Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:22 AM GMT

PDB ID	:	2A0Z
Title	:	The molecular structure of toll-like receptor 3 ligand binding domain
Authors	:	Bell, J.K.; Botos, I.; Hall, P.R.; Askins, J.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on	:	2005-06-17
Resolution	:	2.40 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

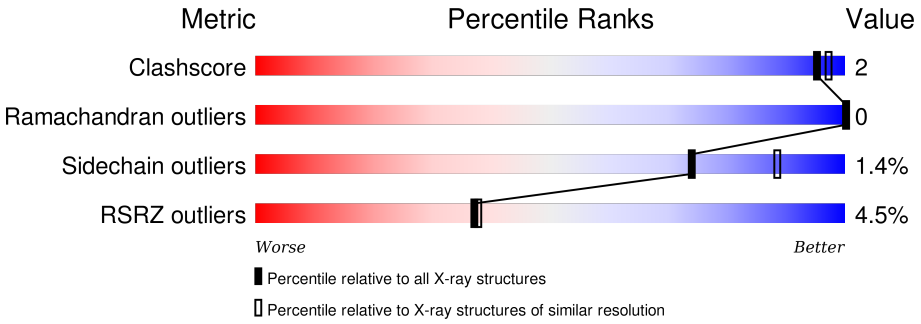
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	705	4% 92% · 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2751	-	-	-	X
2	NAG	A	729	-	-	-	X
8	GLC	A	753	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6183 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	6	0
			5420	3459	919	1023	19			

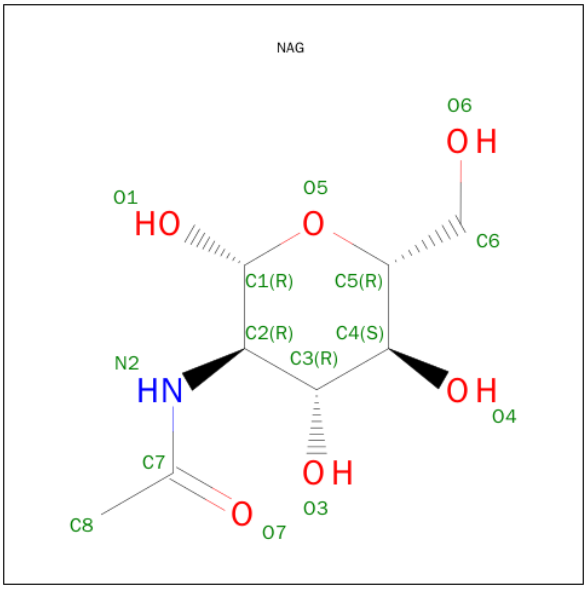
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLU	-	SEE REMARK 999	UNP O15455
A	705	ASN	-	SEE REMARK 999	UNP O15455
A	706	LEU	-	SEE REMARK 999	UNP O15455
A	707	TYR	-	SEE REMARK 999	UNP O15455
A	708	PHE	-	SEE REMARK 999	UNP O15455
A	709	GLN	-	SEE REMARK 999	UNP O15455
A	710	GLY	-	SEE REMARK 999	UNP O15455
A	711	ASP	-	SEE REMARK 999	UNP O15455
A	712	TYR	-	SEE REMARK 999	UNP O15455
A	713	LYS	-	SEE REMARK 999	UNP O15455
A	714	ASP	-	SEE REMARK 999	UNP O15455
A	715	ASP	-	SEE REMARK 999	UNP O15455
A	716	ASP	-	SEE REMARK 999	UNP O15455
A	717	ASP	-	SEE REMARK 999	UNP O15455
A	718	LYS	-	SEE REMARK 999	UNP O15455
A	719	GLY	-	EXPRESSION TAG	UNP O15455
A	720	SER	-	EXPRESSION TAG	UNP O15455
A	721	HIS	-	EXPRESSION TAG	UNP O15455
A	722	HIS	-	EXPRESSION TAG	UNP O15455
A	723	HIS	-	EXPRESSION TAG	UNP O15455
A	724	HIS	-	EXPRESSION TAG	UNP O15455
A	725	HIS	-	EXPRESSION TAG	UNP O15455
A	726	HIS	-	EXPRESSION TAG	UNP O15455

