Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:29 PM GMT

PDB ID	:	4IIF
Title	:	Crystal structure of beta-glucosidase 1 from Aspergillus aculeatus in complex with castanospermine
Authors	:	Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on	:	2012-12-20
Resolution	:	2.45 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 ⓘ symbol.

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

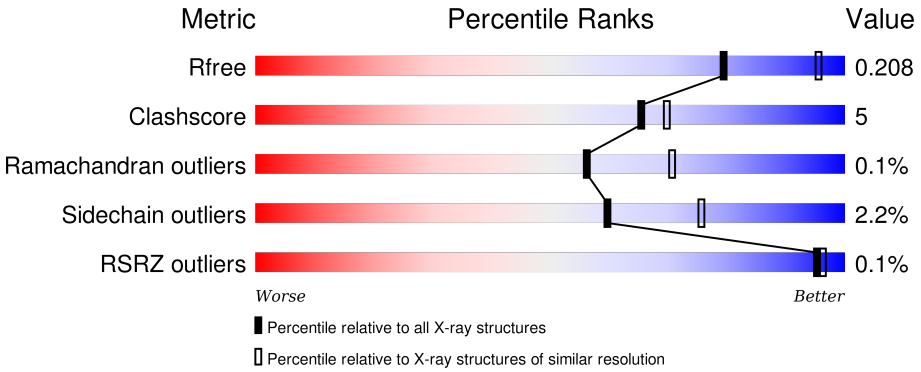
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	89% 9%
1	B	841	87% 11%

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
10	MPD	A	939	-	-	-	X
10	MPD	A	940	-	-	-	X
4	NAG	A	907	-	-	-	X
7	NAG	A	924	-	-	-	X
7	MAN	A	930	-	-	-	X
7	MAN	B	906	-	-	-	X
9	MRD	B	945	-	-	-	X
9	MRD	B	946	-	-	-	X
9	MRD	B	947	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14647 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.

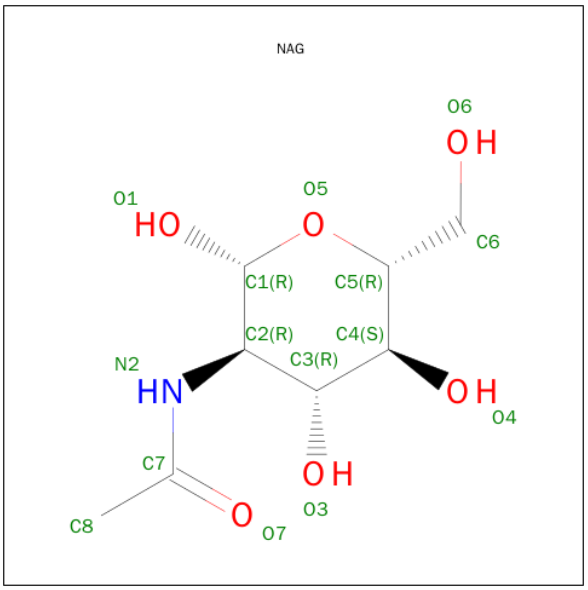
- Molecule 1 is a protein called Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6378	4026	1095	1239	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 (4-MER).

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

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



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

- 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
5	B	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

Continued on next page...

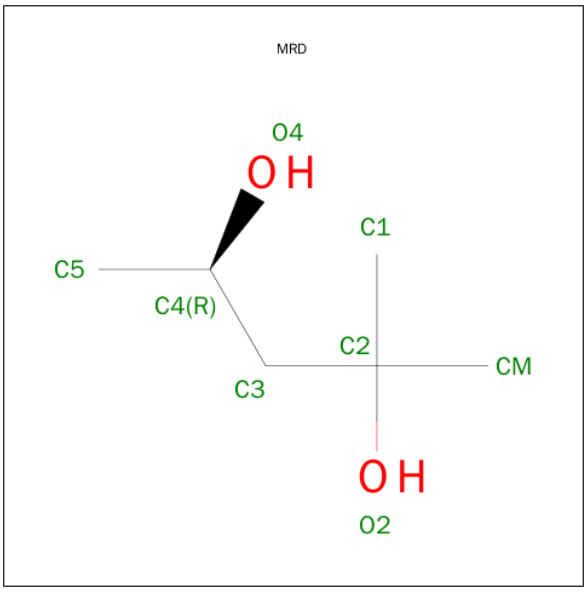
Continued from previous page...

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

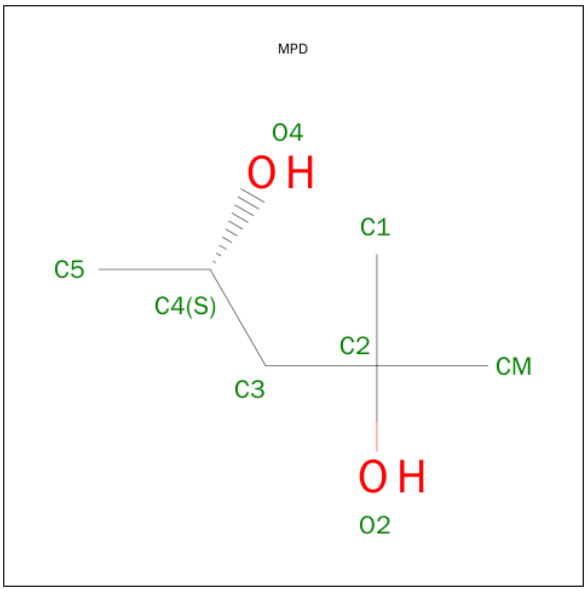
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	6	Total C N O 72 40 2 30	0	0

- Molecule 9 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



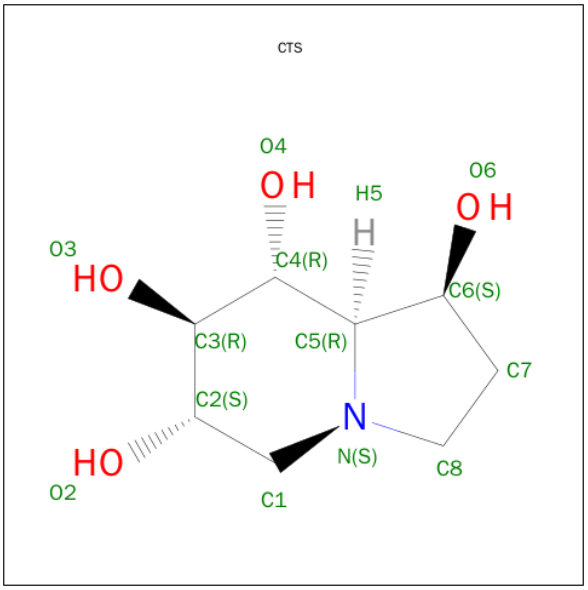
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 8 6 2	0	0
9	B	1	Total C O 8 6 2	0	0
9	B	1	Total C O 8 6 2	0	0
9	B	1	Total C O 8 6 2	0	0

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 11 is CASTANOSPERMINE (three-letter code: CTS) (formula: $C_8H_{15}NO_4$).



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

- Molecule 12 is a polymer of unknown type called SUGAR (8-MER).

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

- Molecule 13 is water.

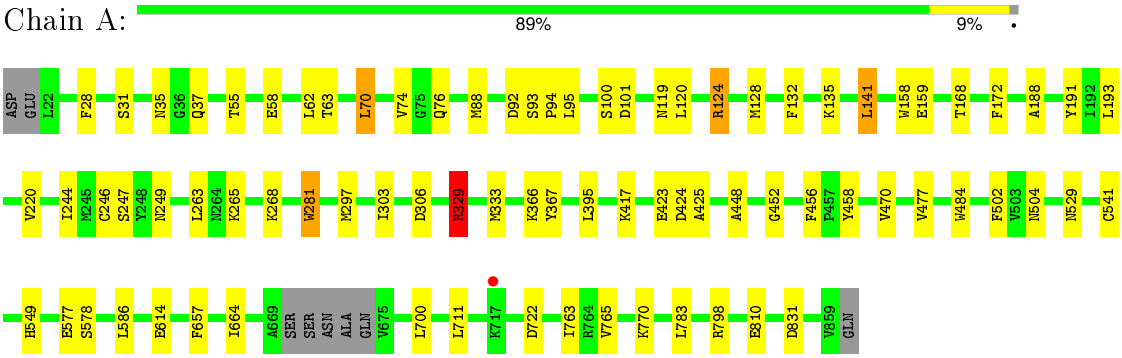
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	380	Total	O	0	0
			380	380		
13	B	450	Total	O	0	0
			450	450		

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.

