



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:29 am GMT

PDB ID : 4QBZ  
Title : Crystal structure of human TLR8 in complex with DS-802  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2014-05-09  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

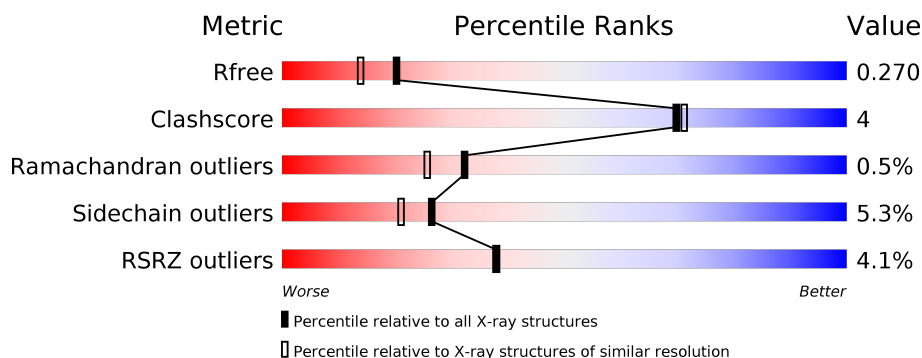
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	811	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>7%</div> </div> </div>
1	B	811	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>7%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	901	-	-	-	X
2	NAG	A	907	-	-	-	X
2	NAG	A	910	-	-	-	X
2	NAG	B	906	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13074 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	754	Total	C	N	O	S	0	0	0
			6071	3882	1029	1141	19			
1	B	751	Total	C	N	O	S	0	1	0
			6062	3878	1031	1134	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

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

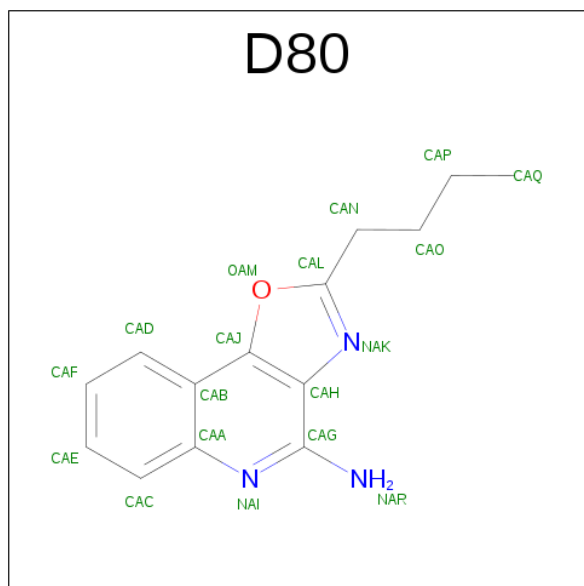
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

- Molecule 6 is 2-BUTYL[1,3]OXAZOLO[4,5-C]QUINOLIN-4-AMINE (three-letter code: D80) (formula: C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	14	3	1		
6	B	1	Total	C	N	O	0	0
			18	14	3	1		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