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

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

- Molecule 3 is SUGAR (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 14 8 1 5	0	0

- 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 39 22 2 15	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total C N O 37 22 2 13	0	0
5	A	3	Total C N O 38 22 2 14	0	0

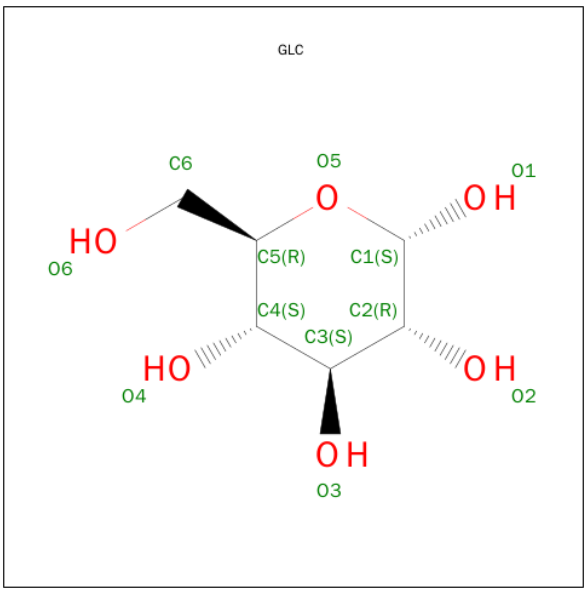
- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

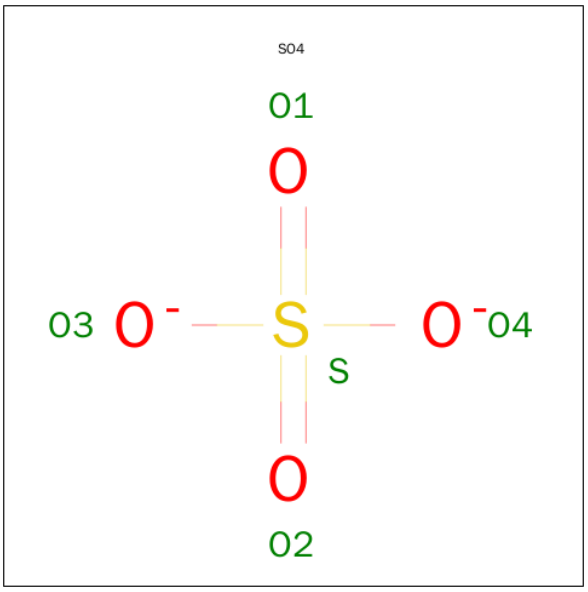
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total C N O 28 16 2 10	0	0

- Molecule 8 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



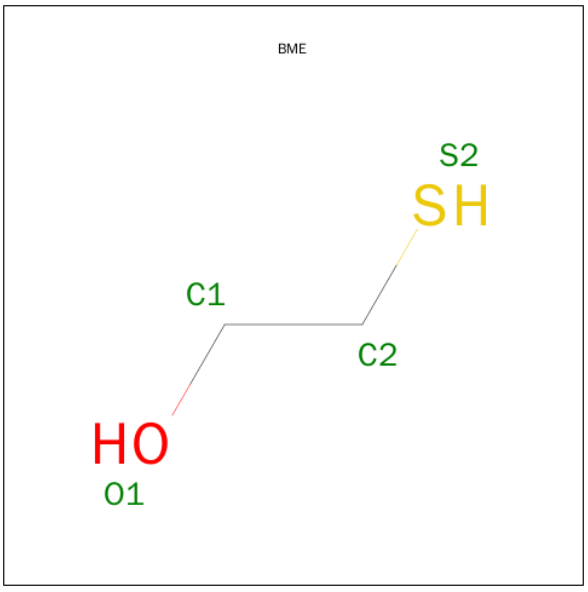
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 12 6 6	0	0
8	A	1	Total C O 12 6 6	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0

- Molecule 10 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O S 4 2 1 1	0	0

- Molecule 11 is water.

