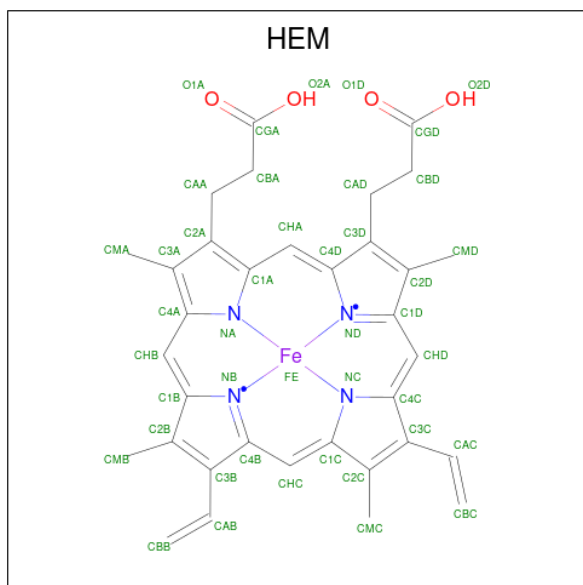
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	714	5621	3513	945	1144	19	0	0	0
1	B	714	5621	3513	945	1144	19	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	THR	SER	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	305	THR	SER	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 (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

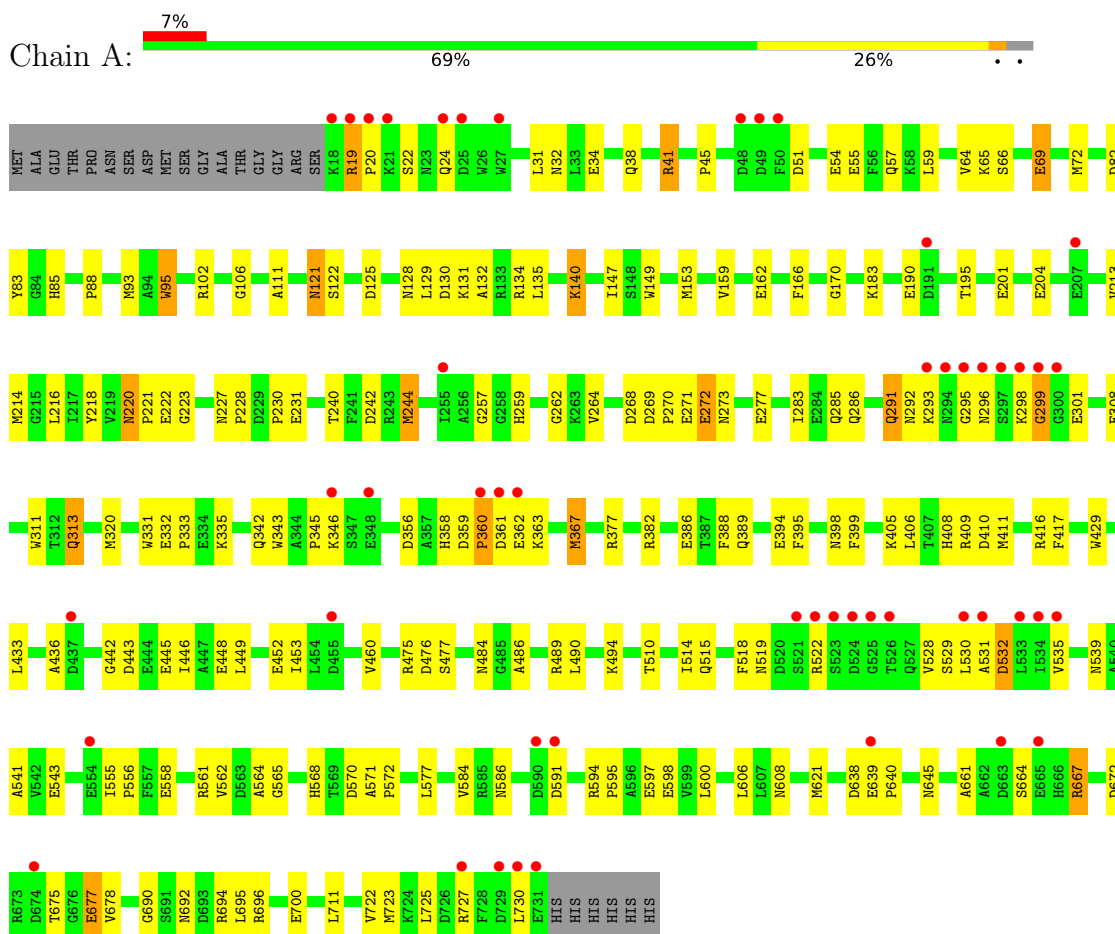
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	169	169	169	0	0
3	B	66	66	66	0	0

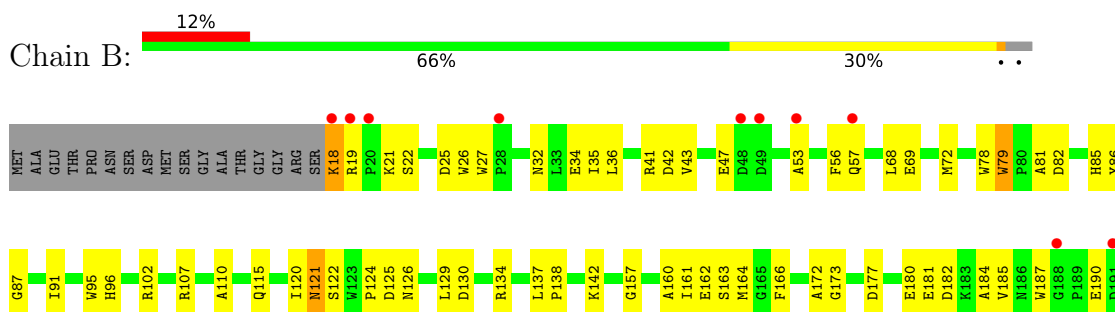
3 Residue-property plots [i](#)

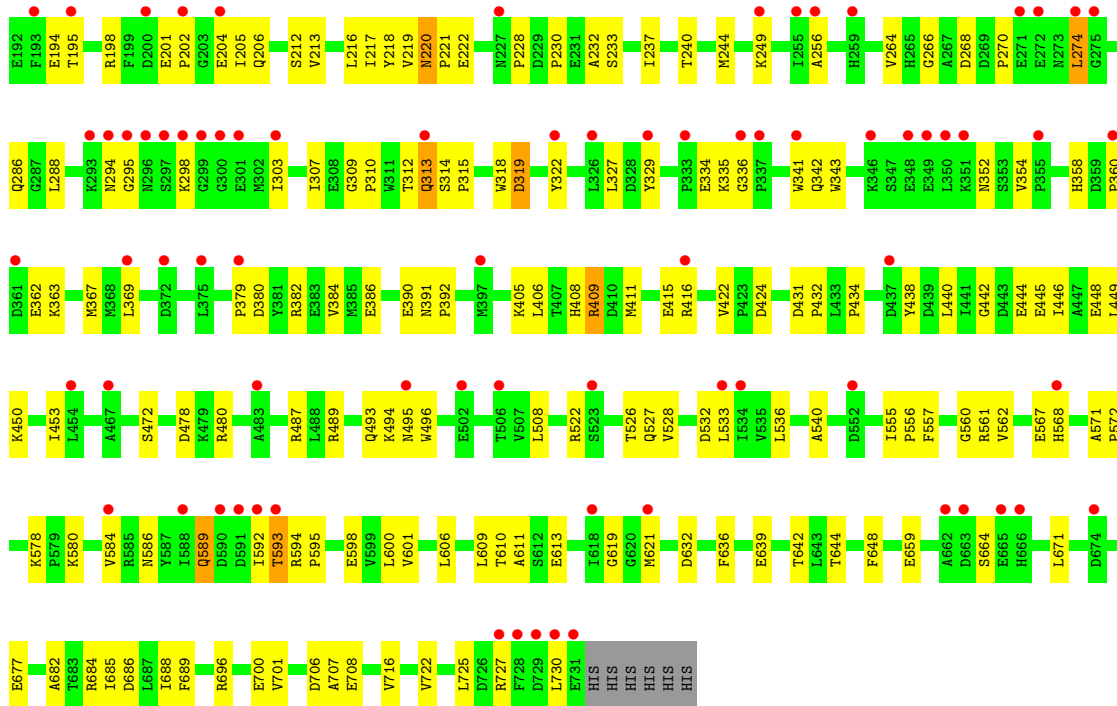
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	315.41Å 81.12Å 75.02Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	24.81 – 2.35 24.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.81-2.35) 99.6 (24.81-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.36Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.309 0.248 , 0.298	Depositor DCC
R_{free} test set	3920 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtrriage
Anisotropy	0.367	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: 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	0.45	0/5757	0.64	0/7822
1	B	0.39	0/5757	0.57	0/7822
All	All	0.42	0/11514	0.61	0/15644

There are no bond length outliers.

