



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:09 PM GMT

PDB ID : 4QI7
Title : Cellobiose dehydrogenase from *Neurospora crassa*, NcCDH
Authors : Tan, T.C.; Gandini, R.; Sygmund, C.; Kittl, R.; Haltrich, D.; Ludwig, R.;
Hallberg, B.M.; Divne, C.
Deposited on : 2014-05-30
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

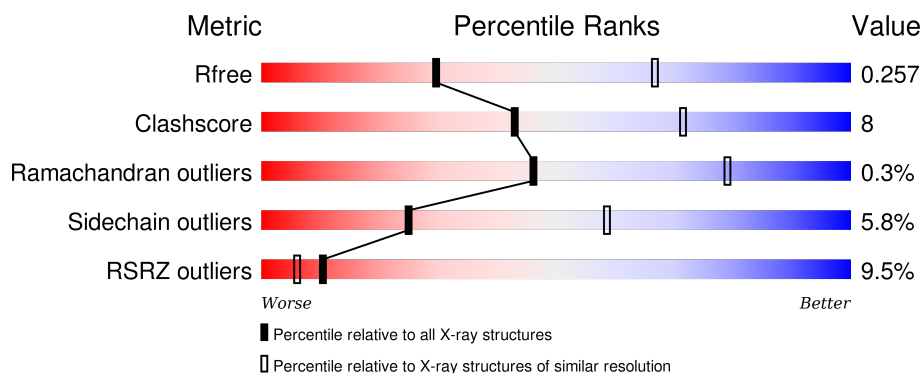
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	806	<div> <div>6%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
1	B	806	<div> <div>13%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	906	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12482 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 Cellobiose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	805	Total	C	N	O	S	0	0	0
			6061	3810	1042	1182	27			
1	B	792	Total	C	N	O	S	0	0	0
			5979	3762	1029	1162	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	-	EXPRESSION TAG	UNP Q7RXM0
B	1	PCA	-	EXPRESSION TAG	UNP Q7RXM0

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



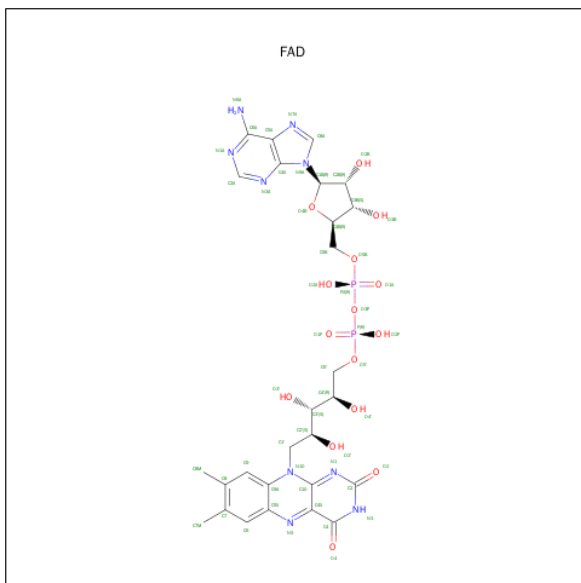
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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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 FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



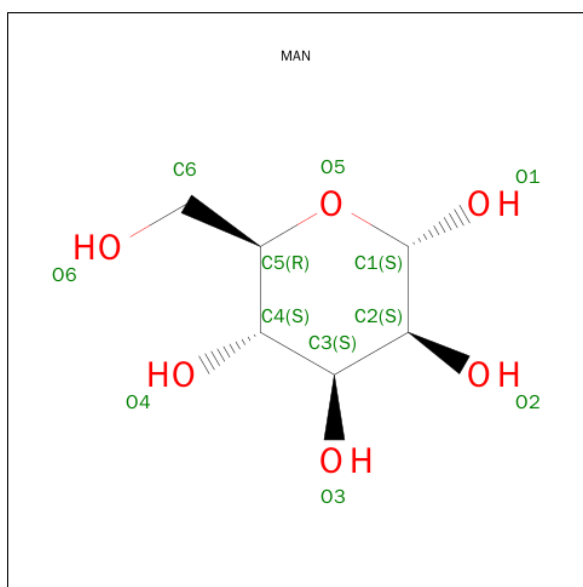
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



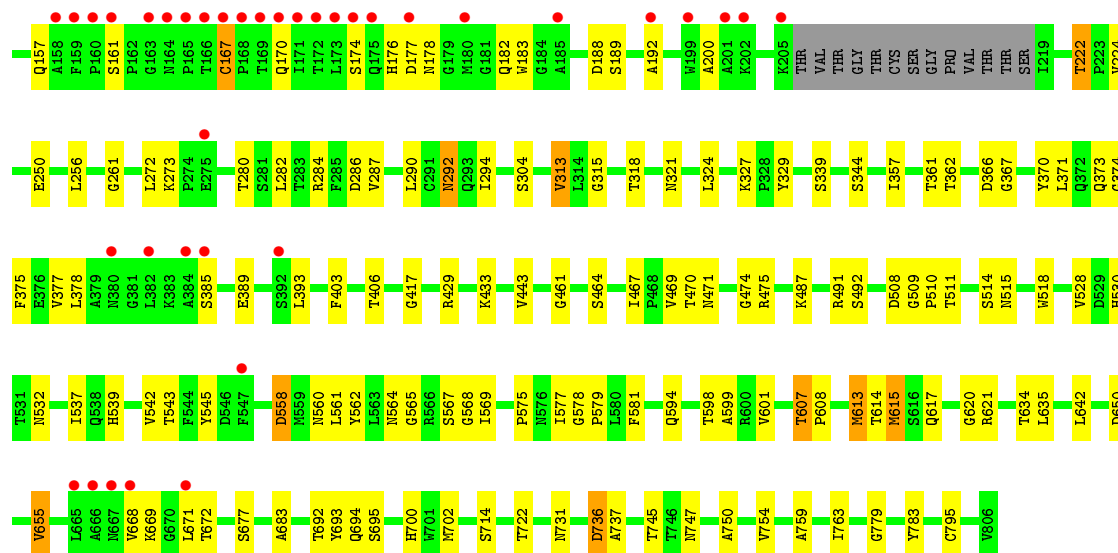
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	8	Total	Pt	0	0
			8	8		
6	A	12	Total	Pt	0	0
			12	12		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	3	Total	Mg	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.60Å 141.85Å 147.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.04 – 2.90 58.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.04-2.90) 99.9 (58.64-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.185 , 0.235 0.214 , 0.257	Depositor DCC
R_{free} test set	1995 reflections (3.30%)	DCC
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.2	EDS
Estimated twinning fraction	0.068 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 62494 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12482	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

