Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 03:35 PM EST

PDB ID	:	3VLK
Title	:	Crystal Structure Analysis of the Ser305Ala variant of KatG from Haloarcula marismortui
Authors	:	Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on	:	2011-12-01
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

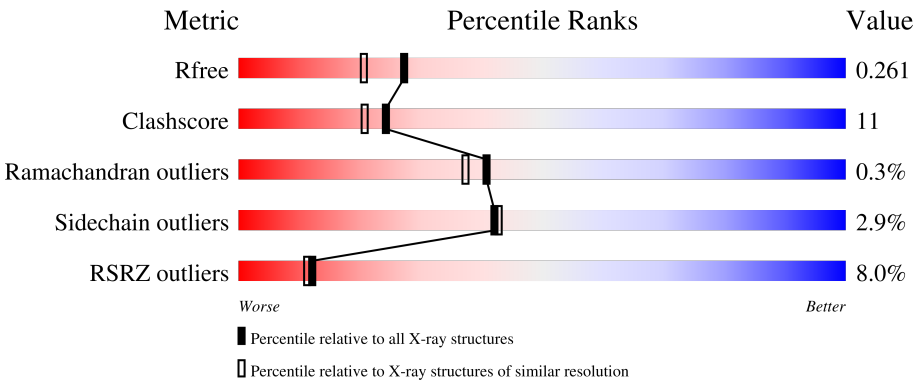
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	9% 77% 19% • •
1	B	737	7% 80% 16% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11488 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.

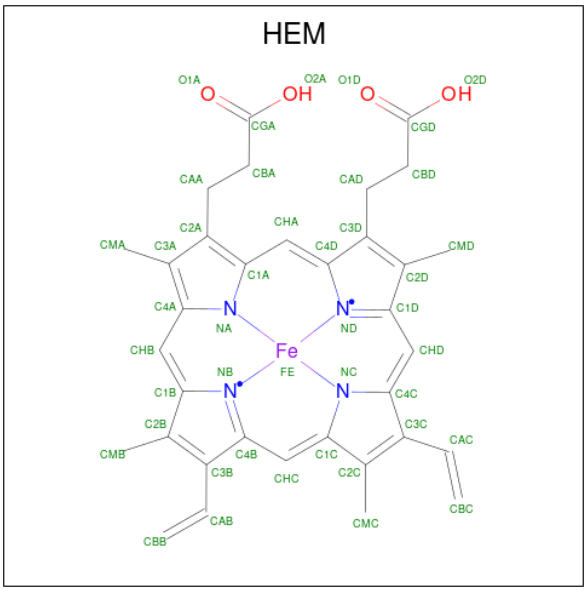
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	714	5619	3512	945	1143	19	0	0	0
1	B	714	5619	3512	945	1143	19	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	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	ALA	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: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is water.

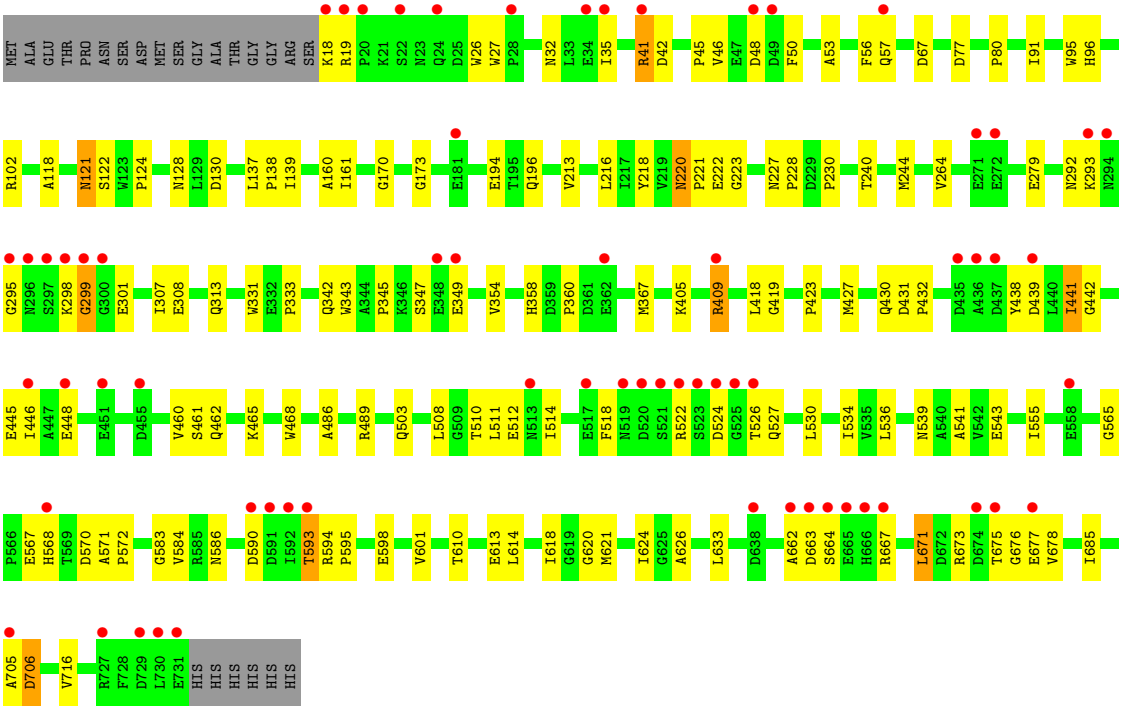
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	162	162	162	0	0
			Total	O		
3	B	2	2	2	0	0

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.