There are no bond angle outliers.

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	5621	0	5267	173	0
1	B	5621	0	5267	167	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	169	0	0	4	0
3	B	66	0	0	4	0
All	All	11563	0	10594	330	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 15.

All (330) 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:218:TYR:HE2	1:B:244:MET:SD	1.36	1.48
1:B:218:TYR:CE2	1:B:244:MET:SD	2.18	1.37
1:A:95:TRP:HH2	1:A:218:TYR:CE1	1.44	1.36
1:A:95:TRP:CH2	1:A:218:TYR:HE1	1.51	1.27
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.61	1.17
1:A:95:TRP:CH2	1:A:218:TYR:CE1	2.29	1.16
1:B:95:TRP:CZ2	1:B:218:TYR:HE1	1.66	1.12
1:A:41:ARG:HD2	1:B:41:ARG:HG2	1.34	1.05
1:B:95:TRP:CH2	1:B:218:TYR:CE1	2.46	1.03
1:A:41:ARG:HB3	1:B:41:ARG:HB3	1.40	1.02
1:B:295:GLY:HA3	1:B:298:LYS:HD3	1.50	0.93
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.55	0.93
1:A:675:THR:HG23	1:A:677:GLU:H	1.33	0.92
1:A:692:ASN:HD22	1:A:695:LEU:H	1.16	0.92
1:A:121:ASN:HD22	1:A:122:SER:N	1.71	0.89
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.56	0.88
1:A:518:PHE:O	1:A:522:ARG:HG2	1.78	0.84
1:B:172:ALA:H	1:B:408:HIS:HE1	1.26	0.84
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.99	0.79
1:A:672:ASP:HB3	1:A:675:THR:HG22	1.63	0.79
1:A:220:ASN:ND2	1:A:222:GLU:H	1.82	0.78
1:A:519:ASN:HD21	1:A:528:VAL:H	1.33	0.77
1:A:201:GLU:HB2	1:A:204:GLU:HG3	1.67	0.77
1:A:320:MET:CE	1:A:389:GLN:HA	2.15	0.76
1:A:489:ARG:O	1:A:494:LYS:HD2	1.87	0.75
1:A:41:ARG:HD2	1:B:41:ARG:CG	2.17	0.73
1:B:233:SER:O	1:B:237:ILE:HG13	1.89	0.73
1:A:727:ARG:HH22	1:A:730:LEU:HD12	1.53	0.72
1:A:565:GLY:H	1:A:568:HIS:HD2	1.35	0.72
1:A:111:ALA:HB2	1:A:410:ASP:OD2	1.91	0.70
1:A:95:TRP:HH2	1:A:218:TYR:CD1	2.09	0.70
1:A:19:ARG:H	1:A:19:ARG:HD3	1.56	0.70
1:B:53:ALA:O	1:B:57:GLN:HG2	1.92	0.69
1:A:692:ASN:ND2	1:A:695:LEU:H	1.89	0.69
1:B:202:PRO:HG2	1:B:232:ALA:HB1	1.74	0.69
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.75	0.68
1:B:18:LYS:HB2	1:B:18:LYS:NZ	2.09	0.68
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.76	0.68
1:A:220:ASN:HD22	1:A:220:ASN:C	1.98	0.67
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.75	0.67
1:B:220:ASN:ND2	1:B:222:GLU:H	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LEU:O	1:B:453:ILE:HG13	1.96	0.66
1:B:177:ASP:HB2	3:B:763:HOH:O	1.95	0.66
1:A:292:ASN:HB3	1:A:295:GLY:O	1.95	0.66
1:A:41:ARG:H	1:A:41:ARG:HD3	1.61	0.65
1:A:308:GLU:H	1:A:342:GLN:HE22	1.45	0.65
1:B:21:LYS:HE2	1:B:25:ASP:HB2	1.79	0.65
1:B:26:TRP:HB2	1:B:27:TRP:CE3	2.33	0.64
1:A:298:LYS:HG2	1:A:301:GLU:HB2	1.80	0.64
1:B:610:THR:OG1	1:B:613:GLU:HG3	1.99	0.63
1:A:271:GLU:O	1:A:272:GLU:HB2	1.96	0.63
1:A:273:ASN:O	1:A:293:LYS:HG2	1.99	0.63
1:B:449:LEU:HD22	1:B:533:LEU:HD21	1.81	0.63
1:A:295:GLY:O	1:A:298:LYS:HD2	1.99	0.63
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.81	0.62
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.80	0.62
1:A:489:ARG:HD3	1:A:530:LEU:HD23	1.82	0.62
1:A:140:LYS:HG2	1:A:149:TRP:CZ2	2.34	0.62
1:A:442:GLY:O	1:A:446:ILE:HG13	2.00	0.62
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.34	0.61
1:B:295:GLY:HA3	1:B:298:LYS:CD	2.26	0.61
1:B:137:LEU:HB3	1:B:138:PRO:HD3	1.82	0.61
1:B:264:VAL:HG22	1:B:309:GLY:O	1.99	0.61
1:A:72:MET:HG3	1:A:85:HIS:CE1	2.35	0.61
1:A:22:SER:OG	1:A:24:GLN:HG2	2.02	0.60
1:B:95:TRP:HZ3	1:B:406:LEU:HD11	1.67	0.60
1:B:600:LEU:HD22	1:B:685:ILE:HG23	1.84	0.59
1:A:220:ASN:HD22	1:A:221:PRO:N	2.00	0.59
1:A:88:PRO:HB3	1:A:262:GLY:HA3	1.85	0.59
1:B:126:ASN:HA	1:B:129:LEU:HD12	1.84	0.59
1:A:299:GLY:HA2	1:A:358:HIS:CE1	2.38	0.59
1:B:68:LEU:O	1:B:72:MET:HG2	2.03	0.58
1:A:696:ARG:O	1:A:700:GLU:HG3	2.04	0.58
1:B:220:ASN:HD22	1:B:222:GLU:H	1.51	0.58
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	2.17	0.57
1:B:220:ASN:HD22	1:B:220:ASN:C	2.07	0.57
1:B:431:ASP:N	1:B:432:PRO:HD3	2.19	0.57
1:B:32:ASN:OD1	1:B:34:GLU:HG2	2.03	0.57
1:B:442:GLY:O	1:B:446:ILE:HG13	2.04	0.57
1:A:220:ASN:HD22	1:A:222:GLU:H	1.52	0.57
1:A:244:MET:O	1:A:409:ARG:NH2	2.37	0.57
1:A:475:ARG:HB2	1:A:606:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:O	1:A:453:ILE:HG13	2.05	0.56
1:B:228:PRO:O	1:B:230:PRO:HD3	2.05	0.56
1:A:162:GLU:HA	1:A:166:PHE:O	2.05	0.56
1:B:172:ALA:H	1:B:408:HIS:CE1	2.17	0.56
1:B:218:TYR:CE2	1:B:244:MET:CE	2.89	0.56
1:A:675:THR:CG2	1:A:677:GLU:HB3	2.36	0.55
1:B:130:ASP:HB2	1:B:288:LEU:HD23	1.87	0.55
1:B:450:LYS:HD2	1:B:540:ALA:HB2	1.88	0.55
1:B:580:LYS:HB3	1:B:589:GLN:NE2	2.21	0.55
1:A:106:GLY:O	1:A:477:SER:HB2	2.07	0.55
1:B:107:ARG:HG2	1:B:185:VAL:HG22	1.87	0.55
1:A:360:PRO:HA	3:A:748:HOH:O	2.07	0.55
1:A:291:GLN:NE2	1:A:296:ASN:HB2	2.22	0.55
1:B:95:TRP:HZ2	1:B:218:TYR:CE1	2.21	0.54
1:B:218:TYR:CZ	1:B:244:MET:SD	2.95	0.54
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.89	0.54
1:B:220:ASN:HD22	1:B:221:PRO:N	2.06	0.54
1:A:490:LEU:HD11	1:A:564:ALA:O	2.08	0.54
1:A:121:ASN:HD22	1:A:121:ASN:C	2.03	0.53
1:A:140:LYS:HD3	1:A:149:TRP:CD2	2.44	0.53
1:A:59:LEU:HD11	1:A:64:VAL:HG21	1.90	0.53
1:A:291:GLN:HE21	1:A:296:ASN:HB2	1.73	0.53
