



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:29 PM GMT

PDB ID : 4IIH
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with thiocellobiose
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 2.00 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 ⓘ](#)) 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

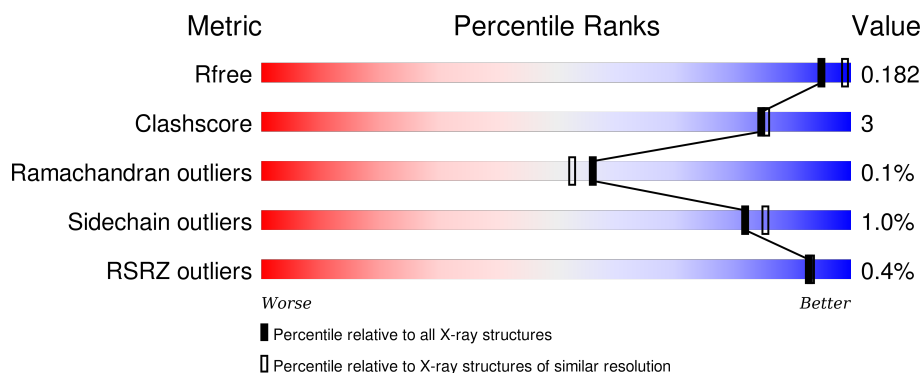
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	 90% 8%
1	B	841	 91% 7%

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	MAN	B	942	-	-	-	X
2	MAN	A	906	-	-	-	X
2	NAG	A	927	-	-	-	X
2	MAN	A	933	-	-	-	X
2	MAN	A	937	-	-	-	X
2	MAN	A	938	-	-	-	X
2	MAN	B	906	-	-	-	X
2	MAN	B	937	-	-	-	X
3	NAG	B	947	-	-	-	X
4	NAG	A	910	-	-	-	X
7	MRD	A	943	-	-	X	X
7	MRD	B	948	-	-	-	X
7	MRD	B	949	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15509 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
			6382	4028	1096	1240	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 (7-MER).

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

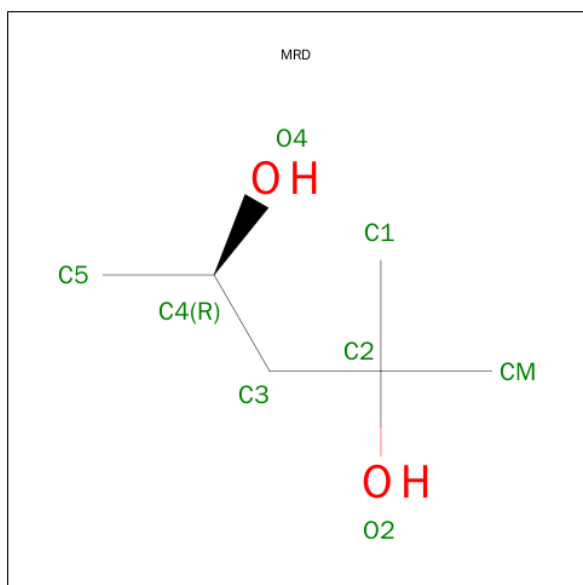
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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).

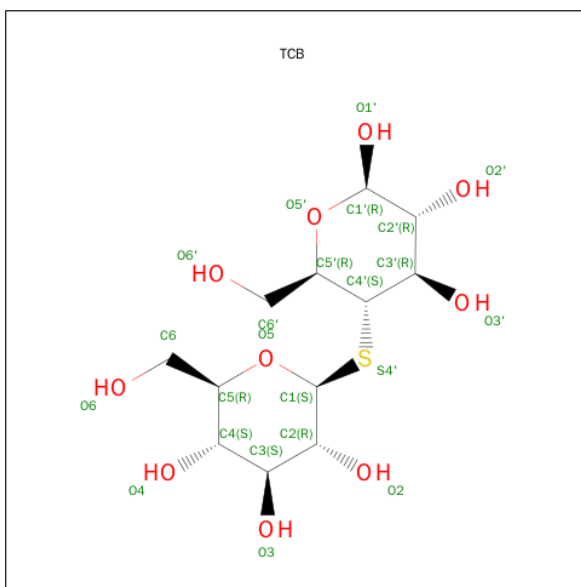
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	10	Total	C	N	O	0	0
			116	64	2	50		
6	B	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 8 is SUGAR (THIOCELLOBIOSE) (three-letter code: TCB) (formula: $C_{12}H_{22}O_{10}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			23	12	10	1		
8	B	1	Total	C	O	S	0	0
			23	12	10	1		

