



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:36 PM GMT

PDB ID : 5AWB  
Title : Crystal structure of human TLR8 in complex with N1-3-aminomethylbenzyl (meta-amine)  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2015-07-03  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

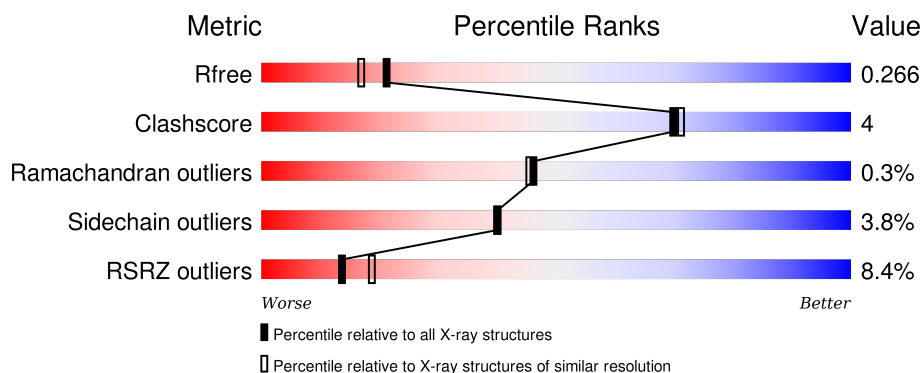
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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>8%</div> <div>80%</div> <div>11%</div> <div>8%</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
3	NAG	A	906	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	913	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6393 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.

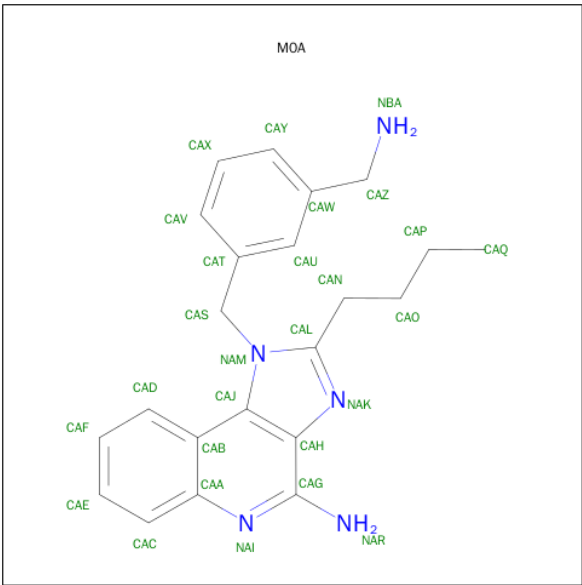
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	0	0
			6017	3851	1021	1126	19			

There are 10 discrepancies between the modelled and reference sequences:

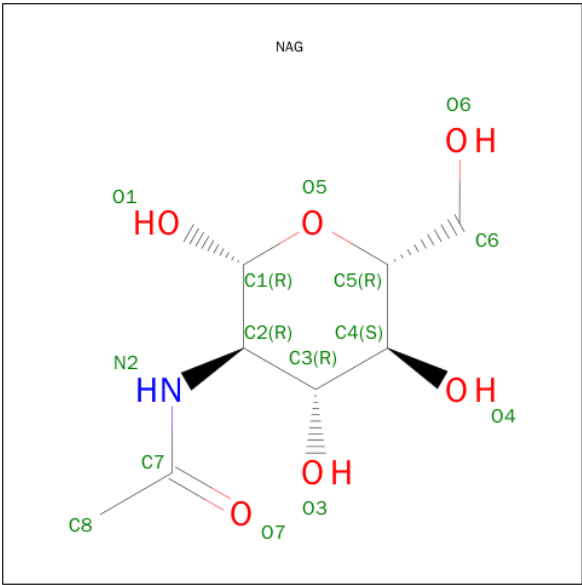
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q9NR97
A	23	SER	-	expression tag	UNP Q9NR97
A	24	PRO	-	expression tag	UNP Q9NR97
A	25	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is 1-[[3-(aminomethyl)phenyl]methyl]-2-butyl-imidazo[4,5-c]quinolin-4-amine (three-letter code: M0A) (formula: C<sub>22</sub>H<sub>25</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			27	22	5		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



