



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 AM GMT

PDB ID : 3EJ6
Title : Neurospora Crassa Catalase-3 Crystal Structure
Authors : Diaz, A.; Valdes, V.-J.; Rudino-Pinera, E.; Horjales, E.; Hansberg, W.
Deposited on : 2008-09-17
Resolution : 2.30 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 (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

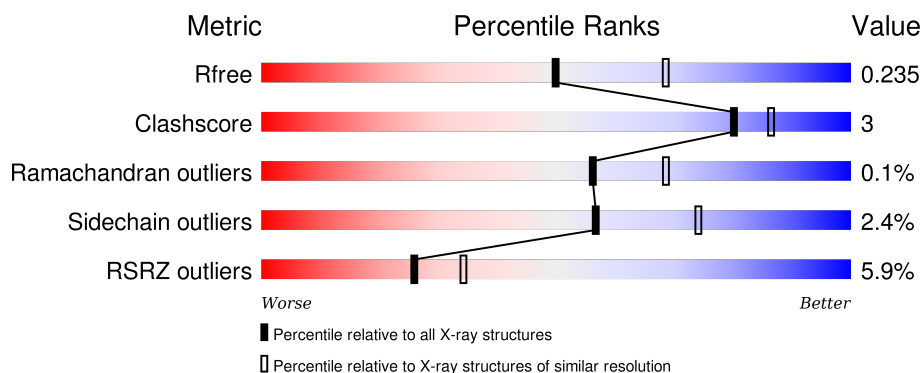
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	688	<div> <div>8%</div> <div>88%</div> <div>11%</div> </div>
1	B	688	<div> <div>6%</div> <div>89%</div> <div>10%</div> </div>
1	C	688	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
1	D	688	<div> <div>6%</div> <div>89%</div> <div>10%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	5007	-	-	-	X
2	NAG	C	5008	-	-	-	X
2	NAG	D	5014	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23009 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	47	0	0
			5340	3381	941	1012	6			
1	B	681	Total	C	N	O	S	72	0	0
			5340	3381	941	1012	6			
1	C	681	Total	C	N	O	S	83	0	0
			5340	3381	941	1012	6			
1	D	681	Total	C	N	O	S	64	0	0
			5340	3381	941	1012	6			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



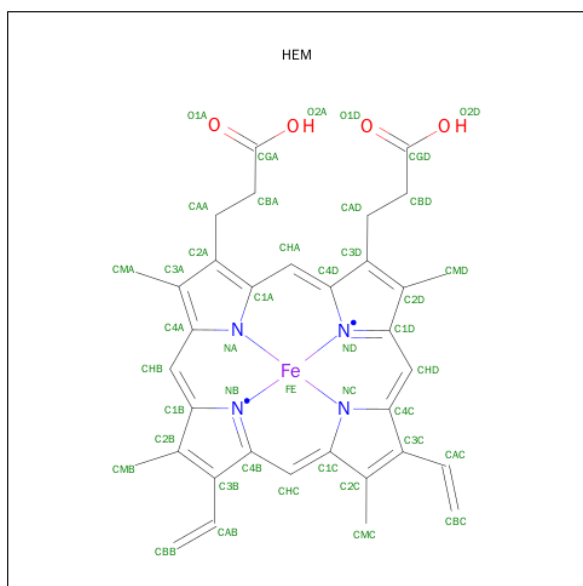
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

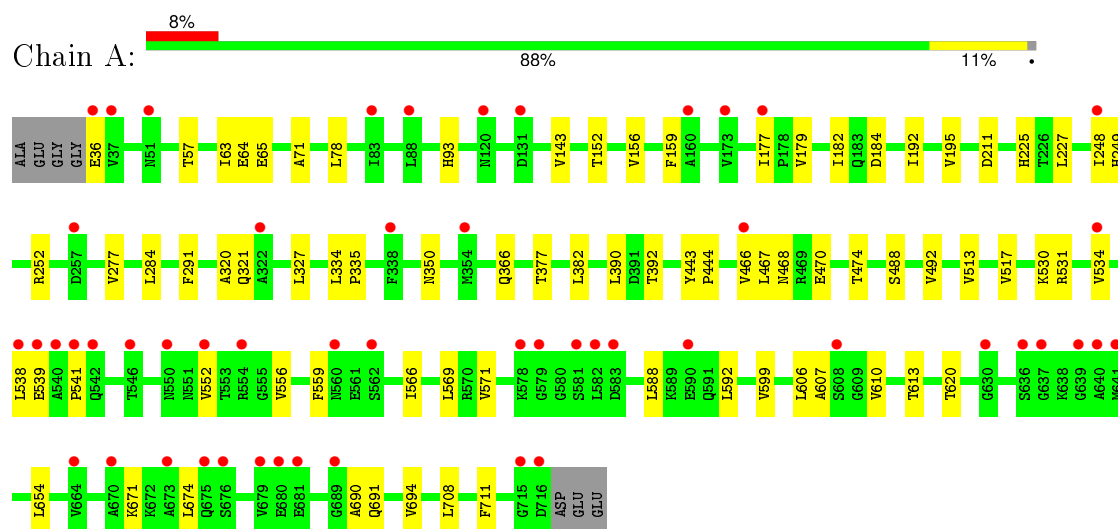
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	319	Total 319	O 319	0	0
4	B	336	Total 336	O 336	0	0
4	C	362	Total 362	O 362	0	0
4	D	348	Total 348	O 348	0	0