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (8-MER).

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

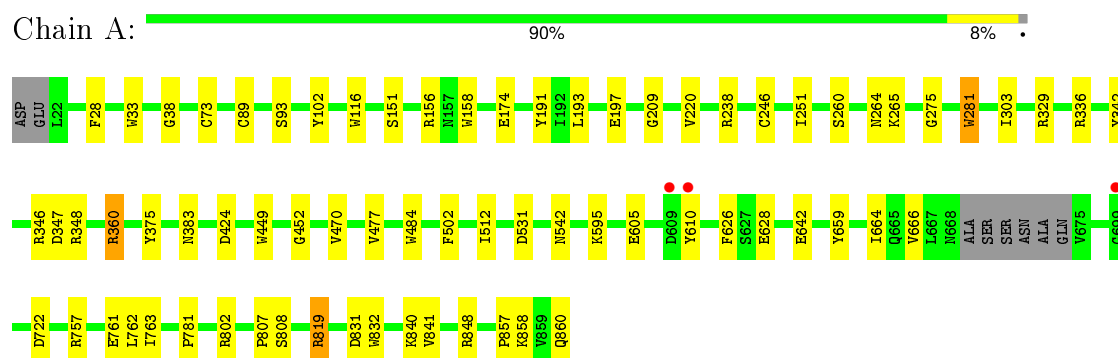
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	748	Total	O	0	0
			748	748		
11	B	859	Total	O	0	0
			859	859		

