



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2016 – 02:35 PM EDT

PDB ID : 5AZ5
Title : Crystal structure of human TLR8 in complex with MB-343
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2015-09-27
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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-20027939

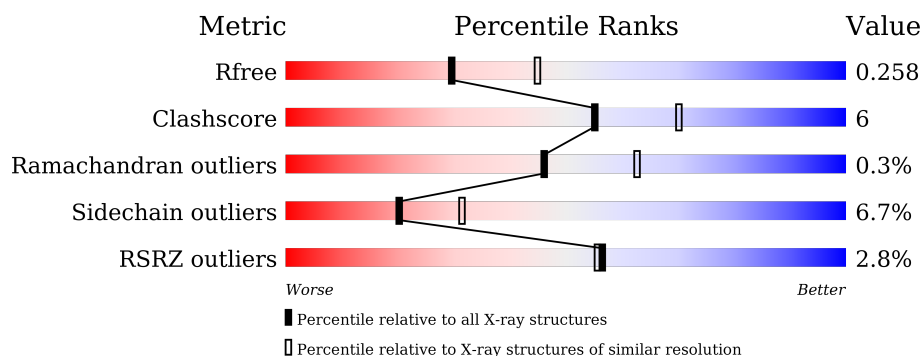
1 Overall quality at a glance

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))
R_{free}	91344	2919 (2.40-2.40)
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 $\leq 5\%$. 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	
1	B	811	
1	C	811	
1	D	811	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MBL	C	901	-	-	-	X
3	NAG	C	914	-	-	-	X
3	NAG	D	1006	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25117 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
			6029	3857	1023	1130	19			
1	B	749	Total	C	N	O	S	0	0	0
			6033	3859	1024	1131	19			
1	C	748	Total	C	N	O	S	0	0	0
			6024	3854	1023	1128	19			
1	D	746	Total	C	N	O	S	0	0	0
			6008	3844	1019	1126	19			

There are 40 discrepancies between the modelled and reference sequences:

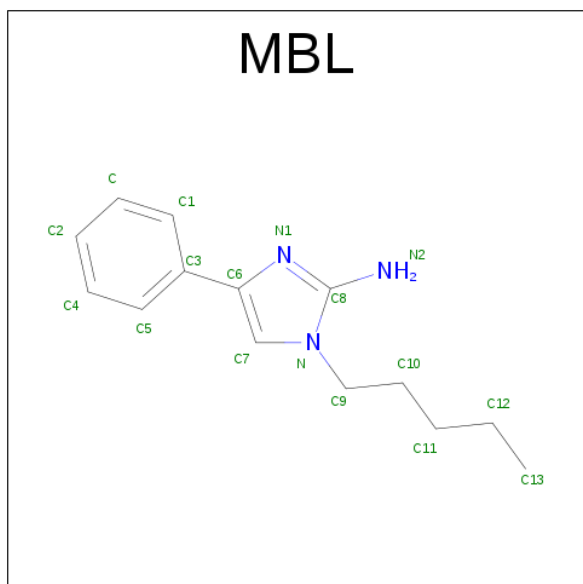
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
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
C	23	ARG	-	expression tag	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP Q9NR97
C	25	PRO	-	expression tag	UNP Q9NR97
C	26	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP Q9NR97
C	832	PRO	-	expression tag	UNP Q9NR97
C	833	ARG	-	expression tag	UNP Q9NR97
D	23	ARG	-	expression tag	UNP Q9NR97
D	24	SER	-	expression tag	UNP Q9NR97
D	25	PRO	-	expression tag	UNP Q9NR97
D	26	TRP	-	expression tag	UNP Q9NR97
D	828	GLU	-	expression tag	UNP Q9NR97
D	829	PHE	-	expression tag	UNP Q9NR97
D	830	LEU	-	expression tag	UNP Q9NR97
D	831	VAL	-	expression tag	UNP Q9NR97
D	832	PRO	-	expression tag	UNP Q9NR97
D	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is 1-pentyl-4-phenyl-imidazol-2-amine (three-letter code: MBL) (formula: $C_{14}H_{19}N_3$).



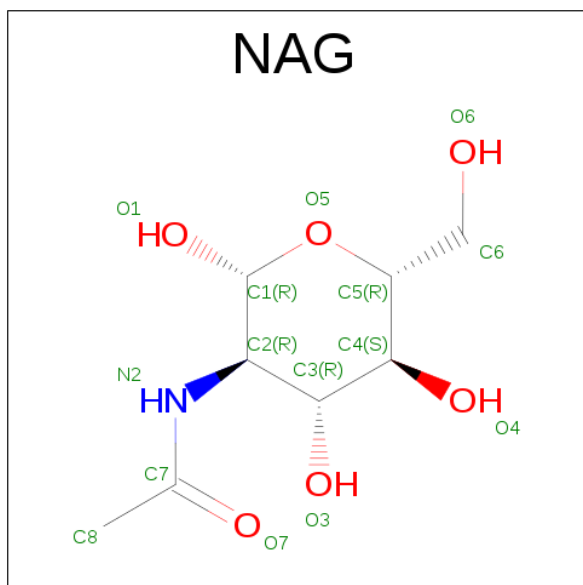
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			17	14	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			17	14	3		
2	C	1	Total	C	N	0	0
			17	14	3		
2	C	1	Total	C	N	0	0
			17	14	3		

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



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

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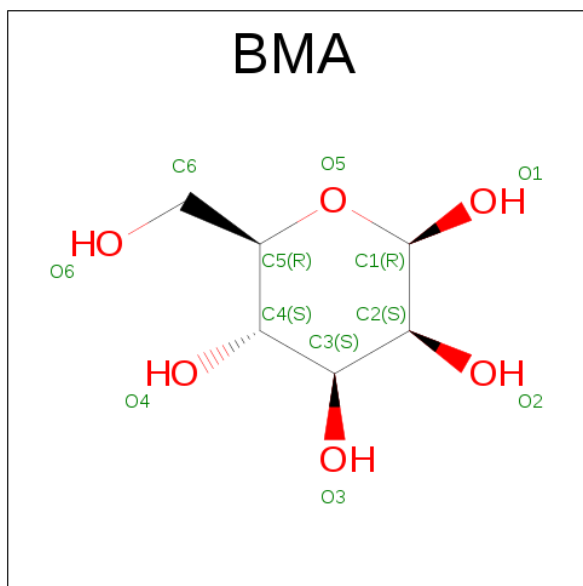
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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

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



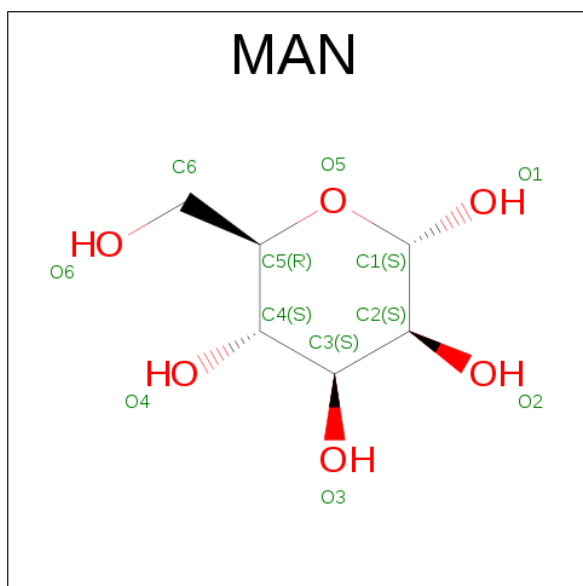
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

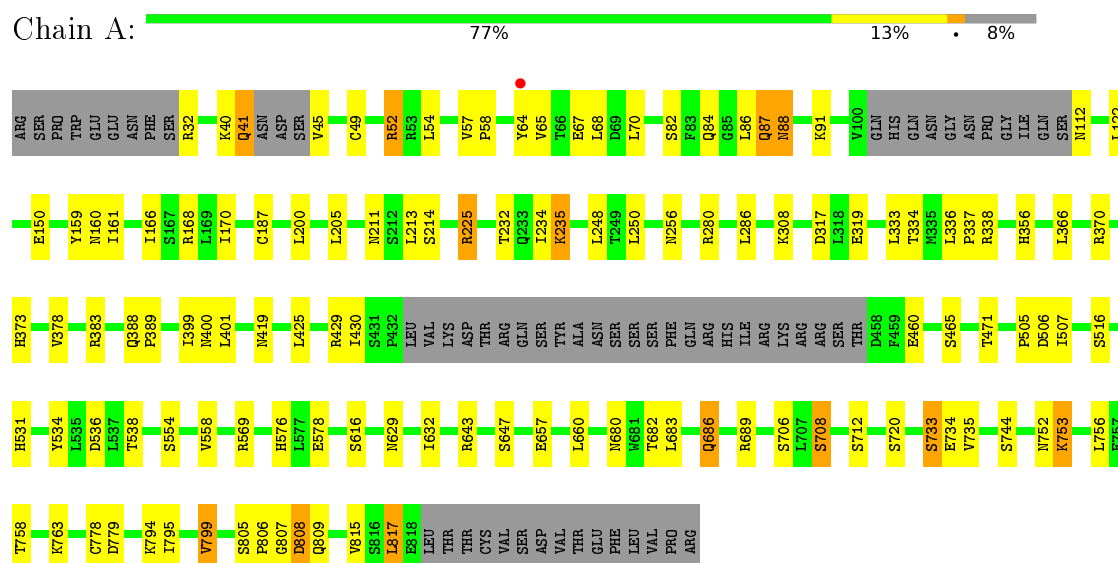
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total 98	O 98	0	0
6	B	83	Total 83	O 83	0	0
6	C	57	Total 57	O 57	0	0
6	D	53	Total 53	O 53	0	0

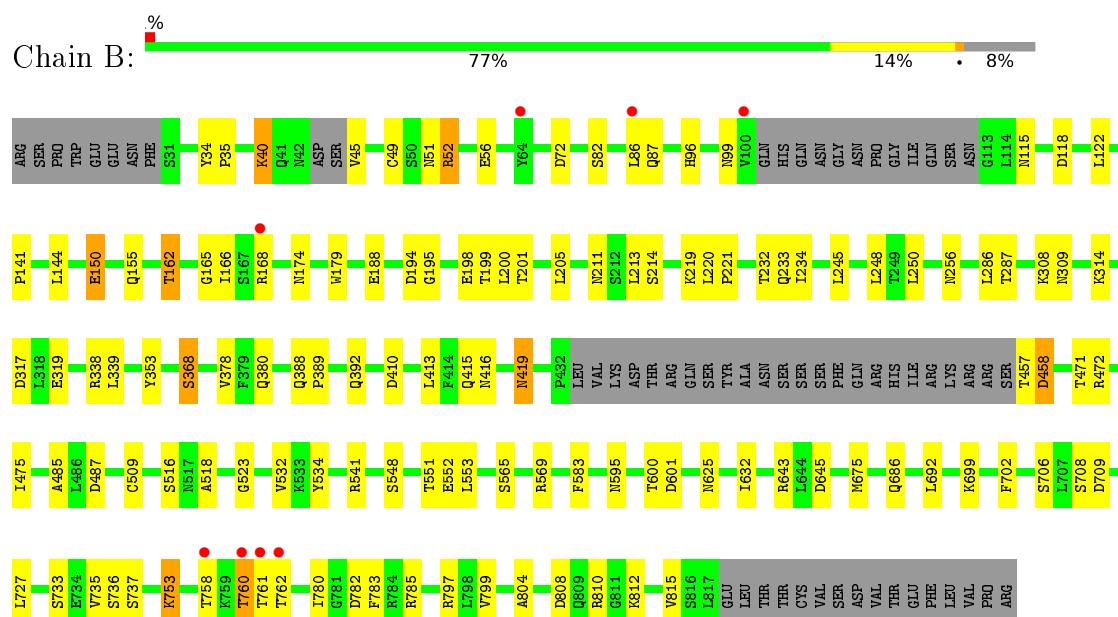
3 Residue-property plots

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.

