Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:09 PM GMT

PDB ID	:	4R6A
Title	:	Crystal structure of human TLR8 in complex with Hybrid-2
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2014-08-22
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:

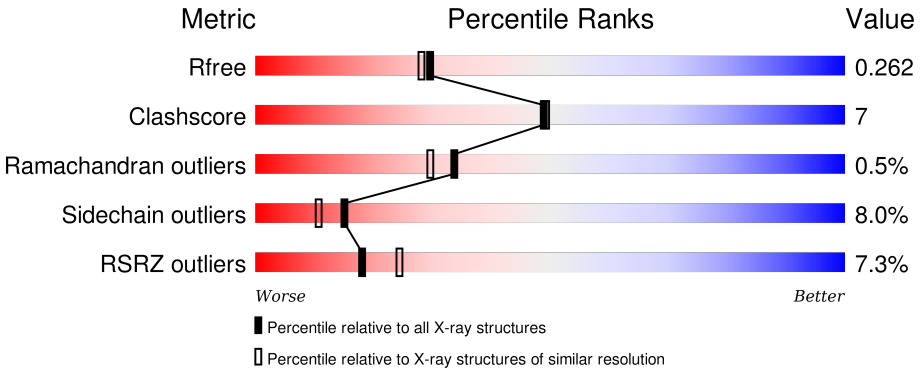
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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	7%, 73%, 16%, •, 8%
1	B	811	7%, 74%, 15%, •, 9%

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	BMA	B	905	-	-	X	-
3	NAG	A	905	-	-	-	X
3	NAG	B	907	-	-	-	X
3	NAG	B	917	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12816 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	746	Total	C	N	O	S	0	0	0
			6009	3844	1021	1125	19			
1	B	740	Total	C	N	O	S	0	0	0
			5964	3819	1013	1113	19			

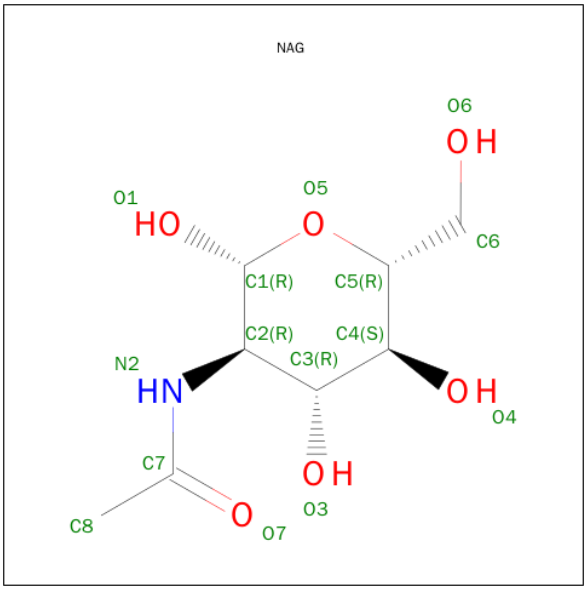
There are 20 discrepancies between the modelled and reference sequences:

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 (4-MER).

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 13 8 1 4	0	0
3	B	1	Total C N O 14 8 1 5	0	0

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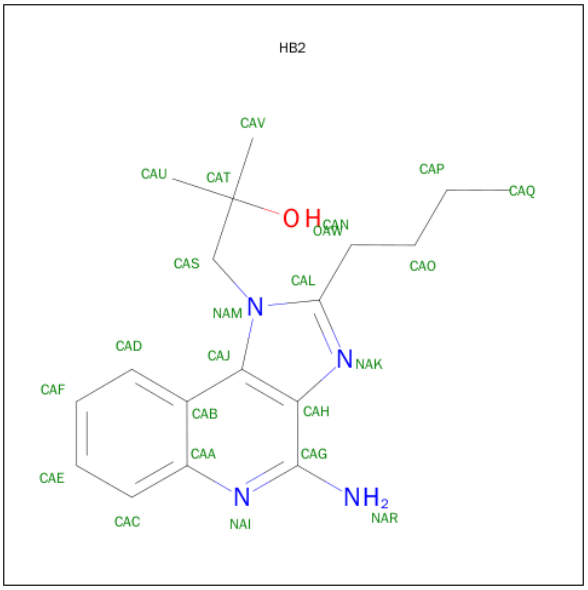
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is 1-(4-AMINO-2-BUTYL-1H-IMIDAZO[4,5-C]QUINOLIN-1-YL)-2-METHYLPROPAN-2-OL (three-letter code: HB2) (formula: $C_{18}H_{24}N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 23 18 4 1	0	0
5	B	1	Total C N O 23 18 4 1	0	0

- Molecule 6 is water.

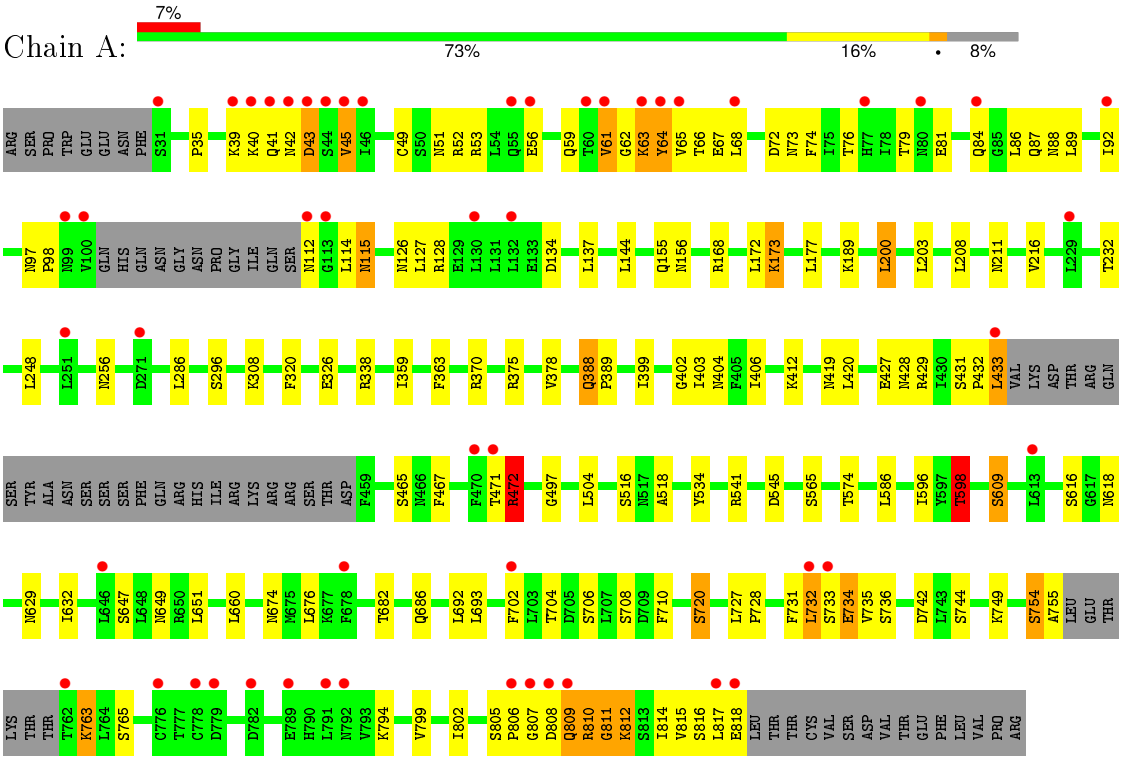
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	196	Total O 196 196	0	0
6	B	206	Total O 206 206	0	0

