Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:05 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

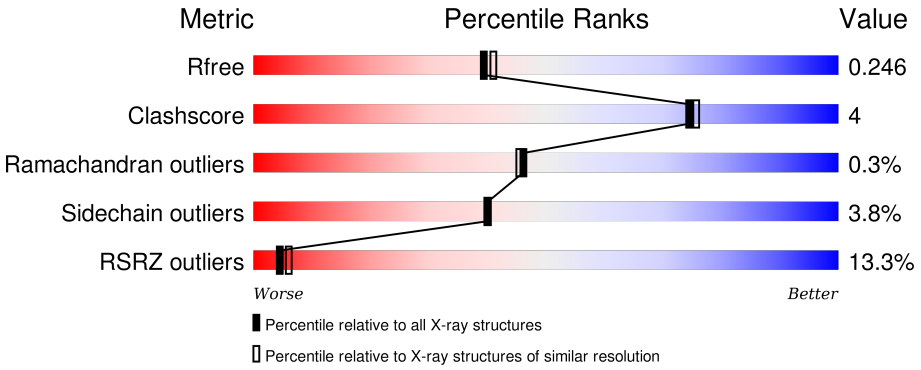
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	811	8% 82% 9% • 7%
1	B	811	16% 79% 12% • 8%

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
4	NAG	A	1015	-	-	-	X
4	NAG	B	917	-	-	-	X
4	NAG	B	921	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13256 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	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

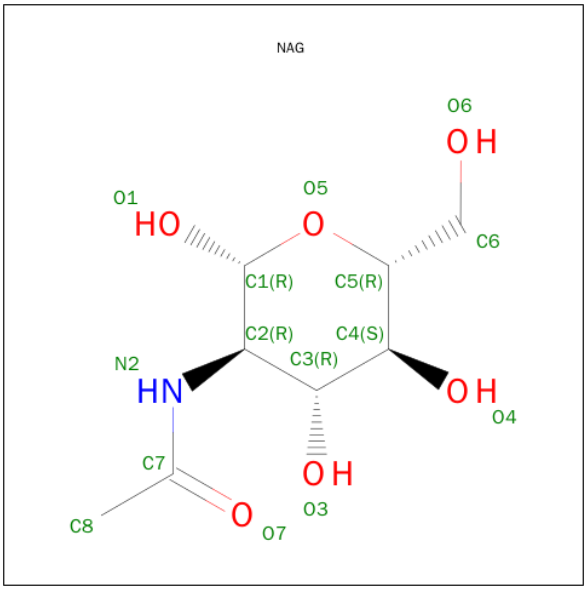
- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

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

- 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 39 22 2 15	0	0
3	B	3	Total C N O 39 22 2 15	0	0

- 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 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0

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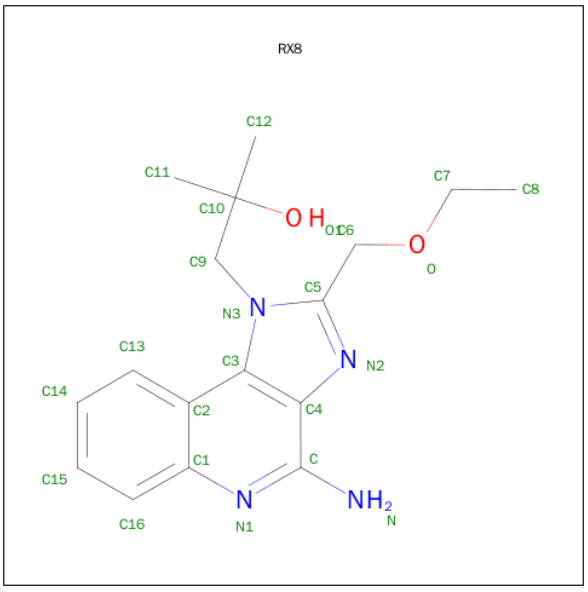
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total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

- 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: $C_{17}H_{22}N_4O_2$).



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

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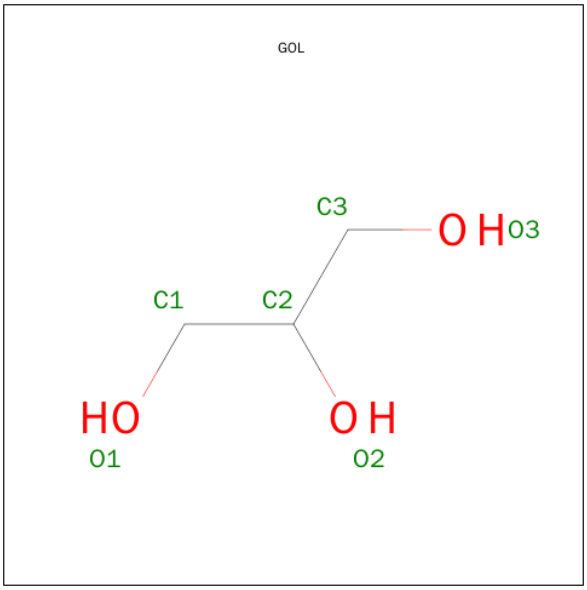
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

