Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:24 PM GMT

PDB ID	:	4CAB
Title	:	The refined structure of catalase DR1998 from Deinococcus radiodurans at 2.6 A resolution
Authors	:	Borges, P.T.; Miranda, C.S.; Santos, S.P.; Frazao, C.; Romao, C.V.
Deposited on	:	2013-10-08
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

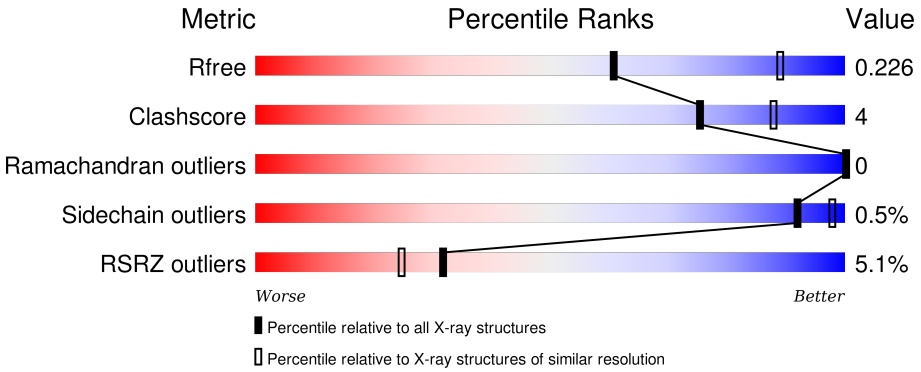
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	536	3% 84% 10% 5%
1	B	536	5% 83% 12% 5%
1	C	536	4% 85% 9% 5%
1	D	536	8% 88% 7% 5%

2 Entry composition

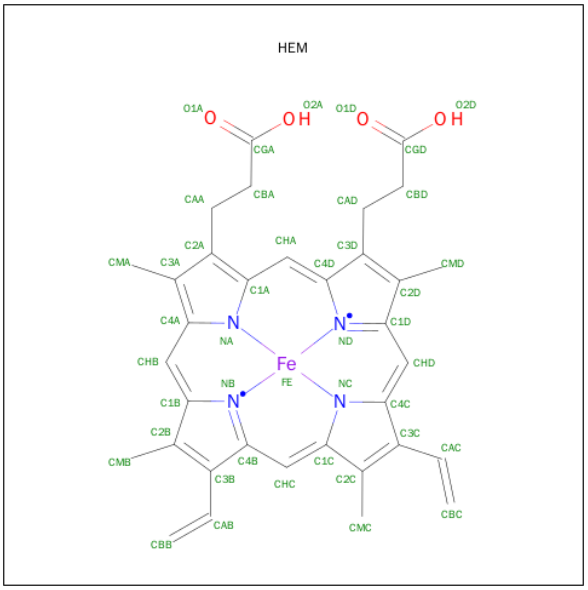
There are 4 unique types of molecules in this entry. The entry contains 17038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	507	Total	C	N	O	S	0	0	0
			4074	2555	732	776	11			
1	B	507	Total	C	N	O	S	0	0	0
			4074	2555	732	776	11			
1	C	507	Total	C	N	O	S	0	1	0
			4080	2559	734	776	11			
1	D	507	Total	C	N	O	S	0	0	0
			4074	2555	732	776	11			

- 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	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Cl	0	0
			3	3		
3	A	3	Total	Cl	0	0
			3	3		
3	D	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		

- Molecule 4 is water.

