



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:00 PM GMT

PDB ID : 2A9E
Title : Helicobacter pylori catalase compound I
Authors : Loewen, P.C.; Carpena, X.; Fita, I.
Deposited on : 2005-07-11
Resolution : 1.76 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

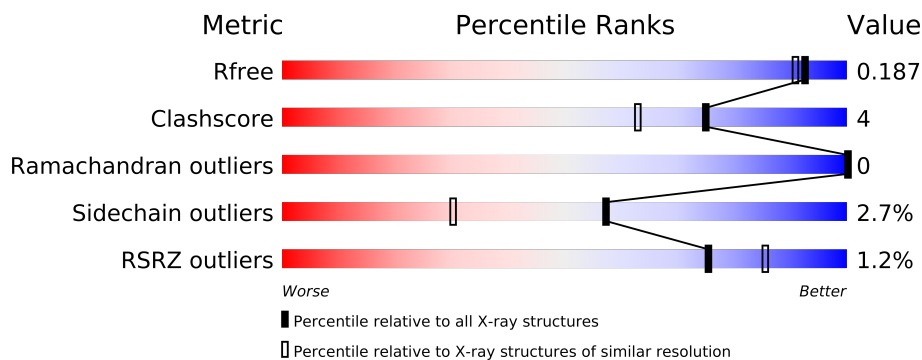
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.76 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}	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	O	A	551	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9112 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

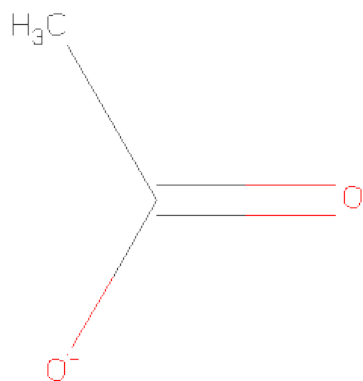
- Molecule 1 is a protein called KatA Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	11	0
			4072	2599	706	753	14			
1	B	491	Total	C	N	O	S	0	11	0
			4064	2594	703	753	14			

There are 8 discrepancies between the modelled and reference sequences:

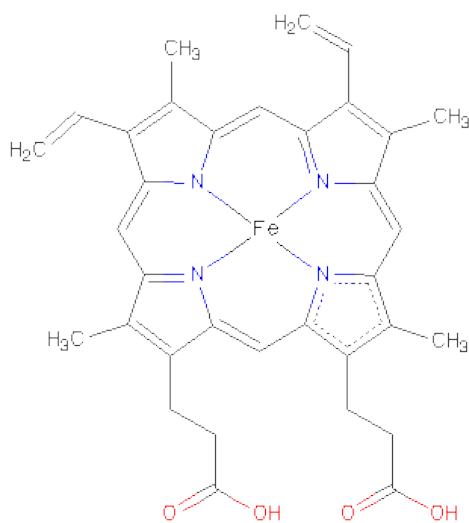
Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MHO	MET	MODIFIED RESIDUE	UNP P77872
A	181	MHO	MET	MODIFIED RESIDUE	UNP P77872
A	292	MHO	MET	MODIFIED RESIDUE	UNP P77872
A	372	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	162	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	181	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	292	MHO	MET	MODIFIED RESIDUE	UNP P77872
B	372	MHO	MET	MODIFIED RESIDUE	UNP P77872

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 5 is water.

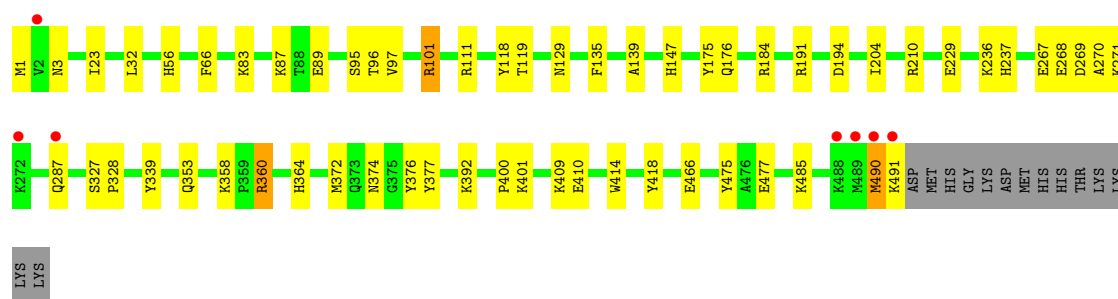
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	440	Total 440	O 440	0	0
5	B	444	Total 444	O 444	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