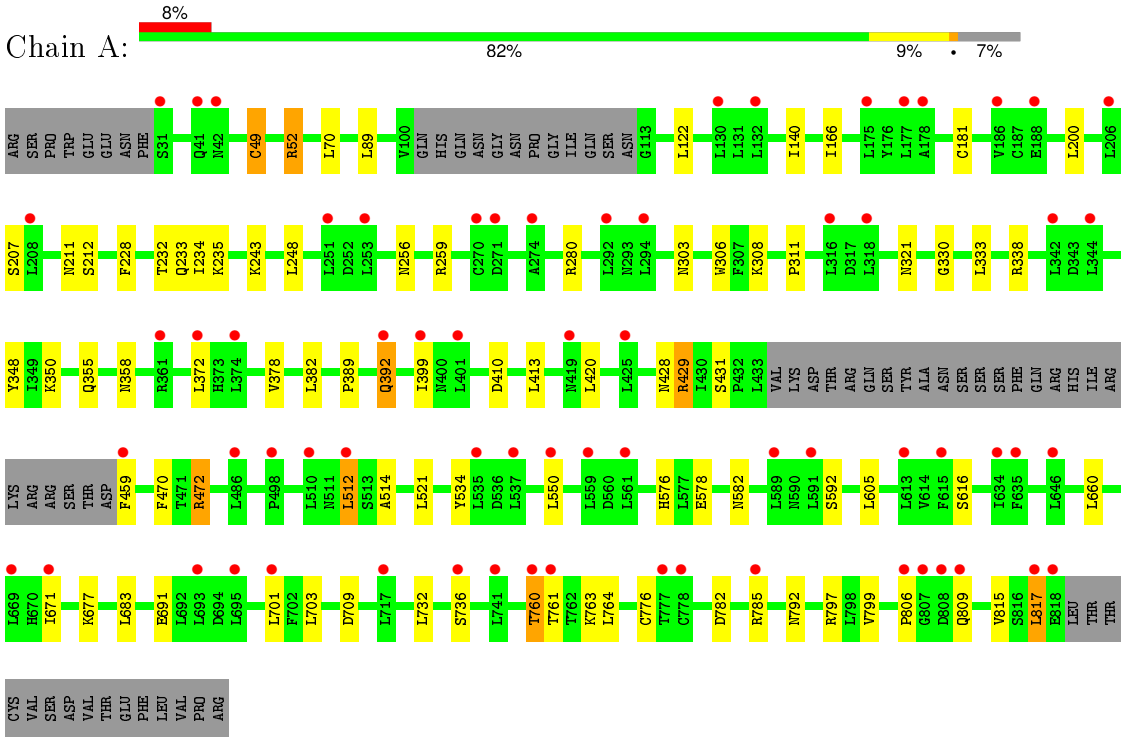
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	419	Total	O	0	0
			419	419		
7	B	248	Total	O	0	0
			248	248		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

