



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:41 am GMT

PDB ID : 4QOP
Title : Structure of Bacillus pumilus catalase with hydroquinone bound.
Authors : Loewen, P.C.
Deposited on : 2014-06-20
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

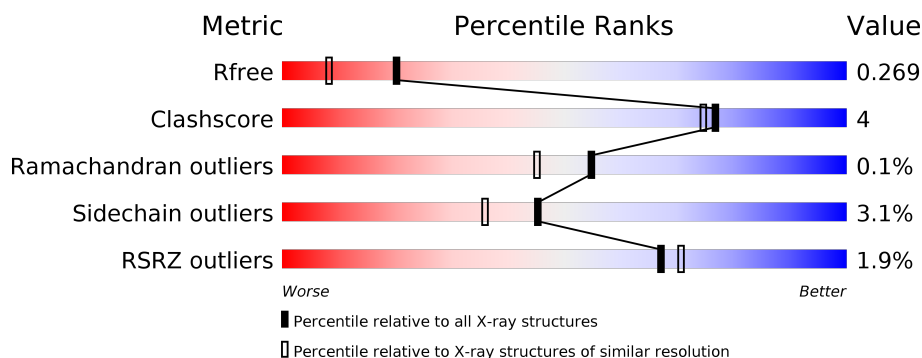
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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. 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	491	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	491	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>••</div> </div> </div>
1	C	491	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	491	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>••</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HQE	A	503	-	-	-	X
3	HQE	B	503	-	-	-	X
3	HQE	C	503	-	-	-	X
3	HQE	D	503	-	-	-	X
4	CL	A	504	-	-	-	X

2 Entry composition [i](#)

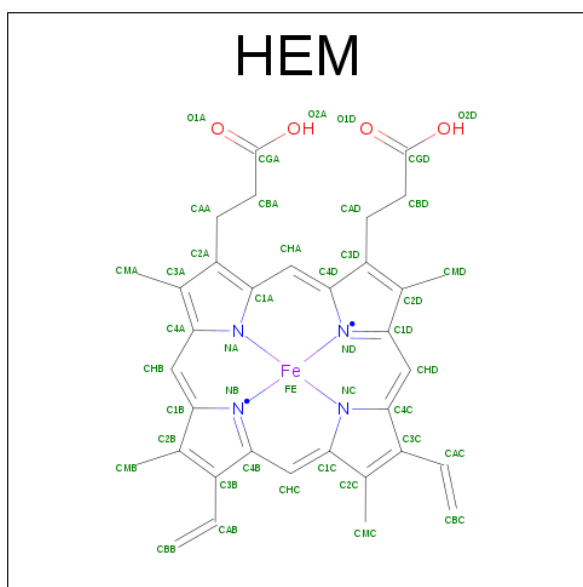
There are 6 unique types of molecules in this entry. The entry contains 17699 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	5	0
			3949	2488	692	755	14			
1	B	480	Total	C	N	O	S	0	5	0
			3951	2491	691	754	15			
1	C	480	Total	C	N	O	S	0	6	0
			3962	2498	695	755	14			
1	D	480	Total	C	N	O	S	0	6	0
			3958	2494	692	758	14			

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



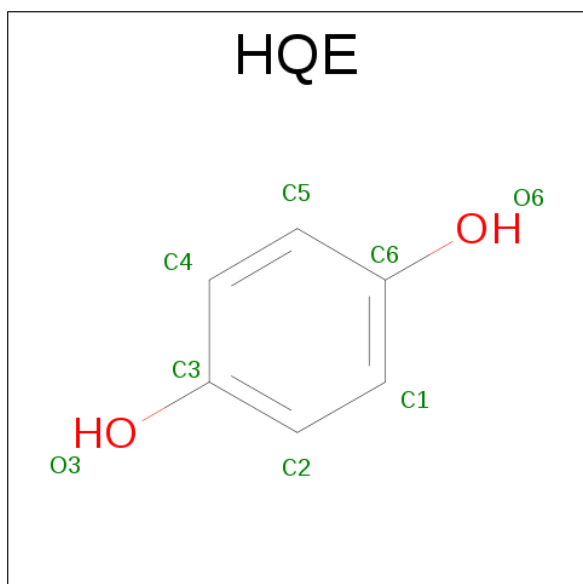
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		