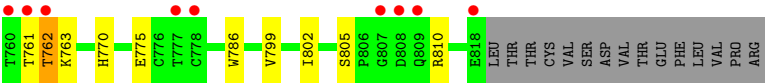
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	277	Total	O	0	0
			277	277		
8	B	229	Total	O	0	0
			229	229		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.15Å 156.72Å 86.16Å 90.00° 77.10° 90.00°	Depositor
Resolution (Å)	26.38 – 2.00 26.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.38-2.00) 99.1 (26.36-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.209 , 0.264 0.218 , 0.270	Depositor DCC
$R_{free}$ test set	6265 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: BMA, NAG, D80, 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	0.51	0/6196	0.92	9/8404 (0.1%)
1	B	0.47	0/6186	0.90	6/8387 (0.1%)
All	All	0.49	0/12382	0.91	15/16791 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	569	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	643	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	630	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	290	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	730	GLY	N-CA-C	-5.74	98.74	113.10
1	A	797	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	630	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	338	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	643	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	431	SER	C-N-CD	5.29	139.51	128.40
1	A	317	ASP	CB-CG-OD2	-5.23	113.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	GLN	CB-CA-C	-5.16	100.09	110.40
1	A	747	LEU	CB-CG-CD2	5.04	119.56	111.00
1	A	569	ARG	CG-CD-NE	5.02	122.34	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ASN	Peptide
1	A	458	ASP	Peptide
1	B	99	ASN	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	6071	0	6055	48	1
1	B	6062	0	6055	58	0
2	A	84	0	78	1	0
2	B	70	0	65	1	0
3	A	61	0	52	1	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	39	0	34	2	0
5	B	39	0	34	0	0
6	A	18	0	15	0	0
6	B	18	0	15	0	0
7	B	50	0	43	0	0
8	A	277	0	0	1	1
8	B	229	0	0	2	0
All	All	13074	0	12496	104	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:GLU:N	1:A:818:GLU:OE1	1.88	1.05
1:A:433:LEU:HD23	1:A:434:VAL:N	1.95	0.82
1:B:99:ASN:HB3	1:B:100:VAL:HG23	1.64	0.80
1:B:317:ASP:OD2	1:B:319:GLU:OE1	2.03	0.76
1:A:31:SER:OG	1:A:32:ARG:N	2.18	0.75
1:B:696:ARG:HG2	1:B:720:SER:HB2	1.69	0.74
1:A:696:ARG:HG2	1:A:720:SER:HB2	1.69	0.73
1:B:799:VAL:O	1:B:802:ILE:HD11	1.93	0.67
1:A:799:VAL:O	1:A:802:ILE:HD11	1.95	0.67
1:B:375[B]:ARG:HD2	1:B:400:ASN:HD21	1.60	0.66
1:A:651:LEU:H	1:A:674:ASN:HD22	1.47	0.63
1:A:462:ASP:OD2	3:A:906:MAN:O6	2.10	0.62
1:B:742:ASP:OD1	1:B:744:SER:HB2	2.00	0.62
1:A:632:ILE:HD11	1:A:657:GLU:HB3	1.81	0.62
1:B:744:SER:OG	1:B:770:HIS:CE1	2.54	0.61
1:A:375:ARG:HD2	1:A:400:ASN:HD21	1.66	0.61
1:B:632:ILE:HD11	1:B:657:GLU:HB3	1.83	0.61
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.37	0.60
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.21	0.59
1:A:731:PHE:O	1:A:732:LEU:HB3	2.02	0.59
1:B:736:SER:O	1:B:763:LYS:HB2	2.01	0.59
1:B:74:PHE:HE1	1:B:100:VAL:HB	1.67	0.59
1:B:682:THR:HG22	1:B:710:PHE:CZ	2.38	0.57
1:A:732:LEU:HA	1:A:735:VAL:CG1	2.35	0.57
1:B:406:ILE:H	1:B:428:ASN:HD22	1.53	0.57
1:A:649:ASN:H	1:A:674:ASN:HD21	1.54	0.56
1:A:287:THR:OG1	8:A:1158:HOH:O	2.17	0.55
1:B:411:PHE:HB3	1:B:504:LEU:HD11	1.88	0.55
1:A:433:LEU:HD23	1:A:433:LEU:C	2.27	0.54