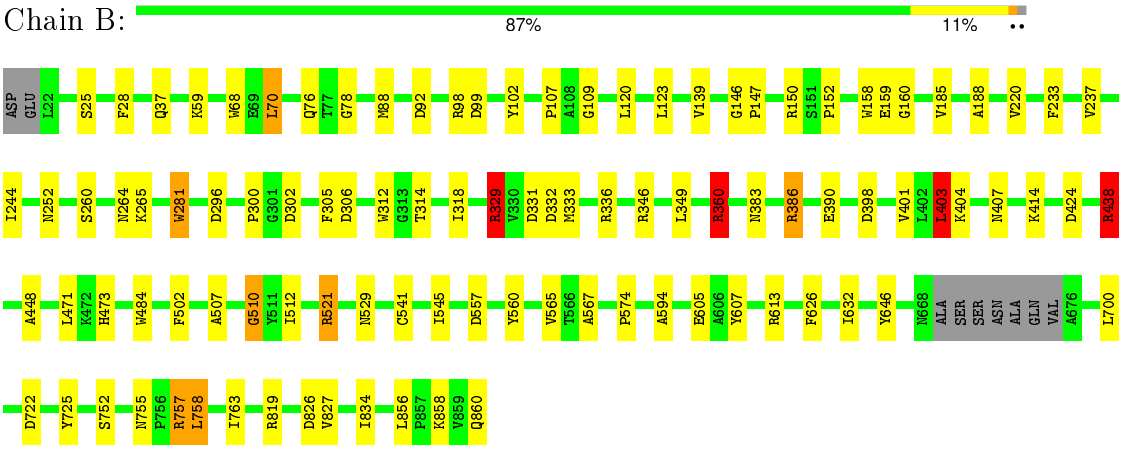
- Molecule 1: Beta-glucosidase 1

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	82.38Å 122.24Å 222.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.45 49.08 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.08-2.45) 99.4 (49.08-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.154 , 0.205 0.157 , 0.208	Depositor DCC
R_{free} test set	4152 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.9	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 82518 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14647	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: MPD, BMA, NAG, CTS, MRD, 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	0.83	3/6541 (0.0%)	0.89	8/8918 (0.1%)
1	B	0.89	2/6538 (0.0%)	0.95	17/8913 (0.2%)
All	All	0.86	5/13079 (0.0%)	0.92	25/17831 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	CYS	CB-SG	6.83	1.93	1.82
1	B	541	CYS	CB-SG	5.52	1.91	1.82
1	B	541	CYS	CA-CB	5.48	1.66	1.53
1	A	423	GLU	CD-OE1	5.33	1.31	1.25
1	A	541	CYS	CA-CB	5.08	1.65	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	ARG	NE-CZ-NH2	-14.40	113.10	120.30
1	B	521	ARG	NE-CZ-NH2	-13.86	113.37	120.30
1	B	329	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	B	521	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	B	438	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	B	329	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	A	329	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	70	LEU	CA-CB-CG	-8.89	94.85	115.30
1	B	360	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	B	70	LEU	CA-CB-CG	-8.56	95.61	115.30
1	B	826	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	124	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	831	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	541	CYS	N-CA-CB	6.90	123.02	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	438	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	798	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	360	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	101	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	329	ARG	CG-CD-NE	-6.02	99.15	111.80
1	B	438	ARG	CG-CD-NE	-5.66	99.92	111.80
1	B	150	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	403	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	403	LEU	CB-CG-CD1	5.42	120.22	111.00
1	A	722	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	510	GLY	N-CA-C	5.12	125.90	113.10