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

- Molecule 3 is BENZENE-1,4-DIOL (three-letter code: HQE) (formula: C₆H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			8	6	2		
3	B	1	Total	C	O		
			8	6	2		
3	C	1	Total	C	O		
			8	6	2		
3	D	1	Total	C	O		
			8	6	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

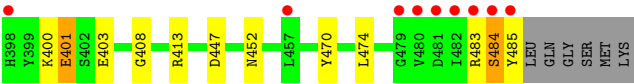
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	392	Total O 392 392	0	0
6	B	361	Total O 361 361	0	0
6	C	388	Total O 388 388	0	0
6	D	354	Total O 354 354	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.28Å 109.45Å 104.20Å 90.00° 92.05° 90.00°	Depositor
Resolution (Å)	104.13 – 1.90 48.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.8 (104.13-1.90) 90.8 (48.44-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.230 , 0.261 0.237 , 0.269	Depositor DCC
R_{free} test set	7647 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17699	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, CL, HQE, NA

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	0.70	0/4068	0.77	4/5516 (0.1%)
1	B	0.71	0/4069	0.77	3/5516 (0.1%)
1	C	0.73	0/4080	0.78	3/5531 (0.1%)
1	D	0.71	0/4076	0.75	2/5526 (0.0%)
All	All	0.71	0/16293	0.77	12/22089 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	413	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	B	440	LEU	CA-CB-CG	6.46	130.16	115.30
1	C	413	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	219	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	413	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	D	252	GLU	CA-CB-CG	5.51	125.53	113.40
1	B	413	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	C	138	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	292	LEU	CB-CG-CD2	5.15	119.75	111.00
1	A	229	MET	CG-SD-CE	5.04	108.27	100.20
1	A	252	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	C	219	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	182	PHE	Peptide

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	3949	0	3748	22	0
1	B	3951	0	3756	19	1
1	C	3962	0	3771	23	1
1	D	3958	0	3758	26	0
2	A	86	0	60	9	0
2	B	86	0	60	12	0
2	C	86	0	60	15	0
2	D	86	0	60	8	0
3	A	8	0	4	2	0
3	B	8	0	6	0	0
3	C	8	0	5	2	0
3	D	8	0	5	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	392	0	0	11	0
6	B	361	0	0	7	0
6	C	388	0	0	8	0
6	D	354	0	0	8	0
All	All	17699	0	15293	111	1

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 4.

