



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:34 AM 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 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/ValidationPDFNotes.html>

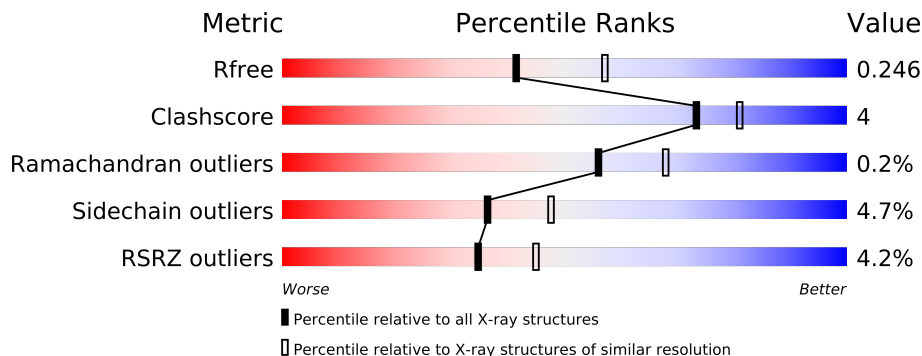
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	811	
1	B	811	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	B	909	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12772 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

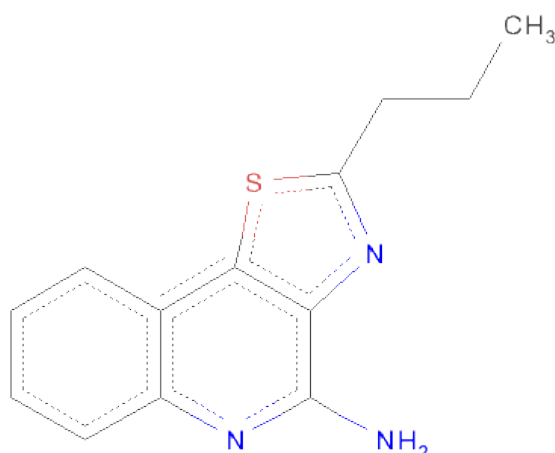
- Molecule 1 is a protein called Toll-like receptor 8.

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 a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		

There are 40 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
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
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

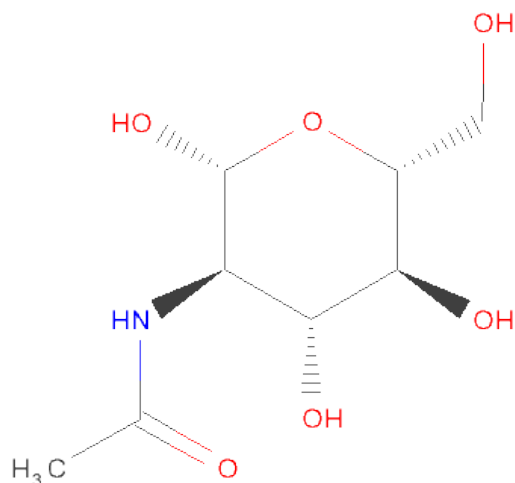
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