5.1 Standard geometry

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

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	0.47	0/6214	0.67	0/8481
1	B	0.46	1/6130 (0.0%)	0.66	0/8362
All	All	0.47	1/12344 (0.0%)	0.66	0/16843

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	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	THR	C-N	-5.71	1.23	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	SER	Peptide
1	B	470	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6061	0	5828	99	0
1	B	5979	0	5749	100	0
2	A	43	0	30	6	0
2	B	43	0	30	9	0
3	A	53	0	31	5	0
3	B	53	0	31	3	0
4	A	98	0	91	5	0
4	B	84	0	78	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
6	A	12	0	0	0	0
6	B	8	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
All	All	12482	0	11908	201	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 8.

All (201) 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:B:4:PRO:HB2	1:B:17:ASN:HD22	1.41	0.83
1:B:176:HIS:CE1	2:B:901:HEM:NA	2.48	0.81
1:A:79:LEU:HD22	2:A:901:HEM:HAC	1.67	0.76
1:A:63:SER:HA	1:A:161:SER:HB3	1.67	0.76
1:B:133:LEU:HD22	1:B:144:ILE:HD11	1.68	0.73
1:A:176:HIS:H	1:A:176:HIS:CD2	2.06	0.73
1:B:176:HIS:CD2	2:B:901:HEM:NC	2.58	0.71
1:B:374:GLY:HA3	1:B:613:MET:HE1	1.73	0.71
1:B:491:ARG:HD3	1:B:635:LEU:HD13	1.72	0.70
1:B:287:VAL:HB	1:B:290:LEU:HD12	1.72	0.70
1:A:265:THR:HA	1:A:283:THR:HG21	1.75	0.68
1:B:469:VAL:HB	1:B:474:GLY:HA3	1.75	0.67
1:A:35:ALA:HB3	1:A:49:ILE:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:THR:HG23	1:B:695:SER:H	1.60	0.66
1:B:47:GLU:OE2	1:B:128:ARG:NE	2.27	0.66
1:B:96:ALA:HB2	1:B:102:PRO:HB3	1.78	0.65
1:B:44:ASP:HA	1:B:146:THR:HG22	1.78	0.65
1:B:594:GLN:HG2	1:B:745:THR:HG23	1.78	0.65
1:A:601:VAL:HG12	1:A:613:MET:HG2	1.79	0.64
1:B:39:ASN:N	1:B:39:ASN:OD1	2.30	0.64
1:A:117:SER:HB2	1:A:124:THR:HB	1.80	0.63
1:A:575:PRO:HB3	1:A:602:GLU:OE2	1.98	0.63
1:A:96:ALA:HB2	1:A:102:PRO:HB3	1.81	0.63
2:A:901:HEM:HMA2	2:A:901:HEM:HBA2	1.81	0.63
1:B:128:ARG:HD2	1:B:200:ALA:HB1	1.83	0.61
1:B:177:ASP:OD1	1:B:178:ASN:N	2.34	0.61
1:A:41:LEU:HD22	1:A:149:LYS:HD3	1.84	0.60
1:A:450:ILE:O	1:A:731:ASN:ND2	2.35	0.60
1:A:491:ARG:HD3	1:A:635:LEU:HD13	1.85	0.58
1:B:63:SER:HA	1:B:161:SER:HB3	1.84	0.58
1:B:121:THR:HG22	1:B:122:HIS:CE1	2.38	0.58
1:B:136:ASP:OD1	1:B:141:THR:HA	2.03	0.58
1:B:250:GLU:HG2	1:B:429:ARG:NH2	2.17	0.58
1:B:594:GLN:OE1	1:B:621:ARG:NH2	2.36	0.58
4:A:904:NAG:H82	1:B:461:GLY:HA3	1.86	0.58
1:A:157:GLN:HB3	1:A:178:ASN:HB3	1.86	0.57
1:B:373:GLN:HB2	1:B:543:THR:HG22	1.85	0.57
1:B:46:THR:HG23	1:B:47:GLU:HB3	1.85	0.57
1:A:536:VAL:HB	1:A:674:ALA:HB3	1.87	0.57
1:B:389:GLU:HB2	1:B:403:PHE:CZ	2.40	0.57
1:A:81:THR:HG22	1:A:92:ASN:O	2.05	0.57
1:B:375:PHE:CE1	1:B:579:PRO:HB3	2.40	0.56
1:B:71:ARG:HD3	1:B:144:ILE:HG22	1.88	0.56
1:B:366:ASP:OD1	1:B:367:GLY:N	2.37	0.56
1:A:327:LYS:HG3	1:A:354:LEU:HD11	1.88	0.55
1:B:564:ASN:OD1	1:B:565:GLY:N	2.39	0.55
1:A:224:VAL:HG23	1:A:464:SER:O	2.07	0.55
1:A:469:VAL:HB	1:A:474:GLY:HA3	1.89	0.55
1:B:545:TYR:CE1	1:B:569:ILE:HG21	2.41	0.55
1:A:676:PRO:HB3	1:A:685:PHE:HB2	1.88	0.55
1:A:148:ASN:N	1:A:149:LYS:HA	2.22	0.55
1:B:642:LEU:HD21	1:B:693:TYR:HB3	1.88	0.55
1:A:283:THR:HG23	1:A:285:PHE:H	1.72	0.54
4:A:906:NAG:O7	4:A:906:NAG:O3	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:HB1	1:A:132:CYS:SG	2.48	0.54
1:A:752:ILE:HD13	3:A:902:FAD:H5'2	1.90	0.54