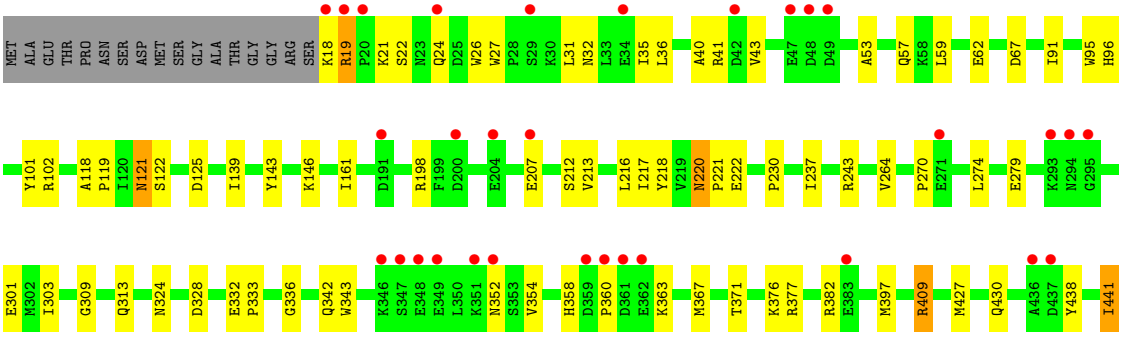
• Molecule 1: Catalase-peroxidase 2

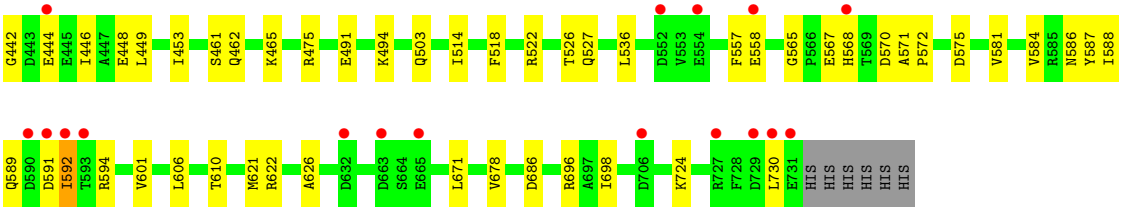
Chain A:



• Molecule 1: Catalase-peroxidase 2

Chain B:




G442 D443 E444 E445 I446 A447 E448 L449 I453 S461 Q462 K465 R475 E491 K494 Q503 I514 F518 R522 T526 Q527 L536 D552 V553 E554 F557 E558 G565 P566 E567 H568 T569 D570 A571 P572 D575 V581 V584 R585 N586 Y587 I588
Q589 D590 D591 I592 T593 R594 V601 L606 T610 M621 R622 A626 D632 D663 S664 E665 L671 V678 D686 R696 A697 I698 D706 K724 H727 F728 D729 L730 E731 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	321.24Å 76.67Å 74.71Å 90.00° 99.54° 90.00°	Depositor
Resolution (Å)	49.97 – 2.00 49.97 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.97-2.00) 98.7 (49.97-1.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.54 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.270 0.234 , 0.261	Depositor DCC
R_{free} test set	8123 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11488	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/5755	0.56	0/7819
1	B	0.31	0/5755	0.54	0/7819
All	All	0.33	0/11510	0.55	0/15638