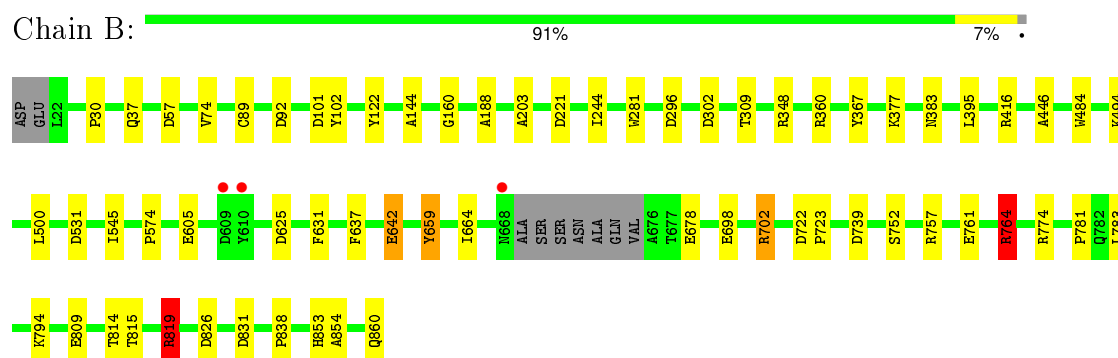
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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, α , β , γ	82.08Å 122.39Å 221.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.00 41.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.07-2.00) 99.6 (41.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.140 , 0.181 0.141 , 0.182	Depositor DCC
R_{free} test set	7569 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 150300 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, BMA, TCB, NAG, 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	1.29	11/6545 (0.2%)	1.07	18/8923 (0.2%)
1	B	1.35	10/6538 (0.2%)	1.11	24/8913 (0.3%)
All	All	1.32	21/13083 (0.2%)	1.09	42/17836 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	642	GLU	CD-OE1	8.91	1.35	1.25
1	B	761	GLU	CD-OE2	-7.47	1.17	1.25
1	A	281	TRP	CB-CG	7.21	1.63	1.50
1	A	761	GLU	CD-OE2	-6.17	1.18	1.25
1	B	605	GLU	CG-CD	6.00	1.60	1.51
1	B	637	PHE	CG-CD1	5.96	1.47	1.38
1	A	151	SER	CB-OG	5.80	1.49	1.42
1	A	174	GLU	CD-OE2	-5.72	1.19	1.25
1	B	702	ARG	CD-NE	-5.70	1.36	1.46
1	B	774	ARG	CZ-NH1	5.64	1.40	1.33
1	B	122	TYR	CE1-CZ	5.46	1.45	1.38
1	A	33	TRP	CE3-CZ3	5.43	1.47	1.38
1	A	832	TRP	CE3-CZ3	5.40	1.47	1.38
1	A	342	TYR	CZ-OH	5.38	1.47	1.37
1	A	158	TRP	CZ3-CH2	5.32	1.48	1.40
1	B	309	THR	CB-CG2	5.23	1.69	1.52
1	B	809	GLU	CD-OE2	-5.15	1.20	1.25
1	A	275	GLY	N-CA	5.14	1.53	1.46
1	A	197	GLU	CD-OE2	5.02	1.31	1.25
1	B	631	PHE	CG-CD2	5.02	1.46	1.38
1	A	209	GLY	N-CA	5.01	1.53	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	B	702	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	757	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	757	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	B	774	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	757	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	B	531	ASP	CB-CG-OD1	8.27	125.74	118.30
1	B	221	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	757	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	B	722	ASP	CB-CG-OD1	7.40	124.96	118.30
1	B	826	ASP	CB-CG-OD1	7.39	124.95	118.30
1	B	764	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	101	ASP	CB-CG-OD1	6.66	124.30	118.30
1	B	348	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	722	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	722	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	819	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	336	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	360	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	360	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	794	LYS	CD-CE-NZ	-6.12	97.62	111.70
1	A	156	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	819	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	B	642	GLU	CG-CD-OE2	-5.96	106.38	118.30
1	B	348	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	531	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	848	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	628	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	B	659	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	B	296	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	346	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	329	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	831	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	347	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	802	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	702	ARG	CB-CG-CD	-5.26	97.92	111.60
1	B	774	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	A	238	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	831	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	73	CYS	CA-CB-SG	-5.09	104.84	114.00
1	B	831	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	416	ARG	NE-CZ-NH1	-5.07	117.77	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	6382	0	6092	31	0
1	B	6375	0	6082	32	0
2	A	249	0	210	2	0
2	B	166	0	139	4	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	67	2	0
4	B	78	0	68	0	0
5	A	28	0	25	3	0
6	A	116	0	96	0	0
6	B	116	0	97	0	0
7	A	16	0	28	9	0
7	B	16	0	28	4	0
8	A	23	0	22	0	0
8	B	23	0	22	4	0
9	B	72	0	61	0	0
10	B	94	0	79	4	0
11	A	748	0	0	3	0
11	B	859	0	0	11	0
All	All	15509	0	13181	79	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 3.

