



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:55 am 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

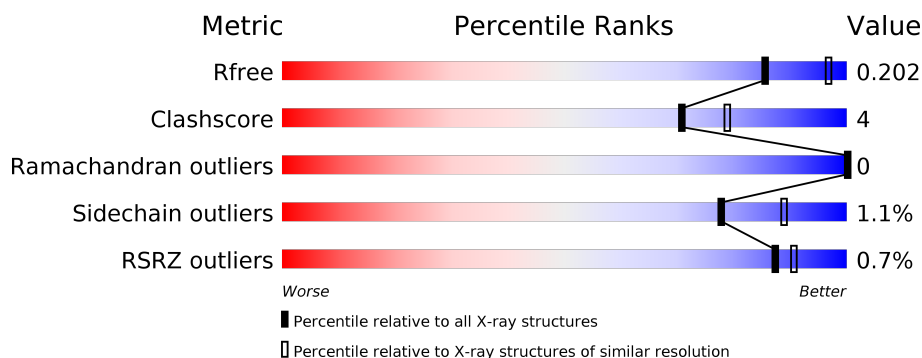
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	841	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 91%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>91%</span> <span>8%</span> </div> </div>
1	B	841	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 89%, yellow 9%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>89%</span> <span>9%</span> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 [i](#)

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.

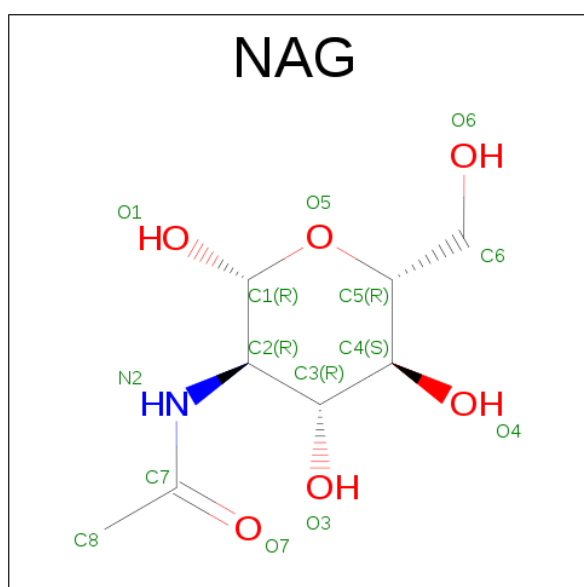
- Molecule 1 is a protein called Beta-glucosidase 1.

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		

*Continued on next page...*

*Continued from previous page...*

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

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

- 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	0	0
			28	16	2	10		

- 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	0	0
			116	64	2	50		
6	B	10	Total	C	N	O	0	0
			116	64	2	50		

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

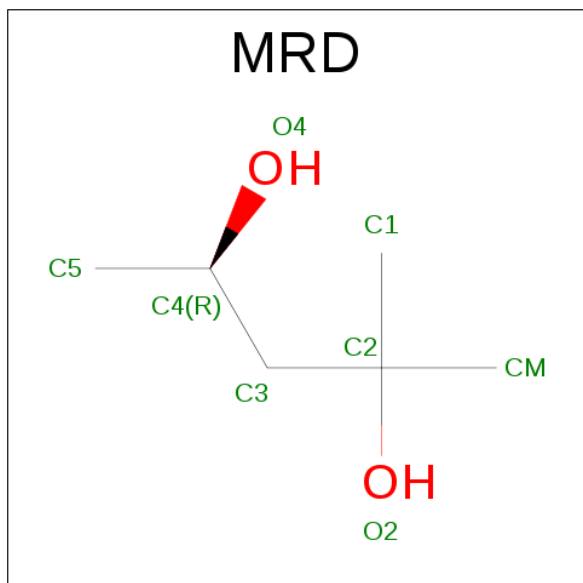
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	7	Total	C	N	O	0	0
			83	46	2	35		
7	A	7	Total	C	N	O	0	0
			83	46	2	35		

*Continued on next page...*

Continued from previous page...

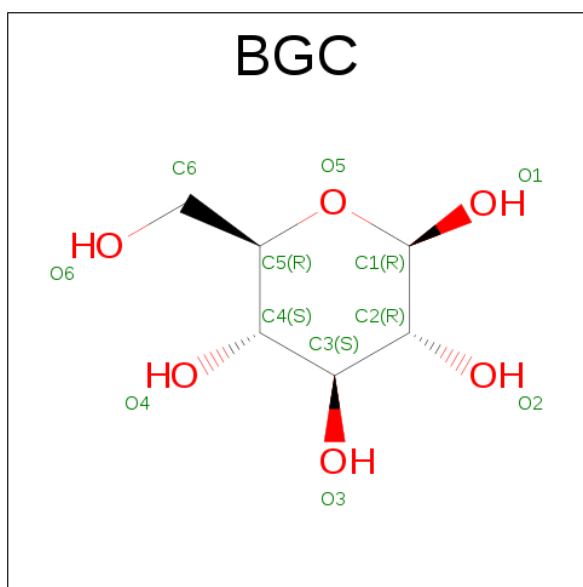
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	7	Total	C	N	O	0	0
			83	46	2	35		
7	B	7	Total	C	N	O	0	0
			83	46	2	35		

- 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	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	B	1	Total	C	O	0	0
			8	6	2		
8	B	1	Total	C	O	0	0
			8	6	2		

- 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	0	0
			12	6	6		
9	A	1	Total	C	O	0	0
			12	6	6		
9	B	1	Total	C	O	0	0
			12	6	6		
9	B	1	Total	C	O	0	0
			12	6	6		

- 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	0	0
			72	40	2	30		

- 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	0	0
			94	52	2	40		

- Molecule 12 is water.