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5619	0	5265	136	0
1	B	5619	0	5265	116	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	162	0	0	2	0
3	B	2	0	0	0	0
All	All	11488	0	10590	240	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 (240) 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:95:TRP:CH2	1:A:218:TYR:HE1	1.03	1.65
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.11	1.65
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.13	1.62
1:A:95:TRP:HH2	1:A:218:TYR:CE1	0.99	1.59
1:A:218:TYR:CE2	1:A:244:MET:SD	2.16	1.38
1:A:218:TYR:HE2	1:A:244:MET:SD	1.50	1.33
1:A:95:TRP:CH2	1:A:218:TYR:CE1	1.88	1.29
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.98	1.15
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.44	1.00
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.46	0.95
1:A:218:TYR:HE2	1:A:244:MET:CG	1.82	0.93
1:A:95:TRP:HH2	1:A:218:TYR:CD1	1.86	0.90
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.54	0.89
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	1.89	0.89
1:A:298:LYS:CE	1:A:301:GLU:HB2	2.06	0.85
1:A:298:LYS:HE3	1:A:301:GLU:HB2	1.61	0.82
1:A:441:ILE:HD13	1:A:441:ILE:H	1.43	0.82
1:B:427:MET:H	1:B:430:GLN:HE21	1.25	0.82
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.64	0.81
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.62	0.81
1:B:567:GLU:HG2	1:B:568:HIS:ND1	1.99	0.78
1:A:427:MET:H	1:A:430:GLN:HE21	1.31	0.78
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.64	0.77
1:A:45:PRO:HD3	1:B:698:ILE:HD12	1.68	0.75
1:A:218:TYR:CZ	1:A:244:MET:SD	2.80	0.74
1:A:298:LYS:CD	1:A:301:GLU:HB2	2.19	0.72
1:B:462:GLN:HE21	1:B:503:GLN:NE2	1.88	0.72
1:A:121:ASN:HD22	1:A:122:SER:N	1.87	0.71
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.76	0.70
1:B:441:ILE:HD13	1:B:441:ILE:H	1.56	0.69
1:B:427:MET:H	1:B:430:GLN:NE2	1.90	0.69
1:B:121:ASN:HD22	1:B:122:SER:N	1.91	0.69
1:B:270:PRO:HA	1:B:274:LEU:HD13	1.73	0.69
1:A:67:ASP:HB3	1:A:139:ILE:HD11	1.75	0.69
1:A:80:PRO:HD2	1:A:298:LYS:O	1.92	0.68
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.76	0.68
1:A:671:LEU:HD22	1:A:678:VAL:HG12	1.75	0.68
1:B:274:LEU:HD11	1:B:303:ILE:HB	1.76	0.67
1:B:444:GLU:O	1:B:448:GLU:HG3	1.94	0.67
1:A:298:LYS:HG3	1:A:299:GLY:H	1.59	0.67
1:A:91:ILE:HD11	1:A:160:ALA:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:H	1:A:430:GLN:NE2	1.92	0.66
1:A:53:ALA:O	1:A:57:GLN:HG2	1.96	0.66
1:A:18:LYS:HB2	1:B:594:ARG:HD3	1.77	0.66
1:A:124:PRO:HG2	1:A:194:GLU:HG3	1.77	0.66
1:A:664:SER:HB3	1:A:667:ARG:HB3	1.78	0.65
1:B:91:ILE:CD1	1:B:161:ILE:HG12	2.27	0.65
1:A:442:GLY:O	1:A:446:ILE:HG12	1.98	0.64
1:A:220:ASN:ND2	1:A:222:GLU:H	1.95	0.64
1:A:567:GLU:HG2	1:A:568:HIS:ND1	2.12	0.64
1:B:462:GLN:NE2	1:B:503:GLN:HE22	1.96	0.64
1:B:143:TYR:O	1:B:146:LYS:HE3	1.98	0.63
1:B:462:GLN:HE21	1:B:503:GLN:HE22	1.43	0.63
1:A:431:ASP:N	1:A:432:PRO:HD3	2.13	0.63
1:A:308:GLU:H	1:A:342:GLN:HE22	1.46	0.63
1:A:220:ASN:HD22	1:A:220:ASN:C	2.03	0.62
1:A:530:LEU:O	1:A:534:ILE:HG12	2.00	0.62
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.65	0.62
1:A:445:GLU:OE2	1:A:526:THR:HG21	2.00	0.61
1:A:298:LYS:HG3	1:A:299:GLY:N	2.15	0.61
1:A:298:LYS:HD2	1:A:301:GLU:HB2	1.82	0.61
1:A:595:PRO:HD2	1:A:598:GLU:OE1	2.00	0.61
1:A:441:ILE:HB	1:A:445:GLU:HB2	1.83	0.61
1:A:539:ASN:O	1:A:543:GLU:HG3	2.02	0.60
1:B:589:GLN:HG2	1:B:591:ASP:OD1	2.01	0.59
1:B:19:ARG:HD3	1:B:19:ARG:N	2.16	0.59
1:B:333:PRO:HG3	1:B:343:TRP:CH2	2.38	0.59
1:A:583:GLY:HA2	1:A:685:ILE:HD13	1.84	0.59
1:A:41:ARG:HH21	1:B:41:ARG:HE	1.49	0.58
1:A:595:PRO:HB2	1:A:598:GLU:HG3	1.85	0.58
1:A:118:ALA:HB2	1:A:279:GLU:CD	2.23	0.58
1:B:475:ARG:HB2	1:B:606:LEU:HD22	1.84	0.58
1:B:35:ILE:CD1	1:B:601:VAL:HG12	2.32	0.58
1:A:565:GLY:H	1:A:568:HIS:CE1	2.22	0.57
1:B:536:LEU:HG	1:B:557:PHE:CE1	2.39	0.57
1:A:95:TRP:CZ3	1:A:218:TYR:CE1	2.76	0.57
1:B:565:GLY:H	1:B:568:HIS:CE1	2.23	0.57
1:A:503:GLN:HB2	3:A:889:HOH:O	2.05	0.57
1:A:518:PHE:O	1:A:522:ARG:HG2	2.05	0.56
1:A:45:PRO:HD3	1:B:698:ILE:CD1	2.35	0.56
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.87	0.56
1:B:31:LEU:HG	1:B:601:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:CE2	1:A:244:MET:CG	2.74	0.56
1:A:41:ARG:HE	1:B:41:ARG:HD3	1.71	0.56
1:A:570:ASP:OD1	1:A:572:PRO:HD2	2.04	0.56
1:A:594:ARG:HD3	1:B:18:LYS:HD2	1.88	0.56
1:A:218:TYR:HE2	1:A:244:MET:HG3	1.68	0.56
1:A:462:GLN:HE21	1:A:503:GLN:HE22	1.54	0.56
1:B:91:ILE:HD11	1:B:161:ILE:HG12	1.88	0.56
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.06	0.56
1:A:41:ARG:HG3	1:B:41:ARG:HB3	1.87	0.55
1:A:593:THR:HG23	1:A:594:ARG:H	1.71	0.55
1:A:91:ILE:CD1	1:A:161:ILE:HG13	2.37	0.55
1:A:41:ARG:HG2	1:B:40:ALA:O	2.07	0.55
1:B:453:ILE:HD13	1:B:514:ILE:HD13	1.89	0.54
1:A:298:LYS:HE3	1:A:301:GLU:CB	2.34	0.54
1:A:298:LYS:CG	1:A:299:GLY:H	2.19	0.54
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.86	0.53
1:A:441:ILE:HD13	1:A:441:ILE:N	2.20	0.53
1:A:445:GLU:HG2	1:A:518:PHE:HZ	1.74	0.53
1:A:91:ILE:CD1	1:A:160:ALA:HB3	2.38	0.53
1:A:170:GLY:HA3	1:A:423:PRO:HG3	1.89	0.53
1:A:220:ASN:HD22	1:A:221:PRO:N	2.07	0.53
1:B:220:ASN:ND2	1:B:222:GLU:H	2.06	0.53
1:A:610:THR:OG1	1:A:613:GLU:HG3	2.09	0.53
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.44	0.53
1:B:220:ASN:HD22	1:B:221:PRO:N	2.07	0.53
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.90	0.52
1:B:53:ALA:O	1:B:57:GLN:HG2	2.10	0.52
1:B:352:ASN:HD22	1:B:363:LYS:HB2	1.74	0.52
1:B:592:ILE:HD13	1:B:592:ILE:N	2.24	0.52
1:A:633:LEU:HD21	1:A:667:ARG:NH2	2.25	0.52
1:A:409:ARG:HD3	1:A:409:ARG:O	2.09	0.52
1:B:438:TYR:CG	1:B:527:GLN:HB2	2.44	0.52
1:B:449:LEU:O	1:B:453:ILE:HG12	2.09	0.52
1:A:218:TYR:CE2	1:A:244:MET:HG3	2.44	0.52