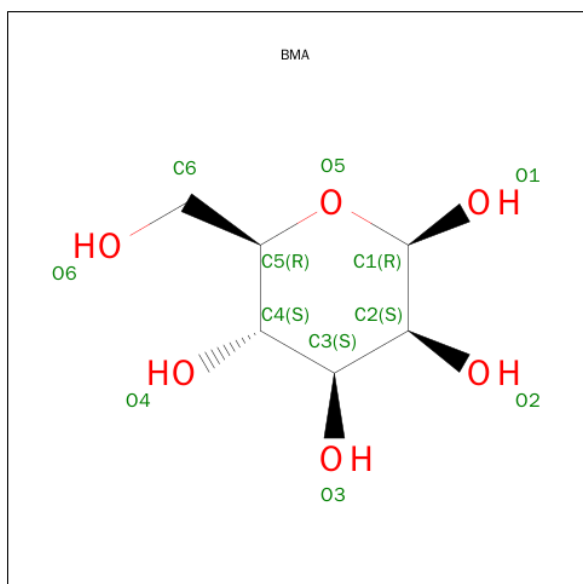
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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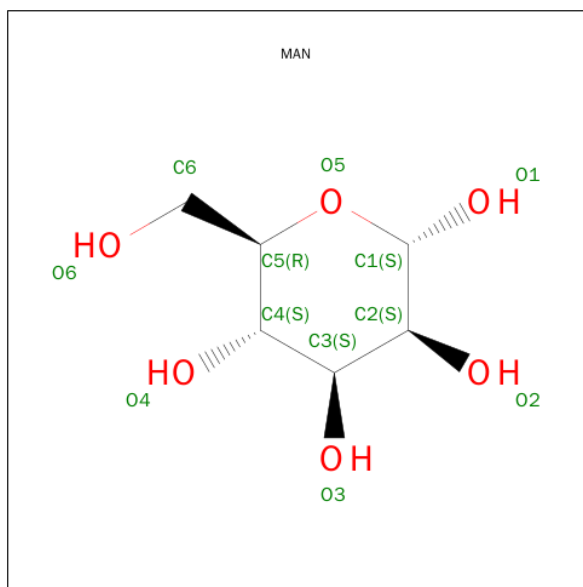
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



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

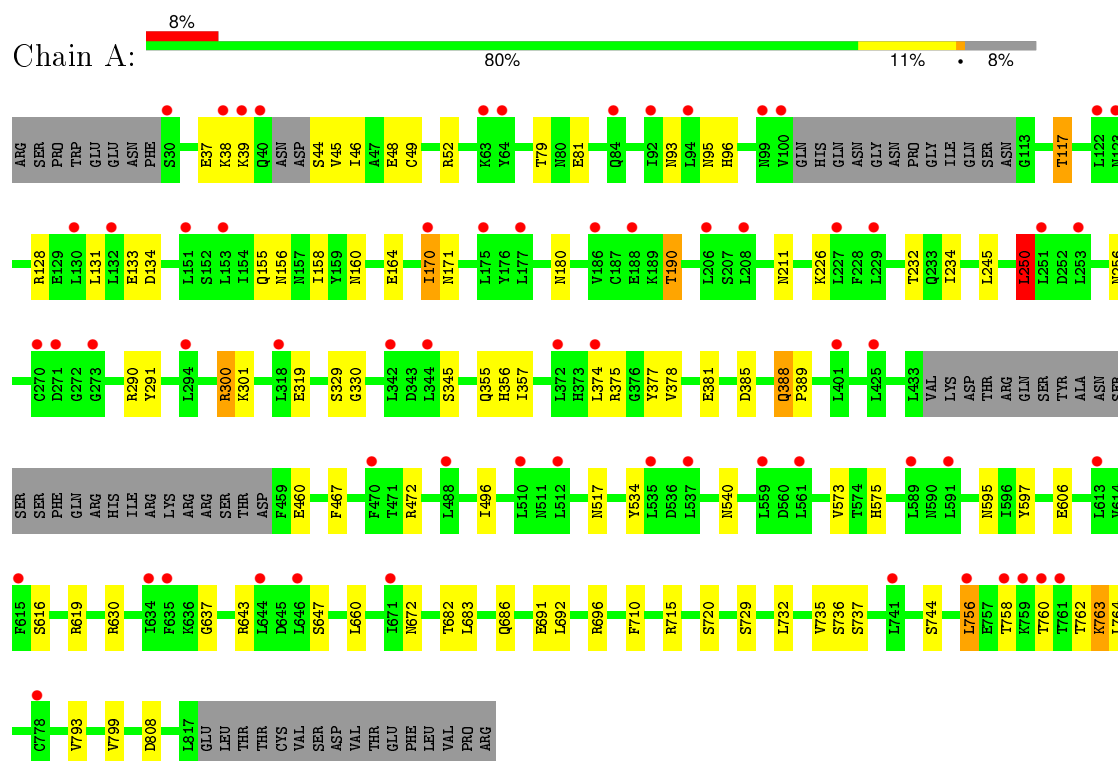
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		