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	6378	0	6089	52	0
1	B	6375	0	6082	75	0
2	A	50	0	43	0	0
2	B	50	0	43	3	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	68	0	0
4	B	39	0	34	0	0
5	A	28	0	25	2	0
5	B	28	0	25	0	0
6	A	116	0	97	0	0
6	B	116	0	97	0	0
7	A	83	0	70	2	0
7	B	166	0	140	3	0
8	A	72	0	61	0	0
9	A	8	0	14	1	0
9	B	24	0	42	6	0
10	A	16	0	28	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	13	0	15	2	0
11	B	13	0	15	2	0
12	B	94	0	79	0	0
13	A	380	0	0	4	0
13	B	450	0	0	7	0
All	All	14647	0	13132	135	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 5.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LEU:HD23	1:B:758:LEU:H	1.22	1.02
1:B:755:ASN:O	1:B:758:LEU:HD23	1.61	0.99
9:B:946:MRD:H1C2	9:B:946:MRD:H5C3	1.47	0.95
1:A:63:THR:HG21	1:A:333:MET:HE2	1.51	0.90
9:B:946:MRD:H1C2	9:B:946:MRD:C5	2.01	0.89
1:B:755:ASN:O	1:B:758:LEU:CD2	2.22	0.87
1:B:758:LEU:HD23	1:B:758:LEU:N	1.90	0.85
1:A:95:LEU:HA	1:A:128:MET:HE1	1.59	0.83
1:B:755:ASN:HB3	1:B:758:LEU:CD2	2.19	0.72
1:B:312:TRP:CH2	1:B:333:MET:HE1	2.24	0.72
1:A:63:THR:CG2	1:A:333:MET:HE2	2.20	0.72
1:A:484:TRP:CE2	7:A:926:BMA:H62	2.26	0.70
1:B:92:ASP:OD2	11:B:948:CTS:O6	2.08	0.69
1:A:124:ARG:CZ	1:A:128:MET:HE3	2.24	0.67
1:B:281:TRP:HB2	11:B:948:CTS:H81	1.75	0.67
1:A:303:ILE:HG21	5:A:910:NAG:H81	1.77	0.65
1:B:755:ASN:HB3	1:B:758:LEU:HD21	1.79	0.64
1:A:770:LYS:HG3	1:A:810:GLU:HG3	1.79	0.64
1:A:159:GLU:HG3	13:A:1021:HOH:O	1.97	0.62
1:B:755:ASN:OD1	1:B:757:ARG:HB2	1.98	0.62
1:B:758:LEU:CD2	1:B:758:LEU:N	2.63	0.61
1:B:312:TRP:CZ3	1:B:333:MET:CE	2.85	0.60
1:B:349:LEU:HD22	13:B:1205:HOH:O	2.02	0.59
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.86	0.57
1:B:386:ARG:HD2	13:B:1314:HOH:O	2.05	0.57
1:B:312:TRP:CZ3	1:B:333:MET:HE1	2.39	0.57
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.86	0.57
1:A:159:GLU:CG	13:A:1021:HOH:O	2.51	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:OE1	1:A:614:GLU:HA	2.06	0.56
1:B:484:TRP:CE2	7:B:930:BMA:H62	2.42	0.55
1:B:296:ASP:HA	1:B:333:MET:HG2	1.89	0.55
1:A:63:THR:HB	1:A:333:MET:CE	2.38	0.54
1:B:312:TRP:CH2	1:B:333:MET:CE	2.90	0.54
1:B:99:ASP:O	1:B:360:ARG:NH2	2.41	0.54
1:B:260:SER:O	1:B:264:ASN:HB2	2.07	0.53
1:A:92:ASP:OD2	11:A:941:CTS:O6	2.21	0.53
1:B:139:VAL:HG22	1:B:185:VAL:HB	1.91	0.53
1:B:424:ASP:HB3	1:B:502:PHE:HB3	1.92	0.52
1:B:755:ASN:O	1:B:758:LEU:HD21	2.09	0.51
1:B:827:VAL:HG11	2:B:910:NAG:O3	2.11	0.51
1:A:93:SER:HB2	1:A:452:GLY:HA2	1.92	0.51
1:A:424:ASP:HB3	1:A:502:PHE:HB3	1.92	0.51
1:B:401:VAL:HG12	1:B:403:LEU:HD13	1.93	0.51
1:A:168:THR:O	1:A:172:PHE:HB2	2.11	0.50
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.41	0.50
1:B:755:ASN:HB3	1:B:758:LEU:HD22	1.94	0.49
1:A:28:PHE:CG	1:A:265:LYS:HB2	2.48	0.49
1:B:107:PRO:HG3	1:B:574:PRO:O	2.13	0.49
9:B:947:MRD:O2	9:B:947:MRD:H5C3	2.13	0.49
1:A:281:TRP:CG	11:A:941:CTS:H72	2.48	0.49
1:A:141:LEU:HD21	1:A:281:TRP:CH2	2.48	0.48
1:B:146:GLY:HA2	1:B:147:PRO:C	2.34	0.48
1:B:763:ILE:HD13	1:B:856:LEU:HD22	1.95	0.48
1:B:158:TRP:CE2	1:B:448:ALA:HB3	2.49	0.48
1:B:403:LEU:HG	1:B:646:TYR:CD2	2.48	0.47
1:A:35:ASN:OD1	1:A:37:GLN:HB2	2.15	0.47
1:A:63:THR:CG2	1:A:333:MET:CE	2.92	0.47
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.49	0.47
1:B:448:ALA:HB1	1:B:507:ALA:O	2.14	0.47
1:A:664:ILE:CD1	1:A:765:VAL:HG22	2.44	0.47
9:A:938:MRD:O2	9:A:938:MRD:H5C3	2.14	0.47
5:A:910:NAG:H83	5:A:910:NAG:H3	1.97	0.46
1:A:191:TYR:O	1:A:246:CYS:HA	2.16	0.46
1:B:102:TYR:HB3	1:B:383:ASN:HA	1.98	0.46
1:B:507:ALA:HB2	1:B:521:ARG:HG3	1.98	0.46
9:B:946:MRD:H4	9:B:946:MRD:H1C1	1.65	0.46
1:B:605:GLU:HB2	13:B:1095:HOH:O	2.15	0.46
1:A:306:ASP:HA	13:A:1012:HOH:O	2.16	0.46
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:NZ	1:B:331:ASP:OD1	2.39	0.45
1:A:128:MET:O	1:A:132:PHE:HD2	1.98	0.45
1:A:247:SER:HB2	1:A:249:ASN:OD1	2.17	0.45
1:B:545:ILE:HG12	1:B:567:ALA:HB3	1.97	0.45
1:A:93:SER:HB2	1:A:94:PRO:CD	2.47	0.45
1:B:827:VAL:CG1	2:B:910:NAG:O3	2.65	0.45
1:A:124:ARG:CZ	1:A:128:MET:CE	2.94	0.45
1:A:577:GLU:O	1:A:578:SER:C	2.56	0.45
1:A:664:ILE:HD12	1:A:765:VAL:HG22	1.98	0.44
1:B:159:GLU:HG3	13:B:1015:HOH:O	2.17	0.44
1:A:188:ALA:HB3	1:A:244:ILE:HD13	1.99	0.44
1:B:28:PHE:CG	1:B:265:LYS:HB2	2.52	0.44
1:B:819:ARG:HG3	1:B:834:ILE:HD11	1.99	0.44
1:B:68:TRP:O	1:B:306:ASP:OD1	2.36	0.44
1:B:37:GLN:NE2	1:B:752:SER:HB2	2.32	0.44
1:B:473:HIS:HE1	13:B:1122:HOH:O	1.99	0.44
1:A:484:TRP:CD2	7:A:926:BMA:H62	2.53	0.44
1:B:346:ARG:HA	1:B:346:ARG:HD2	1.90	0.44
1:B:233:PHE:O	1:B:237:VAL:HG23	2.18	0.43
1:B:438:ARG:HA	1:B:438:ARG:HD3	1.59	0.43
1:A:159:GLU:OE2	1:A:452:GLY:HA3	2.18	0.43
1:B:78:GLY:HA3	7:B:901:NAG:H62	1.99	0.43
1:B:404:LYS:NZ	1:B:565:VAL:O	2.42	0.43
1:A:366:LYS:HE2	1:A:367:TYR:OH	2.19	0.43
1:B:755:ASN:CA	1:B:758:LEU:HD21	2.48	0.43
1:B:300:PRO:HG2	1:B:302:ASP:OD1	2.19	0.43
1:A:329:ARG:HA	1:A:329:ARG:HD2	1.72	0.43
1:A:657:PHE:HA	1:A:770:LYS:O	2.19	0.43
1:A:100:SER:OG	1:A:135:LYS:HE3	2.18	0.43
1:B:109:GLY:HA3	1:B:160:GLY:O	2.19	0.43
1:B:755:ASN:CB	1:B:758:LEU:HD21	2.46	0.43
1:B:819:ARG:NH2	1:B:860:GLN:O	2.51	0.43
1:B:332:ASP:O	1:B:336:ARG:HG3	2.19	0.43
1:B:314:THR:HG22	1:B:318:ILE:HD12	2.01	0.42
1:B:722:ASP:HB3	1:B:725:TYR:HB2	2.01	0.42
1:B:37:GLN:HE22	1:B:752:SER:HB2	1.84	0.42
1:B:76:GLN:HA	1:B:88:MET:O	2.20	0.42
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.54	0.42
1:B:557:ASP:HA	1:B:560:TYR:CD2	2.53	0.42
1:B:438:ARG:HD3	13:B:1102:HOH:O	2.20	0.42
1:A:55:THR:OG1	1:A:58:GLU:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:HG11	1:A:477:VAL:HB	2.02	0.42
2:B:909:NAG:H62	9:B:947:MRD:H5C1	2.02	0.42
1:A:63:THR:O	1:A:297:MET:HA	2.19	0.42
1:A:263:LEU:O	1:A:268:LYS:HG3	2.20	0.41
10:A:939:MPD:HM1	10:A:939:MPD:O4	2.19	0.41
1:B:471:LEU:HA	1:B:471:LEU:HD23	1.85	0.41
1:B:92:ASP:HB2	1:B:98:ARG:HB2	2.00	0.41
1:A:504:ASN:HA	1:A:549:HIS:O	2.20	0.41
1:B:512:ILE:HG21	1:B:512:ILE:HD13	1.83	0.41
1:A:456:PHE:HB3	1:A:458:TYR:O	2.21	0.41
1:A:783:LEU:C	1:A:783:LEU:HD23	2.41	0.41
1:A:425:ALA:HB2	1:A:502:PHE:CD2	2.55	0.41
1:A:31:SER:HB3	1:A:329:ARG:HD3	2.01	0.41
1:A:76:GLN:HA	1:A:88:MET:O	2.21	0.41
1:B:78:GLY:CA	7:B:901:NAG:H62	2.51	0.41
1:B:305:PHE:HE2	9:B:945:MRD:H1C2	1.86	0.41
1:B:152:PRO:HG3	1:B:607:TYR:CG	2.56	0.41
1:B:398:ASP:O	1:B:594:ALA:HB2	2.20	0.41
1:B:613:ARG:NH1	13:B:1051:HOH:O	2.26	0.40
1:B:329:ARG:HD2	1:B:329:ARG:HA	1.71	0.40
1:A:417:LYS:HE3	13:A:1166:HOH:O	2.21	0.40
1:B:25:SER:HB2	1:B:252:ASN:HB2	2.03	0.40
1:B:757:ARG:HH11	1:B:757:ARG:CG	2.34	0.40
1:A:158:TRP:CE2	1:A:448:ALA:HB3	2.56	0.40
1:A:63:THR:CB	1:A:333:MET:CE	3.00	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	829/841 (99%)	798 (96%)	31 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	828/841 (98%)	797 (96%)	30 (4%)	1 (0%)	56 71
All	All	1657/1682 (98%)	1595 (96%)	61 (4%)	1 (0%)	56 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	510	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	670/677 (99%)	657 (98%)	13 (2%)	65 79
1	B	670/677 (99%)	653 (98%)	17 (2%)	55 72
All	All	1340/1354 (99%)	1310 (98%)	30 (2%)	60 75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	70	LEU
1	A	74	VAL
1	A	119	ASN
1	A	120	LEU
1	A	141	LEU
1	A	281	TRP
1	A	329	ARG
1	A	395	LEU
1	A	586	LEU
1	A	700	LEU
1	A	711	LEU
1	A	763	ILE
1	B	70	LEU
1	B	120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	123	LEU
1	B	281	TRP
1	B	329	ARG
1	B	360	ARG
1	B	386	ARG
1	B	390	GLU
1	B	403	LEU
1	B	407	ASN
1	B	414	LYS
1	B	438	ARG
1	B	632	ILE
1	B	700	LEU
1	B	757	ARG
1	B	758	LEU
1	B	858	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	ASN
1	B	37	GLN
1	B	473	HIS

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)

