



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:13 pm GMT

PDB ID : 3W3K
Title : Crystal structure of human TLR8 in complex with CL075
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2012-12-22
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

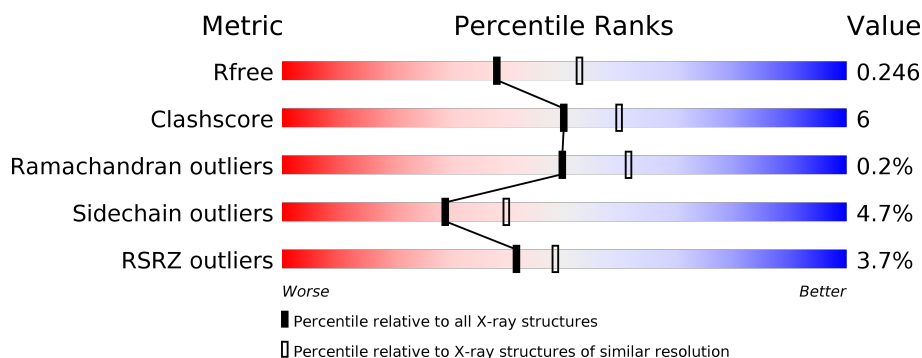
1 Overall quality at a glance

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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (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	811	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>
1	B	811	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12772 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.

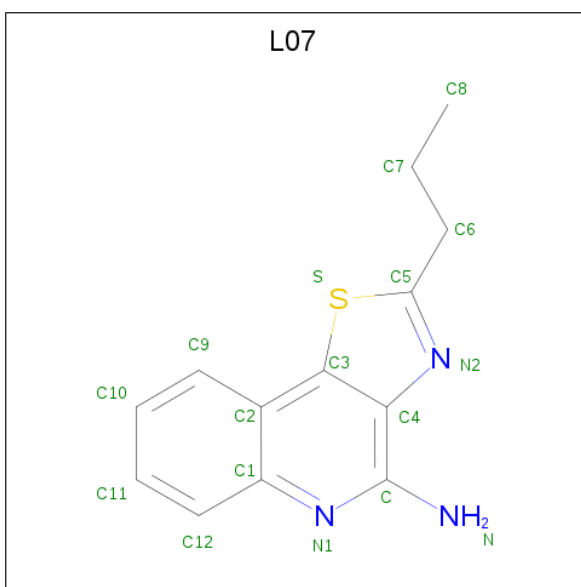
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	0	0
			5986	3834	1017	1116	19			
1	B	747	Total	C	N	O	S	0	0	0
			5997	3841	1018	1119	19			

There are 20 discrepancies between the modelled and reference sequences:

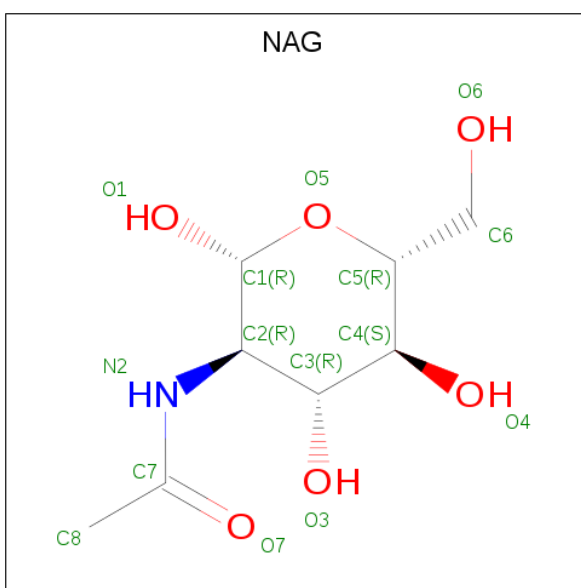
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP 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 2-propyl[1,3]thiazolo[4,5-c]quinolin-4-amine (three-letter code: L07) (formula: C₁₃H₁₃N₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			17	13	3	1		
2	B	1	Total	C	N	S	0	0
			17	13	3	1		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



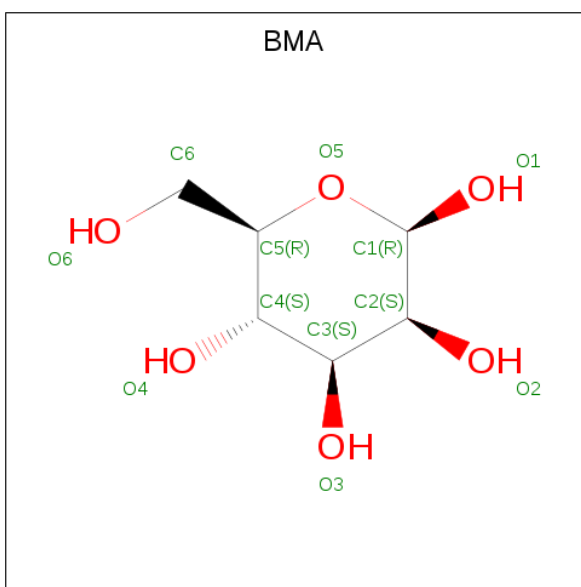
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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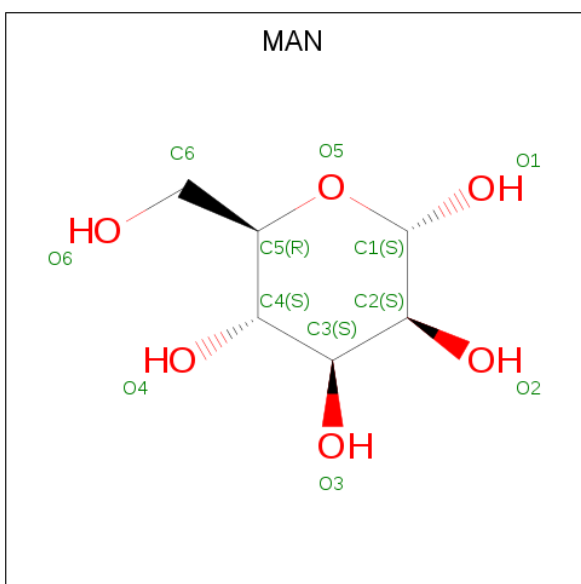
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