All (111) 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:D:401:GLU:OE1	6:D:902:HOH:O	1.88	0.90
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:HBB2	1.56	0.87
1:D:400:LYS:NZ	6:D:933:HOH:O	1.73	0.86
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:CMC	2.11	0.81
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:CMC	2.13	0.77
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:HMC2	1.67	0.77
2:A:502[B]:HEM:HBC2	2:A:502[B]:HEM:HMC2	1.67	0.76
2:B:501[A]:HEM:CMC	2:B:501[A]:HEM:HBC2	2.16	0.76
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:HBB2	1.68	0.75
2:D:502[B]:HEM:HMC1	2:D:502[B]:HEM:HBC2	1.68	0.75
2:C:501[A]:HEM:CMB	2:C:501[A]:HEM:HBB2	2.18	0.74
2:A:501[A]:HEM:CMB	2:A:501[A]:HEM:HBB2	2.15	0.74
2:D:502[B]:HEM:HBC2	2:D:502[B]:HEM:CMC	2.19	0.72
2:C:502[B]:HEM:HBC2	2:C:502[B]:HEM:CMC	2.18	0.71
1:C:455:THR:OG1	1:D:388:ARG:NH1	2.24	0.71
2:C:501[A]:HEM:HBB2	2:C:501[A]:HEM:HMB2	1.74	0.70
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:HMC2	1.73	0.70
1:B:417:GLU:HG3	1:C:28:HIS:CE1	2.28	0.69
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:HMC2	1.72	0.69
1:A:472:GLN:OE1	6:A:863:HOH:O	2.10	0.68
2:C:502[B]:HEM:HBC2	2:C:502[B]:HEM:HMC1	1.75	0.68
2:B:501[A]:HEM:CMB	2:B:501[A]:HEM:HBB2	2.24	0.68
1:C:262:TYR:OH	6:C:970:HOH:O	2.12	0.67
1:A:45:HIS:HD2	6:A:688:HOH:O	1.78	0.67
1:B:275:ASP:HB3	6:B:837:HOH:O	1.93	0.67
2:D:501[A]:HEM:CMC	2:D:501[A]:HEM:HBC2	2.25	0.66
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:HBC2	1.78	0.66
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:HBC2	2.26	0.65
1:B:287:GLU:CD	1:B:292:LEU:HD21	2.18	0.64
1:A:45:HIS:HE1	1:C:351:ASN:OD1	1.81	0.64
1:D:234:GLU:HG3	1:D:235:ILE:N	2.12	0.64
5:A:506:NA:NA	6:A:837:HOH:O	1.71	0.62
1:C:110:ASP:OD1	3:C:503:HQE:H2	1.99	0.62
1:A:417:GLU:HG2	1:D:28:HIS:CD2	2.36	0.61
1:D:332:LEU:HD12	2:D:501[A]:HEM:HBB1	1.82	0.59
1:A:480:VAL:O	6:A:981:HOH:O	2.16	0.58
1:B:237:ALA:HB2	1:C:237:ALA:HB2	1.85	0.57
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:HBC2	1.85	0.57
1:B:100:HIS:HE1	6:C:703:HOH:O	1.86	0.57
1:D:72[B]:SER:OG	1:D:74:GLU:OE1	2.15	0.56
6:A:950:HOH:O	1:D:334:GLN:HG3	2.05	0.56
1:C:336:ARG:HG3	2:C:502[B]:HEM:HMC3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLN:NE2	6:C:730:HOH:O	2.32	0.56
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:CBB	2.36	0.54
2:C:501[A]:HEM:CBC	2:C:501[A]:HEM:HMC2	2.36	0.54
1:C:143:PHE:CD2	2:C:501[A]:HEM:CMB	2.91	0.54
2:C:501[A]:HEM:CBC	2:C:501[A]:HEM:CMC	2.84	0.54
1:B:468:GLU:HG3	6:B:899:HOH:O	2.08	0.53
1:A:9:LEU:HD13	1:C:393:PRO:HB2	1.90	0.53
1:B:420:ASN:ND2	6:B:719:HOH:O	2.39	0.52
1:B:142:LYS:HD3	1:C:21:GLN:HA	1.92	0.52
6:A:798:HOH:O	1:D:100:HIS:HE1	1.91	0.52