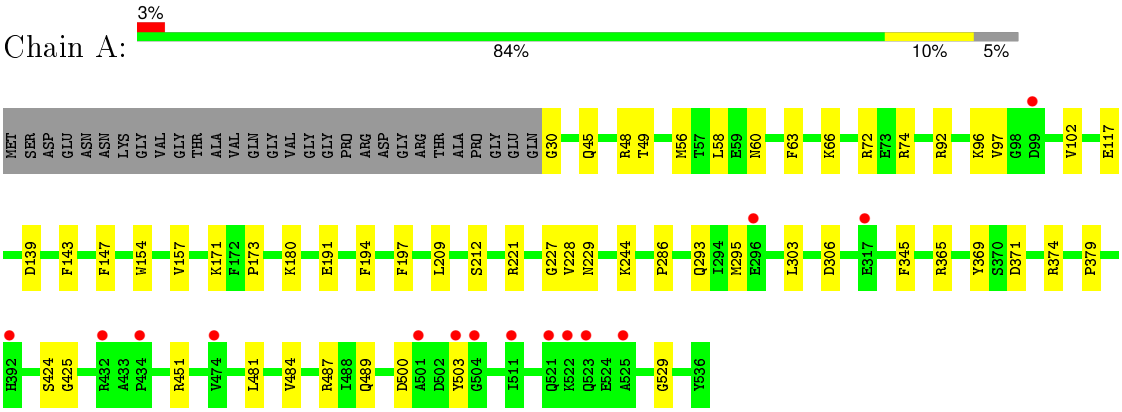
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	118	Total	O	0	0
			118	118		
4	C	176	Total	O	0	0
			176	176		
4	D	113	Total	O	0	0
			113	113		

3 Residue-property plots (i)

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.

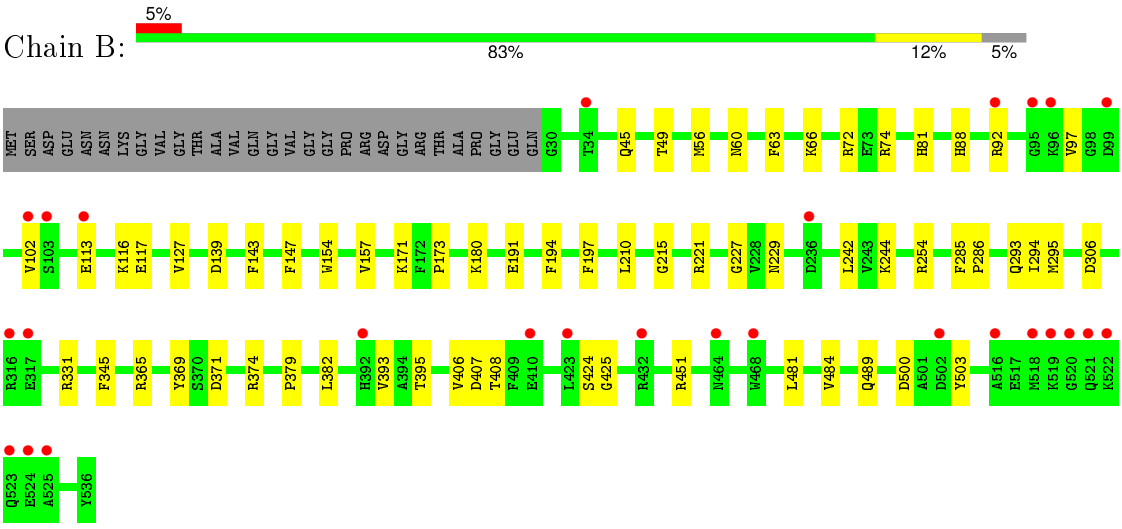
- Molecule 1: CATALASE

Chain A:



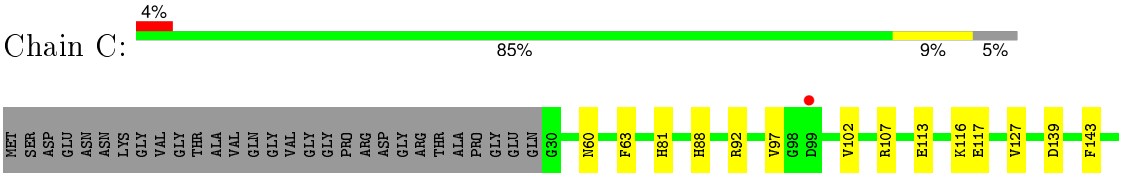
- Molecule 1: CATALASE

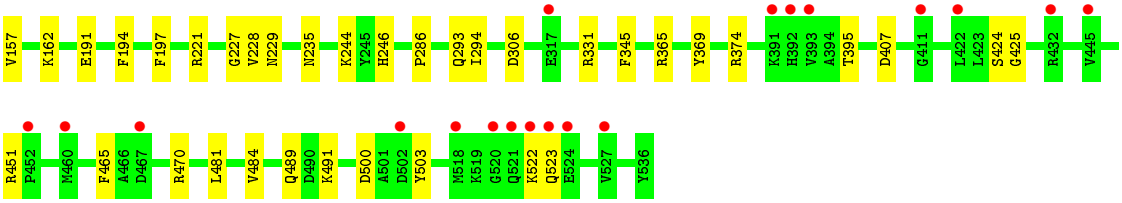
Chain B:



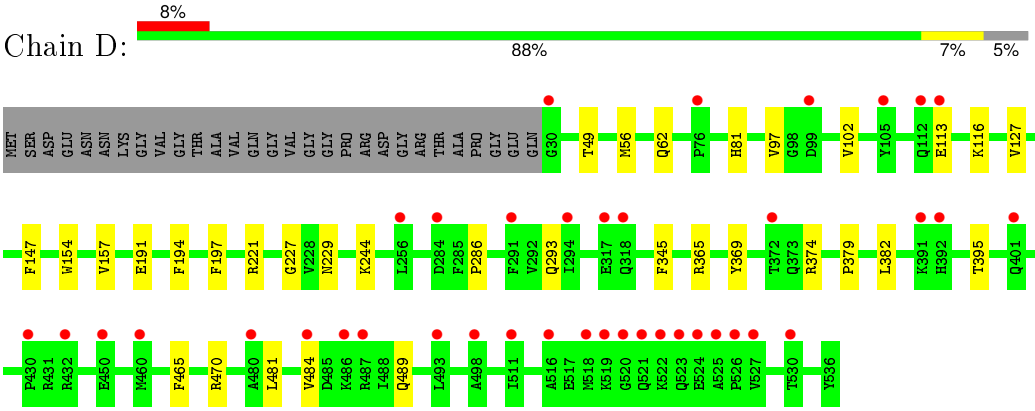
- Molecule 1: CATALASE

Chain C:





- Molecule 1: CATALASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.33Å 311.88Å 145.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.60 49.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.40-2.60) 99.3 (49.40-2.60)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.236 , 0.236 0.227 , 0.226	Depositor DCC
R_{free} test set	1978 reflections (2.91%)	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	1.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 68021 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17038	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.22	0/4181	0.37	0/5669
1	B	0.21	0/4181	0.37	0/5669
1	C	0.22	0/4192	0.38	0/5684
1	D	0.21	0/4181	0.37	0/5669
All	All	0.21	0/16735	0.37	0/22691

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	3873	37	0
1	B	4074	0	3872	39	0
1	C	4080	0	3875	29	0
1	D	4074	0	3872	20	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	1	0
3	C	3	0	0	1	0
3	D	1	0	0	1	0
4	A	147	0	0	2	0
4	B	118	0	0	1	0
4	C	176	0	0	0	0
4	D	113	0	0	1	0
All	All	17038	0	15612	124	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 4.