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 ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

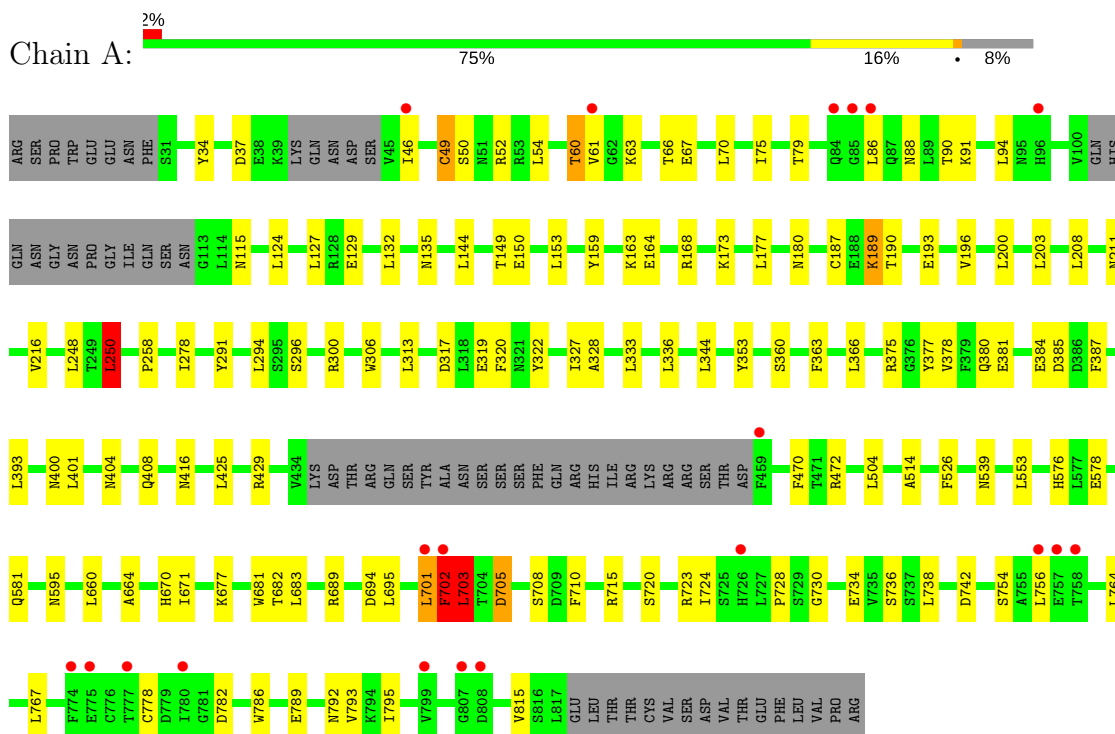
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	174	Total O 174 174	0	0
6	B	186	Total O 186 186	0	0

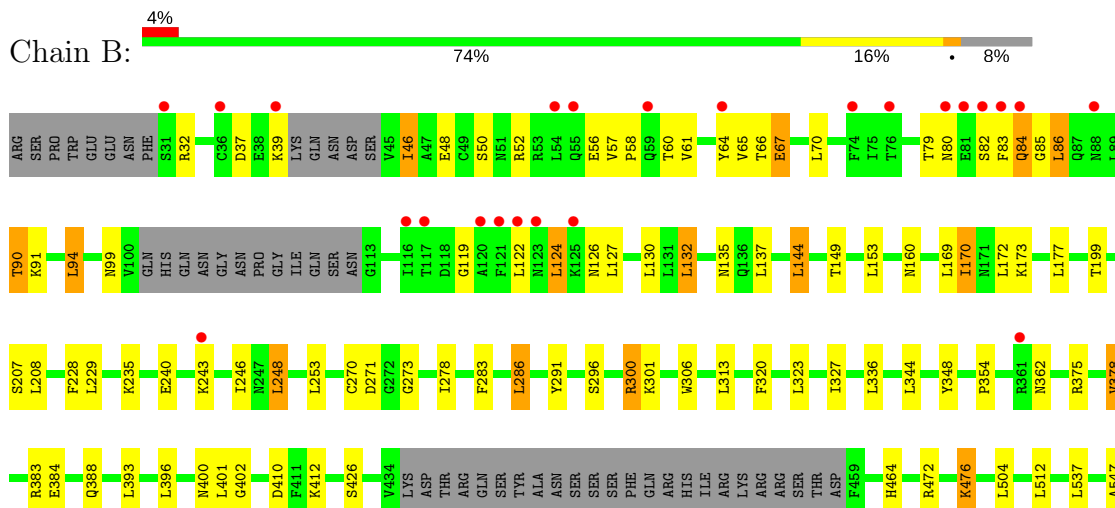
3 Residue-property plots [i](#)