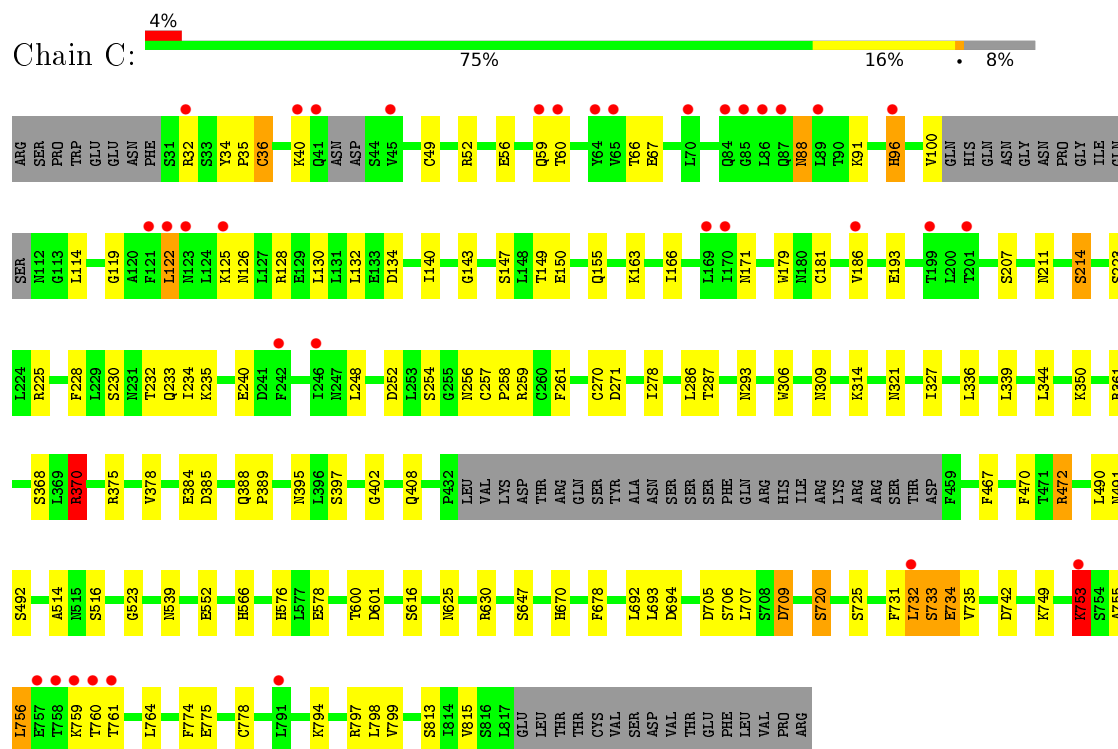
• Molecule 1: Toll-like receptor 8



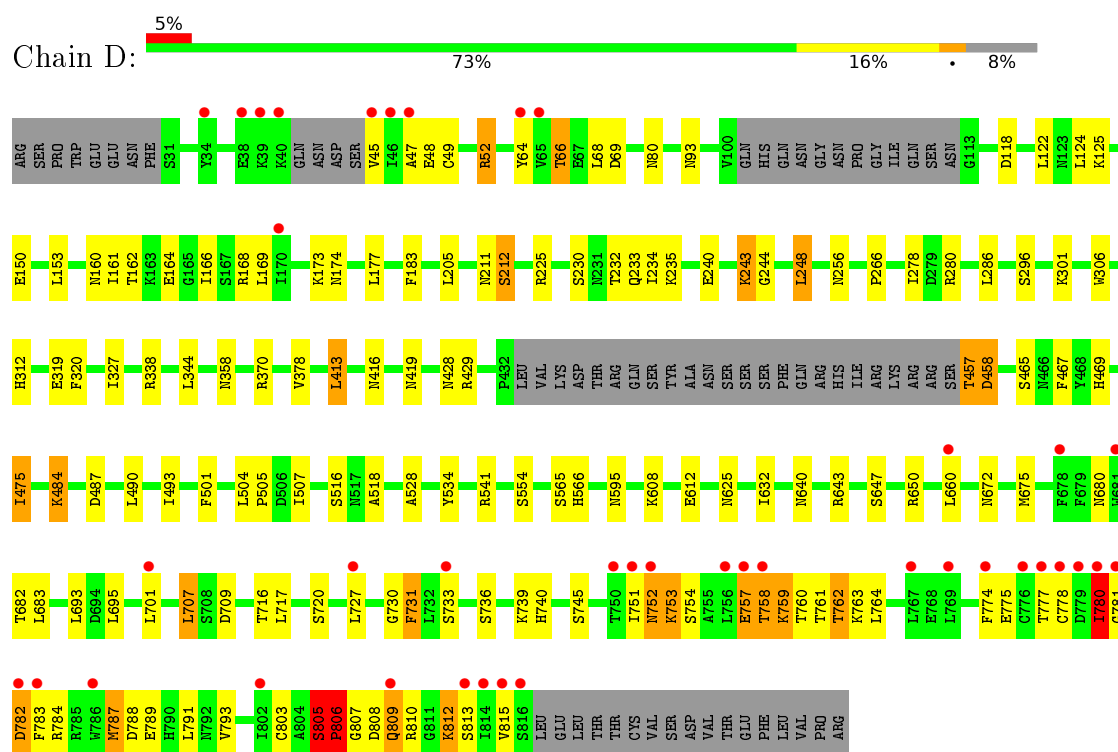
• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.63Å 141.12Å 170.97Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 47.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.40) 95.6 (47.73-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.196 , 0.259 0.200 , 0.258	Depositor DCC
R_{free} test set	7732 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MBL, 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	0.64	0/6153	0.75	2/8343 (0.0%)
1	B	0.58	0/6157	0.73	2/8349 (0.0%)
1	C	0.57	0/6148	0.72	2/8336 (0.0%)
1	D	0.57	0/6132	0.73	4/8315 (0.0%)
All	All	0.59	0/24590	0.73	10/33343 (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	C	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	D	338	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	B	645	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	630	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	370	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	643	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	806	PRO	CA-N-CD	-5.48	103.83	111.50
1	D	338	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	D	805	SER	C-N-CD	5.38	139.71	128.40
1	A	643	ARG	NE-CZ-NH1	5.27	122.94	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	753	LYS	Peptide
1	D	762	THR	Peptide
1	D	780	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	6029	0	6016	53	0
1	B	6033	0	6021	55	0
1	C	6024	0	6015	81	0
1	D	6008	0	5997	126	0
2	A	34	0	0	0	0
2	C	34	0	0	0	0
3	A	126	0	112	3	0
3	B	140	0	125	0	0
3	C	140	0	125	1	0
3	D	126	0	112	4	0
4	A	22	0	18	0	0
4	B	22	0	19	0	0
4	C	22	0	19	0	0
4	D	22	0	20	0	0
5	A	22	0	20	0	0
5	B	11	0	10	0	0
5	C	11	0	10	0	0
6	A	98	0	0	2	0
6	B	83	0	0	2	0
6	C	57	0	0	2	0
6	D	53	0	0	2	0
All	All	25117	0	24639	313	0