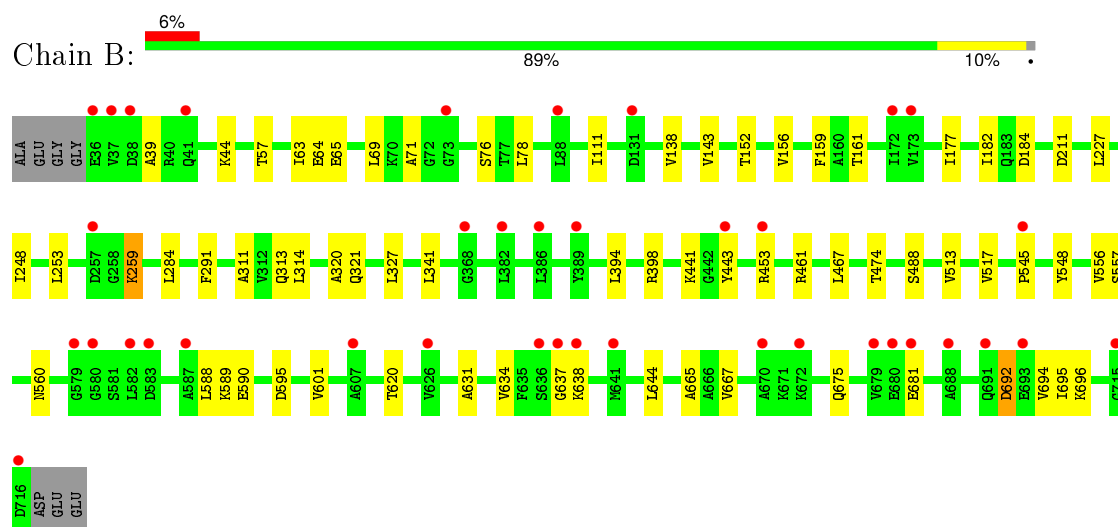
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

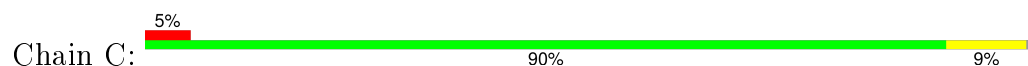
• Molecule 1: Catalase-3

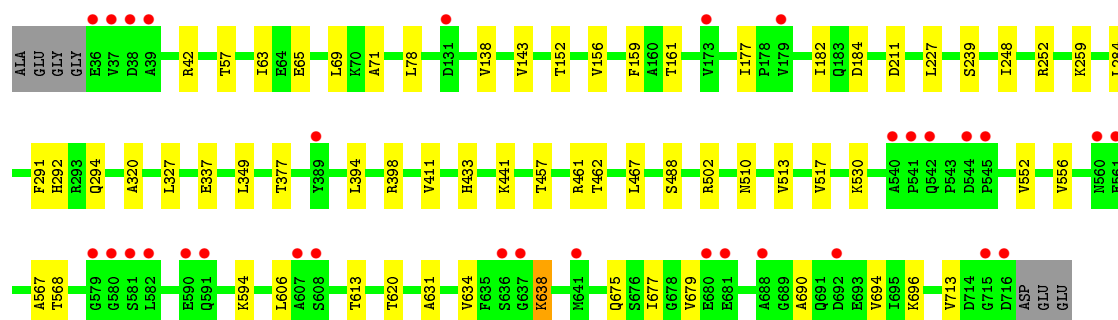


• Molecule 1: Catalase-3

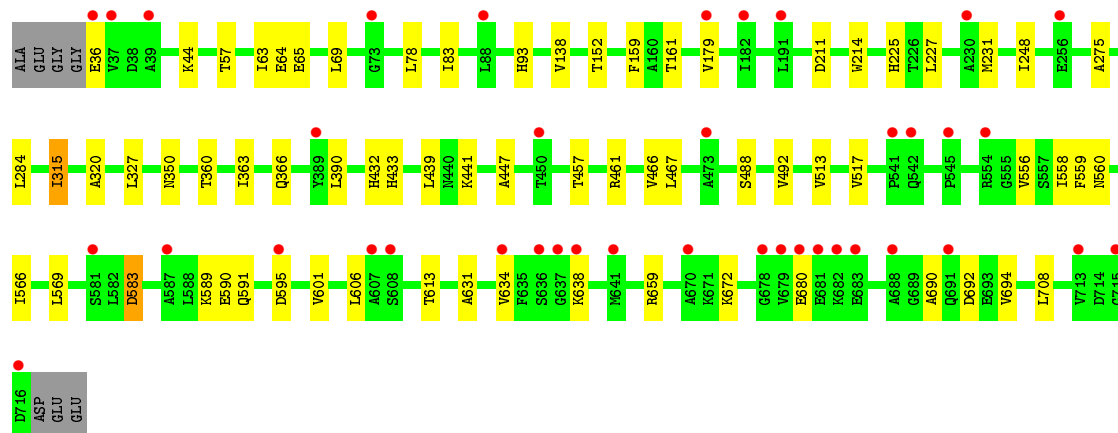
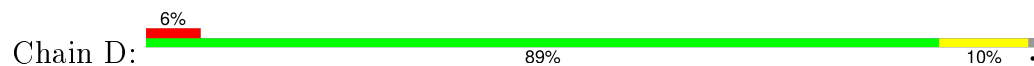


