Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:14 AM GMT

PDB ID	:	2CCD
Title	:	CRYSTAL STRUCTURE OF THE CATALASE-PEROXIDASE (KATG) AND S315T MUTANT FROM MYCOBACTERIUM TUBERCULOSIS
Authors	:	Yu, H.; Sacchettini, J.C.
Deposited on	:	2006-01-16
Resolution	:	2.10 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:

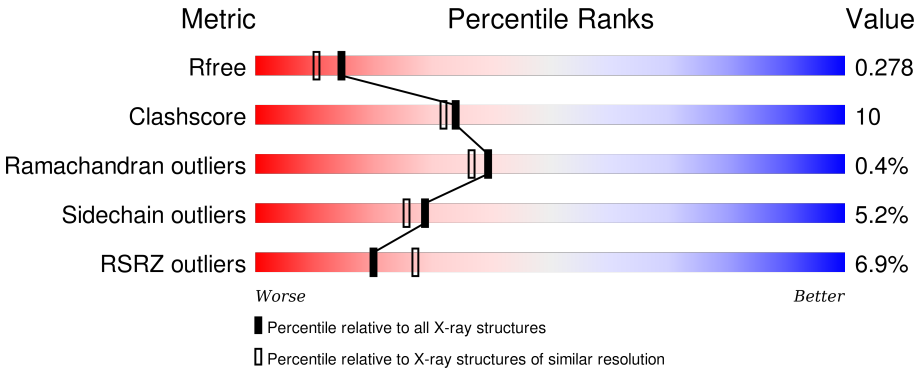
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	740	5% 78% 17%
1	B	740	8% 72% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11715 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.

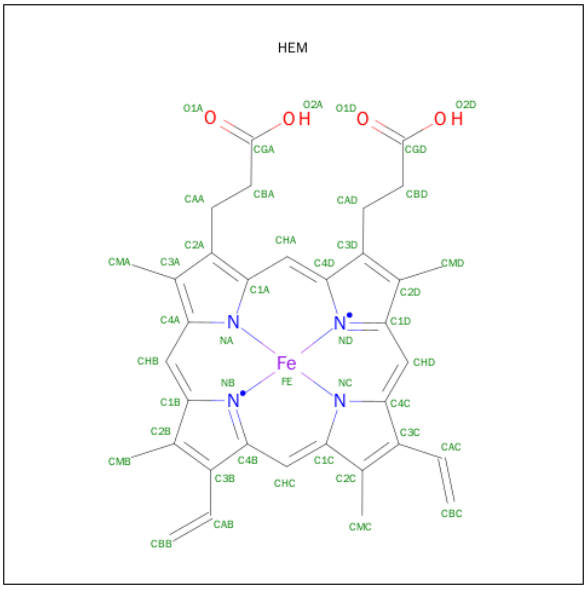
- Molecule 1 is a protein called PEROXIDASE/CATALASE T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5517	3508	949	1041	19			
1	B	715	Total	C	N	O	S	0	0	0
			5517	3508	949	1041	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	THR	SER	ENGINEERED MUTATION	UNP Q08129
B	315	THR	SER	ENGINEERED MUTATION	UNP Q08129

- 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		

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

- Molecule 3 is water.

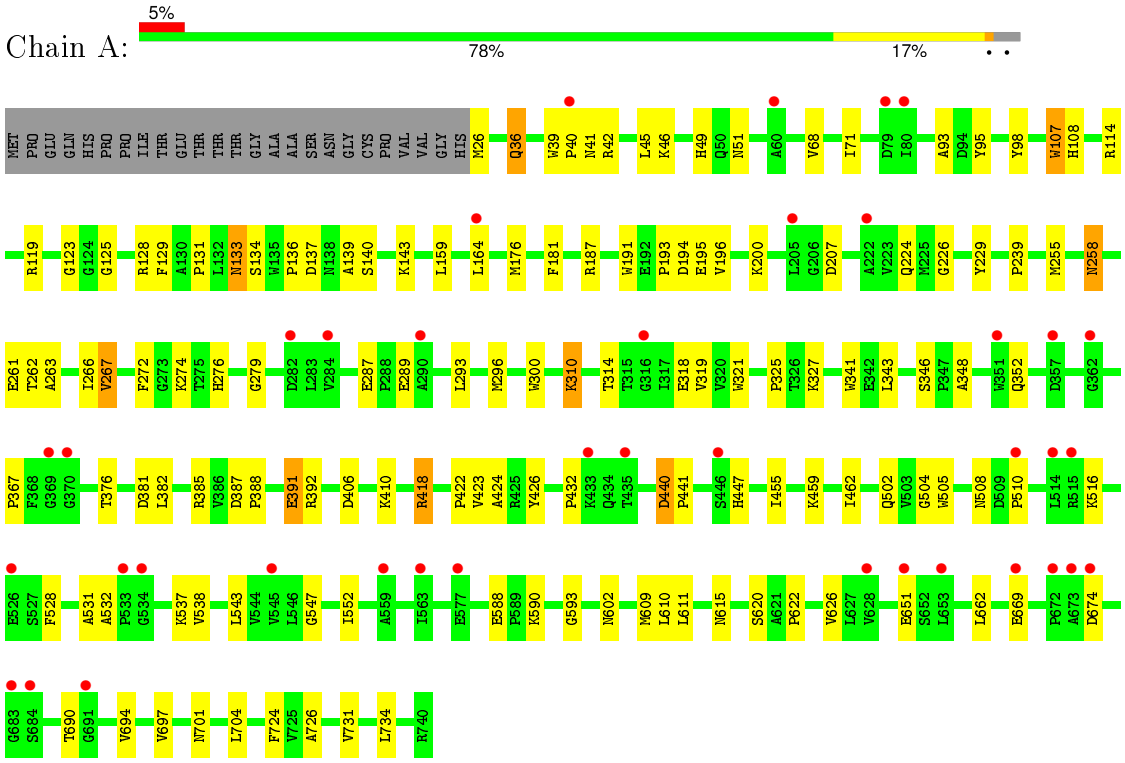
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	340	Total	O	0	0
			340	340		
3	B	255	Total	O	0	0
			255	255		