1:B:411:MET:O	1:B:416:ARG:HD3	2.09	0.53
1:A:298:LYS:HE3	3:A:757:HOH:O	2.07	0.53
1:A:486:ALA:HB2	1:A:531:ALA:HB2	1.89	0.53
1:A:140:LYS:HE3	1:A:147:ILE:O	2.08	0.53
1:B:95:TRP:CD1	1:B:96:HIS:HD2	2.27	0.53
1:A:356:ASP:HB2	1:A:362:GLU:OE2	2.09	0.52
1:A:394:GLU:O	1:A:398:ASN:ND2	2.42	0.52
1:A:230:PRO:HB2	1:A:377:ARG:HG3	1.91	0.52
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.92	0.52
1:B:639:GLU:O	1:B:642:THR:HB	2.10	0.52
1:B:567:GLU:HG2	1:B:568:HIS:HD1	1.75	0.52
1:A:190:GLU:HG2	1:A:195:THR:O	2.10	0.52
1:A:445:GLU:HG2	1:A:518:PHE:HZ	1.75	0.52
1:A:535:VAL:HG13	1:A:723:MET:SD	2.50	0.51
1:A:433:LEU:HD13	1:A:484:ASN:ND2	2.25	0.51
1:B:18:LYS:HB2	1:B:18:LYS:HZ3	1.75	0.51
1:B:440:LEU:CD2	1:B:560:GLY:HA2	2.40	0.51
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.92	0.51
1:A:561:ARG:HG3	1:A:561:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HG22	1:B:166:PHE:HB3	1.93	0.50
1:B:445:GLU:OE2	1:B:526:THR:HG21	2.11	0.50
1:A:32:ASN:OD1	1:A:34:GLU:HG2	2.12	0.50
1:B:595:PRO:HD2	1:B:598:GLU:OE2	2.11	0.50
1:B:567:GLU:HG2	1:B:568:HIS:H	1.75	0.50
1:B:659:GLU:OE2	1:B:671:LEU:HD11	2.12	0.50
1:B:310:PRO:HG3	1:B:354:VAL:HG11	1.93	0.50
1:B:382:ARG:O	1:B:386:GLU:HG3	2.12	0.50
1:A:436:ALA:HB2	1:A:562:VAL:HG12	1.93	0.50
1:B:343:TRP:N	1:B:343:TRP:CD1	2.79	0.50
1:A:38:GLN:NE2	1:A:183:LYS:HG3	2.27	0.50
1:A:292:ASN:OD1	1:A:298:LYS:HE2	2.12	0.50
1:A:411:MET:O	1:A:416:ARG:HD3	2.12	0.50
1:B:180:GLU:HG3	1:B:181:GLU:O	2.12	0.49
1:B:185:VAL:HG11	1:B:187:TRP:CZ2	2.47	0.49
1:A:298:LYS:HE3	1:A:301:GLU:HB3	1.94	0.49
1:A:594:ARG:HD3	1:B:18:LYS:HG2	1.95	0.49
1:B:727:ARG:HH21	1:B:730:LEU:HD21	1.78	0.49
1:B:567:GLU:HG2	1:B:568:HIS:ND1	2.26	0.49
1:A:111:ALA:CB	1:A:410:ASP:OD2	2.59	0.49
1:A:121:ASN:C	1:A:121:ASN:ND2	2.65	0.49
1:A:122:SER:HB3	1:A:277:GLU:HG3	1.95	0.49
1:A:132:ALA:HA	1:A:135:LEU:HD12	1.95	0.49
1:A:140:LYS:HG2	1:A:149:TRP:CE2	2.48	0.49
1:A:283:ILE:HG21	1:B:684:ARG:NH1	2.27	0.49
1:A:722:VAL:HA	1:A:725:LEU:HG	1.94	0.49
1:B:182:ASP:OD1	1:B:184:ALA:HB3	2.13	0.49
1:A:264:VAL:HG12	2:A:800:HEM:HAA1	1.94	0.49
1:A:443:ASP:HA	1:A:446:ILE:HD12	1.94	0.49
1:B:162:GLU:HA	1:B:166:PHE:O	2.13	0.49
1:B:256:ALA:HA	1:B:322:TYR:CE2	2.47	0.49
1:A:445:GLU:O	1:A:448:GLU:HB3	2.13	0.48
1:B:358:HIS:O	1:B:360:PRO:HD3	2.14	0.48
1:A:230:PRO:CB	1:A:377:ARG:HG3	2.43	0.48
1:A:452:GLU:HG2	1:A:514:ILE:HG23	1.95	0.48
1:A:460:VAL:HG13	1:A:541:ALA:HB1	1.95	0.48
1:A:539:ASN:O	1:A:543:GLU:HG3	2.14	0.48
1:A:558:GLU:HB3	1:A:727:ARG:NH1	2.28	0.48
1:B:327:LEU:HD22	1:B:382:ARG:HE	1.79	0.48
1:B:157:GLY:O	1:B:161:ILE:HG13	2.13	0.48
1:B:390:GLU:O	1:B:392:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ARG:HG3	1:B:526:THR:O	2.13	0.48
1:B:567:GLU:CG	1:B:568:HIS:HD1	2.27	0.48
1:A:320:MET:HE1	1:A:389:GLN:HA	1.89	0.48
1:B:32:ASN:CG	1:B:34:GLU:HG2	2.34	0.48
1:B:536:LEU:HG	1:B:557:PHE:CZ	2.49	0.48
1:A:277:GLU:H	1:A:277:GLU:CD	2.17	0.47
1:A:140:LYS:HD3	1:A:149:TRP:CE2	2.49	0.47
1:A:292:ASN:CG	1:A:298:LYS:HE2	2.35	0.47
1:A:298:LYS:CG	1:A:301:GLU:HB2	2.44	0.47
1:A:727:ARG:CZ	1:A:727:ARG:HB3	2.44	0.47
1:B:405:LYS:O	1:B:409:ARG:HB3	2.14	0.47
1:A:332:GLU:CG	1:A:346:LYS:HE2	2.44	0.47
1:A:228:PRO:O	1:A:230:PRO:HD3	2.14	0.47
1:B:198:ARG:HD2	1:B:212:SER:C	2.34	0.47
1:B:87:GLY:O	1:B:91:ILE:HG13	2.14	0.47
1:A:31:LEU:HD13	1:A:597:GLU:HG3	1.97	0.47
1:A:382:ARG:O	1:A:386:GLU:HG2	2.14	0.47
1:B:444:GLU:O	1:B:448:GLU:HG3	2.15	0.47
1:B:494:LYS:HE3	1:B:495:ASN:HD21	1.80	0.47
1:B:682:ALA:HB1	1:B:686:ASP:HB2	1.97	0.47
1:A:190:GLU:HB2	1:A:214:MET:HB2	1.97	0.47
1:A:416:ARG:HB3	1:A:416:ARG:NH1	2.29	0.47
1:B:434:PRO:HD3	1:B:568:HIS:NE2	2.30	0.47
1:A:170:GLY:HA2	3:A:856:HOH:O	2.15	0.46
1:A:313:GLN:O	1:A:313:GLN:HG3	2.15	0.46
1:B:41:ARG:NH1	1:B:43:VAL:HG13	2.30	0.46
1:B:21:LYS:HE2	1:B:25:ASP:CB	2.45	0.46
1:A:675:THR:HG23	1:A:677:GLU:HB3	1.98	0.46
1:A:595:PRO:HD2	1:A:598:GLU:OE2	2.16	0.46
1:A:41:ARG:H	1:A:41:ARG:CD	2.28	0.46
1:A:405:LYS:HA	1:A:429:TRP:CZ2	2.51	0.46
1:A:257:GLY:HA3	1:A:399:PHE:CD2	2.51	0.46
1:A:645:ASN:HA	1:A:711:LEU:HD23	1.98	0.46
1:B:307:ILE:HD13	1:B:369:LEU:HD22	1.98	0.46
1:A:638:ASP:C	1:A:640:PRO:HD3	2.36	0.46
1:A:690:GLY:HA3	1:B:286:GLN:NE2	2.31	0.46
1:B:722:VAL:HA	1:B:725:LEU:HG	1.97	0.46
1:A:677:GLU:HG2	1:A:678:VAL:N	2.30	0.46
1:B:78:TRP:O	1:B:79:TRP:HB2	2.16	0.45
1:B:249:LYS:HD3	1:B:384:VAL:HG13	1.97	0.45
1:A:121:ASN:ND2	1:A:122:SER:N	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASP:CG	1:A:54:GLU:HG3	2.37	0.45
1:A:220:ASN:ND2	1:A:220:ASN:C	2.68	0.45
1:A:223:GLY:HA3	1:A:227:ASN:O	2.17	0.45
1:B:219:VAL:HG13	1:B:240:THR:HG21	1.99	0.45
1:A:320:MET:HE2	1:A:389:GLN:HA	1.96	0.45
1:A:510:THR:O	1:A:514:ILE:HG13	2.17	0.45
1:B:489:ARG:HB3	1:B:508:LEU:HD13	1.97	0.45
1:B:610:THR:O	1:B:611:ALA:C	2.55	0.45
1:B:142:LYS:HG3	3:B:775:HOH:O	2.16	0.45
1:B:487:ARG:HB3	1:B:493:GLN:NE2	2.32	0.45
1:B:82:ASP:OD2	1:B:358:HIS:NE2	2.50	0.45
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.96	0.45
1:B:190:GLU:HG2	1:B:195:THR:O	2.17	0.45
1:B:592:ILE:O	1:B:592:ILE:HG13	2.17	0.45
1:A:242:ASP:C	1:A:244:MET:H	2.20	0.45
1:B:125:ASP:OD2	1:B:217:ILE:HG12	2.17	0.45
