



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:13 AM GMT

PDB ID : 3W3N
Title : Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 3
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2012-12-22
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

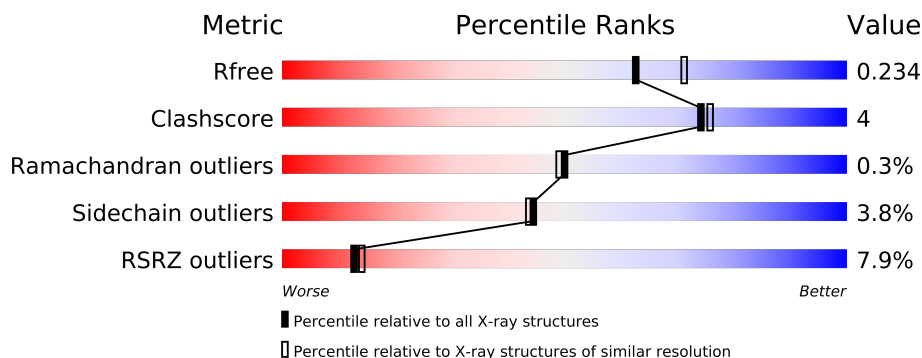
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	1009	-	X
4	NAG	A	1015	-	X
4	NAG	A	1016	-	X
4	NAG	B	917	-	X
4	NAG	B	920	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13256 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			6039	3861	1025	1134	19			
1	B	749	Total	C	N	O	S	0	0	0
			5994	3836	1019	1120	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	24	SER	-	EXPRESSION TAG	UNP Q9NR97
B	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
B	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
B	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
B	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
B	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
B	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

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

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
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	24	SER	-	EXPRESSION TAG	UNP Q9NR97
B	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
B	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
B	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
B	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
B	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
B	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	ARG	-	EXPRESSION TAG	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	SER	-	EXPRESSION TAG	UNP Q9NR97
B	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
B	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
B	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
B	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
B	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
B	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

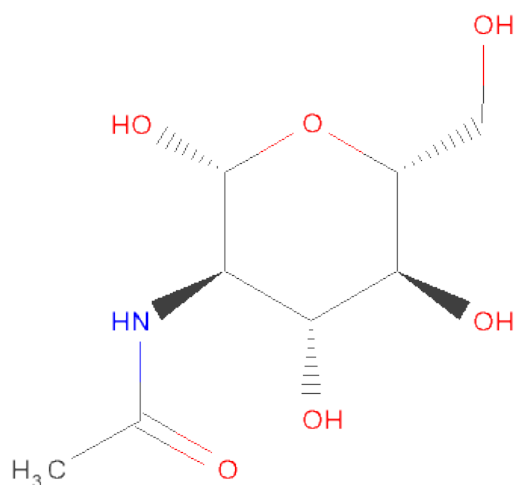
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

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

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	24	SER	-	EXPRESSION TAG	UNP Q9NR97
B	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
B	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
B	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
B	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
B	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
B	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



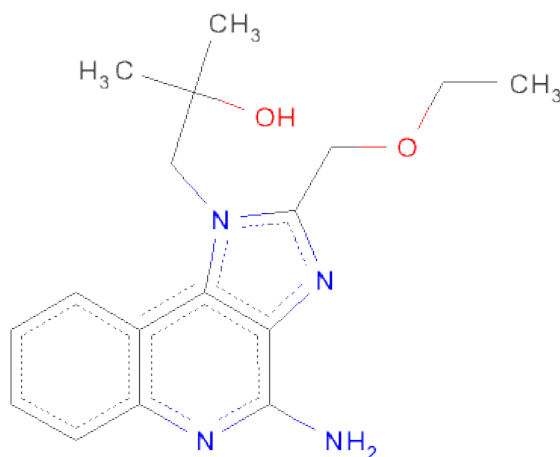
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

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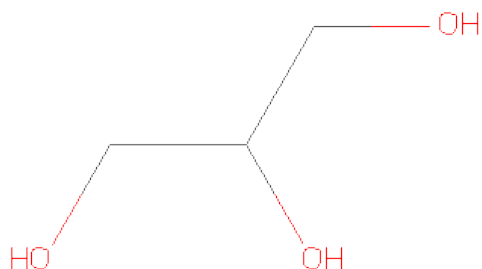
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1-[4-AMINO-2-(ETHOXYMETHYL)-1H-IMIDAZO[4,5-C]QUINOLIN-1-YL]-2-METHYLPROPAN-2-OL (three-letter code: RX8) (formula: C₁₇H₂₂N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	17	4	2		
5	B	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