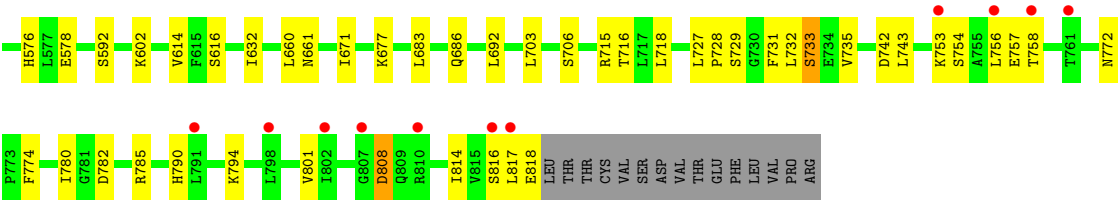
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.41Å 154.02Å 86.86Å 90.00° 103.03° 90.00°	Depositor
Resolution (Å)	37.08 – 2.30 38.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.5 (37.08-2.30) 91.6 (38.51-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.205 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	3784 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12772	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L07, 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	0.34	0/6110	0.62	3/8287 (0.0%)
1	B	0.36	0/6121	0.62	0/8302
All	All	0.35	0/12231	0.62	3/16589 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	250	LEU	CA-CB-CG	6.87	131.11	115.30
1	A	702	PHE	N-CA-C	5.88	126.86	111.00
1	A	703	LEU	CA-CB-CG	5.70	128.41	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	701	LEU	Peptide
1	A	702	PHE	Peptide
1	B	86	LEU	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	5986	0	5952	74	0
1	B	5997	0	5965	81	0
2	A	17	0	13	1	0
2	B	17	0	13	0	0
3	A	126	0	111	1	0
3	B	126	0	112	4	0
4	A	33	0	26	0	0
4	B	22	0	16	0	0
5	A	44	0	40	0	0
5	B	44	0	40	1	0
6	A	174	0	0	5	0
6	B	186	0	0	5	0
All	All	12772	0	12288	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LYS:HD2	1:B:756:LEU:HD11	1.64	0.80
1:A:34:TYR:O	1:A:60:THR:OG1	2.02	0.77
1:A:67:GLU:HG2	1:A:91:LYS:HB3	1.72	0.72
1:B:817:LEU:O	6:B:1151:HOH:O	2.05	0.72
1:B:37:ASP:OD2	1:B:52:ARG:NH1	2.23	0.72
1:A:384:GLU:OE2	1:A:416:ASN:ND2	2.23	0.70
1:A:250:LEU:HB2	1:A:291:TYR:HB2	1.73	0.70
1:B:384:GLU:OE1	1:B:412:LYS:NZ	2.24	0.69
1:B:79:THR:HG23	1:B:82:SER:H	1.60	0.67
1:A:664:ALA:O	6:A:1120:HOH:O	2.12	0.67
1:B:780:ILE:HD11	1:B:817:LEU:HD23	1.76	0.66
1:B:79:THR:OG1	1:B:80:ASN:N	2.28	0.65
1:A:144:LEU:O	1:A:168:ARG:NH2	2.29	0.65
1:B:84:GLN:HE22	1:B:86:LEU:HD13	1.61	0.65
1:B:728:PRO:HG2	1:B:731:PHE:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:OD2	1:A:52:ARG:NH2	2.32	0.63
1:A:94:LEU:HB2	1:A:132:LEU:HD23	1.81	0.62
1:A:705:ASP:OD1	1:A:705:ASP:N	2.29	0.62
1:A:46:ILE:HG22	1:A:67:GLU:HB2	1.83	0.61
1:B:547:ALA:H	3:B:909:NAG:H82	1.67	0.60
1:B:149:THR:HB	1:B:173:LYS:HD3	1.83	0.60
1:A:50:SER:O	1:A:52:ARG:NH1	2.35	0.60
1:A:470:PHE:CD1	1:A:472:ARG:HG2	2.37	0.59
1:B:67:GLU:HG3	1:B:91:LYS:HB3	1.84	0.59
1:B:614:VAL:HG21	3:B:910:NAG:H61	1.86	0.57
1:A:375:ARG:NH1	6:A:1069:HOH:O	2.39	0.56
1:B:46:ILE:HG22	1:B:67:GLU:HB2	1.88	0.56
1:A:124:LEU:HD13	1:A:127:LEU:HD22	1.88	0.55
1:A:381:GLU:HG3	1:A:408:GLN:HG3	1.88	0.55
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.71	0.55
1:A:153:LEU:HB2	1:A:177:LEU:HD23	1.89	0.55
1:B:632:ILE:HG22	1:B:661:ASN:HD22	1.72	0.55
1:B:808:ASP:OD1	1:B:808:ASP:N	2.39	0.55
1:B:235:LYS:HD2	1:B:270:CYS:SG	2.47	0.55