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.

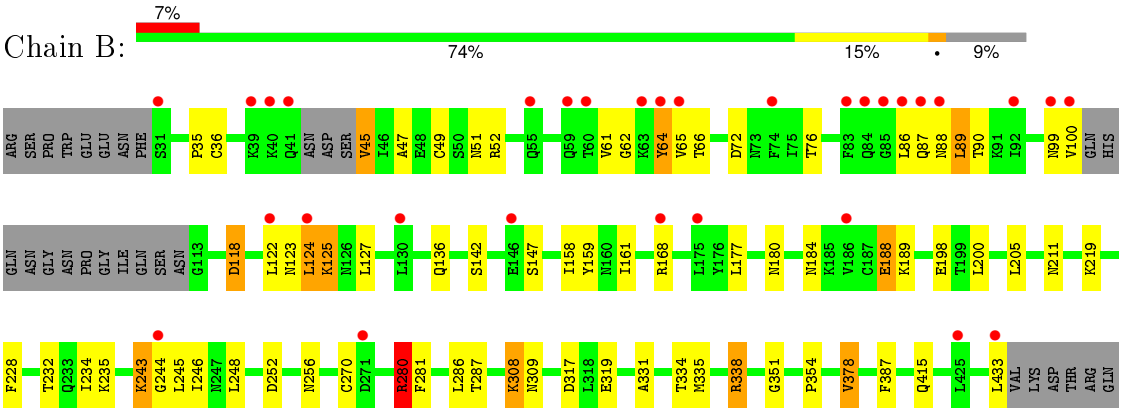
- Molecule 1: Toll-like receptor 8

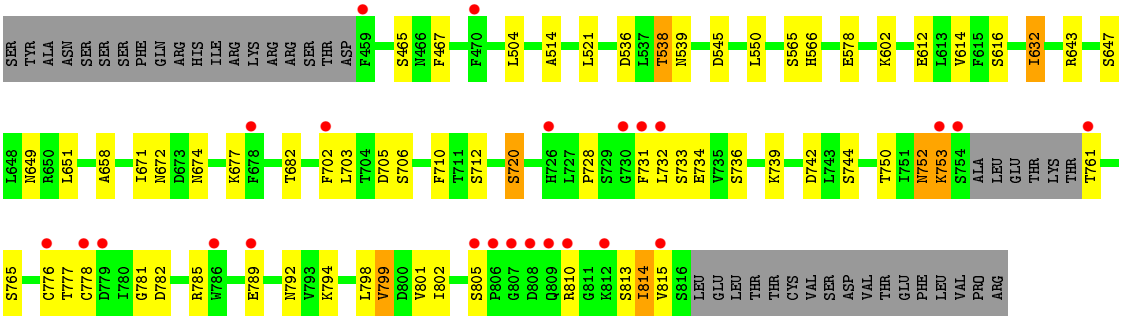
Chain A:



- Molecule 1: Toll-like receptor 8

Chain B:




SER TYR ALA ASN SER SER SER PHE GLN ARG HIS ILE ARG LYS ARG ARG SER THR ASP F459 S465 N466 F467 F470 L504 A514 L521 D536 L537 T538 N539 D545 L550 S565 H566 E578 K602 E612 L613 V614 F615 S616 I632 R643 S647
L648 N649 R650 L651 A658 I671 N672 D673 N674 K677 F678 T682 F702 L703 T704 D705 S706 F710 T711 S712 S720 H726 L727 P728 S729 G730 F731 L732 S733 E734 V735 S736 K739 D742 L743 S744 T750 I751 N752 K753 S754 ALA LEU GLU THR LYS THR T761
S765 C776 T777 C778 D779 I780 G781 D782 R785 W786 E789 N792 V793 K794 L798 V799 D800 V801 I802 S805 P806 G807 D808 Q809 R810 G811 K812 S813 I814 V815 S816 LEU 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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.14Å 122.21Å 107.78Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	26.09 – 2.10 26.09 – 2.09	Depositor EDS
% Data completeness (in resolution range)	86.7 (26.09-2.10) 86.7 (26.09-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.259 0.208 , 0.262	Depositor DCC
R_{free} test set	4671 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.9	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 94384 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12816	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, BMA, NAG, HB2

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	0.59	0/6133	0.77	2/8316 (0.0%)
1	B	0.58	0/6087	0.76	1/8252 (0.0%)
All	All	0.59	0/12220	0.76	3/16568 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	280	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	472	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	598	THR	CB-CA-C	-5.92	95.62	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	GLY	Peptide
1	A	808	ASP	Peptide
1	A	809	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	731	PHE	Peptide

5.2 Too-close contacts (i)

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	6009	0	5988	87	0
1	B	5964	0	5949	78	1
2	A	50	0	43	1	0
2	B	50	0	43	9	0
3	A	56	0	52	1	0
3	B	83	0	78	0	0
4	A	78	0	68	1	0
4	B	78	0	67	2	0
5	A	23	0	24	6	0
5	B	23	0	24	1	0
6	A	196	0	0	7	0
6	B	206	0	0	5	0
All	All	12816	0	12336	177	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 7.