There are 10 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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 7 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.41 Å 154.02 Å 86.86 Å 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 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.205 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	3783 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 75218 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5986	0	0	29	0
1	B	5997	0	0	24	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
3	A	122	0	0	0	0
3	B	122	0	0	0	0
4	A	39	0	0	0	0
5	A	42	0	0	0	0
5	B	42	0	0	0	0
6	B	28	0	0	0	0
7	A	174	0	0	7	0
7	B	186	0	0	7	0
All	All	12772	0	0	52	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:TYR:O	1:A:60:THR:OG1	2.02	0.78
1:B:817:LEU:O	7: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:B:384:GLU:OE1	1:B:412:LYS:NZ	2.24	0.70
1:A:664:ALA:O	7:A:1120:HOH:O	2.12	0.67
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:A:705:ASP:OD1	1:A:705:ASP:N	2.29	0.65
1:A:576:HIS:ND1	1:A:578:GLU:OE2	2.32	0.63
1:A:37:ASP:OD2	1:A:52:ARG:NH2	2.32	0.63
1:A:163:LYS:NZ	1:A:193:GLU:OE2	2.34	0.60
1:A:50:SER:O	1:A:52:ARG:NH1	2.35	0.60
1:A:375:ARG:NH1	7:A:1069:HOH:O	2.39	0.56
1:B:782:ASP:OD1	1:B:785:ARG:NH1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:THR:OG1	1:A:150:GLU:OE1	2.24	0.56
1:A:730:GLY:N	1:A:754:SER:O	2.39	0.56
1:B:808:ASP:OD1	1:B:808:ASP:N	2.39	0.55
1:A:115:ASN:ND2	7:A:1163:HOH:O	2.39	0.55
1:B:194:ASP:OD2	1:B:219:LYS:NZ	2.41	0.54
1:B:32:ARG:NH2	1:B:790:HIS:O	2.40	0.54
1:B:273:GLY:O	1:B:300:ARG:NH2	2.42	0.53
1:B:160:ASN:ND2	7:B:1125:HOH:O	2.42	0.52
1:B:64:TYR:O	7:B:1134:HOH:O	2.18	0.50
1:A:694:ASP:OD2	1:A:696:ARG:NH2	2.43	0.50
1:B:346:PHE:N	1:B:375:ARG:O	2.45	0.50
1:A:792:ASN:ND2	7:A:1144:HOH:O	2.46	0.49
1:B:497:GLY:N	7:B:1180:HOH:O	2.46	0.49
1:B:362:ASN:ND2	7:B:1130:HOH:O	2.48	0.47
1:B:809:GLN:OE1	1:B:812:LYS:NZ	2.48	0.47
1:A:641:LEU:O	1:A:665:SER:OG	2.34	0.46
1:A:702:PHE:O	1:A:702:PHE:CG	2.68	0.46
1:B:84:GLN:NE2	1:B:85:GLY:O	2.49	0.46
1:A:600:THR:OG1	1:B:262:ASN:OD1	2.34	0.46
1:A:242:PHE:N	7:A:1171:HOH:O	2.48	0.46
1:A:595:ASN:O	1:A:595:ASN:ND2	2.49	0.45
1:A:63:LYS:O	1:A:88:ASN:ND2	2.50	0.45
1:A:484:LYS:NZ	7:A:1053:HOH:O	2.49	0.45
1:B:733:SER:OG	1:B:758:THR:N	2.50	0.44
1:A:149:THR:O	1:A:173:LYS:N	2.51	0.44
1:A:668:GLU:OE2	1:A:670:HIS:NE2	2.51	0.43
1:B:185:LYS:NZ	7:B:1162:HOH:O	2.51	0.43
1:A:180:ASN:O	1:A:185:LYS:NZ	2.51	0.43
1:B:730:GLY:N	1:B:754:SER:O	2.52	0.42
1:B:578:GLU:OE1	1:B:578:GLU:N	2.52	0.42
1:B:70:LEU:O	1:B:73:ASN:ND2	2.52	0.42
1:B:120:ALA:N	7:B:1164:HOH:O	2.54	0.41
1:A:576:HIS:NE2	7:A:1042:HOH:O	2.37	0.41
1:A:377:TYR:N	1:A:404:ASN:OD1	2.53	0.41
1:A:671:ILE:O	1:A:674:ASN:ND2	2.54	0.41
1:B:204:GLU:O	1:B:225:ARG:N	2.54	0.41
1:A:667:THR:O	1:A:691:GLU:N	2.53	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%)	59	72
1	B	739/811 (91%)	705 (95%)	32 (4%)	2 (0%)	50	60
All	All	1477/1622 (91%)	1413 (96%)	61 (4%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	VAL
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%)	41	55
1	B	686/755 (91%)	650 (95%)	36 (5%)	32	42
All	All	1370/1510 (91%)	1306 (95%)	64 (5%)	36	47

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	B	818	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

