Full wwPDB X-ray Structure Validation Report

Oct 20, 2016 – 07:44 AM EDT

PDB ID	:	5GKN
Title	:	Catalase structure determined by electron crystallography of thin 3D crystals
Authors	:	Yonekura, K.
Deposited on	:	2016-07-04
Resolution	:	3.20 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 (i)) were used in the production of this report:

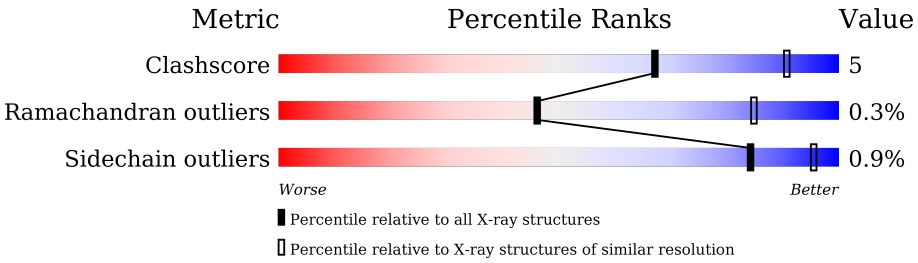
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	527	82% 12% • 5%
1	B	527	82% 12% • 5%
1	C	527	85% 9% 5%
1	D	527	84% 10% • 5%

2 Entry composition

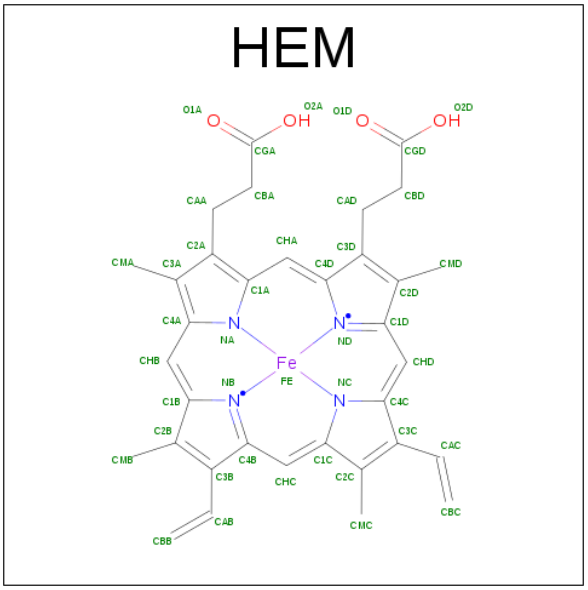
There are 4 unique types of molecules in this entry. The entry contains 16548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	499	Total	C	N	O	S	0	0	0
			4017	2548	717	738	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	717	738	14			
1	C	499	Total	C	N	O	S	0	0	0
			4017	2548	717	738	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	717	738	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	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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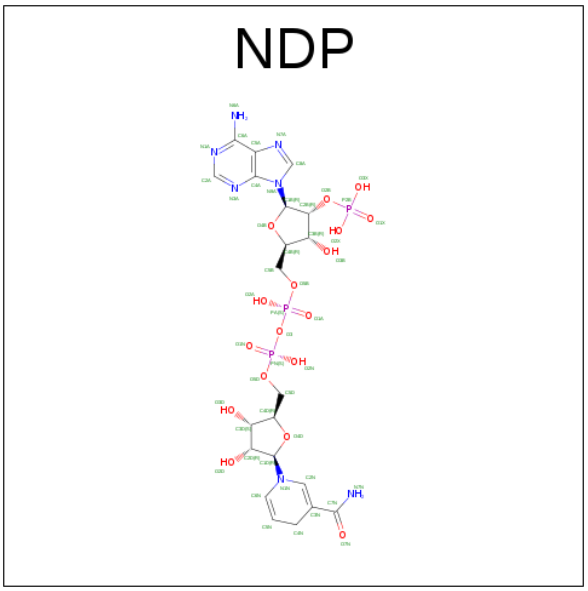
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	18	Total	O	0	0
			18	18		
4	C	30	Total	O	0	0
			30	30		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	33	Total O 33 33	0	0