1:A:542:VAL:HB	1:A:611:TYR:HA	1.89	0.54
1:A:176:HIS:HE1	2:A:901:HEM:C4D	2.26	0.53
1:A:337:PHE:HD1	1:A:707:MET:HE1	1.74	0.53
1:B:702:MET:HG2	1:B:737:ALA:HB1	1.90	0.53
1:A:321:ASN:HB2	3:A:902:FAD:N5	2.24	0.53
1:B:542:VAL:HG22	1:B:613:MET:HE3	1.89	0.53
1:A:747:ASN:HB3	3:A:902:FAD:C2	2.38	0.53
1:A:726:VAL:O	1:A:729:THR:OG1	2.23	0.52
1:B:287:VAL:HG22	1:B:562:TYR:HE2	1.74	0.52
1:B:558:ASP:OD1	1:B:558:ASP:N	2.35	0.52
1:B:537:ILE:HD12	1:B:671:LEU:HD11	1.92	0.52
1:A:692:THR:HG22	1:A:695:SER:HB2	1.91	0.52
1:B:38:SER:HA	1:B:192:ALA:HB1	1.92	0.52
1:A:693:TYR:O	1:A:697:ARG:HB3	2.10	0.51
1:A:44:ASP:OD1	1:A:145:SER:OG	2.28	0.51
1:B:47:GLU:HG2	1:B:48:PHE:N	2.25	0.51
1:B:575:PRO:O	1:B:577:ILE:HG13	2.10	0.51
1:A:229:SER:OG	1:A:470:THR:HG22	2.11	0.51
1:A:89:VAL:O	1:A:113:GLN:NE2	2.39	0.51
1:A:17:ASN:O	1:A:33:GLY:HA2	2.11	0.51
1:B:371:LEU:HD11	1:B:545:TYR:HD1	1.76	0.51
1:B:93:LEU:HD11	1:B:111:ILE:HG13	1.93	0.50
1:A:654:VAL:HG12	1:A:686:VAL:HG21	1.93	0.50
1:B:601:VAL:HG23	1:B:601:VAL:O	2.11	0.50
1:A:721:ASP:HB3	1:A:727:TYR:CZ	2.47	0.50
1:B:406:THR:OG1	1:B:577:ILE:O	2.22	0.50
1:B:321:ASN:HB2	3:B:902:FAD:C4X	2.42	0.50
1:A:544:PHE:HB2	1:A:610:GLY:HA2	1.93	0.50
1:A:72:GLY:HA2	1:A:154:GLY:H	1.77	0.50
1:B:79:LEU:HD22	2:B:901:HEM:HAC	1.93	0.49
1:A:321:ASN:HB2	3:A:902:FAD:C4X	2.42	0.49
1:B:515:ASN:HA	1:B:518:TRP:CD1	2.48	0.49
1:A:642:LEU:O	1:A:646:LYS:HE3	2.13	0.49
1:B:81:THR:HG22	2:B:901:HEM:HBC2	1.95	0.49
1:A:293:GLN:HE22	1:A:296:LYS:HD3	1.78	0.49
1:A:700:HIS:O	1:A:702:MET:HG3	2.13	0.49
1:B:562:TYR:HA	1:B:567:SER:H	1.76	0.48
1:A:262:PHE:HZ	1:A:301:ILE:HD13	1.76	0.48
1:B:273:LYS:HD3	1:B:282:LEU:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:OG	1:A:25:GLN:HG3	2.13	0.48
1:A:747:ASN:HB3	3:A:902:FAD:O2	2.14	0.48
1:B:747:ASN:HB3	3:B:902:FAD:C2	2.44	0.48
1:B:272:LEU:O	1:B:284:ARG:HG2	2.14	0.48
1:A:72:GLY:HA2	1:A:154:GLY:N	2.29	0.48
1:B:44:ASP:HA	1:B:146:THR:CG2	2.44	0.47
1:A:601:VAL:O	1:A:601:VAL:HG23	2.14	0.47
1:A:128:ARG:CZ	1:A:130:GLN:HE21	2.27	0.47
1:B:327:LYS:HB2	1:B:393:LEU:O	2.14	0.47
1:B:176:HIS:CE1	2:B:901:HEM:C1A	3.03	0.47
1:B:74:MET:HB2	2:B:901:HEM:C1D	2.49	0.47
1:A:797:LYS:HB2	1:A:803:TRP:CE2	2.50	0.47
1:B:167:CYS:HB3	1:B:170:GLN:HB2	1.97	0.47
1:B:375:PHE:HE1	1:B:579:PRO:HB3	1.79	0.47
1:A:293:GLN:HG3	1:A:551:TRP:CE3	2.50	0.46
1:B:224:VAL:HG23	1:B:464:SER:O	2.15	0.46
1:A:19:TRP:CE2	1:A:185:ALA:HB1	2.49	0.46
1:B:491:ARG:HD2	1:B:508:ASP:OD2	2.16	0.46
1:B:176:HIS:CD2	2:B:901:HEM:C1C	3.04	0.46
1:B:759:ALA:O	1:B:763:ILE:HG13	2.15	0.46
1:B:578:GLY:N	1:B:599:ALA:O	2.49	0.46
1:B:750:ALA:O	1:B:754:VAL:HG23	2.16	0.46
1:A:122:HIS:HD2	4:A:903:NAG:H5	1.81	0.46
1:B:315:GLY:O	1:B:318:THR:OG1	2.29	0.46
1:A:287:VAL:HB	1:A:290:LEU:HD12	1.98	0.45
1:A:176:HIS:CE1	2:A:901:HEM:C4D	3.04	0.45
1:A:659:VAL:HG12	1:A:663:LYS:HE2	1.99	0.45
1:A:668:VAL:HG12	1:A:671:LEU:HB2	1.98	0.45
1:A:272:LEU:O	1:A:284:ARG:HG2	2.16	0.45
1:A:176:HIS:CD2	2:A:901:HEM:NC	2.84	0.45
1:B:601:VAL:HG12	1:B:613:MET:HE2	1.97	0.45
1:A:238:GLY:H	1:A:242:ILE:HD12	1.81	0.45
1:B:154:GLY:HA2	1:B:182:GLN:HA	1.99	0.45
1:A:287:VAL:HG22	1:A:562:TYR:HE2	1.81	0.45
1:B:378:LEU:HD21	1:B:537:ILE:CD1	2.46	0.45
1:B:560:ASN:O	1:B:564:ASN:ND2	2.50	0.45
1:A:676:PRO:HB3	1:A:685:PHE:CB	2.46	0.45
1:B:357:ILE:HD13	1:B:417:GLY:HA2	1.99	0.44
1:B:370:TYR:CE2	1:B:568:GLY:HA2	2.52	0.44
1:A:138:ASP:HB3	1:A:139:GLY:H	1.67	0.44