• Molecule 1: Catalase-3





• Molecule 1: Catalase-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.84Å 154.51Å 162.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.67 – 2.30 34.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (34.67-2.30) 93.0 (34.68-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.242 0.234 , 0.235	Depositor DCC
R_{free} test set	13602 reflections (9.94%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.6	EDS
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136856 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23009	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/5473	0.45	0/7424
1	B	0.34	2/5473 (0.0%)	0.47	3/7424 (0.0%)
1	C	0.34	2/5473 (0.0%)	0.48	2/7424 (0.0%)
1	D	0.34	3/5473 (0.1%)	0.47	2/7424 (0.0%)
All	All	0.33	7/21892 (0.0%)	0.47	7/29696 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	680	GLU	CB-CG	5.82	1.63	1.52
1	C	259	LYS	CG-CD	-5.71	1.33	1.52
1	B	259	LYS	CB-CG	5.64	1.67	1.52
1	C	638	LYS	CA-CB	5.53	1.66	1.53
1	B	638	LYS	CA-CB	-5.52	1.41	1.53
1	D	590	GLU	CA-CB	5.28	1.65	1.53
1	D	44	LYS	CG-CD	-5.10	1.35	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	LYS	N-CA-CB	5.55	120.59	110.60
1	C	713	VAL	CA-CB-CG1	5.50	119.15	110.90
1	D	692	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	675	GLN	CB-CA-C	-5.42	99.56	110.40
1	B	692	ASP	N-CA-CB	-5.39	100.90	110.60
1	B	259	LYS	CA-CB-CG	-5.29	101.76	113.40
1	D	583	ASP	CA-CB-CG	-5.27	101.81	113.40

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	5340	0	5155	43	0
1	B	5340	0	5153	37	0
1	C	5340	0	5154	35	0
1	D	5340	0	5154	37	0
2	A	14	0	13	0	0
2	B	42	0	39	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	1	0
4	A	319	0	0	0	0
4	B	336	0	0	0	0
4	C	362	0	0	0	0
4	D	348	0	0	0	0
All	All	23009	0	20840	141	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 3.