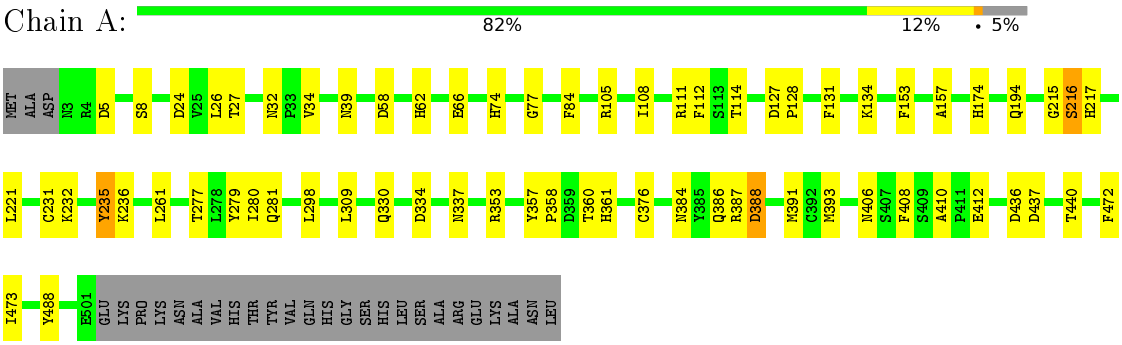
3 Residue-property plots (i)

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.

Note EDS was not executed.

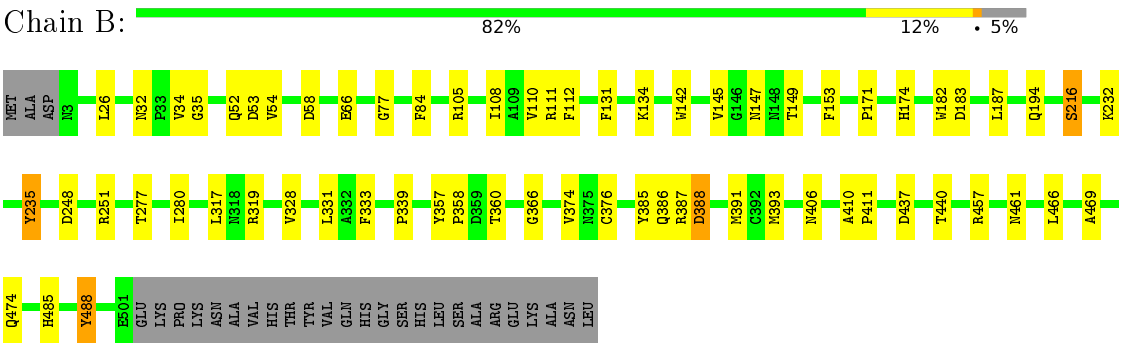
- Molecule 1: Catalase

Chain A:



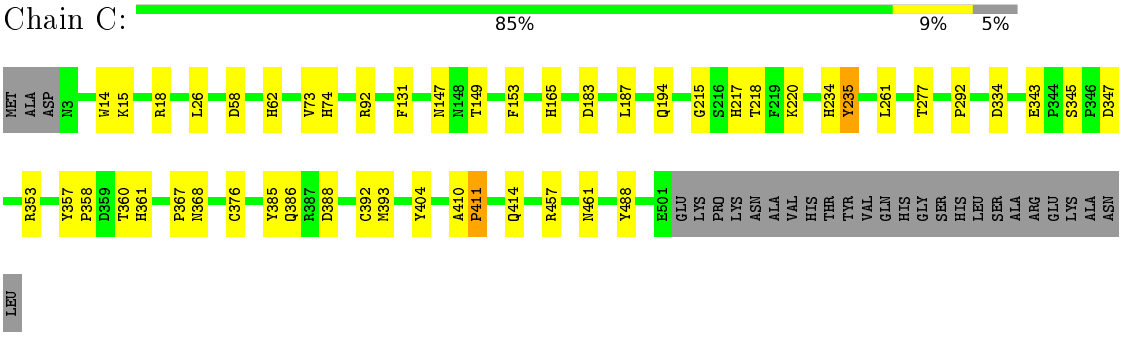
- Molecule 1: Catalase

Chain B:



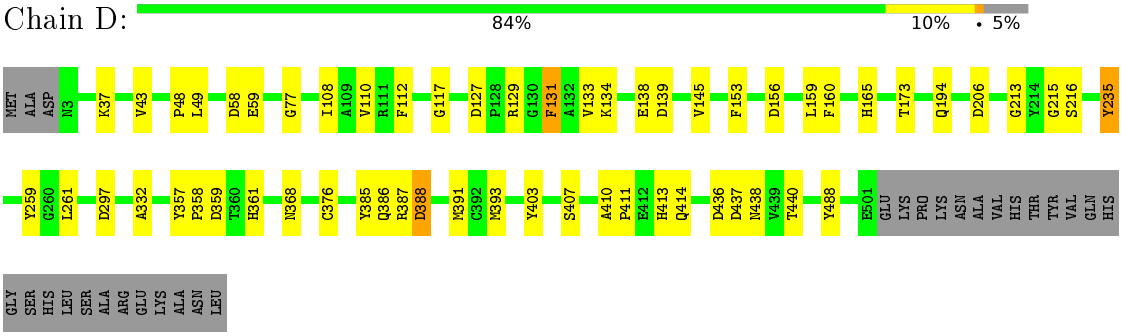
- Molecule 1: Catalase

Chain C:



• Molecule 1: Catalase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.00Å 173.50Å 206.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20	Depositor
% Data completeness (in resolution range)	73.0 (19.99-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.251 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16548	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NDP

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	0.38	1/4137 (0.0%)	0.57	0/5619
1	B	0.41	1/4137 (0.0%)	0.54	0/5619
1	C	0.38	1/4137 (0.0%)	0.54	0/5619
1	D	0.38	1/4137 (0.0%)	0.54	0/5619
All	All	0.39	4/16548 (0.0%)	0.55	0/22476

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	CYS	C-N	13.35	1.59	1.34
1	D	376	CYS	C-N	8.37	1.50	1.34
1	C	376	CYS	C-N	-7.34	1.20	1.34
1	A	376	CYS	C-N	6.44	1.46	1.34

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	4017	0	3843	49	0
1	B	4017	0	3843	51	0
1	C	4017	0	3843	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4017	0	3843	47	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	1	0
3	A	48	0	26	1	0
3	B	48	0	26	0	0
3	C	48	0	26	0	0
3	D	48	0	26	0	0
4	A	35	0	0	1	0
4	B	18	0	0	3	0
4	C	30	0	0	3	0
4	D	33	0	0	5	0
All	All	16548	0	15596	155	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 5.