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.

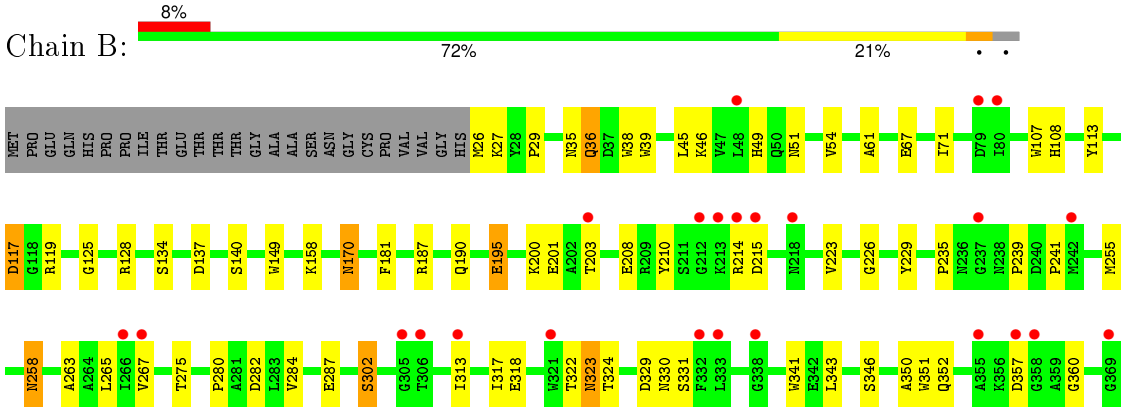
- Molecule 1: PEROXIDASE/CATALASE T

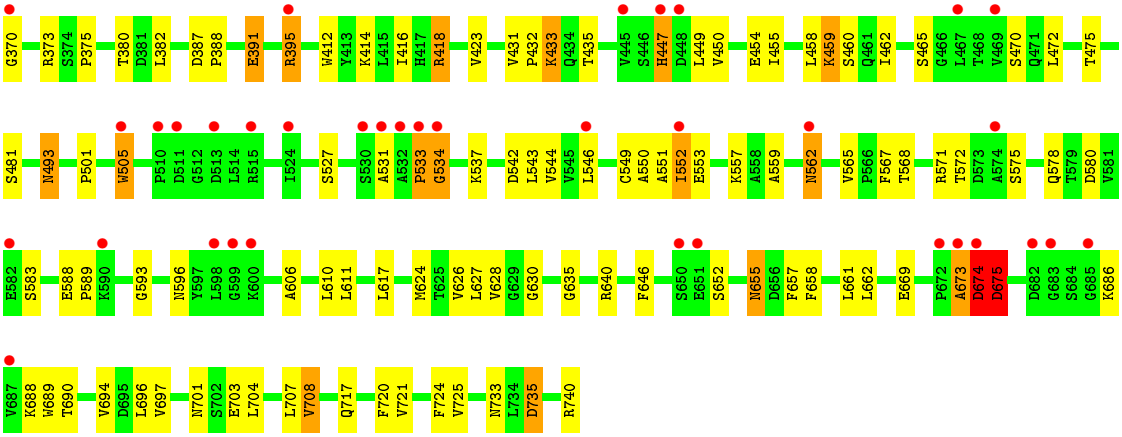
Chain A:



- Molecule 1: PEROXIDASE/CATALASE T

Chain B:




G370 R373 S374 P375 T380 D381 L382 D387 P388 E391 R395 W412 Y413 K414 L415 I416 H417 R418 V423 V431 P432 K433 Q434 T435 V445 S446 H447 D448 I449 V450 E454 I455 L458 K459 S460 Q461 I462 S465 G466 L467 T468 V469 S470 Q471 L472 T475
S481 N493 P501 W505 P510 D511 G512 D513 L514 R515 I524 S527 S530 A531 A532 P533 G534 K537 D542 L543 V544 V545 L546 C549 A550 A551 I552 E553 K557 A558 A559 N562 V565 P566 F567 T568 R571 T572 D573 A574 S575 Q578 T579 D580 V581
E582 S583 E588 P589 K590 G593 N596 Y597 L598 G599 K600 A606 L610 L611 L617 M624 T625 V626 L627 V628 G629 G630 G635 R640 F646 S650 E651 S652 N655 D656 F657 F658 L661 L662 E669 P672 A673 D674 D675 D682 G683 S684 G685 K686
V687 K688 W689 T690 V694 D695 L696 V697 N701 S702 E703 L704 L707 V708 Q717 F720 V721 F724 V725 N733 L734 D735 R740

