



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2017 – 11:45 AM EST

PDB ID : 5WYX
Title : Crystal structure of human TLR8 in complex with CU-CPT8m
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2017-01-16
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

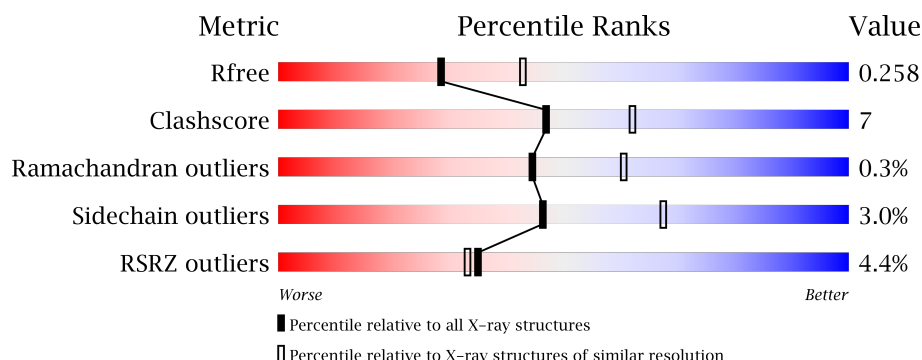
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	811	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>8%</div> </div> </div>
1	B	811	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</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
2	NAG	A	915	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12621 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			6038	3861	1026	1132	19			
1	B	739	Total	C	N	O	S	0	0	0
			5957	3810	1012	1116	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



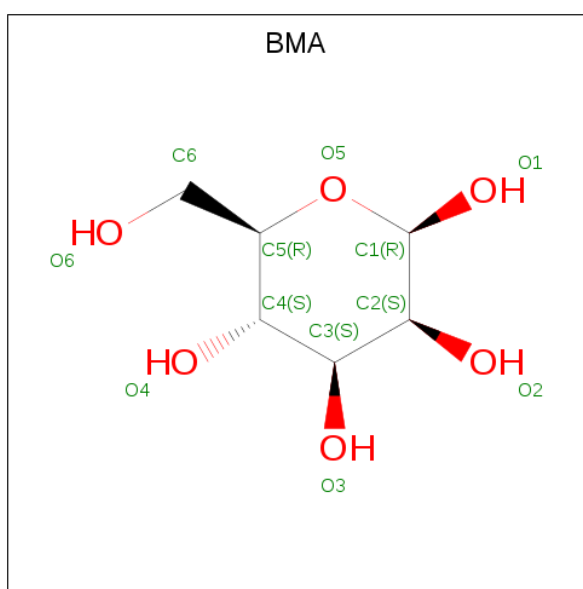
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1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

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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	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		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



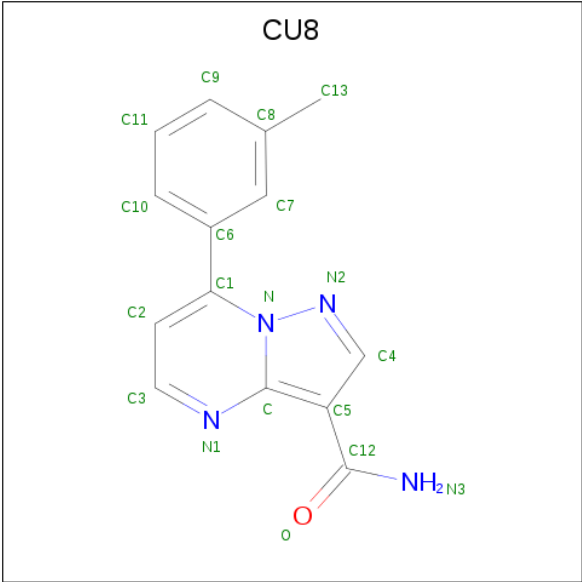
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is 7-(3-methylphenyl)pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: CU8) (formula: C₁₄H₁₂N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	4	1		
5	B	1	Total	C	N	O	0	0
			19	14	4	1		

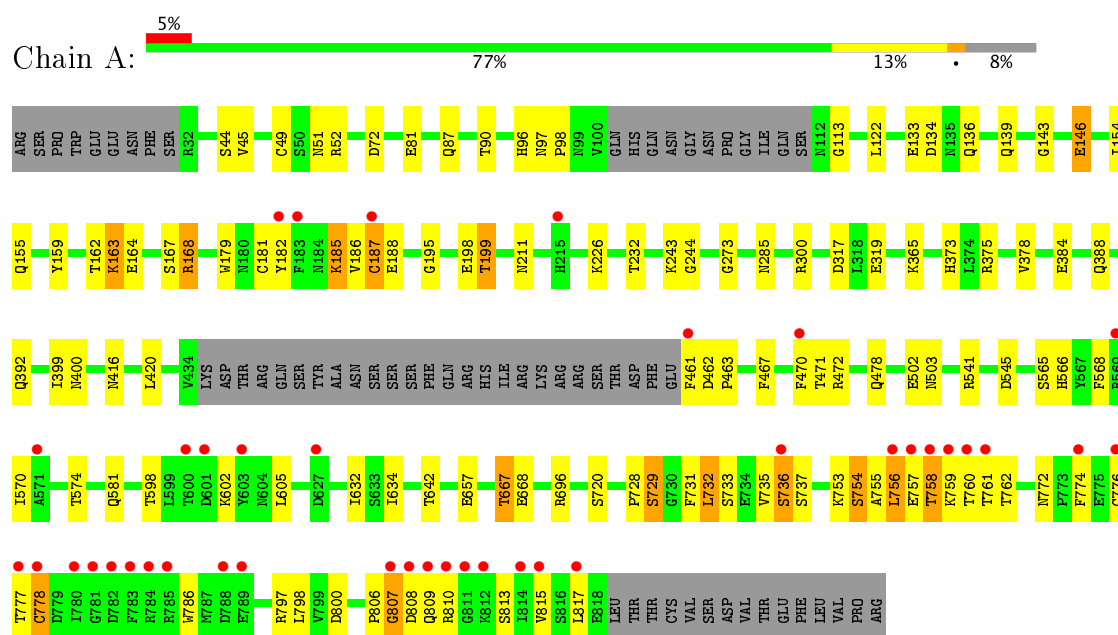
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	104	Total	O	0	0
			104	104		

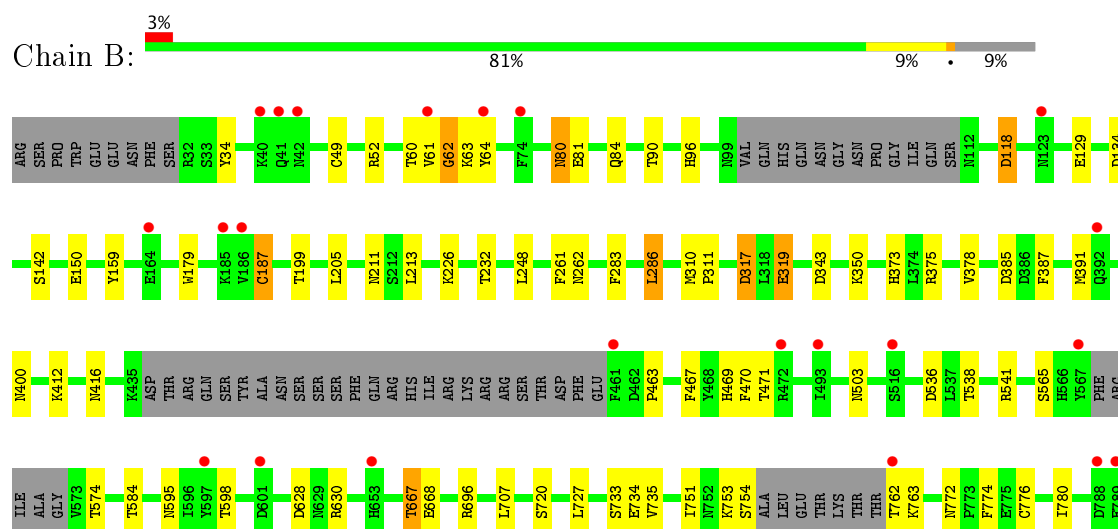
3 Residue-property plots [i](#)

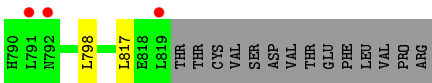
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.14Å 99.15Å 140.25Å 90.00° 108.07° 90.00°	Depositor
Resolution (Å)	40.16 – 2.40 40.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.16-2.40) 99.6 (40.16-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.256 0.206 , 0.258	Depositor DCC
R_{free} test set	3569 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12621	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CU8, BMA, NAG, 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	0.68	0/6162	0.81	2/8358 (0.0%)
1	B	0.68	0/6078	0.78	2/8240 (0.0%)
All	All	0.68	0/12240	0.80	4/16598 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	62	GLY	N-CA-C	-6.09	97.88	113.10
1	B	317	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	778	CYS	CA-CB-SG	5.34	123.61	114.00
1	A	163	LYS	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	LYS	Peptide
1	A	187	CYS	Peptide
1	A	807	GLY	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	6038	0	6032	116	0
1	B	5957	0	5950	59	0
2	A	140	0	125	2	0
2	B	112	0	99	4	0
3	A	22	0	17	0	0
3	B	22	0	18	0	0