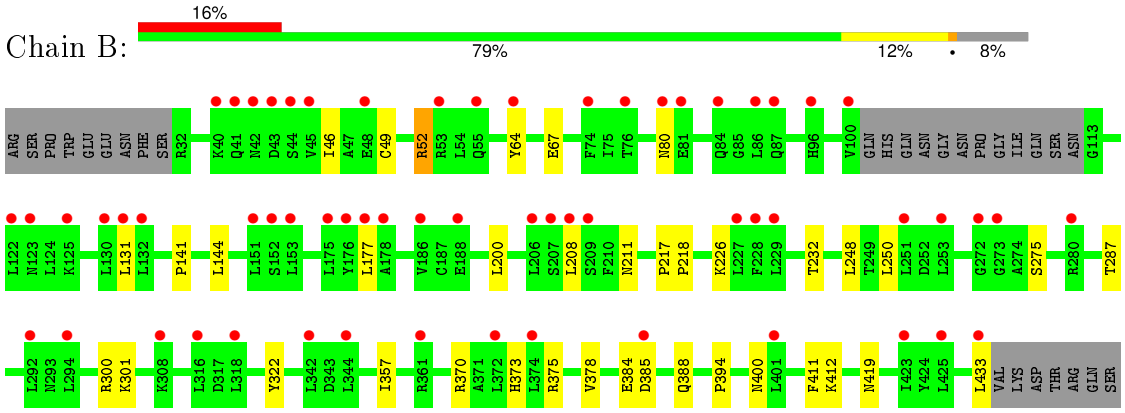
- Molecule 1: Toll-like receptor 8

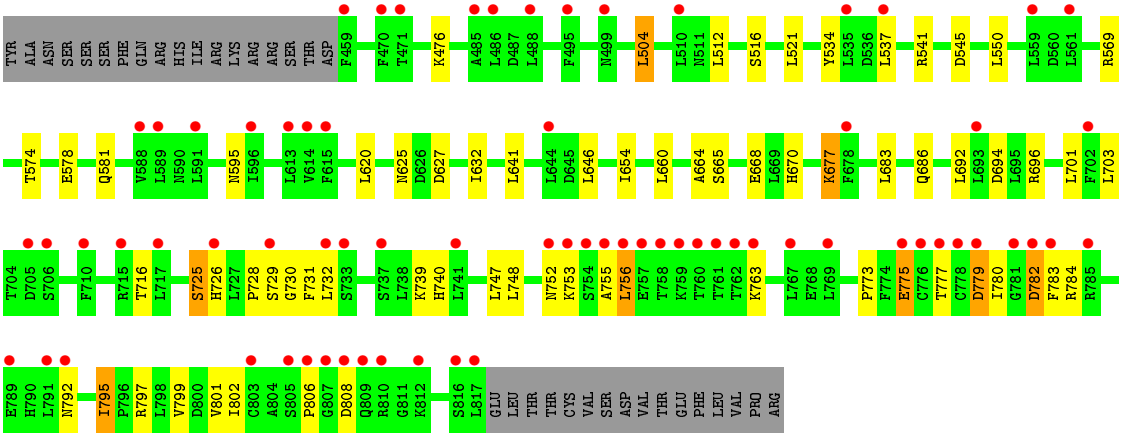
Chain A:



- Molecule 1: Toll-like receptor 8

Chain B:




TYR ALA ASN SER SER SER PHE GLN ARG HIS ILE ARG LYS ARG ARG SER THR ASP F459 F470 T471 K476 A485 L486 D487 L488 F495 W499 L504 L510 N511 L512 S516 L521 Y534 L535 D536 L537 R541 D545 L550 L559 D560 L561 R569
T574 E578 Q581 V588 L589 N590 L591 N595 I596 L613 V614 F615 L620 N625 D626 D627 I632 L641 L644 D645 L646 I654 L660 A664 S665 E668 L669 H670 K677 F678 L683 Q686 L692 L693 D694 L695 R696 L701 F702 L703
T704 D705 S706 F710 R715 T716 L717 S725 H726 L727 P728 S729 G730 F731 L732 S733 S737 L738 K739 H740 L741 L747 L748 N752 K753 S754 A755 L756 E757 T758 K759 T760 T761 T762 K763 L767 E768 L769 P773 F774 E775 C776 T777 C778 D779 I780 G781 D782 F783 R784 R785
E789 H790 L791 N792 L795 P796 R797 L798 V799 D800 V801 I802 C803 A804 S805 P806 G807 D808 Q809 R810 G811 K812 S816 L817 GLU LEU THR THR CYS VAL SER ASP VAL THR GLU PHE LEU VAL PRO ARG

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.200 , 0.233 0.212 , 0.246	Depositor DCC
R_{free} test set	6502 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 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	6039	0	6005	41	0
1	B	5994	0	5937	57	0
2	A	122	0	104	0	0
2	B	122	0	104	0	0
3	A	39	0	34	0	0
3	B	39	0	34	1	0
4	A	84	0	78	1	0
4	B	98	0	91	0	0
5	A	23	0	22	1	0
5	B	23	0	22	3	0
6	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	419	0	0	10	0
7	B	248	0	0	9	0
All	All	13256	0	12439	100	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 4.