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.81Å 149.81Å 154.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	78.5 (20.00-2.10) 78.5 (20.01-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.276 0.237 , 0.278	Depositor DCC
R_{free} test set	3986 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.3	EDS
Estimated twinning fraction	0.032 for -h,l,k 0.026 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	3 of 80299 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11715	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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

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	0.60	2/5667 (0.0%)	0.66	1/7714 (0.0%)
1	B	0.54	0/5667	0.69	5/7714 (0.1%)
All	All	0.57	2/11334 (0.0%)	0.68	6/15428 (0.0%)

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	A	0	1
1	B	0	6
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	ASP	C-N	19.62	1.71	1.34
1	A	440	ASP	CA-C	9.06	1.76	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	674	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	675	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	673	ALA	CB-CA-C	5.90	118.95	110.10
1	A	440	ASP	CA-C-N	-5.79	100.89	117.10
1	B	673	ALA	O-C-N	-5.53	113.85	122.70
1	B	735	ASP	CB-CA-C	-5.51	99.37	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	SER	Mainchain
1	B	140	SER	Mainchain
1	B	673	ALA	Mainchain,Peptide
1	B	674	ASP	Mainchain
1	B	675	ASP	Mainchain
1	B	735	ASP	Peptide

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	5517	0	5347	93	0
1	B	5517	0	5347	133	0
2	A	43	0	30	0	0
2	B	43	0	30	5	0
3	A	340	0	0	9	0
3	B	255	0	0	14	0
All	All	11715	0	10754	221	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 10.