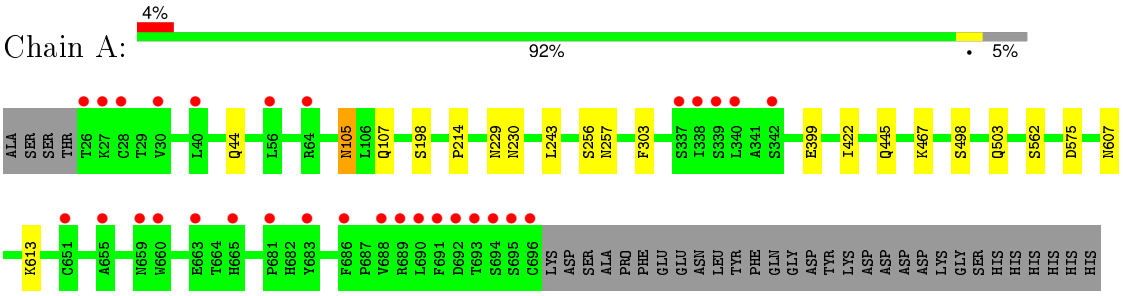
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	363	Total O 363 363	0	0

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 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 3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	141.60Å 160.79Å 122.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.75 – 2.42	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-2.40) 93.6 (48.75-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.232 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 50030 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6183	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BME, GLC, NDG, FUC, SO4, 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	0.71	1/5533 (0.0%)	0.73	0/7511

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SER	CB-OG	7.28	1.51	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5420	0	5399	15	1
2	A	140	0	125	3	0
3	A	14	0	13	0	0
4	A	39	0	34	0	0
5	A	75	0	66	3	0
6	A	61	0	52	0	0
7	A	28	0	25	0	0
8	A	24	0	24	0	0
9	A	15	0	0	0	0
10	A	4	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	363	0	0	1	0
All	All	6183	0	5743	19	1

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 2.

All (19) 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:422:ILE:H	1:A:445:GLN:HE22	1.23	0.86
5:A:5071:NAG:H61	5:A:5072:NAG:H82	1.72	0.70
1:A:230[A]:ASN:ND2	1:A:257:ASN:HD22	1.95	0.64
1:A:422:ILE:N	1:A:445:GLN:HE22	1.98	0.56
1:A:230[A]:ASN:HD22	1:A:257:ASN:HD22	1.52	0.55
1:A:230[A]:ASN:HD22	1:A:257:ASN:ND2	2.06	0.54
1:A:399:GLU:OE2	5:A:3981:NAG:H83	2.08	0.52
1:A:422:ILE:H	1:A:445:GLN:NE2	2.02	0.52
1:A:229[A]:ASN:HD22	1:A:256:SER:H	1.57	0.51
1:A:562:SER:HB3	11:A:6550:HOH:O	2.11	0.51
1:A:229[A]:ASN:ND2	1:A:256:SER:H	2.09	0.51
5:A:5071:NAG:H61	5:A:5072:NAG:C8	2.42	0.47
1:A:44:GLN:OE1	2:A:730:NAG:H62	2.16	0.46
2:A:2521:NAG:H3	2:A:2521:NAG:H82	1.99	0.45
1:A:105:ASN:HD22	1:A:107:GLN:H	1.65	0.44
1:A:105:ASN:ND2	1:A:107:GLN:H	2.16	0.43
2:A:727:NAG:H61	2:A:728:NAG:N2	2.33	0.42
1:A:105:ASN:HD22	1:A:105:ASN:C	2.23	0.42
1:A:105:ASN:HD21	1:A:107:GLN:HG2	1.86	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ASP:OD2	1:A:575:ASP:OD2[4_555]	2.15	0.05

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	674/705 (96%)	634 (94%)	40 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	631/656 (96%)	622 (99%)	9 (1%)	74 88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	214	PRO
1	A	243	LEU
1	A	303	PHE
1	A	467	LYS
1	A	498	SER
1	A	503	GLN
1	A	607	ASN
1	A	613	LYS