25 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	902	1,3	12,14,15	0.68	1 (8%)	15,19,21	1.23	2 (13%)
3	NAG	A	903	3	12,14,15	0.86	1 (8%)	15,19,21	0.97	0
3	BMA	A	904	3	10,11,12	0.72	0	11,15,17	0.91	0
3	MAN	A	905	3	10,11,12	0.76	0	11,15,17	0.92	1 (9%)
3	MAN	A	906	3	10,11,12	0.78	0	11,15,17	0.85	1 (9%)
4	NAG	A	907	1,4	12,14,15	0.65	0	15,19,21	1.30	2 (13%)
4	NAG	A	908	4	12,14,15	0.65	1 (8%)	15,19,21	0.87	0
4	BMA	A	909	4	10,11,12	0.91	0	11,15,17	1.65	3 (27%)
3	NAG	A	911	1,3	12,14,15	0.65	0	15,19,21	0.77	0
3	NAG	A	912	3	12,14,15	0.76	1 (8%)	15,19,21	0.92	1 (6%)
3	BMA	A	913	3	10,11,12	0.74	0	11,15,17	1.03	0
3	MAN	A	914	3	10,11,12	0.78	0	11,15,17	0.93	1 (9%)
3	MAN	A	915	3	10,11,12	0.74	0	11,15,17	0.95	1 (9%)
3	NAG	B	902	1,3	12,14,15	0.60	0	15,19,21	1.34	4 (26%)
3	NAG	B	903	3	12,14,15	0.76	1 (8%)	15,19,21	1.08	2 (13%)
3	BMA	B	904	3	10,11,12	1.00	0	11,15,17	1.12	0
3	MAN	B	905	3	10,11,12	0.69	0	11,15,17	1.10	0
3	MAN	B	906	3	10,11,12	0.77	0	11,15,17	1.01	1 (9%)
6	NAG	B	907	1,6	12,14,15	0.71	1 (8%)	15,19,21	1.23	2 (13%)
6	NAG	B	908	6	12,14,15	0.68	1 (8%)	15,19,21	1.49	3 (20%)
3	NAG	B	910	1,3	12,14,15	0.62	0	15,19,21	1.37	3 (20%)
3	NAG	B	911	3	12,14,15	0.82	1 (8%)	15,19,21	0.98	1 (6%)
3	BMA	B	912	3	10,11,12	0.49	0	11,15,17	1.25	1 (9%)
3	MAN	B	913	3	10,11,12	0.82	1 (10%)	11,15,17	0.84	0
3	MAN	B	914	3	10,11,12	0.81	0	11,15,17	1.10	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	3	-	0/6/23/26	0/1/1/1
3	BMA	A	904	3	-	0/2/19/22	0/1/1/1
3	MAN	A	905	3	-	0/2/19/22	0/1/1/1
3	MAN	A	906	3	-	0/2/19/22	0/1/1/1
4	NAG	A	907	1,4	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	NAG	O5-C5	-2.49	1.40	1.45
3	A	912	NAG	O5-C5	-2.13	1.41	1.45
3	B	911	NAG	O5-C5	-2.12	1.41	1.45
3	A	902	NAG	O5-C5	-2.09	1.41	1.45
6	B	908	NAG	O5-C5	-2.08	1.41	1.45
6	B	907	NAG	O5-C5	-2.07	1.41	1.45
4	A	908	NAG	O5-C5	-2.07	1.41	1.45
3	B	903	NAG	O5-C5	-2.04	1.41	1.45
3	B	913	MAN	O5-C5	-2.02	1.41	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	907	NAG	O5-C5-C6	4.07	111.25	106.98
4	A	909	BMA	C4-C3-C2	3.72	115.50	110.50
6	B	907	NAG	O5-C5-C6	3.35	110.50	106.98
3	B	914	MAN	O5-C5-C6	3.25	110.39	106.98
3	B	903	NAG	O5-C5-C6	3.02	110.15	106.98
3	B	902	NAG	O5-C5-C4	2.84	114.26	110.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	906	MAN	O5-C5-C6	2.78	109.89	106.98
6	B	908	NAG	O5-C5-C4	2.73	114.12	110.65
3	B	912	BMA	O5-C5-C4	-2.70	107.22	110.65
3	B	902	NAG	C3-C2-N2	-2.64	107.74	111.76
4	A	909	BMA	O5-C5-C4	-2.59	107.37	110.65
6	B	908	NAG	C3-C4-C5	2.55	114.77	110.20
3	A	905	MAN	O5-C5-C6	2.36	109.46	106.98
4	A	909	BMA	O5-C5-C6	2.36	109.46	106.98
3	B	910	NAG	O5-C5-C6	-2.33	104.54	106.98
3	A	914	MAN	O5-C5-C6	2.32	109.42	106.98