1:A:797:ARG:HH11	1:A:797:ARG:HG2	1.72	0.54
1:B:287:THR:HA	1:B:309:ASN:O	2.08	0.53
1:B:235:LYS:HD3	1:B:235:LYS:N	2.24	0.53
1:A:287:THR:HA	1:A:309:ASN:O	2.09	0.52
1:A:797:ARG:HH11	1:A:797:ARG:CG	2.22	0.52
1:B:59:GLN:HE21	1:B:59:GLN:HA	1.75	0.52
1:B:715:ARG:HG2	1:B:739:LYS:HE2	1.91	0.52
1:B:431:SER:HB2	1:B:432:PRO:CD	2.40	0.52
1:B:404:ASN:H	1:B:428:ASN:HD21	1.58	0.52
1:A:749:LYS:N	1:A:749:LYS:HD3	2.25	0.51
1:B:98:PRO:HG2	1:B:112:ASN:OD1	2.11	0.50
1:B:300:ARG:HG3	1:B:322:TYR:HB2	1.94	0.50
1:A:60:THR:HG22	1:A:60:THR:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:VAL:HG12	1:B:101:GLN:N	2.28	0.49
1:A:329:SER:OG	1:A:330:GLY:N	2.45	0.49
1:A:234:ILE:O	1:A:256:ASN:HB3	2.12	0.49
1:B:234:ILE:O	1:B:256:ASN:HB3	2.13	0.49
1:B:761:THR:O	1:B:762:THR:HG22	2.13	0.48
2:B:909:NAG:H82	8:B:1045:HOH:O	2.14	0.48
1:B:720:SER:OG	1:B:744:SER:HB2	2.13	0.48
1:A:205:LEU:HD23	1:A:205:LEU:C	2.34	0.48
1:B:60:THR:HG22	1:B:60:THR:O	2.14	0.48
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.97	0.47
1:B:381:GLU:HG3	1:B:408:GLN:HG3	1.96	0.47
1:B:243:LYS:O	1:B:285:ASN:OD1	2.32	0.47
1:A:651:LEU:H	1:A:674:ASN:ND2	2.12	0.47
1:A:805:SER:HB3	1:B:805:SER:HB3	1.97	0.47
1:A:728:PRO:HG2	1:A:731:PHE:HB2	1.97	0.47
1:B:100:VAL:HG12	1:B:101:GLN:HG3	1.97	0.47
1:B:756:LEU:HD13	1:B:786:TRP:HB2	1.96	0.47
1:B:81:GLU:O	1:B:84:GLN:NE2	2.48	0.47
1:B:211:ASN:O	1:B:232:THR:HA	2.15	0.46
1:B:404:ASN:H	1:B:428:ASN:ND2	2.14	0.46
1:B:433:LEU:O	1:B:434:VAL:CG2	2.64	0.46
1:B:660:LEU:HD22	1:B:686:GLN:HG3	1.97	0.46
1:A:300:ARG:HG3	1:A:322:TYR:HB2	1.98	0.46
1:B:128:ARG:HA	1:B:128:ARG:HD3	1.82	0.46
1:B:584:THR:HB	8:B:1129:HOH:O	2.16	0.45
1:A:458:ASP:N	1:A:458:ASP:OD2	2.50	0.45
1:B:736:SER:O	1:B:763:LYS:CB	2.65	0.45
1:A:375:ARG:HA	1:A:402:GLY:O	2.17	0.45
1:A:534:TYR:OH	5:A:913:NAG:H81	2.16	0.44
1:B:375[B]:ARG:HA	1:B:402:GLY:O	2.17	0.44
1:A:683:LEU:HD21	2:A:916:NAG:H61	2.00	0.44
1:A:649:ASN:H	1:A:674:ASN:ND2	2.14	0.44
1:B:431:SER:HB2	1:B:432:PRO:HD2	2.00	0.44
1:B:749:LYS:HZ2	1:B:775:GLU:HB2	1.82	0.44
1:B:459:PHE:CD2	1:B:459:PHE:O	2.70	0.43
1:B:375[A]:ARG:HA	1:B:402:GLY:O	2.17	0.43
1:A:730:GLY:HA2	1:A:754:SER:O	2.18	0.43
1:B:205:LEU:HD23	1:B:205:LEU:C	2.39	0.43
1:A:213:LEU:HB2	1:A:232:THR:HB	2.00	0.43
1:A:514:ALA:HA	1:A:539:ASN:O	2.19	0.42
1:B:317:ASP:OD2	1:B:319:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:O	1:A:232:THR:HA	2.19	0.42
1:B:744:SER:HG	1:B:770:HIS:CE1	2.35	0.42
1:B:514:ALA:HA	1:B:539:ASN:O	2.19	0.42
1:A:810:ARG:CD	1:B:749:LYS:HD2	2.50	0.42
1:A:749:LYS:HD2	1:B:810:ARG:CZ	2.49	0.42
1:B:375[B]:ARG:HD2	1:B:400:ASN:ND2	2.32	0.42
1:A:45:VAL:CG1	1:A:64:TYR:O	2.68	0.42
1:A:534:TYR:CE2	5:A:913:NAG:H81	2.54	0.42
1:A:762:THR:HG22	1:A:763:LYS:N	2.35	0.41
1:B:569:ARG:HE	1:B:569:ARG:HB3	1.52	0.41
1:B:672:ASN:HA	1:B:696:ARG:O	2.19	0.41
1:B:100:VAL:HG12	1:B:101:GLN:CG	2.51	0.41
1:B:45:VAL:CG1	1:B:64:TYR:O	2.69	0.41
1:B:112:ASN:O	1:B:136:GLN:OE1	2.39	0.41
1:A:223:SER:O	1:A:225:ARG:NH1	2.54	0.41
1:A:280:ARG:CZ	1:A:305:ALA:HB1	2.52	0.41
1:A:573:VAL:O	1:A:575:HIS:CE1	2.75	0.40
1:B:49:CYS:HB3	1:B:70:LEU:HD23	2.03	0.40
1:A:431:SER:HB2	1:A:432:PRO:CD	2.50	0.40
1:A:736:SER:O	1:A:763:LYS:HG2	2.21	0.40
1:B:45:VAL:HG13	1:B:64:TYR:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LYS:NZ	8:A:1277:HOH:O[1_556]	2.02	0.18