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

*Continued on next page...*

*Continued from previous page...*

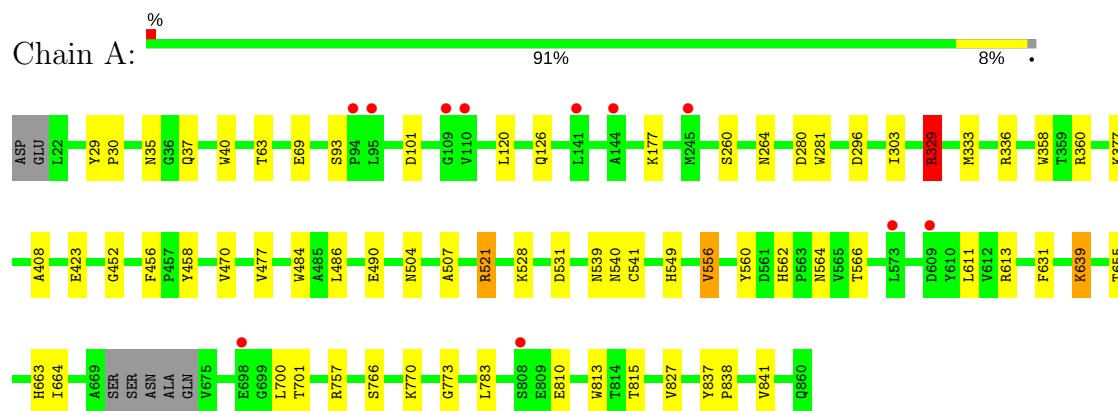
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	689	Total 689	O 689	0	0



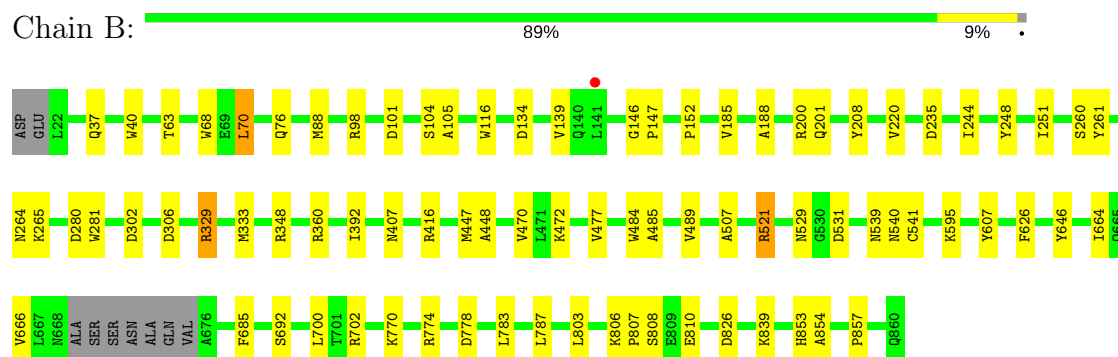
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



#### • Molecule 1: Beta-glucosidase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	4964 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.88	0.53
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: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
1:A:93:SER:HB2	1:A:452:GLY:HA2	1.92	0.51
11:B:940:BMA:H61	12:B:1439:HOH:O	2.11	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:448:ALA:HB1	1:B:507:ALA:O	2.12	0.49
1:B:770:LYS:HG3	1:B:810:GLU:HG3	1.93	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
9:A:943:BGC:H6C2	12:A:1564:HOH:O	2.12	0.48
1:B:251:ILE:CG2	10:B:909:NAG:H82	2.43	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
1:A:329:ARG:HD2	1:A:329:ARG:HA	1.72	0.48
8:A:940:MRD:H5C3	8:A:940:MRD:O2	2.13	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

*Continued on next page...*

*Continued from previous page...*

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:611:LEU:HD12	1:A:613:ARG:NH2	2.30	0.46
1:A:63:THR:HB	1:A:333:MET:CE	2.45	0.46
1:B:329:ARG:HD2	1:B:329:ARG:HA	1.80	0.46
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.98	0.45
1:B:664:ILE:CD1	1:B:854:ALA:HB3	2.46	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:A:766:SER:HA	1:A:813:TRP:O	2.20	0.41
1:B:507:ALA:HB2	1:B:521:ARG:HG3	2.03	0.41
8:B:948:MRD:C5	8:B:948:MRD:H1C2	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

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:A:837:TYR:HA	1:A:838:PRO:HD3	1.97	0.40
1:B:105:ALA:HB1	1:B:447:MET:CE	2.51	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%)	75	87

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	670/677 (99%)	663 (99%)	7 (1%)	80	90
All	All	1341/1354 (99%)	1326 (99%)	15 (1%)	78	89