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

All (313) 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:D:243:LYS:HB3	1:D:244:GLY:HA3	1.20	1.17
1:D:759:LYS:HD2	1:D:760:THR:H	1.09	1.09
1:D:758:THR:HB	1:D:760:THR:HG23	1.32	1.08
1:D:759:LYS:HD2	1:D:760:THR:N	1.79	0.97
1:D:751:ILE:HD12	1:D:783:PHE:CD1	2.01	0.96
1:B:761:THR:HB	1:B:762:THR:O	1.68	0.93
1:D:759:LYS:O	1:D:762:THR:N	2.02	0.92
1:D:780:ILE:CD1	1:D:784:ARG:HG3	2.02	0.90
1:C:732:LEU:HB2	1:C:735:VAL:HG21	1.55	0.89
1:D:780:ILE:HD12	1:D:784:ARG:HG3	1.55	0.89
1:D:758:THR:HB	1:D:760:THR:CG2	2.02	0.88
1:C:732:LEU:HB2	1:C:735:VAL:CG2	2.04	0.88
1:D:751:ILE:HD12	1:D:783:PHE:CG	2.10	0.87
1:B:761:THR:HB	1:B:762:THR:C	1.97	0.83
1:A:45:VAL:HG13	1:A:65:VAL:HA	1.59	0.82
1:C:813:SER:OG	1:C:815:VAL:HG12	1.80	0.81
1:D:243:LYS:CB	1:D:244:GLY:HA3	2.07	0.81
1:D:757:GLU:HA	1:D:758:THR:C	2.03	0.78
1:D:457:THR:OG1	1:D:458:ASP:N	2.17	0.78
1:D:777:THR:O	1:D:780:ILE:HG22	1.86	0.76
1:C:733:SER:HA	1:C:735:VAL:H	1.49	0.75
1:C:732:LEU:HD21	1:C:764:LEU:HD22	1.69	0.74
1:A:686:GLN:HG3	1:A:686:GLN:O	1.85	0.74
1:D:243:LYS:HB3	1:D:244:GLY:CA	2.08	0.74
1:D:761:THR:O	1:D:762:THR:OG1	2.05	0.74
1:A:686:GLN:HB2	6:A:1079:HOH:O	1.88	0.73
1:D:808:ASP:HA	1:D:809:GLN:C	2.08	0.72
1:D:759:LYS:O	1:D:760:THR:OG1	2.09	0.70
1:D:751:ILE:CD1	1:D:783:PHE:CD1	2.75	0.70
1:D:153:LEU:HB2	1:D:177:LEU:HD23	1.73	0.70
1:D:775:GLU:HA	1:D:805:SER:HB2	1.76	0.67
1:C:566:HIS:CE1	1:D:490:LEU:HD22	2.30	0.66
1:D:716:THR:HG23	1:D:740:HIS:HB3	1.78	0.66
1:D:739:LYS:HA	1:D:763:LYS:HG3	1.78	0.65
1:D:780:ILE:C	1:D:780:ILE:HD13	2.17	0.65
1:C:733:SER:OG	1:C:734:GLU:HA	1.98	0.64
1:D:660:LEU:HD21	1:D:683:LEU:HD22	1.79	0.64
1:D:806:PRO:HD2	1:D:807:GLY:H	1.62	0.64
1:A:733:SER:HB2	1:A:758:THR:HG21	1.80	0.64
1:C:278:ILE:HB	1:C:306:TRP:CZ2	2.32	0.64
1:C:707:LEU:HD23	1:C:735:VAL:HG11	1.79	0.64
1:A:536:ASP:OD1	1:A:538:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:PHE:HB3	3:C:902:NAG:H81	1.79	0.63
1:C:753:LYS:HD3	1:C:755:ALA:HB2	1.82	0.62
1:C:368:SER:HA	1:C:395:ASN:HD22	1.65	0.62
1:D:680:ASN:OD1	1:D:682:THR:HB	1.99	0.62
1:D:782:ASP:N	1:D:782:ASP:OD2	2.29	0.62
1:D:806:PRO:CD	1:D:807:GLY:H	2.12	0.62
1:D:150:GLU:HG3	1:D:174:ASN:HB2	1.83	0.61
1:D:733:SER:HB3	1:D:759:LYS:HB3	1.82	0.61
1:A:460:GLU:OE1	6:A:1001:HOH:O	2.15	0.60
1:B:735:VAL:HG13	1:B:735:VAL:O	2.00	0.60
1:B:804:ALA:O	1:B:810:ARG:NH1	2.34	0.60
1:D:761:THR:O	1:D:761:THR:HG22	2.01	0.60
1:D:205:LEU:HD23	1:D:205:LEU:C	2.22	0.60
1:D:780:ILE:O	1:D:780:ILE:HD13	2.02	0.60
1:C:734:GLU:HB2	1:C:760:THR:HG22	1.84	0.59
1:C:731:PHE:O	1:C:756:LEU:N	2.34	0.59
1:C:66:THR:HG22	1:C:88:ASN:O	2.02	0.59
1:C:755:ALA:HB1	1:C:756:LEU:C	2.22	0.59
1:B:761:THR:N	1:B:762:THR:HA	2.17	0.59
1:D:813:SER:OG	1:D:815:VAL:HG12	2.02	0.59
1:C:735:VAL:HG23	1:C:735:VAL:O	2.01	0.59
1:C:370:ARG:HD3	6:C:1021:HOH:O	2.02	0.58
1:C:732:LEU:HD22	6:C:1052:HOH:O	2.04	0.58
1:D:758:THR:OG1	1:D:759:LYS:O	2.20	0.58
3:A:914:NAG:O3	3:A:914:NAG:H82	2.03	0.58
1:D:758:THR:CB	1:D:760:THR:HG23	2.20	0.58
1:D:762:THR:OG1	1:D:763:LYS:O	2.22	0.57
1:B:457:THR:O	1:B:458:ASP:HB2	2.04	0.57
1:C:96:HIS:HD2	1:C:134:ASP:HB3	1.69	0.57
1:D:124:LEU:HB3	6:D:1110:HOH:O	2.05	0.57
1:D:212:SER:OG	1:D:233:GLN:NE2	2.38	0.56
1:D:762:THR:OG1	1:D:763:LYS:N	2.35	0.56
1:D:806:PRO:HD2	1:D:809:GLN:O	2.04	0.56
1:C:733:SER:HA	1:C:735:VAL:N	2.20	0.56
1:D:752:ASN:ND2	1:D:753:LYS:H	2.04	0.56
1:D:760:THR:N	1:D:761:THR:HA	2.21	0.56
1:C:235:LYS:HD2	1:C:270:CYS:SG	2.46	0.55
1:D:809:GLN:HA	1:D:810:ARG:C	2.26	0.55
1:A:67:GLU:OE2	1:A:91:LYS:HE2	2.06	0.55
1:B:234:ILE:O	1:B:256:ASN:HB3	2.07	0.55
1:C:706:SER:HB2	1:C:709:ASP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:SER:CB	1:D:759:LYS:HB3	2.36	0.55
1:A:87:GLN:O	1:A:88:ASN:HB2	2.07	0.54
1:B:753:LYS:N	1:B:753:LYS:HD3	2.22	0.54
1:C:252:ASP:OD1	1:C:293:ASN:HB3	2.06	0.54
1:D:806:PRO:CG	1:D:807:GLY:H	2.21	0.54
1:B:706:SER:HB3	1:B:709:ASP:OD2	2.07	0.54
1:D:211:ASN:O	1:D:232:THR:HA	2.08	0.54
1:B:675:MET:HG2	1:B:699:LYS:HE3	1.90	0.54
1:D:808:ASP:CA	1:D:809:GLN:C	2.76	0.54
1:B:317:ASP:OD1	1:B:319:GLU:OE1	2.25	0.54
1:D:757:GLU:CA	1:D:758:THR:C	2.76	0.54
1:D:758:THR:N	1:D:759:LYS:HA	2.22	0.54
1:A:807:GLY:O	1:A:808:ASP:OD2	2.25	0.54
1:A:471:THR:HG22	1:A:471:THR:O	2.08	0.53
1:C:214:SER:HA	1:C:233:GLN:O	2.08	0.53
1:A:52:ARG:HG2	1:A:799:VAL:HG11	1.89	0.53
1:B:194:ASP:OD1	1:B:219:LYS:NZ	2.33	0.53
1:A:52:ARG:HG3	1:A:799:VAL:HG21	1.90	0.53
1:D:164:GLU:O	1:D:168:ARG:NH1	2.40	0.53
1:D:707:LEU:HD12	1:D:731:PHE:CE1	2.43	0.53
1:C:600:THR:O	1:C:601:ASP:HB2	2.08	0.53
1:C:35:PRO:O	1:C:36:CYS:HB2	2.09	0.53
1:D:48:GLU:O	1:D:52:ARG:NH2	2.42	0.53
1:B:392:GLN:HB2	6:B:1136:HOH:O	2.09	0.52
1:C:490:LEU:HD22	1:D:566:HIS:NE2	2.24	0.52
1:B:523:GLY:O	1:B:552:GLU:HB3	2.09	0.52
1:D:759:LYS:C	1:D:762:THR:H	2.10	0.52
1:A:708:SER:OG	1:A:734:GLU:OE1	2.26	0.52
1:D:751:ILE:CD1	1:D:783:PHE:CE1	2.93	0.52
1:A:333:LEU:HD22	1:A:366:LEU:HD11	1.90	0.52
1:A:205:LEU:C	1:A:205:LEU:HD23	2.30	0.52
1:B:213:LEU:O	1:B:214:SER:HB2	2.09	0.52
1:D:370:ARG:HH22	3:D:1010:NAG:H81	1.75	0.52
1:B:410:ASP:O	1:B:413:LEU:HD23	2.09	0.52
1:D:493:ILE:HG22	1:D:493:ILE:O	2.10	0.52
1:B:211:ASN:O	1:B:232:THR:HA	2.11	0.52
1:C:207:SER:HA	1:C:228:PHE:HB2	1.91	0.51
1:C:35:PRO:O	1:C:36:CYS:CB	2.59	0.51
1:C:140:ILE:HD13	1:C:166:ILE:HD11	1.92	0.51
1:C:692:LEU:HD23	1:C:692:LEU:C	2.30	0.51
1:A:680:ASN:OD1	1:A:682:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ALA:HB2	1:B:541:ARG:HD2	1.91	0.51
1:D:806:PRO:CG	1:D:807:GLY:N	2.73	0.51
1:B:166:ILE:CG2	1:B:200:LEU:HD11	2.41	0.51
1:C:794:LYS:HD3	1:C:794:LYS:N	2.26	0.51
1:D:759:LYS:CD	1:D:759:LYS:N	2.73	0.51
1:A:161:ILE:HD13	1:A:161:ILE:N	2.26	0.50
1:C:732:LEU:C	1:C:735:VAL:HG22	2.32	0.50
1:A:40:LYS:O	1:A:41:GLN:OE1	2.29	0.50
1:D:612:GLU:OE2	1:D:643:ARG:NH1	2.44	0.50
1:D:161:ILE:HD12	1:D:177:LEU:HD13	1.92	0.50
1:D:759:LYS:CD	1:D:759:LYS:H	2.24	0.50
1:C:734:GLU:CB	1:C:760:THR:HG22	2.42	0.50
1:D:428:ASN:O	1:D:429:ARG:HD3	2.11	0.50
1:D:752:ASN:ND2	1:D:753:LYS:N	2.60	0.50
1:D:774:PHE:HB2	1:D:803:CYS:HB3	1.94	0.50
1:C:149:THR:HG22	1:C:171:ASN:O	2.11	0.49
1:D:806:PRO:CD	1:D:807:GLY:N	2.73	0.49
1:D:707:LEU:HD12	1:D:731:PHE:HE1	1.76	0.49
1:D:754:SER:OG	1:D:754:SER:O	2.28	0.49
1:A:809:GLN:HE22	1:A:817:LEU:HD13	1.77	0.49
1:B:761:THR:N	1:B:762:THR:CA	2.75	0.49
1:C:96:HIS:HD2	1:C:134:ASP:CB	2.25	0.49
3:D:1011:NAG:H82	3:D:1011:NAG:O3	2.13	0.49
1:C:130:LEU:HD21	1:C:132:LEU:HD11	1.95	0.49
1:C:692:LEU:HD23	1:C:693:LEU:N	2.27	0.49
1:D:80:ASN:OD1	1:D:80:ASN:N	2.45	0.49
1:C:234:ILE:O	1:C:256:ASN:HB3	2.12	0.49
1:A:430:ILE:HD12	1:A:430:ILE:N	2.27	0.49
1:B:162:THR:HG22	1:B:165:GLY:H	1.78	0.49
1:B:808:ASP:O	1:B:812:LYS:NZ	2.45	0.49
1:D:730:GLY:H	1:D:754:SER:HB2	1.78	0.49
1:A:250:LEU:C	1:A:250:LEU:HD23	2.34	0.48
1:A:516:SER:HB3	1:B:516:SER:OG	2.14	0.48
1:B:205:LEU:C	1:B:205:LEU:HD23	2.33	0.48
1:C:88:ASN:HA	1:C:126:ASN:HD22	1.78	0.48
1:C:52:ARG:HG3	1:C:799:VAL:HG11	1.96	0.48
1:A:752:ASN:OD1	1:A:753:LYS:N	2.46	0.48
1:B:195:GLY:O	1:B:198:GLU:HG2	2.14	0.48
1:C:34:TYR:CD1	1:C:815:VAL:HG11	2.49	0.48
1:D:693:LEU:HD23	1:D:717:LEU:CD1	2.44	0.48
1:D:736:SER:HA	1:D:762:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ILE:CD1	1:D:784:ARG:CG	2.83	0.48
1:A:534:TYR:CE2	1:A:558:VAL:HG11	2.50	0.47
1:A:234:ILE:O	1:A:256:ASN:HB3	2.14	0.47
1:A:54:LEU:HD13	1:A:58:PRO:HG3	1.95	0.47
1:D:278:ILE:HB	1:D:306:TRP:CZ2	2.49	0.47
1:A:506:ASP:OD1	1:A:531:HIS:HD2	1.97	0.47
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.96	0.47
1:B:141:PRO:HB2	1:B:144:LEU:HD21	1.97	0.47
1:C:67:GLU:OE2	1:C:91:LYS:CE	2.63	0.47
1:B:548:SER:O	1:B:551:THR:OG1	2.21	0.47
1:D:225:ARG:O	1:D:248:LEU:HD22	2.14	0.47
1:D:759:LYS:HD2	1:D:759:LYS:N	2.29	0.47
1:B:72:ASP:O	1:B:99:ASN:ND2	2.48	0.47
1:C:223:SER:O	1:C:225:ARG:NH1	2.48	0.47
1:C:670:HIS:HA	1:C:694:ASP:HB3	1.95	0.47
1:C:149:THR:HA	1:C:171:ASN:O	2.15	0.47
1:A:166:ILE:CG2	1:A:200:LEU:HD11	2.45	0.46
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.15	0.46
1:C:516:SER:OG	1:D:516:SER:HB3	2.14	0.46
1:B:40:LYS:HA	1:B:45:VAL:HA	1.97	0.46
1:C:616:SER:HA	1:C:647:SER:O	2.16	0.46
1:D:775:GLU:HA	1:D:805:SER:CB	2.41	0.46
1:D:806:PRO:HG2	1:D:807:GLY:H	1.81	0.46
1:D:809:GLN:HG3	1:D:812:LYS:HD2	1.97	0.46
1:B:52:ARG:HG2	1:B:799:VAL:HG11	1.97	0.46
1:C:385:ASP:HA	1:C:388:GLN:HG2	1.97	0.46
1:D:467:PHE:HB3	3:D:1001:NAG:H81	1.97	0.46
1:D:753:LYS:HG2	1:D:782:ASP:OD1	2.16	0.46
1:C:720:SER:OG	1:C:742:ASP:OD2	2.25	0.46
1:C:88:ASN:N	1:C:88:ASN:HD22	2.14	0.46
1:B:200:LEU:O	1:B:221:PRO:HG3	2.16	0.46
1:C:67:GLU:OE2	1:C:91:LYS:HE3	2.15	0.46
1:D:484:LYS:HE2	1:D:505:PRO:HB2	1.97	0.46
1:D:518:ALA:HB2	1:D:541:ARG:HD2	1.98	0.46
1:A:57:VAL:HG21	1:A:82:SER:HB3	1.98	0.46
1:C:211:ASN:O	1:C:232:THR:HA	2.16	0.46
1:C:119:GLY:HA3	1:C:122:LEU:HD23	1.99	0.45
1:D:759:LYS:HE3	1:D:759:LYS:H	1.81	0.45
1:A:370:ARG:NH2	3:A:913:NAG:H81	2.31	0.45
1:C:388:GLN:N	1:C:389:PRO:CD	2.80	0.45
1:A:211:ASN:O	1:A:232:THR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLN:H	1:C:59:GLN:CD	2.18	0.45
1:C:733:SER:CB	1:C:734:GLU:HA	2.47	0.45
1:C:755:ALA:HA	1:C:756:LEU:CB	2.46	0.45
1:C:259:ARG:NH1	1:C:321:ASN:O	2.50	0.45
1:D:693:LEU:HD21	1:D:695:LEU:HD11	1.99	0.45
1:D:809:GLN:HA	1:D:810:ARG:O	2.16	0.45
1:D:45:VAL:N	1:D:66:THR:HG1	2.15	0.45
1:D:758:THR:CB	1:D:759:LYS:C	2.85	0.45
1:A:401:LEU:HB2	1:A:425:LEU:HD23	1.98	0.45
1:A:52:ARG:HB3	1:A:54:LEU:HG	1.99	0.45
1:A:616:SER:HA	1:A:647:SER:O	2.17	0.45
1:A:720:SER:HA	1:A:744:SER:O	2.17	0.45
1:D:183:PHE:HB3	1:D:266:PRO:HG2	1.99	0.45
1:D:475:ILE:HD13	1:D:487:ASP:HB2	1.99	0.45
1:D:758:THR:HB	1:D:759:LYS:C	2.37	0.45
1:D:780:ILE:HG23	1:D:781:GLY:N	2.32	0.45
1:A:505:PRO:O	1:A:507:ILE:HG12	2.17	0.44
1:B:150:GLU:HG2	1:B:174:ASN:HB2	1.99	0.44
1:B:287:THR:HA	1:B:309:ASN:O	2.17	0.44
1:B:115:ASN:OD1	1:B:115:ASN:C	2.56	0.44
1:B:338:ARG:HA	1:B:368:SER:OG	2.18	0.44
1:D:166:ILE:HA	1:D:169:LEU:HD12	1.98	0.44
1:D:312:HIS:HE1	6:D:1127:HOH:O	1.99	0.44
1:B:475:ILE:CD1	1:B:487:ASP:HB2	2.47	0.44
1:D:327:ILE:HG12	1:D:344:LEU:HD13	2.00	0.44
1:B:457:THR:O	1:B:458:ASP:CB	2.65	0.44
1:D:565:SER:O	1:D:566:HIS:C	2.55	0.44
1:D:780:ILE:CD1	1:D:780:ILE:C	2.85	0.44
1:D:501:PHE:HB2	1:D:528:ALA:HB3	1.99	0.44
1:D:757:GLU:HA	1:D:758:THR:O	2.18	0.44
1:A:213:LEU:O	1:A:214:SER:HB2	2.17	0.43
1:D:808:ASP:N	1:D:808:ASP:OD1	2.50	0.43
1:A:86:LEU:C	1:A:87:GLN:O	2.54	0.43
1:B:692:LEU:HD23	1:B:692:LEU:C	2.39	0.43
1:D:650:ARG:HA	1:D:675:MET:HE3	2.01	0.43
1:B:388:GLN:N	1:B:389:PRO:CD	2.81	0.43
1:C:128:ARG:HG2	1:C:147:SER:O	2.19	0.43
1:C:230:SER:HA	1:C:254:SER:O	2.19	0.43
1:C:287:THR:HA	1:C:309:ASN:O	2.18	0.43
1:A:805:SER:HB2	1:A:806:PRO:HA	2.01	0.43
1:C:336:LEU:HD13	1:C:339:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:753:LYS:HD2	1:C:753:LYS:O	2.19	0.43
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.37	0.43
1:B:34:TYR:CG	1:B:35:PRO:HA	2.54	0.43
1:A:373:HIS:HA	1:A:400:ASN:HB3	2.01	0.42
1:A:471:THR:O	1:A:471:THR:CG2	2.66	0.42
1:C:327:ILE:HG12	1:C:344:LEU:HD13	2.00	0.42
1:D:504:LEU:HA	1:D:504:LEU:HD23	1.87	0.42
1:A:370:ARG:HH22	3:A:913:NAG:H81	1.84	0.42
1:A:68:LEU:HD21	1:A:70:LEU:HD11	2.01	0.42
1:B:782:ASP:HA	1:B:785:ARG:NH1	2.34	0.42
1:D:467:PHE:CB	3:D:1001:NAG:H81	2.49	0.42
1:D:758:THR:HB	1:D:760:THR:CB	2.48	0.42
1:C:155:GLN:HA	1:C:179:TRP:O	2.20	0.42
1:C:181:CYS:O	1:C:211:ASN:HA	2.19	0.42
1:A:807:GLY:O	1:A:808:ASP:CG	2.58	0.42
1:C:472:ARG:HH11	1:C:472:ARG:CG	2.32	0.42
1:A:159:TYR:CE1	1:A:187:CYS:HB2	2.54	0.42
1:B:583:PHE:HB3	6:B:1142:HOH:O	2.19	0.42
1:C:732:LEU:O	1:C:735:VAL:HG13	2.20	0.42
1:D:419:ASN:N	1:D:419:ASN:OD1	2.53	0.42
1:D:760:THR:HG1	1:D:762:THR:H	1.67	0.42
1:C:576:HIS:HB3	1:C:578:GLU:OE1	2.20	0.42
1:B:155:GLN:HA	1:B:179:TRP:O	2.20	0.42
1:B:353:TYR:CZ	1:B:380:GLN:HG2	2.55	0.42
1:D:230:SER:O	1:D:232:THR:HG23	2.20	0.42
1:D:234:ILE:O	1:D:256:ASN:HB3	2.19	0.42
1:B:250:LEU:HD23	1:B:250:LEU:C	2.40	0.42
1:C:375:ARG:HA	1:C:402:GLY:O	2.20	0.42
1:D:296:SER:HA	1:D:320:PHE:O	2.19	0.42
1:D:783:PHE:CE2	1:D:787:MET:SD	3.13	0.41
1:B:600:THR:O	1:B:601:ASP:HB2	2.20	0.41
1:D:505:PRO:O	1:D:507:ILE:HG12	2.20	0.41
1:D:47:ALA:HB3	1:D:68:LEU:HA	2.03	0.41
1:B:532:VAL:HB	1:B:553:LEU:HD22	2.01	0.41
1:D:69:ASP:HA	1:D:93:ASN:HB3	2.02	0.41
1:A:430:ILE:H	1:A:430:ILE:HD12	1.84	0.41
1:B:214:SER:HA	1:B:233:GLN:O	2.20	0.41
1:B:760:THR:HA	1:B:761:THR:C	2.40	0.41
1:B:565:SER:OG	1:B:569:ARG:NH1	2.53	0.41
1:C:491:ASN:HB3	1:C:492:SER:H	1.71	0.41
1:D:788:ASP:HA	1:D:791:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:N	1:A:389:PRO:CD	2.84	0.41
1:B:314:LYS:C	1:B:339:LEU:HD12	2.41	0.41
1:B:419:ASN:HD22	1:B:419:ASN:HA	1.72	0.41
1:C:235:LYS:HD3	1:C:235:LYS:N	2.35	0.41
1:D:647:SER:HA	1:D:672:ASN:O	2.20	0.41
1:A:235:LYS:HE2	1:A:235:LYS:HB2	1.87	0.41
1:B:220:LEU:HB2	1:B:245:LEU:HD21	2.03	0.41
1:B:780:ILE:O	1:B:783:PHE:N	2.54	0.41
1:C:514:ALA:HA	1:C:539:ASN:O	2.19	0.41
1:D:319:GLU:OE1	1:D:469:HIS:HD2	2.04	0.41
1:C:753:LYS:C	1:C:755:ALA:N	2.74	0.41
1:A:356:HIS:CD2	1:A:383:ARG:HE	2.39	0.41
1:C:257:CYS:N	1:C:258:PRO:CD	2.84	0.40
1:C:523:GLY:O	1:C:552:GLU:HB3	2.22	0.40
1:C:749:LYS:O	1:C:774:PHE:HA	2.21	0.40
1:D:764:LEU:O	1:D:793:VAL:HG22	2.21	0.40
1:C:261:PHE:CZ	1:C:350:LYS:HD2	2.57	0.40
1:D:413:LEU:HD12	1:D:413:LEU:C	2.41	0.40
1:B:485:ALA:HA	1:B:509:CYS:O	2.22	0.40
1:D:608:LYS:O	1:D:640:ASN:HB2	2.21	0.40
1:D:707:LEU:CD1	1:D:731:PHE:HE1	2.35	0.40
1:D:758:THR:CB	1:D:760:THR:CG2	2.85	0.40
1:A:336:LEU:N	1:A:337:PRO:CD	2.84	0.40
1:C:119:GLY:HA2	1:C:143:GLY:HA3	2.03	0.40
1:D:806:PRO:HD2	1:D:807:GLY:N	2.32	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%)	47 (6%)	1 (0%)	56 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	741/811 (91%)	694 (94%)	45 (6%)	2 (0%)	46	63
1	C	740/811 (91%)	680 (92%)	56 (8%)	4 (0%)	34	48
1	D	738/811 (91%)	677 (92%)	58 (8%)	3 (0%)	39	56
All	All	2959/3244 (91%)	2743 (93%)	206 (7%)	10 (0%)	46	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	806	PRO
1	B	458	ASP
1	D	709	ASP
1	C	378	VAL
1	B	378	VAL
1	C	36	CYS
1	C	60	THR
1	D	378	VAL
1	A	378	VAL
1	C	186	VAL