1:B:249:ASP:O	1:B:253:LYS:HG2	2.09	0.52
2:A:501[A]:HEM:CBC	2:A:501[A]:HEM:HMC2	2.40	0.52
1:B:19:ASP:OD2	6:D:933:HOH:O	2.18	0.51
1:A:27:GLY:HA3	1:D:408:GLY:HA3	1.93	0.51
1:A:286:SER:OG	1:A:288:GLU:HG2	2.10	0.51
1:B:140:ALA:HA	2:B:501[A]:HEM:HBB1	1.92	0.51
1:A:138:ARG:NH2	6:A:713:HOH:O	2.45	0.49
1:A:392:GLN:NE2	6:A:736:HOH:O	2.35	0.49
2:B:501[A]:HEM:CBC	2:B:501[A]:HEM:HMC2	2.38	0.49
1:A:237:ALA:HB2	1:D:237:ALA:HB2	1.95	0.49
2:C:501[A]:HEM:CBB	2:C:501[A]:HEM:HMB2	2.41	0.49
1:C:410:ARG:NH2	1:D:403:GLU:O	2.45	0.49
1:C:238:ASN:C	6:C:631:HOH:O	2.51	0.49
1:A:142:LYS:HD3	1:D:21:GLN:HA	1.94	0.48
1:A:21:GLN:HA	1:D:142:LYS:HD3	1.94	0.48
1:D:6:HIS:HA	6:D:780:HOH:O	2.13	0.48
2:B:501[A]:HEM:O2A	6:B:685:HOH:O	2.18	0.48
2:C:502[B]:HEM:CBC	2:C:502[B]:HEM:HMC1	2.42	0.48
1:D:302:ARG:NH1	6:D:816:HOH:O	2.26	0.47
1:D:483:ARG:O	1:D:484:SER:CB	2.61	0.47
1:A:100:HIS:HE1	6:D:671:HOH:O	1.96	0.47
1:B:36:ASP:OD1	1:C:413:ARG:NH1	2.42	0.46
1:D:134[B]:ILE:HD13	1:D:134[B]:ILE:H	1.80	0.46
1:B:332:LEU:HD12	2:B:501[A]:HEM:HBB1	1.96	0.46
1:B:21:GLN:HA	1:C:142:LYS:HD3	1.96	0.45
1:D:181:LEU:HD21	3:D:503:HQE:C4	2.46	0.45
1:B:9:LEU:HD13	1:D:393:PRO:HB2	1.99	0.45
2:D:502[B]:HEM:HMC1	2:D:502[B]:HEM:CBC	2.42	0.45
1:C:336:ARG:HG2	2:C:502[B]:HEM:C2C	2.52	0.45
1:A:238:ASN:ND2	6:A:977:HOH:O	2.29	0.45
2:B:502[B]:HEM:HMB1	2:B:502[B]:HEM:HBB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:CG	6:A:668:HOH:O	2.66	0.44
1:A:110:ASP:OD1	3:A:503:HQE:O3	2.35	0.44
1:C:403:GLU:OE2	6:C:732:HOH:O	2.21	0.44
1:B:393:PRO:HB2	1:D:9:LEU:HD13	1.98	0.44
1:B:354:ARG:NH1	6:B:804:HOH:O	2.46	0.43
2:A:502[B]:HEM:CMC	2:A:502[B]:HEM:HBC2	2.42	0.43
1:A:130:ASN:CG	2:A:502[B]:HEM:HMB2	2.39	0.43
1:A:72:SER:OG	1:A:74:GLU:OE1	2.36	0.43
2:C:502[B]:HEM:HBB2	2:C:502[B]:HEM:CMB	2.49	0.43
1:D:483:ARG:O	1:D:484:SER:HB3	2.19	0.42
1:B:442:LYS:NZ	6:B:957:HOH:O	2.52	0.42
1:B:287:GLU:CG	1:B:292:LEU:HD21	2.50	0.42
6:B:821:HOH:O	1:C:331:LYS:HG2	2.19	0.42
1:D:143:PHE:CD2	2:D:501[A]:HEM:CMB	3.02	0.42
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:CBC	2.48	0.42
1:D:354:ARG:NE	6:D:940:HOH:O	2.53	0.42
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:CBC	2.47	0.41
1:D:110:ASP:OD1	3:D:503:HQE:O3	2.37	0.41
3:D:503:HQE:H2	6:D:857:HOH:O	2.19	0.41
1:A:181:LEU:HD21	3:A:503:HQE:C4	2.50	0.41
1:A:393:PRO:HB2	1:C:9[A]:LEU:HD13	2.02	0.41
2:C:502[B]:HEM:HBB2	2:C:502[B]:HEM:HMB1	2.03	0.41
1:D:75:LYS:HG2	1:D:76:HIS:CE1	2.56	0.41
1:C:150:LEU:HD22	3:C:503:HQE:C4	2.51	0.41
1:C:28:HIS:HD2	6:C:829:HOH:O	2.04	0.41
1:A:483:ARG:NH1	6:A:867:HOH:O	2.24	0.40
1:C:121:GLU:HG3	6:C:762:HOH:O	2.21	0.40
1:C:423:LYS:HB3	6:C:972:HOH:O	2.20	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLU:OE1	1:C:417:GLU:OE2[1_455]	2.15	0.05