76 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	901	1,2	14,14,15	0.75	0	15,19,21	0.94	0
2	NAG	A	902	2	14,14,15	0.71	0	15,19,21	1.77	2 (13%)
2	BMA	A	903	2	11,11,12	1.17	0	14,15,17	2.65	6 (42%)
2	MAN	A	904	2	11,11,12	0.92	0	14,15,17	2.83	7 (50%)
4	NAG	A	906	1,4	14,14,15	1.03	1 (7%)	15,19,21	0.96	1 (6%)
4	NAG	A	907	4	14,14,15	0.63	0	15,19,21	1.42	1 (6%)
4	BMA	A	908	4	11,11,12	0.77	0	14,15,17	2.74	10 (71%)
5	NAG	A	909	1,5	14,14,15	0.61	0	15,19,21	1.81	2 (13%)
5	NAG	A	910	5	14,14,15	0.65	1 (7%)	15,19,21	1.69	4 (26%)
6	NAG	A	911	1,6	14,14,15	0.71	0	15,19,21	0.95	0
6	NAG	A	912	6	14,14,15	0.96	1 (7%)	15,19,21	1.53	3 (20%)
6	BMA	A	913	6	11,11,12	1.03	1 (9%)	14,15,17	1.12	1 (7%)
6	MAN	A	914	6	11,11,12	0.84	0	14,15,17	1.09	2 (14%)
6	MAN	A	915	6	11,11,12	1.05	1 (9%)	14,15,17	1.71	2 (14%)
6	MAN	A	916	6	11,11,12	0.68	0	14,15,17	1.60	3 (21%)
6	MAN	A	917	6	11,11,12	1.01	1 (9%)	14,15,17	1.58	5 (35%)
6	MAN	A	918	6	11,11,12	0.73	0	14,15,17	1.74	3 (21%)
6	MAN	A	919	6	11,11,12	1.17	1 (9%)	14,15,17	1.98	4 (28%)
6	MAN	A	920	6	11,11,12	0.77	0	14,15,17	1.44	3 (21%)
4	NAG	A	921	1,4	14,14,15	0.74	0	15,19,21	1.73	1 (6%)
4	NAG	A	922	4	14,14,15	0.80	0	15,19,21	1.55	4 (26%)
4	BMA	A	923	4	11,11,12	0.81	0	14,15,17	1.78	4 (28%)
7	NAG	A	924	1,7	14,14,15	0.71	0	15,19,21	1.70	4 (26%)
7	NAG	A	925	7	14,14,15	0.95	1 (7%)	15,19,21	2.14	4 (26%)
7	BMA	A	926	7	11,11,12	0.76	0	14,15,17	1.77	3 (21%)
7	MAN	A	927	7	11,11,12	0.75	0	14,15,17	2.06	4 (28%)
7	MAN	A	928	7	11,11,12	1.04	1 (9%)	14,15,17	1.78	4 (28%)
7	MAN	A	929	7	11,11,12	0.82	1 (9%)	14,15,17	2.40	6 (42%)
7	MAN	A	930	7	11,11,12	0.83	0	14,15,17	1.57	3 (21%)
8	NAG	A	931	1,8	14,14,15	0.89	1 (7%)	15,19,21	2.11	3 (20%)
8	NAG	A	932	8	14,14,15	0.85	1 (7%)	15,19,21	1.44	2 (13%)
8	BMA	A	933	8	11,11,12	0.66	0	14,15,17	1.97	4 (28%)
8	MAN	A	934	8	11,11,12	1.10	0	14,15,17	2.24	9 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	A	935	8	11,11,12	1.25	1 (9%)	14,15,17	2.13	6 (42%)
8	MAN	A	936	8	11,11,12	0.79	0	14,15,17	1.43	3 (21%)
7	NAG	B	901	1,7	14,14,15	1.15	1 (7%)	15,19,21	1.54	2 (13%)
7	NAG	B	902	7	14,14,15	0.84	0	15,19,21	1.69	3 (20%)
7	BMA	B	903	7	11,11,12	0.84	0	14,15,17	1.66	2 (14%)
7	MAN	B	904	7	11,11,12	0.74	0	14,15,17	1.14	2 (14%)
7	MAN	B	905	7	11,11,12	0.73	0	14,15,17	1.55	2 (14%)
7	MAN	B	906	7	11,11,12	0.73	0	14,15,17	1.21	3 (21%)
7	MAN	B	907	7	11,11,12	1.00	1 (9%)	14,15,17	2.12	6 (42%)
2	NAG	B	909	1,2	14,14,15	1.14	2 (14%)	15,19,21	1.66	4 (26%)
2	NAG	B	910	2	14,14,15	0.77	0	15,19,21	0.91	0
2	BMA	B	911	2	11,11,12	0.78	0	14,15,17	1.27	2 (14%)
2	MAN	B	912	2	11,11,12	1.28	1 (9%)	14,15,17	2.20	5 (35%)
5	NAG	B	913	1,5	14,14,15	0.92	0	15,19,21	1.61	3 (20%)
5	NAG	B	914	5	14,14,15	0.77	0	15,19,21	1.83	4 (26%)
6	NAG	B	915	1,6	14,14,15	0.79	0	15,19,21	1.83	4 (26%)
6	NAG	B	916	6	14,14,15	0.76	0	15,19,21	0.98	0
6	BMA	B	917	6	11,11,12	1.08	1 (9%)	14,15,17	1.29	2 (14%)
6	MAN	B	918	6	11,11,12	0.64	0	14,15,17	1.78	4 (28%)
6	MAN	B	919	6	11,11,12	1.04	1 (9%)	14,15,17	2.53	6 (42%)
6	MAN	B	920	6	11,11,12	0.74	0	14,15,17	2.17	6 (42%)
6	MAN	B	921	6	11,11,12	0.90	0	14,15,17	2.10	4 (28%)
6	MAN	B	922	6	11,11,12	0.84	0	14,15,17	1.60	2 (14%)
6	MAN	B	923	6	11,11,12	0.85	0	14,15,17	1.64	2 (14%)
6	MAN	B	924	6	11,11,12	0.79	0	14,15,17	1.77	2 (14%)
4	NAG	B	925	1,4	14,14,15	0.80	0	15,19,21	1.51	4 (26%)
4	NAG	B	926	4	14,14,15	0.97	1 (7%)	15,19,21	1.12	1 (6%)
4	BMA	B	927	4	11,11,12	0.77	0	14,15,17	2.22	3 (21%)
7	NAG	B	928	1,7	14,14,15	1.05	1 (7%)	15,19,21	1.34	1 (6%)
7	NAG	B	929	7	14,14,15	1.11	2 (14%)	15,19,21	1.68	2 (13%)
7	BMA	B	930	7	11,11,12	0.66	0	14,15,17	1.31	2 (14%)
7	MAN	B	931	7	11,11,12	0.93	0	14,15,17	2.42	5 (35%)
7	MAN	B	932	7	11,11,12	1.07	0	14,15,17	1.85	3 (21%)
7	MAN	B	933	7	11,11,12	0.69	0	14,15,17	1.76	3 (21%)
7	MAN	B	934	7	11,11,12	0.73	0	14,15,17	2.04	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	NAG	B	935	1,12	14,14,15	0.96	1 (7%)	15,19,21	1.79	3 (20%)
12	NAG	B	936	12	14,14,15	0.86	1 (7%)	15,19,21	1.72	3 (20%)
12	BMA	B	937	12	11,11,12	1.08	1 (9%)	14,15,17	1.59	2 (14%)
12	MAN	B	938	12	11,11,12	0.94	0	14,15,17	2.24	7 (50%)
12	MAN	B	939	12	11,11,12	0.65	0	14,15,17	1.86	4 (28%)
12	MAN	B	940	12	11,11,12	0.85	0	14,15,17	1.54	2 (14%)
12	MAN	B	941	12	11,11,12	0.83	1 (9%)	14,15,17	1.67	2 (14%)
12	MAN	B	942	12	11,11,12	0.88	1 (9%)	14,15,17	2.16	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
2	BMA	A	903	2	-	0/2/19/22	0/1/1/1
2	MAN	A	904	2	-	0/2/19/22	0/1/1/1
4	NAG	A	906	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	907	4	-	0/6/23/26	0/1/1/1
4	BMA	A	908	4	-	0/2/19/22	0/1/1/1
5	NAG	A	909	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	910	5	-	0/6/23/26	0/1/1/1
6	NAG	A	911	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	912	6	-	0/6/23/26	0/1/1/1
6	BMA	A	913	6	-	0/2/19/22	0/1/1/1
6	MAN	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
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
4	NAG	A	921	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	922	4	-	0/6/23/26	0/1/1/1
4	BMA	A	923	4	-	0/2/19/22	0/1/1/1
7	NAG	A	924	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	925	7	-	0/6/23/26	0/1/1/1
7	BMA	A	926	7	-	0/2/19/22	0/1/1/1
7	MAN	A	927	7	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
8	NAG	A	931	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	932	8	-	0/6/23/26	0/1/1/1
8	BMA	A	933	8	-	0/2/19/22	0/1/1/1
8	MAN	A	934	8	-	0/2/19/22	0/1/1/1
8	MAN	A	935	8	-	0/2/19/22	0/1/1/1
8	MAN	A	936	8	-	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
2	NAG	B	909	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	910	2	-	0/6/23/26	0/1/1/1
2	BMA	B	911	2	-	0/2/19/22	0/1/1/1
2	MAN	B	912	2	-	0/2/19/22	0/1/1/1
5	NAG	B	913	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	914	5	-	0/6/23/26	0/1/1/1
6	NAG	B	915	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	916	6	-	0/6/23/26	0/1/1/1
6	BMA	B	917	6	-	0/2/19/22	0/1/1/1
6	MAN	B	918	6	-	0/2/19/22	0/1/1/1
6	MAN	B	919	6	-	0/2/19/22	0/1/1/1
6	MAN	B	920	6	-	0/2/19/22	0/1/1/1
6	MAN	B	921	6	-	0/2/19/22	0/1/1/1
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
4	NAG	B	925	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	926	4	-	0/6/23/26	0/1/1/1
4	BMA	B	927	4	-	0/2/19/22	0/1/1/1
7	NAG	B	928	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	929	7	-	0/6/23/26	0/1/1/1
7	BMA	B	930	7	-	0/2/19/22	0/1/1/1
7	MAN	B	931	7	-	0/2/19/22	0/1/1/1
7	MAN	B	932	7	-	0/2/19/22	0/1/1/1
7	MAN	B	933	7	-	0/2/19/22	0/1/1/1
7	MAN	B	934	7	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	935	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	936	12	-	0/6/23/26	0/1/1/1
12	BMA	B	937	12	-	0/2/19/22	0/1/1/1
12	MAN	B	938	12	-	0/2/19/22	0/1/1/1
12	MAN	B	939	12	-	0/2/19/22	0/1/1/1
12	MAN	B	940	12	-	0/2/19/22	0/1/1/1
12	MAN	B	941	12	-	0/2/19/22	0/1/1/1
12	MAN	B	942	12	-	0/2/19/22	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	901	NAG	O5-C1	-2.98	1.38	1.43
7	B	928	NAG	O5-C1	-2.84	1.39	1.43
4	A	906	NAG	O5-C1	-2.78	1.39	1.43
8	A	935	MAN	O5-C1	-2.75	1.39	1.43
6	A	919	MAN	O5-C1	-2.61	1.39	1.43
7	B	929	NAG	O5-C1	-2.57	1.39	1.43
6	A	912	NAG	O5-C1	-2.57	1.39	1.43
6	B	917	BMA	O5-C1	-2.48	1.39	1.43
12	B	937	BMA	O5-C1	-2.37	1.39	1.43
12	B	935	NAG	O5-C1	-2.36	1.39	1.43
7	B	929	NAG	C2-N2	-2.30	1.42	1.46
12	B	936	NAG	O5-C1	-2.26	1.39	1.43
8	A	931	NAG	C1-C2	-2.25	1.49	1.52
7	A	928	MAN	O5-C1	-2.21	1.40	1.43
6	A	913	BMA	O2-C2	-2.20	1.38	1.43
7	A	925	NAG	O5-C1	-2.19	1.40	1.43
2	B	909	NAG	O5-C1	-2.19	1.40	1.43
8	A	932	NAG	O5-C1	-2.16	1.40	1.43
7	A	929	MAN	O5-C1	-2.13	1.40	1.43
6	A	917	MAN	O5-C1	-2.12	1.40	1.43
5	A	910	NAG	O5-C1	-2.10	1.40	1.43
12	B	941	MAN	C2-C3	2.04	1.55	1.52
2	B	909	NAG	C1-C2	2.14	1.55	1.52
7	B	907	MAN	C4-C5	2.14	1.57	1.53
4	B	926	NAG	C1-C2	2.19	1.55	1.52
2	B	912	MAN	C4-C3	2.29	1.58	1.52
12	B	942	MAN	C2-C3	2.38	1.55	1.52
6	B	919	MAN	C2-C3	2.43	1.55	1.52
6	A	915	MAN	C2-C3	2.48	1.55	1.52