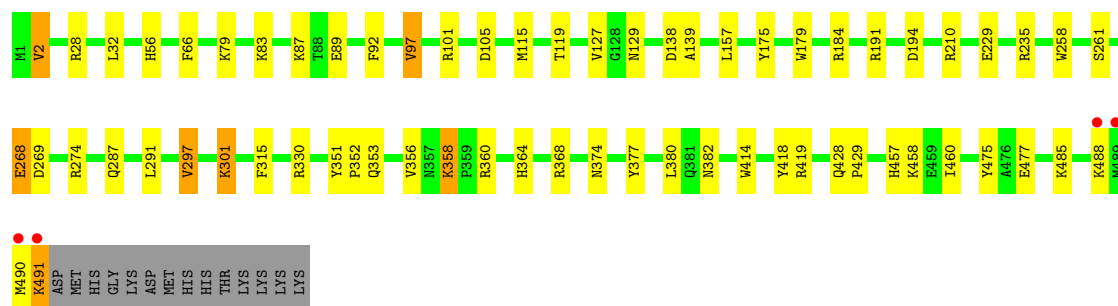
• Molecule 1: KatA Catalase

Chain A: 



• Molecule 1: KatA Catalase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.39Å 154.29Å 95.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.00 – 1.76 37.06 – 1.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.00-1.76) 96.6 (37.06-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.137 , 0.178 0.148 , 0.187	Depositor DCC
R_{free} test set	4674 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 25.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 92078 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9112	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MHO, ACT, O, 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	1.23	11/4211 (0.3%)	1.05	13/5694 (0.2%)
1	B	1.30	16/4200 (0.4%)	1.12	25/5680 (0.4%)
All	All	1.26	27/8411 (0.3%)	1.08	38/11374 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LYS	CE-NZ	8.05	1.69	1.49
1	A	376	TYR	CB-CG	7.92	1.63	1.51
1	A	229	GLU	CG-CD	7.47	1.63	1.51
1	A	466	GLU	CB-CG	-6.62	1.39	1.52
1	A	376	TYR	CG-CD1	6.51	1.47	1.39
1	B	360	ARG	CZ-NH1	6.51	1.41	1.33
1	B	297[A]	VAL	CB-CG1	6.23	1.66	1.52
1	B	297[B]	VAL	CB-CG1	6.23	1.66	1.52
1	A	477	GLU	CG-CD	6.13	1.61	1.51
1	B	419	ARG	C-O	6.10	1.34	1.23
1	B	229	GLU	CG-CD	6.02	1.60	1.51
1	A	376	TYR	CE1-CZ	5.96	1.46	1.38
1	B	477	GLU	CG-CD	5.84	1.60	1.51
1	B	97	VAL	CB-CG2	5.73	1.64	1.52
1	B	235	ARG	CB-CG	-5.55	1.37	1.52
1	A	392	LYS	CD-CE	5.54	1.65	1.51
1	B	301	LYS	CD-CE	5.51	1.65	1.51
1	B	89	GLU	CB-CG	5.43	1.62	1.52
1	B	268[A]	GLU	CB-CG	5.29	1.62	1.52
1	B	268[B]	GLU	CB-CG	5.29	1.62	1.52
1	A	339	TYR	CE1-CZ	5.17	1.45	1.38
1	B	97	VAL	CB-CG1	5.17	1.63	1.52
1	A	401	LYS	CB-CG	-5.13	1.38	1.52
1	A	270	ALA	CA-CB	5.09	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	GLU	CD-OE1	5.08	1.31	1.25
1	B	358	LYS	CG-CD	5.06	1.69	1.52
1	B	179	TRP	CE3-CZ3	5.02	1.47	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	B	28	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	B	330	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	210	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	B	184	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	194	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	2	VAL	CG1-CB-CG2	6.97	122.05	110.90
1	A	101[A]	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	101[B]	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	B	101[A]	ARG	N-CA-C	6.87	129.54	111.00
1	B	101[B]	ARG	N-CA-C	6.87	129.54	111.00
1	B	83	LYS	CD-CE-NZ	6.58	126.84	111.70
1	A	191	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	194	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	191	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	360	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	356	VAL	CG1-CB-CG2	6.33	121.03	110.90
1	B	301	LYS	CD-CE-NZ	6.26	126.11	111.70
1	A	194	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	210	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	210	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	368	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	368	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	101[A]	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	101[B]	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	269	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	B	380	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	B	101[A]	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	101[B]	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	360[A]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	360[B]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	269	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	28	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	191	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	138	ASP	CB-CG-OD2	-5.15	113.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	184	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	105	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4072	0	3893	35	1