1:A:41:ARG:CG	1:B:41:ARG:HB3	2.40	0.52
1:A:67:ASP:HB3	1:A:139:ILE:CD1	2.40	0.52
1:B:35:ILE:HG13	1:B:36:LEU:N	2.25	0.52
1:B:125:ASP:OD2	1:B:217:ILE:HG12	2.10	0.51
1:B:91:ILE:HD12	1:B:161:ILE:HG12	1.92	0.51
1:A:220:ASN:HD22	1:A:222:GLU:H	1.57	0.51
1:B:592:ILE:HD13	1:B:592:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:HG2	1:B:626:ALA:HB1	1.93	0.51
1:A:292:ASN:HB3	1:A:295:GLY:CA	2.40	0.51
1:B:220:ASN:HD22	1:B:220:ASN:C	2.12	0.51
1:B:198:ARG:HD2	1:B:212:SER:C	2.32	0.50
1:A:41:ARG:HH21	1:B:41:ARG:NE	2.08	0.50
1:A:358:HIS:O	1:A:360:PRO:HD3	2.11	0.50
1:B:522:ARG:HD2	1:B:522:ARG:N	2.25	0.50
1:A:95:TRP:CD1	1:A:96:HIS:HD2	2.31	0.49
1:A:405:LYS:O	1:A:409:ARG:HB2	2.13	0.49
1:B:491:GLU:HG2	1:B:494:LYS:HE2	1.94	0.49
1:A:26:TRP:HB2	1:A:27:TRP:CE3	2.48	0.49
1:A:299:GLY:CA	1:A:358:HIS:CD2	2.95	0.49
1:A:32:ASN:ND2	1:A:35:ILE:HG23	2.28	0.49
1:B:21:LYS:HD3	1:B:26:TRP:CE2	2.48	0.49
1:B:237:ILE:HD11	1:B:371:THR:HG22	1.95	0.49
1:A:438:TYR:CG	1:A:527:GLN:HB2	2.48	0.48
1:A:705:ALA:O	1:A:706:ASP:HB3	2.13	0.48
1:B:446:ILE:HD12	1:B:536:LEU:HD11	1.94	0.48
1:B:558:GLU:HG2	1:B:724:LYS:HE3	1.95	0.48
1:A:508:LEU:O	1:A:512:GLU:HG3	2.14	0.48
1:B:336:GLY:HA3	1:B:342:GLN:NE2	2.29	0.48
1:A:46:VAL:HG11	1:A:50:PHE:CD2	2.48	0.48
1:A:441:ILE:H	1:A:441:ILE:CD1	2.17	0.48
1:A:91:ILE:HD11	1:A:161:ILE:HG13	1.95	0.48
1:A:121:ASN:ND2	1:A:122:SER:N	2.59	0.48
1:B:441:ILE:H	1:B:441:ILE:CD1	2.25	0.48
1:B:587:TYR:O	1:B:588:ILE:HD13	2.14	0.48
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.95	0.47
1:B:324:ASN:O	1:B:328:ASP:HB2	2.15	0.47
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.79	0.47
1:A:331:TRP:CZ3	1:A:345:PRO:HD3	2.50	0.47
1:A:298:LYS:CG	1:A:299:GLY:N	2.76	0.47
1:A:486:ALA:O	1:A:489:ARG:HG2	2.13	0.47
1:A:95:TRP:CZ2	1:A:218:TYR:CD1	3.03	0.47
1:A:510:THR:O	1:A:514:ILE:HG12	2.15	0.47
1:B:230:PRO:HB2	1:B:377:ARG:HG3	1.96	0.47
1:A:462:GLN:HE21	1:A:503:GLN:NE2	2.12	0.47
1:A:460:VAL:HG13	1:A:541:ALA:HB1	1.97	0.46
1:A:419:GLY:HA3	3:A:750:HOH:O	2.16	0.46
1:A:465:LYS:HG2	1:A:626:ALA:HB1	1.98	0.46
1:B:62:GLU:OE2	1:B:62:GLU:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:HB3	1:B:24:GLN:HG2	1.98	0.46
1:A:461:SER:O	1:A:465:LYS:HG3	2.15	0.46
1:A:80:PRO:HB2	1:A:358:HIS:CE1	2.51	0.46
1:B:101:TYR:CE2	1:B:409:ARG:HD2	2.51	0.46
1:A:445:GLU:HA	1:A:448:GLU:HB2	1.98	0.46
1:A:56:PHE:CZ	1:A:173:GLY:HA3	2.51	0.45
1:A:555:ILE:HG12	1:A:716:VAL:HG13	1.96	0.45
1:A:511:LEU:HD13	1:A:534:ILE:HD13	1.97	0.45
1:B:301:GLU:O	1:B:303:ILE:HG13	2.17	0.45
1:B:453:ILE:HD13	1:B:514:ILE:CD1	2.46	0.45
1:A:18:LYS:HD2	1:B:594:ARG:HD3	1.98	0.45
1:B:536:LEU:HG	1:B:557:PHE:CD1	2.52	0.45
1:B:376:LYS:O	1:B:382:ARG:HD3	2.16	0.45
1:A:347:SER:HB2	1:A:349:GLU:OE1	2.16	0.45
1:B:67:ASP:HB3	1:B:139:ILE:HD12	1.98	0.45
1:B:518:PHE:O	1:B:522:ARG:CD	2.65	0.45
1:B:442:GLY:O	1:B:446:ILE:HG12	2.17	0.44
1:A:223:GLY:HA3	1:A:227:ASN:O	2.17	0.44
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.05	0.44
1:B:352:ASN:ND2	1:B:363:LYS:HB2	2.32	0.44
1:B:441:ILE:HD13	1:B:441:ILE:N	2.26	0.44
1:B:592:ILE:H	1:B:592:ILE:CD1	2.31	0.44
1:B:41:ARG:HG3	1:B:41:ARG:NH1	2.27	0.44
1:A:292:ASN:HB3	1:A:295:GLY:HA3	2.00	0.44
1:B:40:ALA:HB2	1:B:610:THR:CG2	2.48	0.44
1:B:264:VAL:HG22	1:B:309:GLY:O	2.17	0.44
1:B:518:PHE:O	1:B:522:ARG:HD3	2.18	0.44
1:A:121:ASN:ND2	1:A:121:ASN:C	2.71	0.44
1:B:526:THR:HG22	1:B:527:GLN:N	2.32	0.44
1:B:567:GLU:HG2	1:B:568:HIS:N	2.33	0.43
1:B:121:ASN:HD22	1:B:121:ASN:C	2.21	0.43
1:A:664:SER:CB	1:A:667:ARG:HB3	2.48	0.43
1:B:438:TYR:CD1	1:B:527:GLN:HB2	2.53	0.43
1:B:461:SER:O	1:B:465:LYS:HG3	2.19	0.43
1:B:207:GLU:HA	1:B:243:ARG:NH2	2.34	0.43
1:B:570:ASP:OD1	1:B:572:PRO:HD2	2.18	0.43
1:A:264:VAL:HG12	2:A:800:HEM:CAA	2.48	0.42
1:A:41:ARG:NE	1:B:41:ARG:HD3	2.33	0.42
1:A:614:LEU:O	1:A:618:ILE:HG12	2.19	0.42
1:A:299:GLY:HA3	1:A:358:HIS:CD2	2.54	0.42
1:A:468:TRP:CZ2	1:A:584:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TRP:HB2	1:B:27:TRP:CE3	2.54	0.42
1:B:121:ASN:ND2	1:B:122:SER:N	2.64	0.42
1:B:581:VAL:HG13	1:B:588:ILE:CD1	2.49	0.42
1:B:213:VAL:HB	1:B:216:LEU:HD12	2.02	0.42
1:B:382:ARG:HG2	1:B:382:ARG:NH1	2.34	0.42
1:B:589:GLN:O	1:B:592:ILE:HD12	2.20	0.42
1:B:671:LEU:HD22	1:B:678:VAL:HG22	2.00	0.42
1:A:218:TYR:OH	1:A:244:MET:SD	2.78	0.42
1:A:228:PRO:O	1:A:230:PRO:HD3	2.20	0.42
1:A:240:THR:O	1:A:244:MET:HG3	2.19	0.42
1:A:298:LYS:HG2	1:A:301:GLU:C	2.40	0.42
1:A:620:GLY:O	1:A:624:ILE:HG12	2.20	0.42
1:B:118:ALA:HB2	1:B:279:GLU:HG3	2.00	0.42
1:B:121:ASN:C	1:B:121:ASN:ND2	2.73	0.42
1:B:220:ASN:HD22	1:B:221:PRO:CD	2.33	0.42
1:B:358:HIS:O	1:B:360:PRO:HD3	2.19	0.42
1:A:567:GLU:HG2	1:A:568:HIS:N	2.34	0.41
1:B:41:ARG:NH1	1:B:43:VAL:HG13	2.35	0.41
1:B:332:GLU:HA	1:B:333:PRO:HD3	1.90	0.41
1:B:95:TRP:CD1	1:B:96:HIS:HD2	2.38	0.41
1:B:59:LEU:HD13	1:B:146:LYS:HB3	2.01	0.41
1:A:307:ILE:HG23	1:A:342:GLN:HB3	2.02	0.41
1:A:439:ASP:HB2	1:A:526:THR:HA	2.02	0.41
1:B:32:ASN:O	1:B:35:ILE:HG23	2.21	0.41
1:B:125:ASP:HB2	1:B:216:LEU:HA	2.03	0.41
1:A:137:LEU:HB3	1:A:138:PRO:HD3	2.03	0.41
1:A:593:THR:HG23	1:A:594:ARG:N	2.36	0.41
1:A:662:ALA:O	1:A:663:ASP:HB2	2.20	0.41
1:A:343:TRP:CD1	1:A:343:TRP:N	2.88	0.40
1:A:91:ILE:HD12	1:A:161:ILE:HG13	2.02	0.40
1:B:622:ARG:NE	1:B:686:ASP:OD1	2.46	0.40
1:A:673:ARG:C	1:A:675:THR:H	2.25	0.40
1:B:67:ASP:HB3	1:B:139:ILE:CD1	2.51	0.40
1:B:671:LEU:CD2	1:B:678:VAL:HG22	2.51	0.40
1:A:121:ASN:HD22	1:A:122:SER:H	1.67	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%)	677 (95%)	31 (4%)	4 (1%)	25	19
1	B	712/737 (97%)	683 (96%)	29 (4%)	0	100	100
All	All	1424/1474 (97%)	1360 (96%)	60 (4%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	706	ASP
1	A	524	ASP
1	A	299	GLY
1	A	676	GLY