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	931	MAN	C1-O5-C5	-6.58	103.90	112.25
7	A	925	NAG	C2-N2-C7	-5.91	115.45	123.04
2	A	903	BMA	O5-C5-C6	-5.22	96.05	107.35
5	B	914	NAG	C3-C4-C5	-4.80	101.83	110.20
7	A	927	MAN	O5-C1-C2	-4.69	103.25	110.86
2	A	902	NAG	C3-C4-C5	-4.67	102.06	110.20
7	B	907	MAN	O4-C4-C3	-4.59	100.00	110.34
12	B	937	BMA	O5-C1-C2	-4.45	103.64	110.86
12	B	939	MAN	O2-C2-C1	-4.40	100.39	109.21
7	A	929	MAN	O5-C1-C2	-4.39	103.73	110.86
7	B	905	MAN	O2-C2-C3	-4.28	101.50	110.12
12	B	936	NAG	C2-N2-C7	-4.24	117.59	123.04
7	B	928	NAG	C2-N2-C7	-4.21	117.63	123.04
6	A	916	MAN	O6-C6-C5	-4.13	97.69	111.33
6	B	921	MAN	O6-C6-C5	-4.09	97.82	111.33
7	B	929	NAG	C2-N2-C7	-4.02	117.88	123.04
7	B	903	BMA	C1-C2-C3	-3.89	104.94	109.54
7	A	927	MAN	C1-C2-C3	-3.81	105.03	109.54
7	A	924	NAG	C2-N2-C7	-3.68	118.31	123.04
7	B	929	NAG	C3-C4-C5	-3.63	103.87	110.20
8	A	935	MAN	O2-C2-C3	-3.56	102.96	110.12
6	B	919	MAN	C6-C5-C4	-3.55	104.25	113.02
4	A	907	NAG	C2-N2-C7	-3.54	118.50	123.04
4	A	908	BMA	O2-C2-C3	-3.48	103.12	110.12
4	A	922	NAG	C2-N2-C7	-3.38	118.69	123.04
2	B	909	NAG	C4-C3-C2	-3.35	106.02	111.23
7	A	924	NAG	O3-C3-C2	-3.24	102.70	109.11
6	A	912	NAG	O5-C5-C6	-3.22	100.38	107.35
7	A	926	BMA	C6-C5-C4	-3.20	105.12	113.02
6	B	923	MAN	O2-C2-C3	-3.19	103.71	110.12
4	A	908	BMA	O3-C3-C2	-3.18	104.25	110.00
7	B	934	MAN	C2-C3-C4	-3.18	105.65	111.04
6	B	920	MAN	C1-C2-C3	-3.17	105.79	109.54
12	B	940	MAN	O2-C2-C3	-3.15	103.78	110.12
2	A	904	MAN	O3-C3-C2	-3.15	104.30	110.00
6	B	915	NAG	C3-C4-C5	-3.14	104.72	110.20
2	A	903	BMA	C2-C3-C4	-3.12	105.74	111.04
7	A	924	NAG	C3-C2-N2	-3.11	103.10	110.56
6	A	919	MAN	O6-C6-C5	-3.11	101.06	111.33
7	B	931	MAN	O5-C1-C2	-3.08	105.86	110.86
6	B	915	NAG	O4-C4-C5	-3.08	101.09	109.24
6	A	918	MAN	O3-C3-C2	-3.07	104.45	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	934	MAN	O4-C4-C3	-3.06	103.44	110.34
7	A	925	NAG	C3-C4-C5	-2.97	105.02	110.20
7	B	932	MAN	O4-C4-C3	-2.95	103.69	110.34
7	A	929	MAN	C6-C5-C4	-2.94	105.75	113.02
7	A	925	NAG	C1-O5-C5	-2.93	108.53	112.25
6	B	917	BMA	C2-C3-C4	-2.82	106.25	111.04
6	B	920	MAN	C2-C3-C4	-2.82	106.25	111.04
8	A	935	MAN	C3-C4-C5	-2.81	105.31	110.20
6	A	917	MAN	C1-O5-C5	-2.80	108.70	112.25
7	B	902	NAG	O4-C4-C5	-2.78	101.88	109.24
5	B	913	NAG	C6-C5-C4	-2.76	106.22	113.02
7	A	929	MAN	O6-C6-C5	-2.73	102.31	111.33
8	A	935	MAN	O4-C4-C3	-2.72	104.22	110.34
4	A	908	BMA	O5-C1-C2	-2.71	106.46	110.86
8	A	931	NAG	C6-C5-C4	-2.68	106.40	113.02
6	B	915	NAG	C1-O5-C5	-2.68	108.85	112.25
5	B	914	NAG	O6-C6-C5	-2.65	102.58	111.33
4	B	927	BMA	C2-C3-C4	-2.64	106.56	111.04
6	A	916	MAN	O3-C3-C4	-2.63	104.42	110.34
12	B	939	MAN	O4-C4-C3	-2.54	104.61	110.34
7	B	903	BMA	O6-C6-C5	-2.52	102.99	111.33
6	B	920	MAN	O3-C3-C4	-2.52	104.66	110.34
4	A	906	NAG	C3-C2-N2	-2.50	104.57	110.56
7	A	929	MAN	O2-C2-C3	-2.50	105.10	110.12
5	B	913	NAG	O4-C4-C5	-2.48	102.66	109.24
6	A	916	MAN	O2-C2-C3	-2.45	105.19	110.12
6	B	920	MAN	O6-C6-C5	-2.38	103.48	111.33
4	B	925	NAG	O7-C7-C8	-2.37	117.70	122.06
7	B	902	NAG	O6-C6-C5	-2.37	103.50	111.33
12	B	935	NAG	O4-C4-C5	-2.36	102.98	109.24
7	B	934	MAN	O6-C6-C5	-2.35	103.56	111.33
6	A	919	MAN	O4-C4-C5	-2.35	103.02	109.24
6	B	921	MAN	O3-C3-C4	-2.33	105.09	110.34
7	A	930	MAN	O3-C3-C4	-2.33	105.09	110.34
4	A	908	BMA	O4-C4-C3	-2.31	105.12	110.34
12	B	938	MAN	O4-C4-C5	-2.29	103.17	109.24
6	A	920	MAN	C1-C2-C3	-2.29	106.83	109.54
6	A	919	MAN	C6-C5-C4	-2.29	107.37	113.02
6	A	917	MAN	C2-C3-C4	-2.29	107.16	111.04
7	A	928	MAN	C2-C3-C4	-2.27	107.19	111.04
6	A	917	MAN	O2-C2-C3	-2.26	105.57	110.12
6	A	917	MAN	O5-C1-C2	-2.26	107.19	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	942	MAN	C1-C2-C3	-2.26	106.87	109.54
6	A	914	MAN	C6-C5-C4	-2.25	107.46	113.02
6	A	913	BMA	O2-C2-C3	-2.21	105.67	110.12
7	B	901	NAG	C2-N2-C7	-2.21	120.20	123.04
7	B	930	BMA	C3-C4-C5	-2.19	106.37	110.20
8	A	934	MAN	O5-C1-C2	-2.19	107.31	110.86
4	B	925	NAG	O4-C4-C5	-2.18	103.46	109.24
8	A	936	MAN	O6-C6-C5	-2.17	104.15	111.33
6	A	920	MAN	O4-C4-C3	-2.17	105.45	110.34
6	B	921	MAN	C6-C5-C4	-2.16	107.68	113.02
12	B	939	MAN	O5-C1-C2	-2.16	107.36	110.86
2	B	909	NAG	C3-C2-N2	-2.14	105.43	110.56
6	B	918	MAN	O2-C2-C3	-2.13	105.83	110.12
6	B	924	MAN	C6-C5-C4	-2.11	107.80	113.02
6	B	917	BMA	O3-C3-C4	-2.10	105.60	110.34