1:A:703:LEU:HD21	1:A:724:ILE:HD13	1.88	0.54
1:B:32:ARG:NH2	1:B:790:HIS:O	2.40	0.54
1:B:578:GLU:HG3	1:B:602:LYS:HG2	1.90	0.54
1:B:782:ASP:OD1	1:B:785:ARG:NH1	2.38	0.53
1:A:730:GLY:N	1:A:754:SER:O	2.39	0.52
1:B:153:LEU:HB2	1:B:177:LEU:HD23	1.90	0.52
1:B:160:ASN:ND2	6:B:1125:HOH:O	2.42	0.52
1:B:84:GLN:NE2	1:B:86:LEU:HD13	2.24	0.52
1:A:576:HIS:ND1	1:A:578:GLU:OE2	2.32	0.52
1:B:660:LEU:HD22	1:B:686:GLN:HG3	1.90	0.51
1:A:300:ARG:HG3	1:A:322:TYR:HB2	1.93	0.51
1:A:701:LEU:HA	1:A:723:ARG:O	2.10	0.51
1:B:124:LEU:HG	1:B:127:LEU:HB2	1.92	0.51
1:B:512:LEU:HB2	1:B:537:LEU:HD23	1.93	0.51
1:B:64:TYR:O	6:B:1134:HOH:O	2.18	0.50
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.93	0.50
1:A:526:PHE:HB3	1:A:553:LEU:HD21	1.94	0.50
1:B:772:ASN:HB2	1:B:774:PHE:CE2	2.47	0.50
1:A:715:ARG:O	1:A:738:LEU:HD12	2.12	0.50
1:B:61:VAL:HG22	1:B:65:VAL:HG11	1.93	0.49
1:A:792:ASN:ND2	6:A:1144:HOH:O	2.46	0.49
1:B:119:GLY:HA2	1:B:122:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:HB3	1:A:196:VAL:HG13	1.93	0.49
1:A:63:LYS:NZ	1:A:88:ASN:HD21	2.10	0.49
1:A:514:ALA:HA	1:A:539:ASN:O	2.13	0.49
1:A:578:GLU:O	1:A:581:GLN:HG2	2.13	0.49
1:B:354:PRO:HD2	1:B:378:VAL:O	2.13	0.49
1:B:632:ILE:HG22	1:B:661:ASN:ND2	2.27	0.49
1:B:729:SER:OG	1:B:754:SER:HB2	2.12	0.49
1:B:64:TYR:HB2	6:B:1134:HOH:O	2.14	0.48
1:A:115:ASN:ND2	6:A:1163:HOH:O	2.39	0.48
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.13	0.48
1:A:90:THR:O	1:A:127:LEU:HD12	2.14	0.48
1:B:732:LEU:HD12	1:B:733:SER:N	2.29	0.48
1:B:383:ARG:HA	1:B:410:ASP:OD2	2.14	0.47
1:B:283:PHE:O	1:B:286:LEU:HB2	2.14	0.47
1:B:291:TYR:HB3	3:B:902:NAG:O6	2.14	0.47
1:A:159:TYR:CE1	1:A:187:CYS:HB2	2.48	0.47
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.96	0.47
1:A:681:TRP:CZ2	1:A:703:LEU:HD12	2.50	0.47
1:B:692:LEU:HG	1:B:716:THR:HB	1.95	0.47
1:B:801:VAL:HG23	1:B:814:ILE:HB	1.95	0.47
1:B:169:LEU:HB3	1:B:172:LEU:HG	1.96	0.46
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.50	0.46
1:B:124:LEU:HA	1:B:124:LEU:HD13	1.81	0.46
1:A:702:PHE:O	1:A:702:PHE:CG	2.68	0.46
1:B:273:GLY:O	1:B:300:ARG:NH2	2.42	0.46
1:B:229:LEU:HB2	1:B:253:LEU:HD23	1.98	0.46
1:B:83:PHE:HZ	1:B:94:LEU:HD21	1.81	0.46
1:B:327:ILE:HG12	1:B:344:LEU:HD13	1.98	0.46
1:A:163:LYS:NZ	1:A:193:GLU:OE2	2.34	0.46
1:A:327:ILE:HG12	1:A:344:LEU:HD13	1.97	0.46
1:A:682:THR:HA	1:A:710:PHE:CG	2.51	0.46
1:B:83:PHE:O	1:B:84:GLN:HG3	2.16	0.46
1:B:84:GLN:NE2	1:B:85:GLY:O	2.49	0.46
1:B:375:ARG:HD2	1:B:400:ASN:ND2	2.30	0.46
1:A:333:LEU:HD23	1:A:363:PHE:HA	1.98	0.45
1:A:470:PHE:CE1	1:A:472:ARG:HG2	2.52	0.45
1:A:149:THR:OG1	1:A:150:GLU:OE1	2.24	0.45
1:A:278:ILE:HB	1:A:306:TRP:CZ2	2.51	0.45
1:A:63:LYS:O	1:A:88:ASN:ND2	2.50	0.45
1:B:177:LEU:HB2	1:B:208:LEU:HD23	1.99	0.45