All (124) 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:221:ARG:HD2	1:D:286:PRO:HG3	1.75	0.68
1:A:221:ARG:HD2	1:A:286:PRO:HG3	1.76	0.68
1:B:221:ARG:HD2	1:B:286:PRO:HG3	1.74	0.67
1:C:97:VAL:HG12	1:C:102:VAL:HA	1.78	0.66
1:A:487:ARG:NH1	3:A:1539:CL:CL	2.60	0.66
1:D:97:VAL:HG12	1:D:102:VAL:HA	1.78	0.66
1:A:97:VAL:HG12	1:A:102:VAL:HA	1.78	0.65
1:C:221:ARG:HD2	1:C:286:PRO:HG3	1.78	0.65
2:A:537:HEM:HMC2	2:A:537:HEM:HBC2	1.78	0.64
2:D:537:HEM:HBC2	2:D:537:HEM:HMC2	1.79	0.64
2:B:537:HEM:HBC2	2:B:537:HEM:HMC2	1.79	0.64
1:A:306:ASP:HA	1:A:451:ARG:HH21	1.63	0.64
1:B:97:VAL:HG12	1:B:102:VAL:HA	1.80	0.64
2:C:537:HEM:HBC2	2:C:537:HEM:HMC2	1.78	0.63
1:A:48:ARG:NH1	4:A:2008:HOH:O	2.33	0.61
1:A:173:PRO:HG2	1:B:66:LYS:HE2	1.83	0.61
1:B:365:ARG:HB3	1:B:369:TYR:HE2	1.65	0.60
1:B:374:ARG:NH1	1:B:379:PRO:O	2.34	0.59
1:A:229:ASN:OD1	1:A:365:ARG:NH1	2.34	0.58
1:C:88:HIS:HB2	1:C:331:ARG:HB3	1.86	0.58
1:A:244:LYS:HB2	1:A:293:GLN:HB2	1.85	0.57
1:A:72:ARG:NH2	1:B:371:ASP:OD1	2.32	0.56
1:B:229:ASN:OD1	1:B:365:ARG:NH1	2.33	0.56
1:B:306:ASP:HA	1:B:451:ARG:HH21	1.70	0.56
1:D:191:GLU:HG3	1:D:484:VAL:HG13	1.88	0.56
1:B:244:LYS:HB2	1:B:293:GLN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:O	1:A:489:GLN:NE2	2.39	0.54
1:C:481:LEU:O	1:C:489:GLN:NE2	2.35	0.54
1:A:45:GLN:HA	1:B:171:LYS:HD3	1.89	0.54
1:A:30:GLY:N	4:A:2001:HOH:O	2.41	0.53
1:A:66:LYS:HE2	1:B:173:PRO:HG2	1.89	0.53
1:A:191:GLU:HG3	1:A:484:VAL:HG13	1.90	0.53
1:C:162:LYS:HD3	1:C:246:HIS:CE1	2.45	0.52
1:B:191:GLU:HG3	1:B:484:VAL:HG13	1.92	0.52
1:D:113:GLU:HB2	1:D:116:LYS:HB2	1.91	0.52
1:D:227:GLY:O	1:D:229:ASN:N	2.42	0.52
1:C:113:GLU:HB2	1:C:116:LYS:HB2	1.92	0.51
1:C:191:GLU:HG3	1:C:484:VAL:HG13	1.92	0.51
1:B:481:LEU:O	1:B:489:GLN:NE2	2.38	0.51
1:A:374:ARG:NH1	1:A:379:PRO:O	2.43	0.51
1:C:365:ARG:HB3	1:C:369:TYR:HE2	1.75	0.51
1:B:88:HIS:HB2	1:B:331:ARG:HB3	1.93	0.51
1:D:229:ASN:OD1	1:D:365:ARG:NH1	2.36	0.51
1:B:365:ARG:HB3	1:B:369:TYR:CE2	2.45	0.50
1:D:374:ARG:NH1	1:D:379:PRO:O	2.43	0.50
1:D:481:LEU:O	1:D:489:GLN:NE2	2.36	0.50
1:C:500:ASP:HB3	1:C:503:TYR:HB2	1.94	0.50
1:A:424:SER:OG	1:A:425:GLY:N	2.44	0.50