7	B	904	MAN	C2-C3-C4	-2.07	107.53	111.04
5	A	910	NAG	O7-C7-C8	-2.07	118.27	122.06
2	A	904	MAN	O4-C4-C5	-2.06	103.78	109.24
12	B	935	NAG	C2-N2-C7	-2.05	120.40	123.04
7	B	904	MAN	C1-C2-C3	-2.05	107.12	109.54
6	B	919	MAN	C1-C2-C3	-2.01	107.16	109.54
7	B	933	MAN	C3-C4-C5	-2.01	106.69	110.20
8	A	934	MAN	O3-C3-C2	-2.01	106.37	110.00
7	B	933	MAN	C6-C5-C4	-2.01	108.07	113.02
7	A	925	NAG	C6-C5-C4	2.00	117.95	113.02
6	A	914	MAN	O5-C5-C6	2.01	111.69	107.35
8	A	934	MAN	C1-C2-C3	2.03	111.94	109.54
12	B	938	MAN	C1-O5-C5	2.03	114.82	112.25
2	B	909	NAG	O7-C7-N2	2.04	126.02	121.86
7	B	907	MAN	O5-C5-C6	2.05	111.78	107.35
7	A	928	MAN	O5-C1-C2	2.05	114.19	110.86
8	A	932	NAG	C3-C4-C5	2.06	113.79	110.20
7	B	906	MAN	C1-O5-C5	2.07	114.87	112.25
12	B	936	NAG	O5-C5-C6	2.07	111.83	107.35
7	B	907	MAN	C1-C2-C3	2.09	112.01	109.54
8	A	934	MAN	C6-C5-C4	2.10	118.19	113.02
7	B	931	MAN	C6-C5-C4	2.10	118.19	113.02
7	A	924	NAG	C1-O5-C5	2.11	114.92	112.25
8	A	936	MAN	O3-C3-C2	2.11	113.81	110.00
7	B	931	MAN	C3-C4-C5	2.12	113.89	110.20
6	B	918	MAN	C1-C2-C3	2.12	112.05	109.54
6	A	918	MAN	C1-C2-C3	2.15	112.09	109.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	934	MAN	O4-C4-C5	2.16	114.97	109.24
7	B	930	BMA	O3-C3-C2	2.20	113.97	110.00
7	A	927	MAN	C2-C3-C4	2.22	114.81	111.04
7	A	926	BMA	O5-C5-C6	2.23	112.17	107.35
6	A	912	NAG	C1-O5-C5	2.24	115.09	112.25
8	A	931	NAG	O4-C4-C3	2.24	115.38	110.34
7	B	906	MAN	C1-C2-C3	2.24	112.19	109.54
12	B	938	MAN	O2-C2-C1	2.25	113.71	109.21
6	A	917	MAN	O4-C4-C5	2.30	115.33	109.24
5	B	914	NAG	O4-C4-C5	2.30	115.34	109.24
8	A	933	BMA	O2-C2-C3	2.31	114.77	110.12
7	B	906	MAN	O5-C5-C6	2.32	112.36	107.35
2	A	902	NAG	O5-C5-C6	2.32	112.36	107.35
2	A	904	MAN	O6-C6-C5	2.32	119.01	111.33
12	B	940	MAN	C1-C2-C3	2.34	112.31	109.54
12	B	937	BMA	O2-C2-C1	2.34	113.90	109.21
4	A	923	BMA	O3-C3-C4	2.34	115.61	110.34
4	A	908	BMA	O6-C6-C5	2.35	119.09	111.33
4	B	926	NAG	C2-N2-C7	2.36	126.07	123.04
6	A	920	MAN	O5-C5-C6	2.36	112.46	107.35
6	B	915	NAG	C8-C7-N2	2.38	120.66	116.11
5	B	914	NAG	C2-N2-C7	2.38	126.10	123.04
6	A	912	NAG	C3-C2-N2	2.39	116.29	110.56
4	A	922	NAG	C1-O5-C5	2.39	115.29	112.25
12	B	942	MAN	O2-C2-C3	2.40	114.95	110.12
6	B	918	MAN	O2-C2-C1	2.40	114.02	109.21
4	B	925	NAG	C2-N2-C7	2.43	126.16	123.04
7	A	928	MAN	O3-C3-C2	2.46	114.44	110.00
7	A	929	MAN	O2-C2-C1	2.46	114.14	109.21
7	A	930	MAN	C1-O5-C5	2.47	115.38	112.25
4	A	922	NAG	C4-C3-C2	2.48	115.08	111.23
8	A	935	MAN	O3-C3-C4	2.49	115.93	110.34
4	A	922	NAG	C3-C4-C5	2.50	114.56	110.20
2	B	911	BMA	C3-C4-C5	2.52	114.58	110.20
8	A	933	BMA	O3-C3-C4	2.53	116.03	110.34
12	B	941	MAN	O5-C5-C6	2.54	112.84	107.35
7	B	905	MAN	O5-C5-C6	2.54	112.84	107.35
6	B	922	MAN	O2-C2-C3	2.54	115.23	110.12
8	A	933	BMA	O5-C1-C2	2.55	114.99	110.86
4	A	908	BMA	C1-O5-C5	2.56	115.49	112.25
7	A	927	MAN	O2-C2-C3	2.58	115.32	110.12
4	B	925	NAG	C1-O5-C5	2.61	115.56	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	939	MAN	C1-C2-C3	2.66	112.69	109.54
2	B	911	BMA	C1-O5-C5	2.67	115.63	112.25
4	A	908	BMA	C2-C3-C4	2.68	115.59	111.04
5	A	910	NAG	C1-O5-C5	2.76	115.75	112.25
7	A	930	MAN	O5-C5-C6	2.77	113.34	107.35
12	B	938	MAN	O5-C1-C2	2.77	115.34	110.86
2	A	903	BMA	O3-C3-C4	2.80	116.65	110.34
4	A	923	BMA	C3-C4-C5	2.82	115.12	110.20
7	B	907	MAN	O3-C3-C2	2.85	115.15	110.00
7	B	931	MAN	O5-C5-C6	2.89	113.60	107.35
6	B	919	MAN	O3-C3-C2	2.91	115.26	110.00
2	A	904	MAN	O3-C3-C4	2.94	116.95	110.34
8	A	936	MAN	O3-C3-C4	2.98	117.04	110.34
2	A	903	BMA	C1-O5-C5	2.98	116.03	112.25
5	A	910	NAG	C8-C7-N2	3.02	121.88	116.11
8	A	934	MAN	C1-O5-C5	3.02	116.08	112.25
7	B	932	MAN	C1-C2-C3	3.02	113.12	109.54
2	B	912	MAN	O5-C5-C6	3.05	113.94	107.35
12	B	942	MAN	C3-C4-C5	3.06	115.53	110.20
7	B	907	MAN	C6-C5-C4	3.06	120.57	113.02
8	A	935	MAN	C1-O5-C5	3.07	116.14	112.25
8	A	934	MAN	O6-C6-C5	3.09	121.54	111.33
6	B	919	MAN	O2-C2-C3	3.11	116.37	110.12
2	B	912	MAN	O6-C6-C5	3.13	121.69	111.33
12	B	938	MAN	C2-C3-C4	3.16	116.41	111.04
4	A	908	BMA	O5-C5-C6	3.18	114.24	107.35
7	B	907	MAN	O6-C6-C5	3.18	121.85	111.33
12	B	936	NAG	C1-O5-C5	3.25	116.38	112.25
6	A	918	MAN	C1-O5-C5	3.32	116.46	112.25
5	A	910	NAG	C2-N2-C7	3.33	127.31	123.04
6	B	923	MAN	C1-O5-C5	3.33	116.48	112.25
6	B	919	MAN	O5-C5-C6	3.34	114.58	107.35
4	A	923	BMA	O2-C2-C1	3.41	116.03	109.21
12	B	941	MAN	O3-C3-C4	3.41	118.01	110.34