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	695/755 (92%)	646 (93%)	49 (7%)	18	28
1	B	696/755 (92%)	654 (94%)	42 (6%)	24	37
1	C	695/755 (92%)	652 (94%)	43 (6%)	23	35
1	D	693/755 (92%)	642 (93%)	51 (7%)	17	26
All	All	2779/3020 (92%)	2594 (93%)	185 (7%)	20	31

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG

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Mol	Chain	Res	Type
1	A	41	GLN
1	A	49	CYS
1	A	52	ARG
1	A	64	TYR
1	A	84	GLN
1	A	87	GLN
1	A	88	ASN
1	A	112	ASN
1	A	122	LEU
1	A	150	GLU
1	A	160	ASN
1	A	168	ARG
1	A	170	ILE
1	A	225	ARG
1	A	235	LYS
1	A	248	LEU
1	A	280	ARG
1	A	286	LEU
1	A	308	LYS
1	A	334	THR
1	A	338	ARG
1	A	399	ILE
1	A	419	ASN
1	A	429	ARG
1	A	465	SER
1	A	554	SER
1	A	569	ARG
1	A	629	ASN
1	A	632	ILE
1	A	657	GLU
1	A	686	GLN
1	A	689	ARG
1	A	706	SER
1	A	708	SER
1	A	712	SER
1	A	733	SER
1	A	735	VAL
1	A	753	LYS
1	A	756	LEU
1	A	763	LYS
1	A	778	CYS
1	A	779	ASP

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Mol	Chain	Res	Type
1	A	794	LYS
1	A	795	ILE
1	A	799	VAL
1	A	808	ASP
1	A	815	VAL
1	A	817	LEU
1	B	40	LYS
1	B	49	CYS
1	B	51	ASN
1	B	52	ARG
1	B	56	GLU
1	B	82	SER
1	B	86	LEU
1	B	87	GLN
1	B	96	HIS
1	B	118	ASP
1	B	122	LEU
1	B	150	GLU
1	B	162	THR
1	B	168	ARG
1	B	188	GLU
1	B	199	THR
1	B	201	THR
1	B	248	LEU
1	B	286	LEU
1	B	308	LYS
1	B	368	SER
1	B	415	GLN
1	B	416	ASN
1	B	419	ASN
1	B	471	THR
1	B	472	ARG
1	B	534	TYR
1	B	595	ASN
1	B	625	ASN
1	B	632	ILE
1	B	686	GLN
1	B	702	PHE
1	B	708	SER
1	B	727	LEU
1	B	733	SER
1	B	736	SER

