



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:01 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 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/ValidationPDFNotes.html>

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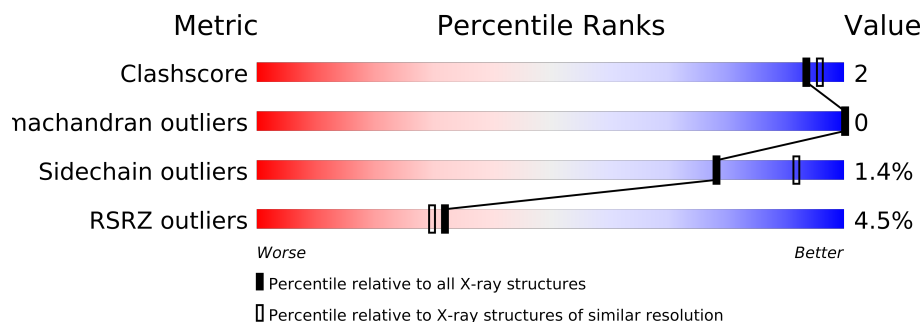
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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  $\geq 3$ , 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	705	

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

Mol	Type	Chain	Res	Geometry	Electron density
10	BME	A	1270	-	X
3	NAG	A	1961	-	X
8	GLC	A	753	-	X
8	GLC	A	754	-	X
9	SO4	A	752	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6183 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 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	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 115 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
A	704	GLU	-	SEE REMARK 999	UNP O15455
A	705	ASN	-	SEE REMARK 999	UNP O15455
A	706	LEU	-	SEE REMARK 999	UNP O15455

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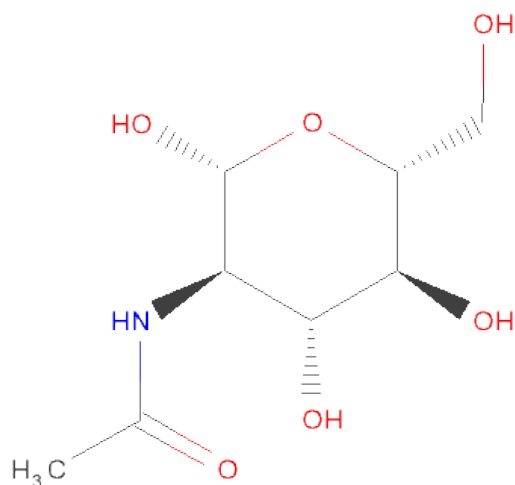
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	TYR	-	SEE REMARK 999	UNP O15455
A	708	PHE	-	SEE REMARK 999	UNP O15455
A	709	GLN	-	SEE REMARK 999	UNP O15455
A	710	GLY	-	SEE REMARK 999	UNP O15455
A	711	ASP	-	SEE REMARK 999	UNP O15455
A	712	TYR	-	SEE REMARK 999	UNP O15455
A	713	LYS	-	SEE REMARK 999	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	726	HIS	-	EXPRESSION TAG	UNP O15455

- 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	0	0
			14	8	1	5		

- 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 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 5 is a polymer of unknown type called SUGAR (3-MER).

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

There are 46 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 6 is a polymer of unknown type called SUGAR (5-MER).

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

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLU	-	SEE REMARK 999	UNP O15455

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Chain	Residue	Modelled	Actual	Comment	Reference
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 7 is a polymer of unknown type called SUGAR (2-MER).

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

There are 23 discrepancies between the modelled and reference sequences:

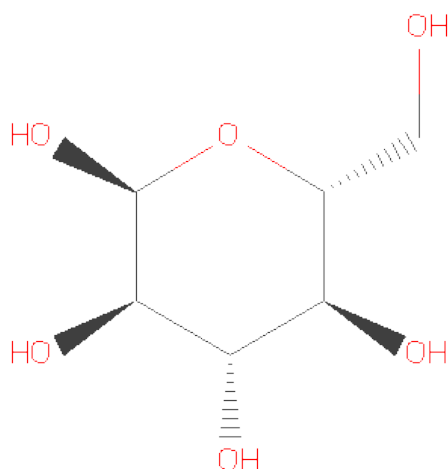
Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLU	-	SEE REMARK 999	UNP O15455
A	705	ASN	-	SEE REMARK 999	UNP O15455
A	706	LEU	-	SEE REMARK 999	UNP O15455
A	707	TYR	-	SEE REMARK 999	UNP O15455
A	708	PHE	-	SEE REMARK 999	UNP O15455
A	709	GLN	-	SEE REMARK 999	UNP O15455
A	710	GLY	-	SEE REMARK 999	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 8 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