All (177) 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:720:SER:OG	1:B:742:ASP:OD2	1.75	1.02
1:B:308:LYS:HG2	1:B:335:MET:HE1	1.43	0.99
1:B:158:ILE:H	1:B:180:ASN:HD22	1.24	0.85
1:B:538:THR:CG2	1:B:539:ASN:HD22	1.93	0.82
1:B:308:LYS:HG2	1:B:335:MET:CE	2.10	0.81
2:B:905:BMA:H61	2:B:906:MAN:H5	1.63	0.80
5:A:915:HB2:H21	1:B:351:GLY:H	1.48	0.79
1:B:798:LEU:HA	1:B:801:VAL:HG12	1.66	0.77
1:B:538:THR:HG23	1:B:539:ASN:ND2	2.01	0.76
1:B:538:THR:HG22	1:B:539:ASN:HD22	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD12	1:B:127:LEU:HB2	1.68	0.75
1:A:63:LYS:HD3	1:A:63:LYS:H	1.50	0.75
1:B:649:ASN:H	1:B:674:ASN:HD21	1.35	0.74
1:B:538:THR:CG2	1:B:539:ASN:ND2	2.51	0.74
1:A:598:THR:HG21	6:A:1050:HOH:O	1.86	0.74
2:B:905:BMA:C6	2:B:906:MAN:H5	2.17	0.73
1:A:42:ASN:N	1:A:43:ASP:HA	2.05	0.71
2:B:905:BMA:C6	2:B:906:MAN:C5	2.69	0.70
1:A:649:ASN:H	1:A:674:ASN:HD21	1.40	0.70
1:A:211:ASN:O	1:A:232:THR:HA	1.93	0.68
2:B:904:NAG:O3	2:B:905:BMA:H2	1.93	0.68
1:A:596:ILE:H	1:A:618:ASN:HD22	1.41	0.67
5:A:915:HB2:H16	5:A:915:HB2:H15	1.77	0.67
5:A:915:HB2:H21	1:B:351:GLY:N	2.09	0.67
1:B:243:LYS:HA	6:B:1080:HOH:O	1.94	0.66
1:A:115:ASN:C	1:A:115:ASN:HD22	2.00	0.65
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.77	0.65
1:A:598:THR:HG23	6:A:1007:HOH:O	1.97	0.64
1:B:798:LEU:HA	1:B:801:VAL:CG1	2.27	0.64
1:A:598:THR:CG2	6:A:1007:HOH:O	2.45	0.64
2:B:905:BMA:H61	2:B:906:MAN:C5	2.28	0.64
1:A:799:VAL:O	1:A:802:ILE:HD11	1.98	0.64
1:A:651:LEU:H	1:A:674:ASN:HD22	1.46	0.63
1:A:763:LYS:HE2	1:A:763:LYS:HA	1.79	0.63
1:B:245:LEU:HA	6:B:1201:HOH:O	1.97	0.63
1:B:198:GLU:HG3	1:B:219:LYS:HB3	1.80	0.62
1:B:338:ARG:NH1	6:B:1110:HOH:O	2.33	0.61
1:A:586:LEU:O	1:A:609:SER:HB3	1.99	0.61
4:B:913:NAG:H61	6:B:1050:HOH:O	2.00	0.61
1:A:810:ARG:O	1:A:812:LYS:N	2.34	0.61
1:B:51:ASN:HA	1:B:72:ASP:O	2.01	0.61
1:B:536:ASP:OD1	1:B:538:THR:HB	2.00	0.60
1:B:159:TYR:CD2	1:B:188:GLU:HG2	2.36	0.60
2:B:905:BMA:O6	2:B:905:BMA:O4	2.12	0.60
1:B:123:ASN:O	1:B:125:LYS:HG3	2.01	0.60
1:A:232:THR:H	1:A:256:ASN:HD21	1.49	0.60
1:B:118:ASP:O	1:B:142:SER:O	2.19	0.59
1:B:649:ASN:H	1:B:674:ASN:ND2	2.00	0.59
5:A:915:HB2:H19	5:A:915:HB2:H8	1.84	0.58
1:B:86:LEU:O	1:B:88:ASN:N	2.37	0.58
1:A:45:VAL:HG13	1:A:66:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:THR:HA	1:B:710:PHE:CD1	2.40	0.57
1:A:406:ILE:H	1:A:428:ASN:HD22	1.52	0.57
1:B:211:ASN:O	1:B:232:THR:HA	2.05	0.57
1:A:763:LYS:CE	1:A:763:LYS:HA	2.35	0.56
1:B:158:ILE:H	1:B:180:ASN:ND2	2.01	0.56
1:A:126:ASN:O	1:A:128:ARG:HD2	2.05	0.56
1:A:41:GLN:C	1:A:43:ASP:HA	2.27	0.56
1:A:35:PRO:O	1:A:52:ARG:NH1	2.39	0.56
1:B:280:ARG:HD3	1:B:281:PHE:CE2	2.41	0.55
1:A:326:GLU:CD	6:A:1168:HOH:O	2.43	0.55
1:A:433:LEU:HD13	1:A:497:GLY:HA3	1.88	0.55
1:B:651:LEU:H	1:B:674:ASN:HD22	1.53	0.55
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.42	0.55
1:A:429:ARG:HG2	6:A:1090:HOH:O	2.07	0.55
1:B:814:ILE:HG13	1:B:815:VAL:N	2.22	0.55
1:B:317:ASP:OD1	1:B:319:GLU:OE1	2.25	0.54
1:B:752:ASN:ND2	1:B:753:LYS:O	2.40	0.54
1:A:816:SER:O	1:A:817:LEU:HD12	2.08	0.54
1:B:682:THR:HG22	1:B:710:PHE:CZ	2.44	0.53
1:B:234:ILE:O	1:B:256:ASN:HB3	2.09	0.52
1:A:734:GLU:CD	1:A:734:GLU:N	2.63	0.52
1:B:467:PHE:HB3	2:B:903:NAG:H81	1.91	0.52
1:A:427:GLU:OE1	1:B:566:HIS:HE1	1.92	0.52
1:A:73:ASN:HB2	1:A:97:ASN:HD21	1.74	0.51
1:A:76:THR:HG22	1:A:98:PRO:HG3	1.91	0.51
1:B:72:ASP:OD1	1:B:99:ASN:ND2	2.43	0.51
1:A:720:SER:OG	1:A:742:ASP:OD2	2.28	0.51
1:B:47:ALA:HB2	1:B:65:VAL:HG21	1.92	0.50
1:B:616:SER:HA	1:B:647:SER:O	2.11	0.50
1:B:52:ARG:HG2	1:B:799:VAL:HG21	1.93	0.50
1:A:660:LEU:CD2	1:A:686:GLN:HG3	2.41	0.49
1:B:99:ASN:O	1:B:100:VAL:C	2.51	0.49
1:A:708:SER:HB3	1:A:734:GLU:HB2	1.94	0.49
1:B:35:PRO:O	1:B:52:ARG:NH1	2.46	0.49
1:A:732:LEU:HD13	1:A:733:SER:HA	1.94	0.49
1:B:100:VAL:O	1:B:100:VAL:HG13	2.13	0.49
1:A:404:ASN:H	1:A:428:ASN:ND2	2.11	0.49
1:B:66:THR:O	1:B:89:LEU:HA	2.13	0.49