## 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	748/811 (92%)	698 (93%)	46 (6%)	4 (0%)	32	26
1	B	744/811 (92%)	693 (93%)	48 (6%)	3 (0%)	38	33
All	All	1492/1622 (92%)	1391 (93%)	94 (6%)	7 (0%)	32	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	B	762	THR
1	B	100	VAL
1	A	330	GLY
1	B	378	VAL
1	A	42	ASN
1	A	378	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	701/755 (93%)	663 (95%)	38 (5%)	26	20
1	B	699/755 (93%)	663 (95%)	36 (5%)	27	22
All	All	1400/1510 (93%)	1326 (95%)	74 (5%)	26	21

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	40	LYS
1	A	41	GLN
1	A	42	ASN
1	A	45	VAL
1	A	49	CYS
1	A	52	ARG
1	A	55	GLN
1	A	56	GLU

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Mol	Chain	Res	Type
1	A	150	GLU
1	A	188	GLU
1	A	200	LEU
1	A	213	LEU
1	A	225	ARG
1	A	248	LEU
1	A	286	LEU
1	A	301	LYS
1	A	317	ASP
1	A	385	ASP
1	A	471	THR
1	A	472	ARG
1	A	504	LEU
1	A	534	TYR
1	A	569	ARG
1	A	584	THR
1	A	632	ILE
1	A	701	LEU
1	A	703	LEU
1	A	720	SER
1	A	732	LEU
1	A	749	LYS
1	A	753	LYS
1	A	756	LEU
1	A	760	THR
1	A	766	MET
1	A	797	ARG
1	A	816	SER
1	A	817	LEU
1	B	45	VAL
1	B	48	GLU
1	B	49	CYS
1	B	52	ARG
1	B	56	GLU
1	B	81	GLU
1	B	84	GLN
1	B	118	ASP
1	B	146	GLU
1	B	150	GLU
1	B	160	ASN
1	B	200	LEU
1	B	225	ARG

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Mol	Chain	Res	Type
1	B	235	LYS
1	B	248	LEU
1	B	280	ARG
1	B	286	LEU
1	B	300	ARG
1	B	329	SER
1	B	334	THR
1	B	385	ASP
1	B	397	SER
1	B	460	GLU
1	B	534	TYR
1	B	569	ARG
1	B	584	THR
1	B	595	ASN
1	B	632	ILE
1	B	701	LEU
1	B	703	LEU
1	B	720	SER
1	B	743	LEU
1	B	744	SER
1	B	747	LEU
1	B	749	LYS
1	B	757	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	135	ASN
1	A	309	ASN
1	A	469	HIS
1	A	674	ASN
1	B	59	GLN
1	B	84	GLN
1	B	135	ASN
1	B	136	GLN
1	B	285	ASN
1	B	428	ASN
1	B	469	HIS
1	B	531	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

19 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$
3	NAG	A	902	1,3	14,14,15	0.82	0	15,19,21	1.47	4 (26%)
3	NAG	A	903	3	14,14,15	0.61	0	15,19,21	1.58	3 (20%)
3	BMA	A	904	3	11,11,12	0.45	0	13,15,17	1.84	3 (23%)
3	BMA	A	905	3	11,11,12	0.29	0	13,15,17	2.66	7 (53%)
3	MAN	A	906	3	11,11,12	0.77	0	14,15,17	3.85	8 (57%)
4	NAG	A	908	1,4	14,14,15	1.03	1 (7%)	15,19,21	1.92	5 (33%)
4	NAG	A	909	4	14,14,15	0.51	0	15,19,21	1.78	4 (26%)
5	NAG	A	912	1,5	14,14,15	0.59	0	15,19,21	1.71	3 (20%)
5	NAG	A	913	5	14,14,15	0.95	1 (7%)	15,19,21	2.36	6 (40%)
5	BMA	A	914	5	11,11,12	0.46	0	13,15,17	2.20	6 (46%)
7	NAG	B	902	1,7	14,14,15	0.63	0	15,19,21	1.95	7 (46%)
7	NAG	B	903	7	14,14,15	0.91	1 (7%)	15,19,21	1.45	2 (13%)
7	BMA	B	904	7	11,11,12	0.49	0	13,15,17	2.13	5 (38%)
7	MAN	B	905	7	11,11,12	0.52	0	13,15,17	2.96	7 (53%)
4	NAG	B	907	1,4	14,14,15	0.79	1 (7%)	15,19,21	2.14	5 (33%)
4	NAG	B	908	4	14,14,15	0.60	0	15,19,21	2.85	6 (40%)
5	NAG	B	911	1,5	14,14,15	0.78	0	15,19,21	1.52	1 (6%)
5	NAG	B	912	5	14,14,15	0.74	0	15,19,21	1.58	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	B	913	5	11,11,12	0.55	0	13,15,17	2.08	4 (30%)