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

- Molecule 1: Toll-like receptor 8





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.90 Å   107.05 Å   72.09 Å 90.00°   106.35°   90.00°	Depositor
Resolution (Å)	27.50 – 2.10 27.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (27.50-2.10) 98.7 (27.50-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.201   ,   0.259 0.209   ,   0.266	Depositor DCC
$R_{free}$ test set	2872 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56545 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, M0A, 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	0.79	0/6141	0.89	7/8328 (0.1%)

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	300	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	A	300	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	290	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	630	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	375	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	643	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	250	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	LYS	Peptide
1	A	496	ILE	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	6017	0	6000	52	0
2	A	27	0	25	2	0
3	A	126	0	112	5	0
4	A	22	0	19	0	0
5	A	11	0	10	0	0
6	A	190	0	0	5	0
All	All	6393	0	6166	55	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 4.

All (55) 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:736:SER:O	1:A:763:LYS:HG2	1.63	0.97
1:A:732:LEU:O	1:A:735:VAL:HG12	1.83	0.79
1:A:517:ASN:H	1:A:540:ASN:HD22	1.31	0.78
1:A:736:SER:O	1:A:763:LYS:CG	2.31	0.78
1:A:158:ILE:H	1:A:180:ASN:HD22	1.33	0.76
1:A:52:ARG:HB2	1:A:799:VAL:HG21	1.69	0.75
1:A:226:LYS:NZ	3:A:903:NAG:H81	2.03	0.73
1:A:95:ASN:ND2	1:A:133:GLU:H	1.89	0.71
1:A:190:THR:HG21	1:A:211:ASN:HB3	1.73	0.68
1:A:691:GLU:OE2	6:A:1001:HOH:O	2.12	0.67
1:A:736:SER:O	1:A:763:LYS:CD	2.44	0.66
1:A:736:SER:O	1:A:763:LYS:HD3	1.97	0.64
1:A:300:ARG:HD3	6:A:1189:HOH:O	1.97	0.64
3:A:903:NAG:H82	6:A:1153:HOH:O	1.97	0.63
1:A:96:HIS:HB3	6:A:1041:HOH:O	2.00	0.60
1:A:234:ILE:O	1:A:256:ASN:HB3	2.00	0.60
1:A:226:LYS:HZ3	3:A:903:NAG:H81	1.67	0.58
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.85	0.58
1:A:211:ASN:O	1:A:232:THR:HA	2.04	0.58
1:A:732:LEU:CD1	1:A:756:LEU:HD12	2.34	0.57
1:A:44:SER:HB2	6:A:1104:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:THR:HG23	1:A:762:THR:O	2.08	0.53
1:A:732:LEU:HD13	1:A:756:LEU:HD12	1.91	0.53
1:A:720:SER:HA	1:A:744:SER:O	2.09	0.52
1:A:226:LYS:HZ2	3:A:903:NAG:H81	1.74	0.52
1:A:597:TYR:HB3	1:A:619:ARG:HB2	1.92	0.51
1:A:764:LEU:O	1:A:793:VAL:HG22	2.11	0.50
2:A:901:M0A:CAS	2:A:901:M0A:H15	2.41	0.50
2:A:901:M0A:H16	2:A:901:M0A:H15	1.95	0.49
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.47	0.48
1:A:606:GLU:HG2	1:A:637:GLY:HA3	1.94	0.48
1:A:692:LEU:HD23	1:A:692:LEU:C	2.34	0.48
1:A:737:SER:HA	1:A:763:LYS:HD3	1.95	0.47
1:A:616:SER:HA	1:A:647:SER:O	2.14	0.47
1:A:758:THR:HB	1:A:760:THR:HG22	1.95	0.47
1:A:735:VAL:O	1:A:735:VAL:HG13	2.14	0.46
1:A:329:SER:OG	1:A:330:GLY:N	2.48	0.45
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.99	0.45
1:A:467:PHE:HB3	3:A:902:NAG:H81	1.98	0.44
1:A:250:LEU:HD22	1:A:291:TYR:HB2	1.98	0.44
1:A:37:GLU:HA	1:A:46:ILE:O	2.17	0.44
1:A:79:THR:HA	1:A:117:THR:OG1	2.17	0.44
1:A:357:ILE:HG13	1:A:377:TYR:CE1	2.53	0.44
1:A:319:GLU:HG2	1:A:345:SER:HB2	1.99	0.43
1:A:356:HIS:CD2	1:A:381:GLU:HG3	2.53	0.43
1:A:93:ASN:HA	1:A:131:LEU:HB2	2.01	0.43
1:A:171:ASN:HD22	1:A:171:ASN:N	2.17	0.42
1:A:190:THR:CG2	1:A:211:ASN:HB3	2.46	0.42
1:A:672:ASN:HA	1:A:696:ARG:O	2.20	0.42
1:A:573:VAL:O	1:A:575:HIS:CE1	2.72	0.42
1:A:388:GLN:N	1:A:389:PRO:CD	2.84	0.41
1:A:156:ASN:HB2	1:A:180:ASN:HD21	1.84	0.41
1:A:170:ILE:HG22	1:A:171:ASN:HD22	1.86	0.41
1:A:134:ASP:HA	1:A:155:GLN:O	2.21	0.41
1:A:95:ASN:HD22	1:A:133: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	740/811 (91%)	692 (94%)	46 (6%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	378	VAL