All (79) 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:819:ARG:HH12	1:A:860:GLN:C	1.51	1.12
1:B:815:THR:HG22	11:B:1525:HOH:O	1.70	0.89
1:A:819:ARG:NH1	1:A:860:GLN:C	2.31	0.84
7:A:942:MRD:H5C2	11:A:1191:HOH:O	1.77	0.84
5:A:913:NAG:H83	5:A:913:NAG:H3	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HH11	7:A:943:MRD:HMC3	1.45	0.80
7:A:943:MRD:HMC2	11:B:1105:HOH:O	1.85	0.74
7:A:943:MRD:HMC1	7:A:943:MRD:H5C3	1.70	0.72
1:B:764:ARG:HD3	1:B:814:THR:HG21	1.74	0.69
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.75	0.68
1:B:764:ARG:HD3	1:B:814:THR:CG2	2.25	0.67
1:B:664:ILE:HD11	1:B:854:ALA:HB3	1.81	0.62
1:B:484:TRP:CE2	2:B:933:BMA:H62	2.34	0.62
7:A:942:MRD:H5C3	7:A:942:MRD:O2	1.99	0.62
10:B:940:BMA:H61	11:B:1464:HOH:O	2.04	0.58
1:A:360:ARG:HH11	7:A:943:MRD:CM	2.15	0.57
5:A:913:NAG:C8	5:A:913:NAG:H3	2.36	0.55
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.88	0.55
7:A:943:MRD:C5	7:A:943:MRD:HMC1	2.37	0.55
1:B:494:LYS:HE2	11:B:1291:HOH:O	2.08	0.53
7:B:949:MRD:C5	7:B:949:MRD:O2	2.57	0.53
1:B:74:VAL:CG2	8:B:950:TCB:H61	2.40	0.52
1:B:74:VAL:HG21	8:B:950:TCB:H61	1.91	0.52
1:B:702:ARG:HD3	11:B:1175:HOH:O	2.10	0.52
1:A:605:GLU:HA	1:A:610:TYR:OH	2.11	0.51
1:A:666:VAL:CG2	1:A:857:PRO:HG3	2.40	0.51
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.76	0.51
1:A:260:SER:O	1:A:264:ASN:HB2	2.12	0.50
1:B:819:ARG:HH22	1:B:860:GLN:C	2.16	0.49
2:A:903:BMA:H61	2:A:907:MAN:H5	1.95	0.48
10:B:940:BMA:H62	10:B:942:MAN:H5	1.95	0.48
1:B:783:LEU:C	1:B:783:LEU:HD23	2.34	0.48
1:B:203:ALA:HB3	11:B:1726:HOH:O	2.13	0.48
1:A:191:TYR:O	1:A:246:CYS:HA	2.13	0.47
1:B:819:ARG:NH2	1:B:860:GLN:C	2.68	0.47
1:B:37:GLN:OE1	1:B:752:SER:HB2	2.15	0.47
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.97	0.47
7:B:948:MRD:H4	11:B:1363:HOH:O	2.15	0.47
1:A:424:ASP:HB3	1:A:502:PHE:HB3	1.96	0.47
7:A:942:MRD:O2	7:A:942:MRD:C5	2.63	0.46
1:B:74:VAL:HB	8:B:950:TCB:H61	1.96	0.46