All (221) 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:440:ASP:CA	1:A:440:ASP:C	1.76	1.49
1:A:440:ASP:C	1:A:441:PRO:N	1.71	1.41
1:B:107:TRP:CH2	1:B:229:TYR:CE1	2.17	1.31
1:A:229:TYR:CE2	1:A:255:MET:SD	2.25	1.30
1:B:107:TRP:HH2	1:B:229:TYR:CE1	1.50	1.28
1:B:107:TRP:CH2	1:B:229:TYR:HE1	1.50	1.27
1:B:350:ALA:HB1	3:B:2106:HOH:O	1.21	1.25
1:B:229:TYR:CE2	1:B:255:MET:SD	2.39	1.16
1:B:447:HIS:HB2	1:B:537:LYS:HE2	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD23	1:B:611:LEU:HD21	1.40	1.02
1:B:447:HIS:CB	1:B:537:LYS:HE2	1.90	1.01
1:A:229:TYR:HE2	1:A:255:MET:SD	1.76	0.95
1:A:516:LYS:NZ	3:A:2240:HOH:O	1.86	0.92
1:B:552:ILE:HG23	1:B:565:VAL:HG21	1.56	0.86
1:B:229:TYR:CZ	1:B:255:MET:SD	2.70	0.85
1:A:229:TYR:HE2	1:A:255:MET:CG	1.91	0.82
1:B:51:ASN:HD21	1:B:190:GLN:HB3	1.44	0.80
1:B:533:PRO:O	1:B:534:GLY:O	2.00	0.79
1:B:117:ASP:OD1	1:B:119:ARG:NH1	2.18	0.77
1:B:701:ASN:HD22	1:B:704:LEU:H	1.32	0.77
1:B:229:TYR:HE2	1:B:255:MET:SD	2.07	0.77
1:B:542:ASP:HB2	1:B:567:PHE:HZ	1.47	0.77
1:B:107:TRP:HH2	1:B:229:TYR:CD1	2.02	0.77
1:B:107:TRP:CH2	1:B:229:TYR:CD1	2.74	0.75
1:B:527:SER:O	1:B:531:ALA:HB2	1.86	0.75
1:B:433:LYS:HD2	1:B:433:LYS:H	1.51	0.74
1:A:440:ASP:C	1:A:440:ASP:CB	2.56	0.73
1:A:505:TRP:HB2	1:A:508:ASN:HD22	1.54	0.72
1:A:51:ASN:HD21	1:A:191:TRP:H	1.35	0.72
1:B:450:VAL:HG12	1:B:455:ILE:HG13	1.72	0.71
1:B:258:ASN:HD22	1:B:258:ASN:C	1.93	0.70
1:A:229:TYR:CZ	1:A:255:MET:SD	2.84	0.70
1:A:406:ASP:O	1:A:410:LYS:HG3	1.91	0.70
1:B:210:TYR:HD2	1:B:214:ARG:O	1.75	0.69
1:B:447:HIS:HB2	1:B:537:LYS:CE	2.18	0.69
1:B:395:ARG:NH2	3:B:2166:HOH:O	2.24	0.69
1:B:447:HIS:HB3	1:B:537:LYS:HE2	1.74	0.68
1:B:553:GLU:HG3	1:B:565:VAL:HG23	1.76	0.67
1:B:210:TYR:CD2	1:B:214:ARG:O	2.48	0.67
1:B:357:ASP:HB3	3:B:2153:HOH:O	1.95	0.66
1:B:610:LEU:HD22	1:B:694:VAL:HG13	1.77	0.65
1:A:318:GLU:H	1:A:352:GLN:HE22	1.43	0.64
1:A:45:LEU:HD23	1:A:611:LEU:HD21	1.79	0.63
1:B:107:TRP:CZ3	1:B:229:TYR:HE1	2.14	0.63
1:B:195:GLU:HB2	3:B:2085:HOH:O	1.99	0.62
1:B:170:ASN:HD22	1:B:412:TRP:HE1	1.46	0.62
1:B:655:ASN:ND2	1:B:717:GLN:HE21	1.96	0.62
1:B:239:PRO:HG3	1:B:351:TRP:CG	2.35	0.61
1:A:133:ASN:HD22	1:A:134:SER:N	1.98	0.60
1:A:505:TRP:HB2	1:A:508:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LYS:HD3	1:B:546:LEU:HD11	1.83	0.60
1:B:26:MET:N	3:B:2002:HOH:O	2.35	0.60
1:A:258:ASN:ND2	1:A:261:GLU:H	2.00	0.59
1:B:542:ASP:HB2	1:B:567:PHE:CZ	2.34	0.58
1:B:125:GLY:O	1:B:128:ARG:HG2	2.02	0.58
1:A:531:ALA:HB2	3:A:2243:HOH:O	2.03	0.58
2:B:1741:HEM:HMB2	2:B:1741:HEM:HBB2	1.86	0.58
1:A:440:ASP:C	1:A:441:PRO:CA	2.68	0.57
1:A:609:MET:HA	1:A:609:MET:HE2	1.86	0.57
1:B:433:LYS:N	1:B:433:LYS:HD2	2.17	0.57
1:B:318:GLU:H	1:B:352:GLN:HE22	1.53	0.57
1:B:239:PRO:O	1:B:241:PRO:HD3	2.05	0.57
1:A:440:ASP:CA	1:A:441:PRO:N	2.68	0.56
1:B:275:THR:HG22	2:B:1741:HEM:CAA	2.35	0.56
1:A:41:ASN:OD1	1:B:27:LYS:NZ	2.36	0.56
1:A:181:PHE:CE2	1:A:432:PRO:HG3	2.41	0.56
1:A:258:ASN:HD22	1:A:258:ASN:C	2.09	0.56
1:B:187:ARG:HA	3:B:2075:HOH:O	2.06	0.55
1:B:113:TYR:HB3	1:B:418:ARG:HH11	1.72	0.55
1:B:658:PHE:HD2	1:B:708:VAL:HB	1.73	0.54
1:B:472:LEU:HB2	1:B:551:ALA:HB2	1.90	0.54
1:B:210:TYR:OH	1:B:223:VAL:HG12	2.08	0.54
1:B:357:ASP:CB	3:B:2153:HOH:O	2.54	0.54
1:B:323:ASN:H	1:B:323:ASN:HD22	1.55	0.54
1:B:350:ALA:CB	3:B:2106:HOH:O	2.02	0.53
1:B:733:ASN:O	1:B:740:ARG:NH1	2.41	0.53