All (100) 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: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:333:LEU:O	7:A:1220:HOH:O	2.05	0.74
1:B:775:GLU:O	1:B:780:ILE:HD11	1.91	0.71
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:459:PHE:HB2	7:A:1160:HOH:O	1.94	0.66
1:B:370:ARG:NH1	7:B:1094:HOH:O	2.17	0.65
1:A:350:LYS:NZ	7:A:1454:HOH:O	2.30	0.64
1:A:732:LEU:HD21	1:A:764:LEU:HD22	1.81	0.63
1:B:52:ARG:HG2	1:B:799:VAL:HG11	1.82	0.62
1:B:660:LEU:HD22	1:B:686:GLN:HG3	1.83	0.61
1:B:46:ILE:HG12	1:B:67:GLU:HB2	1.82	0.61
1:A:677:LYS:O	7:A:1410:HOH:O	2.16	0.61
5:B:901:RX8:H19	5:B:901:RX8:H9	1.82	0.60
1:B:795:ILE:HD11	1:B:801:VAL:HG21	1.83	0.60
1:B:748:LEU:H	1:B:773:PRO:HD2	1.66	0.60
1:B:753:LYS:HA	1:B:756:LEU:HD22	1.82	0.60
1:A:776:CYS:HB3	1:A:817:LEU:HD11	1.84	0.60
4:A:1018:NAG:O7	7:A:1384:HOH:O	2.17	0.59
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.83	0.59
1:B:654:ILE:O	7:B:1210:HOH:O	2.16	0.58
1:B:300:ARG:HG2	1:B:322:TYR:HB2	1.84	0.58
1:A:782:ASP:OD1	1:A:785:ARG:NH1	2.37	0.58
1:B:677:LYS:HD3	7:B:1204:HOH:O	2.03	0.57
1:B:780:ILE:O	1:B:783:PHE:N	2.37	0.57
1:A:355:GLN:NE2	7:A:1476:HOH:O	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1020:RX8:H9	5:A:1020:RX8:H19	1.87	0.56
1:B:574:THR:HG23	5:B:901:RX8:H10	1.88	0.56
1:A:399:ILE:HG12	1:A:420:LEU:HD21	1.86	0.55
1:B:394:PRO:O	1:B:419:ASN:ND2	2.40	0.55
1:B:782:ASP:N	1:B:782:ASP:OD1	2.37	0.55
1:B:357:ILE:HG22	7:B:1031:HOH:O	2.06	0.55
1:A:514:ALA:C	1:B:541:ARG:HH22	2.11	0.54
1:A:392:GLN:NE2	1:A:392:GLN:H	2.08	0.52
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.74	0.52
1:B:739:LYS:HG2	1:B:763:LYS:NZ	2.24	0.52
1:A:212:SER:OG	1:A:233:GLN:NE2	2.42	0.52
1:A:52:ARG:HG2	1:A:799:VAL:HG21	1.91	0.52
1:B:660:LEU:HD21	1:B:683:LEU:HD22	1.92	0.51
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.93	0.51
1:B:694:ASP:OD2	1:B:696:ARG:NH2	2.42	0.50
1:A:470:PHE:CD1	1:A:472:ARG:HG3	2.47	0.50
1:B:739:LYS:HG2	1:B:763:LYS:HZ3	1.77	0.50
1:A:207:SER:HA	1:A:228:PHE:HB2	1.93	0.49
1:B:64:TYR:H	1:B:64:TYR:HD1	1.61	0.49
1:B:627:ASP:HB2	7:B:1187:HOH:O	2.12	0.48
1:B:730:GLY:H	1:B:755:ALA:HA	1.78	0.48
1:B:668:GLU:HG3	1:B:692:LEU:HB3	1.96	0.48
1:B:476:LYS:HD2	3:B:907:NAG:H83	1.94	0.48
1:A:806:PRO:HD2	1:A:809:GLN:HB2	1.95	0.48
1:B:725:SER:HA	1:B:747:LEU:O	2.13	0.48
1:B:792:ASN:N	1:B:792:ASN:OD1	2.47	0.47
1:B:777:THR:H	1:B:780:ILE:CD1	2.27	0.47
1:A:311:PRO:O	1:A:338:ARG:HG3	2.15	0.47
1:A:49:CYS:HB3	1:A:70:LEU:HD23	1.97	0.47
1:B:732:LEU:HD12	1:B:756:LEU:HD12	1.96	0.47
1:A:235:LYS:HE3	1:A:235:LYS:HB3	1.61	0.46
1:A:792:ASN:OD1	1:A:792:ASN:N	2.47	0.46
1:A:348:TYR:CD2	5:B:901:RX8:H3	2.51	0.45
1:B:716:THR:HG23	1:B:740:HIS:HB3	1.98	0.45
1:B:512:LEU:HB2	1:B:537:LEU:HD23	1.98	0.45
1:B:545:ASP:OD1	1:B:574:THR:OG1	2.26	0.45
1:A:140:ILE:HD13	1:A:166:ILE:HD11	1.99	0.45
1:B:177:LEU:HB2	1:B:208:LEU:HD23	2.00	0.43
1:B:385:ASP:HA	1:B:388:GLN:HG2	2.01	0.43
1:B:141:PRO:HB2	1:B:144:LEU:HD21	2.01	0.43
1:B:729:SER:HA	1:B:755:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:PRO:HG2	1:B:808:ASP:OD1	2.19	0.43
1:B:375:ARG:NE	7:B:1195:HOH:O	2.52	0.43
1:A:259:ARG:NH1	1:A:321:ASN:O	2.48	0.42
1:B:373:HIS:HA	1:B:400:ASN:HB3	2.01	0.42
1:A:280:ARG:HH22	1:A:308:LYS:HE2	1.84	0.42
1:B:728:PRO:HG2	1:B:731:PHE:HD2	1.85	0.42
1:A:211:ASN:O	1:A:232:THR:HA	2.19	0.42
1:B:411:PHE:HB3	1:B:504:LEU:HD13	2.02	0.42
1:B:211:ASN:O	1:B:232:THR:HA	2.19	0.42
1:B:217:PRO:HA	1:B:218:PRO:HD3	1.84	0.41
1:B:226:LYS:HG2	1:B:250:LEU:HB3	2.01	0.41
1:B:780:ILE:HG22	1:B:784:ARG:HG2	2.02	0.41
1:A:234:ILE:O	1:A:256:ASN:HB3	2.21	0.41
1:A:512:LEU:HD12	1:A:512:LEU:HA	1.90	0.41
1:B:670:HIS:HA	1:B:694:ASP:HB3	2.02	0.41
1:A:428:ASN:HB3	1:A:429:ARG:H	1.75	0.41
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.20	0.41
1:A:736:SER:O	1:A:763:LYS:HG2	2.21	0.41
1:B:521:LEU:HD13	1:B:550:LEU:HD21	2.03	0.41
1:B:677:LYS:HE3	1:B:677:LYS:HB3	1.85	0.41
1:A:181:CYS:HB3	7:A:1506:HOH:O	2.21	0.41
1:A:592:SER:HA	1:A:616:SER:O	2.21	0.40
1:B:620:LEU:HD11	1:B:646:LEU:HD22	2.03	0.40
1:B:641:LEU:O	1:B:665:SER:OG	2.36	0.40
1:A:303:ASN:HB3	1:A:306:TRP:CE2	2.56	0.40
1:A:709:ASP:OD1	7:A:1460:HOH:O	2.21	0.40
1:B:578:GLU:O	1:B:581:GLN:HG2	2.22	0.40
1:A:382:LEU:HG	1:A:413:LEU:HD21	2.02	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	745/811 (92%)	711 (95%)	32 (4%)	2 (0%)	46 45
1	B	743/811 (92%)	710 (96%)	31 (4%)	2 (0%)	46 45
All	All	1488/1622 (92%)	1421 (96%)	63 (4%)	4 (0%)	46 45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	797	ARG
1	A	378	VAL
1	B	378	VAL
1	A	330	GLY