4	A	33	0	30	0	0
4	B	22	0	20	0	0
5	A	19	0	0	0	0
5	B	19	0	0	0	0
6	A	133	0	0	8	0
6	B	104	0	0	3	0
All	All	12621	0	12291	174	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 7.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:O	1:A:300:ARG:NH2	1.74	1.18
1:A:753:LYS:HA	1:A:756:LEU:HB3	1.45	0.99
1:A:167:SER:HB2	1:A:199:THR:HG21	1.44	0.98
1:A:777:THR:HB	1:A:778:CYS:HA	1.46	0.98
1:B:34:TYR:O	1:B:60:THR:HG21	1.67	0.95
1:B:469:HIS:CD2	1:B:470:PHE:CD2	2.56	0.94
1:A:735:VAL:HA	1:A:736:SER:CB	2.01	0.91
1:A:732:LEU:HD22	1:A:755:ALA:O	1.73	0.87
1:A:735:VAL:HA	1:A:736:SER:HB3	1.57	0.86
1:A:319:GLU:HG2	6:A:1055:HOH:O	1.74	0.85
1:A:167:SER:O	1:A:168:ARG:HB2	1.77	0.84
1:A:167:SER:CB	1:A:199:THR:HG21	2.07	0.83
1:B:62:GLY:HA3	1:B:63:LYS:HG3	1.60	0.82
1:B:469:HIS:CD2	1:B:470:PHE:HD2	1.99	0.81
1:A:732:LEU:CD2	1:A:755:ALA:O	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:CYS:HB3	1:B:817:LEU:HD21	1.68	0.76
1:A:754:SER:N	1:A:756:LEU:O	2.19	0.75
1:A:187:CYS:SG	1:A:188:GLU:O	2.44	0.75
1:A:186:VAL:HA	1:A:187:CYS:C	2.06	0.74
1:A:732:LEU:O	1:A:762:THR:HG21	1.88	0.73
1:B:469:HIS:NE2	1:B:470:PHE:CD2	2.57	0.72
1:B:319:GLU:OE1	1:B:469:HIS:HB2	1.88	0.72
1:A:807:GLY:HA2	1:A:810:ARG:H	1.54	0.72
1:A:777:THR:CB	1:A:778:CYS:HA	2.19	0.69
1:A:753:LYS:CA	1:A:756:LEU:HB3	2.20	0.68
1:B:226:LYS:NZ	2:B:904:NAG:H81	2.07	0.68
1:A:187:CYS:CB	1:A:188:GLU:O	2.42	0.68
1:A:733:SER:OG	1:A:757:GLU:HG2	1.94	0.67
1:A:545:ASP:OD2	6:A:1001:HOH:O	2.11	0.67
1:A:187:CYS:HB2	1:A:188:GLU:O	1.94	0.67
1:A:122:LEU:HD13	1:A:143:GLY:O	1.95	0.67
1:B:62:GLY:CA	1:B:63:LYS:HG3	2.24	0.67
1:B:63:LYS:O	1:B:64:TYR:HB2	1.95	0.66
1:A:807:GLY:HA3	1:A:810:ARG:HB3	1.75	0.65
1:A:154:ILE:HD13	1:A:463:PRO:HG2	1.79	0.65
1:A:809:GLN:NE2	1:A:817:LEU:HD11	2.11	0.65
1:A:777:THR:HB	1:A:778:CYS:CA	2.27	0.64
1:A:807:GLY:HA2	1:A:809:GLN:N	2.13	0.63
1:A:467:PHE:HB3	2:A:902:NAG:H81	1.81	0.63
1:B:735:VAL:HG23	6:B:1014:HOH:O	1.99	0.63
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.63	0.62
1:A:632:ILE:HD12	1:A:657:GLU:HG2	1.82	0.61
1:A:735:VAL:HG13	1:A:736:SER:OG	2.01	0.60
1:A:195:GLY:O	1:A:198:GLU:HG2	2.02	0.60
1:A:732:LEU:O	1:A:762:THR:CG2	2.48	0.60
1:A:760:THR:H	1:A:761:THR:HA	1.65	0.60
1:B:584:THR:HG22	6:B:1092:HOH:O	2.02	0.59
1:A:179:TRP:CD1	1:A:463:PRO:HB3	2.38	0.58
1:A:807:GLY:CA	1:A:810:ARG:H	2.15	0.58
1:A:754:SER:H	1:A:756:LEU:C	2.06	0.57
1:A:541:ARG:HA	1:A:565:SER:O	2.03	0.57
1:A:159:TYR:CD1	1:A:187:CYS:HB3	2.40	0.57
1:A:163:LYS:O	1:A:164:GLU:CB	2.52	0.56
1:B:469:HIS:NE2	1:B:470:PHE:CE2	2.73	0.56
1:A:211:ASN:O	1:A:232:THR:HA	2.05	0.56
1:B:80:ASN:N	1:B:80:ASN:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:CYS:O	1:A:806:PRO:CD	2.55	0.55
1:A:243:LYS:HD2	1:A:285:ASN:HD22	1.72	0.55
1:A:728:PRO:O	1:A:731:PHE:HB3	2.06	0.55
1:A:776:CYS:O	1:A:806:PRO:HD3	2.06	0.55
1:B:226:LYS:HZ2	2:B:904:NAG:H81	1.70	0.55