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	62	GLN
1	A	105	ASN
1	A	107	GLN
1	A	229[A]	ASN
1	A	309	ASN
1	A	311	GLN
1	A	445	GLN
1	A	494	ASN
1	A	659	ASN
1	A	678	ASN

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)

26 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	$\#\|Z\|>2$
2	NAG	A	2521	1,2	14,14,15	0.58	0	15,19,21	0.58	0
2	NAG	A	2522	2	14,14,15	0.56	0	15,19,21	0.68	1 (6%)
4	NAG	A	2651	1,4	14,14,15	0.46	0	15,19,21	0.73	1 (6%)
4	NAG	A	2652	4	14,14,15	0.51	0	15,19,21	0.74	1 (6%)
4	BMA	A	2653	4	11,11,12	0.55	0	14,15,17	0.24	0
2	NAG	A	2751	1,2	14,14,15	0.58	0	15,19,21	0.70	0
2	NAG	A	2752	2	14,14,15	0.59	0	15,19,21	0.73	1 (6%)
2	NAG	A	2911	1,2	14,14,15	0.51	0	15,19,21	0.68	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	2912	2	14,14,15	0.56	0	15,19,21	0.61	0
5	NAG	A	3981	1,9,5	13,13,15	0.84	1 (7%)	15,17,21	0.90	1 (6%)
5	NAG	A	3982	5	14,14,15	0.57	0	15,19,21	0.77	1 (6%)
5	FUC	A	3986	5	10,10,11	0.62	0	14,14,16	0.55	0
6	NAG	A	4131	1,6	14,14,15	0.50	0	15,19,21	0.67	0
6	NAG	A	4132	6	14,14,15	0.54	0	15,19,21	0.68	1 (6%)
6	BMA	A	4133	6	11,11,12	0.62	0	14,15,17	0.50	0
6	MAN	A	4134	6	11,11,12	0.70	0	14,15,17	0.65	1 (7%)
6	BMA	A	4135	6	11,11,12	0.65	0	14,15,17	0.47	0
5	NAG	A	5071	1,5	14,14,15	0.59	0	15,19,21	0.74	0
5	NAG	A	5072	5	14,14,15	0.68	0	15,19,21	0.84	1 (6%)
5	FUC	A	5076	5	10,10,11	0.67	0	14,14,16	0.56	0
7	NAG	A	6361	1,7	14,14,15	1.03	1 (7%)	15,19,21	0.72	0
7	NDG	A	6362	7	14,14,15	0.66	0	15,19,21	0.73	1 (6%)
2	NAG	A	727	1,2	14,14,15	0.67	0	15,19,21	0.55	0
2	NAG	A	728	2	14,14,15	0.54	0	15,19,21	0.75	1 (6%)
2	NAG	A	729	1,2	14,14,15	0.55	0	15,19,21	0.70	1 (6%)
2	NAG	A	730	2	14,14,15	0.65	0	15,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2521	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2522	2	-	0/6/23/26	0/1/1/1
4	NAG	A	2651	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2652	4	-	2/6/23/26	0/1/1/1
4	BMA	A	2653	4	-	0/2/19/22	0/1/1/1
2	NAG	A	2751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2752	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2912	2	-	0/6/23/26	0/1/1/1
5	NAG	A	3981	1,9,5	-	0/6/19/26	0/1/1/1
5	NAG	A	3982	5	-	1/6/23/26	0/1/1/1
5	FUC	A	3986	5	-	0/0/17/20	0/1/1/1
6	NAG	A	4131	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	4132	6	-	0/6/23/26	0/1/1/1
6	BMA	A	4133	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	4134	6	-	0/2/19/22	1/1/1/1
6	BMA	A	4135	6	-	0/2/19/22	0/1/1/1
5	NAG	A	5071	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5072	5	-	0/6/23/26	0/1/1/1
5	FUC	A	5076	5	-	0/0/17/20	0/1/1/1
7	NAG	A	6361	1,7	-	0/6/23/26	0/1/1/1
7	NDG	A	6362	7	-	0/6/23/26	0/1/1/1
2	NAG	A	727	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	728	2	-	0/6/23/26	0/1/1/1
2	NAG	A	729	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	730	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6361	NAG	C1-C2	2.10	1.55	1.52
5	A	3981	NAG	C1-C2	2.15	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3982	NAG	C2-N2-C7	-2.40	119.95	123.04
4	A	2652	NAG	C2-N2-C7	-2.30	120.08	123.04
2	A	2752	NAG	C2-N2-C7	-2.29	120.10	123.04
5	A	3981	NAG	C4-C3-C2	-2.29	110.27	112.53
2	A	728	NAG	C2-N2-C7	-2.20	120.21	123.04
2	A	2911	NAG	C2-N2-C7	-2.16	120.27	123.04
5	A	5072	NAG	C2-N2-C7	-2.15	120.27	123.04
2	A	729	NAG	C2-N2-C7	-2.15	120.27	123.04
4	A	2651	NAG	C2-N2-C7	-2.13	120.31	123.04
6	A	4132	NAG	C2-N2-C7	-2.11	120.33	123.04
2	A	2522	NAG	C2-N2-C7	-2.08	120.36	123.04
7	A	6362	NDG	C2-N2-C7	-2.01	120.46	123.04
6	A	4134	MAN	C1-O5-C5	2.03	114.82	112.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3982	NAG	O7-C7-N2-C2
4	A	2652	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	727	NAG	O7-C7-N2-C2
4	A	2652	NAG	O7-C7-N2-C2
2	A	727	NAG	C8-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4134	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2521	NAG	1	0
5	A	3981	NAG	1	0
5	A	5071	NAG	2	0
5	A	5072	NAG	2	0
2	A	727	NAG	1	0
2	A	728	NAG	1	0
2	A	730	NAG	1	0