1:A:649:ASN:H	1:A:674:ASN:ND2	2.10	0.49
1:B:235:LYS:HD2	1:B:270:CYS:SG	2.53	0.48
1:A:545:ASP:OD1	1:A:574:THR:OG1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ASN:HD22	1:B:672:ASN:H	1.60	0.48
1:A:51:ASN:HA	1:A:72:ASP:O	2.13	0.48
1:A:404:ASN:H	1:A:428:ASN:HD21	1.61	0.48
1:A:370:ARG:HH22	3:A:905:NAG:H61	1.78	0.48
1:A:810:ARG:HG2	1:A:811:GLY:H	1.78	0.48
1:A:296:SER:HA	1:A:320:PHE:O	2.13	0.48
1:A:53:ARG:HA	1:A:74:PHE:CD2	2.48	0.48
5:B:901:HB2:H16	5:B:901:HB2:H15	1.95	0.48
1:A:177:LEU:HB2	1:A:208:LEU:HD23	1.95	0.47
1:A:807:GLY:O	1:A:810:ARG:HB3	2.13	0.47
5:A:915:HB2:CAU	5:A:915:HB2:H8	2.44	0.47
1:B:703:LEU:HD23	1:B:732:LEU:CD2	2.44	0.47
1:B:62:GLY:O	1:B:65:VAL:HG12	2.15	0.47
1:A:616:SER:HA	1:A:647:SER:O	2.14	0.47
1:B:521:LEU:HD13	1:B:550:LEU:HD21	1.96	0.47
1:B:720:SER:HA	1:B:744:SER:O	2.15	0.47
1:A:61:VAL:CG1	1:A:86:LEU:HD11	2.45	0.47
1:A:87:GLN:N	1:A:87:GLN:CD	2.68	0.47
1:B:61:VAL:HG12	1:B:86:LEU:HD22	1.97	0.47
1:A:66:THR:OG1	1:A:67:GLU:N	2.41	0.46
1:B:781:GLY:O	1:B:782:ASP:C	2.53	0.46
1:A:359:ILE:HG23	1:A:363:PHE:CD1	2.50	0.46
1:A:431:SER:HB2	1:A:432:PRO:HD2	1.97	0.46
1:B:415:GLN:NE2	6:B:1171:HOH:O	2.49	0.46
1:B:354:PRO:HD2	1:B:378:VAL:O	2.16	0.46
1:B:244:GLY:HA2	1:B:245:LEU:C	2.35	0.46
1:A:720:SER:HA	1:A:744:SER:O	2.15	0.46
1:A:692:LEU:HD23	1:A:692:LEU:C	2.35	0.46
1:A:137:LEU:H	1:A:156:ASN:HD22	1.62	0.46
1:B:813:SER:O	1:B:814:ILE:C	2.53	0.45
1:A:89:LEU:HD23	1:A:92:ILE:HD11	1.98	0.45
1:B:776:CYS:SG	1:B:814:ILE:HG22	2.57	0.45
1:B:205:LEU:HD23	1:B:205:LEU:C	2.37	0.45
1:A:728:PRO:HG2	1:A:731:PHE:HB2	1.99	0.44
2:B:905:BMA:H62	2:B:906:MAN:C5	2.47	0.44
1:A:754:SER:O	1:A:755:ALA:C	2.54	0.44
1:A:810:ARG:CG	1:A:811:GLY:N	2.80	0.44
1:B:317:ASP:OD1	1:B:319:GLU:HG3	2.16	0.44
1:A:467:PHE:HB3	2:A:901:NAG:H81	2.00	0.44
4:A:907:NAG:H62	4:A:908:BMA:C1	2.48	0.44
5:A:915:HB2:H15	5:A:915:HB2:CAS	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:THR:HG22	6:A:1007:HOH:O	2.14	0.44
1:B:36:CYS:HA	1:B:52:ARG:NH1	2.32	0.44
1:A:45:VAL:HG22	1:A:65:VAL:HA	2.00	0.44
1:B:672:ASN:H	1:B:672:ASN:ND2	2.15	0.44
1:A:692:LEU:HD23	1:A:693:LEU:N	2.33	0.44
1:A:472:ARG:HH11	1:A:472:ARG:CG	2.30	0.44
1:B:785:ARG:CZ	1:B:785:ARG:HB2	2.48	0.43
1:A:134:ASP:HA	1:A:155:GLN:O	2.19	0.43
1:B:161:ILE:HD12	1:B:177:LEU:HD13	2.00	0.43
1:A:388:GLN:N	1:A:389:PRO:CD	2.81	0.43
1:A:61:VAL:CG1	1:A:86:LEU:HD21	2.48	0.43
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.33	0.43
1:B:331:ALA:O	1:B:334:THR:HB	2.18	0.43
1:A:126:ASN:O	1:A:128:ARG:CD	2.67	0.42
1:A:81:GLU:HA	1:A:84:GLN:HB3	2.01	0.42
1:B:798:LEU:HD23	1:B:801:VAL:HG11	2.01	0.42
1:A:596:ILE:H	1:A:618:ASN:ND2	2.14	0.42
1:A:810:ARG:C	1:A:812:LYS:H	2.22	0.42
1:A:403:ILE:HA	1:A:427:GLU:O	2.18	0.42
1:B:287:THR:HA	1:B:309:ASN:O	2.19	0.42
1:B:612:GLU:OE2	1:B:643:ARG:NH1	2.52	0.42
1:A:629:ASN:ND2	1:B:184:ASN:HB3	2.35	0.42
1:B:45:VAL:CG1	1:B:64:TYR:O	2.67	0.42
1:A:518:ALA:HA	1:A:541:ARG:O	2.21	0.41
1:A:61:VAL:CG2	1:A:86:LEU:HD21	2.50	0.41
1:B:467:PHE:CB	2:B:903:NAG:H81	2.51	0.41
1:A:399:ILE:HG23	1:A:399:ILE:O	2.20	0.41
1:A:144:LEU:O	1:A:168:ARG:NH2	2.53	0.41
1:A:817:LEU:O	1:A:818:GLU:C	2.59	0.41
1:A:649:ASN:N	1:A:674:ASN:HD21	2.14	0.41
1:A:200:LEU:HB3	1:A:203:LEU:HB2	2.02	0.41
1:B:244:GLY:HA2	1:B:246:ILE:N	2.36	0.41
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.03	0.41
1:B:614:VAL:HG21	4:B:913:NAG:H61	2.03	0.41
1:A:516:SER:N	6:A:1115:HOH:O	2.45	0.41
1:B:514:ALA:HA	1:B:539:ASN:O	2.21	0.41
1:A:708:SER:CB	1:A:734:GLU:HB2	2.51	0.41
1:B:578:GLU:HG2	1:B:602:LYS:HG3	2.04	0.40
1:A:814:ILE:HG13	1:A:815:VAL:N	2.36	0.40
1:A:375:ARG:HA	1:A:402:GLY:O	2.20	0.40
1:B:632:ILE:HD13	1:B:658:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:ND2	1:A:115:ASN:C	2.72	0.40
1:A:64:TYR:HD2	1:A:64:TYR:HA	1.78	0.40
1:B:705:ASP:HB3	1:B:728:PRO:HB2	2.04	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:B:280:ARG:NH2	1:B:545:ASP:OD2[2_445]	2.18	0.02