6	A	915	MAN	C2-C3-C4	3.44	116.88	111.04
2	B	912	MAN	C1-C2-C3	3.47	113.65	109.54
8	A	935	MAN	C6-C5-C4	3.48	121.59	113.02
4	B	927	BMA	C3-C4-C5	3.51	116.32	110.20
6	A	919	MAN	C1-O5-C5	3.52	116.72	112.25
4	A	923	BMA	C1-O5-C5	3.56	116.77	112.25
8	A	934	MAN	O5-C5-C6	3.62	115.19	107.35
2	B	909	NAG	C1-O5-C5	3.64	116.87	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	913	NAG	C1-O5-C5	3.67	116.91	112.25
6	B	920	MAN	C1-O5-C5	3.68	116.92	112.25
6	B	920	MAN	O3-C3-C2	3.82	116.90	110.00
6	B	922	MAN	C1-O5-C5	3.85	117.13	112.25
12	B	938	MAN	C1-C2-C3	3.90	114.16	109.54
6	A	915	MAN	O2-C2-C3	3.92	118.00	110.12
8	A	932	NAG	C1-O5-C5	3.93	117.24	112.25
2	B	912	MAN	C6-C5-C4	3.96	122.78	113.02
2	B	912	MAN	O3-C3-C4	3.98	119.31	110.34
4	A	908	BMA	C1-C2-C3	4.00	114.28	109.54
5	A	909	NAG	C2-N2-C7	4.01	128.19	123.04
2	A	904	MAN	O5-C1-C2	4.04	117.42	110.86
7	B	901	NAG	C1-O5-C5	4.07	117.41	112.25
7	A	928	MAN	O3-C3-C4	4.09	119.54	110.34
2	A	903	BMA	C1-C2-C3	4.14	114.44	109.54
2	A	904	MAN	C3-C4-C5	4.15	117.44	110.20
12	B	938	MAN	C3-C4-C5	4.16	117.44	110.20
7	B	902	NAG	C1-O5-C5	4.19	117.57	112.25
7	B	933	MAN	C1-O5-C5	4.24	117.63	112.25
7	A	926	BMA	C1-O5-C5	4.33	117.75	112.25
2	A	903	BMA	C3-C4-C5	4.40	117.87	110.20
7	B	932	MAN	C1-O5-C5	4.51	117.98	112.25
6	B	918	MAN	C1-O5-C5	4.59	118.08	112.25
5	A	909	NAG	C1-O5-C5	4.60	118.09	112.25
7	A	929	MAN	C1-O5-C5	4.76	118.29	112.25
4	A	908	BMA	C3-C4-C5	4.79	118.54	110.20
8	A	933	BMA	C1-O5-C5	4.97	118.56	112.25
6	B	924	MAN	C1-O5-C5	5.01	118.61	112.25
12	B	935	NAG	C1-O5-C5	5.09	118.71	112.25
6	B	919	MAN	O2-C2-C1	5.47	120.17	109.21
6	B	921	MAN	C1-O5-C5	5.60	119.36	112.25
7	B	934	MAN	C1-O5-C5	5.66	119.42	112.25
4	A	921	NAG	C1-O5-C5	5.68	119.46	112.25
12	B	942	MAN	C1-O5-C5	6.00	119.86	112.25
4	B	927	BMA	C1-O5-C5	6.29	120.23	112.25
8	A	931	NAG	C1-O5-C5	6.82	120.90	112.25
2	A	904	MAN	C1-O5-C5	6.87	120.96	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	910	NAG	2	0
7	A	926	BMA	2	0
7	B	901	NAG	2	0
2	B	909	NAG	1	0
2	B	910	NAG	2	0
7	B	930	BMA	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	905	1	14,14,15	0.72	0	15,19,21	1.35	1 (6%)
3	NAG	A	937	1	14,14,15	0.97	0	15,19,21	1.94	4 (26%)
9	MRD	A	938	-	6,7,7	0.28	0	7,10,10	0.69	0
10	MPD	A	939	-	6,7,7	0.35	0	7,10,10	0.60	0
10	MPD	A	940	-	6,7,7	0.45	0	7,10,10	0.91	0
11	CTS	A	941	-	14,14,14	1.34	1 (7%)	15,21,21	1.27	3 (20%)
3	NAG	B	908	1	14,14,15	1.04	1 (7%)	15,19,21	1.47	4 (26%)
3	NAG	B	943	1	14,14,15	0.71	0	15,19,21	1.35	1 (6%)
3	NAG	B	944	1	14,14,15	0.69	0	15,19,21	1.60	2 (13%)
9	MRD	B	945	-	6,7,7	0.54	0	7,10,10	0.40	0
9	MRD	B	946	-	6,7,7	0.73	0	7,10,10	1.02	1 (14%)
9	MRD	B	947	-	6,7,7	0.53	0	7,10,10	0.40	0
11	CTS	B	948	-	14,14,14	1.06	1 (7%)	15,21,21	1.29	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	937	1	-	0/6/23/26	0/1/1/1
9	MRD	A	938	-	-	0/5/5/5	0/0/0/0
10	MPD	A	939	-	-	0/5/5/5	0/0/0/0
10	MPD	A	940	-	-	0/5/5/5	0/0/0/0
11	CTS	A	941	-	-	0/0/29/29	0/2/2/2
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	943	1	-	0/6/23/26	0/1/1/1
3	NAG	B	944	1	-	0/6/23/26	0/1/1/1
9	MRD	B	945	-	-	0/5/5/5	0/0/0/0
9	MRD	B	946	-	-	0/5/5/5	0/0/0/0
9	MRD	B	947	-	-	0/5/5/5	0/0/0/0
11	CTS	B	948	-	-	0/0/29/29	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	941	CTS	C6-C5	-4.36	1.49	1.54
3	B	908	NAG	O5-C1	-2.64	1.39	1.43
11	B	948	CTS	C1-C2	2.88	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	937	NAG	C2-N2-C7	-4.95	116.68	123.04
3	A	905	NAG	C4-C3-C2	-3.72	105.45	111.23
3	A	937	NAG	C3-C4-C5	-2.91	105.12	110.20
11	A	941	CTS	O2-C2-C3	-2.34	105.41	110.12
3	B	908	NAG	O7-C7-C8	-2.27	117.90	122.06
9	B	946	MRD	C2-C3-C4	-2.18	106.35	116.66
3	B	908	NAG	C1-O5-C5	-2.16	109.51	112.25
3	B	944	NAG	O4-C4-C3	-2.06	105.70	110.34
11	A	941	CTS	O3-C3-C2	-2.01	106.36	110.00
11	B	948	CTS	O3-C3-C2	2.01	113.63	110.00
3	B	908	NAG	C3-C2-N2	2.15	115.71	110.56
3	A	937	NAG	C8-C7-N2	2.18	120.28	116.11
11	A	941	CTS	C1-C2-C3	2.40	112.83	110.21
3	B	908	NAG	C2-N2-C7	2.87	126.72	123.04
3	A	937	NAG	C1-O5-C5	3.09	116.17	112.25
3	B	943	NAG	C4-C3-C2	4.24	117.82	111.23
3	B	944	NAG	C1-O5-C5	4.66	118.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	938	MRD	1	0
10	A	939	MPD	1	0
11	A	941	CTS	2	0
9	B	945	MRD	1	0
9	B	946	MRD	3	0
9	B	947	MRD	2	0
11	B	948	CTS	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