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	589/607 (97%)	569 (97%)	20 (3%)	37	36
1	B	589/607 (97%)	575 (98%)	14 (2%)	49	51
All	All	1178/1214 (97%)	1144 (97%)	34 (3%)	42	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	41	ARG

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Mol	Chain	Res	Type
1	A	42	ASP
1	A	48	ASP
1	A	77	ASP
1	A	102	ARG
1	A	121	ASN
1	A	196	GLN
1	A	220	ASN
1	A	293	LYS
1	A	367	MET
1	A	409	ARG
1	A	418	LEU
1	A	441	ILE
1	A	536	LEU
1	A	586	ASN
1	A	590	ASP
1	A	593	THR
1	A	671	LEU
1	A	677	GLU
1	B	19	ARG
1	B	102	ARG
1	B	119	PRO
1	B	121	ASN
1	B	220	ASN
1	B	367	MET
1	B	397	MET
1	B	409	ARG
1	B	441	ILE
1	B	575	ASP
1	B	586	ASN
1	B	592	ILE
1	B	696	ARG
1	B	730	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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	324	ASN
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	352	ASN
1	A	358	HIS
1	A	389	GLN
1	A	430	GLN
1	A	503	GLN
1	A	515	GLN
1	A	586	ASN
1	A	608	ASN
1	B	32	ASN
1	B	38	GLN
1	B	121	ASN
1	B	220	ASN
1	B	286	GLN
1	B	324	ASN
1	B	342	GLN
1	B	352	ASN
1	B	389	GLN
1	B	430	GLN
1	B	495	ASN
1	B	503	GLN
1	B	515	GLN
1	B	586	ASN
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	B	800	1	41,50,50	2.12	12 (29%)	45,82,82	8.71	30 (66%)
2	HEM	A	800	1	41,50,50	2.09	14 (34%)	45,82,82	6.93	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	B	800	1	-	2/12/54/54	-
2	HEM	A	800	1	-	3/12/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	FE-NB	5.59	2.24	1.96
2	B	800	HEM	CBB-CAB	5.04	1.55	1.30
2	A	800	HEM	CBB-CAB	4.71	1.53	1.30
2	A	800	HEM	C3C-C2C	-4.62	1.34	1.40
2	B	800	HEM	C3C-C2C	-4.31	1.34	1.40
2	A	800	HEM	CBD-CGD	-4.23	1.40	1.50
2	A	800	HEM	CBC-CAC	4.10	1.56	1.29
2	B	800	HEM	FE-ND	4.05	2.16	1.96
2	B	800	HEM	CBC-CAC	3.93	1.55	1.29
2	B	800	HEM	CBA-CGA	-3.84	1.41	1.50
2	B	800	HEM	CBD-CGD	-3.82	1.41	1.50
2	A	800	HEM	CBA-CGA	-3.81	1.41	1.50
2	A	800	HEM	C3C-CAC	3.37	1.54	1.47
2	A	800	HEM	FE-ND	3.31	2.13	1.96
2	A	800	HEM	O1A-CGA	2.66	1.31	1.22
2	B	800	HEM	C4D-ND	-2.58	1.35	1.40
2	A	800	HEM	C4D-ND	-2.57	1.35	1.40
2	B	800	HEM	O1A-CGA	2.48	1.30	1.22
2	B	800	HEM	CBD-CAD	2.47	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	CHA-C4D	2.37	1.41	1.35
2	A	800	HEM	FE-NB	2.35	2.08	1.96
2	A	800	HEM	C2C-C1C	2.30	1.47	1.42
2	A	800	HEM	CHB-C1B	2.15	1.40	1.35
2	A	800	HEM	CBD-CAD	2.07	1.58	1.52
2	B	800	HEM	CHA-C4D	2.06	1.40	1.35
2	B	800	HEM	C3C-CAC	2.01	1.51	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	800	HEM	C4C-CHD-C1D	24.81	155.31	122.56
2	A	800	HEM	C4C-CHD-C1D	20.75	149.94	122.56
2	B	800	HEM	C4B-CHC-C1C	20.18	149.19	122.56
2	A	800	HEM	C4B-CHC-C1C	19.45	148.23	122.56
2	B	800	HEM	CHD-C1D-ND	-19.31	103.45	124.43
2	B	800	HEM	CHC-C4B-C3B	15.22	147.86	124.57
2	B	800	HEM	CHC-C4B-NB	-14.94	108.20	124.43
2	B	800	HEM	C4A-C3A-C2A	-13.66	97.49	107.00
2	B	800	HEM	CHA-C4D-ND	-13.58	107.60	124.38
2	A	800	HEM	CHC-C4B-NB	-13.17	110.12	124.43
2	A	800	HEM	C4A-C3A-C2A	-13.09	97.89	107.00
2	B	800	HEM	C2C-C3C-C4C	12.10	115.35	106.90
2	B	800	HEM	C4B-C3B-C2B	11.36	116.13	107.11
2	B	800	HEM	C3B-C2B-C1B	-10.98	98.34	106.49
2	A	800	HEM	CHD-C1D-ND	-10.57	112.95	124.43
2	B	800	HEM	C1D-C2D-C3D	-10.52	95.90	106.96
2	B	800	HEM	CHB-C1B-NB	-10.39	111.54	124.38
2	A	800	HEM	CMD-C2D-C1D	10.15	140.50	125.04
2	A	800	HEM	C1D-C2D-C3D	-9.92	96.52	106.96
2	A	800	HEM	CHB-C1B-NB	-8.89	113.40	124.38
2	B	800	HEM	CHA-C4D-C3D	8.71	141.68	125.33
2	B	800	HEM	CAD-C3D-C4D	-8.32	110.11	124.66
2	B	800	HEM	C2D-C1D-ND	8.17	119.66	109.88
2	A	800	HEM	CAD-C3D-C4D	-7.85	110.93	124.66
2	A	800	HEM	CMC-C2C-C3C	7.40	138.53	124.68
2	A	800	HEM	CHC-C4B-C3B	7.40	135.90	124.57
2	B	800	HEM	CHD-C1D-C2D	7.28	136.35	124.98
2	A	800	HEM	CHA-C4D-ND	-7.03	115.69	124.38
2	A	800	HEM	C2D-C1D-ND	6.72	117.93	109.88
2	B	800	HEM	O2A-CGA-O1A	-6.50	107.10	123.30
2	A	800	HEM	CHA-C4D-C3D	6.07	136.72	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	HEM	C2C-C3C-C4C	5.98	111.07	106.90
2	A	800	HEM	C1B-NB-C4B	-5.95	98.92	105.07
2	B	800	HEM	O2A-CGA-CBA	5.87	132.89	114.03
2	A	800	HEM	C4D-C3D-C2D	5.86	115.44	106.90
2	A	800	HEM	C2B-C1B-NB	5.69	116.58	109.84
2	A	800	HEM	CMA-C3A-C2A	5.67	135.63	124.94
2	A	800	HEM	O2A-CGA-O1A	-5.53	109.51	123.30
2	B	800	HEM	C4D-C3D-C2D	5.45	114.83	106.90
2	B	800	HEM	CMC-C2C-C3C	5.24	134.48	124.68
2	B	800	HEM	C3C-C4C-NC	-5.07	101.38	110.94
2	B	800	HEM	CMA-C3A-C2A	5.04	134.44	124.94
2	A	800	HEM	CAA-CBA-CGA	-4.83	100.23	113.76
2	B	800	HEM	CMD-C2D-C1D	4.60	132.05	125.04
2	B	800	HEM	C2B-C1B-NB	4.33	114.97	109.84
2	B	800	HEM	CAA-CBA-CGA	-4.08	102.31	113.76
2	A	800	HEM	O2A-CGA-CBA	4.01	126.90	114.03
2	B	800	HEM	CAD-C3D-C2D	3.85	135.06	127.88
2	A	800	HEM	C3D-C4D-ND	-3.49	106.28	110.17
2	B	800	HEM	C4D-ND-C1D	-3.36	101.60	105.07
2	A	800	HEM	O2D-CGD-O1D	-3.04	115.73	123.30
2	A	800	HEM	CBA-CAA-C2A	2.86	117.49	112.62
2	B	800	HEM	CBD-CAD-C3D	2.77	120.32	112.63
2	A	800	HEM	C3B-C2B-C1B	-2.71	104.48	106.49
2	A	800	HEM	CHD-C1D-C2D	2.64	129.10	124.98
2	A	800	HEM	C3C-C4C-NC	-2.49	106.24	110.94
2	B	800	HEM	CAB-C3B-C4B	-2.43	113.16	124.47
2	A	800	HEM	CAD-C3D-C2D	2.40	132.35	127.88
2	B	800	HEM	CMD-C2D-C3D	2.17	132.01	126.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