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 ⓘ

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 ⓘ

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	1.11	1 (7%)	15,19,21	0.89	0
2	NAG	A	902	2	14,14,15	0.87	1 (7%)	15,19,21	1.53	5 (33%)
2	BMA	A	903	2	11,11,12	1.17	1 (9%)	13,15,17	1.75	3 (23%)
2	MAN	A	904	2	11,11,12	1.19	1 (9%)	13,15,17	3.48	8 (61%)
2	MAN	A	905	2	11,11,12	0.89	0	13,15,17	2.39	5 (38%)
4	NAG	A	907	1,4	14,14,15	1.00	1 (7%)	15,19,21	1.47	2 (13%)
4	NAG	A	908	4	14,14,15	0.75	0	15,19,21	1.74	5 (33%)
4	BMA	A	909	4	11,11,12	0.87	0	13,15,17	3.04	7 (53%)
5	NAG	A	910	1,5	14,14,15	0.73	0	15,19,21	1.33	2 (13%)
5	NAG	A	911	5	14,14,15	0.67	0	15,19,21	2.26	8 (53%)
6	NAG	A	912	1,6	14,14,15	0.89	0	15,19,21	1.35	3 (20%)
6	NAG	A	913	6	14,14,15	0.69	0	15,19,21	1.60	5 (33%)
6	BMA	A	914	6	11,11,12	1.09	1 (9%)	13,15,17	1.36	2 (15%)
6	MAN	A	915	6	11,11,12	0.77	0	13,15,17	1.25	1 (7%)
6	MAN	A	916	6	11,11,12	1.12	2 (18%)	13,15,17	2.46	5 (38%)
6	MAN	A	917	6	11,11,12	0.64	0	13,15,17	2.09	4 (30%)
6	MAN	A	918	6	11,11,12	1.09	1 (9%)	13,15,17	1.59	3 (23%)
6	MAN	A	919	6	11,11,12	0.56	0	13,15,17	0.97	0
6	MAN	A	920	6	11,11,12	0.78	0	13,15,17	1.39	3 (23%)
6	MAN	A	921	6	11,11,12	1.05	1 (9%)	13,15,17	2.30	6 (46%)
4	NAG	A	922	1,4	14,14,15	0.95	1 (7%)	15,19,21	1.41	2 (13%)
4	NAG	A	923	4	14,14,15	0.80	1 (7%)	15,19,21	1.49	1 (6%)
4	BMA	A	924	4	11,11,12	0.75	0	13,15,17	1.50	3 (23%)
7	NAG	A	925	1,7	14,14,15	0.69	0	15,19,21	1.52	2 (13%)
7	NAG	A	926	7	14,14,15	0.80	1 (7%)	15,19,21	2.32	4 (26%)
7	BMA	A	927	7	11,11,12	0.79	0	13,15,17	0.74	0
7	MAN	A	928	7	11,11,12	0.72	0	13,15,17	1.81	3 (23%)
7	MAN	A	929	7	11,11,12	0.86	0	13,15,17	1.64	3 (23%)
7	MAN	A	930	7	11,11,12	1.11	1 (9%)	13,15,17	2.38	5 (38%)

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	0.76	0	13,15,17	1.22	1 (7%)
7	NAG	A	932	1,7	14,14,15	1.00	1 (7%)	15,19,21	1.97	4 (26%)
7	NAG	A	933	7	14,14,15	0.76	0	15,19,21	1.20	2 (13%)
7	BMA	A	934	7	11,11,12	1.20	0	13,15,17	2.60	6 (46%)
7	MAN	A	935	7	11,11,12	0.88	0	13,15,17	1.45	1 (7%)
7	MAN	A	936	7	11,11,12	0.99	0	13,15,17	1.67	3 (23%)
7	MAN	A	937	7	11,11,12	0.68	0	13,15,17	1.53	2 (15%)
7	MAN	A	938	7	11,11,12	0.85	0	13,15,17	2.33	6 (46%)
7	NAG	B	901	1,7	14,14,15	0.90	0	15,19,21	2.08	3 (20%)
7	NAG	B	902	7	14,14,15	0.79	1 (7%)	15,19,21	1.53	3 (20%)
7	BMA	B	903	7	11,11,12	1.08	1 (9%)	13,15,17	1.64	3 (23%)
7	MAN	B	904	7	11,11,12	0.63	0	13,15,17	1.49	2 (15%)
7	MAN	B	905	7	11,11,12	1.01	1 (9%)	13,15,17	1.32	2 (15%)
7	MAN	B	906	7	11,11,12	0.84	0	13,15,17	1.01	0
7	MAN	B	907	7	11,11,12	1.20	1 (9%)	13,15,17	2.64	6 (46%)
10	NAG	B	909	1,10	14,14,15	0.88	0	15,19,21	1.82	3 (20%)
10	NAG	B	910	10	14,14,15	1.12	1 (7%)	15,19,21	1.55	3 (20%)
10	BMA	B	911	10	11,11,12	0.76	0	13,15,17	1.55	2 (15%)
10	MAN	B	912	10	11,11,12	1.60	1 (9%)	13,15,17	2.08	5 (38%)
10	MAN	B	913	10	11,11,12	0.65	0	13,15,17	2.64	3 (23%)
10	MAN	B	914	10	11,11,12	0.86	1 (9%)	13,15,17	0.93	0
4	NAG	B	915	1,4	14,14,15	1.05	1 (7%)	15,19,21	1.85	3 (20%)
4	NAG	B	916	4	14,14,15	0.89	1 (7%)	15,19,21	1.25	3 (20%)
4	BMA	B	917	4	11,11,12	0.61	0	13,15,17	2.63	5 (38%)
6	NAG	B	918	1,6	14,14,15	0.92	0	15,19,21	1.94	5 (33%)
6	NAG	B	919	6	14,14,15	0.74	0	15,19,21	0.97	0
6	BMA	B	920	6	11,11,12	0.98	0	13,15,17	1.37	3 (23%)
6	MAN	B	921	6	11,11,12	0.76	0	13,15,17	1.31	3 (23%)
6	MAN	B	922	6	11,11,12	1.21	2 (18%)	13,15,17	2.44	5 (38%)
6	MAN	B	923	6	11,11,12	0.75	0	13,15,17	2.01	4 (30%)
6	MAN	B	924	6	11,11,12	0.81	0	13,15,17	1.43	2 (15%)
6	MAN	B	925	6	11,11,12	1.05	0	13,15,17	0.95	0
6	MAN	B	926	6	11,11,12	0.89	0	13,15,17	1.91	4 (30%)
6	MAN	B	927	6	11,11,12	1.44	2 (18%)	13,15,17	2.20	4 (30%)
4	NAG	B	928	1,4	14,14,15	0.71	0	15,19,21	1.41	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	0.92	0	15,19,21	1.70	4 (26%)
4	BMA	B	930	4	11,11,12	0.92	0	13,15,17	1.49	1 (7%)
7	NAG	B	931	1,7	14,14,15	1.11	1 (7%)	15,19,21	1.79	5 (33%)
7	NAG	B	932	7	14,14,15	1.26	2 (14%)	15,19,21	1.87	5 (33%)
7	BMA	B	933	7	11,11,12	0.67	0	13,15,17	0.95	1 (7%)
7	MAN	B	934	7	11,11,12	0.96	1 (9%)	13,15,17	1.99	5 (38%)
7	MAN	B	935	7	11,11,12	1.22	2 (18%)	13,15,17	1.81	2 (15%)
7	MAN	B	936	7	11,11,12	0.69	0	13,15,17	1.43	1 (7%)
7	MAN	B	937	7	11,11,12	0.83	0	13,15,17	1.36	1 (7%)
11	NAG	B	938	11,1	14,14,15	0.74	1 (7%)	15,19,21	1.93	2 (13%)
11	NAG	B	939	11	14,14,15	0.69	0	15,19,21	1.16	1 (6%)
11	BMA	B	940	11	11,11,12	0.97	0	13,15,17	3.67	6 (46%)
11	MAN	B	941	11	11,11,12	1.04	0	13,15,17	2.23	6 (46%)
11	MAN	B	942	11	11,11,12	0.70	0	13,15,17	1.94	3 (23%)
11	MAN	B	943	11	11,11,12	0.65	0	13,15,17	1.91	2 (15%)
11	MAN	B	944	11	11,11,12	0.58	0	13,15,17	1.43	4 (30%)
11	MAN	B	945	11	11,11,12	0.91	0	13,15,17	1.83	3 (23%)