All (141) 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:248:ILE:HD12	3:C:4002:HEM:HMB1	1.64	0.79
1:A:654:LEU:HD21	1:A:674:LEU:HD23	1.65	0.78
1:B:248:ILE:HD12	3:B:4001:HEM:HMB1	1.66	0.76
1:A:248:ILE:HD12	3:A:4000:HEM:HMB1	1.66	0.76
1:C:71:ALA:HB2	1:C:78:LEU:HD21	1.72	0.72
1:A:467:LEU:HD22	1:D:78:LEU:HD11	1.73	0.70
1:C:152:THR:HG21	1:C:284:LEU:HD23	1.74	0.69
1:B:78:LEU:HD11	1:C:467:LEU:HD22	1.73	0.69
1:D:606:LEU:CD1	1:D:613:THR:HG23	2.24	0.68
1:B:467:LEU:HD22	1:C:78:LEU:HD11	1.74	0.67
1:D:152:THR:HG21	1:D:284:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ALA:HB3	1:A:610:VAL:HG23	1.80	0.64
1:A:152:THR:HG21	1:A:284:LEU:HD23	1.81	0.62
1:A:320:ALA:HA	1:A:327:LEU:HD12	1.82	0.62
1:B:320:ALA:HA	1:B:327:LEU:HD12	1.84	0.60
1:A:571:VAL:HG11	1:A:592:LEU:HD21	1.84	0.59
1:B:71:ALA:HB2	1:B:78:LEU:HD21	1.84	0.58
1:A:531:ARG:O	1:A:534:VAL:HG12	2.03	0.58
1:C:606:LEU:CD1	1:C:613:THR:HG23	2.34	0.57
1:C:152:THR:HG21	1:C:284:LEU:CD2	2.33	0.57
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.85	0.57
1:B:152:THR:HG21	1:B:284:LEU:HD23	1.86	0.57
1:B:57:THR:HG22	1:B:63:ILE:HD13	1.87	0.57
1:B:665:ALA:HB1	1:B:694:VAL:HG13	1.87	0.56
1:C:320:ALA:HA	1:C:327:LEU:HD12	1.88	0.54
1:A:488:SER:HB2	1:A:556:VAL:HG21	1.90	0.54
1:A:143:VAL:HG23	1:A:156:VAL:O	2.08	0.54
1:A:592:LEU:HD23	1:A:599:VAL:HG22	1.90	0.54
1:A:249:HIS:CD2	1:A:382:LEU:HD13	2.43	0.53
1:C:488:SER:HA	1:C:552:VAL:HG13	1.90	0.53
1:D:57:THR:CG2	1:D:63:ILE:HD13	2.39	0.53
1:D:152:THR:HG21	1:D:284:LEU:CD2	2.39	0.53
1:A:559:PHE:HB3	1:A:708:LEU:HD11	1.91	0.53
1:A:606:LEU:CD1	1:A:613:THR:HG23	2.39	0.52
1:D:138:VAL:HG22	1:D:161:THR:HG23	1.90	0.52
1:A:78:LEU:HD11	1:D:467:LEU:HD22	1.91	0.52
1:C:462:THR:HG22	1:D:466:VAL:HA	1.90	0.52
1:C:143:VAL:HG23	1:C:156:VAL:O	2.09	0.52
1:D:320:ALA:HA	1:D:327:LEU:HD12	1.90	0.52
1:B:488:SER:HB2	1:B:556:VAL:HG21	1.92	0.52
1:D:57:THR:HG22	1:D:63:ILE:HD13	1.92	0.52
1:D:64:GLU:O	1:D:83:ILE:HG21	2.09	0.52
1:A:57:THR:HG23	1:A:63:ILE:HD13	1.91	0.52
1:B:152:THR:HG21	1:B:284:LEU:CD2	2.40	0.51
1:B:57:THR:CG2	1:B:63:ILE:HD13	2.41	0.51
1:D:606:LEU:HD13	1:D:613:THR:HG23	1.92	0.51
1:B:667:VAL:HG22	1:B:694:VAL:HG21	1.93	0.51
1:B:284:LEU:HD21	1:B:291:PHE:CD2	2.46	0.50
1:A:492:VAL:HG11	1:A:708:LEU:HB3	1.93	0.50
1:A:57:THR:CG2	1:A:63:ILE:HD13	2.42	0.50
1:A:152:THR:HG21	1:A:284:LEU:CD2	2.42	0.50
1:A:592:LEU:HD23	1:A:599:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG23	1:B:156:VAL:O	2.12	0.49
1:D:366:GLN:HE22	1:D:390:LEU:HD13	1.78	0.49
1:C:42:ARG:HD2	1:C:411:VAL:HG12	1.95	0.49
1:A:71:ALA:HB2	1:A:78:LEU:HD21	1.93	0.49
1:D:513:VAL:O	1:D:517:VAL:HG23	2.13	0.49
1:A:284:LEU:HD21	1:A:291:PHE:CD2	2.48	0.48
1:A:179:VAL:HG11	1:A:225:HIS:CE1	2.49	0.47
1:A:513:VAL:O	1:A:517:VAL:HG23	2.14	0.47
1:A:321:GLN:NE2	1:A:474:THR:HG21	2.29	0.47
1:A:690:ALA:O	1:A:694:VAL:HG23	2.14	0.47
1:D:492:VAL:HG11	1:D:708:LEU:HB3	1.97	0.47
1:B:513:VAL:O	1:B:517:VAL:HG23	2.15	0.47
1:B:39:ALA:HB2	1:B:111:ILE:HD11	1.97	0.47
1:D:488:SER:HB2	1:D:556:VAL:HG21	1.97	0.47
1:D:566:ILE:HB	1:D:569:LEU:HD12	1.97	0.46
1:C:631:ALA:O	1:C:634:VAL:HG22	2.15	0.46
1:D:315:ILE:HD13	1:D:315:ILE:N	2.31	0.46
1:A:588:LEU:HD13	1:A:691:GLN:HG3	1.97	0.46
1:C:69:LEU:HG	1:C:78:LEU:HD12	1.97	0.46
1:C:252:ARG:NH1	1:C:377:THR:HG22	2.31	0.46
1:D:69:LEU:HG	1:D:78:LEU:HD12	1.97	0.46
1:B:69:LEU:HG	1:B:78:LEU:HD12	1.97	0.46
1:B:321:GLN:NE2	1:B:474:THR:HG21	2.30	0.46
1:A:607:ALA:HB3	1:A:610:VAL:CG2	2.45	0.46
1:B:156:VAL:HG22	1:B:177:ILE:HD12	1.97	0.46