1:A:243:LYS:HD2	1:A:285:ASN:ND2	2.23	0.54
1:B:211:ASN:O	1:B:232:THR:HA	2.07	0.54
1:B:129:GLU:HG2	1:B:150:GLU:HB3	1.89	0.54
1:A:375:ARG:HD2	1:A:400:ASN:HD21	1.73	0.54
1:A:758:THR:OG1	1:A:759:LYS:HA	2.07	0.54
1:B:317:ASP:HB2	1:B:343:ASP:HB3	1.91	0.53
1:A:756:LEU:HG	1:A:786:TRP:CD1	2.44	0.53
1:B:261:PHE:CE2	1:B:350:LYS:HD3	2.43	0.53
1:B:541:ARG:HA	1:B:565:SER:O	2.08	0.53
1:A:732:LEU:HD23	1:A:732:LEU:C	2.29	0.53
1:A:735:VAL:HA	1:A:736:SER:OG	2.07	0.53
1:A:392:GLN:HB2	6:A:1002:HOH:O	2.08	0.52
1:B:470:PHE:O	1:B:471:THR:HB	2.09	0.52
1:A:226:LYS:NZ	2:A:903:NAG:H81	2.24	0.52
1:B:469:HIS:NE2	1:B:470:PHE:HD2	1.99	0.52
1:B:734:GLU:HA	1:B:735:VAL:C	2.28	0.52
1:A:728:PRO:HB2	1:A:731:PHE:HB2	1.92	0.52
1:B:96:HIS:HD2	1:B:134:ASP:OD2	1.93	0.52
1:A:642:THR:CG2	6:A:1117:HOH:O	2.60	0.50
1:A:181:CYS:SG	1:A:187:CYS:N	2.84	0.50
1:A:605:LEU:HD13	1:A:634:ILE:HG12	1.92	0.50
1:A:777:THR:CB	1:A:778:CYS:CA	2.86	0.50
1:A:566:HIS:HE1	1:B:262:ASN:O	1.95	0.50
1:B:34:TYR:O	1:B:60:THR:CG2	2.49	0.50
1:A:566:HIS:HD2	1:A:568:PHE:H	1.59	0.49
1:A:470:PHE:CZ	1:A:472:ARG:HG2	2.48	0.49
1:A:185:LYS:N	1:A:186:VAL:O	2.45	0.49
1:B:776:CYS:HB3	1:B:817:LEU:CD2	2.41	0.49
1:A:113:GLY:HA3	1:A:136:GLN:HB2	1.95	0.49
1:A:162:THR:C	1:A:163:LYS:O	2.47	0.49
1:A:44:SER:HB3	6:A:1122:HOH:O	2.12	0.49
1:A:797:ARG:NH1	1:A:800:ASP:OD2	2.46	0.49
1:A:96:HIS:HD2	1:A:134:ASP:OD2	1.96	0.49
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.95	0.48
1:B:61:VAL:HG12	1:B:62:GLY:N	2.28	0.48
1:A:416:ASN:ND2	6:A:1008:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:LYS:O	1:A:754:SER:OG	2.29	0.48
1:B:261:PHE:CE2	1:B:350:LYS:CD	2.96	0.48
1:A:155:GLN:HE21	1:A:463:PRO:HG3	1.78	0.48
1:A:502:GLU:O	1:A:503:ASN:HB2	2.13	0.47
1:A:185:LYS:CG	1:A:186:VAL:H	2.28	0.47
1:A:729:SER:HA	1:A:754:SER:C	2.34	0.47
1:A:813:SER:OG	1:A:815:VAL:HG22	2.14	0.47
1:B:226:LYS:HZ3	2:B:904:NAG:H81	1.79	0.47
1:B:179:TRP:CD1	1:B:463:PRO:HB3	2.49	0.47
1:A:731:PHE:O	1:A:732:LEU:HD22	2.14	0.47
1:A:146:GLU:CD	1:A:146:GLU:H	2.17	0.47
1:A:754:SER:H	1:A:756:LEU:CA	2.28	0.47
1:B:387:PHE:O	1:B:391:MET:HG3	2.15	0.47
1:B:707:LEU:HD23	1:B:735:VAL:HG11	1.96	0.46
1:B:283:PHE:HA	1:B:286:LEU:HD22	1.96	0.46
1:B:772:ASN:HB2	1:B:774:PHE:CE2	2.50	0.46
1:A:733:SER:HB2	1:A:757:GLU:HB3	1.97	0.46
1:A:807:GLY:HA2	1:A:808:ASP:C	2.36	0.46
1:B:467:PHE:HB3	2:B:903:NAG:H81	1.98	0.46
1:A:461:PHE:CG	1:A:462:ASP:N	2.83	0.45
1:A:817:LEU:HA	6:A:1077:HOH:O	2.16	0.45
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.45
1:A:243:LYS:CB	1:A:244:GLY:HA2	2.46	0.45
1:A:735:VAL:HG12	1:A:737:SER:N	2.31	0.45
1:B:667:THR:HG22	1:B:668:GLU:HG3	1.97	0.45
1:A:182:TYR:HD1	1:A:182:TYR:H	1.63	0.45
1:A:696:ARG:HG2	1:A:720:SER:OG	2.16	0.45
1:A:753:LYS:CB	1:A:756:LEU:HD13	2.46	0.45
1:B:470:PHE:O	1:B:471:THR:CB	2.64	0.45
1:B:412:LYS:HB3	1:B:503:ASN:HB3	1.99	0.44
1:B:310:MET:N	1:B:311:PRO:HD3	2.32	0.44