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	932	NAG	C2-N2	-3.35	1.40	1.46
4	B	915	NAG	O4-C4	-2.71	1.36	1.43
7	B	905	MAN	O5-C1	-2.41	1.39	1.43
7	B	931	NAG	O3-C3	-2.38	1.37	1.43
7	A	930	MAN	O2-C2	-2.38	1.38	1.43
6	A	918	MAN	O5-C1	-2.35	1.39	1.43
4	B	916	NAG	O5-C1	-2.31	1.39	1.43
6	B	927	MAN	O5-C1	-2.29	1.40	1.43
6	A	916	MAN	O5-C1	-2.28	1.40	1.43
4	A	922	NAG	O5-C1	-2.25	1.40	1.43
7	B	902	NAG	O5-C1	-2.23	1.40	1.43
4	A	923	NAG	O5-C1	-2.19	1.40	1.43
7	B	932	NAG	O5-C1	-2.19	1.40	1.43
7	B	903	BMA	O4-C4	-2.17	1.38	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	910	NAG	O5-C5	-2.15	1.38	1.43
6	A	914	BMA	O2-C2	-2.11	1.38	1.43
7	A	926	NAG	C2-N2	-2.10	1.42	1.46
11	B	938	NAG	O5-C1	-2.10	1.40	1.43
6	B	922	MAN	O5-C1	-2.09	1.40	1.43
2	A	903	BMA	O5-C1	-2.07	1.40	1.43
7	B	935	MAN	O2-C2	-2.07	1.38	1.43
6	A	916	MAN	O3-C3	-2.05	1.38	1.43
7	A	932	NAG	C1-C2	-2.01	1.49	1.52
7	B	934	MAN	C2-C3	2.04	1.55	1.52
10	B	914	MAN	C2-C3	2.15	1.55	1.52
2	A	902	NAG	C1-C2	2.30	1.55	1.52
7	B	907	MAN	C4-C5	2.37	1.58	1.53
4	A	907	NAG	C1-C2	2.41	1.55	1.52
6	A	921	MAN	C2-C3	2.45	1.55	1.52
7	B	935	MAN	C2-C3	2.77	1.56	1.52
6	B	922	MAN	C2-C3	3.20	1.56	1.52
2	A	901	NAG	C1-C2	3.55	1.57	1.52
2	A	904	MAN	C2-C3	3.63	1.57	1.52
6	B	927	MAN	C2-C3	3.69	1.57	1.52
10	B	912	MAN	C2-C3	4.65	1.58	1.52

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	940	BMA	C6-C5-C4	-7.08	96.44	113.00
7	A	926	NAG	C2-N2-C7	-6.67	113.21	122.94
7	A	928	MAN	O5-C1-C2	-4.14	104.31	110.79
4	B	915	NAG	O4-C4-C5	-4.09	98.98	109.28
7	A	930	MAN	O2-C2-C3	-4.04	102.24	110.17
10	B	909	NAG	O5-C1-C2	-4.00	105.91	111.47
6	B	918	NAG	C1-C2-N2	-3.92	103.79	110.49
5	A	911	NAG	C3-C4-C5	-3.89	103.36	110.22
11	B	942	MAN	O2-C2-C1	-3.87	101.31	109.18
7	B	907	MAN	O4-C4-C3	-3.86	101.95	110.36
7	B	934	MAN	O5-C1-C2	-3.86	104.74	110.79
7	A	936	MAN	O2-C2-C3	-3.81	102.69	110.17
7	B	931	NAG	C1-C2-N2	-3.66	104.24	110.49
7	A	926	NAG	O6-C6-C5	-3.63	99.12	111.34
7	B	932	NAG	O5-C1-C2	-3.61	106.45	111.47
2	A	904	MAN	O3-C3-C4	-3.52	102.69	110.36
7	A	925	NAG	C1-C2-N2	-3.50	104.52	110.49