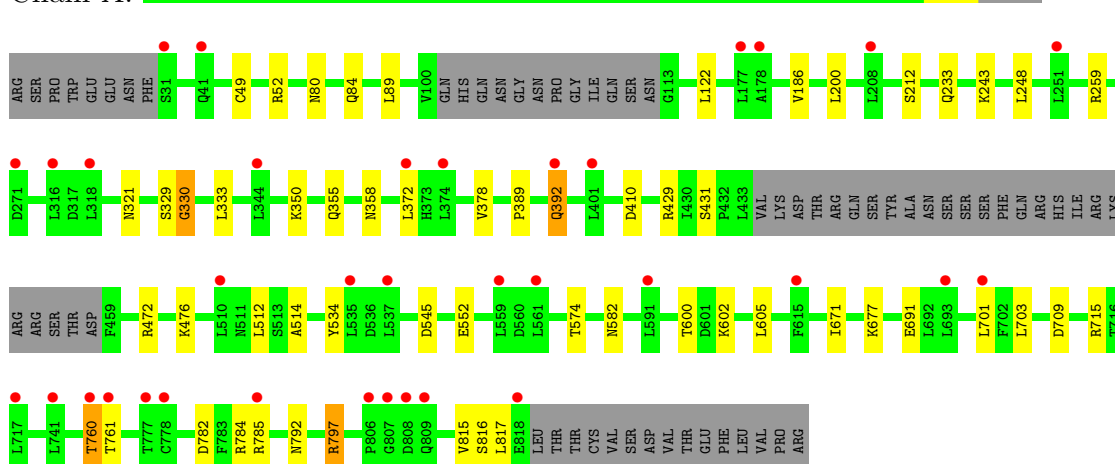
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	419	Total	O	0	0
			419	419		
7	B	248	Total	O	0	0
			248	248		

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.

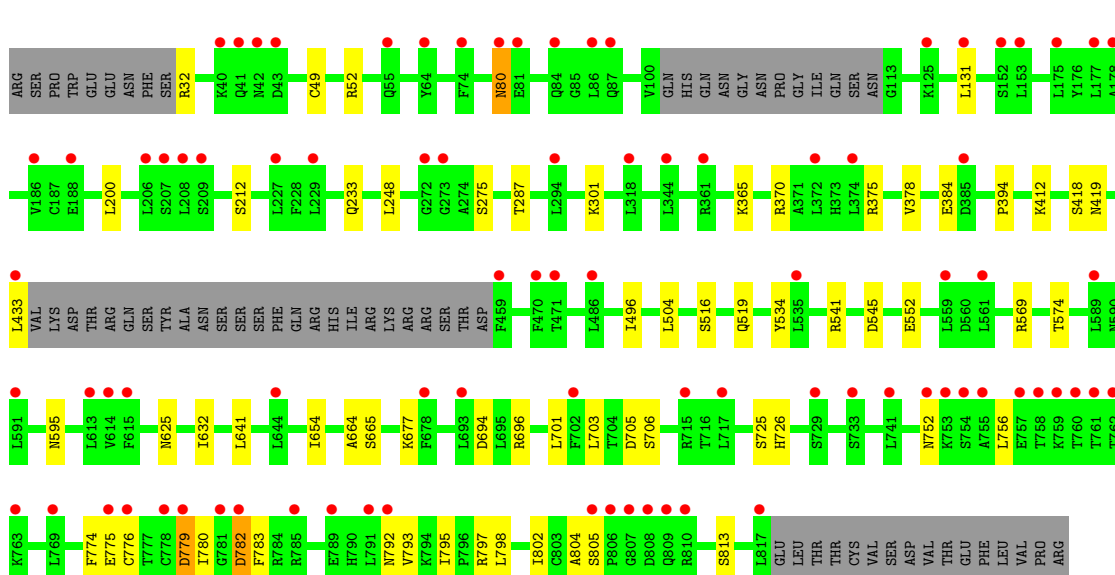
• Molecule 1: Toll-like receptor 8

Chain A:



• Molecule 1: Toll-like receptor 8

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.22Å 100.78Å 265.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.39 – 2.10 28.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (28.39-2.10) 95.7 (28.39-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.200 , 0.233 0.201 , 0.234	Depositor DCC
R_{free} test set	6495 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 129652 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13256	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GOL, BMA, NAG, RX8

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	0.27	0/6164	0.47	0/8361
1	B	0.27	0/6119	0.46	0/8302
All	All	0.27	0/12283	0.46	0/16663

There are no bond length outliers.