1:B:130:LEU:HG	1:B:132:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HB2	1:A:425:LEU:HD23	1.99	0.45
1:A:375:ARG:HD2	1:A:400:ASN:HD21	1.81	0.45
1:B:718:LEU:HA	1:B:742:ASP:HB3	1.99	0.45
1:A:200:LEU:HD12	1:A:203:LEU:HD22	1.99	0.44
1:B:124:LEU:C	1:B:126:ASN:H	2.20	0.44
1:A:173:LYS:O	1:A:203:LEU:HD12	2.17	0.44
1:A:764:LEU:O	1:A:793:VAL:HG22	2.18	0.44
1:B:727:LEU:HD21	1:B:743:LEU:HD13	2.00	0.44
1:A:296:SER:HA	1:A:320:PHE:O	2.18	0.44
1:B:402:GLY:HA2	1:B:426:SER:O	2.17	0.44
1:B:170:ILE:H	1:B:170:ILE:HG13	1.63	0.44
1:B:56:GLU:HG2	1:B:57:VAL:N	2.33	0.44
1:B:58:PRO:HD2	1:B:70:LEU:HD21	1.98	0.44
1:A:429:ARG:HD2	1:A:429:ARG:HA	1.86	0.43
1:B:153:LEU:HD23	1:B:153:LEU:HA	1.78	0.43
1:A:132:LEU:HB3	1:A:135:ASN:HD22	1.82	0.43
1:A:291:TYR:HB3	3:A:902:NAG:O6	2.18	0.43
1:A:595:ASN:O	1:A:595:ASN:ND2	2.49	0.43
1:B:66:THR:HG23	1:B:90:THR:HB	2.00	0.43
1:B:592:SER:HA	1:B:616:SER:O	2.19	0.43
1:B:296:SER:HA	1:B:320:PHE:O	2.18	0.43
1:B:757:GLU:HA	1:B:758:THR:CB	2.49	0.43
1:A:366:LEU:O	1:A:393:LEU:HD22	2.19	0.43
1:B:135:ASN:HB2	1:B:137:LEU:HD13	1.99	0.43
1:B:240:GLU:HG3	1:B:243:LYS:NZ	2.34	0.43
1:A:189:LYS:HE2	1:A:190:THR:O	2.19	0.42
1:B:207:SER:HA	1:B:228:PHE:HB2	2.02	0.42
1:A:49:CYS:HB3	1:A:70:LEU:HD23	2.00	0.42
1:A:387:PHE:HA	1:A:387:PHE:HD1	1.72	0.42
1:B:66:THR:HG22	1:B:67:GLU:N	2.34	0.42
1:B:464:HIS:HB3	5:B:905:MAN:H2	2.02	0.42
1:A:695:LEU:HA	1:A:695:LEU:HD23	1.76	0.42
1:B:576:HIS:HB3	1:B:578:GLU:OE1	2.20	0.42
1:A:129:GLU:HG3	1:A:150:GLU:HB2	2.02	0.42
1:A:258:PRO:HA	1:A:296:SER:O	2.19	0.42
1:B:286:LEU:HD12	1:B:286:LEU:HA	1.90	0.42
1:A:708:SER:HB3	1:A:734:GLU:OE1	2.20	0.41
1:A:177:LEU:HB2	1:A:208:LEU:HD23	2.01	0.41
1:A:576:HIS:NE2	6:A:1042:HOH:O	2.37	0.41
1:A:180:ASN:HB2	1:A:211:ASN:OD1	2.20	0.41
1:B:248:LEU:HA	1:B:248:LEU:HD23	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:LEU:HD21	1:B:683:LEU:HD22	2.02	0.41
1:A:353:TYR:CZ	1:A:380:GLN:HG2	2.55	0.41
1:A:720:SER:HB3	1:A:742:ASP:OD2	2.21	0.41
2:A:901:L07:H2	1:B:348:TYR:CE1	2.56	0.41
1:B:362:ASN:ND2	6:B:1130:HOH:O	2.48	0.41
1:A:313:LEU:HD23	1:A:336:LEU:HD22	2.02	0.41
1:A:377:TYR:N	1:A:404:ASN:OD1	2.53	0.41
1:B:313:LEU:HD23	1:B:336:LEU:HD22	2.03	0.41
1:B:393:LEU:HD12	1:B:396:LEU:HD22	2.02	0.41
1:B:476:LYS:HB2	3:B:907:NAG:O7	2.21	0.41
1:A:328:ALA:O	1:A:360:SER:HB2	2.22	0.40
1:A:767:LEU:HB3	1:A:795:ILE:HD13	2.03	0.40
1:B:144:LEU:HA	1:B:144:LEU:HD12	1.82	0.40
1:A:756:LEU:HD22	1:A:786:TRP:CD1	2.56	0.40
1:A:705:ASP:HB3	1:A:728:PRO:HB2	2.04	0.40
1:B:278:ILE:HB	1:B:306:TRP:CZ2	2.57	0.40
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	738/811 (91%)	708 (96%)	29 (4%)	1 (0%)	53	66
1	B	739/811 (91%)	705 (95%)	32 (4%)	2 (0%)	43	53
All	All	1477/1622 (91%)	1413 (96%)	61 (4%)	3 (0%)	49	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	VAL