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	738/811 (91%)	681 (92%)	53 (7%)	4 (0%)	34	30
1	B	730/811 (90%)	671 (92%)	56 (8%)	3 (0%)	39	37
All	All	1468/1622 (90%)	1352 (92%)	109 (7%)	7 (0%)	34	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	GLY
1	A	39	LYS
1	A	806	PRO
1	B	87	GLN
1	A	378	VAL
1	B	378	VAL
1	B	814	ILE

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	692/755 (92%)	634 (92%)	58 (8%)	14 9
1	B	687/755 (91%)	634 (92%)	53 (8%)	16 12
All	All	1379/1510 (91%)	1268 (92%)	111 (8%)	15 11

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	43	ASP
1	A	45	VAL
1	A	49	CYS
1	A	56	GLU
1	A	59	GLN
1	A	61	VAL
1	A	63	LYS
1	A	64	TYR
1	A	68	LEU
1	A	79	THR
1	A	88	ASN
1	A	112	ASN
1	A	114	LEU
1	A	115	ASN
1	A	127	LEU
1	A	172	LEU
1	A	173	LYS
1	A	189	LYS
1	A	200	LEU
1	A	216	VAL
1	A	248	LEU
1	A	286	LEU
1	A	308	LYS
1	A	338	ARG
1	A	388	GLN
1	A	412	LYS

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	420	LEU
1	A	433	LEU
1	A	465	SER
1	A	471	THR
1	A	472	ARG
1	A	504	LEU
1	A	534	TYR
1	A	565	SER
1	A	598	THR
1	A	609	SER
1	A	632	ILE
1	A	676	LEU
1	A	702	PHE
1	A	704	THR
1	A	706	SER
1	A	720	SER
1	A	727	LEU
1	A	732	LEU
1	A	734	GLU
1	A	735	VAL
1	A	736	SER
1	A	749	LYS
1	A	754	SER
1	A	763	LYS
1	A	765	SER
1	A	794	LYS
1	A	805	SER
1	A	809	GLN
1	A	810	ARG
1	A	812	LYS
1	B	45	VAL
1	B	49	CYS
1	B	64	TYR
1	B	76	THR
1	B	89	LEU
1	B	90	THR
1	B	118	ASP
1	B	122	LEU
1	B	124	LEU
1	B	125	LYS
1	B	136	GLN

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Mol	Chain	Res	Type
1	B	147	SER
1	B	168	ARG
1	B	188	GLU
1	B	189	LYS
1	B	200	LEU
1	B	243	LYS
1	B	248	LEU
1	B	280	ARG
1	B	286	LEU
1	B	308	LYS
1	B	338	ARG
1	B	387	PHE
1	B	433	LEU
1	B	465	SER
1	B	504	LEU
1	B	538	THR
1	B	565	SER
1	B	632	ILE
1	B	671	ILE
1	B	677	LYS
1	B	702	PHE
1	B	706	SER
1	B	712	SER
1	B	720	SER
1	B	733	SER
1	B	734	GLU
1	B	736	SER
1	B	739	LYS
1	B	750	THR
1	B	752	ASN
1	B	753	LYS
1	B	761	THR
1	B	765	SER
1	B	777	THR
1	B	778	CYS
1	B	789	GLU
1	B	792	ASN
1	B	794	LYS
1	B	799	VAL
1	B	802	ILE
1	B	805	SER
1	B	810	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	97	ASN
1	A	115	ASN
1	A	139	GLN
1	A	156	ASN
1	A	174	ASN
1	A	247	ASN
1	A	256	ASN
1	A	419	ASN
1	A	428	ASN
1	A	531	HIS
1	A	618	ASN
1	A	674	ASN
1	A	809	GLN
1	B	97	ASN
1	B	123	ASN
1	B	139	GLN
1	B	180	ASN
1	B	380	GLN
1	B	499	ASN
1	B	539	ASN
1	B	566	HIS
1	B	653	HIS
1	B	672	ASN
1	B	674	ASN