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	935	MAN	O5-C1-C2	-3.47	105.35	110.79
6	B	918	NAG	C1-O5-C5	-3.46	107.40	112.17
6	A	917	MAN	O6-C6-C5	-3.44	99.75	111.34
4	A	908	NAG	C3-C4-C5	-3.39	104.24	110.22
6	A	921	MAN	C3-C4-C5	-3.29	104.42	110.22
7	B	904	MAN	O2-C2-C3	-3.29	103.72	110.17
11	B	941	MAN	C1-O5-C5	-3.28	107.64	112.17
5	A	911	NAG	O5-C1-C2	-3.27	106.92	111.47
7	A	928	MAN	C1-C2-C3	-3.16	105.64	109.65
4	A	909	BMA	C1-C2-C3	-3.15	105.65	109.65
4	A	908	NAG	O5-C1-C2	-3.11	107.14	111.47
7	B	903	BMA	C1-C2-C3	-3.09	105.73	109.65
7	B	934	MAN	C1-O5-C5	-3.09	107.90	112.17
7	A	932	NAG	C1-C2-N2	-3.08	105.22	110.49
6	B	927	MAN	O5-C1-C2	-3.02	106.06	110.79
11	B	941	MAN	O6-C6-C5	-2.99	101.27	111.34
7	B	901	NAG	C2-N2-C7	-2.98	118.60	122.94
6	A	921	MAN	O4-C4-C3	-2.98	103.88	110.36
6	B	923	MAN	O3-C3-C4	-2.95	103.93	110.36
2	A	902	NAG	O4-C4-C5	-2.92	101.91	109.28
7	B	932	NAG	C2-N2-C7	-2.90	118.72	122.94
6	B	922	MAN	C6-C5-C4	-2.88	106.27	113.00
6	A	917	MAN	C1-C2-C3	-2.83	106.06	109.65
4	A	909	BMA	O4-C4-C3	-2.81	104.23	110.36
5	A	911	NAG	O7-C7-C8	-2.80	116.96	122.06
10	B	910	NAG	O5-C1-C2	-2.78	107.61	111.47
7	A	932	NAG	C6-C5-C4	-2.73	106.62	113.00
7	A	930	MAN	O5-C1-C2	-2.71	106.54	110.79
7	B	932	NAG	C1-C2-N2	-2.68	105.90	110.49
6	A	918	MAN	O2-C2-C3	-2.68	104.91	110.17
6	A	917	MAN	O3-C3-C4	-2.67	104.55	110.36
7	A	930	MAN	O6-C6-C5	-2.66	102.41	111.34
4	A	922	NAG	C1-C2-N2	-2.65	105.95	110.49
6	B	923	MAN	O6-C6-C5	-2.64	102.46	111.34
6	B	918	NAG	O4-C4-C5	-2.63	102.66	109.28
11	B	941	MAN	O4-C4-C5	-2.61	102.70	109.28
6	B	924	MAN	C3-C4-C5	-2.61	105.62	110.22
2	A	905	MAN	C2-C3-C4	-2.60	106.34	110.88
11	B	943	MAN	O6-C6-C5	-2.59	102.61	111.34
7	B	901	NAG	O7-C7-C8	-2.57	117.38	122.06
10	B	909	NAG	C3-C4-C5	-2.53	105.76	110.22
6	A	921	MAN	C1-C2-C3	-2.49	106.50	109.65