1	B	4064	0	3874	35	0
2	A	4	0	3	0	0
3	A	43	0	30	4	0
3	B	43	0	30	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	440	0	0	8	3
5	B	444	0	0	3	3
All	All	9112	0	7830	64	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:358:LYS:CE	1:B:358:LYS:NZ	1.69	1.49
1:A:32[A]:LEU:HD23	1:B:32[A]:LEU:HD23	1.20	1.15
1:A:101[B]:ARG:O	5:A:1321:HOH:O	1.69	1.07
1:A:89:GLU:OE1	5:A:1133:HOH:O	1.75	1.02
1:A:32[A]:LEU:HD23	1:B:32[A]:LEU:CD2	1.92	0.98
1:A:32[A]:LEU:CD2	1:B:32[A]:LEU:CD2	2.66	0.74
1:A:353:GLN:HE22	1:A:374:ASN:H	1.41	0.69
1:A:360[A]:ARG:NH1	5:A:1327:HOH:O	1.82	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:274[A]:ARG:HH22	1:B:287:GLN:NE2	1.93	0.65
1:B:364:HIS:HD2	5:B:888:HOH:O	1.80	0.64
1:B:353:GLN:HE22	1:B:374:ASN:H	1.44	0.64
1:A:1:MET:HE3	1:A:3:ASN:HD21	1.68	0.58
1:A:32[A]:LEU:CD2	1:B:32[A]:LEU:HD23	2.12	0.58
1:A:139:ALA:HB2	3:A:550:HEM:HBB1	1.87	0.57
1:A:118:TYR:CD1	1:A:360[B]:ARG:HD3	2.39	0.57
1:B:491:LYS:NZ	1:B:491:LYS:HB2	2.21	0.56
1:B:490:MET:H	1:B:491:LYS:C	2.10	0.55
1:B:490:MET:N	1:B:491:LYS:C	2.61	0.54
1:A:32[A]:LEU:CD2	1:B:32[A]:LEU:HD21	2.38	0.53
1:B:258:TRP:HB2	1:B:297[B]:VAL:HG23	1.90	0.53
1:A:1:MET:CE	1:A:3:ASN:HD21	2.23	0.52
1:B:428:GLN:N	1:B:429:PRO:HD2	2.25	0.52
1:A:139:ALA:CB	3:A:550:HEM:HBB1	2.42	0.50
1:B:491:LYS:HZ2	1:B:491:LYS:HB2	1.77	0.49
1:B:457:HIS:HB2	1:B:460:ILE:HD12	1.93	0.49
1:A:287:GLN:HG2	5:A:1255:HOH:O	2.13	0.49
1:B:428:GLN:N	1:B:429:PRO:CD	2.76	0.49
1:A:56:HIS:CE1	1:A:97:VAL:HG22	2.48	0.48
1:A:490:MET:N	1:A:491:LYS:HA	2.29	0.48
1:A:409:LYS:HG3	5:A:1143:HOH:O	2.15	0.47
1:B:79:LYS:HE3	5:B:937:HOH:O	2.15	0.47
1:A:129:ASN:CG	3:A:550:HEM:HAC	2.35	0.47
1:A:135:PHE:CE2	1:A:176:GLN:HG3	2.51	0.46
1:A:268[B]:GLU:HG2	5:A:1248:HOH:O	2.13	0.46
1:B:261[B]:SER:OG	1:B:291:LEU:HD22	2.14	0.46
1:A:327:SER:HB2	1:A:328:PRO:HD2	1.97	0.46
1:B:139:ALA:CB	3:B:550:HEM:CBB	2.94	0.46
1:B:66:PHE:O	1:B:87:LYS:HA	2.17	0.45
1:B:351:TYR:N	1:B:352:PRO:CD	2.80	0.45
1:B:92:PHE:CZ	1:B:297[A]:VAL:HG11	2.52	0.44
1:B:129:ASN:CG	3:B:550:HEM:HAC	2.38	0.44
1:A:135:PHE:CZ	1:A:176:GLN:HG3	2.53	0.44
1:A:95:SER:O	1:A:111:ARG:HA	2.17	0.44
1:A:360[A]:ARG:CD	5:A:1327:HOH:O	2.67	0.43
1:B:56:HIS:CE1	1:B:97:VAL:HG22	2.54	0.42
1:A:364:HIS:HD2	5:A:1105:HOH:O	2.02	0.42
1:A:236:LYS:HE3	1:A:237:HIS:CE1	2.54	0.42
1:A:204:ILE:HD12	1:A:400:PRO:HG2	2.02	0.42
1:B:92:PHE:CZ	1:B:297[B]:VAL:HG11	2.55	0.42
1:B:358:LYS:HD2	5:B:875:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:ALA:CB	3:B:550:HEM:HBB1	2.49	0.42
1:B:92:PHE:CZ	1:B:115:MET:HG2	2.55	0.41
1:A:147:HIS:HB3	1:B:382:ASN:OD1	2.21	0.41
1:A:358:LYS:HE2	1:A:358:LYS:HB3	1.82	0.41
1:A:23:ILE:HG22	1:A:32[A]:LEU:HD12	2.03	0.41
1:B:139:ALA:HB2	3:B:550:HEM:HBB1	2.02	0.41
1:A:56:HIS:HA	1:A:96:THR:O	2.21	0.41
1:A:66:PHE:O	1:A:87:LYS:HA	2.20	0.41
1:B:92:PHE:CE1	1:B:115:MET:HG2	2.55	0.41
1:A:139:ALA:CB	3:A:550:HEM:CBB	2.98	0.41
1:B:488:LYS:O	1:B:491:LYS:HG3	2.22	0.40
1:B:139:ALA:HA	3:B:550:HEM:HBB1	2.04	0.40
1:B:127:VAL:HG22	1:B:315:PHE:HB3	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1339:HOH:O	5:B:993:HOH:O[2_565]	2.02	0.18
5:A:1295:HOH:O	5:A:1295:HOH:O[2_565]	2.13	0.07
5:A:1318:HOH:O	5:B:916:HOH:O[2_565]	2.14	0.06
1:A:372:MHO:OD1	5:B:688:HOH:O[2_565]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/505 (98%)	478 (96%)	18 (4%)	0	100	100
1	B	495/505 (98%)	478 (97%)	17 (3%)	0	100	100
All	All	991/1010 (98%)	956 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	435/438 (99%)	424 (98%)	11 (2%)	60	33
1	B	434/438 (99%)	421 (97%)	13 (3%)	53	25
All	All	869/876 (99%)	845 (97%)	24 (3%)	57	28