1:B:589:LYS:HD2	1:B:601:VAL:HG23	1.98	0.46
1:A:466:VAL:HG23	1:B:461:ARG:O	2.16	0.46
1:D:360:THR:O	1:D:363:ILE:HG22	2.15	0.45
1:C:284:LEU:HD21	1:C:291:PHE:CD2	2.52	0.45
1:A:392:THR:HG21	3:A:4000:HEM:HBD1	1.99	0.45
1:C:57:THR:CG2	1:C:63:ILE:HD13	2.47	0.45
1:A:566:ILE:HB	1:A:569:LEU:HD12	1.98	0.45
1:D:492:VAL:HG11	1:D:708:LEU:HD22	1.98	0.45
1:D:214:TRP:CZ2	1:D:231:MET:HE3	2.51	0.45
1:B:39:ALA:HB2	1:B:111:ILE:CD1	2.48	0.44
1:C:57:THR:HG22	1:C:63:ILE:HD13	1.99	0.44
1:D:248:ILE:HD12	3:D:4003:HEM:HBB2	1.99	0.44
1:D:566:ILE:HD11	1:D:595:ASP:OD1	2.17	0.44
1:C:248:ILE:CD1	3:C:4002:HEM:HMB1	2.43	0.44
1:A:366:GLN:HE22	1:A:390:LEU:HD13	1.83	0.44
1:B:588:LEU:HD12	1:B:695:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:ILE:C	1:D:560:ASN:H	2.20	0.43
1:C:510:ASN:OD1	1:C:513:VAL:HG23	2.17	0.43
1:A:93:HIS:CE1	1:C:394:LEU:HD13	2.53	0.43
1:D:690:ALA:O	1:D:694:VAL:HG23	2.19	0.43
1:D:432:HIS:CE1	1:D:439:LEU:HB3	2.53	0.43
1:B:557:SER:HB3	1:B:560:ASN:HB2	1.99	0.43
1:C:138:VAL:HG22	1:C:161:THR:HG23	1.99	0.43
1:A:192:ILE:HA	1:A:195:VAL:HG22	2.00	0.43
1:B:441:LYS:O	1:B:443:TYR:CD1	2.71	0.43
1:C:567:ALA:C	1:C:568:THR:HG23	2.39	0.43
1:A:284:LEU:HD13	1:A:620:THR:HB	2.01	0.43
1:D:63:ILE:HD12	1:D:83:ILE:HG23	2.00	0.43
1:C:138:VAL:CG2	1:C:349:LEU:HD21	2.48	0.43
1:B:644:LEU:HD23	1:C:502:ARG:NH1	2.34	0.43
1:C:457:THR:HG23	1:C:461:ARG:HH21	1.84	0.42
1:A:182:ILE:HD12	1:A:184:ASP:O	2.18	0.42
1:B:631:ALA:O	1:B:634:VAL:HG22	2.19	0.42
1:A:443:TYR:HA	1:A:444:PRO:C	2.40	0.42
1:D:589:LYS:HD2	1:D:601:VAL:HG23	2.01	0.42
1:B:182:ILE:HD12	1:B:184:ASP:O	2.19	0.42
1:D:631:ALA:O	1:D:634:VAL:HG22	2.20	0.42
1:B:394:LEU:HD13	1:D:93:HIS:CE1	2.55	0.42
1:A:277:VAL:HG11	1:A:711:PHE:CZ	2.55	0.42
1:B:313:GLN:HG3	1:B:341:LEU:HD23	2.02	0.41
1:D:275:ALA:HB3	1:D:559:PHE:CZ	2.56	0.41
1:C:156:VAL:HG22	1:C:177:ILE:HD12	2.02	0.41
1:B:64:GLU:HG2	1:D:447:ALA:O	2.21	0.41
1:C:284:LEU:HD13	1:C:620:THR:HB	2.02	0.41
1:A:78:LEU:HD22	1:B:76:SER:HB2	2.02	0.41
1:B:253:LEU:HD12	1:B:314:LEU:HD21	2.02	0.41
1:D:179:VAL:HG21	1:D:225:HIS:ND1	2.36	0.41
1:C:488:SER:HB2	1:C:556:VAL:HG21	2.02	0.41
1:C:677:ILE:HG13	1:C:679:VAL:HG23	2.03	0.41
1:C:182:ILE:HD12	1:C:184:ASP:O	2.21	0.41
1:B:284:LEU:HD13	1:B:620:THR:HB	2.03	0.41
1:D:492:VAL:HG21	1:D:708:LEU:HB3	2.03	0.41
1:C:513:VAL:O	1:C:517:VAL:HG23	2.21	0.41
1:C:239:SER:HA	1:C:292:HIS:CD2	2.56	0.41
1:C:138:VAL:HG23	1:C:349:LEU:HD21	2.04	0.40
1:B:311:ALA:HB1	1:B:341:LEU:HB3	2.03	0.40
1:B:545:PRO:HA	1:B:548:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:SER:HA	1:A:552:VAL:HG13	2.03	0.40
1:D:457:THR:HG23	1:D:461:ARG:HH21	1.85	0.40
1:A:156:VAL:HG22	1:A:177:ILE:HD12	2.04	0.40
1:D:214:TRP:HZ2	1:D:231:MET:HE3	1.87	0.40
1:C:690:ALA:O	1:C:694:VAL:HG23	2.22	0.40
1:A:252:ARG:NH1	1:A:377:THR:HG22	2.36	0.40
1:A:334:LEU:HD12	1:A:335:PRO:HD2	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	679/688 (99%)	652 (96%)	26 (4%)	1 (0%)	56	68
1	B	679/688 (99%)	657 (97%)	21 (3%)	1 (0%)	56	68
1	C	679/688 (99%)	659 (97%)	20 (3%)	0	100	100
1	D	679/688 (99%)	645 (95%)	34 (5%)	0	100	100
All	All	2716/2752 (99%)	2613 (96%)	101 (4%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	GLY
1	A	541	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	559/563 (99%)	546 (98%)	13 (2%)	58	75
1	B	559/563 (99%)	545 (98%)	14 (2%)	55	73
1	C	559/563 (99%)	546 (98%)	13 (2%)	58	75
1	D	559/563 (99%)	545 (98%)	14 (2%)	55	73
All	All	2236/2252 (99%)	2182 (98%)	54 (2%)	57	74