1:B:528:VAL:HG12	1:B:702:MET:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLY:N	1:B:510:PRO:HD2	2.32	0.44
1:B:30:PHE:HB2	1:B:157:GLN:NE2	2.31	0.44
1:A:363:PRO:HB2	1:A:571:ALA:O	2.18	0.44
1:A:705:ASN:HB3	1:A:719:VAL:HG11	1.99	0.43
1:B:176:HIS:HE1	2:B:901:HEM:C1A	2.35	0.43
1:B:558:ASP:HA	1:B:561:LEU:HB3	1.99	0.43
1:A:73:ALA:O	1:A:77:ASN:ND2	2.48	0.43
1:B:779:GLY:HA2	1:B:783:TYR:CD2	2.53	0.43
1:B:539:HIS:HB3	1:B:542:VAL:HG23	2.01	0.43
1:B:530:HIS:CD2	1:B:620:GLY:HA2	2.53	0.43
1:B:84:PRO:HD3	1:B:123:PHE:CZ	2.53	0.43
1:A:538:GLN:HG3	1:A:672:THR:HB	2.01	0.43
1:B:487:LYS:O	1:B:491:ARG:HG3	2.18	0.43
1:B:443:VAL:HG22	1:B:492:SER:OG	2.19	0.43
1:A:491:ARG:HD2	1:A:508:ASP:OD1	2.18	0.43
1:A:606:GLU:HB2	1:A:675:TYR:OH	2.19	0.43
1:A:14:ILE:HG23	1:A:199:TRP:CE3	2.53	0.43
1:B:692:THR:OG1	1:B:694:GLN:OE1	2.29	0.42
1:A:409:MET:O	1:A:416:GLY:HA3	2.19	0.42
1:B:148:ASN:O	1:B:149:LYS:HG2	2.18	0.42
1:A:446:GLU:OE2	1:A:794:LYS:NZ	2.45	0.42
1:A:647:ASP:HA	1:A:648:PRO:HD2	1.79	0.42
1:A:273:LYS:HE2	1:A:282:LEU:O	2.19	0.42
1:A:9:HIS:HA	1:A:10:PRO:HD3	1.91	0.42
1:B:256:LEU:HD12	1:B:433:LYS:O	2.19	0.42
1:A:594:GLN:HG2	1:A:745:THR:HG23	2.00	0.42
1:A:651:LYS:O	1:A:655:VAL:HG23	2.18	0.42
1:B:581:PHE:HZ	1:B:615:MET:HE2	1.84	0.42
1:A:779:GLY:HA2	1:A:783:TYR:CD2	2.54	0.42
1:A:669:LYS:HG2	4:A:908:NAG:H83	2.01	0.42
1:B:176:HIS:HD2	2:B:901:HEM:C1C	2.38	0.42
1:B:16:PHE:HE2	1:B:49:ILE:HG22	1.85	0.42
1:A:337:PHE:O	1:A:342:LYS:HE2	2.19	0.42
1:A:290:LEU:HD22	1:A:551:TRP:HE3	1.84	0.42
1:A:238:GLY:N	1:A:242:ILE:HD12	2.34	0.42
1:A:177:ASP:OD1	1:A:177:ASP:N	2.52	0.42
1:A:623:ALA:O	1:A:626:ARG:NH2	2.53	0.42
1:B:188:ASP:OD1	1:B:189:SER:N	2.49	0.42
1:B:261:GLY:HA3	1:B:313:VAL:HA	2.01	0.42
1:B:607:THR:HA	1:B:608:PRO:HD3	1.84	0.42
1:B:292:ASN:OD1	1:B:575:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ASN:O	1:A:739:ILE:HA	2.20	0.41
1:B:70:LEU:HA	1:B:70:LEU:HD23	1.74	0.41
1:A:285:PHE:HZ	1:A:301:ILE:HD12	1.85	0.41
1:A:264:SER:OG	1:A:265:THR:N	2.54	0.41
1:A:247:LYS:HD2	1:A:247:LYS:HA	1.90	0.41
1:A:122:HIS:CD2	4:A:903:NAG:H5	2.55	0.41
1:B:475:ARG:HA	1:B:731:ASN:HB2	2.03	0.41
1:A:575:PRO:HG2	1:A:602:GLU:HG3	2.02	0.41
1:B:736:ASP:HB2	3:B:902:FAD:O2P	2.20	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.71	0.41
1:A:545:TYR:CE1	1:A:569:ILE:HD13	2.56	0.41
1:A:42:THR:OG1	1:A:43:THR:N	2.54	0.41
1:A:489:LEU:HD12	1:A:705:ASN:ND2	2.36	0.41
1:B:58:LYS:HE2	1:B:59:ASN:OD1	2.21	0.41
1:B:655:VAL:HG11	1:B:683:ALA:HA	2.03	0.41
1:A:421:THR:OG1	1:A:422:TYR:N	2.53	0.40
1:A:546:ASP:O	1:A:547:PHE:HB2	2.20	0.40
1:B:700:HIS:O	1:B:702:MET:HG3	2.21	0.40
1:B:599:ALA:HA	1:B:614:THR:O	2.21	0.40
1:A:74:MET:HB2	2:A:901:HEM:C1D	2.56	0.40
1:A:441:LYS:HE2	1:A:441:LYS:HB3	1.71	0.40
1:A:58:LYS:HA	1:A:58:LYS:HD2	1.86	0.40
1:B:532:ASN:HA	1:B:617:GLN:O	2.22	0.40
1:A:799:ASN:HB2	1:A:801:TRP:H	1.87	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	803/806 (100%)	766 (95%)	35 (4%)	2 (0%)	52 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	788/806 (98%)	752 (95%)	34 (4%)	2 (0%)	46 79
All	All	1591/1612 (99%)	1518 (95%)	69 (4%)	4 (0%)	46 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	ASN
1	A	605	PHE
1	B	736	ASP
1	A	219	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	643/643 (100%)	610 (95%)	33 (5%)	29 65
1	B	632/643 (98%)	591 (94%)	41 (6%)	21 52
All	All	1275/1286 (99%)	1201 (94%)	74 (6%)	25 58