5.3.2 Protein sidechains (i)

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%)	43 44
1	B	683/755 (90%)	654 (96%)	29 (4%)	36 35
All	All	1377/1510 (91%)	1324 (96%)	53 (4%)	40 40

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

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Mol	Chain	Res	Type
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
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. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	233	GLN
1	A	392	GLN
1	A	790	HIS
1	B	309	ASN
1	B	499	ASN
1	B	809	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

26 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	1001	1,2	14,14,15	0.54	0	15,19,21	0.57	0
2	NAG	A	1002	2	14,14,15	0.64	0	15,19,21	0.61	0
2	BMA	A	1003	2	11,11,12	0.79	1 (9%)	14,15,17	0.92	0
2	MAN	A	1004	2	11,11,12	0.60	0	14,15,17	0.58	0
2	MAN	A	1005	2	11,11,12	0.61	0	14,15,17	0.81	0
3	NAG	A	1006	1,3	14,14,15	0.53	0	15,19,21	0.78	0
3	NAG	A	1007	3	14,14,15	0.57	0	15,19,21	0.82	0
3	BMA	A	1008	3	11,11,12	0.57	0	14,15,17	0.77	0
2	NAG	A	1010	1,2	14,14,15	0.57	0	15,19,21	0.65	0
2	NAG	A	1011	2	14,14,15	0.57	0	15,19,21	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	A	1012	2	11,11,12	1.29	2 (18%)	14,15,17	1.99	3 (21%)
2	MAN	A	1013	2	11,11,12	0.75	0	14,15,17	1.33	2 (14%)
2	MAN	A	1014	2	11,11,12	0.54	0	14,15,17	1.19	2 (14%)
2	NAG	B	902	1,2	14,14,15	0.49	0	15,19,21	0.61	0
2	NAG	B	903	2	14,14,15	0.64	0	15,19,21	0.70	0
2	BMA	B	904	2	11,11,12	0.80	1 (9%)	14,15,17	1.05	2 (14%)
2	MAN	B	905	2	11,11,12	0.65	0	14,15,17	0.70	0
2	MAN	B	906	2	11,11,12	0.63	0	14,15,17	0.79	0
3	NAG	B	907	1,3	14,14,15	0.49	0	15,19,21	0.96	1 (6%)
3	NAG	B	908	3	14,14,15	0.60	0	15,19,21	0.81	0
3	BMA	B	909	3	11,11,12	0.67	0	14,15,17	0.66	0
2	NAG	B	911	1,2	14,14,15	0.49	0	15,19,21	0.64	0
2	NAG	B	912	2	14,14,15	0.59	0	15,19,21	1.01	1 (6%)
2	BMA	B	913	2	11,11,12	0.82	1 (9%)	14,15,17	0.79	0
2	MAN	B	914	2	11,11,12	0.65	0	14,15,17	0.77	0
2	MAN	B	915	2	11,11,12	0.58	0	14,15,17	0.98	1 (7%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1012	BMA	O5-C1	-2.99	1.38	1.43
2	A	1003	BMA	O5-C1	-2.17	1.40	1.43
2	B	904	BMA	O5-C1	-2.16	1.40	1.43
2	B	913	BMA	O5-C1	-2.09	1.40	1.43
2	A	1012	BMA	C4-C5	2.42	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1013	MAN	C1-O5-C5	-2.93	108.53	112.25
2	A	1013	MAN	O5-C1-C2	-2.90	106.15	110.86
2	A	1014	MAN	O5-C1-C2	-2.82	106.28	110.86
2	B	912	NAG	C2-N2-C7	-2.54	119.78	123.04
2	B	904	BMA	O2-C2-C3	-2.31	105.47	110.12
2	B	915	MAN	O5-C1-C2	-2.28	107.16	110.86
2	A	1011	NAG	C2-N2-C7	-2.26	120.13	123.04
2	A	1012	BMA	O5-C5-C6	-2.15	102.70	107.35
2	A	1014	MAN	C1-O5-C5	2.12	114.94	112.25
2	A	1012	BMA	C3-C4-C5	2.16	113.97	110.20
2	B	904	BMA	C1-C2-C3	2.30	112.27	109.54
3	B	907	NAG	C1-O5-C5	2.56	115.50	112.25
2	A	1012	BMA	C1-O5-C5	6.23	120.15	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	907	NAG	1	0