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Mol	Chain	Res	Type
1	B	378	VAL
1	B	170	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	684/755 (91%)	656 (96%)	28 (4%)	33	46
1	B	686/755 (91%)	650 (95%)	36 (5%)	25	35
All	All	1370/1510 (91%)	1306 (95%)	64 (5%)	29	40

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	54	LEU
1	A	60	THR
1	A	61	VAL
1	A	66	THR
1	A	75	ILE
1	A	79	THR
1	A	86	LEU
1	A	164	GLU
1	A	189	LYS
1	A	216	VAL
1	A	248	LEU
1	A	250	LEU
1	A	294	LEU
1	A	317	ASP
1	A	319	GLU
1	A	385	ASP
1	A	504	LEU
1	A	671	ILE
1	A	677	LYS
1	A	689	ARG

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Mol	Chain	Res	Type
1	A	703	LEU
1	A	705	ASP
1	A	736	SER
1	A	778	CYS
1	A	782	ASP
1	A	789	GLU
1	A	815	VAL
1	B	39	LYS
1	B	46	ILE
1	B	48	GLU
1	B	50	SER
1	B	60	THR
1	B	67	GLU
1	B	84	GLN
1	B	90	THR
1	B	94	LEU
1	B	99	ASN
1	B	124	LEU
1	B	132	LEU
1	B	144	LEU
1	B	199	THR
1	B	246	ILE
1	B	248	LEU
1	B	271	ASP
1	B	286	LEU
1	B	300	ARG
1	B	301	LYS
1	B	388	GLN
1	B	401	LEU
1	B	472	ARG
1	B	476	LYS
1	B	504	LEU
1	B	671	ILE
1	B	677	LYS
1	B	703	LEU
1	B	706	SER
1	B	715	ARG
1	B	733	SER
1	B	735	VAL
1	B	794	LYS
1	B	808	ASP
1	B	816	SER

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Mol	Chain	Res	Type
1	B	818	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	B	84	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](#)

33 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	L07	A	901	-	16,19,19	1.60	3 (18%)	16,27,27	0.91	1 (6%)
3	NAG	A	902	1,3	14,14,15	0.66	0	17,19,21	1.39	2 (11%)
3	NAG	A	903	3,4	14,14,15	0.64	0	17,19,21	0.86	0
4	BMA	A	904	3,5	11,11,12	0.85	0	15,15,17	0.82	0
5	MAN	A	905	4	11,11,12	0.68	0	15,15,17	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	906	4	11,11,12	0.61	0	15,15,17	0.78	0
3	NAG	A	907	1,3	14,14,15	0.55	0	17,19,21	1.22	3 (17%)
3	NAG	A	908	3,4	14,14,15	0.58	0	17,19,21	0.88	0
4	BMA	A	909	3	11,11,12	1.13	1 (9%)	15,15,17	1.37	2 (13%)
3	NAG	A	910	1	14,14,15	0.65	0	17,19,21	0.72	0
3	NAG	A	911	1,3	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
3	NAG	A	912	3,4	14,14,15	0.65	0	17,19,21	0.77	0
4	BMA	A	913	3,5	11,11,12	1.02	1 (9%)	15,15,17	1.00	0
5	MAN	A	914	4	11,11,12	0.63	0	15,15,17	0.88	1 (6%)
5	MAN	A	915	4	11,11,12	0.59	0	15,15,17	1.08	1 (6%)
3	NAG	A	916	1	14,14,15	0.51	0	17,19,21	1.89	6 (35%)
3	NAG	A	917	1	14,14,15	0.52	0	17,19,21	1.72	1 (5%)
2	L07	B	901	-	16,19,19	1.68	3 (18%)	16,27,27	1.04	1 (6%)
3	NAG	B	902	1,3	14,14,15	0.61	0	17,19,21	1.18	3 (17%)
3	NAG	B	903	3,4	14,14,15	0.67	0	17,19,21	0.84	0
4	BMA	B	904	3,5	11,11,12	1.11	1 (9%)	15,15,17	0.85	0
5	MAN	B	905	4	11,11,12	0.53	0	15,15,17	1.32	2 (13%)
5	MAN	B	906	4	11,11,12	0.70	0	15,15,17	1.22	1 (6%)
3	NAG	B	907	1,3	14,14,15	0.67	0	17,19,21	1.15	2 (11%)
3	NAG	B	908	3	14,14,15	0.57	0	17,19,21	1.53	2 (11%)
3	NAG	B	909	1	14,14,15	0.46	0	17,19,21	1.21	2 (11%)
3	NAG	B	910	1,3	14,14,15	0.60	0	17,19,21	1.60	3 (17%)
3	NAG	B	911	3,4	14,14,15	0.76	0	17,19,21	0.92	0
4	BMA	B	912	3,5	11,11,12	0.64	0	15,15,17	0.84	0
5	MAN	B	913	4	11,11,12	0.70	0	15,15,17	1.07	1 (6%)
5	MAN	B	914	4	11,11,12	0.72	0	15,15,17	1.10	2 (13%)
3	NAG	B	915	1	14,14,15	0.64	0	17,19,21	1.11	2 (11%)
3	NAG	B	916	1	14,14,15	0.59	0	17,19,21	1.48	1 (5%)