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	-	0/6/23/26	0/1/1/1
3	BMA	A	904	3	-	0/2/19/22	0/1/1/1
3	BMA	A	905	3	-	0/2/19/22	0/1/1/1
3	MAN	A	906	3	-	0/2/18/22	0/1/1/1
4	NAG	A	908	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	909	4	-	0/6/23/26	0/1/1/1
5	NAG	A	912	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	913	5	-	0/6/23/26	0/1/1/1
5	BMA	A	914	5	-	0/2/19/22	0/1/1/1
7	NAG	B	902	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	903	7	-	0/6/23/26	0/1/1/1
7	BMA	B	904	7	-	0/2/19/22	0/1/1/1
7	MAN	B	905	7	-	0/2/19/22	0/1/1/1
4	NAG	B	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	908	4	-	0/6/23/26	0/1/1/1
5	NAG	B	911	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	912	5	-	0/6/23/26	0/1/1/1
5	BMA	B	913	5	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	908	NAG	O5-C1	-2.67	1.39	1.43
5	A	913	NAG	C8-C7	-2.22	1.45	1.50
4	B	907	NAG	O5-C1	-2.21	1.40	1.43
7	B	903	NAG	O5-C1	-2.14	1.40	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	906	MAN	C2-C3-C4	-8.95	98.89	110.59
7	B	905	MAN	O3-C3-C2	-6.06	99.00	110.02
3	A	906	MAN	C3-C4-C5	-5.53	104.38	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	905	MAN	O5-C1-C2	-5.48	102.20	110.79
3	A	906	MAN	C1-C2-C3	-5.37	101.92	111.13
3	A	906	MAN	O5-C1-C2	-5.30	106.88	110.77
5	A	913	NAG	O7-C7-C8	-4.99	112.97	122.06
5	A	912	NAG	O4-C4-C3	-4.47	100.64	110.36
3	A	905	BMA	O5-C1-C2	-4.38	103.92	110.79
5	B	913	BMA	C2-C3-C4	-4.35	103.29	110.88
5	A	914	BMA	C2-C3-C4	-4.25	103.47	110.88
4	B	907	NAG	C4-C3-C2	-4.23	104.82	111.02
3	A	905	BMA	C2-C3-C4	-3.96	103.97	110.88
4	A	908	NAG	C4-C3-C2	-3.84	105.40	111.02
3	A	905	BMA	C1-C2-C3	-3.79	104.84	109.65
4	B	907	NAG	C1-O5-C5	-3.67	107.11	112.17
3	A	904	BMA	C2-C3-C4	-3.63	104.54	110.88
5	B	911	NAG	O5-C1-C2	-3.56	106.52	111.47
3	A	905	BMA	O4-C4-C3	-3.39	102.97	110.36
4	A	909	NAG	C3-C4-C5	-3.14	104.68	110.22
3	A	903	NAG	O7-C7-C8	-3.13	116.37	122.06
4	A	908	NAG	O3-C3-C2	-3.08	102.79	109.39
5	B	912	NAG	C4-C3-C2	-3.05	106.54	111.02
4	B	907	NAG	O4-C4-C3	-3.02	103.78	110.36
5	B	912	NAG	O4-C4-C3	-3.02	103.78	110.36
4	A	908	NAG	C1-C2-N2	-2.98	105.40	110.49
7	B	905	MAN	O2-C2-C1	-2.96	103.15	109.18
5	A	913	NAG	O3-C3-C4	-2.86	104.13	110.36
7	B	904	BMA	O5-C1-C2	-2.84	106.33	110.79
7	B	904	BMA	O3-C3-C4	-2.80	104.26	110.36
5	A	912	NAG	O5-C1-C2	-2.73	107.67	111.47
4	B	908	NAG	O6-C6-C5	-2.68	102.31	111.34
7	B	903	NAG	O5-C1-C2	-2.68	107.74	111.47
3	A	902	NAG	O6-C6-C5	-2.64	102.47	111.34
3	A	904	BMA	O4-C4-C3	-2.62	104.66	110.36
4	B	908	NAG	O3-C3-C4	-2.56	104.78	110.36
4	B	908	NAG	O7-C7-C8	-2.55	117.41	122.06
5	A	913	NAG	O6-C6-C5	-2.51	102.89	111.34
7	B	902	NAG	C1-C2-N2	-2.46	106.29	110.49
4	A	909	NAG	O7-C7-C8	-2.45	117.60	122.06
7	B	902	NAG	O5-C1-C2	-2.45	108.07	111.47
7	B	902	NAG	O6-C6-C5	-2.34	103.47	111.34
3	A	905	BMA	O2-C2-C1	-2.31	104.48	109.18
4	A	909	NAG	C2-N2-C7	-2.28	119.61	122.94
5	A	914	BMA	O2-C2-C3	-2.26	105.74	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	907	NAG	O6-C6-C5	-2.24	103.82	111.34
4	A	908	NAG	C6-C5-C4	-2.22	107.81	113.00
7	B	902	NAG	O4-C4-C5	-2.22	103.69	109.28
3	A	902	NAG	C2-N2-C7	-2.21	119.71	122.94
5	A	914	BMA	O4-C4-C5	-2.18	103.79	109.28
5	A	914	BMA	O4-C4-C3	-2.16	105.65	110.36
3	A	906	MAN	O6-C6-C5	-2.06	104.42	111.34
5	A	912	NAG	O3-C3-C4	-2.02	105.97	110.36
5	B	912	NAG	O7-C7-N2	2.03	125.82	121.92
3	A	903	NAG	O7-C7-N2	2.22	126.19	121.92
7	B	903	NAG	C6-C5-C4	2.23	118.23	113.00
7	B	902	NAG	O7-C7-N2	2.29	126.33	121.92
7	B	905	MAN	O4-C4-C3	2.29	115.35	110.36
5	B	913	BMA	C3-C4-C5	2.30	114.27	110.22
7	B	904	BMA	C1-C2-C3	2.38	112.67	109.65
7	B	905	MAN	O3-C3-C4	2.38	115.53	110.36
7	B	904	BMA	C1-O5-C5	2.39	115.46	112.17
3	A	902	NAG	C6-C5-C4	2.41	118.64	113.00
3	A	905	BMA	O3-C3-C4	2.42	115.61	110.36
5	B	913	BMA	C1-C2-C3	2.42	112.72	109.65
7	B	905	MAN	C2-C3-C4	2.49	115.21	110.88
4	A	908	NAG	C3-C4-C5	2.60	114.80	110.22
5	A	913	NAG	C2-N2-C7	2.77	126.99	122.94
3	A	902	NAG	O3-C3-C4	2.78	116.41	110.36
3	A	903	NAG	C1-C2-N2	2.80	115.28	110.49
4	B	908	NAG	C8-C7-N2	2.82	121.19	116.11
3	A	906	MAN	O4-C4-C5	2.87	116.52	109.28
7	B	902	NAG	C1-O5-C5	2.88	116.14	112.17
7	B	905	MAN	C1-C2-C3	2.89	113.32	109.65
7	B	902	NAG	O4-C4-C3	2.90	116.67	110.36
3	A	906	MAN	O3-C3-C4	2.96	116.00	110.17
5	A	914	BMA	C1-C2-C3	3.09	113.57	109.65
5	A	913	NAG	C8-C7-N2	3.12	121.73	116.11
5	A	913	NAG	C1-C2-N2	3.22	115.99	110.49
4	B	907	NAG	O3-C3-C4	3.34	117.62	110.36
4	A	909	NAG	C8-C7-N2	3.38	122.21	116.11
4	B	908	NAG	C1-C2-N2	3.41	116.31	110.49
3	A	905	BMA	C3-C4-C5	3.52	116.42	110.22
3	A	904	BMA	O3-C3-C2	3.67	116.69	110.02
5	A	914	BMA	O3-C3-C4	3.72	118.44	110.36
3	A	906	MAN	O3-C3-C2	3.82	119.28	110.02
5	B	913	BMA	O3-C3-C4	3.93	118.91	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	904	BMA	O3-C3-C2	4.91	118.95	110.02
4	B	908	NAG	C1-O5-C5	8.54	123.94	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	906	MAN	1	0
5	A	913	NAG	2	0

## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	901	1	14,14,15	0.64	0	15,19,21	1.56	3 (20%)
2	NAG	A	907	1	14,14,15	0.46	0	15,19,21	1.17	2 (13%)
2	NAG	A	910	1	14,14,15	0.76	0	15,19,21	1.85	3 (20%)
2	NAG	A	911	1	14,14,15	0.42	0	15,19,21	2.78	4 (26%)
2	NAG	A	915	1	14,14,15	0.90	1 (7%)	15,19,21	3.07	6 (40%)
2	NAG	A	916	1	14,14,15	0.62	0	15,19,21	3.00	6 (40%)
6	D80	A	917	-	16,20,20	0.95	1 (6%)	15,28,28	1.19	2 (13%)
6	D80	B	901	-	16,20,20	1.08	1 (6%)	15,28,28	0.83	0
2	NAG	B	906	1	14,14,15	0.42	0	15,19,21	2.45	9 (60%)
2	NAG	B	909	1	14,14,15	0.54	0	15,19,21	2.15	5 (33%)
2	NAG	B	910	1	14,14,15	0.37	0	15,19,21	1.87	2 (13%)
2	NAG	B	914	1	14,14,15	0.73	0	15,19,21	2.38	8 (53%)
2	NAG	B	915	1	14,14,15	0.52	0	15,19,21	3.48	6 (40%)