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	119	THR
1	A	175	TYR
1	A	267	GLU
1	A	271	LYS
1	A	377	TYR
1	A	414	TRP
1	A	418	TYR
1	A	475	TYR
1	A	485	LYS
1	A	490	MET
1	B	2	VAL
1	B	119	THR
1	B	175	TYR
1	B	268[A]	GLU
1	B	268[B]	GLU
1	B	301	LYS
1	B	377	TYR
1	B	414	TRP
1	B	418	TYR
1	B	458	LYS
1	B	475	TYR
1	B	485	LYS
1	B	491	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	149	GLN
1	A	237	HIS
1	A	353	GLN
1	A	364	HIS
1	B	287	GLN
1	B	353	GLN
1	B	364	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MHO	A	162	1	8,8,9	7.95	5 (62%)	7,9,11	3.75	4 (57%)
1	MHO	A	181	1	8,8,9	5.68	4 (50%)	7,9,11	2.92	3 (42%)
1	MHO	A	292	1	8,8,9	6.94	3 (37%)	7,9,11	3.19	5 (71%)
1	MHO	A	372	1	8,8,9	6.88	3 (37%)	7,9,11	2.42	3 (42%)
1	MHO	B	162	1	8,8,9	7.50	5 (62%)	7,9,11	4.40	5 (71%)
1	MHO	B	181	1	8,8,9	5.98	3 (37%)	7,9,11	2.24	4 (57%)
1	MHO	B	292	1	8,8,9	7.29	3 (37%)	7,9,11	2.97	2 (28%)
1	MHO	B	372	1	8,8,9	5.33	4 (50%)	7,9,11	3.27	4 (57%)