1:B:57:ASP:OD1	1:B:57:ASP:N	2.47	0.46
1:A:542:ASN:ND2	11:A:1606:HOH:O	2.36	0.46
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.98	0.46
1:A:807:PRO:O	1:A:808:SER:HB2	2.16	0.46
1:A:303:ILE:HG21	5:A:913:NAG:H81	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:TYR:HB3	1:B:383:ASN:HA	1.98	0.45
1:A:484:TRP:CE2	2:A:929:BMA:H62	2.52	0.45
10:B:940:BMA:H62	10:B:942:MAN:H3	1.99	0.45
1:B:377:LYS:HD3	11:B:1200:HOH:O	2.16	0.45
1:B:723:PRO:HG2	11:B:1452:HOH:O	2.15	0.45
1:B:446:ALA:HA	1:B:574:PRO:HD2	1.98	0.45
1:A:375:TYR:CG	10:B:945:MAN:H62	2.53	0.44
7:B:948:MRD:H1C2	7:B:948:MRD:H4	1.38	0.44
1:B:500:LEU:HD23	1:B:545:ILE:HB	2.00	0.44
1:A:762:LEU:C	1:A:763:ILE:HG12	2.38	0.44
1:B:494:LYS:CE	11:B:1291:HOH:O	2.64	0.44
1:A:360:ARG:HG2	7:A:943:MRD:HMC1	1.99	0.44
1:A:659:TYR:HE1	1:A:781:PRO:HB3	1.83	0.43
1:A:93:SER:HB2	1:A:452:GLY:HA2	2.00	0.43
1:B:367:TYR:CZ	2:B:902:NAG:H83	2.54	0.42
1:A:840:LYS:HB3	1:A:840:LYS:HE2	1.91	0.42
1:A:449:TRP:CD1	1:A:512:ILE:HB	2.55	0.42
1:B:838:PRO:HD2	11:B:1672:HOH:O	2.20	0.42
2:B:933:BMA:H61	2:B:935:MAN:H5	2.02	0.42
1:B:625:ASP:HB3	7:B:949:MRD:HMC2	2.01	0.42
1:B:395:LEU:O	1:B:395:LEU:HD23	2.20	0.42
1:B:144:ALA:O	1:B:160:GLY:HA2	2.20	0.42
1:A:251:ILE:HG21	4:A:909:NAG:H82	2.01	0.41
1:A:220:VAL:HG22	1:A:626:PHE:CG	2.56	0.41
1:A:251:ILE:CG2	4:A:909:NAG:H82	2.50	0.41
1:A:348:ARG:NH1	11:A:1479:HOH:O	2.52	0.41
1:A:28:PHE:CG	1:A:265:LYS:HB2	2.56	0.41
1:B:30:PRO:HG3	1:B:739:ASP:O	2.21	0.41
1:A:116:TRP:CD1	1:A:595:LYS:HB2	2.57	0.40
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.50	0.40
1:B:74:VAL:CB	8:B:950:TCB:H61	2.50	0.40
1:B:484:TRP:CZ2	2:B:933:BMA:H62	2.57	0.40
1:A:102:TYR:HB3	1:A:383:ASN:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	803 (97%)	25 (3%)	1 (0%)	56	53
1	B	828/841 (98%)	804 (97%)	24 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	49 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLY

5.3.2 Protein sidechains

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%)	667 (99%)	4 (1%)	90	93
1	B	670/677 (99%)	660 (98%)	10 (2%)	72	75
All	All	1341/1354 (99%)	1327 (99%)	14 (1%)	82	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	CYS
1	A	281	TRP
1	A	642	GLU
1	A	858	LYS
1	B	89	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	92	ASP
1	B	281	TRP
1	B	302	ASP
1	B	642	GLU
1	B	678	GLU
1	B	698	GLU
1	B	764	ARG
1	B	819	ARG
1	B	853	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

83 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	1.17	2 (14%)	15,19,21	1.15	1 (6%)
2	NAG	A	902	2	14,14,15	1.11	1 (7%)	15,19,21	1.35	2 (13%)
2	BMA	A	903	2	11,11,12	0.71	0	14,15,17	2.01	3 (21%)
2	MAN	A	904	2	11,11,12	0.96	1 (9%)	14,15,17	2.55	8 (57%)
2	MAN	A	905	2	11,11,12	0.87	0	14,15,17	2.17	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	A	906	2	11,11,12	1.01	0	14,15,17	2.13	6 (42%)
2	MAN	A	907	2	11,11,12	0.85	0	14,15,17	1.07	1 (7%)
4	NAG	A	909	1,4	14,14,15	1.02	0	15,19,21	1.22	2 (13%)
4	NAG	A	910	4	14,14,15	1.41	2 (14%)	15,19,21	1.93	6 (40%)
4	BMA	A	911	4	11,11,12	1.24	0	14,15,17	2.87	7 (50%)
5	NAG	A	912	1,5	14,14,15	1.27	2 (14%)	15,19,21	1.86	3 (20%)
5	NAG	A	913	5	14,14,15	1.08	2 (14%)	15,19,21	1.78	6 (40%)
6	NAG	A	914	1,6	14,14,15	1.45	3 (21%)	15,19,21	1.22	1 (6%)
6	NAG	A	915	6	14,14,15	1.02	0	15,19,21	1.60	3 (20%)
6	BMA	A	916	6	11,11,12	0.65	0	14,15,17	1.38	3 (21%)
6	MAN	A	917	6	11,11,12	1.56	4 (36%)	14,15,17	1.96	5 (35%)
6	MAN	A	918	6	11,11,12	1.23	1 (9%)	14,15,17	2.49	6 (42%)
6	MAN	A	919	6	11,11,12	0.83	1 (9%)	14,15,17	1.10	2 (14%)
6	MAN	A	920	6	11,11,12	1.41	3 (27%)	14,15,17	1.58	2 (14%)
6	MAN	A	921	6	11,11,12	0.88	0	14,15,17	1.04	1 (7%)
6	MAN	A	922	6	11,11,12	1.30	2 (18%)	14,15,17	1.30	3 (21%)
6	MAN	A	923	6	11,11,12	0.83	0	14,15,17	1.38	3 (21%)
4	NAG	A	924	1,4	14,14,15	1.01	1 (7%)	15,19,21	1.69	3 (20%)
4	NAG	A	925	4	14,14,15	0.80	0	15,19,21	1.75	2 (13%)
4	BMA	A	926	4	11,11,12	1.28	2 (18%)	14,15,17	2.03	5 (35%)
2	NAG	A	927	1,2	14,14,15	1.09	1 (7%)	15,19,21	1.70	3 (20%)
2	NAG	A	928	2	14,14,15	0.78	0	15,19,21	1.51	3 (20%)
2	BMA	A	929	2	11,11,12	1.35	1 (9%)	14,15,17	1.84	4 (28%)
2	MAN	A	930	2	11,11,12	0.82	0	14,15,17	1.72	4 (28%)
2	MAN	A	931	2	11,11,12	0.65	0	14,15,17	1.55	1 (7%)
2	MAN	A	932	2	11,11,12	0.81	0	14,15,17	2.28	6 (42%)
2	MAN	A	933	2	11,11,12	1.57	1 (9%)	14,15,17	1.67	3 (21%)
2	NAG	A	934	1,2	14,14,15	0.99	0	15,19,21	1.15	2 (13%)
2	NAG	A	935	2	14,14,15	1.29	2 (14%)	15,19,21	1.08	1 (6%)
2	BMA	A	936	2	11,11,12	1.44	1 (9%)	14,15,17	1.90	3 (21%)
2	MAN	A	937	2	11,11,12	1.18	0	14,15,17	1.23	1 (7%)
2	MAN	A	938	2	11,11,12	1.23	0	14,15,17	2.39	6 (42%)
2	MAN	A	939	2	11,11,12	1.00	1 (9%)	14,15,17	1.90	4 (28%)
2	MAN	A	940	2	11,11,12	1.98	2 (18%)	14,15,17	1.26	1 (7%)
2	NAG	B	901	1,2	14,14,15	1.38	3 (21%)	15,19,21	1.89	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	902	2	14,14,15	0.88	0	15,19,21	2.13	5 (33%)