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	64	GLU
1	A	65	GLU
1	A	159	PHE
1	A	211	ASP
1	A	227	LEU
1	A	350	ASN
1	A	468	ASN
1	A	470	GLU
1	A	530	LYS
1	A	538	LEU
1	A	539	GLU
1	A	671	LYS
1	B	44	LYS
1	B	65	GLU
1	B	159	PHE
1	B	211	ASP
1	B	227	LEU
1	B	259	LYS
1	B	398	ARG
1	B	453	ARG
1	B	590	GLU
1	B	595	ASP
1	B	675	GLN
1	B	681	GLU
1	B	692	ASP
1	B	696	LYS
1	C	65	GLU
1	C	159	PHE
1	C	211	ASP

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Mol	Chain	Res	Type
1	C	227	LEU
1	C	294	GLN
1	C	337	GLU
1	C	398	ARG
1	C	433	HIS
1	C	441	LYS
1	C	530	LYS
1	C	594	LYS
1	C	638	LYS
1	C	696	LYS
1	D	36	GLU
1	D	65	GLU
1	D	159	PHE
1	D	211	ASP
1	D	227	LEU
1	D	315	ILE
1	D	350	ASN
1	D	433	HIS
1	D	441	LYS
1	D	583	ASP
1	D	591	GLN
1	D	638	LYS
1	D	659	ARG
1	D	672	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	53	GLN
1	A	89	GLN
1	A	133	GLN
1	A	321	GLN
1	A	350	ASN
1	A	362	GLN
1	A	366	GLN
1	A	393	GLN
1	A	417	ASN
1	A	449	GLN
1	A	510	ASN
1	A	512	GLN
1	A	516	ASN