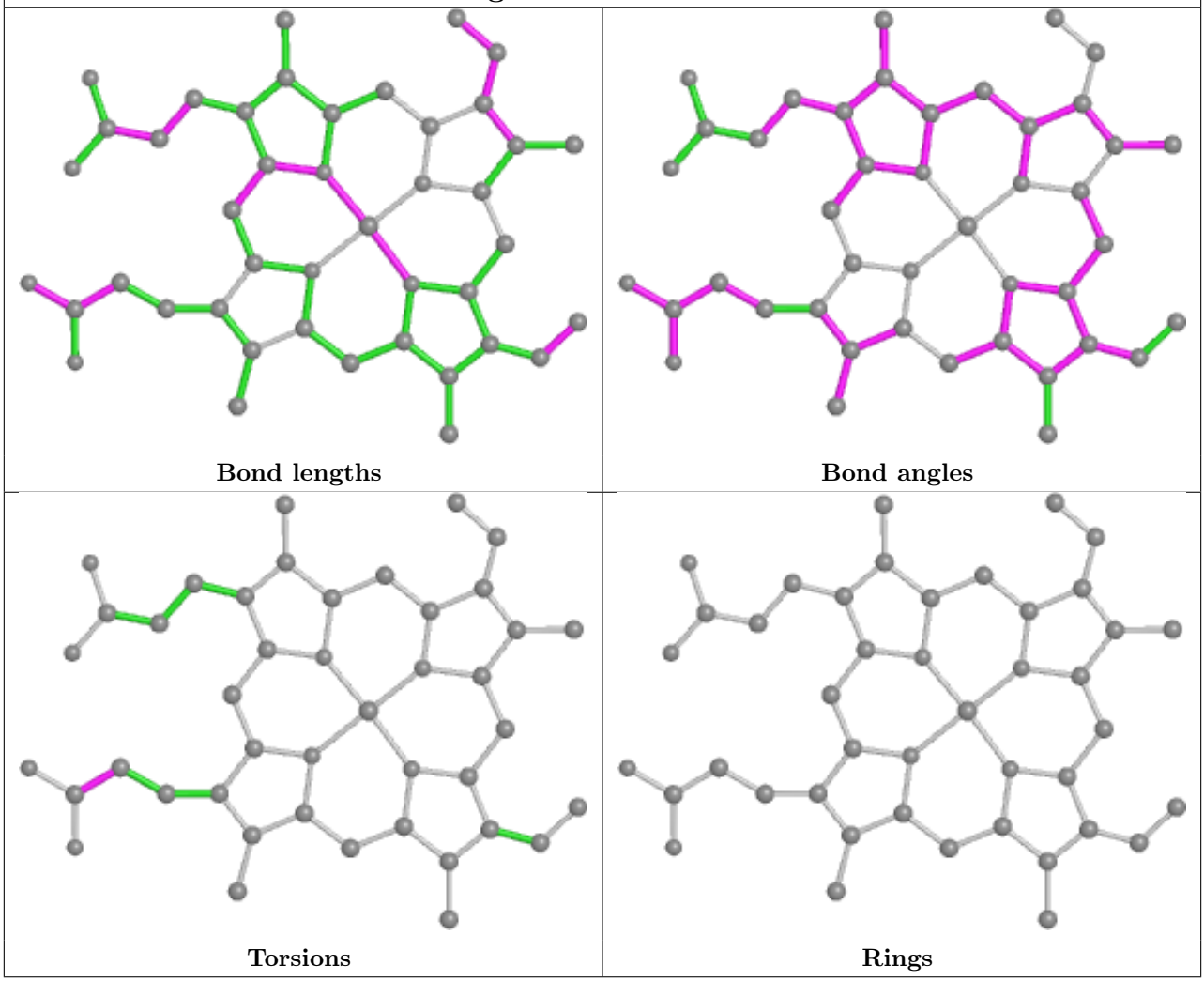
There are no ring outliers.