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

20 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	901	1,2	14,14,15	0.51	0	15,19,21	1.92	5 (33%)
2	NAG	A	902	2	14,14,15	0.80	0	15,19,21	1.34	2 (13%)
2	BMA	A	903	2	11,11,12	0.35	0	15,15,17	0.93	0
2	MAN	A	904	2	11,11,12	0.66	0	15,15,17	1.43	2 (13%)
4	NAG	A	906	1,4	14,14,15	0.98	0	15,19,21	1.62	3 (20%)
4	NAG	A	907	4	14,14,15	0.82	1 (7%)	15,19,21	1.76	4 (26%)
4	BMA	A	908	4	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
4	NAG	A	910	1,4	14,14,15	0.79	0	15,19,21	1.52	5 (33%)
4	NAG	A	911	4	14,14,15	0.65	0	15,19,21	1.28	2 (13%)
4	BMA	A	912	4	11,11,12	0.71	0	15,15,17	2.29	5 (33%)
2	NAG	B	903	1,2	14,14,15	0.64	0	15,19,21	1.19	3 (20%)
2	NAG	B	904	2	14,14,15	0.97	1 (7%)	15,19,21	1.86	4 (26%)
2	BMA	B	905	2	11,11,12	0.85	0	15,15,17	3.25	7 (46%)
2	MAN	B	906	2	11,11,12	0.78	0	15,15,17	2.45	5 (33%)
4	NAG	B	908	1,4	14,14,15	0.85	0	15,19,21	1.46	3 (20%)
4	NAG	B	909	4	14,14,15	0.73	0	15,19,21	1.71	5 (33%)
4	BMA	B	910	4	11,11,12	0.93	1 (9%)	15,15,17	2.00	7 (46%)
4	NAG	B	913	1,4	14,14,15	1.03	1 (7%)	15,19,21	2.48	4 (26%)
4	NAG	B	914	4	14,14,15	0.90	0	15,19,21	1.24	2 (13%)
4	BMA	B	915	4	11,11,12	0.61	0	15,15,17	2.46	3 (20%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
2	BMA	A	903	2	-	0/2/19/22	0/1/1/1
2	MAN	A	904	2	-	0/2/19/22	0/1/1/1
4	NAG	A	906	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	907	4	-	0/6/23/26	0/1/1/1
4	BMA	A	908	4	-	0/2/19/22	0/1/1/1
4	NAG	A	910	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	911	4	-	0/6/23/26	0/1/1/1
4	BMA	A	912	4	-	0/2/19/22	0/1/1/1
2	NAG	B	903	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	904	2	-	0/6/23/26	0/1/1/1
2	BMA	B	905	2	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	0/2/19/22	0/1/1/1
4	NAG	B	908	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	909	4	-	0/6/23/26	0/1/1/1
4	BMA	B	910	4	-	0/2/19/22	0/1/1/1
4	NAG	B	913	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	914	4	-	0/6/23/26	0/1/1/1
4	BMA	B	915	4	-	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	907	NAG	O5-C1	-2.52	1.39	1.43
2	B	904	NAG	O5-C1	-2.42	1.39	1.43
4	B	913	NAG	C2-N2	-2.31	1.42	1.46
4	B	910	BMA	C2-C3	2.62	1.56	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	905	BMA	C2-C3-C4	-8.49	96.25	111.05
4	A	912	BMA	O4-C4-C3	-5.00	99.07	110.36
2	B	905	BMA	C3-C4-C5	-4.71	101.83	110.23
2	B	904	NAG	C1-O5-C5	-4.10	106.11	112.14
2	A	901	NAG	O6-C6-C5	-4.08	97.68	111.30
4	B	913	NAG	O5-C5-C6	-3.75	99.32	107.34
4	A	907	NAG	C6-C5-C4	-3.43	104.39	112.99
4	B	913	NAG	C6-C5-C4	-3.42	104.42	112.99
4	A	906	NAG	O4-C4-C5	-3.40	100.27	109.23
4	B	913	NAG	O3-C3-C4	-3.26	103.00	110.36
4	B	908	NAG	C1-O5-C5	-2.94	107.81	112.14
2	B	904	NAG	O4-C4-C5	-2.93	101.51	109.23
4	B	909	NAG	O7-C7-C8	-2.69	117.12	122.07
2	B	905	BMA	C6-C5-C4	-2.69	106.25	112.99
2	B	906	MAN	O6-C6-C5	-2.66	102.41	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	906	NAG	C4-C3-C2	-2.59	107.32	111.34
4	A	907	NAG	O7-C7-C8	-2.57	117.33	122.07
2	A	902	NAG	C6-C5-C4	-2.51	106.69	112.99
2	B	904	NAG	O3-C3-C2	-2.50	104.03	109.37
4	B	909	NAG	C2-N2-C7	-2.47	119.90	123.11
4	A	908	BMA	C2-C3-C4	-2.46	106.77	111.05
4	B	908	NAG	C4-C3-C2	-2.42	107.58	111.34
2	B	906	MAN	C6-C5-C4	-2.42	106.92	112.99
4	B	909	NAG	C3-C4-C5	-2.39	105.96	110.23
4	B	910	BMA	O4-C4-C3	-2.37	105.01	110.36
4	A	910	NAG	O5-C5-C4	-2.35	106.25	110.13
4	A	910	NAG	O7-C7-C8	-2.33	117.77	122.07
2	B	903	NAG	O4-C4-C5	-2.32	103.12	109.23
4	A	911	NAG	C6-C5-C4	-2.25	107.35	112.99
4	B	909	NAG	O5-C5-C4	-2.22	106.47	110.13
4	B	914	NAG	O3-C3-C4	-2.19	105.42	110.36
4	A	910	NAG	C2-N2-C7	-2.12	120.34	123.11
2	A	901	NAG	O4-C4-C5	-2.11	103.67	109.23
4	B	914	NAG	C6-C5-C4	-2.09	107.75	112.99
4	A	911	NAG	O3-C3-C2	-2.09	104.91	109.37
4	A	912	BMA	O5-C1-C2	-2.07	107.58	110.89
2	B	903	NAG	C1-O5-C5	-2.04	109.13	112.14
2	A	901	NAG	C6-C5-C4	-2.04	107.88	112.99
2	B	903	NAG	O6-C6-C5	-2.03	104.51	111.30
4	A	912	BMA	C1-O5-C5	2.02	115.11	112.14
4	B	910	BMA	C2-C3-C4	2.06	114.64	111.05
4	B	910	BMA	O5-C5-C6	2.10	111.84	107.34
4	A	906	NAG	O3-C3-C4	2.11	115.13	110.36
2	A	902	NAG	C1-O5-C5	2.24	115.43	112.14
4	A	910	NAG	O3-C3-C2	2.32	114.33	109.37
4	B	909	NAG	C8-C7-N2	2.55	120.99	116.10
4	A	910	NAG	C8-C7-N2	2.58	121.05	116.10
4	B	910	BMA	C1-O5-C5	2.59	115.95	112.14
2	A	904	MAN	O2-C2-C3	2.59	115.41	110.19
2	A	904	MAN	O3-C3-C2	2.65	114.86	110.01
4	A	907	NAG	C1-O5-C5	2.75	116.18	112.14
2	B	905	BMA	O3-C3-C2	2.75	115.06	110.01
2	B	904	NAG	O4-C4-C3	2.77	116.59	110.36
4	B	910	BMA	O3-C3-C2	2.77	115.09	110.01
2	B	905	BMA	O5-C5-C4	2.82	114.80	110.13
4	B	908	NAG	O3-C3-C4	2.82	116.72	110.36
4	B	910	BMA	C3-C4-C5	2.95	115.48	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	905	BMA	C1-O5-C5	2.98	116.53	112.14
2	B	906	MAN	O2-C2-C3	3.25	116.74	110.19
4	A	907	NAG	C3-C4-C5	3.29	116.09	110.23
2	A	901	NAG	C1-O5-C5	3.48	117.26	112.14
2	A	901	NAG	O5-C5-C4	3.57	116.04	110.13
4	B	910	BMA	C1-C2-C3	3.58	113.89	109.55
2	B	905	BMA	O3-C3-C4	3.79	118.90	110.36
4	A	912	BMA	O5-C5-C4	3.82	116.46	110.13
2	B	906	MAN	O3-C3-C2	3.96	117.26	110.01
4	B	915	BMA	O5-C5-C4	4.18	117.05	110.13
4	A	912	BMA	C3-C4-C5	4.62	118.47	110.23
4	B	915	BMA	C3-C4-C5	4.74	118.68	110.23
2	B	906	MAN	C1-O5-C5	6.28	121.37	112.14
4	B	915	BMA	C1-O5-C5	6.30	121.40	112.14
4	B	913	NAG	C1-O5-C5	6.78	122.11	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0
4	A	907	NAG	1	0
4	A	908	BMA	1	0
2	B	903	NAG	2	0
2	B	904	NAG	1	0
2	B	905	BMA	7	0
2	B	906	MAN	5	0
4	B	913	NAG	2	0