1:C:522:LYS:HB2	1:C:523:GLN:HA	1.92	0.50
1:A:365:ARG:HB3	1:A:369:TYR:HE2	1.77	0.50
2:C:537:HEM:HMB1	2:C:537:HEM:HBB2	1.94	0.49
1:A:171:LYS:HD3	1:B:45:GLN:HA	1.93	0.49
1:D:62:GLN:NE2	4:D:2003:HOH:O	2.44	0.49
1:C:229:ASN:OD1	1:C:365:ARG:NH1	2.39	0.49
1:B:227:GLY:O	1:B:229:ASN:N	2.45	0.49
2:B:537:HEM:HBB2	2:B:537:HEM:HMB1	1.95	0.49
1:C:227:GLY:O	1:C:229:ASN:N	2.43	0.49
1:D:194:PHE:HA	1:D:197:PHE:HB2	1.95	0.49
1:A:529:GLY:O	1:B:254:ARG:NH2	2.46	0.49
1:C:395:THR:H	1:C:407:ASP:HB3	1.79	0.48
1:A:371:ASP:OD1	1:B:72:ARG:NH2	2.37	0.48
1:B:81:HIS:CE1	1:B:127:VAL:HG22	2.48	0.47
1:A:227:GLY:O	1:A:229:ASN:N	2.42	0.47
1:A:365:ARG:HB3	1:A:369:TYR:CE2	2.50	0.47
2:D:537:HEM:HBB2	2:D:537:HEM:HMB1	1.97	0.47
1:D:365:ARG:HB3	1:D:369:TYR:HE2	1.79	0.47
1:B:113:GLU:HB2	1:B:116:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ASP:HB3	1:A:503:TYR:HB2	1.97	0.47
1:D:382:LEU:HB2	3:D:1537:CL:CL	2.51	0.47
1:A:157:VAL:HG22	1:A:345:PHE:HB3	1.98	0.46
1:A:180:LYS:HE2	1:B:74:ARG:HH21	1.81	0.46
2:A:537:HEM:HBB2	2:A:537:HEM:HMB1	1.96	0.45
1:A:147:PHE:HB2	1:A:154:TRP:HB3	1.98	0.45
1:B:424:SER:OG	1:B:425:GLY:N	2.47	0.45
1:C:228:VAL:O	1:C:244:LYS:NZ	2.48	0.45
1:B:500:ASP:HB3	1:B:503:TYR:HB2	1.99	0.45
1:B:194:PHE:HA	1:B:197:PHE:HB2	1.97	0.45
1:C:81:HIS:CE1	1:C:127:VAL:HG22	2.52	0.45
1:B:157:VAL:HG22	1:B:345:PHE:HB3	1.99	0.45
1:C:365:ARG:HB3	1:C:369:TYR:CE2	2.52	0.45
1:B:92:ARG:HG2	1:B:117:GLU:HG2	1.99	0.44
1:C:194:PHE:HA	1:C:197:PHE:HB2	1.98	0.44
1:C:157:VAL:HG22	1:C:345:PHE:HB3	1.99	0.44
1:D:244:LYS:HB2	1:D:293:GLN:HB2	1.98	0.44
1:B:60:ASN:HB3	1:B:63:PHE:HB3	2.00	0.44
1:D:424:SER:OG	1:D:425:GLY:N	2.50	0.44
1:A:60:ASN:HB3	1:A:63:PHE:HB3	2.00	0.44
1:B:74:ARG:NH2	4:B:2010:HOH:O	2.49	0.43
1:A:92:ARG:HG2	1:A:117:GLU:HG2	1.99	0.43
1:A:365:ARG:HG2	2:A:537:HEM:C1C	2.54	0.43
1:C:60:ASN:HB3	1:C:63:PHE:HB3	2.00	0.43
1:C:306:ASP:HA	1:C:451:ARG:HH21	1.84	0.43
1:C:244:LYS:HB2	1:C:293:GLN:HB2	2.01	0.43
1:B:382:LEU:HB2	3:B:1537:CL:CL	2.56	0.43
1:C:97:VAL:HG21	1:C:294:ILE:HD11	2.01	0.43
1:A:194:PHE:HA	1:A:197:PHE:HB2	2.01	0.43
1:A:228:VAL:O	1:A:244:LYS:NZ	2.50	0.42