1:B:459:LYS:HG3	1:B:550:ALA:HB2	1.90	0.53
1:A:159:LEU:HD21	1:A:164:LEU:HD13	1.91	0.52
1:A:143:LYS:NZ	3:A:2058:HOH:O	2.42	0.52
1:A:731:VAL:HA	1:A:734:LEU:HG	1.92	0.52
1:A:620:SER:HB2	1:A:622:PRO:HD2	1.92	0.52
1:A:133:ASN:HD22	1:A:133:ASN:C	2.12	0.51
1:B:107:TRP:CD1	1:B:108:HIS:HD2	2.28	0.51
1:B:470:SER:OG	1:B:635:GLY:HA3	2.10	0.51
1:A:125:GLY:O	1:A:128:ARG:HG2	2.09	0.51
1:A:609:MET:CE	1:A:609:MET:HA	2.41	0.51
1:B:626:VAL:HG23	1:B:720:PHE:CD1	2.46	0.51
1:A:143:LYS:HD2	1:A:143:LYS:H	1.76	0.51
1:B:284:VAL:HG22	1:B:302:SER:HB2	1.93	0.51
1:A:341:TRP:HB2	1:A:382:LEU:HD21	1.92	0.50
1:B:170:ASN:ND2	1:B:412:TRP:HE1	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ASN:HD21	1:B:572:THR:H	1.59	0.50
1:A:263:ALA:O	1:A:267:VAL:CG1	2.59	0.50
1:B:36:GLN:NE2	1:B:36:GLN:H	2.09	0.50
1:B:113:TYR:HB3	1:B:418:ARG:NH1	2.27	0.50
1:A:26:MET:HA	1:B:200:LYS:O	2.12	0.50
1:A:107:TRP:CD1	1:A:108:HIS:HD2	2.30	0.49
1:A:694:VAL:O	1:A:697:VAL:HG12	2.11	0.49
1:A:263:ALA:O	1:A:267:VAL:HG13	2.13	0.49
1:B:416:ILE:HG22	1:B:416:ILE:O	2.13	0.49
1:A:128:ARG:NH1	3:B:2240:HOH:O	2.45	0.49
1:B:134:SER:HB3	1:B:287:GLU:HG3	1.94	0.49
1:A:195:GLU:HB3	1:B:29:PRO:HB3	1.95	0.49
1:B:662:LEU:HD21	1:B:708:VAL:HG22	1.94	0.49
1:B:67:GLU:HB3	1:B:158:LYS:HA	1.94	0.49
1:B:701:ASN:ND2	1:B:703:GLU:H	2.10	0.49
1:B:258:ASN:ND2	1:B:258:ASN:C	2.65	0.49
1:B:181:PHE:CE2	1:B:432:PRO:HG2	2.48	0.48
1:B:542:ASP:HB3	1:B:571:ARG:HH11	1.78	0.48
1:B:694:VAL:O	1:B:697:VAL:HG12	2.13	0.48
1:B:137:ASP:HB2	1:B:226:GLY:O	2.13	0.48
1:A:620:SER:HB3	1:B:54:VAL:HG22	1.95	0.48
1:A:136:PRO:HD2	1:A:226:GLY:HA3	1.95	0.48
1:A:662:LEU:HD13	1:B:149:TRP:CZ2	2.48	0.48
1:B:552:ILE:HG13	1:B:724:PHE:HE2	1.78	0.48
1:B:701:ASN:ND2	1:B:704:LEU:H	2.05	0.48
1:A:129:PHE:HB3	1:A:193:PRO:HG3	1.95	0.48
1:B:265:LEU:O	2:B:1741:HEM:HBC2	2.13	0.47
1:B:565:VAL:HG13	1:B:725:VAL:HG13	1.96	0.47
1:A:310:LYS:HB2	3:A:2151:HOH:O	2.13	0.47
1:B:721:VAL:O	1:B:725:VAL:HG23	2.15	0.47
1:A:462:ILE:HG21	1:A:547:GLY:HA2	1.96	0.47
1:A:701:ASN:HD22	1:A:704:LEU:H	1.63	0.47
1:A:590:LYS:HB2	1:A:602:ASN:HD21	1.80	0.47
1:A:459:LYS:NZ	3:A:2210:HOH:O	2.43	0.47
1:A:385:ARG:O	1:A:391:GLU:HG2	2.15	0.47
1:B:450:VAL:HG13	1:B:454:GLU:HB2	1.97	0.47
1:A:68:VAL:O	1:A:71:ILE:HG22	2.15	0.47
1:A:423:VAL:HA	1:A:426:TYR:CD2	2.50	0.47
1:A:262:THR:O	1:A:266:ILE:HG13	2.15	0.47
1:A:229:TYR:HE2	1:A:255:MET:HG3	1.75	0.46
1:A:134:SER:HB3	1:A:287:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ILE:HG22	1:A:459:LYS:HE2	1.98	0.46
1:A:36:GLN:O	1:A:40:PRO:HA	2.15	0.46
1:B:201:GLU:OE2	1:B:208:GLU:N	2.46	0.46
1:B:462:ILE:HA	1:B:465:SER:OG	2.15	0.46
1:A:504:GLY:HA2	1:A:510:PRO:HB3	1.97	0.46
1:A:239:PRO:HG2	1:A:343:LEU:HD11	1.98	0.46
1:A:139:ALA:O	1:A:314:THR:HG23	2.15	0.46
1:A:95:TYR:CZ	1:A:325:PRO:HG2	2.51	0.46
1:A:26:MET:N	3:A:2001:HOH:O	2.50	0.45
3:A:2014:HOH:O	1:B:707:LEU:HD11	2.15	0.45
1:B:630:GLY:HA3	1:B:724:PHE:CE1	2.52	0.45
1:B:593:GLY:HA3	1:B:610:LEU:HD13	1.97	0.45
1:B:575:SER:OG	1:B:578:GLN:HG3	2.16	0.45
1:B:229:TYR:HE2	1:B:255:MET:CG	2.30	0.45
1:A:276:HIS:HB2	1:A:314:THR:HB	1.99	0.45
1:A:321:TRP:NE1	1:A:381:ASP:OD2	2.50	0.44
1:A:119:ARG:HH21	1:A:615:ASN:ND2	2.16	0.44
1:A:133:ASN:HD21	1:A:289:GLU:HG2	1.83	0.44
1:B:501:PRO:HB2	1:B:505:TRP:CZ3	2.52	0.44
1:B:258:ASN:HB2	3:B:2119:HOH:O	2.18	0.44
