Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:29 PM GMT

PDB ID	:	4IIG
Title	:	Crystal structure of beta-glucosidase 1 from Aspergillus aculeatus in complex with D-glucose
Authors	:	Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on	:	2012-12-20
Resolution	:	2.30 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:

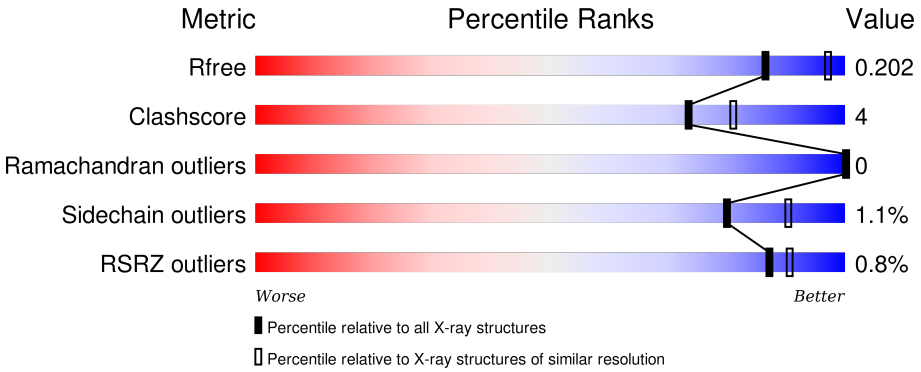
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

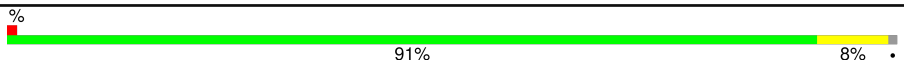
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	841	
1	B	841	

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
11	MAN	B	942	-	-	-	X
3	NAG	B	947	-	-	-	X
7	NAG	A	925	-	-	-	X
7	MAN	A	931	-	-	-	X
7	MAN	A	936	-	-	-	X
8	MRD	A	941	-	-	X	X
8	MRD	B	948	-	-	-	X
8	MRD	B	949	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15202 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.

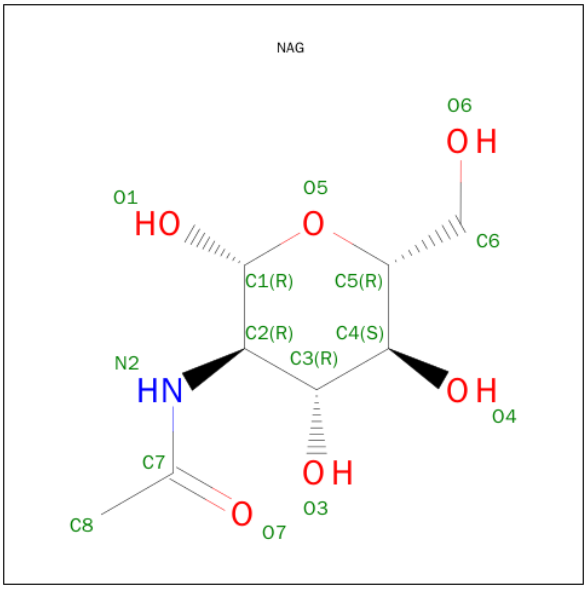
- Molecule 1 is a protein called Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6387	4031	1097	1241	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- 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	0	0
			61	34	2	25		

- 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	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

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

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

- Molecule 6 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total C N O 116 64 2 50	0	0
6	B	10	Total C N O 116 64 2 50	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total C N O 83 46 2 35	0	0
7	A	7	Total C N O 83 46 2 35	0	0

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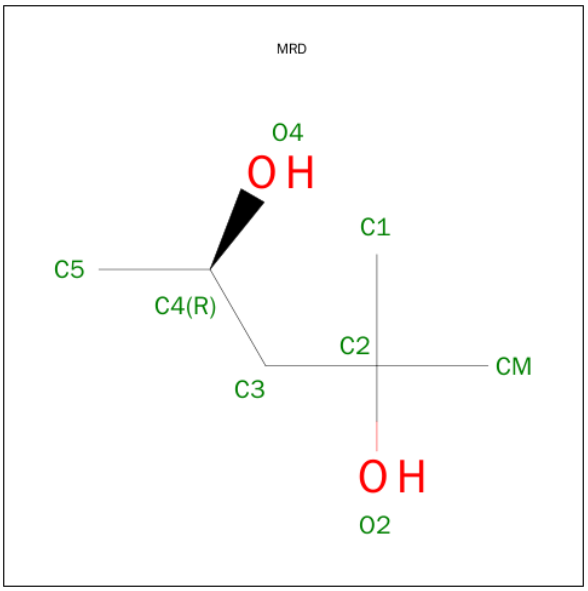
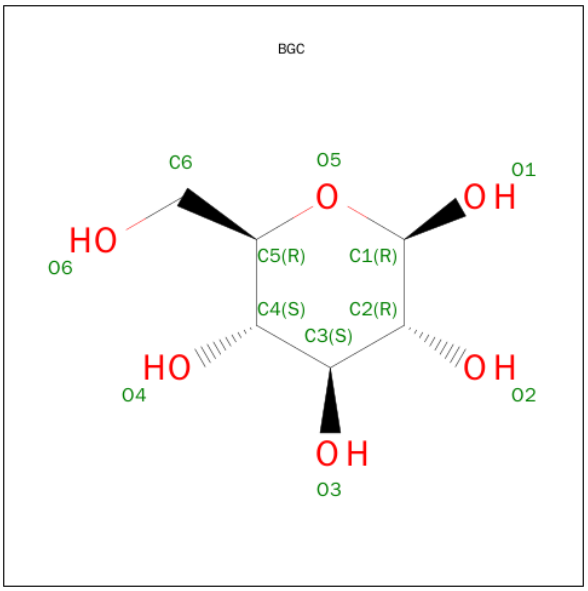
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	7	Total C N O 83 46 2 35	0	0
7	B	7	Total C N O 83 46 2 35	0	0

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 8 6 2	0	0
8	A	1	Total C O 8 6 2	0	0
8	B	1	Total C O 8 6 2	0	0
8	B	1	Total C O 8 6 2	0	0

- Molecule 9 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 12 6 6	0	0
9	A	1	Total C O 12 6 6	0	0
9	B	1	Total C O 12 6 6	0	0
9	B	1	Total C O 12 6 6	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	6	Total C N O 72 40 2 30	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	8	Total C N O 94 52 2 40	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	626	Total O 626 626	0	0

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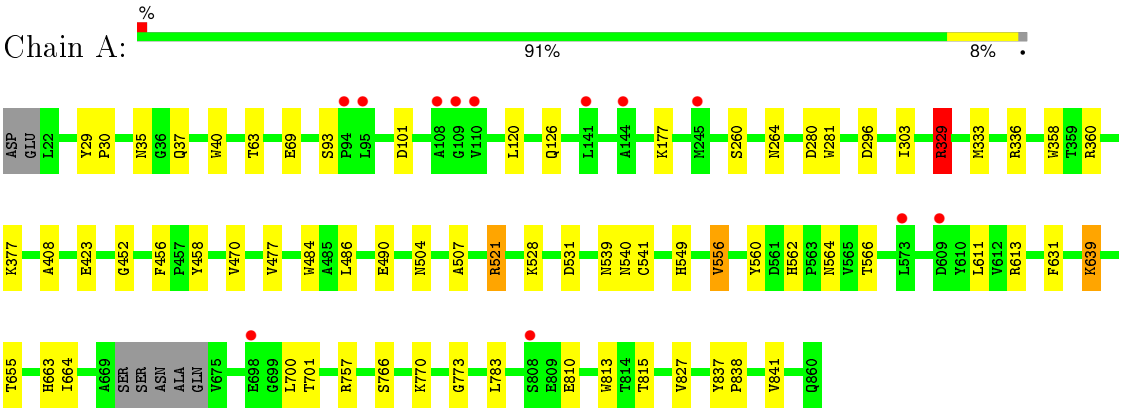
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	689	Total	O	0	0
			689	689		

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.