### 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	692/755 (92%)	666 (96%)	26 (4%)	40	40

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	48	GLU
1	A	49	CYS
1	A	81	GLU
1	A	117	THR
1	A	128	ARG
1	A	160	ASN
1	A	164	GLU
1	A	170	ILE

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Mol	Chain	Res	Type
1	A	190	THR
1	A	245	LEU
1	A	250	LEU
1	A	301	LYS
1	A	355	GLN
1	A	374	LEU
1	A	385	ASP
1	A	388	GLN
1	A	460	GLU
1	A	472	ARG
1	A	534	TYR
1	A	595	ASN
1	A	715	ARG
1	A	729	SER
1	A	756	LEU
1	A	763	LYS
1	A	808	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	95	ASN
1	A	99	ASN
1	A	171	ASN
1	A	180	ASN
1	A	184	ASN
1	A	285	ASN
1	A	540	ASN
1	A	566	HIS
1	A	653	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	14,14,15	0.78	0	15,19,21	1.74	6 (40%)
3	NAG	A	903	3,4	14,14,15	1.08	1 (7%)	15,19,21	2.10	4 (26%)
5	MAN	A	905	4	11,11,12	0.80	0	15,15,17	1.82	4 (26%)
3	NAG	A	906	1	14,14,15	1.38	1 (7%)	15,19,21	2.69	5 (33%)
3	NAG	A	907	1,3	14,14,15	1.18	1 (7%)	15,19,21	1.18	1 (6%)
3	NAG	A	908	3	14,14,15	0.91	1 (7%)	15,19,21	2.08	5 (33%)
3	NAG	A	909	1,3	14,14,15	0.80	0	15,19,21	1.40	1 (6%)
3	NAG	A	910	3,4	14,14,15	0.96	0	15,19,21	1.02	1 (6%)
3	NAG	A	912	1	14,14,15	0.89	0	15,19,21	1.39	2 (13%)
3	NAG	A	913	1	14,14,15	0.82	0	15,19,21	1.64	3 (20%)