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Mol	Chain	Res	Type
1	A	612	GLN
1	B	51	ASN
1	B	53	GLN
1	B	89	GLN
1	B	304	ASN
1	B	321	GLN
1	B	366	GLN
1	B	393	GLN
1	B	417	ASN
1	B	449	GLN
1	B	512	GLN
1	B	516	ASN
1	B	550	ASN
1	B	691	GLN
1	C	51	ASN
1	C	53	GLN
1	C	66	GLN
1	C	89	GLN
1	C	362	GLN
1	C	366	GLN
1	C	449	GLN
1	C	512	GLN
1	C	516	ASN
1	C	612	GLN
1	D	51	ASN
1	D	53	GLN
1	D	89	GLN
1	D	133	GLN
1	D	294	GLN
1	D	342	GLN
1	D	350	ASN
1	D	366	GLN
1	D	417	ASN
1	D	449	GLN
1	D	512	GLN
1	D	516	ASN
1	D	520	GLN
1	D	550	ASN
1	D	612	GLN

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 ⓘ

12 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$
3	HEM	A	4000	1,4	30,50,50	2.20	8 (26%)	24,82,82	2.33	12 (50%)
2	NAG	A	5002	1	14,14,15	0.50	0	15,19,21	0.55	0
3	HEM	B	4001	1	30,50,50	2.21	10 (33%)	24,82,82	2.31	9 (37%)
2	NAG	B	5005	1	14,14,15	0.53	0	15,19,21	0.71	0
2	NAG	B	5006	1	14,14,15	0.49	0	15,19,21	0.59	0
2	NAG	B	5007	1	14,14,15	0.40	0	15,19,21	1.32	1 (6%)
3	HEM	C	4002	1	30,50,50	2.18	9 (30%)	24,82,82	2.35	13 (54%)
2	NAG	C	5008	1	14,14,15	0.52	0	15,19,21	0.64	0
2	NAG	C	5009	1	14,14,15	0.57	0	15,19,21	0.60	0
3	HEM	D	4003	1	30,50,50	2.24	9 (30%)	24,82,82	2.32	10 (41%)
2	NAG	D	5013	1	14,14,15	0.56	0	15,19,21	0.55	0
2	NAG	D	5014	1	14,14,15	0.47	0	15,19,21	0.74	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
3	HEM	A	4000	1,4	-	0/10/54/54	0/0/8/8
2	NAG	A	5002	1	-	1/6/23/26	0/1/1/1
3	HEM	B	4001	1	-	0/10/54/54	0/0/8/8
2	NAG	B	5005	1	-	0/6/23/26	0/1/1/1
2	NAG	B	5006	1	-	0/6/23/26	0/1/1/1
2	NAG	B	5007	1	-	0/6/23/26	0/1/1/1
3	HEM	C	4002	1	-	0/10/54/54	0/0/8/8
2	NAG	C	5008	1	-	0/6/23/26	0/1/1/1
2	NAG	C	5009	1	-	0/6/23/26	0/1/1/1
3	HEM	D	4003	1	-	0/10/54/54	0/0/8/8
2	NAG	D	5013	1	-	0/6/23/26	0/1/1/1
2	NAG	D	5014	1	-	0/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4003	HEM	C3B-C4B	-7.39	1.45	1.51
3	B	4001	HEM	C3B-C4B	-7.15	1.45	1.51
3	A	4000	HEM	C3B-C4B	-7.15	1.45	1.51
3	C	4002	HEM	C3B-C4B	-7.09	1.45	1.51
3	C	4002	HEM	C3D-C4D	-5.25	1.44	1.51
3	B	4001	HEM	C3D-C4D	-5.22	1.44	1.51
3	D	4003	HEM	C3D-C4D	-5.21	1.44	1.51
3	A	4000	HEM	C3D-C4D	-5.20	1.44	1.51
3	B	4001	HEM	C2C-C1C	-3.79	1.45	1.52
3	D	4003	HEM	C2C-C1C	-3.76	1.45	1.52
3	A	4000	HEM	C2C-C1C	-3.75	1.45	1.52
3	C	4002	HEM	C2C-C1C	-3.72	1.45	1.52
3	A	4000	HEM	C2D-C1D	-2.13	1.44	1.51
3	D	4003	HEM	C2D-C1D	-2.12	1.44	1.51
3	C	4002	HEM	C2D-C1D	-2.09	1.45	1.51
3	B	4001	HEM	C2D-C1D	-2.06	1.45	1.51
3	C	4002	HEM	C2B-C1B	-2.02	1.45	1.51
3	A	4000	HEM	FE-ND	2.01	2.08	1.97
3	B	4001	HEM	C3B-CAB	2.01	1.55	1.51
3	C	4002	HEM	FE-ND	2.03	2.08	1.97
3	B	4001	HEM	FE-NB	2.03	2.08	1.97
3	D	4003	HEM	C1C-NC	2.11	1.38	1.36
3	B	4001	HEM	FE-ND	2.16	2.08	1.97
3	D	4003	HEM	FE-ND	2.16	2.08	1.97
3	A	4000	HEM	C1C-NC	2.18	1.38	1.36
3	D	4003	HEM	C4C-NC	2.18	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4001	HEM	C1C-NC	2.20	1.38	1.36
3	C	4002	HEM	C1C-NC	2.22	1.38	1.36
3	C	4002	HEM	C4C-NC	2.23	1.38	1.36
3	B	4001	HEM	C4C-NC	2.24	1.38	1.36
3	A	4000	HEM	C4C-NC	2.29	1.38	1.36
3	D	4003	HEM	FE-NB	2.31	2.09	1.97
3	C	4002	HEM	FE-NC	2.51	2.05	1.95
3	A	4000	HEM	FE-NC	2.71	2.06	1.95
3	B	4001	HEM	FE-NC	2.86	2.07	1.95
3	D	4003	HEM	FE-NC	3.01	2.07	1.95