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	901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	907	1	-	0/6/23/26	0/1/1/1
2	NAG	A	910	1	-	0/6/23/26	0/1/1/1
2	NAG	A	911	1	-	0/6/23/26	0/1/1/1
2	NAG	A	915	1	-	0/6/23/26	0/1/1/1
2	NAG	A	916	1	-	0/6/23/26	0/1/1/1
6	D80	A	917	-	-	0/3/4/4	0/2/3/3
6	D80	B	901	-	-	0/3/4/4	0/2/3/3
2	NAG	B	906	1	-	0/6/23/26	0/1/1/1
2	NAG	B	909	1	-	0/6/23/26	0/1/1/1
2	NAG	B	910	1	-	0/6/23/26	0/1/1/1
2	NAG	B	914	1	-	0/6/23/26	0/1/1/1
2	NAG	B	915	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	917	D80	CAB-CAJ	-2.35	1.38	1.41
2	A	915	NAG	O5-C1	-2.10	1.40	1.43
6	B	901	D80	CAC-CAA	-2.04	1.38	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	916	NAG	C1-O5-C5	-6.70	102.93	112.17
2	A	915	NAG	O3-C3-C4	-6.06	97.17	110.36
2	A	915	NAG	O5-C1-C2	-5.31	104.08	111.47
2	A	916	NAG	O5-C1-C2	-5.19	104.25	111.47
2	B	909	NAG	C6-C5-C4	-4.35	102.81	113.00
2	A	915	NAG	O6-C6-C5	-4.31	96.83	111.34
2	A	910	NAG	O5-C1-C2	-4.30	105.49	111.47
2	B	915	NAG	O5-C1-C2	-4.13	105.72	111.47
2	B	906	NAG	C6-C5-C4	-4.02	103.58	113.00
2	A	915	NAG	O4-C4-C3	-3.90	101.88	110.36
2	B	915	NAG	C2-N2-C7	-3.72	117.52	122.94
2	B	914	NAG	O4-C4-C3	-3.35	103.06	110.36
2	B	915	NAG	C4-C3-C2	-3.30	106.18	111.02
2	B	909	NAG	O6-C6-C5	-3.24	100.43	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	909	NAG	C2-N2-C7	-3.10	118.43	122.94
2	B	914	NAG	C1-C2-N2	-2.99	105.38	110.49
2	A	901	NAG	O6-C6-C5	-2.95	101.42	111.34
2	B	915	NAG	C6-C5-C4	-2.84	106.37	113.00
2	B	914	NAG	O5-C1-C2	-2.79	107.60	111.47
2	A	916	NAG	O3-C3-C4	-2.78	104.30	110.36
2	A	916	NAG	O7-C7-C8	-2.75	117.05	122.06
6	A	917	D80	CAD-CAB-CAJ	-2.70	118.74	122.60
2	A	910	NAG	O6-C6-C5	-2.66	102.37	111.34
2	B	915	NAG	O3-C3-C4	-2.66	104.56	110.36
2	B	914	NAG	O7-C7-C8	-2.65	117.24	122.06
2	A	911	NAG	O4-C4-C3	-2.61	104.67	110.36
2	A	907	NAG	O7-C7-C8	-2.52	117.47	122.06
2	B	906	NAG	C8-C7-N2	-2.52	111.56	116.11
2	A	901	NAG	C6-C5-C4	-2.50	107.14	113.00
2	A	915	NAG	C1-C2-N2	-2.48	106.25	110.49
2	B	906	NAG	C4-C3-C2	-2.43	107.46	111.02
2	B	906	NAG	C1-C2-N2	-2.41	106.37	110.49
2	B	914	NAG	O3-C3-C4	-2.40	105.14	110.36
2	B	906	NAG	O3-C3-C4	-2.37	105.21	110.36
2	B	909	NAG	C4-C3-C2	-2.34	107.59	111.02
2	A	907	NAG	C1-C2-N2	-2.29	106.58	110.49
2	A	916	NAG	O6-C6-C5	-2.06	104.40	111.34
2	B	906	NAG	O7-C7-N2	2.01	125.78	121.92
2	A	911	NAG	C3-C4-C5	2.12	113.96	110.22
2	B	914	NAG	O7-C7-N2	2.20	126.16	121.92
2	A	901	NAG	C1-O5-C5	2.31	115.35	112.17
6	A	917	D80	CAD-CAB-CAA	2.40	121.20	117.59
2	B	906	NAG	C1-O5-C5	2.91	116.18	112.17
2	A	911	NAG	O5-C1-C2	3.06	115.73	111.47
2	B	909	NAG	C1-C2-N2	3.39	116.28	110.49
2	B	910	NAG	C2-N2-C7	3.55	128.12	122.94
2	B	906	NAG	O4-C4-C5	3.55	118.22	109.28
2	A	910	NAG	C1-O5-C5	3.70	117.27	112.17
2	B	914	NAG	C2-N2-C7	4.05	128.85	122.94
2	B	906	NAG	C3-C4-C5	4.13	117.49	110.22
2	B	914	NAG	C1-O5-C5	4.26	118.03	112.17
2	A	915	NAG	C1-O5-C5	4.43	118.28	112.17
2	B	910	NAG	C1-C2-N2	5.17	119.33	110.49
2	A	916	NAG	C1-C2-N2	5.76	120.32	110.49
2	A	911	NAG	C1-O5-C5	9.31	125.00	112.17