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	14,14,15	0.51	0	15,19,21	0.74	0
4	NAG	A	1015	1	14,14,15	0.48	0	15,19,21	1.33	2 (13%)
4	NAG	A	1016	1	14,14,15	0.49	0	15,19,21	0.76	0
4	NAG	A	1017	1	14,14,15	0.46	0	15,19,21	2.06	1 (6%)
4	NAG	A	1018	1	14,14,15	0.56	0	15,19,21	0.94	1 (6%)
4	NAG	A	1019	1	14,14,15	0.53	0	15,19,21	0.98	1 (6%)
5	RX8	A	1020	-	21,25,25	1.59	3 (14%)	21,37,37	0.95	2 (9%)
6	GOL	A	1021	-	5,5,5	0.36	0	5,5,5	0.22	0
5	RX8	B	901	-	21,25,25	1.54	3 (14%)	21,37,37	0.96	1 (4%)
4	NAG	B	910	1	14,14,15	0.49	0	15,19,21	1.14	1 (6%)
4	NAG	B	916	1	14,14,15	0.45	0	15,19,21	1.02	2 (13%)
4	NAG	B	917	1	14,14,15	0.50	0	15,19,21	0.84	0
4	NAG	B	918	1	14,14,15	0.56	0	15,19,21	0.63	0
4	NAG	B	919	1	14,14,15	0.42	0	15,19,21	1.67	4 (26%)
4	NAG	B	920	1	14,14,15	0.47	0	15,19,21	0.83	0
4	NAG	B	921	1	14,14,15	0.43	0	15,19,21	1.35	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/5/9/9	0/3/3/3
6	GOL	A	1021	-	-	0/4/4/4	0/0/0/0
5	RX8	B	901	-	-	0/5/9/9	0/3/3/3
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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	RX8	O1-C10	-2.48	1.37	1.44
5	B	901	RX8	O1-C10	-2.44	1.38	1.44
5	B	901	RX8	C-N	2.72	1.43	1.34
5	A	1020	RX8	C-N	2.78	1.43	1.34
5	B	901	RX8	C2-C3	4.50	1.48	1.40
5	A	1020	RX8	C2-C3	4.72	1.49	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1015	NAG	C2-N2-C7	-2.99	119.19	123.04
4	B	919	NAG	C6-C5-C4	-2.59	106.63	113.02
4	B	916	NAG	C2-N2-C7	-2.57	119.74	123.04
4	B	919	NAG	C2-N2-C7	-2.38	119.98	123.04
5	A	1020	RX8	C2-C1-N1	-2.02	120.78	123.18
4	B	916	NAG	C1-O5-C5	2.09	114.89	112.25
4	B	919	NAG	C3-C4-C5	2.25	114.12	110.20
4	A	1018	NAG	C1-O5-C5	2.38	115.27	112.25
4	A	1019	NAG	C1-O5-C5	2.42	115.32	112.25
5	B	901	RX8	C-N1-C1	2.78	122.28	117.00
5	A	1020	RX8	C-N1-C1	2.81	122.34	117.00
4	A	1015	NAG	C1-O5-C5	3.28	116.41	112.25
4	B	910	NAG	C1-O5-C5	3.34	116.49	112.25
4	B	921	NAG	C1-O5-C5	3.92	117.22	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	919	NAG	C1-O5-C5	4.52	117.98	112.25
4	A	1017	NAG	C1-O5-C5	7.28	121.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1018	NAG	1	0
5	A	1020	RX8	1	0
5	B	901	RX8	3	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	751/811 (92%)	0.35	67 (8%) 12 16	19, 35, 62, 92	0
1	B	749/811 (92%)	0.79	132 (17%) 2 3	21, 46, 87, 107	0
All	All	1500/1622 (92%)	0.57	199 (13%) 4 6	19, 40, 78, 107	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	10.0
1	B	759	LYS	8.3
1	B	64	TYR	7.1
1	B	754	SER	6.6
1	B	778	CYS	6.5
1	A	761	THR	6.4
1	B	808	ASP	6.3
1	B	758	THR	5.8
1	B	753	LYS	5.7
1	A	392	GLN	5.5
1	B	806	PRO	5.2
1	B	757	GLU	5.1
1	B	782	ASP	5.1
1	B	229	LEU	5.1
1	B	84	GLN	5.0
1	A	760	THR	4.9
1	B	294	LEU	4.7
1	B	805	SER	4.7
1	B	42	ASN	4.6
1	B	589	LEU	4.6
1	B	591	LEU	4.6
1	B	760	THR	4.5
1	B	762	THR	4.5
1	B	785	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	810	ARG	4.4
1	B	272	GLY	4.4
1	B	186	VAL	4.2
1	B	776	CYS	4.2
1	B	43	ASP	4.1
1	B	470	PHE	4.1
1	B	678	PHE	4.1
1	B	535	LEU	4.1
1	B	733	SER	4.1
1	B	177	LEU	4.1
1	B	779	ASP	4.0
1	A	374	LEU	4.0
1	B	561	LEU	4.0
1	B	206	LEU	3.9
1	A	591	LEU	3.8
1	B	817	LEU	3.8
1	B	702	PHE	3.8
1	B	227	LEU	3.7
1	B	74	PHE	3.7
1	B	807	GLY	3.7
1	A	778	CYS	3.7
1	B	613	LEU	3.7
1	B	471	THR	3.7
1	A	807	GLY	3.6
1	B	153	LEU	3.6
1	A	372	LEU	3.6
1	A	818	GLU	3.6
1	A	510	LEU	3.6
1	A	559	LEU	3.6
1	B	559	LEU	3.5
1	A	401	LEU	3.5
1	B	208	LEU	3.5
1	A	535	LEU	3.5
1	B	318	LEU	3.5
1	B	87	GLN	3.4
1	B	81	GLU	3.4
1	A	777	THR	3.4
1	B	717	LEU	3.3
1	B	41	GLN	3.3
1	A	251	LEU	3.3
1	A	344	LEU	3.3
1	A	717	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	792	ASN	3.3