1:B:107:TRP:CZ3	1:B:229:TYR:CE1	2.94	0.44
1:B:214:ARG:O	1:B:215:ASP:C	2.56	0.44
1:B:414:LYS:O	1:B:418:ARG:HG2	2.18	0.44
1:B:559:ALA:HB2	1:B:652:SER:OG	2.18	0.43
1:B:688:LYS:HG3	1:B:689:TRP:CE2	2.53	0.43
1:B:324:THR:O	3:B:2142:HOH:O	2.20	0.43
1:A:319:VAL:HG22	1:A:376:THR:HB	2.00	0.43
1:B:275:THR:HG22	2:B:1741:HEM:HAA2	2.01	0.43
1:A:502:GLN:HG2	1:A:505:TRP:CZ3	2.54	0.43
1:A:181:PHE:CE2	1:A:432:PRO:CG	3.01	0.43
1:B:280:PRO:HB2	1:B:282:ASP:OD2	2.19	0.43
1:A:418:ARG:CA	1:A:418:ARG:HE	2.32	0.43
1:A:46:LYS:HG2	1:A:49:HIS:CE1	2.53	0.43
1:A:388:PRO:O	1:A:392:ARG:HG3	2.18	0.43
1:B:493:ASN:ND2	1:B:572:THR:H	2.16	0.43
1:A:279:GLY:O	1:A:348:ALA:HB2	2.18	0.43
1:B:341:TRP:HB2	1:B:382:LEU:HD21	2.01	0.43
1:A:274:LYS:HE3	1:A:367:PRO:HG3	2.01	0.43
1:B:229:TYR:OH	1:B:255:MET:SD	2.74	0.42
1:B:235:PRO:HB3	3:B:2094:HOH:O	2.19	0.42
1:A:119:ARG:HH21	1:A:615:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:PHE:O	1:A:532:ALA:HB2	2.19	0.42
1:B:624:MET:O	1:B:628:VAL:HG23	2.19	0.42
1:B:387:ASP:O	1:B:391:GLU:HB2	2.19	0.42
1:B:505:TRP:CE3	1:B:505:TRP:HA	2.54	0.42
1:B:505:TRP:HE3	1:B:505:TRP:HA	1.85	0.42
1:A:207:ASP:HB2	1:A:224:GLN:HG2	2.02	0.42
1:A:552:ILE:HD13	1:A:724:PHE:HE2	1.85	0.42
1:B:343:LEU:HD11	1:B:351:TRP:CE3	2.54	0.42
1:B:263:ALA:O	1:B:267:VAL:HG23	2.20	0.42
1:B:317:ILE:HG23	1:B:352:GLN:HE21	1.84	0.42
1:B:431:VAL:HA	1:B:432:PRO:HD3	1.91	0.42
1:B:458:LEU:HD22	1:B:543:LEU:HD11	2.01	0.41
1:B:606:ALA:HB1	1:B:694:VAL:HG23	2.02	0.41
1:A:593:GLY:HA3	1:A:610:LEU:HD13	2.00	0.41
1:A:610:LEU:HD22	1:A:694:VAL:HG13	2.02	0.41
1:A:296:MET:HE1	1:B:696:LEU:HB3	2.02	0.41
1:A:387:ASP:HA	1:A:388:PRO:HD2	1.82	0.41
1:B:646:PHE:HE2	1:B:661:LEU:HD13	1.85	0.41
1:A:139:ALA:HA	1:A:300:TRP:CZ3	2.55	0.41
1:A:505:TRP:CE2	1:A:588:GLU:HB2	2.56	0.41
1:A:123:GLY:O	1:A:187:ARG:HB3	2.21	0.41
1:A:422:PRO:HG3	3:A:2220:HOH:O	2.20	0.41
1:A:726:ALA:HB1	3:A:2324:HOH:O	2.20	0.41
1:A:447:HIS:CD2	1:A:537:LYS:HG3	2.55	0.41
1:A:346:SER:HB3	1:A:352:GLN:NE2	2.35	0.41
1:B:580:ASP:HB3	1:B:583:SER:HB3	2.03	0.41
1:B:475:THR:HG22	1:B:544:VAL:HG13	2.02	0.41
1:B:646:PHE:HB2	1:B:657:PHE:HA	2.02	0.41
1:A:176:MET:HB2	1:A:176:MET:HE3	1.86	0.41
1:A:131:PRO:HD3	1:B:35:ASN:HD21	1.86	0.41
1:B:360:GLY:O	1:B:375:PRO:HD3	2.21	0.41
1:B:588:GLU:HA	1:B:589:PRO:HD3	1.94	0.41
1:B:322:THR:HB	1:B:331:SER:OG	2.21	0.41
1:B:61:ALA:HB3	3:B:2019:HOH:O	2.21	0.41
1:B:346:SER:OG	1:B:350:ALA:HB3	2.20	0.41
1:B:549:CYS:HA	1:B:552:ILE:HG22	2.02	0.41
1:B:239:PRO:HG3	1:B:351:TRP:CD1	2.56	0.41
1:A:119:ARG:HD3	1:A:196:VAL:HG22	2.02	0.41
1:B:562:ASN:HD22	1:B:562:ASN:HA	1.66	0.41
1:B:626:VAL:HG23	1:B:720:PHE:HD1	1.86	0.40
1:B:38:TRP:HB2	1:B:39:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HG2	1:B:49:HIS:CE1	2.56	0.40
1:B:388:PRO:HG2	3:B:2161:HOH:O	2.20	0.40
1:B:71:ILE:HG21	1:B:71:ILE:HD13	1.88	0.40
2:B:1741:HEM:HBB2	2:B:1741:HEM:CMB	2.52	0.40
1:A:93:ALA:HB2	1:A:98:TYR:CZ	2.57	0.40
1:A:39:TRP:HB2	1:A:42:ARG:HD2	2.04	0.40
1:B:481:SER:HA	1:B:617:LEU:HD21	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	713/740 (96%)	681 (96%)	30 (4%)	2 (0%)	46	45
1	B	713/740 (96%)	684 (96%)	25 (4%)	4 (1%)	30	24
All	All	1426/1480 (96%)	1365 (96%)	55 (4%)	6 (0%)	39	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	534	GLY
1	A	674	ASP
1	B	370	GLY
1	A	424	ALA
1	B	674	ASP
1	B	533	PRO