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	6039	0	0	25	0
1	B	5994	0	0	26	0
2	A	122	0	0	0	0
2	B	122	0	0	0	0
3	A	39	0	0	0	0
3	B	39	0	0	0	0
4	A	84	0	0	1	0
4	B	98	0	0	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	0	0	0	0
7	A	419	0	0	13	0
7	B	248	0	0	8	0
All	All	13256	0	0	51	0

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

All (51) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:664:ALA:O	7:B:1025:HOH:O	1.89	0.91
1:B:625:ASN:OD1	7:B:1187:HOH:O	1.95	0.83
1:A:355:GLN:NE2	7:A:1476:HOH:O	2.16	0.77
1:B:370:ARG:NH1	7:B:1094:HOH:O	2.17	0.77
1:A:784:ARG:NE	7:A:1444:HOH:O	2.18	0.75
1:A:333:LEU:O	7:A:1220:HOH:O	2.05	0.74
1:A:691:GLU:OE2	7:A:1158:HOH:O	2.09	0.70
1:A:389:PRO:O	1:A:392:GLN:NE2	2.25	0.69
1:A:358:ASN:ND2	7:A:1436:HOH:O	2.26	0.69
1:B:779:ASP:N	1:B:779:ASP:OD1	2.25	0.69
1:B:384:GLU:OE2	7:B:1199:HOH:O	2.12	0.68
1:A:760:THR:OG1	1:A:761:THR:N	2.27	0.68
1:A:350:LYS:NZ	7:A:1454:HOH:O	2.30	0.64
1:A:677:LYS:O	7:A:1410:HOH:O	2.16	0.61
4:A:1018:NAG:O7	7:A:1384:HOH:O	2.17	0.59
1:B:654:ILE:O	7:B:1210:HOH:O	2.16	0.58
1:B:782:ASP:OD1	1:B:782:ASP:N	2.37	0.58
1:A:782:ASP:OD1	1:A:785:ARG:NH1	2.37	0.58
1:B:774:PHE:O	1:B:804:ALA:N	2.38	0.57
1:B:780:ILE:O	1:B:783:PHE:N	2.37	0.57
1:A:715:ARG:NE	7:A:1442:HOH:O	2.39	0.56
1:B:496:ILE:N	1:B:519:GLN:OE1	2.38	0.56
1:B:394:PRO:O	1:B:419:ASN:ND2	2.40	0.55
1:A:212:SER:OG	1:A:233:GLN:NE2	2.42	0.53
1:B:545:ASP:OD1	1:B:574:THR:OG1	2.26	0.53
1:A:476:LYS:NZ	7:A:1513:HOH:O	2.40	0.53
1:B:694:ASP:OD2	1:B:696:ARG:NH2	2.42	0.52
1:A:80:ASN:O	1:A:84:GLN:NE2	2.43	0.52
1:B:776:CYS:N	1:B:805:SER:O	2.44	0.51
1:A:514:ALA:O	1:B:541:ARG:NH2	2.44	0.50
1:B:365:LYS:NZ	7:B:1135:HOH:O	2.44	0.50
1:A:545:ASP:OD1	1:A:574:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:792:ASN:OD1	1:B:792:ASN:N	2.47	0.48
1:B:212:SER:OG	1:B:233:GLN:OE1	2.31	0.48
1:B:32:ARG:NH1	1:B:793:VAL:O	2.48	0.47
1:A:792:ASN:OD1	1:A:792:ASN:N	2.47	0.46
1:A:259:ARG:NH1	1:A:321:ASN:O	2.48	0.46
1:A:797:ARG:N	7:A:1293:HOH:O	2.49	0.45
1:B:798:LEU:O	1:B:813:SER:OG	2.35	0.45
1:B:80:ASN:N	1:B:80:ASN:OD1	2.50	0.44
1:B:641:LEU:O	1:B:665:SER:OG	2.36	0.43
1:A:816:SER:OG	1:A:816:SER:O	2.36	0.43
1:B:375:ARG:NE	7:B:1195:HOH:O	2.52	0.43
1:A:600:THR:O	1:A:602:LYS:N	2.53	0.42
1:A:186:VAL:N	7:A:1484:HOH:O	2.53	0.41
1:A:329:SER:OG	1:A:330:GLY:N	2.54	0.41
1:B:418:SER:N	7:B:1245:HOH:O	2.53	0.41
1:B:705:ASP:OD1	1:B:706:SER:N	2.53	0.41
1:A:552:GLU:N	1:A:552:GLU:OE1	2.54	0.41
1:B:552:GLU:N	1:B:552:GLU:OE1	2.54	0.41
1:A:709:ASP:OD1	7:A:1460:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	745/811 (92%)	711 (95%)	32 (4%)	2 (0%)	50	49
1	B	743/811 (92%)	710 (96%)	31 (4%)	2 (0%)	50	49
All	All	1488/1622 (92%)	1421 (96%)	63 (4%)	4 (0%)	50	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	797	ARG