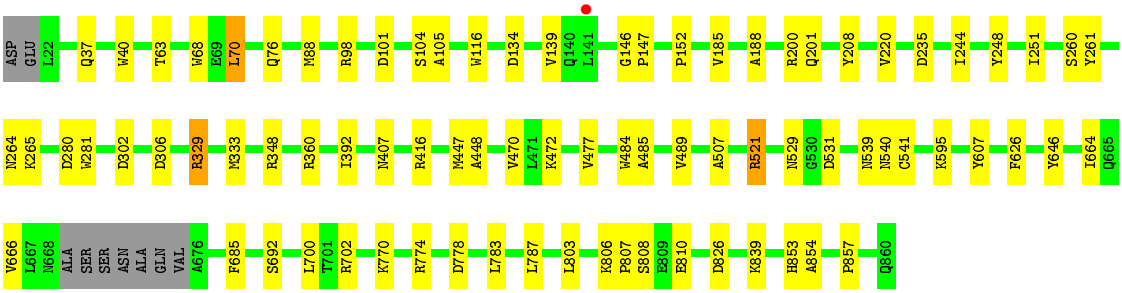
- Molecule 1: Beta-glucosidase 1

Chain A:



- Molecule 1: Beta-glucosidase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.48Å 121.76Å 221.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.99 – 2.30 45.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.99-2.30) 99.1 (45.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.143 , 0.200 0.145 , 0.202	Depositor DCC
R_{free} test set	4996 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 99504 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15202	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: MRD, BGC, NAG, BMA, 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	0.92	2/6550 (0.0%)	0.94	11/8930 (0.1%)
1	B	0.98	5/6538 (0.1%)	0.98	21/8913 (0.2%)
All	All	0.95	7/13088 (0.1%)	0.96	32/17843 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	CYS	CB-SG	9.81	1.99	1.82
1	B	541	CYS	CB-SG	8.09	1.96	1.82
1	A	541	CYS	CA-CB	7.66	1.70	1.53
1	B	208	TYR	CE1-CZ	6.49	1.47	1.38
1	B	541	CYS	CA-CB	6.28	1.67	1.53
1	B	685	PHE	CG-CD1	5.14	1.46	1.38
1	B	646	TYR	CE1-CZ	5.04	1.45	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ARG	NE-CZ-NH2	-20.97	109.81	120.30
1	A	329	ARG	NE-CZ-NH2	-17.88	111.36	120.30
1	B	329	ARG	NE-CZ-NH1	16.60	128.60	120.30
1	B	521	ARG	NE-CZ-NH2	-16.29	112.15	120.30
1	A	521	ARG	NE-CZ-NH2	-16.13	112.23	120.30
1	A	521	ARG	NE-CZ-NH1	12.67	126.63	120.30
1	A	329	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	B	521	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	B	70	LEU	CA-CB-CG	-9.20	94.15	115.30
1	A	329	ARG	CG-CD-NE	-8.21	94.56	111.80
1	B	329	ARG	CD-NE-CZ	7.07	133.49	123.60
1	B	134	ASP	CB-CG-OD2	-6.88	112.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	200	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	134	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	416	ARG	CG-CD-NE	-6.43	98.29	111.80
1	B	101	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	101	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	360	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	826	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	541	CYS	N-CA-CB	6.10	121.58	110.60
1	B	774	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	329	ARG	CD-NE-CZ	5.90	131.87	123.60
1	A	757	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	235	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	B	541	CYS	N-CA-CB	5.68	120.83	110.60
1	A	336	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	329	ARG	CG-CD-NE	-5.59	100.05	111.80
1	B	98	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	B	531	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	348	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	531	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	702	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	6387	0	6097	53	0
1	B	6375	0	6082	42	0
2	A	61	0	52	0	0
3	A	28	0	26	0	0
3	B	42	0	39	1	0
4	A	78	0	68	1	0
4	B	78	0	68	0	0
5	A	28	0	25	4	0
6	A	116	0	97	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	116	0	97	0	0
7	A	166	0	140	4	0
7	B	166	0	140	1	0
8	A	16	0	28	8	0
8	B	16	0	28	2	0
9	A	24	0	24	2	0
9	B	24	0	24	3	0
10	B	72	0	61	2	0
11	B	94	0	79	2	0
12	A	626	0	0	11	0
12	B	689	0	0	7	0
All	All	15202	0	13175	111	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 (111) 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:63:THR:HG21	1:A:333:MET:HE2	1.48	0.95
1:A:63:THR:CG2	1:A:333:MET:HE2	2.01	0.90
8:A:941:MRD:HMC2	12:B:1103:HOH:O	1.74	0.88
1:A:556:VAL:HG13	1:A:560:TYR:HB3	1.57	0.83
1:A:63:THR:HG21	1:A:333:MET:CE	2.08	0.83
1:A:63:THR:CG2	1:A:333:MET:CE	2.56	0.83
1:B:539:ASN:HB2	12:B:1684:HOH:O	1.78	0.82
1:A:377:LYS:HE3	12:A:1445:HOH:O	1.81	0.80
1:A:360:ARG:HH21	8:A:941:MRD:HMC3	1.50	0.77
9:B:951:BGC:H6C2	12:B:1040:HOH:O	1.90	0.71
1:B:201:GLN:HG3	12:B:1680:HOH:O	1.90	0.71
8:A:940:MRD:H5C2	12:A:1188:HOH:O	1.91	0.69
5:A:911:NAG:H82	12:A:1260:HOH:O	1.92	0.68
1:B:63:THR:HG21	1:B:333:MET:HE2	1.76	0.68
1:B:146:GLY:HA2	1:B:147:PRO:C	2.16	0.66
1:B:63:THR:CG2	1:B:333:MET:HE2	2.26	0.66
1:A:507:ALA:HB2	1:A:521:ARG:HG3	1.79	0.65
1:A:539:ASN:HB2	12:A:1290:HOH:O	1.97	0.62
11:B:940:BMA:H62	11:B:942:MAN:H5	1.82	0.61
5:A:911:NAG:C8	12:A:1260:HOH:O	2.46	0.60
1:A:303:ILE:HG21	5:A:911:NAG:H81	1.83	0.60
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:911:NAG:H3	5:A:911:NAG:H83	1.86	0.58
1:A:360:ARG:HH21	8:A:941:MRD:CM	2.17	0.56
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.41	0.56
1:A:63:THR:HG22	1:A:333:MET:HE2	1.86	0.55
7:A:933:NAG:C6	12:A:1603:HOH:O	2.56	0.54
1:A:562:HIS:CE1	1:A:564:ASN:HB2	2.42	0.54
1:A:486:LEU:O	1:A:490:GLU:HG3	2.07	0.54
8:A:941:MRD:HMC1	8:A:941:MRD:H5C3	1.89	0.53
1:B:280:ASP:OD1	9:B:950:BGC:H1	2.08	0.53
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.88	0.53
1:B:260:SER:O	1:B:264:ASN:HB2	2.07	0.52
1:B:68:TRP:O	1:B:306:ASP:OD1	2.27	0.52
3:B:908:NAG:H83	3:B:908:NAG:H3	1.90	0.52
1:A:770:LYS:HG3	1:A:810:GLU:HG2	1.91	0.52
1:A:663:HIS:O	1:A:664:ILE:HD13	2.11	0.51
11:B:940:BMA:H61	12:B:1439:HOH:O	2.11	0.51
1:A:93:SER:HB2	1:A:452:GLY:HA2	1.92	0.51
1:A:63:THR:HB	1:A:333:MET:HE1	1.93	0.50
1:A:484:TRP:CE2	7:A:927:BMA:H62	2.46	0.50
1:B:770:LYS:HG3	1:B:810:GLU:HG3	1.93	0.49
1:B:448:ALA:HB1	1:B:507:ALA:O	2.12	0.49
1:A:296:ASP:O	1:A:333:MET:HE3	2.12	0.49
1:B:76:GLN:HA	1:B:88:MET:O	2.13	0.49
1:B:251:ILE:HG21	10:B:909:NAG:H82	1.95	0.49
1:B:248:TYR:OH	9:B:951:BGC:O6	2.25	0.49
1:B:251:ILE:CG2	10:B:909:NAG:H82	2.43	0.48
9:A:943:BGC:H6C2	12:A:1564:HOH:O	2.12	0.48
1:A:655:THR:OG1	1:A:773:GLY:HA3	2.13	0.48
1:B:484:TRP:CZ2	7:B:933:BMA:H62	2.49	0.48
1:B:261:TYR:CZ	1:B:265:LYS:HD3	2.48	0.48
8:A:940:MRD:H5C3	8:A:940:MRD:O2	2.13	0.48
1:A:329:ARG:HD2	1:A:329:ARG:HA	1.72	0.48
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.48	0.48
1:A:35:ASN:OD1	1:A:37:GLN:HB2	2.14	0.47
1:A:540:ASN:ND2	12:A:1346:HOH:O	2.38	0.47
1:A:504:ASN:HA	1:A:549:HIS:O	2.14	0.47
1:A:280:ASP:OD1	9:A:942:BGC:H1	2.14	0.47
1:A:260:SER:O	1:A:264:ASN:HB2	2.15	0.47
7:A:933:NAG:H62	12:A:1603:HOH:O	2.13	0.46
1:B:664:ILE:HD11	1:B:854:ALA:HB3	1.97	0.46
1:B:63:THR:HG21	1:B:333:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HG2	8:A:941:MRD:HMC1	1.97	0.46
1:B:540:ASN:ND2	12:B:1483:HOH:O	2.42	0.46
1:B:783:LEU:HD23	1:B:783:LEU:C	2.36	0.46
1:A:484:TRP:CZ2	7:A:927:BMA:H62	2.50	0.46
1:A:63:THR:HB	1:A:333:MET:CE	2.45	0.46
1:A:611:LEU:HD12	1:A:613:ARG:NH2	2.30	0.46
1:B:329:ARG:HD2	1:B:329:ARG:HA	1.80	0.46
1:B:664:ILE:CD1	1:B:854:ALA:HB3	2.46	0.45
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.98	0.45
1:A:813:TRP:CZ2	1:A:815:THR:HG21	2.51	0.45
1:A:29:TYR:HB3	1:A:30:PRO:HA	1.98	0.45
1:A:521:ARG:HD2	12:A:1064:HOH:O	2.17	0.45
1:B:139:VAL:HG22	1:B:185:VAL:HB	1.98	0.45
1:A:360:ARG:HD2	8:A:941:MRD:HMC3	1.98	0.45
1:A:456:PHE:HB3	1:A:458:TYR:O	2.17	0.44
1:A:556:VAL:HG13	1:A:560:TYR:CB	2.40	0.44
1:B:152:PRO:HG3	1:B:607:TYR:CG	2.53	0.44
1:A:69:GLU:HG2	1:A:358:TRP:CZ3	2.52	0.44
1:B:472:LYS:NZ	12:B:1436:HOH:O	2.51	0.44
1:B:787:LEU:HA	1:B:839:LYS:HG2	1.98	0.44
1:B:770:LYS:HG3	1:B:810:GLU:CG	2.48	0.44
1:B:472:LYS:HB3	1:B:472:LYS:HE2	1.40	0.44
1:B:37:GLN:O	1:B:40:TRP:HB2	2.18	0.43
1:B:104:SER:HB3	1:B:392:ILE:HD11	2.01	0.43
1:A:69:GLU:HG2	1:A:358:TRP:CE3	2.54	0.43
1:B:807:PRO:O	1:B:808:SER:HB2	2.19	0.43
1:B:116:TRP:NE1	1:B:595:LYS:HB2	2.33	0.43
8:B:949:MRD:C5	8:B:949:MRD:O2	2.67	0.43
1:B:485:ALA:O	1:B:489:VAL:HG23	2.19	0.42
1:A:470:VAL:HG11	1:A:477:VAL:HB	2.01	0.42
1:A:63:THR:CB	1:A:333:MET:CE	2.97	0.42
1:A:783:LEU:C	1:A:783:LEU:HD23	2.40	0.42
1:A:423:GLU:OE1	1:A:528:LYS:HD2	2.19	0.42
1:B:778:ASP:HA	1:B:803:LEU:O	2.20	0.42
1:A:631:PHE:CE1	1:A:639:LYS:HG3	2.54	0.42
1:A:827:VAL:HG11	4:A:908:NAG:O3	2.20	0.41
1:A:126:GLN:HB2	12:A:1090:HOH:O	2.20	0.41
1:B:666:VAL:CG2	1:B:857:PRO:HG2	2.50	0.41
1:B:507:ALA:HB2	1:B:521:ARG:HG3	2.03	0.41
1:A:766:SER:HA	1:A:813:TRP:O	2.20	0.41
8:B:948:MRD:C5	8:B:948:MRD:H1C2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:LYS:HG3	1:B:806:LYS:HZ3	1.50	0.41
1:A:63:THR:CB	1:A:333:MET:HE1	2.51	0.40
1:B:105:ALA:HB1	1:B:447:MET:CE	2.51	0.40
1:A:837:TYR:HA	1:A:838:PRO:HD3	1.97	0.40
1:A:63:THR:HG22	1:A:333:MET:CE	2.44	0.40
1:A:408:ALA:HB2	1:A:566:THR:HB	2.03	0.40
1:A:37:GLN:O	1:A:40:TRP:HB2	2.22	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	830/841 (99%)	794 (96%)	36 (4%)	0	100	100
1	B	828/841 (98%)	802 (97%)	26 (3%)	0	100	100
All	All	1658/1682 (99%)	1596 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	671/677 (99%)	663 (99%)	8 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	670/677 (99%)	663 (99%)	7 (1%)	82 91
All	All	1341/1354 (99%)	1326 (99%)	15 (1%)	80 90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LEU
1	A	177	LYS
1	A	281	TRP
1	A	329	ARG
1	A	556	VAL
1	A	639	LYS
1	A	700	LEU
1	A	701	THR
1	B	70	LEU
1	B	281	TRP
1	B	302	ASP
1	B	407	ASN
1	B	692	SER
1	B	700	LEU
1	B	853	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	540	ASN