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	L07	A	901	-	-	0/2/3/3	0/3/3/3
3	NAG	A	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	904	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	905	4	-	0/2/19/22	0/1/1/1
5	MAN	A	906	4	-	0/2/19/22	0/1/1/1
3	NAG	A	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	908	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	909	3	-	0/2/19/22	0/1/1/1
3	NAG	A	910	1	-	0/6/23/26	0/1/1/1
3	NAG	A	911	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	912	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	913	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	914	4	-	0/2/19/22	0/1/1/1
5	MAN	A	915	4	-	0/2/19/22	0/1/1/1
3	NAG	A	916	1	-	0/6/23/26	0/1/1/1
3	NAG	A	917	1	-	0/6/23/26	0/1/1/1
2	L07	B	901	-	-	0/2/3/3	0/3/3/3
3	NAG	B	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	903	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	904	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	905	4	-	0/2/19/22	0/1/1/1
5	MAN	B	906	4	-	0/2/19/22	0/1/1/1
3	NAG	B	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	908	3	-	0/6/23/26	0/1/1/1
3	NAG	B	909	1	-	0/6/23/26	0/1/1/1
3	NAG	B	910	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	911	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	912	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	913	4	-	0/2/19/22	0/1/1/1
5	MAN	B	914	4	-	0/2/19/22	0/1/1/1
3	NAG	B	915	1	-	0/6/23/26	0/1/1/1
3	NAG	B	916	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	913	BMA	O5-C1	-2.74	1.39	1.43
4	B	904	BMA	O5-C1	-2.20	1.40	1.43
2	B	901	L07	C4-C3	2.01	1.48	1.42
2	A	901	L07	C4-C3	2.05	1.48	1.42
2	A	901	L07	C6-C5	2.61	1.51	1.49
4	A	909	BMA	C2-C3	2.78	1.56	1.52
2	B	901	L07	C6-C5	3.28	1.51	1.49
2	B	901	L07	C2-C1	4.05	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	L07	C2-C1	4.33	1.50	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	905	MAN	O5-C1-C2	-3.28	105.67	110.78
5	B	906	MAN	O5-C1-C2	-3.27	105.68	110.78
3	A	916	NAG	O5-C1-C2	-3.24	107.05	111.52
3	B	915	NAG	C2-N2-C7	-3.10	118.42	122.94
5	B	913	MAN	O5-C1-C2	-3.09	105.96	110.78
3	B	910	NAG	O5-C1-C2	-3.02	107.36	111.52
3	A	907	NAG	O5-C1-C2	-2.93	107.47	111.52
5	A	915	MAN	O5-C1-C2	-2.81	106.40	110.78
3	B	909	NAG	C2-N2-C7	-2.73	118.96	122.94
3	A	907	NAG	C2-N2-C7	-2.54	119.23	122.94
3	B	907	NAG	C2-N2-C7	-2.46	119.35	122.94
3	B	915	NAG	O5-C1-C2	-2.46	108.12	111.52
5	B	914	MAN	C1-O5-C5	-2.38	108.91	112.19
3	A	916	NAG	C2-N2-C7	-2.37	119.49	122.94
3	B	902	NAG	C6-C5-C4	-2.23	107.72	112.99
5	A	914	MAN	O5-C1-C2	-2.22	107.32	110.78
5	B	905	MAN	C1-C2-C3	-2.19	106.89	109.66
3	A	916	NAG	C6-C5-C4	-2.17	107.86	112.99
5	A	905	MAN	O5-C1-C2	-2.11	107.48	110.78
3	A	911	NAG	O5-C1-C2	-2.08	108.65	111.52
5	A	905	MAN	C1-O5-C5	-2.04	109.38	112.19
3	B	902	NAG	O6-C6-C5	-2.03	104.22	111.29
2	B	901	L07	C2-C3-S	2.01	128.30	124.59
5	B	914	MAN	O5-C5-C6	2.05	110.39	107.15
3	B	907	NAG	O5-C5-C6	2.12	110.50	107.15
2	A	901	L07	C2-C3-S	2.12	128.51	124.59
3	B	910	NAG	C3-C4-C5	2.20	114.18	110.24
3	A	902	NAG	C2-N2-C7	2.46	126.53	122.94
3	A	916	NAG	O5-C5-C4	2.50	116.91	110.83
3	B	908	NAG	C3-C4-C5	2.53	114.77	110.24
3	A	907	NAG	O5-C5-C6	2.59	111.25	107.15
3	B	902	NAG	C1-O5-C5	2.66	115.85	112.19
4	A	909	BMA	C2-C3-C4	2.67	115.50	110.87