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	928	MAN	O4-C4-C3	-2.48	104.96	110.36
4	B	929	NAG	C1-C2-N2	-2.47	106.27	110.49
7	A	938	MAN	O3-C3-C2	-2.47	105.54	110.02
6	A	918	MAN	O6-C6-C5	-2.46	103.06	111.34
7	B	932	NAG	O7-C7-N2	-2.46	117.19	121.92
6	B	927	MAN	C6-C5-C4	-2.45	107.28	113.00
6	B	923	MAN	C1-C2-C3	-2.44	106.55	109.65
4	B	915	NAG	O5-C1-C2	-2.44	108.08	111.47
11	B	944	MAN	C6-C5-C4	-2.42	107.34	113.00
6	A	913	NAG	O7-C7-C8	-2.42	117.66	122.06
6	B	922	MAN	O6-C6-C5	-2.37	103.35	111.34
2	A	902	NAG	C3-C4-C5	-2.35	106.08	110.22
10	B	911	BMA	O6-C6-C5	-2.33	103.49	111.34
7	B	903	BMA	O4-C4-C3	-2.30	105.36	110.36
7	B	905	MAN	O6-C6-C5	-2.29	103.63	111.34
11	B	938	NAG	O3-C3-C2	-2.28	104.49	109.39
7	A	932	NAG	O5-C1-C2	-2.28	108.30	111.47
6	B	920	BMA	C2-C3-C4	-2.27	106.91	110.88
10	B	912	MAN	O5-C1-C2	-2.27	107.23	110.79
7	B	931	NAG	O3-C3-C2	-2.27	104.52	109.39
4	B	929	NAG	O5-C1-C2	-2.26	108.33	111.47
7	B	905	MAN	O3-C3-C4	-2.26	105.44	110.36
7	A	931	MAN	C1-O5-C5	-2.23	109.09	112.17
6	A	918	MAN	O3-C3-C4	-2.23	105.51	110.36
7	B	902	NAG	O4-C4-C5	-2.22	103.69	109.28
5	A	910	NAG	O7-C7-C8	-2.21	118.04	122.06
7	A	926	NAG	C3-C4-C5	-2.21	106.33	110.22
6	A	916	MAN	C1-C2-C3	-2.20	106.86	109.65
6	A	914	BMA	O2-C2-C1	-2.20	104.70	109.18
7	B	904	MAN	O3-C3-C4	-2.19	105.58	110.36
7	A	933	NAG	O4-C4-C3	-2.19	105.59	110.36
6	A	921	MAN	O5-C1-C2	-2.18	107.37	110.79
4	B	916	NAG	O6-C6-C5	-2.17	104.05	111.34
7	A	934	BMA	O4-C4-C5	-2.16	103.84	109.28
11	B	944	MAN	C2-C3-C4	-2.16	107.11	110.88
6	A	920	MAN	O6-C6-C5	-2.14	104.14	111.34
2	A	903	BMA	O2-C2-C3	-2.14	105.98	110.17
7	A	930	MAN	C6-C5-C4	-2.12	108.05	113.00
6	B	926	MAN	O6-C6-C5	-2.11	104.25	111.34
5	A	911	NAG	O6-C6-C5	-2.08	104.36	111.34
6	A	913	NAG	O3-C3-C4	-2.07	105.85	110.36
6	B	918	NAG	C2-N2-C7	-2.07	119.92	122.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	921	MAN	O4-C4-C3	-2.07	105.86	110.36
4	A	908	NAG	O6-C6-C5	-2.06	104.41	111.34
6	A	912	NAG	O7-C7-C8	-2.05	118.33	122.06
4	B	929	NAG	C8-C7-N2	-2.05	112.41	116.11
2	A	902	NAG	O6-C6-C5	-2.05	104.45	111.34
6	B	926	MAN	C6-C5-C4	-2.04	108.22	113.00
6	A	913	NAG	O4-C4-C3	-2.03	105.95	110.36
2	A	902	NAG	O7-C7-C8	-2.02	118.37	122.06
4	B	916	NAG	C3-C4-C5	-2.02	106.66	110.22
7	B	902	NAG	O3-C3-C4	2.01	114.72	110.36
6	B	921	MAN	O2-C2-C1	2.01	113.27	109.18
6	A	912	NAG	O5-C1-C2	2.01	114.28	111.47
6	A	916	MAN	C2-C3-C4	2.04	114.43	110.88
11	B	941	MAN	O2-C2-C1	2.04	113.33	109.18
6	B	918	NAG	C4-C3-C2	2.04	114.02	111.02
4	A	924	BMA	C3-C4-C5	2.05	113.83	110.22
7	B	931	NAG	C1-O5-C5	2.05	114.99	112.17
10	B	910	NAG	O3-C3-C4	2.10	114.93	110.36
11	B	945	MAN	C1-O5-C5	2.10	115.07	112.17
6	A	913	NAG	O3-C3-C2	2.11	113.90	109.39
11	B	940	BMA	O2-C2-C1	2.11	113.46	109.18
7	A	937	MAN	O3-C3-C4	2.13	115.00	110.36
2	A	905	MAN	C6-C5-C4	2.14	118.01	113.00
7	B	934	MAN	C2-C3-C4	2.16	114.64	110.88
5	A	911	NAG	O4-C4-C3	2.17	115.07	110.36
7	B	933	BMA	C1-O5-C5	2.17	115.16	112.17
6	A	920	MAN	O3-C3-C2	2.17	113.98	110.02
4	A	908	NAG	C6-C5-C4	2.18	118.11	113.00
7	B	931	NAG	O7-C7-C8	2.18	126.03	122.06
7	A	936	MAN	O2-C2-C1	2.19	113.62	109.18
7	A	929	MAN	O3-C3-C4	2.19	115.12	110.36
7	A	934	BMA	C6-C5-C4	2.20	118.15	113.00
4	B	916	NAG	C2-N2-C7	2.20	126.16	122.94
7	B	907	MAN	C3-C4-C5	2.23	114.14	110.22
5	A	911	NAG	O3-C3-C4	2.24	115.23	110.36
6	B	924	MAN	C1-O5-C5	2.24	115.26	112.17
4	B	917	BMA	C2-C3-C4	2.25	114.79	110.88
2	A	904	MAN	O5-C1-C2	2.26	114.33	110.79
7	B	931	NAG	C4-C3-C2	2.27	114.35	111.02
11	B	942	MAN	O5-C1-C2	2.28	114.37	110.79
6	B	920	BMA	O5-C1-C2	2.29	114.38	110.79
6	B	921	MAN	C1-O5-C5	2.29	115.33	112.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	NAG	O3-C3-C4	2.30	115.36	110.36
6	B	920	BMA	C1-O5-C5	2.32	115.37	112.17
7	B	934	MAN	O2-C2-C1	2.34	113.94	109.18
10	B	912	MAN	O3-C3-C2	2.34	114.29	110.02
7	B	932	NAG	C6-C5-C4	2.35	118.50	113.00
6	A	921	MAN	C1-O5-C5	2.35	115.41	112.17
11	B	944	MAN	O3-C3-C4	2.36	115.48	110.36
4	A	908	NAG	O3-C3-C4	2.36	115.49	110.36
2	A	905	MAN	O5-C1-C2	2.36	114.49	110.79
6	A	916	MAN	O2-C2-C1	2.38	114.02	109.18
7	B	935	MAN	C1-O5-C5	2.44	115.53	112.17
2	A	904	MAN	O2-C2-C3	2.45	114.99	110.17