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)

81 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	1.10	1 (7%)	15,19,21	1.11	1 (6%)
2	NAG	A	902	2	14,14,15	0.86	1 (7%)	15,19,21	1.54	5 (33%)
2	BMA	A	903	2	11,11,12	1.14	1 (9%)	14,15,17	1.79	3 (21%)
2	MAN	A	904	2	11,11,12	1.17	1 (9%)	14,15,17	3.48	8 (57%)
2	MAN	A	905	2	11,11,12	0.87	0	14,15,17	2.42	5 (35%)
4	NAG	A	907	1,4	14,14,15	1.00	1 (7%)	15,19,21	1.35	2 (13%)
4	NAG	A	908	4	14,14,15	0.74	0	15,19,21	1.57	4 (26%)
4	BMA	A	909	4	11,11,12	0.84	0	14,15,17	3.12	8 (57%)
5	NAG	A	910	1,5	14,14,15	0.72	0	15,19,21	1.51	4 (26%)
5	NAG	A	911	5	14,14,15	0.68	0	15,19,21	2.16	8 (53%)
6	NAG	A	912	1,6	14,14,15	0.88	0	15,19,21	1.26	2 (13%)
6	NAG	A	913	6	14,14,15	0.67	0	15,19,21	1.81	5 (33%)
6	BMA	A	914	6	11,11,12	1.07	1 (9%)	14,15,17	1.38	2 (14%)
6	MAN	A	915	6	11,11,12	0.75	0	14,15,17	1.35	2 (14%)
6	MAN	A	916	6	11,11,12	1.09	1 (9%)	14,15,17	2.42	4 (28%)
6	MAN	A	917	6	11,11,12	0.62	0	14,15,17	2.10	4 (28%)
6	MAN	A	918	6	11,11,12	1.07	1 (9%)	14,15,17	1.53	3 (21%)
6	MAN	A	919	6	11,11,12	0.55	0	14,15,17	0.97	0
6	MAN	A	920	6	11,11,12	0.76	0	14,15,17	1.39	3 (21%)
6	MAN	A	921	6	11,11,12	1.03	1 (9%)	14,15,17	2.38	7 (50%)
4	NAG	A	922	1,4	14,14,15	0.93	1 (7%)	15,19,21	1.25	1 (6%)
4	NAG	A	923	4	14,14,15	0.79	1 (7%)	15,19,21	1.32	1 (6%)
4	BMA	A	924	4	11,11,12	0.73	0	14,15,17	1.52	3 (21%)
7	NAG	A	925	1,7	14,14,15	0.67	0	15,19,21	1.52	2 (13%)
7	NAG	A	926	7	14,14,15	0.79	1 (7%)	15,19,21	2.54	4 (26%)
7	BMA	A	927	7	11,11,12	0.77	0	14,15,17	0.74	0
7	MAN	A	928	7	11,11,12	0.70	0	14,15,17	1.83	4 (28%)
7	MAN	A	929	7	11,11,12	0.84	0	14,15,17	1.62	3 (21%)
7	MAN	A	930	7	11,11,12	1.08	1 (9%)	14,15,17	2.35	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	A	931	7	11,11,12	0.73	0	14,15,17	1.60	2 (14%)
7	NAG	A	932	1,7	14,14,15	0.99	1 (7%)	15,19,21	1.85	2 (13%)
7	NAG	A	933	7	14,14,15	0.75	0	15,19,21	1.35	3 (20%)
7	BMA	A	934	7	11,11,12	1.16	0	14,15,17	2.55	6 (42%)
7	MAN	A	935	7	11,11,12	0.86	0	14,15,17	1.77	2 (14%)
7	MAN	A	936	7	11,11,12	0.96	0	14,15,17	1.59	3 (21%)
7	MAN	A	937	7	11,11,12	0.67	0	14,15,17	1.56	3 (21%)
7	MAN	A	938	7	11,11,12	0.83	0	14,15,17	2.31	6 (42%)
7	NAG	B	901	1,7	14,14,15	0.89	0	15,19,21	2.19	3 (20%)
7	NAG	B	902	7	14,14,15	0.78	1 (7%)	15,19,21	1.53	2 (13%)
7	BMA	B	903	7	11,11,12	1.05	1 (9%)	14,15,17	1.59	3 (21%)
7	MAN	B	904	7	11,11,12	0.61	0	14,15,17	1.60	4 (28%)
7	MAN	B	905	7	11,11,12	0.99	1 (9%)	14,15,17	1.27	2 (14%)
7	MAN	B	906	7	11,11,12	0.82	0	14,15,17	1.02	0
7	MAN	B	907	7	11,11,12	1.17	1 (9%)	14,15,17	2.60	7 (50%)
10	NAG	B	909	1,10	14,14,15	0.86	0	15,19,21	1.59	2 (13%)
10	NAG	B	910	10	14,14,15	1.10	1 (7%)	15,19,21	1.36	2 (13%)
10	BMA	B	911	10	11,11,12	0.75	0	14,15,17	1.57	2 (14%)
10	MAN	B	912	10	11,11,12	1.57	1 (9%)	14,15,17	2.09	5 (35%)
10	MAN	B	913	10	11,11,12	0.64	0	14,15,17	2.66	3 (21%)
10	MAN	B	914	10	11,11,12	0.85	1 (9%)	14,15,17	0.99	0
4	NAG	B	915	1,4	14,14,15	1.02	1 (7%)	15,19,21	1.79	3 (20%)
4	NAG	B	916	4	14,14,15	0.88	1 (7%)	15,19,21	1.27	3 (20%)
4	BMA	B	917	4	11,11,12	0.60	0	14,15,17	2.67	5 (35%)
6	NAG	B	918	1,6	14,14,15	0.90	0	15,19,21	1.69	3 (20%)
6	NAG	B	919	6	14,14,15	0.73	0	15,19,21	0.99	0
6	BMA	B	920	6	11,11,12	0.96	0	14,15,17	1.37	3 (21%)
6	MAN	B	921	6	11,11,12	0.74	0	14,15,17	1.34	2 (14%)
6	MAN	B	922	6	11,11,12	1.19	2 (18%)	14,15,17	2.40	5 (35%)
6	MAN	B	923	6	11,11,12	0.73	0	14,15,17	2.00	4 (28%)
6	MAN	B	924	6	11,11,12	0.79	0	14,15,17	1.38	2 (14%)
6	MAN	B	925	6	11,11,12	1.03	0	14,15,17	0.95	0
6	MAN	B	926	6	11,11,12	0.87	0	14,15,17	1.95	4 (28%)
6	MAN	B	927	6	11,11,12	1.41	2 (18%)	14,15,17	2.19	4 (28%)
4	NAG	B	928	1,4	14,14,15	0.70	0	15,19,21	1.29	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	929	4	14,14,15	0.90	0	15,19,21	1.62	2 (13%)
4	BMA	B	930	4	11,11,12	0.90	0	14,15,17	1.60	3 (21%)
7	NAG	B	931	1,7	14,14,15	1.08	1 (7%)	15,19,21	1.62	5 (33%)
7	NAG	B	932	7	14,14,15	1.24	2 (14%)	15,19,21	1.67	4 (26%)
7	BMA	B	933	7	11,11,12	0.65	0	14,15,17	0.95	1 (7%)
7	MAN	B	934	7	11,11,12	0.94	1 (9%)	14,15,17	2.00	5 (35%)
7	MAN	B	935	7	11,11,12	1.20	2 (18%)	14,15,17	1.76	2 (14%)
7	MAN	B	936	7	11,11,12	0.67	0	14,15,17	1.41	1 (7%)
7	MAN	B	937	7	11,11,12	0.81	0	14,15,17	1.36	1 (7%)
11	NAG	B	938	11,1	14,14,15	0.74	1 (7%)	15,19,21	1.98	2 (13%)
11	NAG	B	939	11	14,14,15	0.67	0	15,19,21	1.19	1 (6%)
11	BMA	B	940	11	11,11,12	0.94	0	14,15,17	3.64	6 (42%)
11	MAN	B	941	11	11,11,12	1.02	0	14,15,17	2.20	7 (50%)
11	MAN	B	942	11	11,11,12	0.69	0	14,15,17	1.96	3 (21%)
11	MAN	B	943	11	11,11,12	0.64	0	14,15,17	1.94	2 (14%)
11	MAN	B	944	11	11,11,12	0.56	0	14,15,17	1.57	5 (35%)
11	MAN	B	945	11	11,11,12	0.88	0	14,15,17	1.81	3 (21%)