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Mol	Chain	Res	Type
1	A	378	VAL
1	B	378	VAL
1	A	330	GLY

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	694/755 (92%)	670 (96%)	24 (4%)	48	48
1	B	683/755 (90%)	654 (96%)	29 (4%)	40	38
All	All	1377/1510 (91%)	1324 (96%)	53 (4%)	44	44

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	52	ARG
1	A	89	LEU
1	A	122	LEU
1	A	200	LEU
1	A	243	LYS
1	A	248	LEU
1	A	372	LEU
1	A	392	GLN
1	A	410	ASP
1	A	429	ARG
1	A	431	SER
1	A	472	ARG
1	A	512	LEU
1	A	534	TYR
1	A	582	ASN
1	A	605	LEU
1	A	671	ILE
1	A	701	LEU
1	A	703	LEU
1	A	760	THR
1	A	797	ARG

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Mol	Chain	Res	Type
1	A	815	VAL
1	A	817	LEU
1	B	49	CYS
1	B	52	ARG
1	B	80	ASN
1	B	131	LEU
1	B	200	LEU
1	B	248	LEU
1	B	275	SER
1	B	287	THR
1	B	301	LYS
1	B	412	LYS
1	B	433	LEU
1	B	504	LEU
1	B	516	SER
1	B	534	TYR
1	B	569	ARG
1	B	595	ASN
1	B	632	ILE
1	B	677	LYS
1	B	701	LEU
1	B	703	LEU
1	B	725	SER
1	B	726	HIS
1	B	752	ASN
1	B	756	LEU
1	B	775	GLU
1	B	779	ASP
1	B	782	ASP
1	B	795	ILE
1	B	802	ILE