1 monomer is involved in 1 short contact:

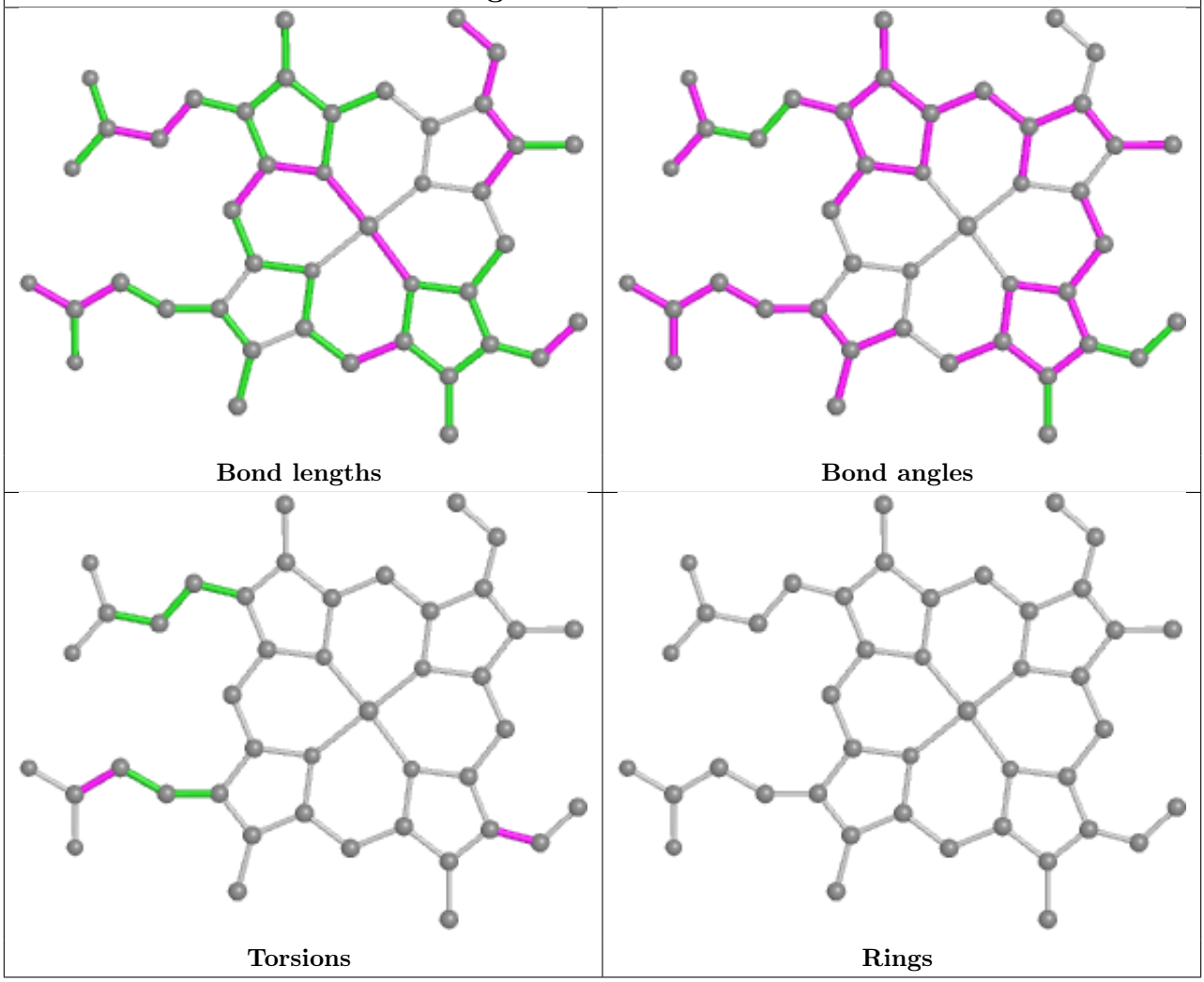
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	HEM	1	0