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
2	MAN	A	905	2	-	0/2/19/22	0/1/1/1
4	NAG	A	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	908	4	-	0/6/23/26	0/1/1/1
4	BMA	A	909	4	-	0/2/19/22	0/1/1/1
5	NAG	A	910	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	911	5	-	0/6/23/26	0/1/1/1
6	NAG	A	912	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	913	6	-	0/6/23/26	0/1/1/1
6	BMA	A	914	6	-	0/2/19/22	0/1/1/1
6	MAN	A	915	6	-	0/2/19/22	0/1/1/1
6	MAN	A	916	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	917	6	-	0/2/19/22	0/1/1/1
6	MAN	A	918	6	-	0/2/19/22	0/1/1/1
6	MAN	A	919	6	-	0/2/19/22	0/1/1/1
6	MAN	A	920	6	-	0/2/19/22	0/1/1/1
6	MAN	A	921	6	-	0/2/19/22	0/1/1/1
4	NAG	A	922	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	923	4	-	0/6/23/26	0/1/1/1
4	BMA	A	924	4	-	0/2/19/22	0/1/1/1
7	NAG	A	925	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	926	7	-	0/6/23/26	0/1/1/1
7	BMA	A	927	7	-	0/2/19/22	0/1/1/1
7	MAN	A	928	7	-	0/2/19/22	0/1/1/1
7	MAN	A	929	7	-	0/2/19/22	0/1/1/1
7	MAN	A	930	7	-	0/2/19/22	0/1/1/1
7	MAN	A	931	7	-	0/2/19/22	0/1/1/1
7	NAG	A	932	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	933	7	-	0/6/23/26	0/1/1/1
7	BMA	A	934	7	-	0/2/19/22	0/1/1/1
7	MAN	A	935	7	-	0/2/19/22	0/1/1/1
7	MAN	A	936	7	-	0/2/19/22	0/1/1/1
7	MAN	A	937	7	-	0/2/19/22	0/1/1/1
7	MAN	A	938	7	-	0/2/19/22	0/1/1/1
7	NAG	B	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	902	7	-	0/6/23/26	0/1/1/1
7	BMA	B	903	7	-	0/2/19/22	0/1/1/1
7	MAN	B	904	7	-	0/2/19/22	0/1/1/1
7	MAN	B	905	7	-	0/2/19/22	0/1/1/1
7	MAN	B	906	7	-	0/2/19/22	0/1/1/1
7	MAN	B	907	7	-	0/2/19/22	0/1/1/1
10	NAG	B	909	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	910	10	-	0/6/23/26	0/1/1/1
10	BMA	B	911	10	-	0/2/19/22	0/1/1/1
10	MAN	B	912	10	-	0/2/19/22	0/1/1/1
10	MAN	B	913	10	-	0/2/19/22	0/1/1/1
10	MAN	B	914	10	-	0/2/19/22	0/1/1/1
4	NAG	B	915	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	916	4	-	0/6/23/26	0/1/1/1
4	BMA	B	917	4	-	0/2/19/22	0/1/1/1
6	NAG	B	918	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	919	6	-	0/6/23/26	0/1/1/1
6	BMA	B	920	6	-	0/2/19/22	0/1/1/1
6	MAN	B	921	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	B	922	6	-	0/2/19/22	0/1/1/1
6	MAN	B	923	6	-	0/2/19/22	0/1/1/1
6	MAN	B	924	6	-	0/2/19/22	0/1/1/1
6	MAN	B	925	6	-	0/2/19/22	0/1/1/1
6	MAN	B	926	6	-	0/2/19/22	0/1/1/1
6	MAN	B	927	6	-	0/2/19/22	0/1/1/1
4	NAG	B	928	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	929	4	-	0/6/23/26	0/1/1/1
4	BMA	B	930	4	-	0/2/19/22	0/1/1/1
7	NAG	B	931	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	932	7	-	0/6/23/26	0/1/1/1
7	BMA	B	933	7	-	0/2/19/22	0/1/1/1
7	MAN	B	934	7	-	0/2/19/22	0/1/1/1
7	MAN	B	935	7	-	0/2/19/22	0/1/1/1
7	MAN	B	936	7	-	0/2/19/22	0/1/1/1
7	MAN	B	937	7	-	0/2/19/22	0/1/1/1
11	NAG	B	938	11,1	-	0/6/23/26	0/1/1/1
11	NAG	B	939	11	-	0/6/23/26	0/1/1/1
11	BMA	B	940	11	-	0/2/19/22	0/1/1/1
11	MAN	B	941	11	-	0/2/19/22	0/1/1/1
11	MAN	B	942	11	-	0/2/19/22	0/1/1/1
11	MAN	B	943	11	-	0/2/19/22	0/1/1/1
11	MAN	B	944	11	-	0/2/19/22	0/1/1/1
11	MAN	B	945	11	-	0/2/19/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	932	NAG	C2-N2	-3.33	1.40	1.46
4	B	915	NAG	O4-C4	-2.61	1.36	1.43
7	B	905	MAN	O5-C1	-2.35	1.39	1.43
7	A	930	MAN	O2-C2	-2.33	1.38	1.43
6	A	918	MAN	O5-C1	-2.30	1.39	1.43
7	B	931	NAG	O3-C3	-2.29	1.37	1.43
4	B	916	NAG	O5-C1	-2.26	1.39	1.43
6	B	927	MAN	O5-C1	-2.24	1.40	1.43
6	A	916	MAN	O5-C1	-2.23	1.40	1.43
4	A	922	NAG	O5-C1	-2.20	1.40	1.43
7	B	902	NAG	O5-C1	-2.19	1.40	1.43
4	A	923	NAG	O5-C1	-2.15	1.40	1.43
7	B	932	NAG	O5-C1	-2.15	1.40	1.43
7	A	926	NAG	C2-N2	-2.09	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	903	BMA	O4-C4	-2.09	1.38	1.43
6	A	914	BMA	O2-C2	-2.06	1.38	1.43
11	B	938	NAG	O5-C1	-2.06	1.40	1.43
10	B	910	NAG	O5-C5	-2.06	1.38	1.43
6	B	922	MAN	O5-C1	-2.05	1.40	1.43
2	A	903	BMA	O5-C1	-2.03	1.40	1.43
7	A	932	NAG	C1-C2	-2.03	1.49	1.52
7	B	935	MAN	O2-C2	-2.03	1.38	1.43
7	B	934	MAN	C2-C3	2.02	1.55	1.52
10	B	914	MAN	C2-C3	2.12	1.55	1.52
2	A	902	NAG	C1-C2	2.28	1.55	1.52
7	B	907	MAN	C4-C5	2.36	1.58	1.53
4	A	907	NAG	C1-C2	2.39	1.55	1.52
6	A	921	MAN	C2-C3	2.42	1.55	1.52
7	B	935	MAN	C2-C3	2.73	1.56	1.52
6	B	922	MAN	C2-C3	3.15	1.56	1.52
2	A	901	NAG	C1-C2	3.52	1.57	1.52
2	A	904	MAN	C2-C3	3.58	1.57	1.52
6	B	927	MAN	C2-C3	3.64	1.57	1.52
10	B	912	MAN	C2-C3	4.58	1.58	1.52