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
1	MHO	A	162	1	-	0/5/7/9	0/0/0/0
1	MHO	A	181	1	-	0/5/7/9	0/0/0/0
1	MHO	A	292	1	-	0/5/7/9	0/0/0/0
1	MHO	A	372	1	-	0/5/7/9	0/0/0/0
1	MHO	B	162	1	-	0/5/7/9	0/0/0/0
1	MHO	B	181	1	-	0/5/7/9	0/0/0/0
1	MHO	B	292	1	-	0/5/7/9	0/0/0/0
1	MHO	B	372	1	-	0/5/7/9	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	MHO	O-C	19.39	1.24	1.11
1	B	162	MHO	O-C	18.32	1.24	1.11
1	A	372	MHO	O-C	17.39	1.23	1.11
1	B	292	MHO	O-C	16.74	1.22	1.11
1	A	292	MHO	O-C	16.51	1.22	1.11
1	B	181	MHO	O-C	15.98	1.22	1.11
1	A	181	MHO	O-C	12.82	1.20	1.11
1	B	292	MHO	OD1-SD	11.20	1.77	1.51
1	B	372	MHO	O-C	11.16	1.19	1.11
1	A	292	MHO	OD1-SD	10.16	1.75	1.51
1	A	181	MHO	OD1-SD	9.02	1.72	1.51
1	B	372	MHO	OD1-SD	8.84	1.72	1.51
1	A	162	MHO	OD1-SD	8.76	1.72	1.51
1	B	162	MHO	OD1-SD	8.37	1.71	1.51
1	A	372	MHO	OD1-SD	7.28	1.68	1.51
1	A	162	MHO	CB-CA	5.88	1.58	1.53
1	B	162	MHO	CB-CA	5.58	1.57	1.53
1	B	181	MHO	OD1-SD	4.85	1.62	1.51
1	A	372	MHO	CB-CA	4.08	1.56	1.53
1	B	372	MHO	CA-C	3.68	1.55	1.48
1	B	292	MHO	CA-C	3.12	1.54	1.48
1	A	162	MHO	CA-C	3.09	1.54	1.48
1	B	372	MHO	CG-SD	-2.85	1.66	1.80
1	A	162	MHO	CG-SD	-2.85	1.66	1.80
1	A	181	MHO	CG-SD	-2.65	1.67	1.80
1	B	181	MHO	CG-SD	-2.64	1.67	1.80
1	A	292	MHO	CG-SD	-2.41	1.68	1.80
1	B	162	MHO	CA-C	2.36	1.52	1.48
1	B	162	MHO	CG-SD	-2.36	1.68	1.80
1	A	181	MHO	CA-C	2.20	1.52	1.48