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	3,4	-	0/6/23/26	0/1/1/1
5	MAN	A	905	4	-	0/2/19/22	0/1/1/1
3	NAG	A	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	908	3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	910	3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	912	1	-	0/6/23/26	0/1/1/1
3	NAG	A	913	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	907	NAG	O5-C1	-3.14	1.38	1.43
3	A	908	NAG	O5-C1	-2.65	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	NAG	C2-N2	-2.09	1.42	1.46
3	A	906	NAG	C1-C2	4.67	1.59	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	913	NAG	O3-C3-C4	-4.17	100.96	110.36
3	A	908	NAG	O3-C3-C2	-3.89	101.05	109.37
3	A	909	NAG	O5-C5-C4	-3.43	104.46	110.13
3	A	912	NAG	O4-C4-C3	-3.21	103.11	110.36
3	A	906	NAG	O3-C3-C4	-2.97	103.66	110.36
3	A	903	NAG	O6-C6-C5	-2.92	101.54	111.30
3	A	906	NAG	C6-C5-C4	-2.92	105.67	112.99
3	A	907	NAG	C4-C3-C2	-2.61	107.28	111.34
3	A	902	NAG	O6-C6-C5	-2.55	102.78	111.30
3	A	902	NAG	C1-O5-C5	-2.54	108.41	112.14
3	A	908	NAG	C3-C4-C5	-2.50	105.78	110.23
5	A	905	MAN	C3-C4-C5	-2.47	105.83	110.23
3	A	908	NAG	C6-C5-C4	-2.33	107.14	112.99
3	A	906	NAG	O7-C7-C8	-2.33	117.79	122.07
3	A	910	NAG	O4-C4-C3	-2.15	105.50	110.36
3	A	902	NAG	C3-C4-C5	-2.12	106.44	110.23
3	A	912	NAG	O3-C3-C4	-2.09	105.65	110.36
3	A	913	NAG	C2-N2-C7	-2.05	120.44	123.11
3	A	903	NAG	C4-C3-C2	-2.01	108.22	111.34
3	A	906	NAG	O5-C5-C4	2.05	113.54	110.13
5	A	905	MAN	O5-C5-C6	2.28	112.23	107.34
3	A	902	NAG	C2-N2-C7	2.37	126.19	123.11
5	A	905	MAN	C1-O5-C5	2.38	115.64	112.14
3	A	902	NAG	O4-C4-C3	2.41	115.79	110.36
3	A	902	NAG	O3-C3-C4	2.71	116.47	110.36
3	A	908	NAG	O4-C4-C3	2.80	116.67	110.36
3	A	913	NAG	C1-O5-C5	2.86	116.34	112.14
3	A	903	NAG	O5-C5-C4	3.90	116.59	110.13
3	A	908	NAG	C1-O5-C5	4.11	118.19	112.14
5	A	905	MAN	O3-C3-C2	4.31	117.91	110.01
3	A	903	NAG	C2-N2-C7	4.55	129.03	123.11
3	A	906	NAG	C1-O5-C5	8.52	124.67	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	NAG	1	0
3	A	903	NAG	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	M0A	A	901	-	27,30,30	1.32	4 (14%)	27,42,42	1.33	3 (11%)
3	NAG	A	902	1,3	14,14,15	0.78	0	15,19,21	1.74	6 (40%)
3	NAG	A	903	3,4	14,14,15	1.08	1 (7%)	15,19,21	2.10	4 (26%)
4	BMA	A	904	3,5	11,11,12	0.55	0	15,15,17	1.73	3 (20%)
5	MAN	A	905	4	11,11,12	0.80	0	15,15,17	1.82	4 (26%)
3	NAG	A	906	1	14,14,15	1.38	1 (7%)	15,19,21	2.69	5 (33%)
3	NAG	A	907	1,3	14,14,15	1.18	1 (7%)	15,19,21	1.18	1 (6%)
3	NAG	A	908	3	14,14,15	0.91	1 (7%)	15,19,21	2.08	5 (33%)
3	NAG	A	909	1,3	14,14,15	0.80	0	15,19,21	1.40	1 (6%)
3	NAG	A	910	3,4	14,14,15	0.96	0	15,19,21	1.02	1 (6%)
4	BMA	A	911	3	11,11,12	0.69	0	15,15,17	3.02	8 (53%)
3	NAG	A	912	1	14,14,15	0.89	0	15,19,21	1.39	2 (13%)
3	NAG	A	913	1	14,14,15	0.82	0	15,19,21	1.64	3 (20%)