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	926	NAG	C2-N2-C7	-7.65	113.21	123.04
11	B	940	BMA	C6-C5-C4	-6.72	96.44	113.02
7	A	928	MAN	O5-C1-C2	-4.04	104.31	110.86
11	B	942	MAN	O2-C2-C1	-3.94	101.31	109.21
5	A	911	NAG	C3-C4-C5	-3.92	103.36	110.20
7	A	930	MAN	O2-C2-C3	-3.92	102.24	110.12
4	B	915	NAG	O4-C4-C5	-3.87	98.98	109.24
6	B	918	NAG	C1-O5-C5	-3.82	107.40	112.25
7	B	934	MAN	O5-C1-C2	-3.77	104.74	110.86
7	B	907	MAN	O4-C4-C3	-3.72	101.95	110.34
7	A	926	NAG	O6-C6-C5	-3.70	99.12	111.33
7	A	936	MAN	O2-C2-C3	-3.69	102.69	110.12
11	B	941	MAN	C1-O5-C5	-3.63	107.64	112.25
6	A	917	MAN	O6-C6-C5	-3.51	99.75	111.33
7	B	901	NAG	C2-N2-C7	-3.46	118.60	123.04
7	B	934	MAN	C1-O5-C5	-3.42	107.90	112.25
4	A	908	NAG	C3-C4-C5	-3.42	104.24	110.20
2	A	904	MAN	O3-C3-C4	-3.39	102.69	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	935	MAN	O5-C1-C2	-3.39	105.35	110.86
7	B	932	NAG	C2-N2-C7	-3.36	118.72	123.04
6	A	921	MAN	C3-C4-C5	-3.32	104.42	110.20
7	A	928	MAN	C1-C2-C3	-3.29	105.64	109.54
4	A	909	BMA	C1-C2-C3	-3.29	105.65	109.54
7	A	925	NAG	C3-C2-N2	-3.25	102.78	110.56
7	B	903	BMA	C1-C2-C3	-3.22	105.73	109.54
7	B	904	MAN	O2-C2-C3	-3.18	103.72	110.12
11	B	941	MAN	O6-C6-C5	-3.05	101.27	111.33
6	B	927	MAN	O5-C1-C2	-2.96	106.06	110.86
6	A	917	MAN	C1-C2-C3	-2.94	106.06	109.54
6	A	921	MAN	O4-C4-C3	-2.87	103.88	110.34
6	B	923	MAN	O3-C3-C4	-2.84	103.93	110.34
5	A	911	NAG	O7-C7-C8	-2.78	116.96	122.06
2	A	905	MAN	C2-C3-C4	-2.77	106.34	111.04
7	B	932	NAG	C3-C2-N2	-2.77	103.93	110.56
2	A	902	NAG	O4-C4-C5	-2.76	101.91	109.24
6	B	922	MAN	C6-C5-C4	-2.73	106.27	113.02
4	A	909	BMA	O4-C4-C3	-2.71	104.23	110.34
7	A	930	MAN	O6-C6-C5	-2.70	102.41	111.33
6	B	923	MAN	O6-C6-C5	-2.68	102.46	111.33
7	A	930	MAN	O5-C1-C2	-2.66	106.54	110.86
11	B	943	MAN	O6-C6-C5	-2.64	102.61	111.33
6	B	924	MAN	C3-C4-C5	-2.62	105.62	110.20
7	B	931	NAG	C3-C2-N2	-2.62	104.28	110.56
4	A	907	NAG	C3-C2-N2	-2.60	104.34	110.56
7	A	932	NAG	C6-C5-C4	-2.59	106.62	113.02
6	A	918	MAN	O2-C2-C3	-2.59	104.91	110.12
6	A	917	MAN	O3-C3-C4	-2.57	104.55	110.34
6	A	921	MAN	C1-C2-C3	-2.57	106.50	109.54
7	B	901	NAG	O7-C7-C8	-2.55	117.38	122.06
10	B	909	NAG	C3-C4-C5	-2.55	105.76	110.20
6	B	923	MAN	C1-C2-C3	-2.53	106.55	109.54
6	A	918	MAN	O6-C6-C5	-2.50	103.06	111.33
7	A	931	MAN	C1-O5-C5	-2.48	109.09	112.25
6	B	918	NAG	O4-C4-C5	-2.48	102.66	109.24
7	A	938	MAN	O3-C3-C2	-2.47	105.54	110.00
11	B	941	MAN	O4-C4-C5	-2.47	102.70	109.24
6	B	920	BMA	C2-C3-C4	-2.43	106.91	111.04
6	B	918	NAG	C2-N2-C7	-2.43	119.92	123.04
6	B	922	MAN	O6-C6-C5	-2.41	103.35	111.33
6	A	913	NAG	O7-C7-C8	-2.40	117.66	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	928	MAN	O4-C4-C3	-2.39	104.96	110.34
10	B	911	BMA	O6-C6-C5	-2.37	103.49	111.33
2	A	902	NAG	C3-C4-C5	-2.36	106.08	110.20
11	B	938	NAG	O3-C3-C2	-2.33	104.49	109.11
7	B	905	MAN	O6-C6-C5	-2.33	103.63	111.33
6	B	927	MAN	C6-C5-C4	-2.33	107.28	113.02
11	B	944	MAN	C2-C3-C4	-2.32	107.11	111.04
7	B	931	NAG	O3-C3-C2	-2.32	104.52	109.11
6	A	913	NAG	O5-C5-C6	-2.31	102.34	107.35
11	B	944	MAN	C6-C5-C4	-2.30	107.34	113.02
7	B	932	NAG	O7-C7-N2	-2.29	117.19	121.86
6	A	916	MAN	C1-C2-C3	-2.27	106.86	109.54
6	A	914	BMA	O2-C2-C1	-2.25	104.70	109.21
10	B	912	MAN	O5-C1-C2	-2.24	107.23	110.86
7	A	926	NAG	C3-C4-C5	-2.22	106.33	110.20
7	B	903	BMA	O4-C4-C3	-2.21	105.36	110.34
4	B	916	NAG	O6-C6-C5	-2.20	104.05	111.33
5	A	910	NAG	O7-C7-C8	-2.19	118.04	122.06
6	A	920	MAN	O6-C6-C5	-2.18	104.14	111.33
7	B	905	MAN	O3-C3-C4	-2.17	105.44	110.34
6	A	921	MAN	O5-C1-C2	-2.15	107.37	110.86
6	B	926	MAN	O6-C6-C5	-2.14	104.25	111.33
6	A	918	MAN	O3-C3-C4	-2.14	105.51	110.34
7	B	904	MAN	O3-C3-C4	-2.11	105.58	110.34
5	A	911	NAG	O6-C6-C5	-2.11	104.36	111.33
7	A	933	NAG	O4-C4-C3	-2.11	105.59	110.34
4	A	908	NAG	O6-C6-C5	-2.10	104.41	111.33
7	B	902	NAG	O4-C4-C5	-2.09	103.69	109.24
2	A	902	NAG	O6-C6-C5	-2.08	104.45	111.33
2	A	903	BMA	O2-C2-C3	-2.06	105.98	110.12
7	A	934	BMA	O4-C4-C5	-2.04	103.84	109.24
6	A	912	NAG	O7-C7-C8	-2.03	118.33	122.06
7	A	933	NAG	C2-N2-C7	-2.03	120.43	123.04
4	B	916	NAG	C3-C4-C5	-2.03	106.66	110.20
7	A	930	MAN	C6-C5-C4	-2.01	108.05	113.02
2	A	902	NAG	O7-C7-C8	-2.01	118.37	122.06
5	A	911	NAG	O5-C5-C6	2.00	111.68	107.35
7	A	937	MAN	O2-C2-C1	2.01	113.23	109.21
7	B	931	NAG	C4-C3-C2	2.01	114.35	111.23
11	B	941	MAN	C1-C2-C3	2.02	111.94	109.54
2	A	905	MAN	C6-C5-C4	2.02	118.01	113.02
6	B	921	MAN	O2-C2-C1	2.03	113.27	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	910	NAG	O3-C3-C4	2.04	114.93	110.34
4	B	930	BMA	C1-C2-C3	2.04	111.96	109.54
7	B	904	MAN	C1-O5-C5	2.05	114.85	112.25
11	B	941	MAN	O2-C2-C1	2.05	113.33	109.21
4	A	908	NAG	C6-C5-C4	2.06	118.11	113.02
7	A	937	MAN	O3-C3-C4	2.07	115.00	110.34
7	A	934	BMA	C6-C5-C4	2.08	118.15	113.02
4	A	924	BMA	C3-C4-C5	2.08	113.83	110.20
6	B	926	MAN	C1-C2-C3	2.09	112.01	109.54
5	A	911	NAG	O4-C4-C3	2.10	115.07	110.34
7	B	934	MAN	C2-C3-C4	2.12	114.64	111.04
7	A	929	MAN	O3-C3-C4	2.12	115.12	110.34
11	B	940	BMA	O2-C2-C1	2.12	113.46	109.21
7	A	928	MAN	O5-C5-C6	2.12	111.95	107.35
4	B	929	NAG	O5-C5-C6	2.13	111.97	107.35
2	A	904	MAN	O5-C1-C2	2.14	114.33	110.86
7	B	931	NAG	O7-C7-C8	2.16	126.03	122.06
7	B	931	NAG	C1-O5-C5	2.16	114.99	112.25
11	B	942	MAN	O5-C1-C2	2.16	114.37	110.86
7	B	907	MAN	O5-C5-C6	2.17	112.04	107.35
6	B	920	BMA	O5-C1-C2	2.17	114.38	110.86
5	A	911	NAG	O3-C3-C4	2.17	115.23	110.34
5	A	910	NAG	C2-N2-C7	2.18	125.84	123.04
7	A	936	MAN	O2-C2-C1	2.20	113.62	109.21
6	A	920	MAN	O3-C3-C2	2.20	113.98	110.00
4	B	917	BMA	C2-C3-C4	2.21	114.79	111.04
11	B	945	MAN	C1-O5-C5	2.22	115.07	112.25
4	B	915	NAG	O3-C3-C2	2.22	113.52	109.11
7	B	932	NAG	C6-C5-C4	2.22	118.50	113.02
2	A	902	NAG	O3-C3-C4	2.23	115.36	110.34
2	A	905	MAN	O5-C1-C2	2.24	114.49	110.86
7	B	907	MAN	C3-C4-C5	2.26	114.14	110.20
11	B	944	MAN	O3-C3-C4	2.29	115.48	110.34
4	A	908	NAG	O3-C3-C4	2.29	115.49	110.34
7	B	933	BMA	C1-O5-C5	2.29	115.16	112.25
4	B	930	BMA	O5-C5-C6	2.33	112.38	107.35