All (155) 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:C:92:ARG:NH2	4:C:701:HOH:O	1.91	1.03
1:C:367:PRO:O	4:C:702:HOH:O	1.91	0.89
1:B:111:ARG:NH1	1:B:328:VAL:O	2.14	0.81
1:A:386:GLN:NE2	1:C:58:ASP:OD2	2.13	0.81
1:A:66:GLU:OE2	1:D:165:HIS:NE2	2.15	0.80
1:D:437:ASP:OD2	1:D:440:THR:OG1	1.99	0.80
1:D:117:GLY:O	4:D:701:HOH:O	2.02	0.78
1:A:360:THR:HG21	2:A:601:HEM:HBA1	1.66	0.77
1:C:360:THR:HG21	2:C:601:HEM:HBA1	1.66	0.76
1:A:58:ASP:OD2	1:C:386:GLN:NE2	2.18	0.75
1:C:353:ARG:NH1	2:C:601:HEM:HBC2	2.04	0.73
1:A:384:ASN:O	4:A:701:HOH:O	2.06	0.73
1:B:248:ASP:OD1	1:B:251:ARG:NH1	2.21	0.73
1:C:217:HIS:ND1	1:C:347:ASP:OD2	2.17	0.71
1:D:49:LEU:O	4:D:702:HOH:O	2.07	0.71
1:B:58:ASP:OD1	1:D:386:GLN:NE2	2.22	0.68
1:B:34:VAL:O	1:D:414:GLN:N	2.25	0.68
1:D:359:ASP:OD1	4:D:703:HOH:O	2.12	0.68
1:B:360:THR:HG21	2:B:601:HEM:HBA1	1.77	0.66
1:C:353:ARG:HH12	2:C:601:HEM:HBC2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ARG:NH1	4:B:702:HOH:O	2.29	0.65
1:B:437:ASP:OD2	1:B:440:THR:OG1	2.12	0.65
1:B:32:ASN:ND2	1:D:139:ASP:O	2.30	0.65
1:B:469:ALA:O	1:B:474:GLN:NE2	2.30	0.65
1:B:386:GLN:NE2	1:D:58:ASP:OD2	2.31	0.64
1:A:236:LYS:NZ	3:A:602:NDP:O3X	2.26	0.63
1:A:74:HIS:O	1:A:111:ARG:NH2	2.32	0.62
1:B:149:THR:HG21	1:B:194:GLN:OE1	1.99	0.61
1:A:215:GLY:O	1:A:217:HIS:N	2.32	0.60
1:A:330:GLN:HE22	1:C:392:CYS:HB3	1.66	0.60
1:B:171:PRO:O	4:B:701:HOH:O	2.16	0.60
1:A:34:VAL:O	1:C:414:GLN:N	2.31	0.60
1:A:174:HIS:HB3	1:D:261:LEU:HD21	1.84	0.60
1:B:52:GLN:O	1:B:54:VAL:N	2.36	0.59
1:A:437:ASP:OD2	1:A:440:THR:OG1	2.15	0.59
1:B:153:PHE:CE2	1:B:194:GLN:HG3	2.38	0.59
1:A:5:ASP:OD1	1:A:8:SER:OG	2.17	0.56
1:C:388:ASP:OD2	4:C:703:HOH:O	2.18	0.56
1:B:393:MET:HG3	1:D:393:MET:HG3	1.88	0.56
1:A:393:MET:HG3	1:C:393:MET:SD	2.46	0.55
1:C:360:THR:CG2	2:C:601:HEM:HBA1	2.37	0.54
1:D:127:ASP:O	1:D:129:ARG:NH1	2.41	0.54
1:D:215:GLY:O	1:D:216:SER:OG	2.19	0.53
1:D:388:ASP:OD1	1:D:388:ASP:N	2.43	0.51
1:C:73:VAL:HG12	1:C:74:HIS:CD2	2.46	0.51
1:A:26:LEU:HG	1:A:34:VAL:CG2	2.41	0.50
1:B:393:MET:HG3	1:D:393:MET:SD	2.51	0.50
1:B:174:HIS:HB3	1:C:261:LEU:HD21	1.93	0.50
1:A:235:TYR:CD2	1:A:235:TYR:N	2.80	0.50
1:A:408:PHE:HD1	1:C:15:LYS:HB2	1.77	0.50
1:A:62:HIS:CG	1:C:386:GLN:HB3	2.47	0.50
1:B:366:GLY:HA3	1:D:391:MET:SD	2.51	0.50
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.95	0.49
1:D:297:ASP:OD1	1:D:297:ASP:C	2.51	0.49
1:C:385:TYR:HH	1:C:404:TYR:HD1	1.60	0.49