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	MHO	CE-SD-CG	8.79	117.84	96.87
1	A	162	MHO	CE-SD-CG	6.07	111.34	96.87
1	A	181	MHO	OD1-SD-CG	-5.43	92.06	105.87
1	B	372	MHO	OD1-SD-CE	5.34	115.55	106.28
1	A	292	MHO	C-CA-N	-5.27	108.57	113.83
1	B	292	MHO	C-CA-N	-5.08	108.76	113.83
1	B	372	MHO	CE-SD-CG	5.05	108.92	96.87
1	B	292	MHO	OD1-SD-CE	5.05	115.04	106.28
1	B	162	MHO	OD1-SD-CG	-4.79	93.67	105.87
1	A	292	MHO	OD1-SD-CG	-4.62	94.12	105.87
1	A	162	MHO	OD1-SD-CE	4.55	114.18	106.28
1	A	162	MHO	C-CA-N	-4.31	109.53	113.83
1	A	372	MHO	CG-CB-CA	4.30	121.57	113.06
1	A	372	MHO	CE-SD-CG	4.12	106.70	96.87
1	A	181	MHO	OD1-SD-CE	-4.02	99.30	106.28
1	B	162	MHO	C-CA-N	-3.94	109.90	113.83
1	A	162	MHO	OD1-SD-CG	-3.90	95.94	105.87
1	B	372	MHO	CG-CB-CA	3.61	120.20	113.06
1	A	181	MHO	CB-CG-SD	3.21	119.70	111.26
1	B	162	MHO	CG-CB-CA	3.14	119.29	113.06
1	A	292	MHO	CG-CB-CA	3.02	119.04	113.06
1	B	181	MHO	CG-CB-CA	-3.00	107.11	113.06
1	B	162	MHO	OD1-SD-CE	-2.87	101.31	106.28
1	B	181	MHO	OD1-SD-CE	-2.81	101.39	106.28
1	B	181	MHO	OD1-SD-CG	-2.79	98.78	105.87
1	A	292	MHO	OD1-SD-CE	-2.74	101.52	106.28
1	A	372	MHO	C-CA-N	-2.25	111.58	113.83
1	B	372	MHO	C-CA-N	-2.14	111.69	113.83
1	B	181	MHO	CE-SD-CG	2.08	101.83	96.87
1	A	292	MHO	CB-CA-N	-2.08	104.59	110.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	550	1,4	49,50,50	2.61	18 (36%)	46,82,82	2.19	9 (19%)
2	ACT	A	900	-	1,3,3	4.57	1 (100%)	0,3,3	0.00	-
3	HEM	B	550	1,4	49,50,50	4.89	18 (36%)	46,82,82	2.78	19 (41%)

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
3	HEM	A	550	1,4	-	0/14/114/114	0/0/8/8
2	ACT	A	900	-	-	0/0/0/0	0/0/0/0
3	HEM	B	550	1,4	-	0/14/114/114	0/0/8/8