3	B	909	NAG	C1-O5-C5	2.78	116.01	112.19
4	A	909	BMA	C1-C2-C3	2.85	113.27	109.66
3	A	916	NAG	C3-C4-C5	2.90	115.42	110.24
3	B	910	NAG	C1-O5-C5	3.22	116.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	NAG	C1-O5-C5	3.50	117.00	112.19
3	B	908	NAG	C1-O5-C5	3.82	117.44	112.19
3	A	916	NAG	C1-O5-C5	4.51	118.40	112.19
3	B	916	NAG	C1-O5-C5	5.15	119.28	112.19
3	A	917	NAG	C1-O5-C5	6.09	120.57	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	L07	1	0
3	A	902	NAG	1	0
3	B	902	NAG	1	0
5	B	905	MAN	1	0
3	B	907	NAG	1	0
3	B	909	NAG	1	0
3	B	910	NAG	1	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	746/811 (91%)	0.22	20 (2%) 54 62	27, 52, 87, 113	0
1	B	747/811 (92%)	0.25	35 (4%) 31 39	27, 52, 94, 117	0
All	All	1493/1622 (92%)	0.24	55 (3%) 41 48	27, 52, 92, 117	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	758	THR	7.0
1	B	761	THR	5.6
1	B	82	SER	5.4
1	A	808	ASP	5.0
1	A	807	GLY	4.5
1	A	702	PHE	4.5
1	A	459	PHE	4.5
1	A	84	GLN	4.2
1	B	817	LEU	4.1
1	A	758	THR	4.0
1	B	117	THR	3.9
1	B	64	TYR	3.9
1	A	756	LEU	3.8
1	A	701	LEU	3.8
1	B	81	GLU	3.7
1	B	59	GLN	3.4
1	B	74	PHE	3.4
1	A	777	THR	3.3
1	B	122	LEU	3.3
1	B	756	LEU	3.2
1	A	757	GLU	3.2
1	B	123	ASN	3.1
1	B	125	LYS	3.0
1	B	88	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	83	PHE	3.0
1	A	85	GLY	3.0
1	B	807	GLY	2.9
1	B	243	LYS	2.9
1	B	120	ALA	2.9
1	B	31	SER	2.9
1	B	121	PHE	2.8
1	B	54	LEU	2.8
1	B	80	ASN	2.8
1	B	361	ARG	2.8
1	B	55	GLN	2.7
1	A	774	PHE	2.7
1	B	802	ILE	2.5
1	A	780	ILE	2.5
1	B	76	THR	2.4
1	B	116	ILE	2.4
1	B	810	ARG	2.4
1	A	775	GLU	2.4
1	A	86	LEU	2.3
1	A	799	VAL	2.3
1	B	84	GLN	2.2
1	B	798	LEU	2.2
1	A	46	ILE	2.2
1	B	816	SER	2.1
1	B	39	LYS	2.1
1	B	791	LEU	2.1
1	A	96	HIS	2.1
1	B	36	CYS	2.1
1	A	726	HIS	2.0
1	A	61	VAL	2.0
1	B	753	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
5	MAN	A	914	11/12	0.65	0.31	83,85,86,87	0
4	BMA	A	909	11/12	0.71	0.26	77,83,88,88	0
5	MAN	B	905	11/12	0.71	0.24	74,78,83,83	0
5	MAN	B	914	11/12	0.80	0.36	86,88,90,91	0
5	MAN	B	913	11/12	0.82	0.43	87,88,90,90	0
5	MAN	A	915	11/12	0.82	0.28	80,83,85,87	0
3	NAG	B	909	14/15	0.83	0.16	66,74,76,76	0
3	NAG	A	908	14/15	0.85	0.17	61,67,76,81	0
4	BMA	A	904	11/12	0.85	0.13	51,60,68,70	0
5	MAN	A	905	11/12	0.85	0.25	67,73,81,82	0
4	BMA	A	913	11/12	0.86	0.21	63,72,80,80	0
4	BMA	B	912	11/12	0.87	0.21	67,77,83,84	0
3	NAG	B	908	14/15	0.88	0.15	64,73,77,78	0
5	MAN	B	906	11/12	0.88	0.18	85,85,87,87	0
3	NAG	A	916	14/15	0.89	0.20	82,88,89,94	0
5	MAN	A	906	11/12	0.89	0.24	74,75,78,82	0
4	BMA	B	904	11/12	0.90	0.16	58,66,74,80	0
3	NAG	B	915	14/15	0.91	0.14	58,63,67,69	0
3	NAG	A	910	14/15	0.92	0.14	60,67,72,74	0
3	NAG	B	916	14/15	0.93	0.15	42,56,64,66	0
3	NAG	A	917	14/15	0.93	0.15	58,66,74,79	0
3	NAG	B	903	14/15	0.95	0.12	38,47,54,56	0
3	NAG	B	902	14/15	0.96	0.16	34,40,47,47	0
3	NAG	A	902	14/15	0.96	0.14	37,39,48,55	0
3	NAG	A	912	14/15	0.96	0.12	40,47,58,60	0
3	NAG	A	903	14/15	0.96	0.11	36,40,52,56	0
3	NAG	A	911	14/15	0.96	0.11	27,37,40,43	0
3	NAG	B	910	14/15	0.96	0.14	23,34,39,46	0
3	NAG	B	907	14/15	0.97	0.12	29,35,42,53	0
3	NAG	B	911	14/15	0.97	0.12	36,41,52,57	0
3	NAG	A	907	14/15	0.97	0.11	30,32,41,51	0
2	L07	A	901	17/17	0.98	0.14	28,36,40,41	0
2	L07	B	901	17/17	0.98	0.15	27,36,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.