1:A:807:GLY:HA2	1:A:810:ARG:N	2.28	0.44
1:B:205:LEU:HD23	1:B:205:LEU:C	2.37	0.44
1:B:159:TYR:CG	1:B:187:CYS:HB2	2.53	0.44
1:B:696:ARG:HG2	1:B:720:SER:OG	2.18	0.44
1:A:735:VAL:CA	1:A:736:SER:CB	2.84	0.44
1:A:574:THR:HG22	1:A:598:THR:HG23	2.00	0.44
1:A:181:CYS:HB2	1:A:187:CYS:HB3	1.93	0.44
1:A:733:SER:CB	1:A:757:GLU:HB3	2.48	0.43
1:B:584:THR:CG2	6:B:1092:HOH:O	2.63	0.43
1:B:118:ASP:N	1:B:118:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:N	1:A:756:LEU:N	2.66	0.43
1:A:756:LEU:HD23	1:A:756:LEU:C	2.39	0.43
1:A:185:LYS:O	1:A:187:CYS:O	2.35	0.43
1:A:667:THR:HG22	1:A:668:GLU:HG3	2.01	0.43
1:B:733:SER:O	1:B:734:GLU:C	2.57	0.43
1:A:97:ASN:HA	1:A:98:PRO:HA	1.81	0.43
1:B:471:THR:HG22	1:B:471:THR:O	2.19	0.43
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.81	0.43
1:A:133:GLU:CG	1:A:154:ILE:HG13	2.49	0.43
1:B:536:ASP:OD1	1:B:538:THR:HG23	2.18	0.43
1:A:568:PHE:C	1:A:570:ILE:H	2.21	0.42
1:A:733:SER:OG	1:A:757:GLU:CG	2.64	0.42
1:A:735:VAL:HG12	1:A:737:SER:H	1.84	0.42
1:A:754:SER:HA	1:A:755:ALA:C	2.40	0.42
1:B:310:MET:N	1:B:311:PRO:CD	2.83	0.42
1:A:51:ASN:HA	1:A:72:ASP:O	2.19	0.42
1:A:133:GLU:HG2	1:A:154:ILE:HG13	2.00	0.42
1:B:574:THR:HG22	1:B:598:THR:HG23	2.01	0.41
1:A:757:GLU:HG3	1:A:758:THR:N	2.34	0.41
1:B:628:ASP:HB2	1:B:630:ARG:HD3	2.02	0.41
1:B:707:LEU:HD23	1:B:735:VAL:CG1	2.50	0.41
1:A:155:GLN:HE21	1:A:463:PRO:CG	2.34	0.41
1:A:735:VAL:CA	1:A:736:SER:HB3	2.39	0.41
1:B:753:LYS:O	1:B:754:SER:C	2.59	0.41
1:B:727:LEU:HD23	1:B:751:ILE:HG23	2.03	0.41
1:A:776:CYS:C	1:A:777:THR:HG23	2.41	0.41
1:A:365:LYS:NZ	6:A:1015:HOH:O	2.53	0.41
1:A:776:CYS:HB3	1:A:777:THR:CG2	2.50	0.41
1:A:772:ASN:HB2	1:A:774:PHE:CE2	2.56	0.41
1:A:399:ILE:HG13	1:A:420:LEU:HD21	2.02	0.40
1:B:375:ARG:HD2	1:B:400:ASN:ND2	2.32	0.40
1:A:375:ARG:HD2	1:A:400:ASN:ND2	2.35	0.40
1:B:763:LYS:HA	1:B:763:LYS:HD3	1.90	0.40
1:A:753:LYS:HB3	1:A:756:LEU:HD13	2.03	0.40
1:A:798:LEU:HD23	1:A:798:LEU:HA	1.96	0.40
1:B:319:GLU:HG3	1:B:319:GLU:H	1.64	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	744/811 (92%)	692 (93%)	48 (6%)	4 (0%)	32	46
1	B	729/811 (90%)	686 (94%)	42 (6%)	1 (0%)	55	72
All	All	1473/1622 (91%)	1378 (94%)	90 (6%)	5 (0%)	44	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ARG
1	A	736	SER
1	A	378	VAL
1	B	378	VAL
1	A	754	SER

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	697/755 (92%)	676 (97%)	21 (3%)	46	67
1	B	689/755 (91%)	668 (97%)	21 (3%)	46	67
All	All	1386/1510 (92%)	1344 (97%)	42 (3%)	46	67

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	49	CYS
1	A	52	ARG
1	A	81	GLU
1	A	87	GLN
1	A	90	THR
1	A	139	GLN
1	A	146	GLU
1	A	199	THR
1	A	317	ASP
1	A	384	GLU
1	A	388	GLN
1	A	471	THR
1	A	478	GLN
1	A	581	GLN
1	A	602	LYS
1	A	667	THR
1	A	729	SER
1	A	732	LEU
1	A	756	LEU
1	A	758	THR
1	B	49	CYS
1	B	52	ARG
1	B	80	ASN
1	B	81	GLU
1	B	84	GLN
1	B	90	THR