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	564/584 (97%)	543 (96%)	21 (4%)	41	41
1	B	564/584 (97%)	526 (93%)	38 (7%)	20	16
All	All	1128/1168 (97%)	1069 (95%)	59 (5%)	29	25

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	107	TRP
1	A	114	ARG
1	A	133	ASN
1	A	137	ASP
1	A	194	ASP
1	A	200	LYS
1	A	258	ASN
1	A	267	VAL
1	A	272	PHE
1	A	293	LEU
1	A	310	LYS
1	A	327	LYS
1	A	391	GLU
1	A	418	ARG
1	A	538	VAL
1	A	543	LEU
1	A	626	VAL
1	A	651	GLU
1	A	669	GLU
1	A	690	THR
1	B	36	GLN
1	B	117	ASP
1	B	170	ASN
1	B	195	GLU
1	B	203	THR
1	B	258	ASN

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Mol	Chain	Res	Type
1	B	302	SER
1	B	313	ILE
1	B	323	ASN
1	B	329	ASP
1	B	330	ASN
1	B	373	ARG
1	B	380	THR
1	B	391	GLU
1	B	395	ARG
1	B	418	ARG
1	B	423	VAL
1	B	433	LYS
1	B	435	THR
1	B	447	HIS
1	B	449	LEU
1	B	459	LYS
1	B	460	SER
1	B	493	ASN
1	B	505	TRP
1	B	552	ILE
1	B	557	LYS
1	B	562	ASN
1	B	568	THR
1	B	596	ASN
1	B	627	LEU
1	B	640	ARG
1	B	655	ASN
1	B	669	GLU
1	B	675	ASP
1	B	686	LYS
1	B	690	THR
1	B	708	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	51	ASN
1	A	133	ASN
1	A	218	ASN
1	A	258	ASN
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	434	GLN
1	A	508	ASN
1	A	535	ASN
1	A	561	HIS
1	A	562	ASN
1	A	602	ASN
1	A	615	ASN
1	A	701	ASN
1	A	722	GLN
1	B	35	ASN
1	B	36	GLN
1	B	50	GLN
1	B	51	ASN
1	B	116	HIS
1	B	170	ASN
1	B	258	ASN
1	B	323	ASN
1	B	330	ASN
1	B	352	GLN
1	B	434	GLN
1	B	439	GLN
1	B	493	ASN
1	B	500	GLN
1	B	525	GLN
1	B	562	ASN
1	B	596	ASN
1	B	655	ASN
1	B	701	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	1741	1	30,50,50	2.31	8 (26%)	24,82,82	2.34	9 (37%)
2	HEM	B	1741	1	30,50,50	2.28	9 (30%)	24,82,82	2.72	9 (37%)

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	1741	1	-	0/10/54/54	0/0/8/8
2	HEM	B	1741	1	-	0/10/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1741	HEM	C3B-C4B	-6.88	1.45	1.51
2	A	1741	HEM	C3B-C4B	-6.14	1.46	1.51
2	A	1741	HEM	C3D-C4D	-5.12	1.45	1.51
2	B	1741	HEM	C2C-C1C	-4.56	1.43	1.52
2	B	1741	HEM	C3D-C4D	-4.36	1.46	1.51
2	A	1741	HEM	C2C-C1C	-3.81	1.45	1.52
2	B	1741	HEM	FE-NC	2.00	2.03	1.95
2	B	1741	HEM	C3B-CAB	2.16	1.55	1.51
2	B	1741	HEM	C4C-NC	2.28	1.38	1.36
2	A	1741	HEM	C3B-CAB	2.29	1.55	1.51
2	B	1741	HEM	C3C-CAC	2.35	1.55	1.51
2	A	1741	HEM	C4C-NC	2.50	1.39	1.36
2	A	1741	HEM	C3C-CAC	2.77	1.56	1.51
2	B	1741	HEM	C1C-NC	3.62	1.40	1.36
2	B	1741	HEM	FE-ND	3.70	2.17	1.97
2	A	1741	HEM	FE-NB	4.12	2.19	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1741	HEM	FE-NC	4.44	2.13	1.95