2	B	915	NAG	C1-O5-C5	10.77	127.00	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	916	NAG	1	0
2	B	909	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	754/811 (92%)	-0.00	29 (3%)	41 41	20, 34, 59, 90	0
1	B	751/811 (92%)	0.10	33 (4%)	35 35	22, 38, 68, 96	0
All	All	1505/1622 (92%)	0.05	62 (4%)	38 38	20, 36, 63, 96	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	LEU	6.3
1	B	760	THR	6.2
1	B	100	VAL	6.0
1	A	100	VAL	5.4
1	B	459	PHE	5.3
1	B	434	VAL	4.9
1	A	470	PHE	4.8
1	B	808	ASP	4.7
1	B	41	GLN	4.6
1	A	64	TYR	4.6
1	A	43	ASP	4.6
1	A	457	THR	4.6
1	B	761	THR	4.2
1	A	434	VAL	4.0
1	B	112	ASN	3.9
1	A	818	GLU	3.9
1	B	31	SER	3.8
1	A	808	ASP	3.8
1	B	818	GLU	3.6
1	A	31	SER	3.6
1	B	759	LYS	3.6
1	B	472	ARG	3.4
1	A	40	LYS	3.3
1	B	778	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	470	PHE	3.2
1	B	762	THR	3.2
1	B	678	PHE	3.1
1	B	39	LYS	3.1
1	A	42	ASN	3.1
1	B	702	PHE	3.0
1	A	41	GLN	3.0
1	A	374	LEU	3.0
1	B	101	GLN	2.8
1	B	85	GLY	2.8
1	B	63	LYS	2.8
1	A	253	LEU	2.7
1	B	46	ILE	2.6
1	A	294	LEU	2.6
1	A	791	LEU	2.6
1	B	589	LEU	2.6
1	A	759	LYS	2.5
1	A	99	ASN	2.5
1	A	44	SER	2.5
1	A	807	GLY	2.4
1	B	374	LEU	2.3
1	A	153	LEU	2.3
1	B	752	ASN	2.3
1	B	753	LYS	2.3
1	B	809	GLN	2.3
1	B	510	LEU	2.2
1	B	471	THR	2.2
1	B	535	LEU	2.2
1	B	807	GLY	2.2
1	A	760	THR	2.1
1	A	208	LEU	2.1
1	A	63	LYS	2.1
1	A	271	ASP	2.1
1	A	458	ASP	2.1
1	A	471	THR	2.1
1	B	777	THR	2.1
1	B	64	TYR	2.1
1	A	620	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	903	14/15	0.95	0.12	0.20	27,33,39,48	0
7	NAG	B	903	14/15	0.92	0.10	-0.24	29,35,42,44	0
7	NAG	B	902	14/15	0.94	0.10	-0.65	28,31,37,47	0
4	NAG	B	907	14/15	0.96	0.09	-0.98	24,26,30,32	0
4	NAG	A	908	14/15	0.96	0.08	-1.05	22,25,30,32	0
5	NAG	B	911	14/15	0.95	0.07	-1.73	24,28,29,30	0
3	NAG	A	902	14/15	0.96	0.08	-1.78	23,26,30,38	0
5	NAG	A	912	14/15	0.97	0.06	-2.00	20,23,27,27	0
4	NAG	A	909	14/15	0.90	0.17	-	36,44,54,55	0
5	NAG	A	913	14/15	0.93	0.12	-	25,30,38,38	0
5	BMA	A	914	11/12	0.87	0.20	-	42,47,50,61	0
3	MAN	A	906	11/12	0.76	0.29	-	44,63,72,94	0
5	BMA	B	913	11/12	0.85	0.21	-	44,51,61,63	0
4	NAG	B	908	14/15	0.87	0.22	-	40,51,56,56	0
3	BMA	A	905	11/12	0.90	0.27	-	59,65,68,70	0
5	NAG	B	912	14/15	0.93	0.12	-	31,33,39,45	0
7	MAN	B	905	11/12	0.61	0.24	-	58,67,77,79	0
3	BMA	A	904	11/12	0.95	0.23	-	42,46,51,55	0
7	BMA	B	904	11/12	0.89	0.20	-	41,46,48,52	0

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	910	14/15	0.94	0.19	7.55	45,56,60,67	0
2	NAG	B	906	14/15	0.88	0.19	4.83	33,43,46,57	0
2	NAG	A	901	14/15	0.79	0.27	3.81	48,57,63,66	0
2	NAG	A	907	14/15	0.94	0.15	2.91	33,39,44,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	915	14/15	0.91	0.13	0.97	33,43,48,50	0
2	NAG	B	914	14/15	0.94	0.12	0.79	27,40,53,55	0
6	D80	B	901	18/18	0.96	0.09	-0.51	21,24,28,30	0
6	D80	A	917	18/18	0.96	0.08	-1.09	21,25,28,28	0
2	NAG	B	910	14/15	0.87	0.27	-	55,62,65,66	0
2	NAG	A	911	14/15	0.86	0.29	-	57,62,68,71	0
2	NAG	A	916	14/15	0.91	0.23	-	45,51,63,67	0
2	NAG	B	909	14/15	0.91	0.18	-	41,54,64,67	0
2	NAG	B	915	14/15	0.87	0.19	-	48,54,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.