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	550	HEM	C3D-C4D	29.43	1.51	1.44
3	B	550	HEM	C2B-C1B	8.67	1.46	1.44
3	B	550	HEM	C2D-C1D	7.34	1.46	1.44
3	A	550	HEM	C2D-C1D	6.44	1.46	1.44
3	A	550	HEM	C3D-C4D	6.41	1.46	1.44
3	A	550	HEM	C2B-C1B	5.82	1.46	1.44
3	A	550	HEM	C4A-C3A	5.69	1.47	1.40
3	A	550	HEM	C3C-CAC	5.18	1.56	1.40
3	B	550	HEM	FE-NA	4.84	2.13	1.92
3	A	550	HEM	C3B-C2B	-4.68	1.35	1.43
3	B	550	HEM	C3B-C2B	-4.65	1.35	1.43
2	A	900	ACT	CH3-C	-4.57	1.42	1.48
3	A	550	HEM	FE-NC	4.01	2.12	1.97
3	B	550	HEM	C3C-CAC	3.88	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	550	HEM	CMC-C2C	3.75	1.59	1.47
3	A	550	HEM	CMC-C2C	3.68	1.58	1.47
3	A	550	HEM	FE-NA	3.58	2.07	1.92
3	A	550	HEM	C3B-CAB	3.50	1.51	1.40
3	A	550	HEM	CMB-C2B	3.25	1.57	1.47
3	B	550	HEM	C3B-CAB	3.22	1.50	1.40
3	B	550	HEM	C4A-C3A	3.11	1.44	1.40
3	B	550	HEM	C3C-C2C	-2.98	1.38	1.43
3	B	550	HEM	CMD-C2D	2.77	1.56	1.47
3	B	550	HEM	FE-NC	2.69	2.07	1.97
3	B	550	HEM	C3D-C2D	2.62	1.48	1.43
3	A	550	HEM	C3C-C2C	-2.45	1.39	1.43
3	B	550	HEM	O1D-CGD	2.41	1.30	1.22
3	A	550	HEM	FE-ND	-2.36	1.89	1.97
3	A	550	HEM	CMA-C3A	2.36	1.56	1.51
3	A	550	HEM	C1A-C2A	2.28	1.47	1.43
3	B	550	HEM	CMA-C3A	2.26	1.56	1.51
3	A	550	HEM	C3D-C2D	2.18	1.47	1.43
3	B	550	HEM	O1A-CGA	2.17	1.30	1.22
3	A	550	HEM	CMD-C2D	2.17	1.54	1.47
3	B	550	HEM	CHB-C1B	2.12	1.38	1.35
3	B	550	HEM	C2C-C1C	2.09	1.49	1.43
3	A	550	HEM	C2C-C1C	2.04	1.49	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	HEM	C3B-C4B-NB	-11.10	106.06	114.00
3	A	550	HEM	C3B-C4B-NB	-7.13	108.90	114.00
3	A	550	HEM	C4C-NC-C1C	6.72	112.52	105.53
3	B	550	HEM	CHC-C1C-NC	-5.09	120.31	124.73
3	B	550	HEM	C4D-ND-C1D	5.03	110.31	105.16
3	A	550	HEM	C1A-CHA-C4D	-4.54	121.50	127.47
3	B	550	HEM	C1B-NB-C4B	4.33	109.59	105.16
3	B	550	HEM	CMA-C3A-C4A	-4.28	122.04	128.62
3	A	550	HEM	CBA-CAA-C2A	-3.87	105.87	112.69
3	B	550	HEM	CHC-C4B-NB	3.81	127.75	124.58
3	A	550	HEM	CMA-C3A-C4A	-3.67	122.97	128.62
3	B	550	HEM	C3A-C4A-NA	-3.62	106.68	109.41
3	B	550	HEM	C4A-NA-C1A	3.27	111.07	106.76
3	A	550	HEM	CHA-C4D-ND	3.10	128.56	124.31
3	B	550	HEM	CHA-C4D-ND	3.06	128.52	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	HEM	CMA-C3A-C2A	3.00	130.60	124.94
3	B	550	HEM	C4C-NC-C1C	2.94	108.59	105.53
3	B	550	HEM	O1A-CGA-CBA	-2.80	113.39	123.03
3	B	550	HEM	CHD-C4C-NC	2.77	127.14	124.73
3	B	550	HEM	CBD-CAD-C3D	-2.75	108.37	114.37
3	B	550	HEM	C1A-CHA-C4D	-2.74	123.87	127.47
3	A	550	HEM	CHD-C4C-NC	2.72	127.10	124.73
3	B	550	HEM	CAD-CBD-CGD	-2.72	105.01	113.48
3	B	550	HEM	CHD-C1D-ND	2.71	126.83	124.58
3	B	550	HEM	CMA-C3A-C2A	2.63	129.90	124.94
3	B	550	HEM	CAD-C3D-C4D	2.18	128.45	124.53
3	A	550	HEM	O2D-CGD-CBD	2.15	121.83	114.22
3	B	550	HEM	C2A-C1A-NA	-2.05	106.89	109.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	491/505 (97%)	-0.25	7 (1%) 72 83	3, 6, 14, 46	1 (0%)
1	B	491/505 (97%)	-0.32	4 (0%) 83 90	3, 6, 14, 45	2 (0%)
All	All	982/1010 (97%)	-0.29	11 (1%) 75 86	3, 6, 14, 46	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	MET	7.0
1	B	491	LYS	6.4
1	A	489	MET	6.0
1	B	490	MET	5.5
1	B	489	MET	5.4
1	A	491	LYS	5.0
1	A	488	LYS	3.2
1	A	272	LYS	3.0
1	A	2	VAL	3.0
1	A	287	GLN	2.5
1	B	488	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	MHO	B	372	9/10	0.10	2.74	7,8,15,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MHO	B	162	9/10	0.09	1.59	2,3,12,15	0
1	MHO	A	372	9/10	0.08	1.42	6,9,18,20	0
1	MHO	A	162	9/10	0.08	0.04	3,4,12,20	0
1	MHO	A	292	9/10	0.07	-0.05	4,7,19,23	0
1	MHO	B	181	9/10	0.07	-0.11	2,4,9,10	0
1	MHO	B	292	9/10	0.07	-0.26	4,7,21,23	0
1	MHO	A	181	9/10	0.06	-1.06	3,4,10,11	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	O	A	551	1/1	0.17	5.87	16,16,16,16	0
4	O	B	551	1/1	0.11	1.53	10,10,10,10	0
3	HEM	A	550	43/43	0.13	1.34	2,3,8,18	1
3	HEM	B	550	43/43	0.11	1.13	2,2,8,12	0
2	ACT	A	900	4/4	0.08	0.63	10,11,11,14	0

6.5 Other polymers

There are no such residues in this entry.