1:B:210:LEU:O	1:B:215:GLY:HA3	2.20	0.42
1:B:242:LEU:HB2	1:B:295:MET:HB3	2.01	0.42
1:A:209:LEU:O	1:A:212:SER:OG	2.30	0.42
1:D:147:PHE:HB2	1:D:154:TRP:HB3	2.01	0.42
1:C:107:ARG:NH1	1:C:235:ASN:O	2.52	0.42
1:C:424:SER:OG	1:C:425:GLY:N	2.49	0.42
1:B:406:VAL:HG12	1:B:408:THR:HG23	2.01	0.42
1:C:491:LYS:HD3	1:C:491:LYS:HA	1.86	0.42
1:D:395:THR:H	1:D:407:ASP:HB3	1.84	0.42
1:C:374:ARG:NH1	3:C:1538:CL:CL	2.88	0.42
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:PHE:O	1:D:470:ARG:NH1	2.53	0.42
1:A:74:ARG:HH21	1:B:180:LYS:HE2	1.85	0.41
1:B:49:THR:HG22	1:B:56:MET:HA	2.02	0.41
1:A:96:LYS:HA	1:A:102:VAL:N	2.35	0.41
1:B:395:THR:H	1:B:407:ASP:HB3	1.85	0.41
1:B:285:PHE:HA	1:B:286:PRO:HD3	1.83	0.41
1:A:295:MET:HE3	1:A:303:LEU:HD11	2.02	0.41
1:D:49:THR:HG22	1:D:56:MET:HA	2.03	0.41
1:D:157:VAL:HG22	1:D:345:PHE:HB3	2.03	0.41
1:C:162:LYS:HD3	1:C:246:HIS:HE1	1.84	0.41
1:A:49:THR:HG22	1:A:56:MET:HA	2.03	0.41
1:B:97:VAL:HG21	1:B:294:ILE:HD11	2.03	0.40
1:B:147:PHE:HB2	1:B:154:TRP:HB3	2.03	0.40
1:C:465:PHE:O	1:C:470:ARG:NH1	2.54	0.40
1:D:81:HIS:CE1	1:D:127:VAL:HG22	2.56	0.40
1:C:92:ARG:HG2	1:C:117:GLU:HG2	2.03	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	505/536 (94%)	479 (95%)	26 (5%)	0	100	100
1	B	505/536 (94%)	478 (95%)	27 (5%)	0	100	100
1	C	506/536 (94%)	480 (95%)	26 (5%)	0	100	100
1	D	505/536 (94%)	480 (95%)	25 (5%)	0	100	100
All	All	2021/2144 (94%)	1917 (95%)	104 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	431/451 (96%)	429 (100%)	2 (0%)	92	98
1	B	431/451 (96%)	428 (99%)	3 (1%)	88	96
1	C	432/451 (96%)	430 (100%)	2 (0%)	92	98
1	D	431/451 (96%)	430 (100%)	1 (0%)	95	99
All	All	1725/1804 (96%)	1717 (100%)	8 (0%)	92	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASP
1	A	143	PHE
1	B	139	ASP
1	B	143	PHE
1	B	393	VAL
1	C	139	ASP
1	C	143	PHE
1	D	143	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	537	1	30,50,50	2.24	7 (23%)	24,82,82	2.28	6 (25%)
2	HEM	B	537	1	30,50,50	2.27	7 (23%)	24,82,82	2.28	7 (29%)
2	HEM	C	537	1	30,50,50	2.19	8 (26%)	24,82,82	2.31	7 (29%)
2	HEM	D	537	1	30,50,50	2.22	8 (26%)	24,82,82	2.28	7 (29%)