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1001	1,2	12,14,15	0.70	1 (8%)	15,19,21	0.80	0
2	NAG	A	1002	2	12,14,15	0.74	0	15,19,21	0.91	1 (6%)
2	BMA	A	1003	2	10,11,12	0.51	0	11,15,17	1.01	0
2	MAN	A	1004	2	10,11,12	0.79	0	11,15,17	0.71	1 (9%)
2	MAN	A	1005	2	10,11,12	0.78	0	11,15,17	0.97	1 (9%)
3	NAG	A	1006	1,3	12,14,15	0.66	0	15,19,21	1.10	2 (13%)
3	NAG	A	1007	3	12,14,15	0.71	1 (8%)	15,19,21	0.73	0
3	BMA	A	1008	3	10,11,12	0.43	0	11,15,17	0.98	0
2	NAG	A	1010	1,2	12,14,15	0.73	1 (8%)	15,19,21	0.84	0
2	NAG	A	1011	2	12,14,15	0.71	0	15,19,21	0.91	0
2	BMA	A	1012	2	10,11,12	0.92	1 (10%)	11,15,17	1.71	3 (27%)
2	MAN	A	1013	2	10,11,12	0.83	1 (10%)	11,15,17	0.89	0
2	MAN	A	1014	2	10,11,12	0.73	0	11,15,17	0.91	0
2	NAG	B	902	1,2	12,14,15	0.67	0	15,19,21	0.96	1 (6%)
2	NAG	B	903	2	12,14,15	0.76	1 (8%)	15,19,21	1.08	1 (6%)
2	BMA	B	904	2	10,11,12	0.57	0	11,15,17	0.97	1 (9%)
2	MAN	B	905	2	10,11,12	0.82	1 (10%)	11,15,17	0.96	1 (9%)
2	MAN	B	906	2	10,11,12	0.80	0	11,15,17	1.03	1 (9%)
3	NAG	B	907	1,3	12,14,15	0.66	0	15,19,21	0.88	1 (6%)
3	NAG	B	908	3	12,14,15	0.72	1 (8%)	15,19,21	0.70	0
3	BMA	B	909	3	10,11,12	0.55	0	11,15,17	1.02	0
2	NAG	B	911	1,2	12,14,15	0.64	0	15,19,21	0.83	1 (6%)
2	NAG	B	912	2	12,14,15	0.72	0	15,19,21	0.96	0
2	BMA	B	913	2	10,11,12	0.62	0	11,15,17	0.88	0
2	MAN	B	914	2	10,11,12	0.81	1 (10%)	11,15,17	0.66	0
2	MAN	B	915	2	10,11,12	0.78	0	11,15,17	0.96	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	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1005	2	-	0/2/19/22	0/1/1/1
3	NAG	A	1006	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1008	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1012	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1013	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1014	2	-	0/2/19/22	0/1/1/1
2	NAG	B	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	903	2	-	0/6/23/26	0/1/1/1
2	BMA	B	904	2	-	0/2/19/22	0/1/1/1
2	MAN	B	905	2	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	0/2/19/22	0/1/1/1
3	NAG	B	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	908	3	-	0/6/23/26	0/1/1/1
3	BMA	B	909	3	-	0/2/19/22	0/1/1/1
2	NAG	B	911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	912	2	-	0/6/23/26	0/1/1/1
2	BMA	B	913	2	-	0/2/19/22	0/1/1/1
2	MAN	B	914	2	-	0/2/19/22	0/1/1/1
2	MAN	B	915	2	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1012	BMA	C4-C5	2.36	1.58	1.53
3	B	908	NAG	O5-C5	-2.22	1.41	1.45
3	A	1007	NAG	O5-C5	-2.20	1.41	1.45
2	A	1001	NAG	O5-C5	-2.18	1.41	1.45
2	B	903	NAG	O5-C5	-2.18	1.41	1.45
2	B	905	MAN	O5-C5	-2.10	1.41	1.45
2	A	1013	MAN	O5-C5	-2.07	1.41	1.45
2	B	914	MAN	O5-C5	-2.00	1.41	1.45
2	A	1010	NAG	O5-C5	-2.00	1.41	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1012	BMA	O5-C5-C6	-4.08	102.70	106.98
2	B	903	NAG	O5-C5-C6	3.31	110.45	106.98
2	B	906	MAN	O5-C5-C6	2.94	110.07	106.98
2	A	1005	MAN	O5-C5-C6	2.88	110.00	106.98
3	A	1006	NAG	O5-C5-C6	2.87	109.99	106.98
2	B	902	NAG	O5-C5-C6	2.86	109.98	106.98
2	A	1012	BMA	O5-C5-C4	2.52	113.85	110.65
2	B	905	MAN	O5-C5-C6	2.44	109.54	106.98
2	A	1002	NAG	C3-C2-N2	-2.21	108.39	111.76
2	B	904	BMA	O2-C2-C3	-2.18	105.47	110.18
2	B	911	NAG	O5-C5-C6	2.18	109.27	106.98
3	A	1006	NAG	C3-C2-N2	-2.17	108.45	111.76
2	A	1012	BMA	C3-C4-C5	2.11	113.97	110.20
3	B	907	NAG	O5-C5-C6	2.02	109.10	106.98
2	A	1004	MAN	O5-C5-C6	2.02	109.10	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