1	B	118	ASP
1	B	142	SER
1	B	187	CYS
1	B	199	THR
1	B	213	LEU
1	B	248	LEU
1	B	286	LEU
1	B	319	GLU
1	B	385	ASP
1	B	416	ASN
1	B	595	ASN
1	B	667	THR
1	B	762	THR
1	B	780	ILE
1	B	798	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	96	HIS
1	A	155	GLN
1	A	285	ASN
1	A	469	HIS
1	A	499	ASN
1	A	566	HIS
1	A	581	GLN
1	A	604	ASN
1	B	77	HIS
1	B	87	GLN
1	B	96	HIS
1	B	99	ASN
1	B	160	ASN
1	B	585	ASN
1	B	686	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

29 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	NAG	A	901	1	14,14,15	0.48	0	15,19,21	2.57	5 (33%)
2	NAG	A	902	1,2	14,14,15	0.93	1 (7%)	15,19,21	1.95	3 (20%)
2	NAG	A	903	3,2	14,14,15	0.59	0	15,19,21	1.56	3 (20%)
3	BMA	A	904	2,4	11,11,12	0.90	0	13,15,17	1.58	4 (30%)
4	MAN	A	905	3	11,11,12	0.80	0	13,15,17	1.59	3 (23%)
2	NAG	A	906	1	14,14,15	0.76	0	15,19,21	1.91	5 (33%)
2	NAG	A	907	1,2	14,14,15	1.10	1 (7%)	15,19,21	1.75	3 (20%)
2	NAG	A	908	2	14,14,15	1.09	1 (7%)	15,19,21	1.50	5 (33%)
2	NAG	A	909	1,2	14,14,15	0.59	0	15,19,21	1.61	3 (20%)
2	NAG	A	910	3,2	14,14,15	1.03	1 (7%)	15,19,21	1.58	3 (20%)
3	BMA	A	911	2,4	11,11,12	0.66	0	13,15,17	1.74	4 (30%)
4	MAN	A	912	3	11,11,12	0.67	0	13,15,17	1.52	4 (30%)
4	MAN	A	913	3	11,11,12	0.63	0	13,15,17	1.27	2 (15%)
2	NAG	A	914	1	14,14,15	0.84	0	15,19,21	1.59	2 (13%)
2	NAG	A	915	1	14,14,15	0.65	0	15,19,21	1.69	3 (20%)
5	CU8	A	916	-	17,21,21	1.64	3 (17%)	19,30,30	2.05	4 (21%)
5	CU8	B	901	-	17,21,21	1.60	3 (17%)	19,30,30	1.99	5 (26%)
2	NAG	B	902	1	14,14,15	0.64	0	15,19,21	1.66	5 (33%)
2	NAG	B	903	1,2	14,14,15	0.73	0	15,19,21	1.64	3 (20%)
2	NAG	B	904	3,2	14,14,15	1.05	1 (7%)	15,19,21	2.14	7 (46%)
3	BMA	B	905	2,4	11,11,12	0.93	0	13,15,17	1.29	1 (7%)
4	MAN	B	906	3	11,11,12	1.17	1 (9%)	13,15,17	2.42	4 (30%)
2	NAG	B	907	1,2	14,14,15	1.15	1 (7%)	15,19,21	1.75	4 (26%)
2	NAG	B	908	2	14,14,15	0.70	0	15,19,21	1.15	1 (6%)
2	NAG	B	909	1,2	14,14,15	0.82	0	15,19,21	1.45	3 (20%)
2	NAG	B	910	3,2	14,14,15	0.90	1 (7%)	15,19,21	1.64	5 (33%)
3	BMA	B	911	2,4	11,11,12	0.88	0	13,15,17	1.88	4 (30%)
4	MAN	B	912	3	11,11,12	0.68	0	13,15,17	0.88	1 (7%)
2	NAG	B	913	1	14,14,15	0.91	1 (7%)	15,19,21	1.12	2 (13%)

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	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	903	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	904	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	905	3	-	0/2/19/22	0/1/1/1
2	NAG	A	906	1	-	0/6/23/26	0/1/1/1
2	NAG	A	907	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	908	2	-	0/6/23/26	0/1/1/1
2	NAG	A	909	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	910	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	911	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	912	3	-	0/2/19/22	0/1/1/1
4	MAN	A	913	3	-	0/2/19/22	0/1/1/1
2	NAG	A	914	1	-	0/6/23/26	0/1/1/1
2	NAG	A	915	1	-	0/6/23/26	0/1/1/1