1:A:84:PHE:O	1:A:105:ARG:HA	2.13	0.48
1:C:218:THR:O	1:C:345:SER:OG	2.22	0.48
1:A:261:LEU:HD21	1:D:173:THR:O	2.12	0.48
1:A:235:TYR:HA	1:A:277:THR:O	2.13	0.48
1:B:360:THR:CG2	2:B:601:HEM:HBA1	2.42	0.48
1:B:216:SER:OG	2:B:601:HEM:HBC1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASP:N	1:B:388:ASP:OD1	2.46	0.47
1:C:183:ASP:OD1	1:D:407:SER:OG	2.28	0.47
1:A:127:ASP:OD1	1:A:128:PRO:HD2	2.14	0.47
1:A:74:HIS:HA	1:A:114:THR:O	2.15	0.47
1:C:334:ASP:OD1	1:C:361:HIS:HD2	1.97	0.47
1:A:279:TYR:CD1	1:A:309:LEU:HB3	2.50	0.47
1:B:232:LYS:HE3	4:B:704:HOH:O	2.15	0.47
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.98	0.46
1:D:77:GLY:HA2	1:D:112:PHE:O	2.15	0.46
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.80	0.46
1:C:149:THR:HG21	1:C:194:GLN:HE22	1.79	0.46
1:C:220:LYS:N	1:C:343:GLU:O	2.43	0.46
1:D:357:TYR:HB2	1:D:358:PRO:HD3	1.98	0.46
1:A:108:ILE:HA	1:A:134:LYS:O	2.16	0.46
1:C:215:GLY:O	1:C:217:HIS:N	2.47	0.46
1:A:334:ASP:OD1	1:A:361:HIS:HD2	1.97	0.46
1:B:387:ARG:O	1:B:388:ASP:HB2	2.16	0.45
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.99	0.45
1:C:410:ALA:O	1:C:411:PRO:O	2.35	0.45
1:D:410:ALA:HB1	1:D:411:PRO:CD	2.47	0.45
1:D:436:ASP:O	1:D:438:ASN:OD1	2.35	0.45
1:B:77:GLY:HA2	1:B:112:PHE:O	2.17	0.45
1:C:147:ASN:CG	2:C:601:HEM:HAC	2.37	0.45
1:A:26:LEU:HG	1:A:34:VAL:HG21	1.99	0.45
1:D:138:GLU:OE1	4:D:704:HOH:O	2.21	0.45
1:B:393:MET:HG3	1:D:393:MET:CG	2.47	0.45
1:A:39:ASN:HA	1:D:156:ASP:OD2	2.17	0.45
1:A:153:PHE:CE2	1:A:194:GLN:HG3	2.51	0.44
1:D:131:PHE:CD2	1:D:235:TYR:HE1	2.34	0.44
1:B:331:LEU:HD21	1:B:374:VAL:HG22	1.99	0.44
1:B:66:GLU:OE2	1:C:165:HIS:NE2	2.47	0.44
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.82	0.44
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.48	0.44
1:D:110:VAL:HG22	1:D:133:VAL:HG22	2.00	0.44
1:B:110:VAL:HG21	1:B:317:LEU:HD21	2.00	0.44
1:A:217:HIS:CE1	1:A:298:LEU:HD22	2.53	0.44
1:C:357:TYR:HB2	1:C:358:PRO:HD3	2.00	0.44
1:A:216:SER:HB3	1:A:298:LEU:HD11	2.00	0.43
1:B:35:GLY:C	1:D:413:HIS:HD1	2.20	0.43
1:D:213:GLY:HA3	1:D:235:TYR:CE1	2.54	0.43
1:D:332:ALA:HB1	1:D:361:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HA	1:A:32:ASN:O	2.17	0.43
1:A:387:ARG:O	1:A:388:ASP:HB2	2.18	0.43
1:D:145:VAL:N	4:D:707:HOH:O	2.42	0.43
1:A:77:GLY:HA2	1:A:112:PHE:O	2.18	0.43
1:C:153:PHE:CE1	1:C:194:GLN:HG3	2.53	0.43
1:B:182:TRP:CD2	1:B:466:LEU:HD13	2.54	0.43