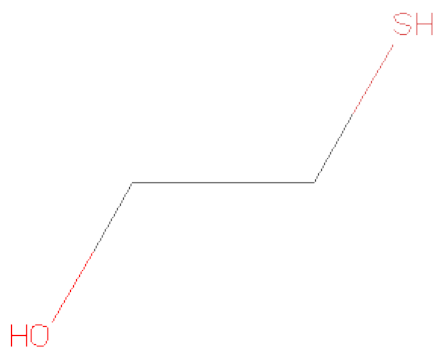
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		
8	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 10 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

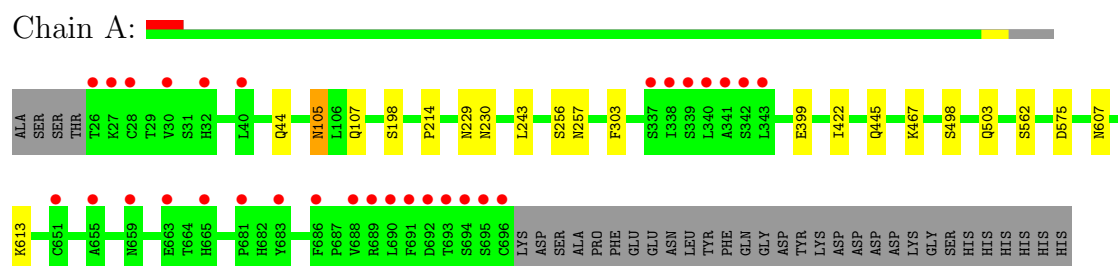
- Molecule 11 is water.

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

### 3 Residue-property plots

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 93.5 (48.75-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.232 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities 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: 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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	15	0	0	0	0
10	A	4	0	5	0	0
11	A	363	0	0	1	0
All	All	6183	0	5743	19	1

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 2.

All (19) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	78	92

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

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Mol	Chain	Res	Type
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 ⓘ

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 ⓘ

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	12,14,15	0.51	0	15,19,21	0.55	0
2	NAG	A	2522	2	12,14,15	0.45	0	15,19,21	0.63	0
4	NAG	A	2651	1,4	12,14,15	0.44	0	15,19,21	0.71	0
4	NAG	A	2652	4	12,14,15	0.49	0	15,19,21	0.67	0
4	BMA	A	2653	4	10,11,12	0.44	0	11,15,17	0.22	0
2	NAG	A	2751	1,2	12,14,15	0.49	0	15,19,21	0.61	0
2	NAG	A	2752	2	12,14,15	0.47	0	15,19,21	0.69	0
2	NAG	A	2911	1,2	12,14,15	0.54	0	15,19,21	0.69	0
2	NAG	A	2912	2	12,14,15	0.46	0	15,19,21	0.59	0
5	NAG	A	3981	1,9,5	11,13,15	0.62	0	9,17,21	0.63	0
5	NAG	A	3982	5	12,14,15	0.45	0	15,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FUC	A	3986	5	9,10,11	0.49	0	10,14,16	0.19	0
6	NAG	A	4131	1,6	12,14,15	0.45	0	15,19,21	0.62	0
6	NAG	A	4132	6	12,14,15	0.48	0	15,19,21	0.68	0
6	BMA	A	4133	6	10,11,12	0.59	0	11,15,17	0.56	0
6	MAN	A	4134	6	10,11,12	0.49	0	11,15,17	0.18	0
6	BMA	A	4135	6	10,11,12	0.50	0	11,15,17	0.28	0
5	NAG	A	5071	1,5	12,14,15	0.55	0	15,19,21	0.71	0
5	NAG	A	5072	5	12,14,15	0.60	0	15,19,21	0.83	0
5	FUC	A	5076	5	9,10,11	0.52	0	10,14,16	0.22	0
7	NAG	A	6361	1,7	12,14,15	0.89	0	15,19,21	0.72	0
7	NDG	A	6362	7	12,14,15	0.45	0	15,19,21	0.70	0
2	NAG	A	727	1,2	12,14,15	0.59	0	15,19,21	0.49	0
2	NAG	A	728	2	12,14,15	0.44	0	15,19,21	0.66	0
2	NAG	A	729	1,2	12,14,15	0.54	0	15,19,21	0.65	0
2	NAG	A	730	2	12,14,15	0.51	0	15,19,21	0.48	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
6	MAN	A	4134	6	-	0/2/19/22	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	727	NAG	C8-C7-N2-C2
4	A	2652	NAG	O7-C7-N2-C2
2	A	727	NAG	O7-C7-N2-C2
4	A	2652	NAG	C8-C7-N2-C2
5	A	3982	NAG	O7-C7-N2-C2

There are no ring outliers.