1:A:298:LYS:HE3	1:A:301:GLU:CB	2.47	0.44
1:B:107:ARG:NH2	1:B:184:ALA:HB1	2.32	0.44
1:A:134:ARG:CZ	1:B:696:ARG:NH2	2.81	0.44
1:A:149:TRP:O	1:A:153:MET:HG3	2.18	0.44
1:B:110:ALA:HB1	3:B:742:HOH:O	2.18	0.44
1:A:259:HIS:CD2	1:A:311:TRP:CZ2	3.06	0.44
1:A:308:GLU:O	1:A:367:MET:HG2	2.18	0.44
1:B:115:GLN:HA	1:B:120:ILE:HG21	2.00	0.44
1:B:205:ILE:HG22	1:B:206:GLN:N	2.33	0.44
1:A:93:MET:HB2	1:A:129:LEU:HD22	1.99	0.44
1:A:240:THR:O	1:A:244:MET:HG3	2.17	0.44
1:A:332:GLU:HG3	1:A:346:LYS:HE2	1.98	0.44
1:A:405:LYS:O	1:A:409:ARG:HB2	2.17	0.44
1:A:555:ILE:HA	1:A:556:PRO:HD3	1.90	0.44
1:B:72:MET:O	1:B:85:HIS:HA	2.17	0.44
1:B:95:TRP:CD1	1:B:96:HIS:CD2	3.06	0.44
1:A:664:SER:HG	1:A:667:ARG:H	1.66	0.44
1:A:664:SER:OG	1:A:667:ARG:HB2	2.18	0.44
1:A:690:GLY:HA3	1:B:286:GLN:HE22	1.82	0.44
1:B:440:LEU:HD21	1:B:560:GLY:HA2	1.99	0.44
1:A:475:ARG:CZ	1:A:577:LEU:CD2	2.96	0.43
1:B:619:GLY:HA3	1:B:648:PHE:CZ	2.53	0.43
1:B:41:ARG:HD2	1:B:41:ARG:O	2.18	0.43
1:A:65:LYS:HE3	1:A:159:VAL:HG22	2.01	0.43
1:A:298:LYS:HG2	1:A:301:GLU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ARG:HG3	1:A:561:ARG:NH1	2.33	0.43
1:A:696:ARG:NH2	1:B:134:ARG:CZ	2.81	0.43
1:B:329:TYR:CD1	1:B:329:TYR:N	2.87	0.43
1:A:332:GLU:HG3	1:A:346:LYS:HG2	1.99	0.43
1:B:528:VAL:O	1:B:528:VAL:HG13	2.17	0.43
1:B:201:GLU:HB2	1:B:204:GLU:HG3	2.01	0.43
1:B:270:PRO:HB3	1:B:303:ILE:HG22	2.00	0.43
1:B:335:LYS:HE3	1:B:341:TRP:CE2	2.54	0.43
1:A:286:GLN:N	3:A:833:HOH:O	2.51	0.43
1:A:356:ASP:HB2	1:A:362:GLU:CD	2.39	0.43
1:A:362:GLU:HG2	1:A:363:LYS:N	2.34	0.43
1:A:296:ASN:C	1:A:298:LYS:H	2.23	0.43
1:B:115:GLN:HA	1:B:120:ILE:CG2	2.49	0.43
1:B:555:ILE:HG12	1:B:716:VAL:CG1	2.49	0.43
1:A:66:SER:O	1:A:69:GLU:HB2	2.18	0.42
1:A:515:GLN:HE21	1:A:515:GLN:HB3	1.64	0.42
1:B:318:TRP:O	1:B:319:ASP:HB3	2.18	0.42
1:A:692:ASN:ND2	1:A:694:ARG:H	2.16	0.42
1:B:95:TRP:HZ3	1:B:406:LEU:CD1	2.33	0.42
1:A:59:LEU:HD11	1:A:64:VAL:CG2	2.49	0.42
1:B:438:TYR:CG	1:B:527:GLN:HB2	2.54	0.42
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.19	0.42
1:A:597:GLU:HG2	1:A:598:GLU:N	2.35	0.42
1:B:688:ILE:HG23	1:B:689:PHE:N	2.33	0.42
1:A:82:ASP:HB3	1:A:83:TYR:CD1	2.54	0.42
1:A:406:LEU:HD12	1:A:409:ARG:NH1	2.34	0.42
1:A:692:ASN:ND2	1:A:694:ARG:N	2.67	0.42
1:B:172:ALA:HB2	1:B:422:VAL:HG22	2.02	0.42
1:A:359:ASP:HA	1:A:360:PRO:HD3	1.76	0.42
1:A:417:PHE:CD2	1:A:417:PHE:N	2.88	0.42
1:A:476:ASP:CB	1:A:608:ASN:HD21	2.33	0.42
1:B:536:LEU:HG	1:B:557:PHE:CE2	2.55	0.42
1:B:606:LEU:HD23	1:B:606:LEU:HA	1.87	0.42
1:A:331:TRP:CZ3	1:A:345:PRO:HG3	2.54	0.42
1:A:388:PHE:CG	1:A:395:PHE:HB2	2.55	0.42
1:A:408:HIS:HB3	1:A:417:PHE:CE1	2.55	0.41
1:B:434:PRO:O	1:B:562:VAL:HG21	2.20	0.41
1:B:701:VAL:O	1:B:707:ALA:HB2	2.19	0.41
1:A:19:ARG:HD3	1:A:19:ARG:N	2.28	0.41
1:A:597:GLU:O	1:A:600:LEU:HB3	2.20	0.41
1:A:268:ASP:OD1	1:A:269:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:H	1:B:47:GLU:HG2	1.70	0.41
1:B:121:ASN:HD22	1:B:122:SER:N	2.17	0.41
1:B:295:GLY:HA3	1:B:298:LYS:CE	2.50	0.41
1:A:134:ARG:HD3	1:A:134:ARG:HA	1.88	0.41
1:B:81:ALA:HB2	1:B:86:TYR:CZ	2.55	0.41
1:B:160:ALA:O	1:B:164:MET:HG3	2.21	0.41
1:B:295:GLY:CA	1:B:298:LYS:HD3	2.35	0.41
1:B:314:SER:N	1:B:315:PRO:HD3	2.35	0.41
1:A:529:SER:OG	1:A:532:ASP:HB2	2.20	0.41
1:B:440:LEU:HD22	1:B:560:GLY:HA2	2.03	0.41
1:B:532:ASP:OD1	1:B:561:ARG:HB2	2.20	0.41
1:B:584:VAL:HG13	1:B:621:MET:CG	2.40	0.41
1:B:593:THR:HG23	1:B:594:ARG:H	1.86	0.41
1:A:231:GLU:CD	1:A:231:GLU:H	2.24	0.41
1:A:672:ASP:CB	1:A:675:THR:HG22	2.41	0.41
1:B:36:LEU:HD22	1:B:609:LEU:O	2.20	0.41
1:B:294:ASN:O	1:B:298:LYS:HE3	2.21	0.41
1:B:352:ASN:HB3	1:B:363:LYS:CB	2.51	0.41
1:B:696:ARG:O	1:B:700:GLU:HG3	2.20	0.41
1:B:124:PRO:HG2	1:B:194:GLU:HG3	2.02	0.41
1:B:478:ASP:CG	1:B:480:ARG:HG3	2.41	0.41
1:B:312:THR:HB	3:B:793:HOH:O	2.21	0.40
1:B:555:ILE:HA	1:B:556:PRO:HD3	1.98	0.40
1:A:269:ASP:HA	1:A:270:PRO:HD3	1.85	0.40
1:B:18:LYS:HB2	1:B:18:LYS:HZ2	1.85	0.40
1:B:56:PHE:CZ	1:B:173:GLY:HA3	2.56	0.40
1:B:95:TRP:HH2	1:B:218:TYR:CZ	2.36	0.40
1:B:268:ASP:H	1:B:303:ILE:HG12	1.85	0.40
1:B:270:PRO:CB	1:B:274:LEU:HD22	2.51	0.40
1:B:336:GLY:HA3	1:B:342:GLN:NE2	2.36	0.40
1:B:352:ASN:N	1:B:352:ASN:HD22	2.19	0.40
1:B:493:GLN:HG2	1:B:496:TRP:CH2	2.56	0.40
1:B:644:THR:HB	1:B:708:GLU:OE1	2.21	0.40
1:A:134:ARG:NE	1:B:696:ARG:HH21	2.19	0.40
1:B:578:LYS:HE2	1:B:578:LYS:HB3	1.87	0.40
1:B:636:PHE:HZ	1:B:682:ALA:HB2	1.86	0.40
1:A:486:ALA:HB3	1:A:489:ARG:NH1	2.37	0.40
1:B:69:GLU:HG3	1:B:163:SER:HB3	2.02	0.40
1:A:486:ALA:O	1:A:489:ARG:HG2	2.22	0.40
1:A:570:ASP:OD1	1:A:570:ASP:C	2.59	0.40
1:A:661:ALA:O	1:A:664:SER:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:HA	1:B:221:PRO:HD2	1.98	0.40
1:B:380:ASP:O	1:B:384:VAL:HG23	2.22	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	712/737 (97%)	655 (92%)	52 (7%)	5 (1%)	22	23
1	B	712/737 (97%)	651 (91%)	54 (8%)	7 (1%)	15	15
All	All	1424/1474 (97%)	1306 (92%)	106 (7%)	12 (1%)	19	20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLU
1	A	299	GLY
1	A	591	ASP
1	B	22	SER
1	B	379	PRO
1	B	472	SER
1	B	706	ASP
1	A	20	PRO
1	B	266	GLY
1	B	319	ASP
1	A	360	PRO
1	B	79	TRP