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	M0A	A	901	-	-	0/10/10/10	0/4/4/4
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
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
3	NAG	A	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	908	3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	910	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	911	3	-	0/2/19/22	0/1/1/1
3	NAG	A	912	1	-	0/6/23/26	0/1/1/1
3	NAG	A	913	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	907	NAG	O5-C1	-3.14	1.38	1.43
3	A	908	NAG	O5-C1	-2.65	1.39	1.43
2	A	901	M0A	CAC-CAA	-2.31	1.37	1.41
2	A	901	M0A	CAJ-CAH	-2.29	1.35	1.43
3	A	903	NAG	C2-N2	-2.09	1.42	1.46
2	A	901	M0A	CAU-CAW	2.21	1.43	1.39
2	A	901	M0A	CAS-CAT	3.68	1.60	1.51
3	A	906	NAG	C1-C2	4.67	1.59	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	913	NAG	O3-C3-C4	-4.17	100.96	110.36
4	A	911	BMA	O4-C4-C3	-3.90	101.56	110.36
3	A	908	NAG	O3-C3-C2	-3.89	101.05	109.37
3	A	909	NAG	O5-C5-C4	-3.43	104.46	110.13
3	A	912	NAG	O4-C4-C3	-3.21	103.11	110.36
4	A	911	BMA	C6-C5-C4	-3.17	105.03	112.99
3	A	906	NAG	O3-C3-C4	-2.97	103.66	110.36
3	A	903	NAG	O6-C6-C5	-2.92	101.54	111.30
3	A	906	NAG	C6-C5-C4	-2.92	105.67	112.99
2	A	901	M0A	CAV-CAT-CAU	-2.88	114.38	118.53
4	A	911	BMA	O2-C2-C1	-2.87	103.48	109.23
4	A	904	BMA	O2-C2-C1	-2.63	103.97	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	907	NAG	C4-C3-C2	-2.61	107.28	111.34
4	A	904	BMA	O5-C1-C2	-2.57	106.79	110.89
3	A	902	NAG	O6-C6-C5	-2.55	102.78	111.30
3	A	902	NAG	C1-O5-C5	-2.54	108.41	112.14
3	A	908	NAG	C3-C4-C5	-2.50	105.78	110.23
5	A	905	MAN	C3-C4-C5	-2.47	105.83	110.23
3	A	908	NAG	C6-C5-C4	-2.33	107.14	112.99
3	A	906	NAG	O7-C7-C8	-2.33	117.79	122.07
4	A	911	BMA	C2-C3-C4	-2.16	107.28	111.05
3	A	910	NAG	O4-C4-C3	-2.15	105.50	110.36
3	A	902	NAG	C3-C4-C5	-2.12	106.44	110.23
3	A	912	NAG	O3-C3-C4	-2.09	105.65	110.36
3	A	913	NAG	C2-N2-C7	-2.05	120.44	123.11
3	A	903	NAG	C4-C3-C2	-2.01	108.22	111.34
2	A	901	M0A	CAD-CAB-CAA	2.03	120.97	117.58
3	A	906	NAG	O5-C5-C4	2.05	113.54	110.13
5	A	905	MAN	O5-C5-C6	2.28	112.23	107.34
3	A	902	NAG	C2-N2-C7	2.37	126.19	123.11
5	A	905	MAN	C1-O5-C5	2.38	115.64	112.14
3	A	902	NAG	O4-C4-C3	2.41	115.79	110.36
3	A	902	NAG	O3-C3-C4	2.71	116.47	110.36
3	A	908	NAG	O4-C4-C3	2.80	116.67	110.36
3	A	913	NAG	C1-O5-C5	2.86	116.34	112.14
4	A	904	BMA	C1-C2-C3	3.34	113.59	109.55
2	A	901	M0A	CAS-CAT-CAU	3.81	126.50	120.26
4	A	911	BMA	O3-C3-C2	3.85	117.06	110.01
3	A	903	NAG	O5-C5-C4	3.90	116.59	110.13
4	A	911	BMA	C3-C4-C5	4.05	117.45	110.23
3	A	908	NAG	C1-O5-C5	4.11	118.19	112.14
5	A	905	MAN	O3-C3-C2	4.31	117.91	110.01
4	A	911	BMA	O5-C5-C4	4.43	117.48	110.13