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	112	THR
1	A	169	THR
1	A	176	HIS
1	A	189	SER
1	A	222	THR
1	A	242	ILE
1	A	280	THR
1	A	292	ASN
1	A	320	ILE
1	A	329	TYR
1	A	356	ARG

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Mol	Chain	Res	Type
1	A	361	THR
1	A	364	SER
1	A	368	LYS
1	A	430	SER
1	A	453	VAL
1	A	466	ILE
1	A	467	ILE
1	A	533	THR
1	A	538	GLN
1	A	543	THR
1	A	545	TYR
1	A	553	ASN
1	A	581	PHE
1	A	605	PHE
1	A	614	THR
1	A	691	VAL
1	A	709	THR
1	A	722	THR
1	A	743	VAL
1	A	782	THR
1	A	795	CYS
1	B	32	VAL
1	B	34	MET
1	B	39	ASN
1	B	71	ARG
1	B	85	SER
1	B	167	CYS
1	B	174	SER
1	B	183	TRP
1	B	222	THR
1	B	280	THR
1	B	286	ASP
1	B	292	ASN
1	B	294	ILE
1	B	304	SER
1	B	313	VAL
1	B	324	LEU
1	B	329	TYR
1	B	339	SER
1	B	344	SER
1	B	361	THR
1	B	362	THR

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Mol	Chain	Res	Type
1	B	377	VAL
1	B	385	SER
1	B	467	ILE
1	B	511	THR
1	B	514	SER
1	B	558	ASP
1	B	598	THR
1	B	607	THR
1	B	613	MET
1	B	615	MET
1	B	634	THR
1	B	650	ASP
1	B	655	VAL
1	B	668	VAL
1	B	669	LYS
1	B	672	THR
1	B	677	SER
1	B	714	SER
1	B	722	THR
1	B	795	CYS

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	152	GLN
1	A	705	ASN
1	B	17	ASN
1	B	182	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

Of 45 ligands modelled in this entry, 24 are monoatomic - leaving 21 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	901	1	24,50,50	3.23	10 (41%)	16,82,82	2.59	10 (62%)
3	FAD	A	902	-	52,58,58	1.26	6 (11%)	52,89,89	2.00	8 (15%)
4	NAG	A	903	1	14,14,15	0.31	0	15,19,21	0.18	0
4	NAG	A	904	1	14,14,15	0.32	0	15,19,21	0.49	0
4	NAG	A	905	1	14,14,15	0.29	0	15,19,21	0.43	0
4	NAG	A	906	1	14,14,15	0.86	1 (7%)	15,19,21	1.49	1 (6%)
4	NAG	A	907	1	14,14,15	0.25	0	15,19,21	0.80	1 (6%)
4	NAG	A	908	1	14,14,15	0.41	0	15,19,21	0.63	1 (6%)
4	NAG	A	909	1	14,14,15	0.28	0	15,19,21	0.45	0
5	MAN	A	910	1	11,11,12	1.07	1 (9%)	15,15,17	1.52	3 (20%)
5	MAN	A	911	1	11,11,12	1.94	2 (18%)	15,15,17	0.96	0
2	HEM	B	901	1	24,50,50	3.22	9 (37%)	16,82,82	2.23	8 (50%)
3	FAD	B	902	-	52,58,58	1.19	4 (7%)	52,89,89	2.07	8 (15%)
4	NAG	B	903	1	14,14,15	0.21	0	15,19,21	0.55	0
4	NAG	B	904	1	14,14,15	0.38	0	15,19,21	0.53	0
4	NAG	B	905	1	14,14,15	0.35	0	15,19,21	0.38	0
4	NAG	B	906	1	14,14,15	0.23	0	15,19,21	0.68	1 (6%)
4	NAG	B	907	1	14,14,15	0.53	0	15,19,21	0.62	0
4	NAG	B	908	1	14,14,15	0.63	1 (7%)	15,19,21	0.58	0
5	MAN	B	909	1	11,11,12	1.90	3 (27%)	15,15,17	1.10	1 (6%)
5	MAN	B	910	1	11,11,12	2.47	6 (54%)	15,15,17	1.24	1 (6%)