1:A:386:GLN:HB3	1:C:62:HIS:ND1	2.34	0.43
1:A:232:LYS:O	1:A:280:ILE:HA	2.19	0.43
1:B:142:TRP:HB2	1:B:339:PRO:HD3	2.01	0.42
1:B:26:LEU:O	1:B:34:VAL:HG22	2.18	0.42
1:A:393:MET:SD	1:C:393:MET:HG3	2.59	0.42
1:C:187:LEU:HD11	1:D:407:SER:OG	2.19	0.42
1:B:111:ARG:NH1	1:B:328:VAL:HG12	2.34	0.42
1:B:66:GLU:HA	1:D:388:ASP:HB2	2.00	0.42
1:C:334:ASP:OD1	1:C:361:HIS:CD2	2.72	0.42
1:B:235:TYR:HA	1:B:277:THR:O	2.20	0.42
1:B:391:MET:HE2	1:D:368:ASN:HB2	2.02	0.42
1:A:357:TYR:HB2	1:A:358:PRO:HD3	2.01	0.42
1:B:108:ILE:HA	1:B:134:LYS:O	2.20	0.42
1:B:485:HIS:HB3	1:B:488:TYR:HB2	2.01	0.42
1:A:231:CYS:HA	1:A:281:GLN:O	2.20	0.42
1:D:387:ARG:O	1:D:388:ASP:HB2	2.20	0.42
1:A:391:MET:HE2	1:C:368:ASN:HB2	2.01	0.41
1:D:410:ALA:HB1	1:D:411:PRO:HD2	2.01	0.41
1:D:385:TYR:CE2	1:D:403:TYR:O	2.73	0.41
1:B:84:PHE:O	1:B:105:ARG:HA	2.20	0.41
1:B:183:ASP:O	1:B:187:LEU:HD12	2.20	0.41
1:D:37:LYS:NZ	1:D:59:GLU:OE2	2.49	0.41
1:A:360:THR:CG2	2:A:601:HEM:HBA1	2.42	0.41
1:B:232:LYS:O	1:B:280:ILE:HA	2.20	0.41
1:B:385:TYR:HA	1:B:387:ARG:HH12	1.85	0.41
1:A:221:LEU:HG	1:A:231:CYS:SG	2.60	0.41
1:C:234:HIS:CD2	1:C:234:HIS:N	2.87	0.41
1:D:153:PHE:CE2	1:D:194:GLN:HG3	2.55	0.41
1:A:157:ALA:CB	2:A:601:HEM:HBB1	2.51	0.41
1:B:457:ARG:O	1:B:461:ASN:ND2	2.54	0.41
1:A:472:PHE:CE1	1:A:473:ILE:HG13	2.55	0.41
1:A:353:ARG:NH1	2:A:601:HEM:HBC2	2.36	0.41
1:C:235:TYR:HA	1:C:277:THR:O	2.20	0.41
1:C:457:ARG:O	1:C:461:ASN:ND2	2.54	0.41
1:B:147:ASN:CG	2:B:601:HEM:HAC	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:MET:SD	1:D:393:MET:HG3	2.61	0.41
1:A:334:ASP:HB2	1:A:337:ASN:ND2	2.36	0.40
1:D:206:ASP:OD1	1:D:259:TYR:OH	2.27	0.40
1:D:160:PHE:CD2	2:D:601:HEM:CMB	3.04	0.40
1:A:412:GLU:O	1:C:26:LEU:N	2.37	0.40
1:C:14:TRP:CH2	1:C:18:ARG:HD3	2.56	0.40
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.52	0.40
1:A:24:ASP:O	1:C:411:PRO:HA	2.21	0.40
1:D:43:VAL:HG13	1:D:43:VAL:O	2.20	0.40
1:B:26:LEU:HA	1:D:411:PRO:CB	2.51	0.40
1:B:26:LEU:HG	1:B:34:VAL:CG2	2.52	0.40
1:D:108:ILE:HA	1:D:134:LYS:O	2.21	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	497/527 (94%)	465 (94%)	30 (6%)	2 (0%)	39	80
1	B	497/527 (94%)	467 (94%)	28 (6%)	2 (0%)	39	80
1	C	497/527 (94%)	471 (95%)	25 (5%)	1 (0%)	52	88
1	D	497/527 (94%)	465 (94%)	31 (6%)	1 (0%)	52	88
All	All	1988/2108 (94%)	1868 (94%)	114 (6%)	6 (0%)	46	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	388	ASP
1	A	216	SER
1	A	388	ASP