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Mol	Chain	Res	Type
1	B	737	SER
1	B	753	LYS
1	B	758	THR
1	B	760	THR
1	B	797	ARG
1	B	815	VAL
1	C	32	ARG
1	C	40	LYS
1	C	49	CYS
1	C	56	GLU
1	C	88	ASN
1	C	96	HIS
1	C	100	VAL
1	C	114	LEU
1	C	122	LEU
1	C	125	LYS
1	C	150	GLU
1	C	163	LYS
1	C	193	GLU
1	C	214	SER
1	C	240	GLU
1	C	248	LEU
1	C	271	ASP
1	C	286	LEU
1	C	314	LYS
1	C	361	ARG
1	C	370	ARG
1	C	384	GLU
1	C	397	SER
1	C	408	GLN
1	C	470	PHE
1	C	472	ARG
1	C	625	ASN
1	C	678	PHE
1	C	705	ASP
1	C	709	ASP
1	C	720	SER
1	C	725	SER
1	C	732	LEU
1	C	733	SER
1	C	734	GLU
1	C	753	LYS

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Mol	Chain	Res	Type
1	C	756	LEU
1	C	759	LYS
1	C	761	THR
1	C	775	GLU
1	C	778	CYS
1	C	797	ARG
1	C	798	LEU
1	D	49	CYS
1	D	52	ARG
1	D	64	TYR
1	D	66	THR
1	D	118	ASP
1	D	122	LEU
1	D	125	LYS
1	D	160	ASN
1	D	162	THR
1	D	173	LYS
1	D	212	SER
1	D	235	LYS
1	D	240	GLU
1	D	243	LYS
1	D	248	LEU
1	D	280	ARG
1	D	286	LEU
1	D	301	LYS
1	D	358	ASN
1	D	413	LEU
1	D	416	ASN
1	D	457	THR
1	D	458	ASP
1	D	465	SER
1	D	475	ILE
1	D	484	LYS
1	D	534	TYR
1	D	554	SER
1	D	595	ASN
1	D	625	ASN
1	D	632	ILE
1	D	701	LEU
1	D	707	LEU
1	D	720	SER
1	D	727	LEU

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Mol	Chain	Res	Type
1	D	731	PHE
1	D	745	SER
1	D	752	ASN
1	D	753	LYS
1	D	757	GLU
1	D	758	THR
1	D	759	LYS
1	D	778	CYS
1	D	780	ILE
1	D	782	ASP
1	D	787	MET
1	D	789	GLU
1	D	805	SER
1	D	806	PRO
1	D	809	GLN
1	D	812	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	77	HIS
1	A	88	ASN
1	A	96	HIS
1	A	285	ASN
1	A	356	HIS
1	A	419	ASN
1	A	531	HIS
1	A	629	ASN
1	A	686	GLN
1	A	809	GLN
1	B	51	ASN
1	B	55	GLN
1	B	87	GLN
1	B	99	ASN
1	B	285	ASN
1	B	419	ASN
1	C	88	ASN
1	C	96	HIS
1	C	126	ASN
1	C	184	ASN
1	C	191	ASN

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Mol	Chain	Res	Type
1	C	355	GLN
1	C	388	GLN
1	C	566	HIS
1	C	593	HIS
1	C	604	ASN
1	C	625	ASN
1	D	123	ASN
1	D	233	GLN
1	D	312	HIS
1	D	355	GLN
1	D	358	ASN
1	D	469	HIS
1	D	752	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 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	0.85	0	15,19,21	1.28	3 (20%)
3	NAG	A	903	3,4	14,14,15	0.82	0	15,19,21	1.68	6 (40%)
5	MAN	A	905	4	11,11,12	0.79	0	15,15,17	1.28	3 (20%)
3	NAG	A	906	1,3	14,14,15	0.62	0	15,19,21	1.53	3 (20%)
3	NAG	A	907	3	14,14,15	0.83	1 (7%)	15,19,21	1.48	2 (13%)
3	NAG	A	908	1,3	14,14,15	0.60	0	15,19,21	1.50	4 (26%)
3	NAG	A	909	3,4	14,14,15	1.04	1 (7%)	15,19,21	1.29	2 (13%)
5	MAN	A	911	4	11,11,12	0.55	0	15,15,17	1.42	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	912	1	14,14,15	0.58	0	15,19,21	1.83	2 (13%)
3	NAG	A	913	1	14,14,15	0.72	0	15,19,21	1.27	1 (6%)
3	NAG	A	914	1	14,14,15	0.71	0	15,19,21	1.66	3 (20%)
3	NAG	B	1001	1,3	14,14,15	0.77	0	15,19,21	1.57	3 (20%)
3	NAG	B	1002	3,4	14,14,15	0.52	0	15,19,21	1.24	2 (13%)
5	MAN	B	1004	4	11,11,12	0.86	0	15,15,17	1.83	5 (33%)
3	NAG	B	1005	1,3	14,14,15	0.88	0	15,19,21	1.46	2 (13%)
3	NAG	B	1006	3	14,14,15	0.87	1 (7%)	15,19,21	1.83	5 (33%)
3	NAG	B	1007	1,3	14,14,15	0.86	0	15,19,21	0.94	0
3	NAG	B	1008	3,4	14,14,15	1.11	1 (7%)	15,19,21	1.20	2 (13%)
3	NAG	B	1010	1	14,14,15	0.75	1 (7%)	15,19,21	1.89	5 (33%)
3	NAG	B	1011	1	14,14,15	0.64	0	15,19,21	1.04	0
3	NAG	B	1012	1	14,14,15	0.88	1 (7%)	15,19,21	1.53	3 (20%)
3	NAG	B	1013	1	14,14,15	0.69	0	15,19,21	1.76	3 (20%)
3	NAG	C	902	1,3	14,14,15	0.72	0	15,19,21	1.41	3 (20%)
3	NAG	C	903	3,4	14,14,15	0.65	0	15,19,21	1.86	6 (40%)
3	NAG	C	905	1,3	14,14,15	0.68	0	15,19,21	1.13	1 (6%)
3	NAG	C	906	3	14,14,15	0.57	0	15,19,21	1.24	2 (13%)
3	NAG	C	907	1	14,14,15	0.85	0	15,19,21	1.29	2 (13%)
3	NAG	C	908	1,3	14,14,15	0.52	0	15,19,21	1.18	2 (13%)
3	NAG	C	909	3,4	14,14,15	0.92	1 (7%)	15,19,21	1.01	1 (6%)
5	MAN	C	911	4	11,11,12	1.02	1 (9%)	15,15,17	1.49	3 (20%)
3	NAG	C	912	1	14,14,15	0.69	0	15,19,21	1.60	1 (6%)
3	NAG	C	913	1	14,14,15	0.90	1 (7%)	15,19,21	1.27	3 (20%)
3	NAG	C	914	1	14,14,15	0.84	1 (7%)	15,19,21	0.87	0
3	NAG	D	1001	1,3	14,14,15	0.92	1 (7%)	15,19,21	1.15	1 (6%)
3	NAG	D	1002	3,4	14,14,15	0.60	0	15,19,21	1.06	0
3	NAG	D	1004	1,3	14,14,15	0.71	1 (7%)	15,19,21	1.41	2 (13%)
3	NAG	D	1005	3	14,14,15	0.72	0	15,19,21	1.33	2 (13%)
3	NAG	D	1006	1	14,14,15	0.51	0	15,19,21	1.46	2 (13%)
3	NAG	D	1007	1,3	14,14,15	0.63	0	15,19,21	1.36	1 (6%)
3	NAG	D	1008	3,4	14,14,15	0.73	0	15,19,21	1.30	3 (20%)
3	NAG	D	1010	1	14,14,15	0.73	0	15,19,21	1.24	2 (13%)
3	NAG	D	1011	1	14,14,15	0.65	0	15,19,21	1.81	4 (26%)

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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	907	3	-	0/6/23/26	0/1/1/1
3	NAG	A	908	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	3,4	-	0/6/23/26	0/1/1/1
5	MAN	A	911	4	-	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
3	NAG	A	914	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3,4	-	0/6/23/26	0/1/1/1
5	MAN	B	1004	4	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1006	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1008	3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1013	1	-	0/6/23/26	0/1/1/1
3	NAG	C	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	903	3,4	-	0/6/23/26	0/1/1/1
3	NAG	C	905	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	906	3	-	0/6/23/26	0/1/1/1
3	NAG	C	907	1	-	0/6/23/26	0/1/1/1
3	NAG	C	908	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	909	3,4	-	0/6/23/26	0/1/1/1
5	MAN	C	911	4	-	0/2/19/22	0/1/1/1
3	NAG	C	912	1	-	0/6/23/26	0/1/1/1
3	NAG	C	913	1	-	0/6/23/26	0/1/1/1
3	NAG	C	914	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1002	3,4	-	0/6/23/26	0/1/1/1
3	NAG	D	1004	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1005	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1006	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1008	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1011	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1008	NAG	O5-C1	-3.14	1.38	1.43
3	A	909	NAG	O5-C1	-2.91	1.39	1.43
3	D	1001	NAG	O5-C1	-2.67	1.39	1.43
3	C	909	NAG	O5-C1	-2.66	1.39	1.43
3	B	1012	NAG	O5-C1	-2.55	1.39	1.43
3	A	907	NAG	O5-C1	-2.42	1.39	1.43
3	B	1006	NAG	O5-C1	-2.34	1.39	1.43
3	D	1004	NAG	O5-C1	-2.18	1.40	1.43
3	C	913	NAG	O5-C1	-2.10	1.40	1.43
3	B	1010	NAG	O5-C1	-2.09	1.40	1.43
3	C	914	NAG	C1-C2	2.12	1.55	1.52
5	C	911	MAN	C2-C3	2.79	1.56	1.52