6	A	915	MAN	O5-C5-C6	2.34	112.41	107.35
7	A	933	NAG	C4-C3-C2	2.34	114.87	111.23
7	B	934	MAN	O2-C2-C1	2.36	113.94	109.21
7	A	936	MAN	C6-C5-C4	2.37	118.87	113.02
6	B	924	MAN	C1-O5-C5	2.37	115.26	112.25
10	B	912	MAN	O3-C3-C2	2.37	114.29	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	910	NAG	O5-C5-C6	2.39	112.51	107.35
6	A	916	MAN	O2-C2-C1	2.40	114.02	109.21
6	A	913	NAG	O3-C3-C2	2.42	113.90	109.11
2	A	904	MAN	O2-C2-C3	2.42	114.99	110.12
6	B	921	MAN	C1-O5-C5	2.43	115.33	112.25
4	B	916	NAG	C2-N2-C7	2.43	126.16	123.04
4	A	909	BMA	O5-C5-C6	2.44	112.62	107.35
6	B	920	BMA	C1-O5-C5	2.46	115.37	112.25
4	A	909	BMA	O2-C2-C3	2.46	115.06	110.12
7	A	938	MAN	O2-C2-C3	2.46	115.06	110.12
6	A	921	MAN	C1-O5-C5	2.49	115.41	112.25
6	B	926	MAN	C3-C4-C5	2.52	114.58	110.20
6	A	913	NAG	C3-C2-N2	2.52	116.60	110.56
7	A	938	MAN	O5-C1-C2	2.52	114.95	110.86
5	A	911	NAG	C8-C7-N2	2.56	121.00	116.11
7	A	926	NAG	O3-C3-C4	2.57	116.13	110.34
7	B	935	MAN	C1-O5-C5	2.58	115.53	112.25
11	B	945	MAN	C2-C3-C4	2.59	115.45	111.04
11	B	944	MAN	C1-O5-C5	2.60	115.55	112.25
7	B	903	BMA	C3-C4-C5	2.62	114.76	110.20
2	A	905	MAN	O3-C3-C4	2.63	116.26	110.34
2	A	901	NAG	O5-C5-C6	2.68	113.16	107.35
11	B	944	MAN	O5-C5-C6	2.74	113.28	107.35
7	B	904	MAN	O5-C5-C6	2.77	113.35	107.35
6	B	927	MAN	O4-C4-C3	2.80	116.63	110.34
6	A	912	NAG	C8-C7-N2	2.85	121.56	116.11
7	A	938	MAN	C1-O5-C5	2.86	115.88	112.25
10	B	913	MAN	O5-C1-C2	2.87	115.50	110.86
2	A	904	MAN	C2-C3-C4	2.88	115.93	111.04
7	A	934	BMA	O5-C1-C2	2.90	115.56	110.86
7	B	937	MAN	C1-O5-C5	2.94	115.97	112.25
7	A	929	MAN	O3-C3-C2	2.96	115.34	110.00
5	A	910	NAG	C1-O5-C5	2.96	116.01	112.25
4	B	930	BMA	C1-O5-C5	2.99	116.05	112.25
4	A	909	BMA	C2-C3-C4	3.01	116.16	111.04
6	A	921	MAN	O5-C5-C6	3.04	113.94	107.35
11	B	940	BMA	O2-C2-C3	3.06	116.28	110.12
6	A	914	BMA	C1-C2-C3	3.09	113.19	109.54
10	B	912	MAN	C3-C4-C5	3.10	115.59	110.20
7	A	934	BMA	O2-C2-C3	3.11	116.38	110.12
6	A	915	MAN	O2-C2-C1	3.13	115.48	109.21
7	B	936	MAN	C1-O5-C5	3.13	116.22	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	941	MAN	C2-C3-C4	3.14	116.38	111.04
4	B	917	BMA	C1-C2-C3	3.22	113.35	109.54
6	A	920	MAN	C1-O5-C5	3.23	116.34	112.25
4	B	917	BMA	C3-C4-C5	3.28	115.91	110.20
6	A	913	NAG	C1-O5-C5	3.32	116.46	112.25
4	A	924	BMA	O2-C2-C1	3.32	115.87	109.21
7	B	934	MAN	C3-C4-C5	3.38	116.09	110.20
7	B	902	NAG	C1-O5-C5	3.47	116.65	112.25
2	A	904	MAN	C1-C2-C3	3.48	113.66	109.54
4	A	924	BMA	C1-O5-C5	3.48	116.66	112.25
2	A	903	BMA	O3-C3-C4	3.48	118.17	110.34
7	A	929	MAN	C1-O5-C5	3.50	116.69	112.25
11	B	940	BMA	C3-C4-C5	3.54	116.37	110.20
4	B	917	BMA	O5-C1-C2	3.57	116.64	110.86
6	B	922	MAN	O3-C3-C2	3.65	116.59	110.00
11	B	940	BMA	C2-C3-C4	3.67	117.28	111.04
10	B	910	NAG	C6-C5-C4	3.70	122.15	113.02
11	B	939	NAG	C1-O5-C5	3.72	116.97	112.25
4	A	907	NAG	C2-N2-C7	3.77	127.89	123.04
7	A	925	NAG	C1-O5-C5	3.78	117.04	112.25
7	B	907	MAN	C1-C2-C3	3.78	114.01	109.54
4	A	909	BMA	O6-C6-C5	3.78	123.84	111.33
10	B	912	MAN	C2-C3-C4	3.84	117.56	111.04
10	B	912	MAN	O2-C2-C3	3.87	117.90	110.12
7	A	931	MAN	O5-C5-C6	3.91	115.82	107.35
4	B	928	NAG	C1-O5-C5	3.93	117.24	112.25
7	B	907	MAN	C6-C5-C4	3.94	122.73	113.02
4	A	922	NAG	C1-O5-C5	3.94	117.25	112.25
2	A	903	BMA	C1-C2-C3	4.06	114.34	109.54
5	A	911	NAG	C2-N2-C7	4.06	128.26	123.04
7	B	907	MAN	O6-C6-C5	4.07	124.79	111.33
7	A	938	MAN	C3-C4-C5	4.10	117.34	110.20
11	B	945	MAN	C3-C4-C5	4.10	117.35	110.20
7	A	937	MAN	C1-O5-C5	4.11	117.47	112.25
7	A	935	MAN	O5-C5-C6	4.18	116.41	107.35
7	B	907	MAN	O3-C3-C4	4.19	119.77	110.34
11	B	941	MAN	C3-C4-C5	4.21	117.54	110.20
4	A	909	BMA	C3-C4-C5	4.23	117.56	110.20
4	A	923	NAG	C4-C3-C2	4.23	117.80	111.23
7	A	934	BMA	O3-C3-C4	4.26	119.92	110.34
6	B	926	MAN	C1-O5-C5	4.27	117.67	112.25
7	A	938	MAN	C2-C3-C4	4.27	118.30	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	904	MAN	C3-C4-C5	4.31	117.71	110.20
10	B	909	NAG	C1-O5-C5	4.31	117.72	112.25
4	B	915	NAG	C1-O5-C5	4.35	117.77	112.25
4	B	929	NAG	C2-N2-C7	4.45	128.76	123.04
10	B	913	MAN	C3-C4-C5	4.47	118.00	110.20
6	B	922	MAN	O2-C2-C3	4.49	119.14	110.12
10	B	911	BMA	C1-O5-C5	4.50	117.96	112.25
2	A	904	MAN	O3-C3-C2	4.59	118.29	110.00
6	B	922	MAN	C1-O5-C5	4.90	118.46	112.25
11	B	942	MAN	C1-C2-C3	4.97	115.42	109.54
6	A	916	MAN	O2-C2-C3	5.01	120.19	110.12
7	B	935	MAN	O3-C3-C2	5.15	119.30	110.00
7	A	932	NAG	C1-O5-C5	5.17	118.81	112.25
6	A	917	MAN	C1-O5-C5	5.20	118.84	112.25
6	B	923	MAN	C1-O5-C5	5.34	119.02	112.25
6	A	916	MAN	C1-O5-C5	5.36	119.05	112.25
6	A	921	MAN	O3-C3-C2	5.43	119.80	110.00
6	B	927	MAN	C1-O5-C5	5.63	119.39	112.25
7	A	934	BMA	C1-O5-C5	5.74	119.53	112.25
11	B	943	MAN	C1-O5-C5	6.08	119.97	112.25
7	A	930	MAN	C1-O5-C5	6.29	120.22	112.25
7	B	901	NAG	C1-O5-C5	6.41	120.38	112.25
11	B	938	NAG	C1-O5-C5	6.79	120.87	112.25
2	A	905	MAN	C1-O5-C5	6.86	120.95	112.25
4	B	917	BMA	C1-O5-C5	7.21	121.40	112.25
10	B	913	MAN	C1-O5-C5	7.83	122.18	112.25
4	A	909	BMA	C1-O5-C5	7.95	122.33	112.25
2	A	904	MAN	C1-O5-C5	8.82	123.44	112.25
11	B	940	BMA	C1-O5-C5	9.40	124.18	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	908	NAG	1	0
5	A	911	NAG	4	0
7	A	927	BMA	2	0
7	A	933	NAG	2	0
10	B	909	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	933	BMA	1	0
11	B	940	BMA	2	0
11	B	942	MAN	1	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	$\#\|Z\| > 2$
3	NAG	A	906	1	14,14,15	0.90	1 (7%)	15,19,21	1.30	2 (13%)
3	NAG	A	939	1	14,14,15	0.59	0	15,19,21	1.69	3 (20%)
8	MRD	A	940	-	6,7,7	0.39	0	7,10,10	0.45	0
8	MRD	A	941	-	6,7,7	0.79	0	7,10,10	0.89	0
9	BGC	A	942	-	12,12,12	0.75	0	17,17,17	1.05	2 (11%)
9	BGC	A	943	-	12,12,12	0.97	1 (8%)	17,17,17	2.62	10 (58%)
3	NAG	B	908	1	14,14,15	0.78	0	15,19,21	1.79	5 (33%)
3	NAG	B	946	1	14,14,15	0.56	0	15,19,21	1.34	1 (6%)
3	NAG	B	947	1	14,14,15	0.72	0	15,19,21	1.42	3 (20%)
8	MRD	B	948	-	6,7,7	0.59	0	7,10,10	0.76	0
8	MRD	B	949	-	6,7,7	0.47	0	7,10,10	0.74	0
9	BGC	B	950	-	12,12,12	0.80	0	17,17,17	1.26	2 (11%)
9	BGC	B	951	-	12,12,12	1.07	1 (8%)	17,17,17	2.65	10 (58%)