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4003	HEM	C3C-CAC-CBC	-2.99	119.86	124.46
3	B	4001	HEM	C3C-CAC-CBC	-2.85	120.09	124.46
3	A	4000	HEM	C3C-CAC-CBC	-2.84	120.10	124.46
3	C	4002	HEM	C3C-CAC-CBC	-2.82	120.14	124.46
3	A	4000	HEM	C3B-CAB-CBB	-2.63	120.42	124.46
3	C	4002	HEM	C3B-CAB-CBB	-2.62	120.43	124.46
3	D	4003	HEM	C3B-CAB-CBB	-2.61	120.45	124.46
3	B	4001	HEM	C3B-CAB-CBB	-2.44	120.72	124.46
3	C	4002	HEM	CBA-CAA-C2A	-2.20	108.58	112.53
3	A	4000	HEM	CBD-CAD-C3D	-2.16	107.27	113.55
3	C	4002	HEM	CBD-CAD-C3D	-2.15	107.29	113.55
3	C	4002	HEM	C3B-C4B-NB	-2.11	107.60	111.63
3	A	4000	HEM	CBA-CAA-C2A	-2.09	108.79	112.53
3	A	4000	HEM	C3B-C4B-NB	-2.07	107.68	111.63
3	C	4002	HEM	C2C-C1C-CHC	2.02	126.75	123.68
3	D	4003	HEM	C2C-C1C-CHC	2.09	126.86	123.68
3	D	4003	HEM	C3B-C4B-CHC	2.19	126.25	123.16
3	B	4001	HEM	C3B-C4B-CHC	2.27	126.36	123.16
3	A	4000	HEM	C3B-C4B-CHC	2.50	126.68	123.16
3	B	4001	HEM	C2D-C3D-C4D	2.56	105.84	101.50
3	C	4002	HEM	C2D-C3D-C4D	2.59	105.89	101.50
3	A	4000	HEM	C2D-C3D-C4D	2.69	106.06	101.50
3	D	4003	HEM	C2D-C3D-C4D	2.71	106.09	101.50
3	C	4002	HEM	C3B-C4B-CHC	2.73	127.00	123.16
3	B	4001	HEM	CMD-C2D-C3D	2.86	126.99	114.35
3	C	4002	HEM	CMD-C2D-C3D	2.90	127.18	114.35
3	A	4000	HEM	CMD-C2D-C3D	2.91	127.23	114.35
3	D	4003	HEM	CMD-C2D-C3D	2.92	127.25	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4002	HEM	CMC-C2C-C3C	3.59	125.50	116.53
3	A	4000	HEM	CMC-C2C-C3C	3.60	125.52	116.53
3	A	4000	HEM	CMB-C2B-C3B	3.60	125.53	116.53
3	B	4001	HEM	CMC-C2C-C3C	3.67	125.69	116.53
3	D	4003	HEM	CMC-C2C-C3C	3.67	125.70	116.53
3	C	4002	HEM	CMB-C2B-C3B	3.70	125.76	116.53
3	B	4001	HEM	CMB-C2B-C3B	3.86	126.16	116.53
3	D	4003	HEM	CMB-C2B-C3B	3.90	126.26	116.53
2	B	5007	NAG	C1-O5-C5	4.09	117.43	112.25
3	C	4002	HEM	CAD-C3D-C4D	4.13	127.04	112.47
3	A	4000	HEM	CAD-C3D-C4D	4.14	127.09	112.47
3	D	4003	HEM	CAD-C3D-C4D	4.15	127.12	112.47
3	B	4001	HEM	CAD-C3D-C4D	4.17	127.19	112.47
3	D	4003	HEM	CAD-C3D-C2D	4.72	126.79	113.22
3	A	4000	HEM	CAD-C3D-C2D	4.74	126.85	113.22
3	B	4001	HEM	CAD-C3D-C2D	4.78	126.97	113.22
3	C	4002	HEM	CAD-C3D-C2D	4.81	127.06	113.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5002	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4000	HEM	2	0
3	B	4001	HEM	1	0
3	C	4002	HEM	2	0
3	D	4003	HEM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	681/688 (98%)	0.66	52 (7%)	17	24	23, 23, 23, 24	13 (1%)
1	B	681/688 (98%)	0.53	38 (5%)	28	36	23, 23, 23, 24	20 (2%)
1	C	681/688 (98%)	0.48	32 (4%)	35	44	23, 23, 23, 24	22 (3%)
1	D	681/688 (98%)	0.52	39 (5%)	27	36	23, 23, 23, 25	16 (2%)
All	All	2724/2752 (98%)	0.54	161 (5%)	26	34	23, 23, 23, 25	71 (2%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	VAL	8.6
1	D	37	VAL	8.6
1	B	37	VAL	8.4
1	A	36	GLU	8.1
1	C	36	GLU	8.0
1	B	36	GLU	7.9
1	A	541	PRO	7.9
1	D	716	ASP	7.6
1	A	37	VAL	7.6
1	D	36	GLU	7.0
1	B	715	GLY	6.6
1	B	680	GLU	6.3
1	C	715	GLY	6.0
1	A	716	ASP	6.0
1	C	716	ASP	5.9
1	B	716	ASP	5.7
1	A	540	ALA	5.0
1	C	540	ALA	4.8
1	A	641	MET	4.6
1	D	715	GLY	4.5
1	C	641	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	579	GLY	4.2
1	D	682	LYS	4.2
1	D	641	MET	4.2
1	B	579	GLY	4.1
1	A	608	SER	4.0
1	A	552	VAL	4.0
1	A	675	GLN	3.8
1	C	579	GLY	3.7
1	A	542	GLN	3.7
1	D	680	GLU	3.7
1	B	636	SER	3.6
1	D	636	SER	3.6
1	D	681	GLU	3.6
1	C	542	GLN	3.5
1	B	587	ALA	3.5
1	B	688	ALA	3.5
1	D	638	LYS	3.4
1	A	582	LEU	3.3
1	C	580	GLY	3.3
1	A	715	GLY	3.3
1	C	173	VAL	3.1
1	A	322	ALA	3.1
1	A	257	ASP	3.1
1	B	641	MET	3.1
1	A	554	ARG	3.1
1	B	453	ARG	3.1
1	B	681	GLU	3.0
1	C	681	GLU	3.0
1	D	39	ALA	3.0
1	A	637	GLY	3.0
1	A	177	ILE	3.0
1	A	636	SER	3.0
1	D	581	SER	3.0
1	A	680	GLU	3.0
1	D	595	ASP	2.9
1	B	257	ASP	2.9
1	A	539	GLU	2.9
1	D	637	GLY	2.9
1	A	639	GLY	2.8
1	B	637	GLY	2.8
1	B	386	LEU	2.8
1	A	673	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	2.8
1	B	38	ASP	2.8
1	C	38	ASP	2.8
1	A	583	ASP	2.7
1	B	172	ILE	2.7
1	A	630	GLY	2.7
1	A	679	VAL	2.7
1	D	542	GLN	2.7
1	C	541	PRO	2.7
1	B	41	GLN	2.6
1	D	554	ARG	2.6
1	D	678	GLY	2.6
1	D	230	ALA	2.6
1	A	120	ASN	2.6
1	D	688	ALA	2.6
1	A	248	ILE	2.6
1	A	676	SER	2.5
1	B	693	GLU	2.5
1	B	580	GLY	2.5
1	C	39	ALA	2.5
1	A	670	ALA	2.5
1	C	688	ALA	2.5
1	A	354	MET	2.5
1	A	173	VAL	2.5
1	B	173	VAL	2.5
1	A	590	GLU	2.5
1	A	160	ALA	2.4
1	D	545	PRO	2.4
1	C	179	VAL	2.4
1	B	691	GLN	2.4
1	C	591	GLN	2.4
1	D	691	GLN	2.4
1	C	131	ASP	2.4
1	B	638	LYS	2.4
1	B	672	LYS	2.4
1	D	541	PRO	2.4
1	A	131	ASP	2.4
1	C	637	GLY	2.4
1	A	581	SER	2.4
1	D	608	SER	2.4
1	D	679	VAL	2.4
1	A	560	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	583	ASP	2.3
1	C	607	ALA	2.3
1	D	450	THR	2.3
1	A	538	LEU	2.3
1	B	582	LEU	2.3
1	C	582	LEU	2.3
1	C	692	ASP	2.3
1	B	545	PRO	2.3
1	B	607	ALA	2.3
1	B	670	ALA	2.3
1	D	634	VAL	2.3
1	A	338	PHE	2.2
1	B	73	GLY	2.2
1	C	544	ASP	2.2
1	C	581	SER	2.2
1	D	389	TYR	2.2
1	A	640	ALA	2.2
1	C	608	SER	2.2
1	A	689	GLY	2.2
1	D	73	GLY	2.2
1	B	131	ASP	2.2
1	D	191	LEU	2.2
1	C	636	SER	2.2
1	C	680	GLU	2.2
1	D	473	ALA	2.2
1	D	587	ALA	2.2
1	A	534	VAL	2.2
1	A	546	THR	2.2
1	B	382	LEU	2.1
1	C	389	TYR	2.1
1	A	550	ASN	2.1
1	C	545	PRO	2.1
1	D	713	VAL	2.1
1	D	683	GLU	2.1
1	D	670	ALA	2.1
1	D	256	GLU	2.1
1	D	182	ILE	2.1
1	B	626	VAL	2.1
1	A	681	GLU	2.1
1	B	443	TYR	2.1
1	C	561	GLU	2.1
1	C	590	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	562	SER	2.1
1	C	560	ASN	2.0
1	B	88	LEU	2.0
1	A	578	LYS	2.0
1	D	179	VAL	2.0
1	D	607	ALA	2.0
1	A	51	ASN	2.0
1	A	83	ILE	2.0
1	B	368	GLY	2.0
1	A	466	VAL	2.0
1	A	664	VAL	2.0
1	B	679	VAL	2.0
1	D	88	LEU	2.0
1	B	389	TYR	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
2	NAG	D	5014	14/15	0.67	0.32	9.41	23,23,23,23	0
2	NAG	B	5007	14/15	0.48	0.47	6.59	24,24,24,24	0
2	NAG	C	5008	14/15	0.78	0.24	2.37	23,23,23,23	0
3	HEM	D	4003	43/43	0.92	0.20	0.04	22,22,22,22	0
3	HEM	C	4002	43/43	0.94	0.19	-0.01	22,22,23,23	0
3	HEM	B	4001	43/43	0.94	0.16	-0.71	22,22,22,23	0
3	HEM	A	4000	43/43	0.92	0.14	-1.39	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	5006	14/15	0.77	0.40	-	23,23,23,23	0
2	NAG	A	5002	14/15	0.67	0.47	-	23,24,24,24	0
2	NAG	B	5005	14/15	0.81	0.41	-	23,24,24,24	0
2	NAG	C	5009	14/15	0.70	0.39	-	24,24,24,24	0
2	NAG	D	5013	14/15	0.71	0.37	-	24,24,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.