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	833/841 (99%)	-0.51	1 (0%) 95 96	17, 26, 42, 72	0
1	B	832/841 (98%)	-0.66	0 100 100	16, 23, 35, 58	0
All	All	1665/1682 (98%)	-0.58	1 (0%) 95 96	16, 24, 39, 72	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	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	MAN	A	930	11/12	0.96	0.12	2.87	32,36,44,45	0
7	NAG	A	924	14/15	0.95	0.15	2.72	26,33,47,49	0
4	NAG	A	907	14/15	0.95	0.13	2.64	27,35,37,37	0
7	MAN	B	906	11/12	0.95	0.19	2.64	31,37,41,48	0
12	MAN	B	939	11/12	0.97	0.19	1.88	30,38,52,60	0
7	MAN	B	934	11/12	0.96	0.16	1.48	30,39,43,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	921	14/15	0.95	0.12	0.80	35,39,47,49	0
8	MAN	A	935	11/12	0.95	0.13	0.79	33,40,46,48	0
6	MAN	B	921	11/12	0.96	0.10	0.56	27,28,33,37	0
7	NAG	B	928	14/15	0.96	0.10	0.40	22,33,45,46	0
6	MAN	A	919	11/12	0.96	0.09	0.35	29,30,37,45	0
8	MAN	A	934	11/12	0.93	0.14	0.17	35,37,41,43	0
6	MAN	A	918	11/12	0.97	0.11	-0.01	28,29,34,35	0
6	NAG	A	911	14/15	0.97	0.16	-0.02	27,32,39,40	0
6	NAG	B	916	14/15	0.97	0.11	-0.20	19,22,26,30	0
8	NAG	A	931	14/15	0.97	0.12	-0.34	26,29,33,37	0
7	NAG	B	901	14/15	0.99	0.10	-0.36	19,20,24,28	0
6	NAG	A	912	14/15	0.97	0.13	-0.37	28,31,34,39	0
6	NAG	B	915	14/15	0.98	0.10	-0.38	22,26,29,30	0
4	NAG	B	925	14/15	0.96	0.10	-0.41	28,33,41,43	0
4	NAG	A	906	14/15	0.96	0.10	-0.47	26,30,32,34	0
12	NAG	B	935	14/15	0.97	0.11	-0.49	23,25,29,34	0
2	NAG	A	901	14/15	0.98	0.09	-0.64	25,32,35,36	0
6	MAN	A	917	11/12	0.97	0.10	-0.73	28,31,33,35	0
2	NAG	A	902	14/15	0.97	0.11	-0.79	31,41,51,61	0
5	NAG	A	909	14/15	0.97	0.11	-0.85	25,28,32,33	0
5	NAG	B	913	14/15	0.98	0.09	-0.87	18,22,26,27	0
7	NAG	B	902	14/15	0.98	0.10	-1.69	21,26,30,31	0
2	NAG	B	910	14/15	0.96	0.08	-1.70	25,34,39,41	0
2	NAG	B	909	14/15	0.97	0.08	-1.94	22,26,28,32	0
6	MAN	B	924	11/12	0.97	0.08	-1.99	26,28,30,31	0
6	MAN	B	923	11/12	0.98	0.08	-2.38	19,21,23,24	0
6	MAN	A	920	11/12	0.93	0.12	-	38,41,46,48	0
12	MAN	B	942	11/12	0.85	0.26	-	53,67,74,75	0
12	MAN	B	938	11/12	0.83	0.26	-	62,71,81,81	0
4	NAG	A	922	14/15	0.87	0.24	-	53,63,73,84	0
7	MAN	B	932	11/12	0.91	0.14	-	33,35,40,46	0
6	MAN	A	916	11/12	0.99	0.08	-	22,26,28,30	0
7	BMA	B	930	11/12	0.92	0.18	-	40,47,56,68	0
7	MAN	A	928	11/12	0.95	0.15	-	35,40,47,48	0
4	BMA	A	908	11/12	0.89	0.25	-	39,48,55,56	0
5	NAG	B	914	14/15	0.91	0.15	-	30,38,49,52	0
7	NAG	B	929	14/15	0.94	0.16	-	23,32,39,40	0
6	BMA	B	917	11/12	0.98	0.10	-	24,25,27,30	0
2	MAN	A	904	11/12	0.80	0.15	-	54,63,71,71	0
7	MAN	B	931	11/12	0.77	0.28	-	70,80,84,88	0
2	BMA	A	903	11/12	0.83	0.13	-	40,53,60,60	0
8	BMA	A	933	11/12	0.92	0.13	-	43,49,55,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BMA	B	911	11/12	0.90	0.13	-	49,53,58,59	0
6	MAN	A	914	11/12	0.97	0.11	-	35,38,43,44	0
12	NAG	B	936	14/15	0.93	0.15	-	29,36,45,45	0
7	NAG	A	925	14/15	0.94	0.15	-	27,33,39,42	0
6	MAN	B	920	11/12	0.99	0.09	-	19,21,24,25	0
6	MAN	B	922	11/12	0.94	0.16	-	36,41,44,44	0
6	MAN	B	919	11/12	0.86	0.15	-	39,49,55,55	0
12	MAN	B	941	11/12	0.93	0.29	-	61,66,71,72	0
12	MAN	B	940	11/12	0.94	0.18	-	39,42,48,50	0
8	NAG	A	932	14/15	0.96	0.17	-	26,35,48,51	0
5	NAG	A	910	14/15	0.96	0.12	-	33,38,50,56	0
8	MAN	A	936	11/12	0.88	0.21	-	50,55,65,70	0
4	NAG	B	926	14/15	0.94	0.10	-	38,40,45,50	0
4	BMA	B	927	11/12	0.89	0.20	-	51,63,70,72	0
7	MAN	A	929	11/12	0.97	0.10	-	26,29,37,43	0
2	MAN	B	912	11/12	0.84	0.23	-	56,69,79,79	0
12	BMA	B	937	11/12	0.93	0.20	-	42,48,58,67	0
7	MAN	B	904	11/12	0.96	0.14	-	38,44,52,56	0
7	MAN	B	907	11/12	0.90	0.16	-	30,38,44,49	0
6	MAN	B	918	11/12	0.96	0.10	-	28,30,33,42	0
7	MAN	B	933	11/12	0.97	0.17	-	30,34,38,47	0
6	BMA	A	913	11/12	0.97	0.10	-	28,33,34,38	0
6	MAN	A	915	11/12	0.94	0.14	-	43,49,59,59	0
7	MAN	A	927	11/12	0.77	0.27	-	60,63,68,68	0
7	BMA	B	903	11/12	0.95	0.10	-	32,35,39,40	0
7	BMA	A	926	11/12	0.91	0.16	-	35,44,50,55	0
7	MAN	B	905	11/12	0.97	0.17	-	39,46,51,59	0
4	BMA	A	923	11/12	0.61	0.36	-	66,80,85,85	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, 95th 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
10	MPD	A	939	8/8	0.93	0.19	7.49	34,42,48,49	0
9	MRD	B	947	8/8	0.90	0.18	6.19	54,59,63,70	0
10	MPD	A	940	8/8	0.86	0.22	5.38	49,58,69,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	MRD	B	946	8/8	0.96	0.15	5.24	32,38,42,44	0
9	MRD	B	945	8/8	0.84	0.29	4.87	46,66,73,75	0
3	NAG	B	944	14/15	0.97	0.21	1.63	35,39,42,46	0
11	CTS	B	948	13/13	0.99	0.17	1.09	20,23,27,28	0
9	MRD	A	938	8/8	0.96	0.14	1.00	38,40,42,43	0
3	NAG	A	937	14/15	0.96	0.24	1.00	39,44,47,52	0
11	CTS	A	941	13/13	0.99	0.15	-0.16	24,26,29,29	0
3	NAG	B	908	14/15	0.87	0.23	-	50,64,80,82	0
3	NAG	B	943	14/15	0.90	0.23	-	54,68,84,84	0
3	NAG	A	905	14/15	0.91	0.22	-	55,67,69,75	0

6.5 Other polymers (i)

There are no such residues in this entry.