1	B	152	SER	3.3
1	B	809	GLN	3.3
1	B	131	LEU	3.3
1	B	775	GLU	3.3
1	B	756	LEU	3.2
1	A	177	LEU	3.2
1	A	561	LEU	3.2
1	B	791	LEU	3.2
1	B	80	ASN	3.2
1	B	100	VAL	3.2
1	B	372	LEU	3.2
1	B	615	PHE	3.2
1	B	209	SER	3.1
1	B	816	SER	3.1
1	A	208	LEU	3.1
1	A	693	LEU	3.1
1	A	701	LEU	3.1
1	B	175	LEU	3.1
1	A	316	LEU	3.1
1	A	292	LEU	3.1
1	B	741	LEU	3.1
1	B	374	LEU	3.0
1	A	271	ASP	3.0
1	B	486	LEU	3.0
1	B	178	ALA	3.0
1	A	186	VAL	3.0
1	B	789	GLU	3.0
1	B	644	LEU	3.0
1	B	763	LYS	3.0
1	A	741	LEU	2.9
1	A	809	GLN	2.9
1	A	537	LEU	2.9
1	B	86	LEU	2.9
1	B	732	LEU	2.9
1	A	615	PHE	2.9
1	B	44	SER	2.9
1	B	151	LEU	2.9
1	A	178	ALA	2.9
1	A	31	SER	2.8
1	B	344	LEU	2.8
1	A	342	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	808	ASP	2.8
1	A	806	PRO	2.8
1	A	318	LEU	2.8
1	A	669	LEU	2.8
1	B	292	LEU	2.8
1	B	537	LEU	2.8
1	B	769	LEU	2.8
1	A	419	ASN	2.8
1	B	273	GLY	2.8
1	A	294	LEU	2.8
1	A	817	LEU	2.8
1	B	122	LEU	2.8
1	B	614	VAL	2.8
1	B	188	GLU	2.7
1	B	385	ASP	2.7
1	B	752	ASN	2.7
1	B	251	LEU	2.7
1	B	715	ARG	2.7
1	A	42	ASN	2.7
1	A	613	LEU	2.7
1	A	589	LEU	2.7
1	B	316	LEU	2.6
1	B	207	SER	2.6
1	A	646	LEU	2.6
1	B	596	ILE	2.6
1	A	486	LEU	2.6
1	B	401	LEU	2.6
1	A	361	ARG	2.6
1	B	125	LYS	2.6
1	B	253	LEU	2.6
1	A	274	ALA	2.6
1	B	76	THR	2.6
1	B	308	LYS	2.6
1	B	40	LYS	2.5
1	B	425	LEU	2.5
1	B	777	THR	2.5
1	A	206	LEU	2.5
1	B	767	LEU	2.5
1	B	781	GLY	2.5
1	A	41	GLN	2.5
1	B	729	SER	2.4
1	A	498	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	2.4
1	A	425	LEU	2.4
1	B	132	LEU	2.4
1	B	228	PHE	2.4
1	B	693	LEU	2.4
1	B	755	ALA	2.4
1	A	270	CYS	2.4
1	B	726	HIS	2.4
1	A	459	PHE	2.4
1	B	812	LYS	2.4
1	A	785	ARG	2.4
1	B	423	ILE	2.4
1	B	433	LEU	2.4
1	A	399	ILE	2.4
1	B	488	LEU	2.4
1	A	634	ILE	2.3
1	B	706	SER	2.3
1	B	783	PHE	2.3
1	B	48	GLU	2.3
1	B	130	LEU	2.3
1	B	361	ARG	2.3
1	B	499	ASN	2.3
1	B	459	PHE	2.2
1	B	588	VAL	2.2
1	B	55	GLN	2.2
1	B	342	LEU	2.2
1	A	188	GLU	2.2
1	B	803	CYS	2.2
1	A	512	LEU	2.2
1	A	550	LEU	2.2
1	B	123	ASN	2.2
1	B	705	ASP	2.1
1	A	635	PHE	2.1
1	A	132	LEU	2.1
1	A	175	LEU	2.1
1	A	695	LEU	2.1
1	B	280	ARG	2.1
1	B	176	TYR	2.1
1	B	485	ALA	2.1
1	A	130	LEU	2.1
1	B	96	HIS	2.0
1	B	510	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	737	SER	2.0
1	B	495	PHE	2.0
1	B	45	VAL	2.0
1	B	53	ARG	2.0
1	A	736	SER	2.0
1	B	710	PHE	2.0
1	A	671	ILE	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	1002	14/15	0.96	0.10	-0.41	19,23,32,35	0
2	NAG	B	902	14/15	0.95	0.14	-0.76	27,29,35,37	0
2	NAG	B	903	14/15	0.95	0.10	-1.03	30,33,37,38	0
2	NAG	B	911	14/15	0.91	0.12	-1.29	23,31,34,41	0
2	NAG	A	1001	14/15	0.97	0.09	-1.53	17,21,29,31	0
3	NAG	B	907	14/15	0.96	0.08	-1.94	22,28,36,37	0
3	NAG	A	1006	14/15	0.96	0.08	-2.69	20,23,28,34	0
2	NAG	A	1010	14/15	0.97	0.08	-3.15	18,21,27,28	0
3	BMA	B	909	11/12	0.85	0.33	-	69,72,73,74	0
3	BMA	A	1008	11/12	0.89	0.32	-	63,67,69,69	0
2	NAG	B	912	14/15	0.88	0.12	-	30,34,43,43	0
2	MAN	B	914	11/12	0.68	0.37	-	73,79,84,86	0
2	BMA	A	1003	11/12	0.92	0.13	-	32,43,54,56	0
3	NAG	A	1007	14/15	0.92	0.16	-	36,49,53,56	0
2	MAN	B	906	11/12	0.89	0.31	-	70,73,76,77	0
2	MAN	A	1004	11/12	0.79	0.22	-	33,39,47,55	0
2	BMA	B	904	11/12	0.93	0.20	-	39,56,63,64	0
2	MAN	B	905	11/12	0.81	0.24	-	45,60,66,67	0
3	NAG	B	908	14/15	0.86	0.19	-	44,57,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BMA	B	913	11/12	0.87	0.24	-	49,63,71,74	0
2	MAN	A	1014	11/12	0.85	0.35	-	69,73,76,76	0
2	BMA	A	1012	11/12	0.93	0.23	-	40,55,67,75	0
2	MAN	A	1013	11/12	0.65	0.38	-	67,73,81,82	0
2	MAN	A	1005	11/12	0.83	0.29	-	56,66,71,76	0
2	NAG	A	1011	14/15	0.94	0.10	-	21,26,36,47	0
2	MAN	B	915	11/12	0.86	0.41	-	72,78,86,87	0