5	CU8	A	916	-	-	0/4/8/8	0/3/3/3
5	CU8	B	901	-	-	0/4/8/8	0/3/3/3
2	NAG	B	902	1	-	0/6/23/26	0/1/1/1
2	NAG	B	903	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	904	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	905	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	906	3	-	0/2/19/22	0/1/1/1
2	NAG	B	907	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	908	2	-	0/6/23/26	0/1/1/1
2	NAG	B	909	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	910	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	911	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	912	3	-	0/2/19/22	0/1/1/1
2	NAG	B	913	1	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	CU8	C1-N	-4.18	1.32	1.41
5	A	916	CU8	C1-N	-4.12	1.32	1.41
5	A	916	CU8	O-C12	-3.20	1.17	1.24
5	B	901	CU8	O-C12	-2.89	1.18	1.24
2	B	904	NAG	O5-C1	-2.61	1.39	1.43
2	A	910	NAG	O5-C1	-2.49	1.39	1.43
2	A	902	NAG	C1-C2	-2.31	1.49	1.52
5	A	916	CU8	C5-C12	-2.27	1.46	1.50
2	B	910	NAG	O5-C1	-2.16	1.40	1.43
5	B	901	CU8	C12-N3	-2.07	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	907	NAG	O5-C1	-2.06	1.40	1.43
2	B	907	NAG	C2-N2	-2.03	1.42	1.46
2	A	908	NAG	O5-C1	-2.02	1.40	1.43
2	B	913	NAG	C1-C2	2.76	1.56	1.52
4	B	906	MAN	C2-C3	3.63	1.57	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	NAG	O5-C1-C2	-5.21	104.22	111.47
5	B	901	CU8	C2-C3-N1	-5.06	116.73	124.58
5	A	916	CU8	C2-C3-N1	-4.93	116.93	124.58
2	B	904	NAG	O5-C1-C2	-4.91	104.64	111.47
2	B	903	NAG	O5-C1-C2	-4.07	105.81	111.47
2	A	909	NAG	O5-C1-C2	-3.51	106.58	111.47
2	A	910	NAG	C4-C3-C2	-3.50	105.89	111.02
3	B	911	BMA	C2-C3-C4	-3.41	104.93	110.88
2	A	915	NAG	O5-C1-C2	-3.40	106.74	111.47
2	A	903	NAG	O5-C1-C2	-3.37	106.78	111.47
2	A	906	NAG	C4-C3-C2	-3.37	106.09	111.02
2	A	906	NAG	C2-N2-C7	-3.31	118.12	122.94
3	B	905	BMA	O5-C1-C2	-3.21	105.77	110.79
2	B	904	NAG	O7-C7-C8	-3.16	116.30	122.06
2	B	910	NAG	C4-C3-C2	-3.14	106.42	111.02
2	A	907	NAG	C1-C2-N2	-3.09	105.22	110.49
2	A	902	NAG	O7-C7-C8	-2.93	116.72	122.06
2	B	910	NAG	O6-C6-C5	-2.91	101.55	111.34
2	A	907	NAG	C6-C5-C4	-2.90	106.22	113.00
4	A	912	MAN	O5-C1-C2	-2.90	106.25	110.79
2	A	908	NAG	O5-C1-C2	-2.88	107.46	111.47
2	B	907	NAG	C1-C2-N2	-2.86	105.61	110.49
2	B	904	NAG	C3-C4-C5	-2.82	105.25	110.22
2	B	908	NAG	O5-C1-C2	-2.78	107.61	111.47
2	A	901	NAG	C4-C3-C2	-2.78	106.95	111.02
2	B	902	NAG	C1-C2-N2	-2.78	105.75	110.49
2	A	907	NAG	C1-O5-C5	-2.75	108.38	112.17
5	B	901	CU8	C6-C7-C8	-2.60	119.47	121.30
2	B	907	NAG	C4-C3-C2	-2.58	107.24	111.02
3	A	911	BMA	O5-C1-C2	-2.58	106.75	110.79
5	A	916	CU8	C6-C7-C8	-2.55	119.50	121.30
4	B	906	MAN	O5-C1-C2	-2.54	106.81	110.79
2	B	913	NAG	O5-C1-C2	-2.54	107.94	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	911	BMA	O4-C4-C3	-2.54	104.84	110.36
2	A	910	NAG	C6-C5-C4	-2.52	107.11	113.00
3	A	904	BMA	O4-C4-C3	-2.50	104.92	110.36