11	B	944	MAN	C1-O5-C5	2.46	115.55	112.17
6	B	926	MAN	C3-C4-C5	2.48	114.58	110.22
4	A	909	BMA	O2-C2-C3	2.49	115.06	110.17
7	A	938	MAN	O2-C2-C3	2.49	115.06	110.17
7	A	936	MAN	C6-C5-C4	2.51	118.87	113.00
7	B	903	BMA	C3-C4-C5	2.58	114.76	110.22
11	B	945	MAN	C2-C3-C4	2.62	115.45	110.88
7	A	933	NAG	C4-C3-C2	2.63	114.87	111.02
7	A	926	NAG	O3-C3-C4	2.65	116.13	110.36
7	A	938	MAN	O5-C1-C2	2.66	114.95	110.79
7	A	938	MAN	C1-O5-C5	2.69	115.88	112.17
5	A	911	NAG	C8-C7-N2	2.71	121.00	116.11
2	A	905	MAN	O3-C3-C4	2.71	116.26	110.36
7	B	937	MAN	C1-O5-C5	2.76	115.97	112.17
5	A	910	NAG	C1-O5-C5	2.79	116.01	112.17
6	A	914	BMA	C1-C2-C3	2.79	113.19	109.65
4	B	930	BMA	C1-O5-C5	2.82	116.05	112.17
6	B	927	MAN	O4-C4-C3	2.88	116.63	110.36
2	A	904	MAN	C2-C3-C4	2.90	115.93	110.88
7	A	929	MAN	O3-C3-C2	2.92	115.34	110.02
4	B	917	BMA	C1-C2-C3	2.92	113.35	109.65
7	B	936	MAN	C1-O5-C5	2.94	116.22	112.17
10	B	913	MAN	O5-C1-C2	3.01	115.50	110.79
6	A	912	NAG	C8-C7-N2	3.02	121.56	116.11
6	A	920	MAN	C1-O5-C5	3.03	116.34	112.17
4	A	909	BMA	C2-C3-C4	3.03	116.16	110.88
7	A	934	BMA	O5-C1-C2	3.05	115.56	110.79
10	B	912	MAN	C3-C4-C5	3.05	115.59	110.22
6	A	915	MAN	O2-C2-C1	3.10	115.48	109.18
11	B	940	BMA	O2-C2-C3	3.11	116.28	110.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	913	NAG	C1-O5-C5	3.11	116.46	112.17
11	B	941	MAN	C2-C3-C4	3.15	116.38	110.88
2	A	904	MAN	C1-C2-C3	3.16	113.66	109.65
7	A	934	BMA	O2-C2-C3	3.16	116.38	110.17
4	B	917	BMA	C3-C4-C5	3.23	115.91	110.22
7	B	902	NAG	C1-O5-C5	3.25	116.65	112.17
4	A	924	BMA	C1-O5-C5	3.26	116.66	112.17
7	A	929	MAN	C1-O5-C5	3.28	116.69	112.17
4	A	924	BMA	O2-C2-C1	3.29	115.87	109.18
7	B	934	MAN	C3-C4-C5	3.34	116.09	110.22
4	A	907	NAG	C2-N2-C7	3.39	127.89	122.94
7	B	907	MAN	C1-C2-C3	3.44	114.01	109.65
4	A	907	NAG	C1-C2-N2	3.48	116.43	110.49
11	B	939	NAG	C1-O5-C5	3.48	116.97	112.17
11	B	940	BMA	C3-C4-C5	3.49	116.37	110.22
7	A	925	NAG	C1-O5-C5	3.54	117.04	112.17
2	A	903	BMA	O3-C3-C4	3.59	118.17	110.36
6	B	922	MAN	O3-C3-C2	3.61	116.59	110.02
5	A	911	NAG	C2-N2-C7	3.65	128.26	122.94
11	B	940	BMA	C2-C3-C4	3.67	117.28	110.88
4	B	928	NAG	C1-O5-C5	3.68	117.24	112.17
4	A	922	NAG	C1-O5-C5	3.69	117.25	112.17
2	A	903	BMA	C1-C2-C3	3.70	114.34	109.65
4	A	909	BMA	O6-C6-C5	3.71	123.84	111.34
4	B	917	BMA	O5-C1-C2	3.74	116.64	110.79
10	B	912	MAN	C2-C3-C4	3.83	117.56	110.88
7	A	937	MAN	C1-O5-C5	3.85	117.47	112.17
10	B	910	NAG	C6-C5-C4	3.91	122.15	113.00
10	B	912	MAN	O2-C2-C3	3.93	117.90	110.17
4	B	929	NAG	C2-N2-C7	3.99	128.76	122.94
6	B	926	MAN	C1-O5-C5	3.99	117.67	112.17
7	B	907	MAN	O6-C6-C5	4.00	124.79	111.34
10	B	909	NAG	C1-O5-C5	4.03	117.72	112.17
7	A	938	MAN	C3-C4-C5	4.05	117.34	110.22
11	B	945	MAN	C3-C4-C5	4.05	117.35	110.22
4	B	915	NAG	C1-O5-C5	4.06	117.77	112.17
7	B	907	MAN	C6-C5-C4	4.16	122.73	113.00
11	B	941	MAN	C3-C4-C5	4.16	117.54	110.22
4	A	909	BMA	C3-C4-C5	4.17	117.56	110.22
10	B	911	BMA	C1-O5-C5	4.20	117.96	112.17
2	A	904	MAN	C3-C4-C5	4.25	117.71	110.22
7	A	938	MAN	C2-C3-C4	4.26	118.30	110.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	907	MAN	O3-C3-C4	4.33	119.77	110.36
7	A	934	BMA	O3-C3-C4	4.39	119.92	110.36
10	B	913	MAN	C3-C4-C5	4.41	118.00	110.22
2	A	904	MAN	O3-C3-C2	4.54	118.29	110.02
11	B	942	MAN	C1-C2-C3	4.55	115.42	109.65
6	B	922	MAN	O2-C2-C3	4.57	119.14	110.17
6	B	922	MAN	C1-O5-C5	4.57	118.46	112.17
4	A	923	NAG	C4-C3-C2	4.63	117.80	111.02
7	A	932	NAG	C1-O5-C5	4.82	118.81	112.17
6	A	917	MAN	C1-O5-C5	4.84	118.84	112.17
6	B	923	MAN	C1-O5-C5	4.98	119.02	112.17
6	A	916	MAN	C1-O5-C5	5.00	119.05	112.17
6	A	916	MAN	O2-C2-C3	5.10	120.19	110.17
7	B	935	MAN	O3-C3-C2	5.10	119.30	110.02
6	B	927	MAN	C1-O5-C5	5.24	119.39	112.17
7	A	934	BMA	C1-O5-C5	5.34	119.53	112.17
6	A	921	MAN	O3-C3-C2	5.37	119.80	110.02
11	B	943	MAN	C1-O5-C5	5.66	119.97	112.17
7	A	930	MAN	C1-O5-C5	5.85	120.22	112.17
7	B	901	NAG	C1-O5-C5	5.96	120.38	112.17
11	B	938	NAG	C1-O5-C5	6.31	120.87	112.17
2	A	905	MAN	C1-O5-C5	6.37	120.95	112.17
4	B	917	BMA	C1-O5-C5	6.70	121.40	112.17
10	B	913	MAN	C1-O5-C5	7.27	122.18	112.17
4	A	909	BMA	C1-O5-C5	7.38	122.33	112.17
2	A	904	MAN	C1-O5-C5	8.18	123.44	112.17
11	B	940	BMA	C1-O5-C5	8.72	124.18	112.17