## 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	0.46	0	2,2,2	1.80	1 (50%)
3	NAG	A	1961	1	12,14,15	0.46	0	15,19,21	0.73	0
9	SO4	A	750	-	4,4,4	0.19	0	6,6,6	0.12	0
9	SO4	A	751	-	4,4,4	0.20	0	6,6,6	0.07	0
9	SO4	A	752	5	4,4,4	0.54	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GLC	A	753	-	12,12,12	1.91	2 (16%)	17,17,17	1.62	3 (17%)
8	GLC	A	754	-	12,12,12	1.83	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	O5-C1	5.63	1.54	1.43
8	A	754	GLC	O5-C1	5.56	1.54	1.43
8	A	753	GLC	C4-C5	2.06	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	754	GLC	O5-C5-C6	3.55	115.06	106.34
8	A	753	GLC	O5-C5-C6	3.46	114.83	106.34
8	A	753	GLC	C6-C5-C4	-3.38	104.83	113.00
8	A	754	GLC	C6-C5-C4	-3.33	104.95	113.00
10	A	1270	BME	C1-C2-S2	-2.54	108.65	113.03
8	A	753	GLC	O6-C6-C5	-2.39	103.13	111.36
8	A	754	GLC	O6-C6-C5	-2.16	103.92	111.36

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, 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	671/705 (95%)	-0.06	30 (4%) 32 30	22, 39, 76, 95	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	THR	9.2
1	A	693	THR	5.5
1	A	695	SER	5.4
1	A	694	SER	5.3
1	A	696	CYS	5.1
1	A	692	ASP	5.1
1	A	690	LEU	4.8
1	A	338	ILE	4.5
1	A	339	SER	4.1
1	A	342	SER	4.1
1	A	27	LYS	4.0
1	A	688	VAL	3.9
1	A	691	PHE	3.8
1	A	686	PHE	3.5
1	A	28	CYS	3.4
1	A	340	LEU	3.2
1	A	659	ASN	3.2
1	A	341	ALA	3.1
1	A	30	VAL	3.0
1	A	663	GLU	3.0
1	A	651	CYS	2.8
1	A	683	TYR	2.8
1	A	689	ARG	2.6
1	A	40	LEU	2.4
1	A	681	PRO	2.3
1	A	655	ALA	2.3
1	A	343	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	HIS	2.2
1	A	665	HIS	2.1
1	A	337	SER	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	FUC	A	3986	10/11	0.28	6.85	84,85,86,87	0
4	BMA	A	2653	11/12	0.32	6.59	91,92,93,93	0
2	NAG	A	727	14/15	0.36	5.56	88,90,92,95	0
2	NAG	A	729	14/15	0.29	3.77	81,85,89,93	0
2	NAG	A	2911	14/15	0.23	2.81	68,73,76,83	0
7	NAG	A	6361	14/15	0.25	1.89	79,85,87,91	0
2	NAG	A	2521	14/15	0.21	1.10	59,65,68,72	0
2	NAG	A	2751	14/15	0.16	1.05	59,63,69,75	0
5	NAG	A	3981	13/15	0.13	0.43	72,75,83,86	0
6	NAG	A	4131	14/15	0.11	-0.08	32,35,39,45	0
4	NAG	A	2652	14/15	0.14	-0.17	84,86,88,90	0
5	NAG	A	5071	14/15	0.10	-0.79	37,53,66,68	0
4	NAG	A	2651	14/15	0.19	-3.94	68,74,76,80	0
2	NAG	A	728	14/15	0.56	-	98,99,100,100	0
2	NAG	A	2522	14/15	0.44	-	76,79,80,81	0
2	NAG	A	2752	14/15	0.30	-	80,84,85,86	0
5	NAG	A	3982	14/15	0.24	-	89,91,92,92	0
6	BMA	A	4135	11/12	0.42	-	99,99,100,100	0
2	NAG	A	730	14/15	0.45	-	97,99,100,100	0
6	MAN	A	4134	11/12	0.43	-	97,99,100,100	0
2	NAG	A	2912	14/15	0.54	-	88,90,92,92	0
5	NAG	A	5072	14/15	0.28	-	73,77,79,80	0
6	NAG	A	4132	14/15	0.18	-	55,59,67,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	A	4133	11/12	0.28	-	84,91,94,97	0
7	NDG	A	6362	14/15	0.31	-	95,97,98,98	0
5	FUC	A	5076	10/11	0.31	-	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<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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1961	14/15	0.29	10.17	74,78,79,81	0
9	SO4	A	752	5/5	0.29	8.76	88,92,92,93	0
8	GLC	A	753	12/12	0.25	8.33	54,59,62,67	0
10	BME	A	1270	4/4	0.33	5.85	57,57,61,64	0
8	GLC	A	754	12/12	0.30	5.09	99,100,100,100	0
9	SO4	A	750	5/5	0.11	-0.50	43,44,46,48	0
9	SO4	A	751	5/5	0.11	-2.85	67,69,69,70	0

## 6.5 Other polymers

There are no such residues in this entry.