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	912	NAG	C4-C3-C2	-4.21	104.81	111.34
3	B	1005	NAG	C3-C4-C5	-4.10	102.91	110.23
3	A	907	NAG	C3-C4-C5	-4.10	102.92	110.23
3	C	903	NAG	C2-N2-C7	-3.53	118.52	123.11
3	B	1006	NAG	C3-C4-C5	-3.51	103.96	110.23
3	D	1011	NAG	C4-C3-C2	-3.23	106.33	111.34
3	A	913	NAG	O4-C4-C3	-3.10	103.36	110.36
3	B	1001	NAG	C2-N2-C7	-3.08	119.09	123.11
3	A	906	NAG	C3-C4-C5	-3.08	104.74	110.23
3	D	1008	NAG	C4-C3-C2	-3.04	106.62	111.34
3	B	1002	NAG	C3-C4-C5	-3.02	104.85	110.23
3	D	1005	NAG	O3-C3-C4	-2.95	103.70	110.36
3	A	914	NAG	C4-C3-C2	-2.95	106.76	111.34
3	C	908	NAG	O5-C5-C4	-2.94	105.26	110.13
3	C	903	NAG	C1-O5-C5	-2.90	107.87	112.14
5	A	911	MAN	O5-C1-C2	-2.89	106.28	110.89
3	B	1008	NAG	O6-C6-C5	-2.79	101.97	111.30
3	B	1001	NAG	C3-C4-C5	-2.77	105.29	110.23
3	C	903	NAG	O3-C3-C4	-2.70	104.26	110.36
3	D	1010	NAG	O5-C5-C4	-2.67	105.70	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	MAN	O5-C1-C2	-2.66	106.65	110.89
5	A	911	MAN	C1-C2-C3	-2.61	106.39	109.55
3	A	903	NAG	O7-C7-C8	-2.57	117.33	122.07
3	A	909	NAG	C4-C3-C2	-2.57	107.34	111.34
3	D	1006	NAG	O7-C7-C8	-2.57	117.34	122.07
3	C	902	NAG	C2-N2-C7	-2.54	119.81	123.11
3	C	907	NAG	O5-C5-C4	-2.51	105.98	110.13
3	B	1006	NAG	O5-C5-C4	-2.47	106.04	110.13
3	A	903	NAG	C1-O5-C5	-2.47	108.51	112.14
3	A	908	NAG	O7-C7-C8	-2.41	117.64	122.07
3	B	1005	NAG	O5-C5-C4	-2.40	106.17	110.13
3	C	905	NAG	O7-C7-C8	-2.36	117.72	122.07
3	C	902	NAG	O4-C4-C5	-2.35	103.03	109.23
3	A	909	NAG	O6-C6-C5	-2.35	103.47	111.30
5	B	1004	MAN	O3-C3-C4	-2.34	105.08	110.36
3	A	914	NAG	O7-C7-N2	-2.34	117.08	121.84
3	B	1010	NAG	C2-N2-C7	-2.33	120.07	123.11
3	C	909	NAG	O4-C4-C3	-2.33	105.10	110.36
3	A	902	NAG	O7-C7-C8	-2.29	117.85	122.07
3	B	1006	NAG	C4-C3-C2	-2.25	107.85	111.34
3	C	907	NAG	O4-C4-C3	-2.24	105.32	110.36
3	B	1008	NAG	C4-C3-C2	-2.24	107.87	111.34
3	A	903	NAG	C3-C4-C5	-2.22	106.28	110.23
3	B	1010	NAG	O3-C3-C4	-2.17	105.46	110.36
3	C	903	NAG	O6-C6-C5	-2.13	104.20	111.30
3	C	913	NAG	O7-C7-C8	-2.11	118.19	122.07
3	C	903	NAG	O4-C4-C3	-2.10	105.62	110.36
3	A	903	NAG	O6-C6-C5	-2.10	104.29	111.30
3	D	1011	NAG	O7-C7-N2	-2.09	117.59	121.84
3	B	1012	NAG	O6-C6-C5	-2.09	104.33	111.30
3	D	1001	NAG	C3-C4-C5	-2.08	106.51	110.23
3	B	1010	NAG	O7-C7-N2	-2.05	117.68	121.84
3	A	902	NAG	O6-C6-C5	-2.04	104.50	111.30
3	D	1008	NAG	O6-C6-C5	-2.02	104.55	111.30
3	A	908	NAG	O5-C5-C4	-2.01	106.81	110.13
5	A	911	MAN	O3-C3-C2	2.01	113.68	110.01
3	A	907	NAG	O5-C5-C6	2.03	111.68	107.34
3	A	908	NAG	O7-C7-N2	2.03	125.99	121.84
3	A	903	NAG	C2-N2-C7	2.04	125.76	123.11
3	C	913	NAG	O3-C3-C4	2.05	114.98	110.36
3	D	1008	NAG	O7-C7-N2	2.06	126.04	121.84
3	D	1005	NAG	O4-C4-C5	2.07	114.67	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	MAN	O2-C2-C3	2.07	114.36	110.19
3	C	908	NAG	C1-O5-C5	2.08	115.19	112.14
3	B	1002	NAG	C1-O5-C5	2.10	115.23	112.14
3	C	903	NAG	O4-C4-C5	2.11	114.78	109.23
3	A	906	NAG	O3-C3-C4	2.13	115.17	110.36
3	C	906	NAG	O4-C4-C5	2.14	114.87	109.23
3	D	1004	NAG	O5-C5-C4	2.15	113.69	110.13
3	C	902	NAG	O3-C3-C4	2.16	115.23	110.36
5	A	905	MAN	C1-O5-C5	2.18	115.34	112.14
5	C	911	MAN	O3-C3-C4	2.18	115.27	110.36
3	D	1010	NAG	O3-C3-C4	2.18	115.28	110.36
5	A	911	MAN	C1-O5-C5	2.26	115.47	112.14
3	B	1012	NAG	C1-O5-C5	2.27	115.47	112.14
3	B	1006	NAG	C8-C7-N2	2.29	120.50	116.10
5	C	911	MAN	O2-C2-C3	2.32	114.86	110.19
3	C	906	NAG	C1-O5-C5	2.32	115.56	112.14
3	A	902	NAG	C1-O5-C5	2.48	115.79	112.14
5	A	905	MAN	O2-C2-C1	2.51	114.27	109.23
3	A	908	NAG	C2-N2-C7	2.56	126.43	123.11
3	C	913	NAG	C1-O5-C5	2.57	115.92	112.14
3	B	1001	NAG	O5-C5-C6	2.58	112.87	107.34
3	B	1013	NAG	C1-O5-C5	2.61	115.98	112.14
3	A	903	NAG	O7-C7-N2	2.73	127.41	121.84
3	D	1011	NAG	C2-N2-C7	2.74	126.66	123.11
5	B	1004	MAN	C2-C3-C4	2.75	115.85	111.05
3	B	1006	NAG	O4-C4-C5	2.76	116.50	109.23
5	B	1004	MAN	C3-C4-C5	2.77	115.17	110.23
3	B	1013	NAG	O5-C5-C6	2.87	113.47	107.34
5	B	1004	MAN	C1-C2-C3	2.92	113.09	109.55
3	D	1004	NAG	C1-O5-C5	2.98	116.52	112.14
3	B	1012	NAG	O5-C5-C4	3.04	115.17	110.13
3	B	1010	NAG	O5-C5-C4	3.27	115.55	110.13
3	D	1006	NAG	C8-C7-N2	3.27	122.37	116.10
5	C	911	MAN	O3-C3-C2	3.32	116.08	110.01
3	B	1013	NAG	C2-N2-C7	3.54	127.71	123.11
3	D	1011	NAG	C8-C7-N2	3.55	122.90	116.10
3	A	906	NAG	O5-C5-C4	3.67	116.21	110.13
3	A	914	NAG	C8-C7-N2	3.94	123.65	116.10
3	D	1007	NAG	C1-O5-C5	4.39	118.60	112.14
3	B	1010	NAG	C1-O5-C5	4.44	118.68	112.14
3	A	912	NAG	C1-O5-C5	4.71	119.07	112.14
3	C	912	NAG	C1-O5-C5	5.14	119.70	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	913	NAG	2	0
3	A	914	NAG	1	0
3	C	902	NAG	1	0
3	D	1001	NAG	2	0
3	D	1010	NAG	1	0
3	D	1011	NAG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

54 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	MBL	A	901	-	15,18,18	0.69	0	16,23,23	0.98	1 (6%)
3	NAG	A	902	1,3	14,14,15	0.85	0	15,19,21	1.28	3 (20%)
3	NAG	A	903	3,4	14,14,15	0.82	0	15,19,21	1.68	6 (40%)
4	BMA	A	904	3,5	11,11,12	0.73	0	15,15,17	1.78	5 (33%)
5	MAN	A	905	4	11,11,12	0.79	0	15,15,17	1.28	3 (20%)
3	NAG	A	906	1,3	14,14,15	0.62	0	15,19,21	1.53	3 (20%)
3	NAG	A	907	3	14,14,15	0.83	1 (7%)	15,19,21	1.48	2 (13%)
3	NAG	A	908	1,3	14,14,15	0.60	0	15,19,21	1.50	4 (26%)
3	NAG	A	909	3,4	14,14,15	1.04	1 (7%)	15,19,21	1.29	2 (13%)
4	BMA	A	910	3,5	11,11,12	0.58	0	15,15,17	1.70	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	911	4	11,11,12	0.55	0	15,15,17	1.42	4 (26%)
3	NAG	A	912	1	14,14,15	0.58	0	15,19,21	1.83	2 (13%)
3	NAG	A	913	1	14,14,15	0.72	0	15,19,21	1.27	1 (6%)
3	NAG	A	914	1	14,14,15	0.71	0	15,19,21	1.66	3 (20%)
2	MBL	A	915	-	15,18,18	0.66	0	16,23,23	1.26	2 (12%)
3	NAG	B	1001	1,3	14,14,15	0.77	0	15,19,21	1.57	3 (20%)
3	NAG	B	1002	3,4	14,14,15	0.52	0	15,19,21	1.24	2 (13%)
4	BMA	B	1003	3,5	11,11,12	0.67	0	15,15,17	1.82	3 (20%)
5	MAN	B	1004	4	11,11,12	0.86	0	15,15,17	1.83	5 (33%)
3	NAG	B	1005	1,3	14,14,15	0.88	0	15,19,21	1.46	2 (13%)
3	NAG	B	1006	3	14,14,15	0.87	1 (7%)	15,19,21	1.83	5 (33%)
3	NAG	B	1007	1,3	14,14,15	0.86	0	15,19,21	0.94	0
3	NAG	B	1008	3,4	14,14,15	1.11	1 (7%)	15,19,21	1.20	2 (13%)
4	BMA	B	1009	3	11,11,12	0.56	0	15,15,17	1.66	3 (20%)
3	NAG	B	1010	1	14,14,15	0.75	1 (7%)	15,19,21	1.89	5 (33%)
3	NAG	B	1011	1	14,14,15	0.64	0	15,19,21	1.04	0
3	NAG	B	1012	1	14,14,15	0.88	1 (7%)	15,19,21	1.53	3 (20%)
3	NAG	B	1013	1	14,14,15	0.69	0	15,19,21	1.76	3 (20%)
2	MBL	C	901	-	15,18,18	0.58	0	16,23,23	1.27	3 (18%)
3	NAG	C	902	1,3	14,14,15	0.72	0	15,19,21	1.41	3 (20%)
3	NAG	C	903	3,4	14,14,15	0.65	0	15,19,21	1.86	6 (40%)
4	BMA	C	904	3	11,11,12	0.71	0	15,15,17	1.48	3 (20%)
3	NAG	C	905	1,3	14,14,15	0.68	0	15,19,21	1.13	1 (6%)
3	NAG	C	906	3	14,14,15	0.57	0	15,19,21	1.24	2 (13%)
3	NAG	C	907	1	14,14,15	0.85	0	15,19,21	1.29	2 (13%)
3	NAG	C	908	1,3	14,14,15	0.52	0	15,19,21	1.18	2 (13%)
3	NAG	C	909	3,4	14,14,15	0.92	1 (7%)	15,19,21	1.01	1 (6%)
4	BMA	C	910	3,5	11,11,12	0.69	0	15,15,17	1.54	3 (20%)
5	MAN	C	911	4	11,11,12	1.02	1 (9%)	15,15,17	1.49	3 (20%)
3	NAG	C	912	1	14,14,15	0.69	0	15,19,21	1.60	1 (6%)
3	NAG	C	913	1	14,14,15	0.90	1 (7%)	15,19,21	1.27	3 (20%)
3	NAG	C	914	1	14,14,15	0.84	1 (7%)	15,19,21	0.87	0
2	MBL	C	915	-	15,18,18	0.88	0	16,23,23	1.51	4 (25%)
3	NAG	D	1001	1,3	14,14,15	0.92	1 (7%)	15,19,21	1.15	1 (6%)
3	NAG	D	1002	3,4	14,14,15	0.60	0	15,19,21	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	D	1003	3	11,11,12	1.18	1 (9%)	15,15,17	1.97	4 (26%)
3	NAG	D	1004	1,3	14,14,15	0.71	1 (7%)	15,19,21	1.41	2 (13%)
3	NAG	D	1005	3	14,14,15	0.72	0	15,19,21	1.33	2 (13%)
3	NAG	D	1006	1	14,14,15	0.51	0	15,19,21	1.46	2 (13%)
3	NAG	D	1007	1,3	14,14,15	0.63	0	15,19,21	1.36	1 (6%)
3	NAG	D	1008	3,4	14,14,15	0.73	0	15,19,21	1.30	3 (20%)
4	BMA	D	1009	3	11,11,12	0.58	0	15,15,17	1.41	2 (13%)
3	NAG	D	1010	1	14,14,15	0.73	0	15,19,21	1.24	2 (13%)
3	NAG	D	1011	1	14,14,15	0.65	0	15,19,21	1.81	4 (26%)