16 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
4	NAG	A	1009	1	12,14,15	0.69	1 (8%)	15,19,21	0.79	0
4	NAG	A	1015	1	12,14,15	0.65	0	15,19,21	1.06	2 (13%)
4	NAG	A	1016	1	12,14,15	0.67	0	15,19,21	0.85	1 (6%)
4	NAG	A	1017	1	12,14,15	0.61	0	15,19,21	1.08	1 (6%)
4	NAG	A	1018	1	12,14,15	0.74	1 (8%)	15,19,21	0.81	0
4	NAG	A	1019	1	12,14,15	0.57	0	15,19,21	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	RX8	A	1020	-	25,25,25	1.57	4 (16%)	37,37,37	1.50	5 (13%)
6	GOL	A	1021	-	5,5,5	0.35	0	5,5,5	0.25	0
5	RX8	B	901	-	25,25,25	1.52	4 (16%)	37,37,37	1.38	5 (13%)
4	NAG	B	910	1	12,14,15	0.65	0	15,19,21	0.95	1 (6%)
4	NAG	B	916	1	12,14,15	0.64	0	15,19,21	0.93	1 (6%)
4	NAG	B	917	1	12,14,15	0.68	1 (8%)	15,19,21	0.94	0
4	NAG	B	918	1	12,14,15	0.73	1 (8%)	15,19,21	0.90	1 (6%)
4	NAG	B	919	1	12,14,15	0.57	0	15,19,21	1.46	3 (20%)
4	NAG	B	920	1	12,14,15	0.64	0	15,19,21	1.03	1 (6%)
4	NAG	B	921	1	12,14,15	0.58	0	15,19,21	1.11	1 (6%)

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
4	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1017	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1018	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1019	1	-	0/6/23/26	0/1/1/1
5	RX8	A	1020	-	-	2/9/9/9	0/0/3/3
6	GOL	A	1021	-	-	0/4/4/4	0/0/0/0
5	RX8	B	901	-	-	2/9/9/9	0/0/3/3
4	NAG	B	910	1	-	0/6/23/26	0/1/1/1
4	NAG	B	916	1	-	0/6/23/26	0/1/1/1
4	NAG	B	917	1	-	0/6/23/26	0/1/1/1
4	NAG	B	918	1	-	0/6/23/26	0/1/1/1
4	NAG	B	919	1	-	0/6/23/26	0/1/1/1
4	NAG	B	920	1	-	0/6/23/26	0/1/1/1
4	NAG	B	921	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)
5	A	1020	RX8	C2-C3	4.72	1.49	1.40
5	B	901	RX8	C2-C3	4.49	1.48	1.40
5	B	901	RX8	C2-C1	-2.91	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	RX8	C2-C1	-2.74	1.37	1.41
5	A	1020	RX8	C-N	2.63	1.43	1.35
5	B	901	RX8	C-N	2.58	1.43	1.35
5	A	1020	RX8	O1-C10	-2.37	1.37	1.44
5	B	901	RX8	O1-C10	-2.34	1.38	1.44
4	A	1018	NAG	O5-C5	-2.23	1.41	1.45
4	B	918	NAG	O5-C5	-2.13	1.41	1.45
4	A	1009	NAG	O5-C5	-2.05	1.41	1.45
4	B	917	NAG	O5-C5	-2.02	1.41	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1020	RX8	C-N1-C1	4.56	122.34	118.42
5	B	901	RX8	C-N1-C1	4.48	122.28	118.42
5	A	1020	RX8	C9-N3-C5	-4.32	124.78	127.34
5	B	901	RX8	C9-N3-C5	-3.67	125.16	127.34
5	A	1020	RX8	C6-O-C7	3.50	120.07	112.57
4	B	919	NAG	O5-C5-C4	3.18	114.69	110.65
4	B	920	NAG	O5-C5-C6	3.01	110.14	106.98
5	B	901	RX8	C6-O-C7	2.96	118.91	112.57
4	B	919	NAG	C6-C5-C4	-2.64	106.63	113.00
5	A	1020	RX8	C2-C1-N1	-2.46	120.78	123.02
4	B	921	NAG	O5-C5-C4	2.42	113.73	110.65
4	A	1019	NAG	C3-C2-N2	-2.42	108.08	111.76
4	B	918	NAG	O5-C5-C6	2.40	109.50	106.98
5	B	901	RX8	C2-C1-N1	-2.39	120.85	123.02
4	A	1015	NAG	C2-N2-C7	-2.32	119.19	123.09
4	A	1016	NAG	O5-C5-C6	2.23	109.33	106.98
5	A	1020	RX8	C2-C3-N3	2.22	135.11	130.42
4	B	916	NAG	O5-C5-C6	2.22	109.31	106.98
4	B	919	NAG	C3-C4-C5	2.19	114.12	110.20
5	B	901	RX8	C3-C2-C1	-2.14	117.92	119.75
4	A	1017	NAG	O5-C5-C4	2.10	113.32	110.65
4	A	1015	NAG	O5-C5-C6	2.08	109.16	106.98
4	A	1019	NAG	O5-C5-C6	2.06	109.15	106.98
4	B	910	NAG	C3-C2-N2	-2.02	108.69	111.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	RX8	O-C6-C5-N2
5	B	901	RX8	O-C6-C5-N3
5	A	1020	RX8	O-C6-C5-N2
5	A	1020	RX8	O-C6-C5-N3