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	901	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	902	-	-	0/30/50/50	0/6/6/6
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	0/6/23/26	0/1/1/1
4	NAG	A	908	1	-	0/6/23/26	0/1/1/1
4	NAG	A	909	1	-	0/6/23/26	0/1/1/1
5	MAN	A	910	1	-	0/2/19/22	0/1/1/1
5	MAN	A	911	1	-	0/2/19/22	0/1/1/1
2	HEM	B	901	1	-	0/6/54/54	0/0/8/8
3	FAD	B	902	-	-	0/30/50/50	0/6/6/6
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1	-	0/6/23/26	0/1/1/1
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
4	NAG	B	908	1	-	0/6/23/26	0/1/1/1
5	MAN	B	909	1	-	0/2/19/22	0/1/1/1
5	MAN	B	910	1	-	0/2/19/22	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	FAD	C2B-C1B	-2.53	1.49	1.53
5	A	910	MAN	O5-C1	-2.07	1.40	1.43
5	B	909	MAN	C2-C3	2.00	1.55	1.52
2	A	901	HEM	C4A-CHB	2.05	1.45	1.40
2	A	901	HEM	C1D-CHD	2.07	1.45	1.40
5	B	910	MAN	O5-C5	2.11	1.48	1.43
3	A	902	FAD	C5X-N5	2.18	1.38	1.35
4	B	908	NAG	C1-C2	2.21	1.55	1.52
2	B	901	HEM	C4A-CHB	2.27	1.46	1.40
2	A	901	HEM	C1A-CHA	2.31	1.46	1.40
5	B	910	MAN	O3-C3	2.36	1.48	1.43
2	B	901	HEM	C1A-CHA	2.36	1.46	1.40
2	B	901	HEM	C4B-CHC	2.38	1.46	1.40
3	A	902	FAD	C2A-N1A	2.38	1.38	1.33
3	B	902	FAD	C2A-N1A	2.50	1.38	1.33
2	A	901	HEM	C4B-CHC	2.53	1.46	1.40
4	A	906	NAG	O5-C1	2.61	1.48	1.43
5	A	911	MAN	C4-C3	2.61	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	910	MAN	C1-C2	2.62	1.58	1.52
5	B	910	MAN	C4-C3	2.71	1.59	1.52
2	A	901	HEM	C3D-C2D	2.76	1.45	1.37
3	B	902	FAD	C4X-N5	2.86	1.37	1.33
3	A	902	FAD	C4X-N5	3.00	1.38	1.33
2	B	901	HEM	C3D-C2D	3.01	1.46	1.37
3	B	902	FAD	C4-N3	3.16	1.38	1.33
5	B	910	MAN	C4-C5	3.20	1.60	1.53
3	A	902	FAD	C4-N3	3.24	1.38	1.33
3	B	902	FAD	C2A-N3A	3.30	1.38	1.32
2	B	901	HEM	C2A-C3A	3.34	1.47	1.37
2	A	901	HEM	C2A-C3A	3.57	1.48	1.37
5	B	909	MAN	O2-C2	3.63	1.51	1.43
3	A	902	FAD	C2A-N3A	3.88	1.39	1.32
5	A	911	MAN	C2-C3	3.98	1.57	1.52
5	B	909	MAN	C1-C2	4.33	1.62	1.52
2	A	901	HEM	C3B-C2B	4.48	1.46	1.40
2	B	901	HEM	C3B-C2B	4.79	1.46	1.40
2	A	901	HEM	C3C-C2C	5.14	1.46	1.40
5	B	910	MAN	C2-C3	5.54	1.60	1.52
2	B	901	HEM	C3C-C2C	6.59	1.48	1.40
2	B	901	HEM	C4C-NC	7.91	1.47	1.36
2	A	901	HEM	C1C-NC	8.08	1.47	1.36
2	B	901	HEM	C1C-NC	8.82	1.48	1.36
2	A	901	HEM	C4C-NC	9.71	1.49	1.36