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Mol	Chain	Res	Type
1	B	53	ASP
1	D	388	ASP
1	C	411	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	431/454 (95%)	427 (99%)	4 (1%)	84	95
1	B	431/454 (95%)	427 (99%)	4 (1%)	84	95
1	C	431/454 (95%)	427 (99%)	4 (1%)	84	95
1	D	431/454 (95%)	427 (99%)	4 (1%)	84	95
All	All	1724/1816 (95%)	1708 (99%)	16 (1%)	84	95

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	PHE
1	A	235	TYR
1	A	436	ASP
1	A	488	TYR
1	B	131	PHE
1	B	216	SER
1	B	235	TYR
1	B	488	TYR
1	C	131	PHE
1	C	235	TYR
1	C	292	PRO
1	C	488	TYR
1	D	131	PHE
1	D	159	LEU
1	D	235	TYR
1	D	488	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	B	397	GLN
1	B	461	ASN
1	D	101	HIS

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

8 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	601	1	24,50,50	0.98	2 (8%)	16,82,82	2.01	5 (31%)
3	NDP	A	602	-	44,52,52	1.03	2 (4%)	55,80,80	1.49	4 (7%)
2	HEM	B	601	1	24,50,50	1.09	2 (8%)	16,82,82	2.55	7 (43%)
3	NDP	B	602	-	44,52,52	1.06	4 (9%)	55,80,80	1.63	10 (18%)
2	HEM	C	601	1	24,50,50	1.03	2 (8%)	16,82,82	2.15	6 (37%)
3	NDP	C	602	-	44,52,52	1.02	2 (4%)	55,80,80	1.47	7 (12%)
2	HEM	D	601	1	24,50,50	0.85	1 (4%)	16,82,82	1.85	5 (31%)
3	NDP	D	602	-	44,52,52	1.00	3 (6%)	55,80,80	1.59	8 (14%)