5.6 Ligand geometry (i)

12 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	$\#\|Z\|>2$
3	NAG	A	905	1	14,14,15	0.66	0	15,19,21	1.78	3 (20%)
3	NAG	A	909	1	14,14,15	1.19	2 (14%)	15,19,21	2.65	5 (33%)
3	NAG	A	913	1	14,14,15	0.55	0	15,19,21	1.02	2 (13%)
3	NAG	A	914	1	14,14,15	0.69	0	15,19,21	1.85	5 (33%)
5	HB2	A	915	-	22,25,25	1.14	1 (4%)	22,37,37	1.39	4 (18%)
5	HB2	B	901	-	22,25,25	1.07	1 (4%)	22,37,37	1.07	1 (4%)
3	NAG	B	902	1	14,14,15	0.70	0	15,19,21	1.39	2 (13%)
3	NAG	B	907	1	14,14,15	0.85	1 (7%)	15,19,21	1.08	2 (13%)
3	NAG	B	911	1	14,14,15	1.02	1 (7%)	15,19,21	1.80	2 (13%)
3	NAG	B	912	1	13,13,15	0.83	0	14,17,21	2.21	5 (35%)
3	NAG	B	916	1	14,14,15	0.71	0	15,19,21	1.02	0
3	NAG	B	917	1	14,14,15	0.59	0	15,19,21	1.14	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
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	909	1	-	0/6/23/26	0/1/1/1
3	NAG	A	913	1	-	0/6/23/26	0/1/1/1
3	NAG	A	914	1	-	0/6/23/26	0/1/1/1
5	HB2	A	915	-	-	0/7/9/9	0/3/3/3
5	HB2	B	901	-	-	0/7/9/9	0/3/3/3
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
3	NAG	B	907	1	-	0/6/23/26	0/1/1/1
3	NAG	B	911	1	-	0/6/23/26	0/1/1/1
3	NAG	B	912	1	-	0/5/22/26	0/1/1/1
3	NAG	B	916	1	-	0/6/23/26	0/1/1/1
3	NAG	B	917	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)
3	B	911	NAG	O5-C1	-2.94	1.38	1.43
3	A	909	NAG	C2-N2	-2.57	1.41	1.46
3	A	909	NAG	O5-C1	-2.10	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	907	NAG	C1-C2	2.18	1.55	1.52
5	A	915	HB2	CAS-CAT	3.28	1.57	1.54
5	B	901	HB2	CAS-CAT	3.61	1.58	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	909	NAG	O7-C7-N2	-4.63	112.40	121.84
3	A	914	NAG	O5-C5-C4	-4.22	103.14	110.13
3	A	909	NAG	O5-C5-C4	-3.35	104.58	110.13
3	B	912	NAG	C6-C5-C4	-3.17	105.03	112.99
3	B	907	NAG	C4-C3-C2	-3.07	106.58	111.34
3	A	914	NAG	C3-C4-C5	-2.67	105.47	110.23
5	A	915	HB2	CAF-CAE-CAC	-2.37	117.03	120.45
3	A	913	NAG	C4-C3-C2	-2.34	107.70	111.34
3	B	907	NAG	C2-N2-C7	-2.34	120.06	123.11
3	B	911	NAG	C6-C5-C4	-2.33	107.14	112.99
3	A	914	NAG	C1-O5-C5	-2.18	108.93	112.14
5	A	915	HB2	CAB-CAA-NAI	-2.17	120.58	123.15
3	A	909	NAG	C1-O5-C5	-2.16	108.96	112.14
3	A	914	NAG	O5-C5-C6	2.20	112.04	107.34
3	A	913	NAG	C1-O5-C5	2.21	115.38	112.14
3	B	902	NAG	C1-O5-C5	2.48	115.79	112.14
5	B	901	HB2	CAG-NAI-CAA	2.52	121.01	116.79
3	A	905	NAG	O5-C5-C4	2.68	114.58	110.13
3	B	902	NAG	C3-C4-C5	2.72	115.08	110.23
3	B	912	NAG	C3-C4-C5	2.78	115.19	110.23
5	A	915	HB2	CAU-CAT-CAS	2.97	117.10	109.89
3	A	914	NAG	C6-C5-C4	3.01	120.53	112.99
3	A	909	NAG	C8-C7-N2	3.15	122.14	116.10
3	B	912	NAG	C1-C2-N2	3.18	115.82	110.45
3	B	917	NAG	C1-O5-C5	3.29	116.97	112.14
5	A	915	HB2	CAG-NAI-CAA	3.29	122.32	116.79
3	B	912	NAG	C1-O5-C5	3.32	117.02	112.14
3	A	905	NAG	C3-C4-C5	3.43	116.35	110.23
3	A	905	NAG	C1-O5-C5	3.81	117.74	112.14
3	B	912	NAG	O5-C5-C4	4.91	118.27	110.13
3	B	911	NAG	C1-O5-C5	4.94	119.40	112.14
3	A	909	NAG	C2-N2-C7	6.72	131.85	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	NAG	1	0
5	A	915	HB2	6	0
5	B	901	HB2	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^{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	746/811 (91%)	0.31	53 (7%)	19	26	15, 33, 74, 122	0
1	B	740/811 (91%)	0.38	55 (7%)	17	24	17, 33, 81, 105	0
All	All	1486/1622 (91%)	0.34	108 (7%)	18	24	15, 33, 77, 122	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	7.5
1	A	809	GLN	7.4
1	B	100	VAL	6.8
1	A	42	ASN	6.7
1	A	818	GLU	6.4
1	B	808	ASP	6.1