3	A	911	BMA	C1-O5-C5	-2.48	108.74	112.17
4	A	913	MAN	O2-C2-C1	-2.48	104.14	109.18
3	B	911	BMA	O4-C4-C5	-2.46	103.08	109.28
5	B	901	CU8	C10-C6-C1	-2.40	117.17	121.05
2	A	915	NAG	C1-C2-N2	-2.38	106.42	110.49
2	A	906	NAG	O5-C1-C2	-2.37	108.18	111.47
2	A	906	NAG	O3-C3-C2	-2.35	104.35	109.39
2	A	903	NAG	C1-O5-C5	-2.33	108.95	112.17
4	A	905	MAN	O3-C3-C4	-2.31	105.32	110.36
2	B	907	NAG	O3-C3-C2	-2.29	104.48	109.39
2	A	909	NAG	O4-C4-C3	-2.29	105.38	110.36
2	B	909	NAG	O5-C1-C2	-2.26	108.33	111.47
2	B	904	NAG	C1-O5-C5	-2.25	109.06	112.17
4	B	912	MAN	O5-C1-C2	-2.24	107.28	110.79
4	A	912	MAN	C1-O5-C5	-2.21	109.12	112.17
2	B	910	NAG	C6-C5-C4	-2.21	107.83	113.00
2	A	903	NAG	O7-C7-C8	-2.20	118.06	122.06
2	A	908	NAG	C3-C4-C5	-2.16	106.42	110.22
2	B	910	NAG	O4-C4-C5	-2.14	103.88	109.28
2	B	913	NAG	O7-C7-C8	-2.13	118.17	122.06
2	A	914	NAG	O6-C6-C5	-2.10	104.27	111.34
2	A	910	NAG	O4-C4-C5	-2.10	104.00	109.28
4	A	912	MAN	O2-C2-C1	-2.09	104.92	109.18
2	B	904	NAG	O4-C4-C3	-2.02	105.96	110.36
2	A	908	NAG	C4-C3-C2	-2.01	108.07	111.02
2	B	902	NAG	C6-C5-C4	-2.00	108.31	113.00
2	A	901	NAG	C2-N2-C7	2.01	125.88	122.94
2	B	904	NAG	C8-C7-N2	2.03	119.78	116.11
2	B	909	NAG	C1-C2-N2	2.04	113.97	110.49
4	A	912	MAN	C2-C3-C4	2.05	114.45	110.88
2	B	903	NAG	O7-C7-N2	2.10	125.96	121.92
4	A	913	MAN	O3-C3-C2	2.10	113.85	110.02
2	A	908	NAG	C1-C2-N2	2.11	114.09	110.49
5	A	916	CU8	C4-N2-N	2.16	107.28	103.94
5	B	901	CU8	C3-N1-C	2.18	119.76	116.80
4	A	905	MAN	C2-C3-C4	2.18	114.68	110.88
2	A	901	NAG	O5-C1-C2	2.20	114.53	111.47
4	B	906	MAN	O2-C2-C3	2.24	114.58	110.17
3	A	904	BMA	O6-C6-C5	2.27	118.97	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	BMA	C1-O5-C5	2.30	115.34	112.17
2	A	902	NAG	C4-C3-C2	2.33	114.43	111.02
2	A	909	NAG	C8-C7-N2	2.40	120.44	116.11
2	A	908	NAG	C1-O5-C5	2.46	115.56	112.17
2	B	910	NAG	C1-O5-C5	2.55	115.67	112.17
2	B	903	NAG	O3-C3-C2	2.57	114.89	109.39
2	B	902	NAG	C3-C4-C5	2.59	114.77	110.22
2	B	904	NAG	C1-C2-N2	2.62	114.97	110.49
4	A	905	MAN	C3-C4-C5	2.70	114.97	110.22
2	B	902	NAG	C4-C3-C2	2.78	115.09	111.02
2	B	902	NAG	O5-C1-C2	2.82	115.40	111.47
3	B	911	BMA	O3-C3-C4	2.90	116.68	110.36
3	A	904	BMA	C3-C4-C5	2.99	115.49	110.22
2	B	909	NAG	C1-O5-C5	3.04	116.35	112.17
3	A	911	BMA	O3-C3-C2	3.21	115.86	110.02
2	A	901	NAG	C8-C7-N2	3.30	122.07	116.11
4	B	906	MAN	C2-C3-C4	3.35	116.72	110.88
2	B	907	NAG	O3-C3-C4	3.36	117.66	110.36
3	B	911	BMA	C1-C2-C3	3.75	114.41	109.65
5	B	901	CU8	C3-C2-C1	3.83	120.74	117.35
2	A	914	NAG	C1-O5-C5	3.94	117.60	112.17
5	A	916	CU8	C3-C2-C1	4.19	121.06	117.35
2	A	915	NAG	C1-O5-C5	4.23	117.99	112.17
2	A	906	NAG	C1-O5-C5	4.35	118.16	112.17
4	B	906	MAN	C1-C2-C3	6.01	117.27	109.65
2	A	901	NAG	C1-O5-C5	7.79	122.90	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	NAG	1	0
2	A	903	NAG	1	0
2	B	903	NAG	1	0