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	FAD	N3A-C2A-N1A	-9.88	121.11	128.87
3	A	902	FAD	N3A-C2A-N1A	-9.20	121.64	128.87
3	A	902	FAD	N3-C2-N1	-4.88	119.48	127.69
3	B	902	FAD	N3-C2-N1	-4.83	119.56	127.69
2	A	901	HEM	C3B-CAB-CBB	-4.15	118.06	126.40
3	B	902	FAD	C4X-C4-N3	-3.28	119.23	123.52
2	A	901	HEM	CBD-CAD-C3D	-3.17	106.91	112.47
3	A	902	FAD	C4X-C4-N3	-3.09	119.49	123.52
2	B	901	HEM	CBA-CAA-C2A	-2.95	107.30	112.49
2	A	901	HEM	CMA-C3A-C4A	-2.89	123.40	128.31
2	A	901	HEM	C3C-CAC-CBC	-2.77	120.82	126.40
2	B	901	HEM	C3B-CAB-CBB	-2.56	121.25	126.40
3	B	902	FAD	C1'-N10-C9A	-2.45	115.99	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	FAD	C2B-C1B-N9A	-2.45	106.91	113.47
5	A	910	MAN	O2-C2-C3	-2.39	105.36	110.19
2	B	901	HEM	C3C-CAC-CBC	-2.29	121.79	126.40
2	B	901	HEM	CBD-CAD-C3D	-2.06	108.85	112.47
3	B	902	FAD	O4B-C1B-N9A	2.09	112.06	108.11
5	B	909	MAN	C1-C2-C3	2.10	112.09	109.55
3	B	902	FAD	C4X-N5-C5X	2.12	119.22	116.72
2	A	901	HEM	CMD-C2D-C3D	2.12	129.68	125.24
2	A	901	HEM	C3C-C4C-NC	2.15	115.00	110.94
4	A	908	NAG	C1-O5-C5	2.17	115.33	112.14
2	B	901	HEM	CMD-C2D-C3D	2.23	129.89	125.24
3	A	902	FAD	C4X-N5-C5X	2.29	119.42	116.72
4	B	906	NAG	C1-O5-C5	2.39	115.66	112.14
2	A	901	HEM	CBA-CAA-C2A	2.54	116.97	112.49
4	A	907	NAG	C1-O5-C5	2.67	116.07	112.14
5	A	910	MAN	C1-C2-C3	2.73	112.86	109.55
2	B	901	HEM	CMC-C2C-C3C	2.84	130.64	125.09
2	A	901	HEM	CMA-C3A-C2A	2.94	131.38	125.24
2	B	901	HEM	CMB-C2B-C3B	3.01	130.98	125.09
3	A	902	FAD	O4B-C1B-N9A	3.07	113.91	108.11
3	A	902	FAD	C5X-C9A-N10	3.10	119.90	117.58
3	B	902	FAD	C5X-C9A-N10	3.11	119.91	117.58
5	A	910	MAN	O5-C1-C2	3.37	116.29	110.89
2	A	901	HEM	CMB-C2B-C3B	3.52	131.98	125.09
5	B	910	MAN	O3-C3-C2	3.58	116.56	110.01
2	A	901	HEM	C3B-C4B-NB	4.72	115.32	109.21
4	A	906	NAG	C1-O5-C5	4.85	119.27	112.14
2	B	901	HEM	C3B-C4B-NB	5.23	115.97	109.21
3	B	902	FAD	C4-N3-C2	6.22	120.35	115.16
3	A	902	FAD	C4-N3-C2	6.29	120.41	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	6	0
3	A	902	FAD	5	0
4	A	903	NAG	2	0
4	A	904	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	906	NAG	1	0
4	A	908	NAG	1	0
2	B	901	HEM	9	0
3	B	902	FAD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	805/806 (99%)	0.27	47 (5%) 26 20	22, 69, 122, 179	0
1	B	792/806 (98%)	0.61	105 (13%) 4 2	25, 75, 149, 196	0
All	All	1597/1612 (99%)	0.44	152 (9%) 10 6	22, 71, 138, 196	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	8.0
1	B	136	ASP	6.6
1	B	132	CYS	6.2
1	B	171	ILE	6.1
1	B	140	VAL	5.9
1	B	92	ASN	5.5
1	B	138	ASP	5.2
1	B	168	PRO	5.2
1	B	42	THR	5.1
1	A	90	TYR	5.1
1	B	34	MET	5.1
1	A	88	GLU	5.0
1	B	85	SER	4.9
1	A	167	CYS	4.6
1	A	86	ASP	4.6
1	A	12	THR	4.5
1	B	95	PHE	4.5
1	B	41	LEU	4.5
1	A	212	SER	4.5
1	B	43	THR	4.4
1	A	166	THR	4.4
1	B	146	THR	4.4
1	B	141	THR	4.2
1	B	137	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	36	LEU	4.1
1	B	164	ASN	4.1
1	A	211	CYS	4.1
1	A	64	GLY	4.1
1	A	168	PRO	4.0
1	B	47	GLU	4.0
1	B	159	PHE	4.0
1	B	167	CYS	4.0
1	B	174	SER	4.0
1	B	133	LEU	4.0
1	B	158	ALA	4.0
1	B	44	ASP	4.0
1	B	65	TRP	3.9
1	A	13	GLY	3.9
1	B	37	PRO	3.9
1	B	160	PRO	3.9
1	B	97	THR	3.9
1	B	81	THR	3.8
1	B	667	ASN	3.7
1	B	111	ILE	3.7
1	B	99	TYR	3.6
1	B	94	MET	3.6
1	B	175	GLN	3.5
1	B	52	LEU	3.5
1	B	145	SER	3.5
1	B	108	ASP	3.5
1	B	105	TYR	3.4
1	B	170	GLN	3.4
1	B	385	SER	3.4
1	B	169	THR	3.4
1	A	120	ALA	3.3
1	B	665	LEU	3.3
1	A	55	SER	3.3
1	A	85	SER	3.3
1	B	68	VAL	3.2
1	B	109	ALA	3.2
1	B	106	ALA	3.2
1	B	76	ASN	3.2
1	B	78	LEU	3.2
1	B	125	LEU	3.2
1	B	48	PHE	3.1
1	A	170	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	380	ASN	3.1
1	B	110	LYS	3.1
1	B	139	GLY	3.0
1	B	185	ALA	3.0
1	B	384	ALA	3.0