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	483/491 (98%)	467 (97%)	16 (3%)	0	100	100
1	B	483/491 (98%)	470 (97%)	13 (3%)	0	100	100
1	C	484/491 (99%)	473 (98%)	11 (2%)	0	100	100
1	D	484/491 (99%)	471 (97%)	12 (2%)	1 (0%)	51	41
All	All	1934/1964 (98%)	1881 (97%)	52 (3%)	1 (0%)	55	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	484	SER

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	426/432 (99%)	415 (97%)	11 (3%)	51	43
1	B	426/432 (99%)	410 (96%)	16 (4%)	38	27
1	C	427/432 (99%)	415 (97%)	12 (3%)	49	40
1	D	427/432 (99%)	414 (97%)	13 (3%)	46	37
All	All	1706/1728 (99%)	1654 (97%)	52 (3%)	45	37

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	114	PHE
1	A	120	THR
1	A	241	GLN
1	A	253	LYS
1	A	401	GLU
1	A	420	ASN
1	A	447	ASP
1	A	452	ASN
1	A	470	TYR
1	A	474	LEU
1	B	110	ASP
1	B	114	PHE
1	B	120	THR
1	B	219	ARG
1	B	241	GLN
1	B	253	LYS
1	B	272	ASP
1	B	292	LEU
1	B	401	GLU
1	B	420	ASN
1	B	440	LEU
1	B	447	ASP
1	B	452	ASN
1	B	470	TYR
1	B	474	LEU
1	B	485	TYR
1	C	72	SER
1	C	110	ASP
1	C	114	PHE
1	C	120	THR
1	C	241	GLN
1	C	401	GLU
1	C	409	ASP
1	C	420	ASN
1	C	447	ASP
1	C	452	ASN
1	C	470	TYR
1	C	485	TYR
1	D	75	LYS
1	D	110	ASP
1	D	114	PHE
1	D	120	THR

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Mol	Chain	Res	Type
1	D	234	GLU
1	D	241	GLN
1	D	388	ARG
1	D	401	GLU
1	D	447	ASP
1	D	452	ASN
1	D	470	TYR
1	D	474	LEU
1	D	485	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	100	HIS
1	A	157	ASN
1	A	226	ASN
1	A	398	HIS
1	A	407	HIS
1	A	420	ASN
1	A	452	ASN
1	A	472	GLN
1	B	100	HIS
1	B	157	ASN
1	B	226	ASN
1	B	367	ASN
1	B	420	ASN
1	B	452	ASN
1	C	100	HIS
1	C	157	ASN
1	C	226	ASN
1	C	420	ASN
1	D	100	HIS
1	D	157	ASN
1	D	226	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z > 2$
2	HEM	A	501[A]	1	28,50,50	0.93	1 (3%)	17,82,82	1.78	4 (23%)
2	HEM	A	502[B]	1	28,50,50	0.84	2 (7%)	17,82,82	1.49	3 (17%)
3	HQE	A	503	-	8,8,8	0.36	0	10,10,10	0.37	0
2	HEM	B	501[A]	1,6	28,50,50	0.95	1 (3%)	17,82,82	1.36	1 (5%)
2	HEM	B	502[B]	1,6	28,50,50	0.81	2 (7%)	17,82,82	1.64	5 (29%)
3	HQE	B	503	-	8,8,8	0.69	0	10,10,10	0.38	0
2	HEM	C	501[A]	1,6	28,50,50	1.05	2 (7%)	17,82,82	1.88	6 (35%)
2	HEM	C	502[B]	1	28,50,50	0.92	1 (3%)	17,82,82	1.99	7 (41%)
3	HQE	C	503	-	8,8,8	0.47	0	10,10,10	0.74	0
2	HEM	D	501[A]	1,6	28,50,50	1.05	1 (3%)	17,82,82	1.80	5 (29%)
2	HEM	D	502[B]	1	28,50,50	1.04	2 (7%)	17,82,82	2.00	6 (35%)
3	HQE	D	503	-	8,8,8	0.61	0	10,10,10	0.64	0