4	A	907	NAG	C2-N2-C7	-2.30	119.23	123.09
3	B	903	NAG	C3-C2-N2	-2.26	108.31	111.76
3	B	910	NAG	C3-C4-C5	2.23	114.18	110.20
6	B	907	NAG	C2-N2-C7	-2.23	119.35	123.09
3	B	902	NAG	C6-C5-C4	-2.18	107.72	113.00
3	A	902	NAG	O5-C5-C4	2.18	113.42	110.65
3	A	912	NAG	C3-C2-N2	-2.16	108.47	111.76
3	B	910	NAG	O4-C4-C3	-2.08	105.69	110.35
3	A	906	MAN	O5-C5-C6	2.08	109.16	106.98
3	B	902	NAG	O6-C6-C5	-2.07	104.22	111.36
3	A	915	MAN	O5-C5-C6	2.05	109.13	106.98
3	A	902	NAG	C2-N2-C7	2.05	126.53	123.09
3	B	911	NAG	C3-C2-N2	-2.02	108.69	111.76
6	B	908	NAG	O5-C5-C6	-2.00	104.88	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	L07	A	901	-	19,19,19	1.92	2 (10%)	25,27,27	1.69	3 (12%)
5	NAG	A	910	1	12,14,15	0.81	1 (8%)	15,19,21	0.75	0
5	NAG	A	916	1	12,14,15	0.63	0	15,19,21	1.74	4 (26%)
5	NAG	A	917	1	12,14,15	0.59	0	15,19,21	1.11	1 (6%)
2	L07	B	901	-	19,19,19	1.92	2 (10%)	25,27,27	1.82	4 (16%)
5	NAG	B	909	1	12,14,15	0.63	0	15,19,21	1.09	2 (13%)
5	NAG	B	915	1	12,14,15	0.88	1 (8%)	15,19,21	0.98	1 (6%)
5	NAG	B	916	1	12,14,15	0.70	1 (8%)	15,19,21	1.16	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	L07	A	901	-	-	0/3/3/3	0/0/3/3
5	NAG	A	910	1	-	0/6/23/26	0/1/1/1
5	NAG	A	916	1	-	0/6/23/26	0/1/1/1
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
2	L07	B	901	-	-	0/3/3/3	0/0/3/3
5	NAG	B	909	1	-	0/6/23/26	0/1/1/1
5	NAG	B	915	1	-	0/6/23/26	0/1/1/1
5	NAG	B	916	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	L07	C2-C1	6.10	1.50	1.41
2	B	901	L07	C2-C1	5.70	1.49	1.41
2	B	901	L07	C3-S	-4.18	1.68	1.74
2	A	901	L07	C3-S	-3.69	1.69	1.74
5	A	910	NAG	O5-C5	-2.36	1.41	1.45
5	B	915	NAG	O5-C5	-2.13	1.41	1.45
5	B	916	NAG	O5-C5	-2.03	1.41	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	L07	C-N1-C1	5.08	122.80	118.42
2	A	901	L07	C5-N2-C4	4.96	114.35	107.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	916	NAG	O5-C5-C4	4.93	116.91	110.65
2	B	901	L07	C5-N2-C4	4.89	114.25	107.11
2	A	901	L07	C-N1-C1	4.20	122.04	118.42
2	B	901	L07	C6-C5-S	-3.66	118.05	121.29
2	A	901	L07	C6-C5-S	-3.64	118.07	121.29
5	A	916	NAG	C3-C4-C5	2.92	115.42	110.20
5	B	916	NAG	C3-C2-N2	-2.85	107.42	111.76
5	B	915	NAG	C2-N2-C7	-2.78	118.42	123.09
5	A	917	NAG	O5-C5-C4	2.70	114.09	110.65
5	B	909	NAG	C2-N2-C7	-2.46	118.96	123.09
5	B	916	NAG	O5-C5-C4	2.20	113.44	110.65
5	A	916	NAG	C2-N2-C7	-2.15	119.49	123.09
5	A	916	NAG	C6-C5-C4	-2.13	107.86	113.00
5	B	909	NAG	O5-C5-C6	2.12	109.20	106.98
2	B	901	L07	C2-C1-N1	-2.01	121.19	123.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	746/811 (91%)	0.23	22 (2%)	49 59	27, 52, 87, 113	0
1	B	747/811 (92%)	0.27	42 (5%)	24 33	27, 52, 94, 117	0
All	All	1493/1622 (92%)	0.25	64 (4%)	35 44	27, 52, 92, 117	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	THR	6.2