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	590/608 (97%)	565 (96%)	25 (4%)	30	36
1	B	590/608 (97%)	569 (96%)	21 (4%)	35	43
All	All	1180/1216 (97%)	1134 (96%)	46 (4%)	32	40

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	41	ARG
1	A	45	PRO
1	A	55	GLU
1	A	57	GLN
1	A	69	GLU
1	A	95	TRP
1	A	102	ARG
1	A	121	ASN
1	A	125	ASP
1	A	131	LYS
1	A	140	LYS
1	A	220	ASN
1	A	244	MET
1	A	285	GLN
1	A	291	GLN
1	A	313	GLN
1	A	335	LYS
1	A	361	ASP
1	A	367	MET
1	A	532	ASP
1	A	586	ASN
1	A	639	GLU
1	A	667	ARG
1	A	677	GLU
1	B	18	LYS
1	B	19	ARG

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Mol	Chain	Res	Type
1	B	42	ASP
1	B	102	ARG
1	B	121	ASN
1	B	220	ASN
1	B	274	LEU
1	B	313	GLN
1	B	334	GLU
1	B	362	GLU
1	B	367	MET
1	B	391	ASN
1	B	409	ARG
1	B	415	GLU
1	B	424	ASP
1	B	586	ASN
1	B	589	GLN
1	B	593	THR
1	B	632	ASP
1	B	664	SER
1	B	677	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	206	GLN
1	A	220	ASN
1	A	286	GLN
1	A	291	GLN
1	A	342	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	24	GLN
1	B	96	HIS
1	B	121	ASN
1	B	220	ASN
1	B	227	ASN
1	B	286	GLN

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Mol	Chain	Res	Type
1	B	324	ASN
1	B	342	GLN
1	B	352	ASN
1	B	364	GLN
1	B	389	GLN
1	B	408	HIS
1	B	493	GLN
1	B	495	ASN
1	B	515	GLN
1	B	527	GLN
1	B	586	ASN
1	B	589	GLN
1	B	608	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	HEM	A	800	1	41,50,50	2.49	12 (29%)	45,82,82	10.83	30 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	800	1	41,50,50	2.28	11 (26%)	45,82,82	9.80	29 (64%)