5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
10	BME	A	1270	1	3,3,3	0.43	0	2,2,2	0.53	0
3	NAG	A	1961	1	14,14,15	0.66	0	15,19,21	0.75	1 (6%)
9	SO4	A	750	-	4,4,4	0.15	0	6,6,6	0.13	0
9	SO4	A	751	-	4,4,4	0.16	0	6,6,6	0.08	0
9	SO4	A	752	5	4,4,4	0.48	0	6,6,6	0.23	0
8	GLC	A	753	-	12,12,12	2.00	2 (16%)	17,17,17	1.62	4 (23%)
8	GLC	A	754	-	12,12,12	1.91	1 (8%)	17,17,17	1.57	3 (17%)

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
10	BME	A	1270	1	-	0/1/1/1	0/0/0/0
3	NAG	A	1961	1	-	0/6/23/26	0/1/1/1
9	SO4	A	750	-	-	0/0/0/0	0/0/0/0
9	SO4	A	751	-	-	0/0/0/0	0/0/0/0
9	SO4	A	752	5	-	0/0/0/0	0/0/0/0
8	GLC	A	753	-	-	0/2/22/22	0/1/1/1
8	GLC	A	754	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	753	GLC	C4-C5	2.11	1.57	1.53
8	A	754	GLC	O5-C1	5.89	1.54	1.43
8	A	753	GLC	O5-C1	5.95	1.54	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	753	GLC	C6-C5-C4	-3.32	104.83	113.02
8	A	754	GLC	C6-C5-C4	-3.27	104.95	113.02
8	A	753	GLC	O6-C6-C5	-2.48	103.13	111.33
3	A	1961	NAG	C2-N2-C7	-2.35	120.01	123.04
8	A	754	GLC	O6-C6-C5	-2.24	103.92	111.33
8	A	753	GLC	O1-C1-C2	2.18	115.04	109.21
8	A	753	GLC	O5-C5-C6	3.35	114.83	106.36
8	A	754	GLC	O5-C5-C6	3.45	115.06	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