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1741	HEM	CAA-CBA-CGA	-4.14	105.16	112.75
2	B	1741	HEM	CMA-C3A-C4A	-2.80	123.72	128.36
2	A	1741	HEM	CAA-C2A-C1A	-2.54	124.25	127.01
2	A	1741	HEM	CAA-CBA-CGA	-2.52	108.13	112.75
2	A	1741	HEM	C3B-CAB-CBB	-2.39	120.78	124.46
2	B	1741	HEM	CAA-C2A-C1A	-2.01	124.82	127.01
2	A	1741	HEM	CMA-C3A-C4A	-2.00	125.05	128.36
2	A	1741	HEM	CMD-C2D-C3D	2.55	125.62	114.35
2	B	1741	HEM	CMD-C2D-C3D	2.91	127.20	114.35
2	B	1741	HEM	C4B-CHC-C1C	3.21	131.19	125.82
2	A	1741	HEM	CMB-C2B-C3B	4.16	126.93	116.53
2	A	1741	HEM	CAD-C3D-C4D	4.45	128.17	112.47
2	B	1741	HEM	CAD-C3D-C2D	4.55	126.30	113.22
2	B	1741	HEM	CAD-C3D-C4D	4.82	129.48	112.47
2	A	1741	HEM	CAD-C3D-C2D	5.16	128.04	113.22
2	A	1741	HEM	CMC-C2C-C3C	5.20	129.52	116.53
2	B	1741	HEM	CMB-C2B-C3B	5.60	130.52	116.53
2	B	1741	HEM	CMC-C2C-C3C	5.81	131.04	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1741	HEM	5	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	715/740 (96%)	0.74	39 (5%)	29	37	7, 19, 31, 38	0
1	B	715/740 (96%)	0.89	60 (8%)	14	19	8, 20, 34, 40	0
All	All	1430/1480 (96%)	0.81	99 (6%)	20	27	7, 20, 33, 40	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	531	ALA	7.8
1	B	533	PRO	7.2
1	B	532	ALA	5.6
1	A	369	GLY	4.8
1	B	673	ALA	4.6
1	A	510	PRO	4.0
1	B	212	GLY	3.9
1	B	505	TRP	3.9
1	B	582	GLU	3.7
1	B	650	SER	3.6
1	A	533	PRO	3.4
1	A	684	SER	3.3
1	B	79	ASP	3.3
1	A	534	GLY	3.3
1	A	79	ASP	3.3
1	B	672	PRO	3.3
1	B	511	ASP	3.2
1	A	370	GLY	3.1
1	B	598	LEU	3.1
1	B	48	LEU	3.0
1	A	433	LYS	3.0
1	B	306	THR	3.0
1	A	683	GLY	3.0
1	A	674	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	515	ARG	2.9
1	B	447	HIS	2.9
1	A	80	ILE	2.9
1	A	351	TRP	2.9
1	B	469	VAL	2.8
1	B	237	GLY	2.8
1	B	685	GLY	2.8
1	B	674	ASP	2.8
1	A	205	LEU	2.8
1	B	213	LYS	2.8
1	B	448	ASP	2.7
1	A	282	ASP	2.7
1	B	513	ASP	2.7
1	B	355	ALA	2.7
1	B	530	SER	2.7
1	A	435	THR	2.6
1	A	559	ALA	2.6
1	B	682	ASP	2.6
1	A	222	ALA	2.6
1	B	370	GLY	2.6
1	B	215	ASP	2.6
1	B	534	GLY	2.6
1	B	552	ILE	2.5
1	B	599	GLY	2.5
1	A	60	ALA	2.5
1	B	467	LEU	2.5
1	B	574	ALA	2.5
1	B	214	ARG	2.5
1	B	333	LEU	2.5
1	A	672	PRO	2.5
1	A	284	VAL	2.5
1	B	395	ARG	2.4
1	A	164	LEU	2.4
1	B	357	ASP	2.4
1	A	446	SER	2.4
1	A	362	GLY	2.4
1	B	651	GLU	2.4
1	A	653	LEU	2.4
1	B	332	PHE	2.4
1	B	600	LYS	2.4
1	A	514	LEU	2.3
1	B	510	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	ILE	2.3
1	A	526	GLU	2.3
1	A	669	GLU	2.3
1	B	445	VAL	2.3
1	A	40	PRO	2.3
1	A	290	ALA	2.3
1	A	691	GLY	2.3
1	B	338	GLY	2.2
1	B	80	ILE	2.2
1	B	687	VAL	2.2
1	B	321	TRP	2.2
1	A	577	GLU	2.2
1	B	524	ILE	2.2
1	B	546	LEU	2.2
1	A	563	ILE	2.2
1	A	316	GLY	2.1
1	B	683	GLY	2.1
1	B	218	ASN	2.1
1	B	369	GLY	2.1
1	B	267	VAL	2.1
1	B	203	THR	2.1
1	A	673	ALA	2.1
1	B	305	GLY	2.1
1	B	358	GLY	2.1
1	B	590	LYS	2.0
1	B	242	MET	2.0
1	A	357	ASP	2.0
1	A	651	GLU	2.0
1	A	628	VAL	2.0
1	B	313	ILE	2.0
1	B	515	ARG	2.0
1	B	562	ASN	2.0
1	A	545	VAL	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

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
2	HEM	B	1741	43/43	0.95	0.14	-0.70	3,7,10,15	0
2	HEM	A	1741	43/43	0.96	0.14	-1.05	2,7,10,12	0

6.5 Other polymers

There are no such residues in this entry.