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	-	5/12/54/54	-
2	HEM	B	800	1	-	3/12/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	FE-ND	7.41	2.33	1.96
2	A	800	HEM	FE-ND	7.00	2.31	1.96
2	A	800	HEM	FE-NB	6.92	2.31	1.96
2	A	800	HEM	CBB-CAB	5.30	1.56	1.30
2	B	800	HEM	CBB-CAB	5.19	1.56	1.30
2	A	800	HEM	C3C-C2C	-4.69	1.33	1.40
2	A	800	HEM	CBA-CGA	-4.44	1.40	1.50
2	B	800	HEM	CBD-CGD	-4.24	1.40	1.50
2	A	800	HEM	CBD-CGD	-4.23	1.40	1.50
2	B	800	HEM	FE-NB	4.08	2.17	1.96
2	B	800	HEM	C3C-C2C	-4.07	1.34	1.40
2	A	800	HEM	CBC-CAC	4.00	1.55	1.29
2	B	800	HEM	CBC-CAC	3.94	1.55	1.29
2	B	800	HEM	CBA-CGA	-3.88	1.41	1.50
2	A	800	HEM	C3C-CAC	2.79	1.53	1.47
2	A	800	HEM	CBD-CAD	2.49	1.59	1.52
2	B	800	HEM	C4D-ND	-2.47	1.36	1.40
2	B	800	HEM	O1A-CGA	2.45	1.30	1.22
2	B	800	HEM	C3C-CAC	2.45	1.52	1.47
2	A	800	HEM	C4D-ND	-2.44	1.36	1.40
2	A	800	HEM	CHA-C4D	2.36	1.41	1.35
2	A	800	HEM	O1A-CGA	2.30	1.29	1.22
2	B	800	HEM	CBD-CAD	2.16	1.58	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	C4C-CHD-C1D	39.38	174.53	122.56
2	B	800	HEM	C4B-CHC-C1C	31.73	164.44	122.56
2	A	800	HEM	C4B-CHC-C1C	30.02	162.18	122.56
2	B	800	HEM	C4C-CHD-C1D	27.15	158.38	122.56
2	A	800	HEM	CHD-C1D-ND	-22.20	100.32	124.43
2	B	800	HEM	CHC-C4B-NB	-21.09	101.52	124.43
2	A	800	HEM	CHC-C4B-NB	-20.28	102.39	124.43
2	B	800	HEM	CHA-C4D-ND	-20.15	99.48	124.38
2	A	800	HEM	CHA-C4D-ND	-19.63	100.12	124.38
2	B	800	HEM	CHC-C4B-C3B	19.60	154.57	124.57
2	A	800	HEM	CHB-C1B-NB	-16.53	103.96	124.38
2	A	800	HEM	CHA-C4D-C3D	15.17	153.81	125.33
2	B	800	HEM	CHD-C1D-ND	-14.57	108.61	124.43
2	A	800	HEM	CHD-C1D-C2D	14.20	147.16	124.98
2	A	800	HEM	CHC-C4B-C3B	14.09	146.13	124.57
2	B	800	HEM	CHB-C1B-NB	-13.26	108.00	124.38
2	B	800	HEM	O2D-CGD-O1D	-12.52	92.10	123.30
2	B	800	HEM	CHA-C4D-C3D	11.87	147.61	125.33
2	A	800	HEM	C4A-C3A-C2A	-11.72	98.84	107.00
2	B	800	HEM	C4B-C3B-C2B	10.05	115.09	107.11
2	B	800	HEM	CHD-C1D-C2D	9.88	140.41	124.98
2	B	800	HEM	C3B-C2B-C1B	-9.39	99.52	106.49
2	A	800	HEM	CMC-C2C-C3C	9.26	142.00	124.68
2	A	800	HEM	CAD-C3D-C4D	-7.87	110.90	124.66
2	A	800	HEM	C2C-C3C-C4C	7.67	112.26	106.90
2	B	800	HEM	CAD-C3D-C4D	-7.07	112.31	124.66
2	B	800	HEM	O1D-CGD-CBD	6.70	144.61	123.08
2	B	800	HEM	C4A-C3A-C2A	-6.42	102.53	107.00
2	B	800	HEM	O2A-CGA-O1A	-6.07	108.17	123.30
2	B	800	HEM	CAD-C3D-C2D	6.01	139.07	127.88
2	A	800	HEM	CHB-C1B-C2B	5.94	143.16	126.72
2	A	800	HEM	CMB-C2B-C1B	-5.71	116.34	125.04
2	A	800	HEM	CBA-CAA-C2A	5.47	121.95	112.62
2	B	800	HEM	C2C-C3C-C4C	-5.40	103.13	106.90
2	A	800	HEM	C1D-C2D-C3D	-5.37	101.32	106.96
2	B	800	HEM	CBA-CAA-C2A	5.35	121.76	112.62
2	A	800	HEM	C3C-C4C-NC	-5.29	100.95	110.94
2	A	800	HEM	CAD-C3D-C2D	4.46	136.18	127.88
2	A	800	HEM	O1D-CGD-CBD	-4.19	109.61	123.08
2	A	800	HEM	C4D-C3D-C2D	4.13	112.92	106.90
2	A	800	HEM	C3D-C4D-ND	-3.94	105.78	110.17
2	B	800	HEM	CAA-CBA-CGA	-3.84	102.99	113.76
2	B	800	HEM	C2B-C1B-NB	3.75	114.28	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CHB-C1B-C2B	3.40	136.12	126.72
2	B	800	HEM	O1A-CGA-CBA	3.40	133.99	123.08
2	A	800	HEM	CMA-C3A-C2A	3.12	130.83	124.94
2	B	800	HEM	O2D-CGD-CBD	2.88	123.30	114.03
2	B	800	HEM	CAA-C2A-C3A	2.59	134.68	127.25
2	A	800	HEM	CBB-CAB-C3B	-2.55	114.95	127.62
2	A	800	HEM	C4D-ND-C1D	2.34	107.49	105.07
2	A	800	HEM	O2D-CGD-CBD	2.30	121.41	114.03
2	A	800	HEM	O2D-CGD-O1D	2.28	128.98	123.30
2	A	800	HEM	CMD-C2D-C1D	2.28	128.51	125.04
2	B	800	HEM	C4D-ND-C1D	2.27	107.42	105.07
2	B	800	HEM	C1B-NB-C4B	2.25	107.39	105.07
2	A	800	HEM	C2D-C1D-ND	2.18	112.49	109.88
2	B	800	HEM	CAB-C3B-C4B	-2.13	114.54	124.47
2	B	800	HEM	CMC-C2C-C3C	2.08	128.58	124.68
2	A	800	HEM	C2B-C1B-NB	2.05	112.27	109.84

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	C2B-C3B-CAB-CBB
2	A	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAD-CBD-CGD-O2D
2	A	800	HEM	CAD-CBD-CGD-O1D

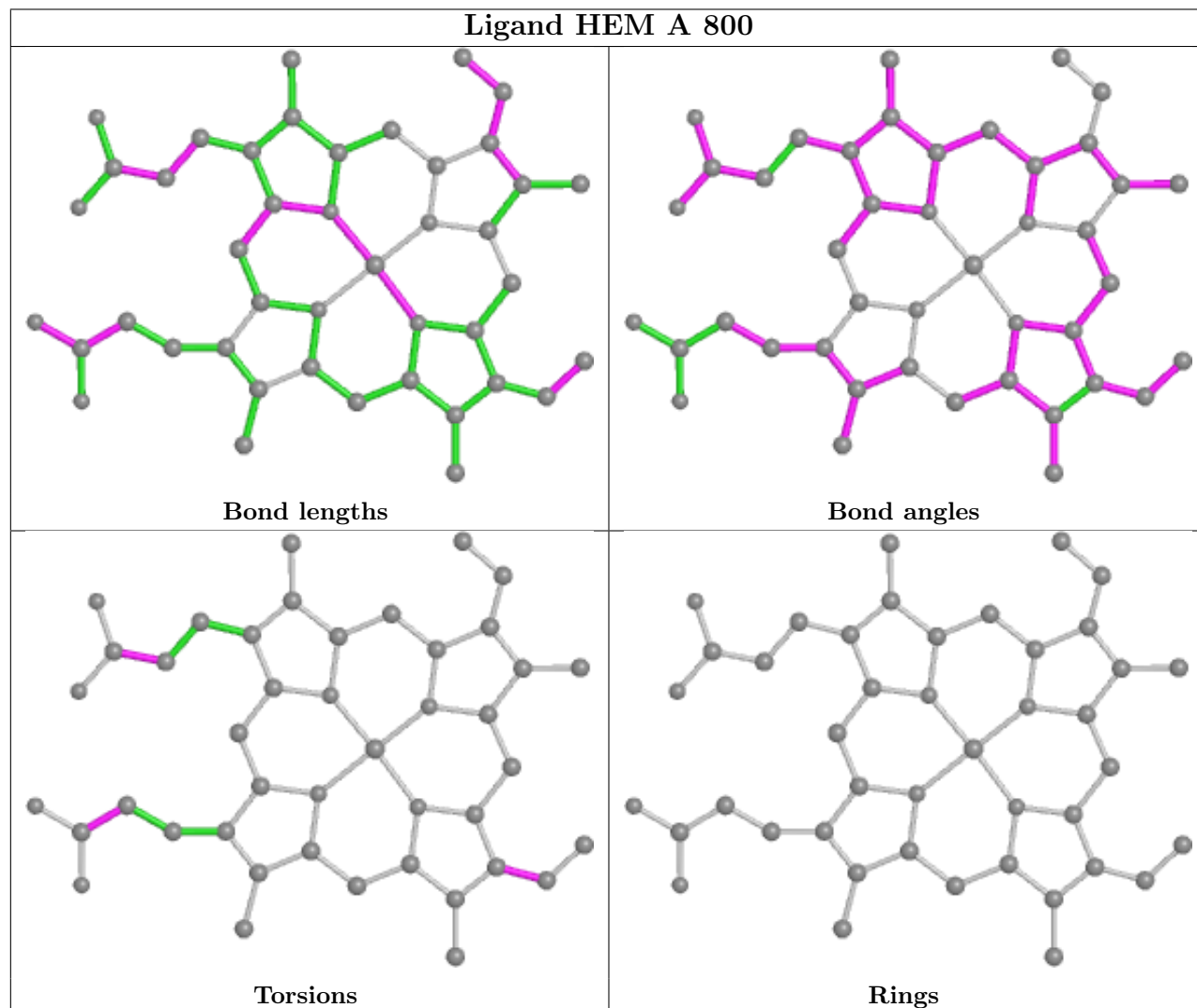
There are no ring outliers.