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	MBL	A	901	-	-	0/9/9/9	0/2/2/2
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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	907	3	-	0/6/23/26	0/1/1/1
3	NAG	A	908	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	910	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	911	4	-	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
3	NAG	A	914	1	-	0/6/23/26	0/1/1/1
2	MBL	A	915	-	-	0/9/9/9	0/2/2/2
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	1003	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	1004	4	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1006	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1008	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	1009	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1010	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1013	1	-	0/6/23/26	0/1/1/1
2	MBL	C	901	-	-	0/9/9/9	0/2/2/2
3	NAG	C	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	903	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	904	3	-	0/2/19/22	0/1/1/1
3	NAG	C	905	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	906	3	-	0/6/23/26	0/1/1/1
3	NAG	C	907	1	-	0/6/23/26	0/1/1/1
3	NAG	C	908	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	909	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	910	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	911	4	-	0/2/19/22	0/1/1/1
3	NAG	C	912	1	-	0/6/23/26	0/1/1/1
3	NAG	C	913	1	-	0/6/23/26	0/1/1/1
3	NAG	C	914	1	-	0/6/23/26	0/1/1/1
2	MBL	C	915	-	-	0/9/9/9	0/2/2/2
3	NAG	D	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	D	1003	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1004	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1005	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1006	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1008	3,4	-	0/6/23/26	0/1/1/1
4	BMA	D	1009	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1011	1	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1008	NAG	O5-C1	-3.14	1.38	1.43
3	A	909	NAG	O5-C1	-2.91	1.39	1.43
3	D	1001	NAG	O5-C1	-2.67	1.39	1.43
3	C	909	NAG	O5-C1	-2.66	1.39	1.43
3	B	1012	NAG	O5-C1	-2.55	1.39	1.43
3	A	907	NAG	O5-C1	-2.42	1.39	1.43
3	B	1006	NAG	O5-C1	-2.34	1.39	1.43
3	D	1004	NAG	O5-C1	-2.18	1.40	1.43
3	C	913	NAG	O5-C1	-2.10	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1010	NAG	O5-C1	-2.09	1.40	1.43
3	C	914	NAG	C1-C2	2.12	1.55	1.52
4	D	1003	BMA	O3-C3	2.59	1.49	1.43
5	C	911	MAN	C2-C3	2.79	1.56	1.52

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	912	NAG	C4-C3-C2	-4.21	104.81	111.34
3	B	1005	NAG	C3-C4-C5	-4.10	102.91	110.23
3	A	907	NAG	C3-C4-C5	-4.10	102.92	110.23
3	C	903	NAG	C2-N2-C7	-3.53	118.52	123.11
4	A	904	BMA	O4-C4-C3	-3.51	102.44	110.36
3	B	1006	NAG	C3-C4-C5	-3.51	103.96	110.23
3	D	1011	NAG	C4-C3-C2	-3.23	106.33	111.34
3	A	913	NAG	O4-C4-C3	-3.10	103.36	110.36
3	B	1001	NAG	C2-N2-C7	-3.08	119.09	123.11
3	A	906	NAG	C3-C4-C5	-3.08	104.74	110.23
3	D	1008	NAG	C4-C3-C2	-3.04	106.62	111.34
3	B	1002	NAG	C3-C4-C5	-3.02	104.85	110.23
2	A	915	MBL	C7-C6-C3	-3.01	125.27	129.49
3	D	1005	NAG	O3-C3-C4	-2.95	103.70	110.36
3	A	914	NAG	C4-C3-C2	-2.95	106.76	111.34
3	C	908	NAG	O5-C5-C4	-2.94	105.26	110.13
3	C	903	NAG	C1-O5-C5	-2.90	107.87	112.14
5	A	911	MAN	O5-C1-C2	-2.89	106.28	110.89
3	B	1008	NAG	O6-C6-C5	-2.79	101.97	111.30
3	B	1001	NAG	C3-C4-C5	-2.77	105.29	110.23
3	C	903	NAG	O3-C3-C4	-2.70	104.26	110.36
3	D	1010	NAG	O5-C5-C4	-2.67	105.70	110.13
5	B	1004	MAN	O5-C1-C2	-2.66	106.65	110.89
2	C	915	MBL	C7-C6-C3	-2.65	125.78	129.49
4	B	1009	BMA	O4-C4-C3	-2.62	104.45	110.36
4	D	1003	BMA	C2-C3-C4	-2.62	106.49	111.05
5	A	911	MAN	C1-C2-C3	-2.61	106.39	109.55
3	A	903	NAG	O7-C7-C8	-2.57	117.33	122.07
3	A	909	NAG	C4-C3-C2	-2.57	107.34	111.34
3	D	1006	NAG	O7-C7-C8	-2.57	117.34	122.07
3	C	902	NAG	C2-N2-C7	-2.54	119.81	123.11
3	C	907	NAG	O5-C5-C4	-2.51	105.98	110.13
4	A	910	BMA	O4-C4-C3	-2.48	104.77	110.36
3	B	1006	NAG	O5-C5-C4	-2.47	106.04	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	NAG	C1-O5-C5	-2.47	108.51	112.14
3	A	908	NAG	O7-C7-C8	-2.41	117.64	122.07
3	B	1005	NAG	O5-C5-C4	-2.40	106.17	110.13
3	C	905	NAG	O7-C7-C8	-2.36	117.72	122.07
3	C	902	NAG	O4-C4-C5	-2.35	103.03	109.23
3	A	909	NAG	O6-C6-C5	-2.35	103.47	111.30
5	B	1004	MAN	O3-C3-C4	-2.34	105.08	110.36
3	A	914	NAG	O7-C7-N2	-2.34	117.08	121.84
3	B	1010	NAG	C2-N2-C7	-2.33	120.07	123.11
3	C	909	NAG	O4-C4-C3	-2.33	105.10	110.36
4	A	910	BMA	O5-C5-C4	-2.29	106.33	110.13
3	A	902	NAG	O7-C7-C8	-2.29	117.85	122.07
3	B	1006	NAG	C4-C3-C2	-2.25	107.85	111.34
3	C	907	NAG	O4-C4-C3	-2.24	105.32	110.36
3	B	1008	NAG	C4-C3-C2	-2.24	107.87	111.34
2	C	901	MBL	C7-C6-C3	-2.23	126.36	129.49
3	A	903	NAG	C3-C4-C5	-2.22	106.28	110.23
2	C	915	MBL	C10-C9-N	-2.20	107.60	112.36
3	B	1010	NAG	O3-C3-C4	-2.17	105.46	110.36
3	C	903	NAG	O6-C6-C5	-2.13	104.20	111.30
3	C	913	NAG	O7-C7-C8	-2.11	118.19	122.07
3	C	903	NAG	O4-C4-C3	-2.10	105.62	110.36
3	A	903	NAG	O6-C6-C5	-2.10	104.29	111.30
3	D	1011	NAG	O7-C7-N2	-2.09	117.59	121.84
3	B	1012	NAG	O6-C6-C5	-2.09	104.33	111.30
3	D	1001	NAG	C3-C4-C5	-2.08	106.51	110.23
4	B	1003	BMA	O2-C2-C1	-2.05	105.14	109.23
3	B	1010	NAG	O7-C7-N2	-2.05	117.68	121.84
3	A	902	NAG	O6-C6-C5	-2.04	104.50	111.30
3	D	1008	NAG	O6-C6-C5	-2.02	104.55	111.30
3	A	908	NAG	O5-C5-C4	-2.01	106.81	110.13
5	A	911	MAN	O3-C3-C2	2.01	113.68	110.01
3	A	907	NAG	O5-C5-C6	2.03	111.68	107.34
3	A	908	NAG	O7-C7-N2	2.03	125.99	121.84
2	C	901	MBL	C9-N-C8	2.04	129.62	126.08
3	A	903	NAG	C2-N2-C7	2.04	125.76	123.11
3	C	913	NAG	O3-C3-C4	2.05	114.98	110.36
3	D	1008	NAG	O7-C7-N2	2.06	126.04	121.84
3	D	1005	NAG	O4-C4-C5	2.07	114.67	109.23
5	A	905	MAN	O2-C2-C3	2.07	114.36	110.19
3	C	908	NAG	C1-O5-C5	2.08	115.19	112.14
3	B	1002	NAG	C1-O5-C5	2.10	115.23	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	NAG	O4-C4-C5	2.11	114.78	109.23
3	A	906	NAG	O3-C3-C4	2.13	115.17	110.36
3	C	906	NAG	O4-C4-C5	2.14	114.87	109.23
3	D	1004	NAG	O5-C5-C4	2.15	113.69	110.13
4	C	904	BMA	O3-C3-C4	2.16	115.22	110.36
3	C	902	NAG	O3-C3-C4	2.16	115.23	110.36
4	B	1003	BMA	O6-C6-C5	2.17	118.56	111.30
5	A	905	MAN	C1-O5-C5	2.18	115.34	112.14
5	C	911	MAN	O3-C3-C4	2.18	115.27	110.36
3	D	1010	NAG	O3-C3-C4	2.18	115.28	110.36
4	C	910	BMA	O3-C3-C4	2.21	115.35	110.36
4	D	1003	BMA	O6-C6-C5	2.22	118.70	111.30
2	A	915	MBL	C3-C6-N1	2.22	123.61	120.58
5	A	911	MAN	C1-O5-C5	2.26	115.47	112.14
3	B	1012	NAG	C1-O5-C5	2.27	115.47	112.14
3	B	1006	NAG	C8-C7-N2	2.29	120.50	116.10
4	D	1009	BMA	C1-C2-C3	2.30	112.33	109.55
4	C	904	BMA	C3-C4-C5	2.31	114.35	110.23
5	C	911	MAN	O2-C2-C3	2.32	114.86	110.19
4	B	1009	BMA	O3-C3-C4	2.32	115.59	110.36
3	C	906	NAG	C1-O5-C5	2.32	115.56	112.14
4	A	904	BMA	O6-C6-C5	2.35	119.15	111.30
2	C	901	MBL	C3-C6-N1	2.37	123.81	120.58
4	C	910	BMA	O5-C1-C2	2.41	114.74	110.89
2	A	901	MBL	C3-C6-N1	2.45	123.92	120.58
3	A	902	NAG	C1-O5-C5	2.48	115.79	112.14
5	A	905	MAN	O2-C2-C1	2.51	114.27	109.23
4	D	1003	BMA	O3-C3-C2	2.52	114.62	110.01
4	A	910	BMA	O2-C2-C3	2.54	115.31	110.19
3	A	908	NAG	C2-N2-C7	2.56	126.43	123.11
3	C	913	NAG	C1-O5-C5	2.57	115.92	112.14
3	B	1001	NAG	O5-C5-C6	2.58	112.87	107.34
2	C	915	MBL	C9-N-C8	2.60	130.60	126.08
3	B	1013	NAG	C1-O5-C5	2.61	115.98	112.14
4	D	1009	BMA	O5-C5-C6	2.69	113.10	107.34
3	A	903	NAG	O7-C7-N2	2.73	127.41	121.84
3	D	1011	NAG	C2-N2-C7	2.74	126.66	123.11
5	B	1004	MAN	C2-C3-C4	2.75	115.85	111.05
3	B	1006	NAG	O4-C4-C5	2.76	116.50	109.23
5	B	1004	MAN	C3-C4-C5	2.77	115.17	110.23
4	A	904	BMA	O5-C5-C6	2.80	113.33	107.34
4	A	904	BMA	C3-C4-C5	2.86	115.32	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1013	NAG	O5-C5-C6	2.87	113.47	107.34
5	B	1004	MAN	C1-C2-C3	2.92	113.09	109.55
4	A	904	BMA	C1-O5-C5	2.93	116.46	112.14
3	D	1004	NAG	C1-O5-C5	2.98	116.52	112.14
3	B	1012	NAG	O5-C5-C4	3.04	115.17	110.13
2	C	915	MBL	C3-C6-N1	3.06	124.76	120.58
3	B	1010	NAG	O5-C5-C4	3.27	115.55	110.13
3	D	1006	NAG	C8-C7-N2	3.27	122.37	116.10
5	C	911	MAN	O3-C3-C2	3.32	116.08	110.01
4	C	904	BMA	C1-C2-C3	3.52	113.81	109.55
3	B	1013	NAG	C2-N2-C7	3.54	127.71	123.11
3	D	1011	NAG	C8-C7-N2	3.55	122.90	116.10
3	A	906	NAG	O5-C5-C4	3.67	116.21	110.13
4	C	910	BMA	C1-O5-C5	3.70	117.58	112.14
4	A	910	BMA	C1-C2-C3	3.70	114.04	109.55
3	A	914	NAG	C8-C7-N2	3.94	123.65	116.10
4	B	1009	BMA	C1-O5-C5	4.15	118.24	112.14
3	D	1007	NAG	C1-O5-C5	4.39	118.60	112.14
3	B	1010	NAG	C1-O5-C5	4.44	118.68	112.14
3	A	912	NAG	C1-O5-C5	4.71	119.07	112.14
4	D	1003	BMA	C1-C2-C3	4.73	115.28	109.55
3	C	912	NAG	C1-O5-C5	5.14	119.70	112.14
4	B	1003	BMA	C1-C2-C3	5.24	115.90	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	913	NAG	2	0
3	A	914	NAG	1	0
3	C	902	NAG	1	0
3	D	1001	NAG	2	0
3	D	1010	NAG	1	0
3	D	1011	NAG	1	0