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

Ligand HEM B 800



Ligand HEM A 800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	714/737 (96%)	0.48	66 (9%)	9	8	7, 19, 43, 56	2 (0%)
1	B	714/737 (96%)	0.36	48 (6%)	17	17	10, 21, 39, 54	0
All	All	1428/1474 (96%)	0.42	114 (7%)	12	11	7, 20, 41, 56	2 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	GLY	17.1
1	A	296	ASN	12.1
1	B	730	LEU	11.5
1	A	730	LEU	10.6
1	A	297	SER	9.5
1	A	298	LYS	9.2
1	A	294	ASN	8.6
1	B	48	ASP	8.2
1	A	300	GLY	8.1
1	B	729	ASP	7.8
1	A	299	GLY	7.3
1	A	525	GLY	6.9
1	B	20	PRO	6.7
1	B	731	GLU	6.6
1	A	729	ASP	6.6
1	A	18	LYS	6.3
1	A	19	ARG	6.3
1	B	663	ASP	6.3
1	A	20	PRO	5.9
1	A	675	THR	5.8
1	A	523	SER	5.7
1	A	663	ASP	5.5
1	B	18	LYS	5.5
1	A	665	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	19	ARG	5.2
1	B	361	ASP	5.1
1	A	409	ARG	5.0
1	A	181	GLU	4.9
1	A	674	ASP	4.7
1	B	593	THR	4.7
1	B	590	ASP	4.6
1	B	348	GLU	4.5
1	A	731	GLU	4.5
1	A	272	GLU	4.5
1	A	437	ASP	4.4
1	B	437	ASP	4.4
1	A	24	GLN	4.3
1	A	520	ASP	4.3
1	A	666	HIS	4.3
1	B	592	ILE	4.2
1	B	293	LYS	4.1
1	B	591	ASP	4.1
1	A	526	THR	3.9
1	A	667	ARG	3.8
1	A	590	ASP	3.8
1	B	347	SER	3.7
1	A	48	ASP	3.7
1	A	591	ASP	3.6
1	A	49	ASP	3.6
1	A	517	GLU	3.6
1	B	352	ASN	3.6
1	A	513	ASN	3.6
1	A	662	ALA	3.6
1	A	664	SER	3.5
1	A	524	ASP	3.5
1	A	439	ASP	3.5
1	B	295	GLY	3.4
1	B	200	ASP	3.3
1	A	293	LYS	3.3
1	B	349	GLU	3.3
1	B	360	PRO	3.3
1	B	191	ASP	3.2
1	A	522	ARG	3.2
1	A	727	ARG	3.2
1	B	727	ARG	3.1
1	B	359	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	28	PRO	3.0
1	A	568	HIS	3.0
1	A	558	GLU	2.9
1	A	638	ASP	2.8
1	B	552	ASP	2.8
1	A	22	SER	2.8
1	A	677	GLU	2.8
1	B	49	ASP	2.8
1	B	665	GLU	2.7
1	B	294	ASN	2.7
1	B	362	GLU	2.7
1	A	592	ILE	2.7
1	A	348	GLU	2.6
1	B	47	GLU	2.6
1	A	57	GLN	2.6
1	A	448	GLU	2.6
1	B	554	GLU	2.6
1	A	593	THR	2.6
1	A	34	GLU	2.5
1	B	24	GLN	2.5
1	A	519	ASN	2.5
1	A	451	GLU	2.5
1	B	436	ALA	2.5
1	B	271	GLU	2.4
1	B	346	LYS	2.4
1	A	521	SER	2.4
1	A	362	GLU	2.4
1	B	444	GLU	2.4
1	A	705	ALA	2.4
1	A	455	ASP	2.4
1	B	558	GLU	2.4
1	A	349	GLU	2.3
1	A	446	ILE	2.3
1	A	435	ASP	2.3
1	B	706	ASP	2.3
1	B	42	ASP	2.3
1	A	436	ALA	2.2
1	B	351	LYS	2.2
1	B	207	GLU	2.2
1	B	568	HIS	2.2
1	A	35	ILE	2.2
1	B	383	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	632	ASP	2.2
1	B	204	GLU	2.1
1	A	41	ARG	2.1
1	B	29	SER	2.1
1	A	271	GLU	2.1
1	B	34	GLU	2.1

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)

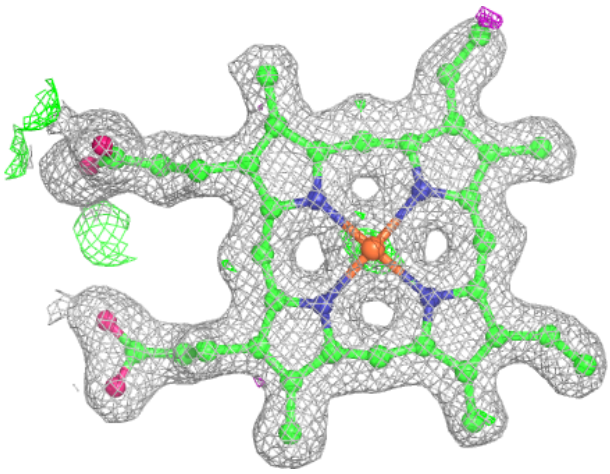
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

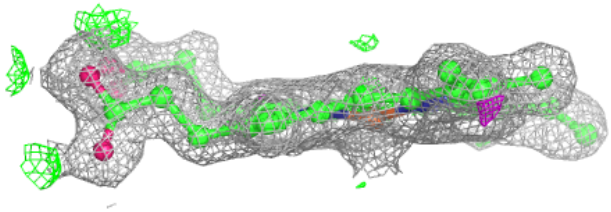
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	800	43/43	0.96	0.14	10,14,17,18	0
2	HEM	A	800	43/43	0.97	0.13	3,9,12,13	0

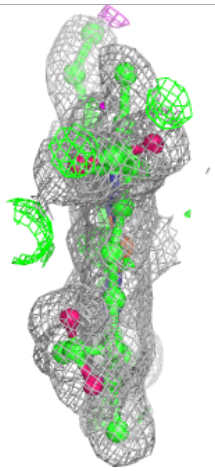
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM B 800:

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

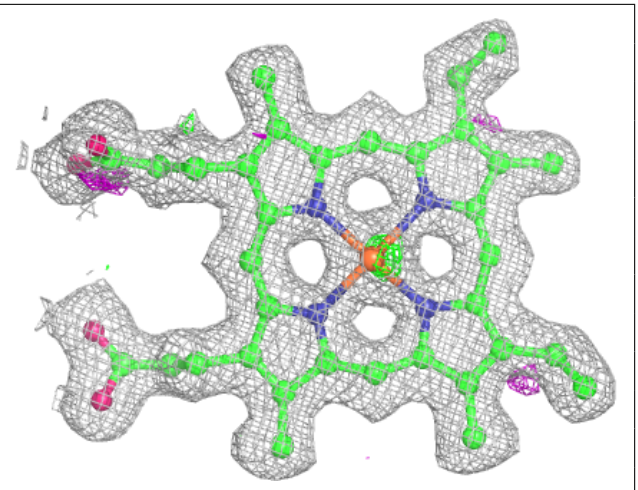


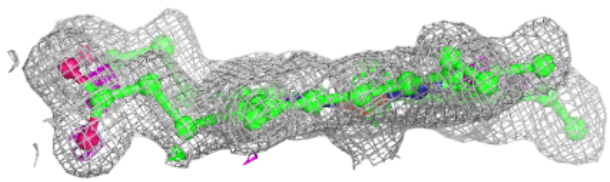


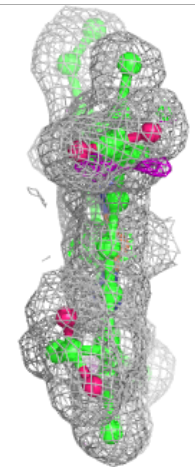


Electron density around HEM A 800:

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.