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	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	939	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MRD	A	940	-	-	0/5/5/5	0/0/0/0
8	MRD	A	941	-	-	0/5/5/5	0/0/0/0
9	BGC	A	942	-	-	0/2/22/22	0/1/1/1
9	BGC	A	943	-	-	0/2/22/22	0/1/1/1
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	946	1	-	0/6/23/26	0/1/1/1
3	NAG	B	947	1	-	0/6/23/26	0/1/1/1
8	MRD	B	948	-	-	0/5/5/5	0/0/0/0
8	MRD	B	949	-	-	0/5/5/5	0/0/0/0
9	BGC	B	950	-	-	0/2/22/22	0/1/1/1
9	BGC	B	951	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	906	NAG	C1-C2	2.02	1.55	1.52
9	A	943	BGC	C1-C2	2.10	1.56	1.52
9	B	951	BGC	C1-C2	2.77	1.58	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	943	BGC	C3-C4-C5	-4.35	102.62	110.20
9	B	951	BGC	O1-C1-O5	-3.70	100.12	110.25
9	B	951	BGC	C3-C4-C5	-3.43	104.21	110.20
3	A	939	NAG	C3-C4-C5	-3.25	104.54	110.20
9	A	943	BGC	O1-C1-O5	-3.14	101.65	110.25
9	A	943	BGC	O2-C2-C3	-3.01	103.56	110.34
9	A	943	BGC	C4-C3-C2	-2.98	105.23	110.79
9	B	950	BGC	O1-C1-O5	-2.88	102.38	110.25
9	B	951	BGC	C4-C3-C2	-2.80	105.56	110.79
3	B	947	NAG	C2-N2-C7	-2.54	119.78	123.04
3	A	906	NAG	O7-C7-C8	-2.38	117.70	122.06
9	A	943	BGC	O5-C5-C4	-2.32	105.33	109.68
9	A	942	BGC	O3-C3-C2	-2.30	105.16	110.34
3	B	947	NAG	O4-C4-C3	-2.09	105.62	110.34
9	A	942	BGC	O1-C1-O5	-2.08	104.56	110.25
9	B	951	BGC	O2-C2-C3	-2.07	105.67	110.34
3	B	947	NAG	C3-C2-N2	-2.02	105.72	110.56
3	B	908	NAG	O7-C7-N2	-2.01	117.77	121.86
3	A	939	NAG	O3-C3-C2	2.01	113.10	109.11
3	A	906	NAG	C2-N2-C7	2.10	125.73	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	951	BGC	C1-C2-C3	2.13	113.60	110.43
3	B	908	NAG	O5-C5-C6	2.14	111.98	107.35
9	A	943	BGC	O5-C5-C6	2.16	111.82	106.36
9	A	943	BGC	O3-C3-C4	2.33	115.59	110.34
9	B	951	BGC	O3-C3-C4	2.45	115.85	110.34
9	A	943	BGC	O4-C4-C5	2.80	116.65	109.24
9	B	951	BGC	O5-C5-C6	2.85	113.55	106.36
3	B	908	NAG	C2-N2-C7	2.91	126.78	123.04
9	B	950	BGC	C1-O5-C5	3.01	119.03	113.47
9	B	951	BGC	O2-C2-C1	3.02	116.46	109.82
3	B	946	NAG	C4-C3-C2	3.03	115.94	111.23
3	B	908	NAG	C8-C7-N2	3.10	122.03	116.11
9	A	943	BGC	C6-C5-C4	3.13	120.73	113.02
3	B	908	NAG	C1-O5-C5	3.21	116.32	112.25
9	B	951	BGC	C6-C5-C4	3.51	121.68	113.02
3	A	939	NAG	C1-O5-C5	3.52	116.71	112.25
9	A	943	BGC	O5-C1-C2	5.18	118.06	109.80
9	B	951	BGC	O5-C1-C2	5.68	118.86	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	940	MRD	2	0
8	A	941	MRD	6	0
9	A	942	BGC	1	0
9	A	943	BGC	1	0
3	B	908	NAG	1	0
8	B	948	MRD	1	0
8	B	949	MRD	1	0
9	B	950	BGC	1	0
9	B	951	BGC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	834/841 (99%)	-0.33	12 (1%) 78 83	13, 22, 37, 67	0
1	B	832/841 (98%)	-0.48	1 (0%) 95 97	12, 19, 32, 62	0
All	All	1666/1682 (99%)	-0.40	13 (0%) 87 90	12, 20, 35, 67	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	LEU	3.3
1	A	110	VAL	3.2
1	A	95	LEU	2.9
1	A	109	GLY	2.5
1	A	144	ALA	2.5
1	B	141	LEU	2.3
1	A	245	MET	2.3
1	A	94	PRO	2.3
1	A	609	ASP	2.3
1	A	808	SER	2.3
1	A	141	LEU	2.2
1	A	698	GLU	2.1
1	A	108	ALA	2.0