1	A	808	ASP	5.7
1	B	758	THR	5.3
1	B	761	THR	5.2
1	A	807	GLY	4.8
1	B	82	SER	4.6
1	B	74	PHE	4.5
1	A	459	PHE	4.5
1	B	756	LEU	4.2
1	B	817	LEU	4.2
1	A	84	GLN	4.1
1	B	39	LYS	4.0
1	B	46	ILE	4.0
1	A	702	PHE	3.9
1	A	756	LEU	3.7
1	B	121	PHE	3.7
1	B	76	THR	3.7
1	B	117	THR	3.6
1	A	777	THR	3.6
1	A	757	GLU	3.5
1	B	122	LEU	3.4
1	B	243	LYS	3.4
1	B	64	TYR	3.4
1	A	809	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	ILE	3.1
1	B	120	ALA	3.1
1	B	83	PHE	3.1
1	A	61	VAL	3.1
1	B	54	LEU	3.1
1	B	810	ARG	3.1
1	A	799	VAL	3.0
1	B	802	ILE	3.0
1	B	803	CYS	2.9
1	B	125	LYS	2.9
1	B	807	GLY	2.9
1	B	36	CYS	2.8
1	B	88	ASN	2.8
1	B	31	SER	2.6
1	A	85	GLY	2.6
1	A	701	LEU	2.5
1	A	805	SER	2.5
1	B	81	GLU	2.5
1	A	186	VAL	2.4
1	B	733	SER	2.4
1	A	726	HIS	2.4
1	B	77	HIS	2.4
1	B	753	LYS	2.4
1	B	791	LEU	2.3
1	B	100	VAL	2.3
1	B	38	GLU	2.3
1	B	470	PHE	2.2
1	B	361	ARG	2.2
1	A	433	LEU	2.2
1	B	89	LEU	2.2
1	A	159	TYR	2.2
1	B	459	PHE	2.1
1	B	806	PRO	2.1
1	B	84	GLN	2.1
1	B	99	ASN	2.1
1	A	754	SER	2.1
1	A	361	ARG	2.0
1	B	816	SER	2.0
1	A	39	LYS	2.0
1	B	128	ARG	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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MAN	A	905	11/12	0.23	44.20	67,73,81,82	0
3	MAN	B	905	11/12	0.23	29.67	74,78,83,83	0
3	NAG	B	902	14/15	0.16	0.89	34,40,47,47	0
3	NAG	B	910	14/15	0.13	0.63	23,34,39,46	0
4	NAG	A	908	14/15	0.17	0.06	61,67,76,81	0
3	NAG	A	902	14/15	0.14	-0.11	37,39,48,55	0
3	NAG	B	911	14/15	0.12	-0.15	36,41,52,57	0
6	NAG	B	907	14/15	0.12	-0.15	29,35,42,53	0
6	NAG	B	908	14/15	0.16	-0.26	64,73,77,78	0
3	NAG	A	903	14/15	0.11	-0.40	36,40,52,56	0
4	NAG	A	907	14/15	0.11	-0.91	30,32,41,51	0
3	NAG	A	912	14/15	0.11	-0.95	40,47,58,60	0
3	NAG	B	903	14/15	0.12	-1.22	38,47,54,56	0
3	NAG	A	911	14/15	0.10	-1.40	27,37,40,43	0
3	MAN	B	906	11/12	0.24	-	85,85,87,87	0
4	BMA	A	909	11/12	0.22	-	77,83,88,88	0
3	MAN	B	914	11/12	0.38	-	86,88,90,91	0
3	BMA	B	912	11/12	0.17	-	67,77,83,84	0
3	BMA	B	904	11/12	0.15	-	58,66,74,80	0
3	BMA	A	913	11/12	0.22	-	63,72,80,80	0
3	MAN	B	913	11/12	0.38	-	87,88,90,90	0
3	BMA	A	904	11/12	0.13	-	51,60,68,70	0
3	MAN	A	914	11/12	0.32	-	83,85,86,87	0
3	MAN	A	906	11/12	0.27	-	74,75,78,82	0
3	MAN	A	915	11/12	0.31	-	80,83,85,87	0

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	909	14/15	0.15	2.27	66,74,76,76	0
5	NAG	A	916	14/15	0.21	1.32	82,88,89,94	0
5	NAG	B	915	14/15	0.14	0.84	58,63,67,69	0
5	NAG	B	916	14/15	0.13	0.55	42,56,64,66	0
2	L07	B	901	17/17	0.13	0.35	27,36,38,38	0
5	NAG	A	917	14/15	0.14	0.01	58,66,74,79	0
2	L07	A	901	17/17	0.13	-0.24	28,36,40,41	0
5	NAG	A	910	14/15	0.11	-0.75	60,67,72,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.