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
7	B	933	BMA	1	0
11	B	940	BMA	2	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	942	MAN	1	0

## 5.6 Ligand geometry

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	0.92	1 (7%)	15,19,21	1.42	3 (20%)
3	NAG	A	939	1	14,14,15	0.60	0	15,19,21	1.85	3 (20%)
8	MRD	A	940	-	7,7,7	0.53	0	9,10,10	0.42	0
8	MRD	A	941	-	7,7,7	0.76	0	9,10,10	0.67	0
9	BGC	A	942	-	12,12,12	0.78	0	17,17,17	1.03	1 (5%)
9	BGC	A	943	-	12,12,12	0.97	1 (8%)	17,17,17	2.61	10 (58%)
3	NAG	B	908	1	14,14,15	0.80	0	15,19,21	1.68	4 (26%)
3	NAG	B	946	1	14,14,15	0.58	0	15,19,21	1.75	2 (13%)
3	NAG	B	947	1	14,14,15	0.73	0	15,19,21	1.20	2 (13%)
8	MRD	B	948	-	7,7,7	0.60	0	9,10,10	0.73	0
8	MRD	B	949	-	7,7,7	0.51	0	9,10,10	0.73	0
9	BGC	B	950	-	12,12,12	0.83	0	17,17,17	1.23	2 (11%)
9	BGC	B	951	-	12,12,12	1.05	1 (8%)	17,17,17	2.63	9 (52%)

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
8	MRD	A	940	-	-	0/5/5/5	0/0/0/0
8	MRD	A	941	-	-	0/5/5/5	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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)
9	A	943	BGC	C1-C2	2.03	1.56	1.52
3	A	906	NAG	C1-C2	2.04	1.55	1.52
9	B	951	BGC	C1-C2	2.64	1.58	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	946	NAG	O5-C1-C2	-4.49	105.22	111.47
9	A	943	BGC	C3-C4-C5	-4.31	102.62	110.22
9	B	951	BGC	C3-C4-C5	-3.41	104.21	110.22
9	B	951	BGC	O1-C1-O5	-3.41	100.12	110.20
3	A	939	NAG	C3-C4-C5	-3.22	104.54	110.22
9	A	943	BGC	C4-C3-C2	-3.18	105.23	110.84
9	A	943	BGC	O2-C2-C3	-3.12	103.56	110.36
9	B	951	BGC	C4-C3-C2	-2.99	105.56	110.84
9	A	943	BGC	O1-C1-O5	-2.89	101.65	110.20
9	B	950	BGC	O1-C1-O5	-2.64	102.38	110.20
3	A	906	NAG	O7-C7-C8	-2.39	117.70	122.06
9	A	942	BGC	O3-C3-C2	-2.39	105.16	110.36
9	A	943	BGC	O5-C5-C4	-2.35	105.33	109.66
3	B	947	NAG	O4-C4-C3	-2.18	105.62	110.36
3	B	947	NAG	C2-N2-C7	-2.17	119.78	122.94
9	B	951	BGC	O2-C2-C3	-2.16	105.67	110.36
3	B	908	NAG	O7-C7-N2	-2.15	117.77	121.92
3	A	906	NAG	C6-C5-C4	-2.02	108.27	113.00
9	A	943	BGC	O5-C5-C6	2.26	111.82	106.41
3	A	906	NAG	C1-C2-N2	2.36	114.53	110.49
9	A	943	BGC	O3-C3-C4	2.40	115.59	110.36
9	B	951	BGC	O3-C3-C4	2.52	115.85	110.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C2-N2-C7	2.63	126.78	122.94
9	A	943	BGC	O4-C4-C5	2.92	116.65	109.28
9	B	951	BGC	O5-C5-C6	2.98	113.55	106.41
3	B	908	NAG	C1-O5-C5	3.01	116.32	112.17
9	B	950	BGC	C1-O5-C5	3.13	119.03	113.39
9	B	951	BGC	O2-C2-C1	3.23	116.46	109.75
3	B	908	NAG	C8-C7-N2	3.28	122.03	116.11
3	A	939	NAG	C1-O5-C5	3.30	116.71	112.17
9	A	943	BGC	C6-C5-C4	3.30	120.73	113.00
3	B	946	NAG	C4-C3-C2	3.36	115.94	111.02
3	A	939	NAG	O5-C1-C2	3.63	116.52	111.47
9	B	951	BGC	C6-C5-C4	3.71	121.68	113.00
9	A	943	BGC	O5-C1-C2	4.84	118.06	110.04
9	B	951	BGC	O5-C1-C2	5.32	118.86	110.04

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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	834/841 (99%)	-0.37	11 (1%) 77 81	13, 22, 37, 67	0
1	B	832/841 (98%)	-0.52	1 (0%) 95 97	12, 19, 32, 62	0
All	All	1666/1682 (99%)	-0.45	12 (0%) 87 90	12, 20, 35, 67	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	LEU	3.1
1	A	110	VAL	3.0
1	A	95	LEU	2.8
1	A	109	GLY	2.4
1	A	144	ALA	2.4
1	B	141	LEU	2.2
1	A	245	MET	2.2
1	A	94	PRO	2.2
1	A	609	ASP	2.2
1	A	808	SER	2.2
1	A	141	LEU	2.1
1	A	698	GLU	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<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	A	925	14/15	0.95	0.12	6.38	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	1.88	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
7	BMA	A	927	11/12	0.91	0.17	-	32,38,45,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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 [i](#)

There are no such residues in this entry.