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	917	14/15	0.93	0.31	6.34	50,60,73,76	0
4	NAG	A	1015	14/15	0.89	0.29	4.13	52,64,74,75	0
4	NAG	B	921	14/15	0.77	0.30	2.52	68,72,74,77	0
4	NAG	B	916	14/15	0.90	0.27	1.69	64,75,83,83	0
6	GOL	A	1021	6/6	0.76	0.15	1.01	66,71,73,74	0
5	RX8	B	901	23/23	0.94	0.12	0.36	22,29,41,45	0
4	NAG	B	918	14/15	0.92	0.13	0.26	44,52,56,57	0
4	NAG	A	1018	14/15	0.97	0.12	0.03	36,42,50,51	0
4	NAG	B	919	14/15	0.91	0.22	-0.07	52,57,63,69	0
5	RX8	A	1020	23/23	0.96	0.10	-0.53	22,32,41,42	0
4	NAG	A	1019	14/15	0.94	0.10	-0.74	29,31,34,34	0
4	NAG	A	1016	14/15	0.87	0.34	-	62,65,67,69	0
4	NAG	B	910	14/15	0.91	0.12	-	44,60,67,75	0
4	NAG	A	1017	14/15	0.86	0.37	-	62,68,75,78	0
4	NAG	A	1009	14/15	0.91	0.20	-	48,56,68,73	0
4	NAG	B	920	14/15	0.89	0.33	-	77,82,86,87	0

6.5 Other polymers

There are no such residues in this entry.