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	537	1	-	0/10/54/54	0/0/8/8
2	HEM	B	537	1	-	0/10/54/54	0/0/8/8
2	HEM	C	537	1	-	0/10/54/54	0/0/8/8
2	HEM	D	537	1	-	0/10/54/54	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	537	HEM	C3B-C4B	-7.83	1.44	1.51
2	C	537	HEM	C3B-C4B	-7.61	1.45	1.51
2	A	537	HEM	C3B-C4B	-7.59	1.45	1.51
2	D	537	HEM	C3B-C4B	-7.58	1.45	1.51
2	B	537	HEM	C3D-C4D	-4.90	1.45	1.51
2	D	537	HEM	C3D-C4D	-4.90	1.45	1.51
2	A	537	HEM	C3D-C4D	-4.89	1.45	1.51
2	C	537	HEM	C3D-C4D	-4.71	1.45	1.51
2	C	537	HEM	C2C-C1C	-3.90	1.45	1.52
2	D	537	HEM	C2C-C1C	-3.89	1.45	1.52
2	B	537	HEM	C2C-C1C	-3.89	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	537	HEM	C2C-C1C	-3.82	1.45	1.52
2	B	537	HEM	C2D-C1D	-2.32	1.44	1.51
2	A	537	HEM	C2D-C1D	-2.26	1.44	1.51
2	C	537	HEM	C2D-C1D	-2.24	1.44	1.51
2	D	537	HEM	C2D-C1D	-2.24	1.44	1.51
2	C	537	HEM	FE-NB	2.02	2.08	1.97
2	D	537	HEM	FE-NB	2.07	2.08	1.97
2	B	537	HEM	C3B-CAB	2.16	1.55	1.51
2	A	537	HEM	C3B-CAB	2.16	1.55	1.51
2	C	537	HEM	FE-NC	2.18	2.04	1.95
2	C	537	HEM	C3B-CAB	2.20	1.55	1.51
2	B	537	HEM	C3C-CAC	2.22	1.55	1.51
2	D	537	HEM	C3B-CAB	2.22	1.55	1.51
2	A	537	HEM	C3C-CAC	2.23	1.55	1.51
2	D	537	HEM	C3C-CAC	2.23	1.55	1.51
2	C	537	HEM	C3C-CAC	2.24	1.55	1.51
2	D	537	HEM	FE-NC	2.58	2.06	1.95
2	A	537	HEM	FE-NC	3.42	2.09	1.95
2	B	537	HEM	FE-NC	3.47	2.09	1.95