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	501[A]	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	502[B]	1	-	0/6/54/54	0/0/8/8
3	HQE	A	503	-	-	0/0/0/0	0/1/1/1
2	HEM	B	501[A]	1,6	-	0/6/54/54	0/0/8/8
2	HEM	B	502[B]	1,6	-	0/6/54/54	0/0/8/8
3	HQE	B	503	-	-	0/0/0/0	0/1/1/1
2	HEM	C	501[A]	1,6	-	0/6/54/54	0/0/8/8
2	HEM	C	502[B]	1	-	0/6/54/54	0/0/8/8
3	HQE	C	503	-	-	0/0/0/0	0/1/1/1
2	HEM	D	501[A]	1,6	-	0/6/54/54	0/0/8/8
2	HEM	D	502[B]	1	-	0/6/54/54	0/0/8/8
3	HQE	D	503	-	-	0/0/0/0	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501[A]	HEM	C3B-C2B	-3.48	1.35	1.40
2	D	501[A]	HEM	C1B-NB	-3.45	1.32	1.36
2	A	501[A]	HEM	C3B-C2B	-2.83	1.36	1.40
2	A	502[B]	HEM	C1B-NB	-2.54	1.33	1.36
2	D	502[B]	HEM	C3C-C2C	-2.32	1.37	1.40
2	B	501[A]	HEM	C3B-C2B	-2.26	1.37	1.40
2	B	502[B]	HEM	C3C-C2C	-2.14	1.37	1.40
2	A	502[B]	HEM	C3B-C2B	-2.11	1.37	1.40
2	B	502[B]	HEM	C3B-C2B	-2.07	1.37	1.40
2	C	501[A]	HEM	C3C-C2C	-2.03	1.37	1.40
2	D	502[B]	HEM	C1B-NB	-2.02	1.34	1.36
2	C	502[B]	HEM	C1A-NA	2.29	1.41	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502[B]	HEM	CMD-C2D-C1D	-4.01	122.31	128.46
2	C	501[A]	HEM	CAD-CBD-CGD	-3.79	106.19	112.66
2	A	501[A]	HEM	CAD-CBD-CGD	-3.66	106.42	112.66
2	D	501[A]	HEM	CMA-C3A-C4A	-3.36	123.30	128.46
2	C	502[B]	HEM	CBD-CAD-C3D	-3.16	106.43	112.47
2	A	502[B]	HEM	CAA-CBA-CGA	-3.09	107.37	112.66
2	C	501[A]	HEM	C3B-C4B-NB	-3.00	105.33	109.21
2	D	502[B]	HEM	CBD-CAD-C3D	-2.85	107.04	112.47
2	C	502[B]	HEM	CMD-C2D-C1D	-2.82	124.13	128.46
2	C	501[A]	HEM	CMA-C3A-C4A	-2.75	124.23	128.46
2	D	501[A]	HEM	C3B-C4B-NB	-2.73	105.68	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	HEM	C3C-C4C-NC	-2.70	105.85	110.94
2	C	501[A]	HEM	CMD-C2D-C1D	-2.58	124.50	128.46
2	D	502[B]	HEM	CMA-C3A-C4A	-2.57	124.51	128.46
2	C	502[B]	HEM	CAA-CBA-CGA	-2.52	108.36	112.66
2	B	502[B]	HEM	CBD-CAD-C3D	-2.31	108.06	112.47
2	C	502[B]	HEM	C3C-C4C-NC	-2.25	106.69	110.94
2	B	501[A]	HEM	C3C-C4C-NC	-2.13	106.93	110.94
2	D	501[A]	HEM	CMD-C2D-C1D	-2.06	125.30	128.46
2	B	502[B]	HEM	CMD-C2D-C1D	-2.04	125.33	128.46
2	C	502[B]	HEM	C4C-C3C-C2C	2.03	108.32	106.90
2	A	502[B]	HEM	CMC-C2C-C3C	2.09	128.77	124.89
2	B	502[B]	HEM	CAD-CBD-CGD	2.18	116.38	112.66
2	B	502[B]	HEM	CMC-C2C-C3C	2.21	128.99	124.89
2	C	501[A]	HEM	C4C-C3C-C2C	2.27	108.48	106.90
2	C	502[B]	HEM	CMB-C2B-C3B	2.38	129.32	124.89
2	C	501[A]	HEM	C4A-C3A-C2A	2.46	108.70	107.00
2	A	502[B]	HEM	CMB-C2B-C3B	2.49	129.51	124.89
2	D	501[A]	HEM	C4A-C3A-C2A	2.53	108.76	107.00
2	A	501[A]	HEM	CAA-CBA-CGA	2.54	117.01	112.66
2	D	502[B]	HEM	CMB-C2B-C3B	2.60	129.72	124.89
2	D	502[B]	HEM	CMD-C2D-C3D	2.81	130.25	124.94
2	B	502[B]	HEM	C4A-C3A-C2A	2.83	108.96	107.00
2	D	502[B]	HEM	C4A-C3A-C2A	2.89	109.01	107.00
2	A	501[A]	HEM	C4A-C3A-C2A	2.94	109.04	107.00
2	D	501[A]	HEM	CMB-C2B-C3B	3.20	130.83	124.89
2	C	502[B]	HEM	CAD-CBD-CGD	3.72	119.01	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	HEM	6	0
2	A	502[B]	HEM	3	0
3	A	503	HQE	2	0
2	B	501[A]	HEM	8	0
2	B	502[B]	HEM	4	0
2	C	501[A]	HEM	8	0
2	C	502[B]	HEM	7	0
3	C	503	HQE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501[A]	HEM	5	0
2	D	502[B]	HEM	3	0
3	D	503	HQE	3	0