1	A	41	GLN	5.7
1	A	64	TYR	5.4
1	B	806	PRO	5.4
1	B	776	CYS	5.3
1	A	791	LEU	5.1
1	B	41	GLN	5.0
1	B	64	TYR	5.0
1	B	807	GLY	4.7
1	B	40	LYS	4.5
1	B	810	ARG	4.5
1	B	731	PHE	4.5
1	A	817	LEU	4.5
1	B	732	LEU	4.1
1	B	470	PHE	4.1
1	A	43	ASP	4.1
1	B	761	THR	4.0
1	A	732	LEU	3.9
1	B	753	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	805	SER	3.7
1	B	39	LYS	3.7
1	A	433	LEU	3.6
1	A	100	VAL	3.6
1	A	44	SER	3.6
1	A	808	ASP	3.5
1	A	45	VAL	3.5
1	A	84	GLN	3.4
1	A	792	ASN	3.3
1	B	702	PHE	3.3
1	A	733	SER	3.3
1	A	782	ASP	3.2
1	A	39	LYS	3.2
1	B	86	LEU	3.1
1	A	470	PHE	3.1
1	A	40	LYS	3.1
1	A	778	CYS	3.0
1	B	59	GLN	3.0
1	A	779	ASP	3.0
1	A	613	LEU	3.0
1	B	812	LYS	3.0
1	B	244	GLY	3.0
1	B	65	VAL	2.9
1	B	809	GLN	2.9
1	B	130	LEU	2.9
1	A	61	VAL	2.9
1	A	113	GLY	2.9
1	B	678	PHE	2.8
1	B	92	ILE	2.8
1	B	63	LYS	2.8
1	B	84	GLN	2.8
1	B	433	LEU	2.8
1	B	168	ARG	2.7
1	A	702	PHE	2.7
1	A	776	CYS	2.7
1	B	779	ASP	2.7
1	A	678	PHE	2.7
1	B	175	LEU	2.7
1	A	31	SER	2.6
1	A	130	LEU	2.6
1	A	762	THR	2.6
1	B	124	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	229	LEU	2.6
1	B	74	PHE	2.5
1	A	99	ASN	2.5
1	B	85	GLY	2.5
1	A	63	LYS	2.5
1	A	471	THR	2.5
1	B	754	SER	2.5
1	B	459	PHE	2.5
1	B	88	ASN	2.4
1	B	31	SER	2.4
1	B	778	CYS	2.4
1	B	60	THR	2.4
1	B	146	GLU	2.4
1	A	646	LEU	2.4
1	A	807	GLY	2.4
1	A	55	GLN	2.3
1	A	806	PRO	2.3
1	B	87	GLN	2.3
1	B	815	VAL	2.3
1	B	786	TRP	2.3
1	A	271	ASP	2.3
1	A	65	VAL	2.3
1	A	46	ILE	2.3
1	B	186	VAL	2.3
1	B	55	GLN	2.3
1	A	92	ILE	2.3
1	A	68	LEU	2.2
1	B	99	ASN	2.2
1	B	726	HIS	2.2
1	B	425	LEU	2.2
1	A	80	ASN	2.2
1	B	83	PHE	2.2
1	A	77	HIS	2.2
1	A	60	THR	2.1
1	B	122	LEU	2.1
1	B	730	GLY	2.1
1	B	789	GLU	2.1
1	A	132	LEU	2.1
1	A	56	GLU	2.1
1	B	271	ASP	2.1
1	A	789	GLU	2.0
1	A	251	LEU	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	902	14/15	0.96	0.12	-0.10	19,27,32,39	0
2	NAG	B	904	14/15	0.96	0.12	-0.22	25,30,35,35	0
4	NAG	B	908	14/15	0.96	0.10	-0.87	17,20,24,26	0
4	NAG	B	913	14/15	0.95	0.09	-1.34	20,23,24,29	0
4	NAG	A	906	14/15	0.97	0.08	-1.38	18,22,26,28	0
2	NAG	B	903	14/15	0.98	0.08	-1.71	19,22,25,30	0
4	NAG	A	910	14/15	0.96	0.09	-1.86	20,22,25,26	0
2	NAG	A	901	14/15	0.96	0.09	-2.03	21,22,23,29	0
4	NAG	A	907	14/15	0.92	0.18	-	35,43,48,52	0
4	BMA	B	910	11/12	0.80	0.28	-	46,53,57,66	0
4	NAG	B	914	14/15	0.93	0.11	-	25,28,33,36	0
2	BMA	B	905	11/12	0.82	0.25	-	41,45,55,56	0
4	BMA	B	915	11/12	0.82	0.22	-	40,47,54,59	0
4	BMA	A	908	11/12	0.83	0.40	-	59,67,74,78	0
2	MAN	B	906	11/12	0.80	0.32	-	41,50,58,58	0
2	MAN	A	904	11/12	0.83	0.30	-	39,43,46,49	0
2	BMA	A	903	11/12	0.92	0.20	-	32,38,42,42	0
4	NAG	A	911	14/15	0.95	0.10	-	23,28,41,42	0
4	NAG	B	909	14/15	0.94	0.21	-	33,42,50,51	0
4	BMA	A	912	11/12	0.83	0.31	-	47,54,63,73	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^{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
3	NAG	A	905	14/15	0.89	0.21	5.13	40,46,55,55	0
3	NAG	B	907	14/15	0.91	0.20	3.16	31,41,43,44	0
3	NAG	B	917	14/15	0.83	0.28	2.61	54,61,66,67	0
3	NAG	A	913	14/15	0.94	0.15	1.37	28,34,41,51	0
3	NAG	B	902	14/15	0.83	0.20	0.64	38,45,49,50	0
3	NAG	B	916	14/15	0.90	0.14	0.50	28,37,40,44	0
3	NAG	A	909	14/15	0.91	0.11	0.36	29,34,41,43	0
3	NAG	B	911	14/15	0.94	0.11	0.34	26,31,36,40	0
5	HB2	B	901	23/23	0.96	0.11	0.07	12,14,22,23	0
5	HB2	A	915	23/23	0.96	0.10	-0.81	15,19,23,29	0
3	NAG	B	912	13/15	0.80	0.29	-	37,52,66,77	0
3	NAG	A	914	14/15	0.90	0.23	-	44,50,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.