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/811 (92%)	0.13	35 (4%) 30 33	19, 35, 62, 92	0
1	B	749/811 (92%)	0.55	87 (11%) 5 6	21, 46, 87, 107	0
All	All	1500/1622 (92%)	0.34	122 (8%) 13 13	19, 40, 78, 107	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	759	LYS	8.7
1	B	761	THR	7.2
1	B	64	TYR	6.6
1	B	758	THR	5.7
1	B	754	SER	5.6
1	B	753	LYS	5.2
1	B	84	GLN	5.2
1	B	42	ASN	5.2
1	B	778	CYS	5.1
1	A	392	GLN	5.1
1	A	761	THR	5.0
1	B	757	GLU	4.9
1	B	733	SER	4.8
1	B	808	ASP	4.6
1	B	805	SER	4.5
1	B	782	ASP	4.4
1	B	785	ARG	4.2
1	B	760	THR	4.1
1	B	229	LEU	4.1
1	B	762	THR	4.1
1	B	43	ASP	4.0
1	B	272	GLY	4.0
1	B	186	VAL	3.8
1	B	779	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	806	PRO	3.7
1	B	470	PHE	3.7
1	B	294	LEU	3.7
1	A	760	THR	3.7
1	B	807	GLY	3.6
1	B	810	ARG	3.5
1	B	678	PHE	3.5
1	B	589	LEU	3.4
1	B	591	LEU	3.4
1	B	702	PHE	3.4
1	B	535	LEU	3.3
1	A	807	GLY	3.2
1	B	74	PHE	3.1
1	B	776	CYS	3.1
1	B	80	ASN	3.0
1	B	613	LEU	3.0
1	B	81	GLU	3.0
1	B	792	ASN	2.9
1	B	227	LEU	2.9
1	B	471	THR	2.9
1	A	818	GLU	2.8
1	B	775	GLU	2.8
1	A	374	LEU	2.8
1	A	559	LEU	2.8
1	B	41	GLN	2.8
1	A	31	SER	2.8
1	A	809	GLN	2.8
1	B	717	LEU	2.8
1	A	401	LEU	2.7
1	B	206	LEU	2.7
1	B	561	LEU	2.7
1	B	188	GLU	2.7
1	B	763	LYS	2.7
1	B	131	LEU	2.7
1	A	271	ASP	2.7
1	A	591	LEU	2.7
1	B	177	LEU	2.7
1	B	789	GLU	2.6
1	B	208	LEU	2.6
1	B	209	SER	2.6
1	B	809	GLN	2.6
1	B	729	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	510	LEU	2.6
1	B	152	SER	2.6
1	B	559	LEU	2.6
1	B	752	ASN	2.6
1	A	717	LEU	2.5
1	B	86	LEU	2.5
1	A	372	LEU	2.5
1	B	459	PHE	2.5
1	B	153	LEU	2.5
1	B	125	LYS	2.4
1	A	344	LEU	2.4
1	A	535	LEU	2.4
1	B	175	LEU	2.4
1	B	741	LEU	2.4
1	A	178	ALA	2.4
1	B	87	GLN	2.4
1	A	318	LEU	2.4
1	B	644	LEU	2.3
1	A	561	LEU	2.3
1	A	701	LEU	2.3
1	A	808	ASP	2.3
1	B	715	ARG	2.3
1	B	178	ALA	2.3
1	A	806	PRO	2.3
1	A	177	LEU	2.3
1	A	615	PHE	2.2
1	A	777	THR	2.2
1	B	318	LEU	2.2
1	A	785	ARG	2.2
1	B	614	VAL	2.2
1	A	41	GLN	2.2
1	B	40	LYS	2.2
1	A	778	CYS	2.2
1	B	615	PHE	2.2
1	B	55	GLN	2.2
1	A	208	LEU	2.2
1	A	693	LEU	2.2
1	A	741	LEU	2.1
1	B	361	ARG	2.1
1	A	316	LEU	2.1
1	B	791	LEU	2.1
1	B	769	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	817	LEU	2.1
1	B	273	GLY	2.1