3	A	903	NAG	C2-N2-C7	4.55	129.03	123.11
4	A	911	BMA	C1-O5-C5	6.51	121.72	112.14
3	A	906	NAG	C1-O5-C5	8.52	124.67	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	M0A	2	0
3	A	902	NAG	1	0
3	A	903	NAG	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	748/811 (92%)	0.27	63 (8%) 14 19	29, 47, 77, 108	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	VAL	6.2
1	A	123	ASN	4.7
1	A	374	LEU	4.7
1	A	758	THR	4.4
1	A	470	PHE	4.2
1	A	64	TYR	4.1
1	A	761	THR	3.7
1	A	535	LEU	3.6
1	A	186	VAL	3.3
1	A	646	LEU	3.3
1	A	759	LYS	3.3
1	A	177	LEU	3.3
1	A	229	LEU	3.3
1	A	153	LEU	3.2
1	A	39	LYS	3.2
1	A	30	SER	3.2
1	A	559	LEU	3.2
1	A	132	LEU	3.1
1	A	273	GLY	3.1
1	A	206	LEU	3.1
1	A	253	LEU	3.1
1	A	38	LYS	3.0
1	A	122	LEU	3.0
1	A	188	GLU	3.0
1	A	130	LEU	3.0
1	A	344	LEU	3.0
1	A	591	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	271	ASP	2.8
1	A	644	LEU	2.8
1	A	251	LEU	2.8
1	A	615	PHE	2.8
1	A	778	CYS	2.8
1	A	175	LEU	2.8
1	A	510	LEU	2.7
1	A	227	LEU	2.7
1	A	671	ILE	2.6
1	A	512	LEU	2.6
1	A	372	LEU	2.6
1	A	634	ILE	2.6
1	A	760	THR	2.6
1	A	613	LEU	2.5
1	A	425	LEU	2.5
1	A	756	LEU	2.5
1	A	63	LYS	2.5
1	A	294	LEU	2.4
1	A	488	LEU	2.3
1	A	151	LEU	2.3
1	A	401	LEU	2.3
1	A	635	PHE	2.3
1	A	99	ASN	2.3
1	A	208	LEU	2.3
1	A	537	LEU	2.2
1	A	318	LEU	2.2
1	A	561	LEU	2.2
1	A	40	GLN	2.2
1	A	92	ILE	2.2
1	A	170	ILE	2.2
1	A	270	CYS	2.1
1	A	342	LEU	2.1
1	A	94	LEU	2.1
1	A	589	LEU	2.1
1	A	741	LEU	2.1
1	A	84	GLN	2.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	913	14/15	0.87	0.23	6.93	57,65,75,77	0
3	NAG	A	906	14/15	0.96	0.17	2.23	54,59,65,74	0
3	NAG	A	912	14/15	0.94	0.12	0.61	42,52,58,61	0
3	NAG	A	907	14/15	0.95	0.09	-1.31	34,36,40,45	0
3	NAG	A	903	14/15	0.96	0.08	-1.42	32,40,48,57	0
3	NAG	A	909	14/15	0.97	0.07	-1.89	28,34,37,37	0
3	NAG	A	902	14/15	0.96	0.09	-1.93	34,40,43,46	0
3	NAG	A	910	14/15	0.95	0.13	-	36,40,48,50	0
5	MAN	A	905	11/12	0.88	0.29	-	52,60,62,64	0
3	NAG	A	908	14/15	0.93	0.18	-	48,57,69,73	0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	913	14/15	0.87	0.23	6.93	57,65,75,77	0
3	NAG	A	906	14/15	0.96	0.17	2.23	54,59,65,74	0
3	NAG	A	912	14/15	0.94	0.12	0.61	42,52,58,61	0
2	M0A	A	901	27/27	0.96	0.10	-0.58	29,36,42,47	0
3	NAG	A	907	14/15	0.95	0.09	-1.31	34,36,40,45	0
3	NAG	A	903	14/15	0.96	0.08	-1.42	32,40,48,57	0
3	NAG	A	909	14/15	0.97	0.07	-1.89	28,34,37,37	0
3	NAG	A	902	14/15	0.96	0.09	-1.93	34,40,43,46	0
4	BMA	A	904	11/12	0.89	0.20	-	56,61,63,64	0
5	MAN	A	905	11/12	0.88	0.29	-	52,60,62,64	0
3	NAG	A	908	14/15	0.93	0.18	-	48,57,69,73	0
3	NAG	A	910	14/15	0.95	0.13	-	36,40,48,50	0
4	BMA	A	911	11/12	0.93	0.24	-	53,60,67,67	0

## 6.5 Other polymers

There are no such residues in this entry.