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	537	HEM	CAA-CBA-CGA	-2.68	107.84	112.75
2	D	537	HEM	CAA-CBA-CGA	-2.17	108.76	112.75
2	B	537	HEM	CAA-CBA-CGA	-2.09	108.92	112.75
2	D	537	HEM	C2D-C3D-C4D	2.30	105.39	101.50
2	A	537	HEM	C2D-C3D-C4D	2.31	105.42	101.50
2	C	537	HEM	C2D-C3D-C4D	2.34	105.47	101.50
2	B	537	HEM	C2D-C3D-C4D	2.35	105.48	101.50
2	D	537	HEM	CMD-C2D-C3D	3.05	127.82	114.35
2	C	537	HEM	CMD-C2D-C3D	3.05	127.85	114.35
2	A	537	HEM	CMD-C2D-C3D	3.06	127.89	114.35
2	B	537	HEM	CMD-C2D-C3D	3.15	128.27	114.35
2	B	537	HEM	CAD-C3D-C4D	4.39	127.95	112.47
2	A	537	HEM	CAD-C3D-C4D	4.41	128.03	112.47
2	D	537	HEM	CAD-C3D-C4D	4.42	128.06	112.47
2	C	537	HEM	CAD-C3D-C4D	4.50	128.34	112.47
2	C	537	HEM	CAD-C3D-C2D	4.51	126.19	113.22
2	D	537	HEM	CAD-C3D-C2D	4.64	126.54	113.22
2	A	537	HEM	CAD-C3D-C2D	4.64	126.56	113.22
2	B	537	HEM	CAD-C3D-C2D	4.64	126.56	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	537	HEM	CMC-C2C-C3C	4.78	128.47	116.53
2	B	537	HEM	CMC-C2C-C3C	4.80	128.51	116.53
2	D	537	HEM	CMC-C2C-C3C	4.84	128.61	116.53
2	C	537	HEM	CMC-C2C-C3C	4.85	128.63	116.53
2	B	537	HEM	CMB-C2B-C3B	4.85	128.64	116.53
2	D	537	HEM	CMB-C2B-C3B	4.90	128.77	116.53
2	A	537	HEM	CMB-C2B-C3B	4.94	128.86	116.53
2	C	537	HEM	CMB-C2B-C3B	5.00	129.00	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	537	HEM	3	0
2	B	537	HEM	2	0
2	C	537	HEM	2	0
2	D	537	HEM	2	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, 95^{th} 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	507/536 (94%)	0.47	15 (2%)	54	47	13, 23, 37, 121	0
1	B	507/536 (94%)	0.62	27 (5%)	30	23	17, 27, 38, 117	0
1	C	507/536 (94%)	0.47	20 (3%)	43	35	8, 22, 36, 105	0
1	D	507/536 (94%)	0.72	41 (8%)	15	10	16, 28, 40, 110	0
All	All	2028/2144 (94%)	0.57	103 (5%)	32	25	8, 25, 38, 121	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	522	LYS	8.8
1	D	523	GLN	8.1
1	D	520	GLY	7.6
1	B	521	GLN	7.3
1	D	392	HIS	6.9
1	B	525	ALA	5.2
1	D	522	LYS	5.1
1	C	392[A]	HIS	5.1
1	B	432	ARG	5.0
1	B	523	GLN	5.0
1	C	521	GLN	4.8
1	B	520	GLY	4.7
1	B	522	LYS	4.6
1	C	523	GLN	4.3
1	B	392	HIS	4.0
1	B	518	MET	3.9
1	B	113	GLU	3.8
1	D	317	GLU	3.7
1	B	524	GLU	3.6
1	A	99	ASP	3.5
1	A	522	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	317	GLU	3.4
1	D	521	GLN	3.4
1	D	460	MET	3.3
1	D	518	MET	3.2
1	D	524	GLU	3.2
1	D	294	ILE	3.2
1	B	423	LEU	3.2
1	C	432	ARG	3.1
1	C	99	ASP	3.0
1	A	523	GLN	3.0
1	A	432	ARG	3.0
1	C	524	GLU	3.0
1	D	498	ALA	3.0
1	C	422	LEU	3.0
1	D	527	VAL	2.9
1	B	96	LYS	2.9
1	D	493	LEU	2.9
1	A	521	GLN	2.8
1	A	525	ALA	2.8
1	D	525	ALA	2.8
1	A	392	HIS	2.8
1	B	502	ASP	2.8
1	B	516	ALA	2.7
1	D	519	LYS	2.7
1	D	113	GLU	2.7
1	C	411	GLY	2.7
1	B	95	GLY	2.7
1	C	467	ASP	2.6
1	D	432	ARG	2.6
1	A	434	PRO	2.6
1	A	504	GLY	2.6
1	D	99	ASP	2.6
1	B	34	THR	2.5
1	B	99	ASP	2.5
1	C	502	ASP	2.5
1	D	511	ILE	2.5
1	A	317	GLU	2.5
1	C	520	GLY	2.5
1	D	526	PRO	2.5
1	D	291	PHE	2.4
1	B	236	ASP	2.4
1	D	486	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	452	PRO	2.4
1	D	76	PRO	2.4
1	C	518	MET	2.4
1	D	530	THR	2.3
1	D	130	GLY	2.3
1	D	318	GLN	2.3
1	A	511	ILE	2.3
1	B	519	LYS	2.3
1	B	317	GLU	2.3
1	B	102	VAL	2.3
1	D	484	VAL	2.3
1	D	450	GLU	2.2
1	B	464	ASN	2.2
1	B	410	GLU	2.2
1	D	284	ASP	2.2
1	D	430	PRO	2.2
1	D	112	GLN	2.2
1	A	503	TYR	2.2
1	D	391	LYS	2.2
1	A	501	ALA	2.2
1	B	92	ARG	2.2
1	D	487	ARG	2.2
1	B	103	SER	2.2
1	D	30	GLY	2.2
1	C	527	VAL	2.1
1	C	393	VAL	2.1
1	D	256	LEU	2.1
1	D	401	GLN	2.1
1	D	131	THR	2.1
1	A	474	VAL	2.1
1	C	445	VAL	2.1
1	D	480	ALA	2.1
1	C	460	MET	2.1
1	D	516	ALA	2.1
1	B	316	ARG	2.1
1	D	105	TYR	2.1
1	B	468	TRP	2.0
1	C	391	LYS	2.0
1	A	296	GLU	2.0
1	D	372	THR	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, 95^{th} 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	CL	A	1539	1/1	0.92	0.31	1.15	37,37,37,37	0
2	HEM	A	537	43/43	0.95	0.20	0.50	20,21,22,22	0
2	HEM	C	537	43/43	0.96	0.17	-0.42	15,19,21,22	0
2	HEM	D	537	43/43	0.95	0.19	-0.49	19,21,22,25	0
2	HEM	B	537	43/43	0.95	0.17	-0.61	17,18,20,20	0
3	CL	B	1537	1/1	0.98	0.12	-2.47	19,19,19,19	0
3	CL	D	1537	1/1	0.99	0.09	-3.02	7,7,7,7	0
3	CL	A	1537	1/1	0.98	0.09	-5.10	7,7,7,7	0
3	CL	C	1538	1/1	0.99	0.04	-5.26	10,10,10,10	0
3	CL	B	1002	1/1	0.98	0.10	-	16,16,16,16	0
3	CL	C	1002	1/1	0.96	0.15	-	13,13,13,13	0
3	CL	B	1538	1/1	0.93	0.15	-	43,43,43,43	0
3	CL	C	1537	1/1	0.84	0.15	-	26,26,26,26	0
3	CL	A	1538	1/1	0.98	0.10	-	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.