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	480/491 (97%)	0.19	8 (1%) 70 73	17, 28, 43, 69	0
1	B	480/491 (97%)	0.13	6 (1%) 77 80	17, 26, 42, 73	0
1	C	480/491 (97%)	0.17	11 (2%) 61 64	16, 24, 42, 107	0
1	D	480/491 (97%)	0.27	12 (2%) 58 62	17, 27, 46, 119	0
All	All	1920/1964 (97%)	0.19	37 (1%) 67 70	16, 26, 44, 119	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	TYR	8.4
1	C	485	TYR	6.2
1	C	484	SER	5.6
1	C	483	ARG	4.8
1	B	485	TYR	4.2
1	D	484	SER	4.0
1	D	483	ARG	4.0
1	A	484	SER	3.7
1	C	6	HIS	3.7
1	B	372[A]	PHE	3.5
1	D	481	ASP	3.3
1	D	372[A]	PHE	3.2
1	D	6	HIS	3.1
1	C	372[A]	PHE	3.0
1	A	485	TYR	3.0
1	B	484	SER	2.9
1	D	480	VAL	2.9
1	D	482	ILE	2.8
1	A	480	VAL	2.8
1	B	398	HIS	2.6
1	D	348	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	482	ILE	2.6
1	D	398	HIS	2.6
1	A	372[A]	PHE	2.5
1	D	457	LEU	2.5
1	C	350	ALA	2.4
1	A	482	ILE	2.4
1	D	479	GLY	2.3
1	B	256	TYR	2.3
1	C	398	HIS	2.3
1	A	479	GLY	2.2
1	C	271	TYR	2.2
1	C	480	VAL	2.2
1	B	6	HIS	2.1
1	C	399	TYR	2.1
1	A	253	LYS	2.0
1	A	288	GLU	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HQE	B	503	8/8	0.86	0.28	12.74	46,48,51,60	0
3	HQE	D	503	8/8	0.69	0.28	7.90	59,65,72,76	0
3	HQE	C	503	8/8	0.84	0.17	4.54	41,45,46,52	0
3	HQE	A	503	8/8	0.86	0.18	2.94	46,50,54,57	0
4	CL	A	504	1/1	0.98	0.21	2.80	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	B	502[B]	43/43	0.95	0.12	0.12	13,17,19,20	43
2	HEM	D	502[B]	43/43	0.95	0.12	-0.02	15,18,20,21	43
2	HEM	D	501[A]	43/43	0.96	0.12	-0.06	18,22,24,26	43
2	HEM	C	501[A]	43/43	0.96	0.12	-0.07	15,20,23,24	43
2	HEM	B	501[A]	43/43	0.95	0.11	-0.20	16,20,23,26	43
2	HEM	C	502[B]	43/43	0.96	0.12	-0.23	12,14,16,16	43
4	CL	B	504	1/1	0.98	0.10	-0.32	24,24,24,24	0
2	HEM	A	501[A]	43/43	0.95	0.12	-0.39	14,18,19,20	43
2	HEM	A	502[B]	43/43	0.95	0.11	-0.42	18,22,23,25	43
4	CL	D	504	1/1	0.99	0.10	-1.03	25,25,25,25	0
5	NA	A	506	1/1	0.99	0.10	-1.17	12,12,12,12	0
4	CL	C	505	1/1	0.99	0.08	-2.12	28,28,28,28	0
4	CL	A	505	1/1	0.99	0.05	-2.20	22,22,22,22	0
4	CL	C	504	1/1	1.00	0.12	-2.50	27,27,27,27	0
5	NA	B	505	1/1	0.92	0.12	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.