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, 95^{th} 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	671/705 (95%)	-0.04	30 (4%) 37 38	22, 39, 76, 95	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	THR	8.6
1	A	693	THR	5.3
1	A	696	CYS	5.1
1	A	694	SER	5.0
1	A	692	ASP	4.8
1	A	690	LEU	4.7
1	A	695	SER	4.3
1	A	688	VAL	3.9
1	A	339	SER	3.5
1	A	338	ILE	3.3
1	A	691	PHE	3.3
1	A	27	LYS	3.3
1	A	686	PHE	3.2
1	A	663	GLU	3.2
1	A	342	SER	3.2
1	A	340	LEU	2.9
1	A	659	ASN	2.9
1	A	30	VAL	2.9
1	A	651	CYS	2.7
1	A	683	TYR	2.6
1	A	28	CYS	2.6
1	A	665	HIS	2.6
1	A	689	ARG	2.5
1	A	40	LEU	2.1
1	A	337	SER	2.1
1	A	64	ARG	2.1
1	A	655	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	660	TRP	2.0
1	A	681	PRO	2.0
1	A	56	LEU	2.0

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

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

6.3 Carbohydrates (i)

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	2751	14/15	0.88	0.16	6.00	59,63,69,75	0
2	NAG	A	729	14/15	0.78	0.39	3.80	81,85,89,93	0
6	NAG	A	4131	14/15	0.98	0.14	-0.22	32,35,39,45	0
7	NDG	A	6362	14/15	0.82	0.35	-	95,97,98,98	0
7	NAG	A	6361	14/15	0.64	0.29	-	79,85,87,91	0
5	NAG	A	3982	14/15	0.83	0.33	-	89,91,92,92	0
2	NAG	A	2522	14/15	0.81	0.24	-	76,79,80,81	0
4	NAG	A	2651	14/15	0.91	0.15	-	68,74,76,80	0
2	NAG	A	728	14/15	0.78	0.43	-	98,99,100,100	0
5	NAG	A	5071	14/15	0.95	0.12	-	37,53,66,68	0
4	BMA	A	2653	11/12	0.77	0.27	-	91,92,93,93	0
5	NAG	A	3981	13/15	0.85	0.18	-	72,75,83,86	0
2	NAG	A	730	14/15	0.75	0.50	-	97,99,100,100	0
2	NAG	A	2911	14/15	0.86	0.20	-	68,73,76,83	0
4	NAG	A	2652	14/15	0.81	0.19	-	84,86,88,90	0
2	NAG	A	2752	14/15	0.78	0.29	-	80,84,85,86	0
2	NAG	A	727	14/15	0.77	0.29	-	88,90,92,95	0
6	BMA	A	4135	11/12	0.65	0.36	-	99,99,100,100	0
2	NAG	A	2521	14/15	0.83	0.17	-	59,65,68,72	0
6	MAN	A	4134	11/12	0.77	0.33	-	97,99,100,100	0
2	NAG	A	2912	14/15	0.66	0.43	-	88,90,92,92	0
5	NAG	A	5072	14/15	0.86	0.23	-	73,77,79,80	0
6	NAG	A	4132	14/15	0.92	0.14	-	55,59,67,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	BMA	A	4133	11/12	0.86	0.26	-	84,91,94,97	0
5	FUC	A	3986	10/11	0.78	0.35	-	84,85,86,87	0
5	FUC	A	5076	10/11	0.84	0.23	-	73,76,77,77	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	GLC	A	753	12/12	0.73	0.23	6.76	54,59,62,67	0
9	SO4	A	751	5/5	0.97	0.12	-1.67	67,69,69,70	0
10	BME	A	1270	4/4	0.94	0.26	-	57,57,61,64	0
9	SO4	A	752	5/5	0.76	0.31	-	88,92,92,93	0
9	SO4	A	750	5/5	0.99	0.12	-	43,44,46,48	0
3	NAG	A	1961	14/15	0.73	0.23	-	74,78,79,81	0
8	GLC	A	754	12/12	0.66	0.25	-	99,100,100,100	0

6.5 Other polymers

There are no such residues in this entry.