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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
7	NAG	A	925	14/15	0.95	0.12	6.46	22,28,42,46	0
7	MAN	A	931	11/12	0.97	0.15	6.34	27,30,38,42	0
11	MAN	B	942	11/12	0.95	0.21	4.01	25,38,53,57	0
7	MAN	A	936	11/12	0.96	0.13	2.73	35,37,44,48	0
4	NAG	A	908	14/15	0.95	0.14	1.89	26,33,36,42	0
7	MAN	A	935	11/12	0.93	0.13	1.87	30,36,44,58	0
7	NAG	B	931	14/15	0.96	0.09	1.20	19,28,41,42	0
7	MAN	B	906	11/12	0.97	0.15	1.13	34,36,41,50	0
10	NAG	B	910	14/15	0.96	0.10	0.86	25,29,34,41	0
4	NAG	B	928	14/15	0.96	0.09	0.57	26,36,45,53	0
6	MAN	B	927	11/12	0.98	0.09	0.22	19,21,22,28	0
6	MAN	A	920	11/12	0.96	0.10	0.11	23,27,36,40	0
6	MAN	A	919	11/12	0.98	0.10	-0.11	24,26,28,29	0
6	NAG	B	918	14/15	0.98	0.09	-0.18	21,25,27,27	0
6	NAG	B	919	14/15	0.96	0.09	-0.18	17,22,28,33	0
6	MAN	A	918	11/12	0.96	0.10	-0.29	19,24,26,26	0
7	MAN	B	937	11/12	0.97	0.10	-0.41	25,31,35,37	0
10	NAG	B	909	14/15	0.97	0.09	-0.42	20,25,27,27	0
6	NAG	A	913	14/15	0.97	0.11	-0.42	25,27,29,29	0
2	NAG	A	901	14/15	0.97	0.08	-0.46	22,25,28,28	0
6	NAG	A	912	14/15	0.98	0.10	-0.51	24,27,31,31	0
2	NAG	A	902	14/15	0.97	0.09	-0.59	25,33,43,46	0
11	NAG	B	938	14/15	0.97	0.10	-0.60	19,23,26,28	0
7	NAG	A	932	14/15	0.95	0.11	-0.79	24,26,32,34	0
6	MAN	B	926	11/12	0.98	0.07	-0.80	16,19,19,21	0
7	NAG	B	901	14/15	0.98	0.08	-0.93	15,18,21,22	0
4	NAG	A	922	14/15	0.94	0.09	-1.03	29,37,50,54	0
4	NAG	A	907	14/15	0.96	0.07	-1.24	22,27,30,36	0
5	NAG	A	910	14/15	0.98	0.07	-1.46	22,24,26,30	0
4	NAG	B	915	14/15	0.99	0.06	-1.60	15,19,23,25	0
7	NAG	B	902	14/15	0.98	0.07	-2.00	18,23,28,34	0
7	MAN	B	935	11/12	0.96	0.14	-	31,34,38,41	0
4	BMA	B	930	11/12	0.84	0.24	-	66,74,79,83	0
6	MAN	A	916	11/12	0.92	0.15	-	37,42,54,57	0
6	BMA	B	920	11/12	0.97	0.08	-	22,24,25,28	0
7	MAN	B	905	11/12	0.95	0.20	-	33,42,54,77	0
11	MAN	B	944	11/12	0.91	0.22	-	51,59,66,74	0
7	MAN	A	937	11/12	0.87	0.22	-	56,60,68,69	0
7	NAG	A	926	14/15	0.94	0.13	-	21,29,35,41	0
11	MAN	B	943	11/12	0.96	0.12	-	32,36,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	BMA	A	927	11/12	0.91	0.17	-	32,38,45,56	0
6	MAN	A	915	11/12	0.98	0.11	-	29,32,34,35	0
11	BMA	B	940	11/12	0.92	0.18	-	36,44,55,61	0
7	MAN	B	907	11/12	0.92	0.12	-	36,39,42,42	0
6	MAN	B	924	11/12	0.97	0.10	-	25,26,32,32	0
4	BMA	A	909	11/12	0.86	0.23	-	40,48,60,62	0
11	NAG	B	939	14/15	0.95	0.15	-	25,33,41,43	0
10	BMA	B	911	11/12	0.92	0.13	-	49,54,62,75	0
6	MAN	B	922	11/12	0.90	0.14	-	39,47,51,55	0
10	MAN	B	914	11/12	0.90	0.34	-	80,84,89,92	0
7	MAN	B	904	11/12	0.96	0.13	-	30,34,40,41	0
4	BMA	A	924	11/12	0.54	0.31	-	79,91,96,96	0
7	BMA	B	903	11/12	0.95	0.08	-	26,31,33,35	0
4	BMA	B	917	11/12	0.87	0.30	-	61,76,90,93	0
6	MAN	B	921	11/12	0.98	0.10	-	25,27,29,35	0
11	MAN	B	945	11/12	0.79	0.26	-	51,61,66,77	0
6	MAN	B	925	11/12	0.95	0.14	-	30,33,36,36	0
7	MAN	A	929	11/12	0.92	0.15	-	34,36,43,44	0
11	MAN	B	941	11/12	0.84	0.25	-	66,72,81,81	0
6	BMA	A	914	11/12	0.97	0.09	-	23,25,27,30	0
7	MAN	B	936	11/12	0.97	0.11	-	32,33,36,46	0
10	MAN	B	913	11/12	0.79	0.25	-	73,77,80,83	0
7	BMA	B	933	11/12	0.93	0.17	-	31,37,44,52	0
6	MAN	B	923	11/12	0.98	0.06	-	18,19,21,23	0
7	NAG	A	933	14/15	0.95	0.21	-	30,32,42,51	0
5	NAG	A	911	14/15	0.96	0.13	-	30,37,45,51	0
6	MAN	A	921	11/12	0.96	0.18	-	34,35,44,44	0
7	MAN	A	930	11/12	0.97	0.12	-	26,28,39,51	0
7	MAN	A	938	11/12	0.77	0.25	-	51,63,68,69	0
2	MAN	A	905	11/12	0.84	0.17	-	55,60,69,70	0
7	MAN	B	934	11/12	0.69	0.29	-	72,78,86,87	0
7	MAN	A	928	11/12	0.89	0.27	-	62,64,74,76	0
2	MAN	A	904	11/12	0.70	0.23	-	70,78,89,90	0
7	BMA	A	934	11/12	0.91	0.14	-	37,44,51,52	0
4	NAG	B	929	14/15	0.93	0.18	-	41,47,57,60	0
2	BMA	A	903	11/12	0.91	0.12	-	43,56,61,62	0
10	MAN	B	912	11/12	0.49	0.25	-	69,83,89,91	0
4	NAG	A	923	14/15	0.86	0.17	-	52,64,80,85	0
6	MAN	A	917	11/12	0.98	0.09	-	19,21,23,24	0
4	NAG	B	916	14/15	0.95	0.14	-	21,32,46,50	0
7	NAG	B	932	14/15	0.93	0.17	-	23,30,37,38	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
8	MRD	A	941	8/8	0.89	0.22	5.04	34,39,47,47	0
8	MRD	B	949	8/8	0.94	0.15	3.96	45,47,49,54	0
8	MRD	B	948	8/8	0.97	0.13	3.09	30,37,40,41	0
3	NAG	B	947	14/15	0.97	0.21	2.07	29,34,43,45	0
9	BGC	B	951	12/12	0.87	0.22	1.96	31,43,51,52	0
3	NAG	A	939	14/15	0.95	0.19	1.70	32,46,50,56	0
9	BGC	A	943	12/12	0.87	0.20	1.33	36,46,50,53	0
9	BGC	A	942	12/12	0.98	0.21	0.17	19,22,24,30	0
8	MRD	A	940	8/8	0.96	0.10	-0.03	33,38,39,40	0
9	BGC	B	950	12/12	0.99	0.18	-0.19	14,18,20,26	0
3	NAG	B	908	14/15	0.88	0.29	-	49,59,68,69	0
3	NAG	B	946	14/15	0.93	0.26	-	50,64,70,78	0
3	NAG	A	906	14/15	0.88	0.36	-	58,69,76,76	0

6.5 Other polymers

There are no such residues in this entry.