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	748/811 (92%)	-0.28	1 (0%) 95 95	34, 50, 80, 110	0
1	B	749/811 (92%)	-0.22	8 (1%) 82 82	33, 55, 99, 145	0
1	C	748/811 (92%)	0.04	34 (4%) 37 38	34, 64, 105, 168	0
1	D	746/811 (91%)	0.05	40 (5%) 29 30	36, 63, 121, 169	0
All	All	2991/3244 (92%)	-0.10	83 (2%) 56 55	33, 57, 104, 169	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	8.1
1	C	84	GLN	7.6
1	C	85	GLY	6.5
1	B	64	TYR	6.2
1	C	753	LYS	6.1
1	D	751	ILE	6.0
1	D	776	CYS	5.9
1	C	758	THR	5.5
1	C	759	LYS	5.3
1	D	64	TYR	5.2
1	C	64	TYR	5.1
1	C	86	LEU	4.9
1	D	783	PHE	4.8
1	C	122	LEU	4.7
1	C	121	PHE	4.5
1	D	678	PHE	4.2
1	C	41	GLN	4.1
1	D	814	ILE	4.0
1	D	39	LYS	4.0
1	D	815	VAL	3.9
1	D	65	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	778	CYS	3.8
1	C	757	GLU	3.8
1	C	65	VAL	3.7
1	C	791	LEU	3.6
1	C	125	LYS	3.6
1	D	750	THR	3.5
1	D	758	THR	3.4
1	C	123	ASN	3.3
1	D	756	LEU	3.3
1	C	760	THR	3.2
1	C	87	GLN	3.2
1	D	813	SER	3.2
1	D	774	PHE	3.1
1	B	762	THR	3.1
1	D	757	GLU	3.1
1	D	660	LEU	3.1
1	D	40	LYS	3.1
1	C	199	THR	3.1
1	C	761	THR	3.0
1	B	100	VAL	2.8
1	D	45	VAL	2.8
1	D	779	ASP	2.8
1	D	727	LEU	2.8
1	D	38	GLU	2.8
1	D	777	THR	2.7
1	D	46	ILE	2.7
1	D	780	ILE	2.7
1	A	64	TYR	2.7
1	C	40	LYS	2.6
1	D	767	LEU	2.6
1	C	246	ILE	2.6
1	D	781	GLY	2.6
1	D	802	ILE	2.5
1	D	752	ASN	2.5
1	C	59	GLN	2.5
1	D	701	LEU	2.4
1	D	782	ASP	2.4
1	C	45	VAL	2.4
1	D	34	TYR	2.4
1	C	201	THR	2.4
1	B	168	ARG	2.4
1	C	96	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	186	VAL	2.3
1	D	681	TRP	2.3
1	D	170	ILE	2.3
1	D	816	SER	2.2
1	C	60	THR	2.2
1	C	242	PHE	2.2
1	D	769	LEU	2.2
1	D	786	TRP	2.2
1	C	170	ILE	2.2
1	C	732	LEU	2.2
1	D	47	ALA	2.2
1	B	758	THR	2.1
1	C	70	LEU	2.1
1	C	169	LEU	2.1
1	D	733	SER	2.1
1	B	760	THR	2.1
1	B	86	LEU	2.1
1	C	32	ARG	2.1
1	D	809	GLN	2.1
1	C	89	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	D	1006	14/15	0.94	0.21	2.86	73,83,92,96	0
3	NAG	C	914	14/15	0.93	0.15	2.45	59,64,67,70	0
3	NAG	A	914	14/15	0.89	0.17	1.70	61,68,72,78	0
3	NAG	C	912	14/15	0.93	0.15	0.79	56,66,74,82	0
3	NAG	B	1012	14/15	0.93	0.14	0.58	56,65,75,78	0
3	NAG	C	903	14/15	0.95	0.14	0.31	53,57,64,66	0
3	NAG	D	1011	14/15	0.92	0.11	-0.01	79,87,95,106	0
3	NAG	C	902	14/15	0.98	0.14	-0.02	44,47,56,57	0
3	NAG	B	1010	14/15	0.95	0.13	-0.23	50,57,64,72	0
3	NAG	D	1007	14/15	0.93	0.13	-0.24	42,49,54,54	0
3	NAG	A	903	14/15	0.98	0.13	-0.24	35,40,48,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	1005	14/15	0.98	0.14	-0.27	34,41,45,49	0
3	NAG	A	913	14/15	0.97	0.12	-0.30	56,60,64,64	0
3	NAG	C	913	14/15	0.96	0.13	-0.37	61,76,82,85	0
3	NAG	D	1004	14/15	0.97	0.14	-0.37	45,50,54,61	0
3	NAG	D	1010	14/15	0.95	0.12	-0.63	51,54,64,65	0
3	NAG	A	902	14/15	0.98	0.14	-0.70	29,35,37,38	0
3	NAG	A	908	14/15	0.96	0.12	-0.73	38,41,46,49	0
3	NAG	B	1013	14/15	0.92	0.10	-0.92	66,73,78,78	0
3	NAG	C	909	14/15	0.97	0.13	-0.97	38,42,51,55	0
3	NAG	C	905	14/15	0.98	0.14	-1.04	40,46,50,54	0
3	NAG	B	1001	14/15	0.98	0.15	-1.06	35,42,48,50	0
3	NAG	A	906	14/15	0.99	0.12	-1.11	36,40,47,48	0
3	NAG	C	908	14/15	0.98	0.12	-1.27	35,38,41,46	0
3	NAG	B	1002	14/15	0.97	0.13	-1.89	45,49,58,63	0
3	NAG	D	1001	14/15	0.98	0.12	-1.91	39,43,45,47	0
3	NAG	D	1002	14/15	0.97	0.11	-1.96	42,50,58,58	0
3	NAG	B	1007	14/15	0.97	0.11	-1.97	29,38,41,43	0
5	MAN	B	1004	11/12	0.89	0.15	-	57,75,79,81	0
5	MAN	A	905	11/12	0.91	0.13	-	55,63,68,69	0
3	NAG	D	1005	14/15	0.89	0.14	-	65,75,87,88	0
3	NAG	D	1008	14/15	0.98	0.10	-	47,55,63,63	0
3	NAG	A	912	14/15	0.90	0.18	-	76,83,94,96	0
3	NAG	B	1006	14/15	0.95	0.12	-	54,64,70,71	0
3	NAG	C	907	14/15	0.94	0.12	-	66,77,87,95	0
3	NAG	B	1011	14/15	0.93	0.22	-	74,88,92,95	0
3	NAG	B	1008	14/15	0.98	0.14	-	36,44,51,52	0
3	NAG	A	909	14/15	0.98	0.17	-	33,45,49,58	0
3	NAG	A	907	14/15	0.90	0.17	-	48,66,70,70	0
5	MAN	C	911	11/12	0.80	0.16	-	76,93,101,102	0
3	NAG	C	906	14/15	0.90	0.17	-	70,82,92,93	0
5	MAN	A	911	11/12	0.91	0.13	-	78,91,95,96	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	D	1006	14/15	0.94	0.21	2.86	73,83,92,96	0
3	NAG	C	914	14/15	0.93	0.15	2.45	59,64,67,70	0
2	MBL	C	901	17/17	0.97	0.17	2.25	50,57,61,63	0
3	NAG	A	914	14/15	0.89	0.17	1.70	61,68,72,78	0
3	NAG	C	912	14/15	0.93	0.15	0.79	56,66,74,82	0
3	NAG	B	1012	14/15	0.93	0.14	0.58	56,65,75,78	0
3	NAG	C	903	14/15	0.95	0.14	0.31	53,57,64,66	0
2	MBL	C	915	17/17	0.97	0.15	0.10	44,47,55,56	0
3	NAG	D	1011	14/15	0.92	0.11	-0.01	79,87,95,106	0
3	NAG	C	902	14/15	0.98	0.14	-0.02	44,47,56,57	0
2	MBL	A	915	17/17	0.97	0.16	-0.04	39,44,49,49	0
3	NAG	B	1010	14/15	0.95	0.13	-0.23	50,57,64,72	0
3	NAG	D	1007	14/15	0.93	0.13	-0.24	42,49,54,54	0
3	NAG	A	903	14/15	0.98	0.13	-0.24	35,40,48,52	0
3	NAG	B	1005	14/15	0.98	0.14	-0.27	34,41,45,49	0
3	NAG	A	913	14/15	0.97	0.12	-0.30	56,60,64,64	0
3	NAG	D	1004	14/15	0.97	0.14	-0.37	45,50,54,61	0
3	NAG	C	913	14/15	0.96	0.13	-0.37	61,76,82,85	0
2	MBL	A	901	17/17	0.96	0.16	-0.50	43,48,54,54	0
3	NAG	D	1010	14/15	0.95	0.12	-0.63	51,54,64,65	0
3	NAG	A	902	14/15	0.98	0.14	-0.70	29,35,37,38	0
3	NAG	A	908	14/15	0.96	0.12	-0.73	38,41,46,49	0
3	NAG	B	1013	14/15	0.92	0.10	-0.92	66,73,78,78	0
3	NAG	C	909	14/15	0.97	0.13	-0.97	38,42,51,55	0
3	NAG	C	905	14/15	0.98	0.14	-1.04	40,46,50,54	0
3	NAG	B	1001	14/15	0.98	0.15	-1.06	35,42,48,50	0
3	NAG	A	906	14/15	0.99	0.12	-1.11	36,40,47,48	0
3	NAG	C	908	14/15	0.98	0.12	-1.27	35,38,41,46	0
3	NAG	B	1002	14/15	0.97	0.13	-1.89	45,49,58,63	0
3	NAG	D	1001	14/15	0.98	0.12	-1.91	39,43,45,47	0
3	NAG	D	1002	14/15	0.97	0.11	-1.96	42,50,58,58	0
3	NAG	B	1007	14/15	0.97	0.11	-1.97	29,38,41,43	0
4	BMA	C	904	11/12	0.85	0.13	-	64,70,79,83	0
3	NAG	C	906	14/15	0.90	0.17	-	70,82,92,93	0
5	MAN	B	1004	11/12	0.89	0.15	-	57,75,79,81	0
4	BMA	A	904	11/12	0.89	0.10	-	50,59,62,62	0
5	MAN	A	905	11/12	0.91	0.13	-	55,63,68,69	0
4	BMA	D	1009	11/12	0.86	0.13	-	69,73,80,81	0
4	BMA	C	910	11/12	0.96	0.10	-	57,65,69,84	0
3	NAG	D	1008	14/15	0.98	0.10	-	47,55,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BMA	B	1003	11/12	0.93	0.13	-	55,66,72,82	0
3	NAG	D	1005	14/15	0.89	0.14	-	65,75,87,88	0
3	NAG	B	1006	14/15	0.95	0.12	-	54,64,70,71	0
3	NAG	A	912	14/15	0.90	0.18	-	76,83,94,96	0
3	NAG	B	1011	14/15	0.93	0.22	-	74,88,92,95	0
3	NAG	C	907	14/15	0.94	0.12	-	66,77,87,95	0
3	NAG	A	909	14/15	0.98	0.17	-	33,45,49,58	0
3	NAG	A	907	14/15	0.90	0.17	-	48,66,70,70	0
4	BMA	B	1009	11/12	0.92	0.10	-	53,66,72,72	0
3	NAG	B	1008	14/15	0.98	0.14	-	36,44,51,52	0
5	MAN	A	911	11/12	0.91	0.13	-	78,91,95,96	0
4	BMA	D	1003	11/12	0.87	0.13	-	50,63,71,72	0
5	MAN	C	911	11/12	0.80	0.16	-	76,93,101,102	0
4	BMA	A	910	11/12	0.94	0.11	-	55,68,79,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.