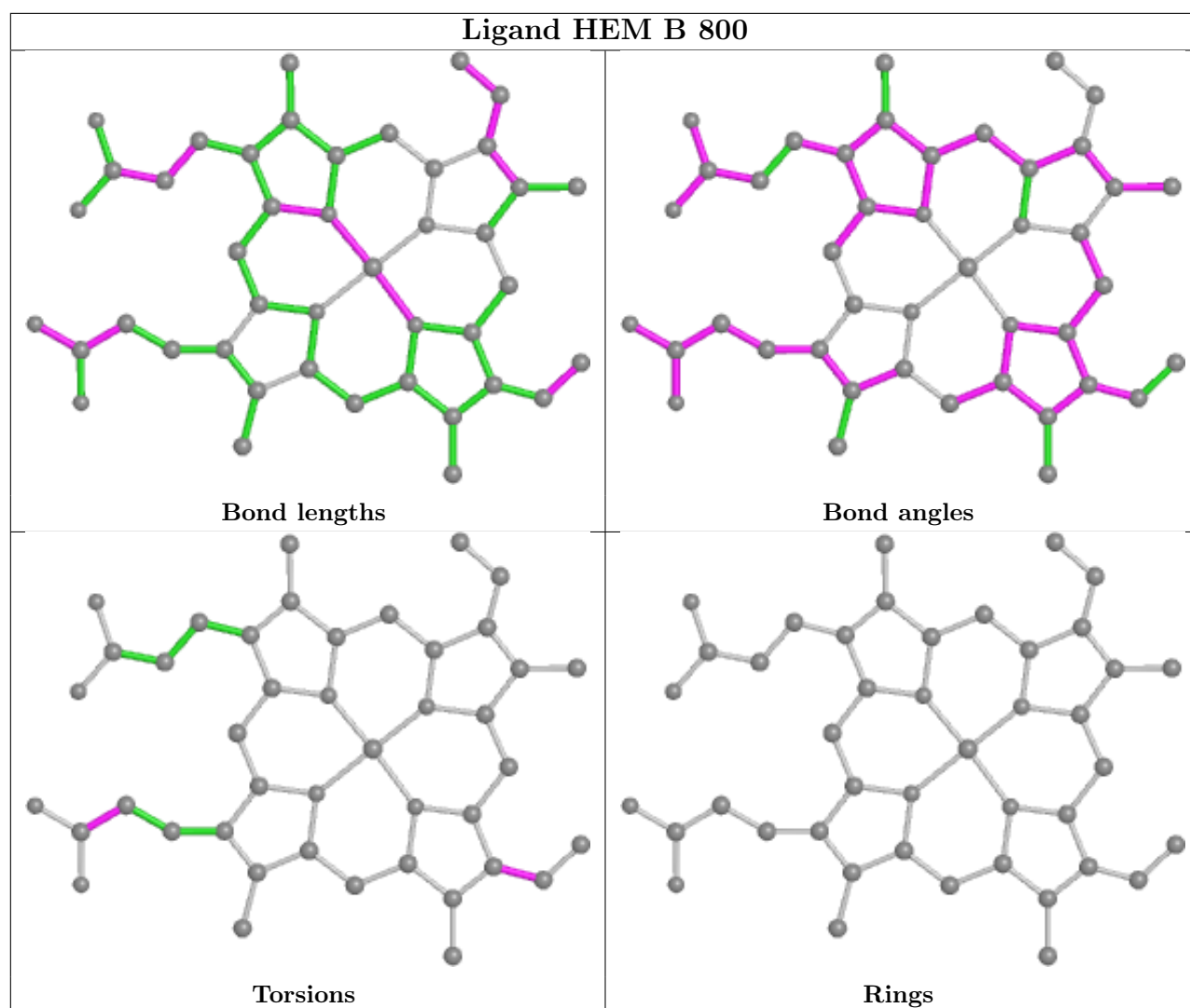
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	HEM	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.





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	714/737 (96%)	0.44	50 (7%) 16 24	20, 38, 65, 93	0
1	B	714/737 (96%)	0.79	86 (12%) 4 7	26, 49, 74, 99	0
All	All	1428/1474 (96%)	0.61	136 (9%) 8 13	20, 43, 71, 99	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	ASN	12.8
1	B	296	ASN	12.1
1	A	298	LYS	11.3
1	A	299	GLY	10.5
1	A	295	GLY	10.3
1	B	730	LEU	10.3
1	A	297	SER	8.3
1	A	300	GLY	8.0
1	B	200	ASP	7.0
1	B	299	GLY	6.9
1	A	730	LEU	6.8
1	A	19	ARG	6.2
1	B	729	ASP	6.1
1	B	361	ASP	5.6
1	B	297	SER	5.5
1	A	729	ASP	5.5
1	A	20	PRO	5.3
1	B	19	ARG	5.3
1	B	300	GLY	5.2
1	B	295	GLY	5.2
1	A	18	LYS	5.0
1	A	361	ASP	4.8
1	A	731	GLU	4.7
1	B	191	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	48	ASP	4.6
1	B	294	ASN	4.4
1	A	360	PRO	4.4
1	A	294	ASN	4.4
1	A	525	GLY	4.3
1	B	731	GLU	4.3
1	B	348	GLU	4.3
1	B	350	LEU	4.3
1	A	24	GLN	4.2
1	B	301	GLU	4.2
1	A	665	GLU	4.1
1	A	523	SER	4.0
1	B	341	TRP	3.9
1	B	18	LYS	3.9
1	A	27	TRP	3.7
1	B	20	PRO	3.6
1	B	666	HIS	3.5
1	B	293	LYS	3.5
1	B	204	GLU	3.5
1	B	336	GLY	3.4
1	B	437	ASP	3.4
1	B	274	LEU	3.3
1	B	360	PRO	3.3
1	A	591	ASP	3.3
1	A	437	ASP	3.3
1	B	49	ASP	3.3
1	B	271	GLU	3.2
1	A	554	GLU	3.2
1	A	590	ASP	3.2
1	A	293	LYS	3.1
1	B	188	GLY	3.1
1	A	50	PHE	3.1
1	B	322	TYR	3.1
1	A	362	GLU	3.1
1	B	663	ASP	3.0
1	A	348	GLU	3.0
1	A	727	ARG	3.0
1	B	349	GLU	3.0
1	B	568	HIS	3.0
1	B	298	LYS	3.0
1	A	663	ASP	2.9
1	B	590	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	533	LEU	2.8
1	B	337	PRO	2.8
1	A	48	ASP	2.8
1	B	662	ALA	2.8
1	B	355	PRO	2.7
1	B	313	GLN	2.7
1	A	21	LYS	2.7
1	B	249	LYS	2.7
1	B	727	ARG	2.7
1	B	523	SER	2.7
1	A	639	GLU	2.7
1	B	467	ALA	2.7
1	B	195	THR	2.6
1	B	454	LEU	2.5
1	A	49	ASP	2.5
1	B	351	LYS	2.5
1	B	227	ASN	2.5
1	B	618	ILE	2.5
1	B	534	ILE	2.5
1	B	333	PRO	2.5
1	A	191	ASP	2.5
1	B	375	LEU	2.5
1	B	552	ASP	2.4
1	B	533	LEU	2.4
1	B	369	LEU	2.4
1	A	534	ILE	2.4
1	B	591	ASP	2.4
1	B	272	GLU	2.4
1	B	372	ASP	2.3
1	B	256	ALA	2.3
1	B	303	ILE	2.3
1	A	535	VAL	2.3
1	B	592	ILE	2.3
1	B	506	THR	2.3
1	B	275	GLY	2.3
1	B	259	HIS	2.3
1	B	665	GLU	2.2
1	A	255	ILE	2.2
1	B	588	ILE	2.2
1	B	326	LEU	2.2
1	A	346	LYS	2.2
1	B	28	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	202	PRO	2.2
1	B	346	LYS	2.2
1	A	25	ASP	2.2
1	A	530	LEU	2.2
1	A	522	ARG	2.2
1	B	728	PHE	2.2
1	B	193	PHE	2.2
1	A	526	THR	2.2
1	B	416	ARG	2.2
1	B	379	PRO	2.2
1	B	329	TYR	2.1
1	B	584	VAL	2.1
1	A	531	ALA	2.1
1	B	53	ALA	2.1
1	B	255	ILE	2.1
1	B	483	ALA	2.1
1	A	674	ASP	2.1
1	B	593	THR	2.1
1	A	455	ASP	2.1
1	B	674	ASP	2.1
1	A	207	GLU	2.1
1	A	521	SER	2.1
1	B	57	GLN	2.0
1	B	621	MET	2.0
1	B	495	ASN	2.0
1	B	397	MET	2.0
1	B	502	GLU	2.0
1	A	524	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