1	B	127	PHE	3.0
1	A	61	ALA	2.9
1	A	84	PRO	2.9
1	B	19	TRP	2.9
1	A	215	VAL	2.9
1	B	23	ASP	2.9
1	B	69	SER	2.9
1	B	173	LEU	2.9
1	B	80	ILE	2.9
1	B	144	ILE	2.9
1	B	46	THR	2.8
1	B	166	THR	2.8
1	A	275	GLU	2.8
1	B	666	ALA	2.8
1	A	665	LEU	2.7
1	B	134	SER	2.7
1	B	17	ASN	2.7
1	B	90	TYR	2.7
1	B	135	TRP	2.7
1	B	93	LEU	2.7
1	B	45	ALA	2.6
1	B	130	GLN	2.6
1	A	59	ASN	2.6
1	A	56	SER	2.6
1	B	40	ALA	2.6
1	A	121	THR	2.6
1	B	59	ASN	2.6
1	A	63	SER	2.5
1	A	62	ASN	2.5
1	A	89	VAL	2.5
1	B	275	GLU	2.5
1	B	201	ALA	2.5
1	B	161	SER	2.4
1	A	208	THR	2.4
1	B	165	PRO	2.4
1	A	82	ALA	2.4
1	A	210	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	392	SER	2.4
1	B	172	THR	2.4
1	B	29	GLY	2.4
1	A	387	TRP	2.4
1	B	671	LEU	2.3
1	B	131	ASN	2.3
1	A	213	GLY	2.3
1	B	61	ALA	2.3
1	B	39	ASN	2.3
1	B	71	ARG	2.3
1	A	87	GLY	2.3
1	A	667	ASN	2.3
1	A	57	ALA	2.2
1	B	180	MET	2.2
1	A	216	THR	2.2
1	B	382	LEU	2.2
1	B	177	ASP	2.2
1	B	79	LEU	2.2
1	A	123	PHE	2.2
1	A	83	TRP	2.2
1	A	52	LEU	2.2
1	A	127	PHE	2.2
1	B	83	TRP	2.2
1	B	100	ALA	2.2
1	B	668	VAL	2.2
1	A	201	ALA	2.2
1	A	111	ILE	2.1
1	A	165	PRO	2.1
1	B	112	THR	2.1
1	B	88	GLU	2.1
1	B	143	GLY	2.1
1	B	107	GLY	2.1
1	B	163	GLY	2.1
1	B	199	TRP	2.1
1	B	63	SER	2.1
1	A	67	GLY	2.1
1	A	48	PHE	2.1
1	B	547	PHE	2.1
1	A	113	GLN	2.0
1	A	377	VAL	2.0
1	A	380	ASN	2.0
1	B	202	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	205	LYS	2.0
1	B	192	ALA	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
4	NAG	A	906	14/15	0.76	0.37	5.48	72,105,123,124	0
2	HEM	A	901	43/43	0.96	0.24	0.56	55,78,100,129	0
5	MAN	B	909	11/12	0.88	0.29	0.38	73,81,96,96	0
4	NAG	A	903	14/15	0.90	0.30	0.25	96,105,116,123	0
4	NAG	B	903	14/15	0.84	0.22	0.12	98,111,115,117	0
6	PT	B	918	1/1	0.95	0.19	0.08	132,132,132,132	0
3	FAD	A	902	53/53	0.97	0.19	-0.16	20,52,93,102	0
3	FAD	B	902	53/53	0.97	0.18	-0.19	20,54,90,97	0
4	NAG	B	907	14/15	0.86	0.28	-0.26	86,119,129,129	0
4	NAG	A	908	14/15	0.91	0.25	-0.28	83,106,124,129	0
2	HEM	B	901	43/43	0.96	0.33	-0.32	60,86,110,126	0
5	MAN	A	910	11/12	0.91	0.17	-0.45	91,100,115,119	0
7	MG	A	926	1/1	0.95	0.25	-	56,56,56,56	0
7	MG	A	925	1/1	0.94	0.43	-	54,54,54,54	0
6	PT	A	919	1/1	0.98	0.18	-	107,107,107,107	0
6	PT	A	912	1/1	0.99	0.25	-	84,84,84,84	0
6	PT	B	916	1/1	0.96	0.18	-	106,106,106,106	1
6	PT	A	913	1/1	0.95	0.19	-	120,120,120,120	0
5	MAN	A	911	11/12	0.90	0.30	-	89,101,108,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	904	14/15	0.86	0.24	-	85,104,111,123	0
4	NAG	B	908	14/15	0.90	0.22	-	75,91,103,106	0
7	MG	B	919	1/1	0.92	0.24	-	54,54,54,54	0
6	PT	B	917	1/1	0.98	0.19	-	102,102,102,102	0
6	PT	B	914	1/1	0.94	0.15	-	134,134,134,134	1
6	PT	A	917	1/1	0.97	0.14	-	151,151,151,151	1
6	PT	A	922	1/1	0.97	0.23	-	133,133,133,133	0
6	PT	A	916	1/1	0.96	0.15	-	117,117,117,117	1
6	PT	B	913	1/1	0.93	0.07	-	146,146,146,146	1
6	PT	A	923	1/1	0.99	0.12	-	92,92,92,92	1
6	PT	A	921	1/1	0.87	0.42	-	282,282,282,282	0
4	NAG	A	904	14/15	0.84	0.41	-	90,104,121,121	0
6	PT	A	914	1/1	0.89	0.19	-	156,156,156,156	1
4	NAG	A	905	14/15	0.97	0.15	-	79,96,105,113	0
6	PT	B	912	1/1	0.84	0.21	-	147,147,147,147	1
4	NAG	B	906	14/15	0.94	0.15	-	59,75,109,118	0
5	MAN	B	910	11/12	0.87	0.30	-	61,92,106,106	0
6	PT	A	918	1/1	0.95	0.16	-	123,123,123,123	1
4	NAG	B	905	14/15	0.95	0.22	-	81,99,103,107	0
6	PT	B	915	1/1	0.78	0.15	-	164,164,164,164	1
4	NAG	A	907	14/15	0.95	0.12	-	63,76,109,116	0
6	PT	A	920	1/1	0.92	0.15	-	114,114,114,114	1
4	NAG	A	909	14/15	0.95	0.27	-	66,83,98,100	0
7	MG	A	924	1/1	0.83	0.62	-	73,73,73,73	0
6	PT	B	911	1/1	1.00	0.22	-	71,71,71,71	0
6	PT	A	915	1/1	0.90	0.07	-	155,155,155,155	1

6.5 Other polymers [i](#)

There are no such residues in this entry.