2	B	904	NAG	3	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	750/811 (92%)	0.18	40 (5%)	27 25	29, 57, 103, 151	0
1	B	739/811 (91%)	0.11	25 (3%)	46 44	30, 55, 98, 134	0
All	All	1489/1622 (91%)	0.15	65 (4%)	35 33	29, 56, 99, 151	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	LEU	7.8
1	A	182	TYR	4.9
1	A	183	PHE	4.6
1	B	185	LYS	4.6
1	B	461	PHE	4.6
1	A	780	ILE	4.5
1	A	461	PHE	4.2
1	A	758	THR	4.1
1	A	759	LYS	4.0
1	A	776	CYS	3.8
1	A	760	THR	3.6
1	A	812	LYS	3.4
1	A	777	THR	3.3
1	A	809	GLN	3.3
1	A	783	PHE	3.3
1	A	571	ALA	3.2
1	B	493	ILE	3.1
1	B	819	LEU	3.1
1	A	808	ASP	3.0
1	B	601	ASP	3.0
1	A	782	ASP	3.0
1	B	392	GLN	2.8
1	B	792	ASN	2.8
1	A	778	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	807	GLY	2.7
1	A	789	GLU	2.7
1	A	736	SER	2.7
1	B	567	TYR	2.7
1	A	774	PHE	2.6
1	B	61	VAL	2.6
1	B	791	LEU	2.6
1	B	597	TYR	2.6
1	B	123	ASN	2.6
1	A	817	LEU	2.5
1	B	40	LYS	2.5
1	A	569	ARG	2.5
1	A	788	ASP	2.4
1	A	811	GLY	2.4
1	A	810	ARG	2.4
1	B	64	TYR	2.4
1	B	762	THR	2.4
1	A	785	ARG	2.4
1	B	41	GLN	2.4
1	B	186	VAL	2.4
1	A	215	HIS	2.4
1	A	627	ASP	2.3
1	A	601	ASP	2.3
1	B	789	GLU	2.3
1	A	603	TYR	2.3
1	A	757	GLU	2.2
1	A	600	THR	2.2
1	B	42	ASN	2.2
1	B	164	GLU	2.2
1	A	761	THR	2.2
1	A	815	VAL	2.1
1	B	653	HIS	2.1
1	A	814	ILE	2.1
1	B	74	PHE	2.1
1	B	516	SER	2.1
1	B	788	ASP	2.1
1	A	470	PHE	2.1
1	A	187	CYS	2.1
1	A	784	ARG	2.1
1	A	781	GLY	2.0
1	B	472	ARG	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	A	915	14/15	0.77	0.23	2.97	76,90,106,106	0
2	NAG	A	901	14/15	0.87	0.18	0.48	76,85,90,92	0
2	NAG	B	913	14/15	0.93	0.15	0.39	53,61,71,72	0
2	NAG	B	909	14/15	0.97	0.13	0.06	33,36,37,38	0
5	CU8	B	901	19/19	0.97	0.22	0.02	36,42,49,53	0
5	CU8	A	916	19/19	0.96	0.14	-0.45	33,39,51,53	0
2	NAG	A	902	14/15	0.96	0.13	-0.52	35,40,47,47	0
2	NAG	A	914	14/15	0.97	0.13	-0.60	40,44,57,61	0
2	NAG	A	909	14/15	0.98	0.12	-0.70	27,35,38,38	0
2	NAG	A	903	14/15	0.97	0.12	-0.73	38,46,52,61	0
2	NAG	B	903	14/15	0.98	0.13	-1.00	33,37,46,55	0
2	NAG	B	907	14/15	0.97	0.12	-1.17	34,38,46,51	0
2	NAG	A	906	14/15	0.96	0.10	-1.26	52,62,69,72	0
2	NAG	A	907	14/15	0.98	0.11	-1.27	31,36,41,41	0
2	NAG	B	904	14/15	0.97	0.13	-1.48	33,45,58,64	0
2	NAG	B	910	14/15	0.98	0.12	-1.80	36,41,45,50	0
4	MAN	A	905	11/12	0.86	0.23	-	74,84,88,91	0
3	BMA	A	911	11/12	0.95	0.10	-	49,59,69,73	0
4	MAN	B	912	11/12	0.69	0.22	-	73,96,113,114	0
4	MAN	A	913	11/12	0.91	0.18	-	87,95,108,110	0
3	BMA	B	911	11/12	0.83	0.15	-	53,59,80,103	0
2	NAG	B	902	14/15	0.83	0.24	-	79,87,98,100	0
4	MAN	A	912	11/12	0.83	0.19	-	79,84,89,96	0
4	MAN	B	906	11/12	0.72	0.20	-	79,91,97,98	0
2	NAG	A	908	14/15	0.89	0.16	-	49,62,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	908	14/15	0.88	0.18	-	55,71,82,95	0
3	BMA	B	905	11/12	0.87	0.13	-	63,68,84,85	0
2	NAG	A	910	14/15	0.98	0.12	-	31,37,46,53	0
3	BMA	A	904	11/12	0.84	0.19	-	55,67,79,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.