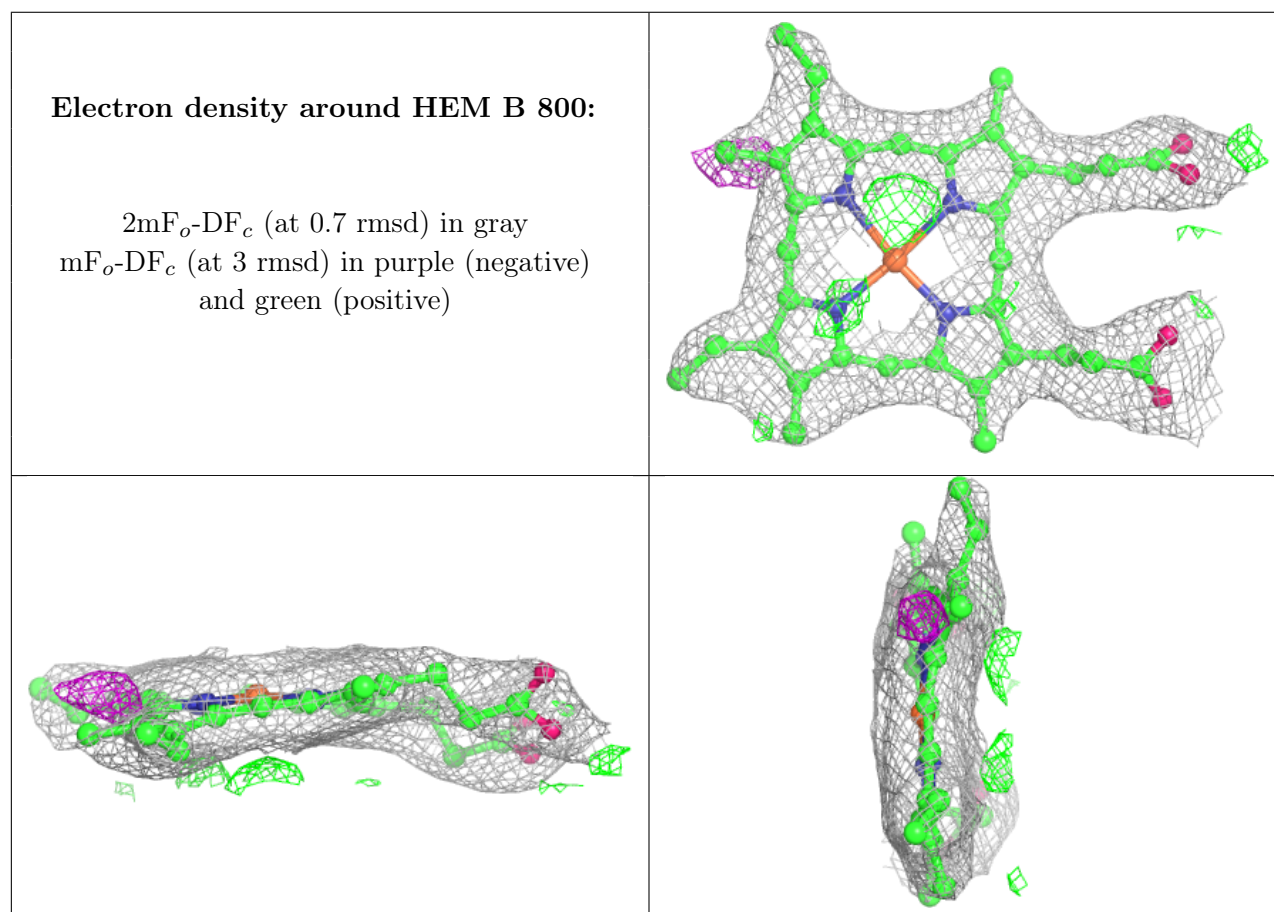
6.4 Ligands [i](#)

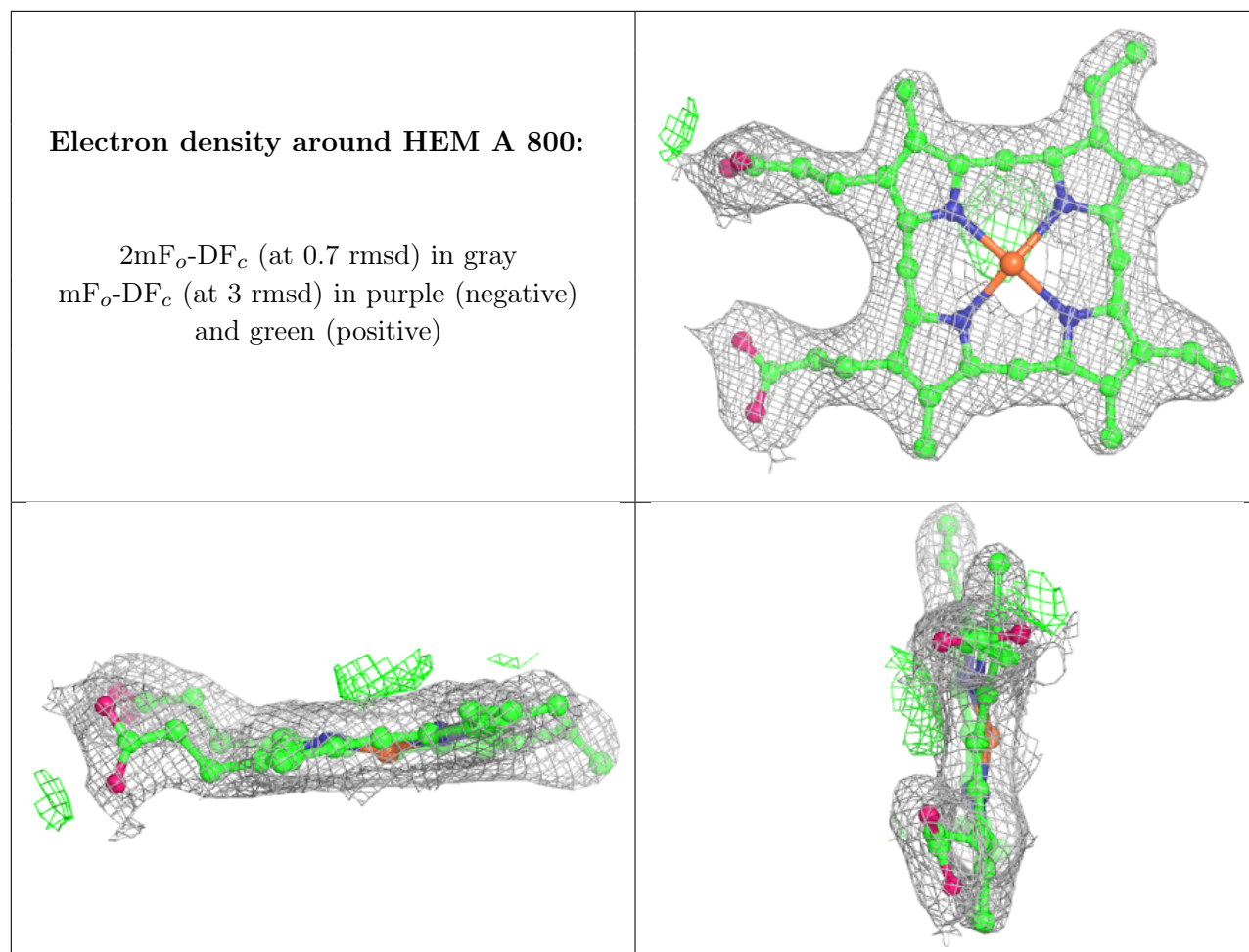
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	B	800	43/43	0.95	0.25	47,50,55,60	0
2	HEM	A	800	43/43	0.97	0.17	22,29,33,37	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.