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	601	1	-	0/6/54/54	0/0/8/8
3	NDP	A	602	-	-	0/30/77/77	0/5/5/5
2	HEM	B	601	1	-	0/6/54/54	0/0/8/8
3	NDP	B	602	-	-	0/30/77/77	0/5/5/5
2	HEM	C	601	1	-	0/6/54/54	0/0/8/8
3	NDP	C	602	-	-	0/30/77/77	0/5/5/5
2	HEM	D	601	1	-	0/6/54/54	0/0/8/8
3	NDP	D	602	-	-	0/30/77/77	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C3B-C2B	-2.90	1.36	1.40
2	A	601	HEM	C3B-C2B	-2.88	1.36	1.40
2	A	601	HEM	C1B-NB	-2.58	1.33	1.36
2	B	601	HEM	C1B-NB	-2.49	1.33	1.36
2	C	601	HEM	C1B-NB	-2.29	1.33	1.36
3	B	602	NDP	C2N-N1N	-2.26	1.33	1.37
2	D	601	HEM	C1B-NB	-2.25	1.33	1.36
2	B	601	HEM	C3D-C2D	-2.06	1.31	1.37
3	D	602	NDP	C2A-N3A	2.05	1.35	1.32
3	B	602	NDP	C2A-N3A	2.19	1.36	1.32
3	D	602	NDP	C5A-C4A	2.64	1.46	1.40
3	B	602	NDP	C5A-C4A	2.79	1.46	1.40
3	C	602	NDP	C5A-C4A	2.88	1.47	1.40
3	A	602	NDP	C5A-C4A	2.94	1.47	1.40
3	A	602	NDP	C6N-C5N	3.23	1.39	1.33
3	B	602	NDP	C6N-C5N	3.45	1.39	1.33
3	C	602	NDP	C6N-C5N	3.46	1.39	1.33
3	D	602	NDP	C6N-C5N	3.56	1.39	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	NDP	N3A-C2A-N1A	-7.73	122.80	128.87
3	D	602	NDP	N3A-C2A-N1A	-7.49	122.99	128.87
3	C	602	NDP	N3A-C2A-N1A	-7.25	123.18	128.87
3	B	602	NDP	N3A-C2A-N1A	-6.39	123.85	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	C3B-CAB-CBB	-4.96	116.42	126.40
2	C	601	HEM	C3C-CAC-CBC	-4.60	117.14	126.40
2	B	601	HEM	C3C-CAC-CBC	-4.31	117.74	126.40
2	B	601	HEM	CAA-CBA-CGA	-4.26	104.50	112.78
2	A	601	HEM	CBD-CAD-C3D	-4.05	105.36	112.47
2	D	601	HEM	C3C-CAC-CBC	-3.97	118.41	126.40
2	C	601	HEM	CAA-CBA-CGA	-3.51	105.94	112.78
2	A	601	HEM	C3C-CAC-CBC	-3.49	119.39	126.40
3	A	602	NDP	C1B-N9A-C4A	-3.30	123.13	126.81
2	C	601	HEM	CAD-CBD-CGD	-3.18	106.59	112.78
2	B	601	HEM	CAD-CBD-CGD	-3.15	106.65	112.78
2	D	601	HEM	CAD-CBD-CGD	-3.11	106.73	112.78
3	A	602	NDP	O2B-P2B-O1X	-3.00	100.32	107.48
2	B	601	HEM	CAD-C3D-C2D	-2.99	120.46	129.00
2	A	601	HEM	C3B-CAB-CBB	-2.97	120.42	126.40
2	D	601	HEM	C3B-CAB-CBB	-2.88	120.61	126.40
2	C	601	HEM	C3B-CAB-CBB	-2.85	120.67	126.40
3	C	602	NDP	C1B-N9A-C4A	-2.64	123.86	126.81
3	B	602	NDP	C1D-N1N-C2N	-2.62	116.29	120.85
2	A	601	HEM	CAA-CBA-CGA	-2.62	107.69	112.78
2	A	601	HEM	CMA-C3A-C4A	-2.61	123.88	128.31
2	B	601	HEM	CBD-CAD-C3D	-2.41	108.23	112.47
2	D	601	HEM	CBA-CAA-C2A	-2.36	108.34	112.49
3	C	602	NDP	O7N-C7N-N7N	-2.36	116.67	122.73
2	D	601	HEM	CBD-CAD-C3D	-2.17	108.66	112.47
3	B	602	NDP	C1B-N9A-C4A	-2.16	124.40	126.81
3	C	602	NDP	C1D-N1N-C2N	-2.16	117.10	120.85
2	C	601	HEM	CBA-CAA-C2A	-2.14	108.73	112.49
3	D	602	NDP	O4B-C1B-C2B	-2.11	102.80	106.60
3	D	602	NDP	N6A-C6A-N1A	2.03	121.92	118.52
3	A	602	NDP	C2B-C3B-C4B	2.04	106.69	101.85
3	C	602	NDP	C2A-N1A-C6A	2.06	122.45	118.77
3	C	602	NDP	C2B-C3B-C4B	2.08	106.78	101.85
3	B	602	NDP	O4D-C4D-C3D	2.09	109.39	105.16
2	B	601	HEM	CMB-C2B-C3B	2.17	129.33	125.09
3	D	602	NDP	C3D-C2D-C1D	2.25	105.95	101.44
3	B	602	NDP	C3B-C2B-C1B	2.38	107.19	102.63
3	D	602	NDP	O4D-C1D-N1N	2.39	112.65	108.09
3	B	602	NDP	C4B-O4B-C1B	2.39	112.18	109.64
3	C	602	NDP	C3D-C2D-C1D	2.41	106.28	101.44
3	B	602	NDP	O4D-C1D-N1N	2.42	112.70	108.09
2	C	601	HEM	CMC-C2C-C3C	2.45	129.88	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	NDP	O4B-C1B-N9A	2.55	112.92	108.11
3	D	602	NDP	O4B-C1B-N9A	2.63	113.08	108.11
3	B	602	NDP	C3D-C2D-C1D	2.73	106.92	101.44
3	D	602	NDP	O3X-P2B-O2X	2.73	117.48	107.44
3	D	602	NDP	C3B-C2B-C1B	2.76	107.91	102.63
3	B	602	NDP	O3X-P2B-O2X	2.86	117.93	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	4	0
3	A	602	NDP	1	0
2	B	601	HEM	4	0
2	C	601	HEM	5	0
2	D	601	HEM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	376:CYS	C	377:PRO	N	1.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.