1	B	781	GLY	2.1
1	A	251	LEU	2.1
1	B	693	LEU	2.1
1	B	385	ASP	2.1
1	B	755	ALA	2.1
1	B	207	SER	2.1
1	B	344	LEU	2.0
1	A	537	LEU	2.0
1	B	372	LEU	2.0
1	B	374	LEU	2.0
1	B	433	LEU	2.0
1	B	486	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MAN	A	1004	11/12	0.20	5.83	33,39,47,55	0
2	MAN	B	905	11/12	0.22	3.16	45,60,66,67	0
3	NAG	B	908	14/15	0.20	0.85	44,57,67,72	0
2	NAG	A	1002	14/15	0.09	-0.48	19,23,32,35	0
2	NAG	B	902	14/15	0.14	-0.53	27,29,35,37	0
2	NAG	B	912	14/15	0.11	-0.61	30,34,43,43	0
2	NAG	B	903	14/15	0.10	-0.94	30,33,37,38	0
2	NAG	B	911	14/15	0.12	-1.09	23,31,34,41	0
2	NAG	A	1011	14/15	0.09	-1.11	21,26,36,47	0
3	NAG	A	1007	14/15	0.13	-1.14	36,49,53,56	0
2	NAG	A	1001	14/15	0.08	-1.52	17,21,29,31	0
3	NAG	A	1006	14/15	0.07	-2.35	20,23,28,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	907	14/15	0.07	-2.58	22,28,36,37	0
2	NAG	A	1010	14/15	0.07	-2.89	18,21,27,28	0
2	MAN	B	906	11/12	0.30	-	70,73,76,77	0
2	MAN	A	1005	11/12	0.28	-	56,66,71,76	0
2	BMA	B	904	11/12	0.17	-	39,56,63,64	0
2	MAN	B	915	11/12	0.35	-	72,78,86,87	0
3	BMA	B	909	11/12	0.34	-	69,72,73,74	0
3	BMA	A	1008	11/12	0.30	-	63,67,69,69	0
2	MAN	A	1014	11/12	0.35	-	69,73,76,76	0
2	BMA	A	1012	11/12	0.21	-	40,55,67,75	0
2	BMA	B	913	11/12	0.21	-	49,63,71,74	0
2	MAN	B	914	11/12	0.35	-	73,79,84,86	0
2	BMA	A	1003	11/12	0.12	-	32,43,54,56	0
2	MAN	A	1013	11/12	0.37	-	67,73,81,82	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	1009	14/15	0.17	9.77	48,56,68,73	0
4	NAG	B	920	14/15	0.32	5.72	77,82,86,87	0
4	NAG	A	1015	14/15	0.27	5.47	52,64,74,75	0
4	NAG	A	1016	14/15	0.31	5.06	62,65,67,69	0
4	NAG	B	917	14/15	0.26	4.46	50,60,73,76	0
4	NAG	B	921	14/15	0.25	1.52	68,72,74,77	0
6	GOL	A	1021	6/6	0.16	1.42	66,71,73,74	0
4	NAG	B	910	14/15	0.12	1.41	44,60,67,75	0
4	NAG	B	916	14/15	0.24	1.35	64,75,83,83	0
4	NAG	A	1017	14/15	0.37	1.04	62,68,75,78	0
5	RX8	B	901	23/23	0.12	0.50	22,29,41,45	0
4	NAG	B	919	14/15	0.23	0.14	52,57,63,69	0
4	NAG	B	918	14/15	0.12	-0.06	44,52,56,57	0
4	NAG	A	1018	14/15	0.10	-0.15	36,42,50,51	0
5	RX8	A	1020	23/23	0.10	-0.33	22,32,41,42	0
4	NAG	A	1019	14/15	0.09	-0.87	29,31,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.