2	BMA	B	903	2	11,11,12	1.86	2 (18%)	14,15,17	1.80	4 (28%)
2	MAN	B	904	2	11,11,12	0.68	0	14,15,17	1.76	4 (28%)
2	MAN	B	905	2	11,11,12	1.06	1 (9%)	14,15,17	1.13	0
2	MAN	B	906	2	11,11,12	0.87	0	14,15,17	1.41	2 (14%)
2	MAN	B	907	2	11,11,12	0.67	0	14,15,17	1.95	5 (35%)
9	NAG	B	909	1,9	14,14,15	0.88	0	15,19,21	1.50	2 (13%)
9	NAG	B	910	9	14,14,15	1.62	6 (42%)	15,19,21	1.84	6 (40%)
9	BMA	B	911	9	11,11,12	1.13	1 (9%)	14,15,17	2.00	5 (35%)
9	MAN	B	912	9	11,11,12	1.27	1 (9%)	14,15,17	1.39	2 (14%)
9	MAN	B	913	9	11,11,12	0.82	0	14,15,17	1.68	3 (21%)
9	MAN	B	914	9	11,11,12	0.84	0	14,15,17	2.19	3 (21%)
4	NAG	B	915	1,4	14,14,15	0.85	0	15,19,21	0.93	1 (6%)
4	NAG	B	916	4	14,14,15	0.80	0	15,19,21	1.73	4 (26%)
4	BMA	B	917	4	11,11,12	0.91	0	14,15,17	2.00	5 (35%)
6	NAG	B	918	1,6	14,14,15	1.28	1 (7%)	15,19,21	1.28	1 (6%)
6	NAG	B	919	6	14,14,15	1.53	2 (14%)	15,19,21	1.45	2 (13%)
6	BMA	B	920	6	11,11,12	1.15	1 (9%)	14,15,17	1.28	1 (7%)
6	MAN	B	921	6	11,11,12	0.91	1 (9%)	14,15,17	2.50	6 (42%)
6	MAN	B	922	6	11,11,12	1.12	1 (9%)	14,15,17	2.30	4 (28%)
6	MAN	B	923	6	11,11,12	0.90	0	14,15,17	1.28	2 (14%)
6	MAN	B	924	6	11,11,12	0.93	0	14,15,17	2.11	5 (35%)
6	MAN	B	925	6	11,11,12	1.16	0	14,15,17	1.98	5 (35%)
6	MAN	B	926	6	11,11,12	0.80	0	14,15,17	2.12	4 (28%)
6	MAN	B	927	6	11,11,12	1.16	1 (9%)	14,15,17	1.51	1 (7%)
4	NAG	B	928	1,4	14,14,15	1.14	1 (7%)	15,19,21	1.48	4 (26%)
4	NAG	B	929	4	14,14,15	1.35	3 (21%)	15,19,21	3.15	8 (53%)
4	BMA	B	930	4	11,11,12	1.38	1 (9%)	14,15,17	3.05	8 (57%)
2	NAG	B	931	1,2	14,14,15	1.03	1 (7%)	15,19,21	0.82	0
2	NAG	B	932	2	14,14,15	1.13	1 (7%)	15,19,21	1.65	4 (26%)
2	BMA	B	933	2	11,11,12	1.33	2 (18%)	14,15,17	2.17	4 (28%)
2	MAN	B	934	2	11,11,12	1.26	2 (18%)	14,15,17	2.37	6 (42%)
2	MAN	B	935	2	11,11,12	0.86	0	14,15,17	1.75	5 (35%)
2	MAN	B	936	2	11,11,12	1.21	1 (9%)	14,15,17	1.81	5 (35%)
2	MAN	B	937	2	11,11,12	0.96	0	14,15,17	1.85	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	B	938	1,10	14,14,15	0.96	1 (7%)	15,19,21	1.92	3 (20%)
10	NAG	B	939	10	14,14,15	0.79	0	15,19,21	1.00	1 (6%)
10	BMA	B	940	10	11,11,12	1.27	2 (18%)	14,15,17	3.56	6 (42%)
10	MAN	B	941	10	11,11,12	1.09	1 (9%)	14,15,17	2.26	6 (42%)
10	MAN	B	942	10	11,11,12	1.04	1 (9%)	14,15,17	2.13	5 (35%)
10	MAN	B	943	10	11,11,12	1.07	0	14,15,17	1.86	3 (21%)
10	MAN	B	944	10	11,11,12	0.86	0	14,15,17	3.74	8 (57%)
10	MAN	B	945	10	11,11,12	1.02	1 (9%)	14,15,17	2.88	8 (57%)

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
2	MAN	A	906	2	-	0/2/19/22	0/1/1/1
2	MAN	A	907	2	-	0/2/19/22	0/1/1/1
4	NAG	A	909	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	910	4	-	0/6/23/26	0/1/1/1
4	BMA	A	911	4	-	0/2/19/22	0/1/1/1
5	NAG	A	912	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	913	5	-	0/6/23/26	0/1/1/1
6	NAG	A	914	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	915	6	-	0/6/23/26	0/1/1/1
6	BMA	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
6	MAN	A	921	6	-	0/2/19/22	0/1/1/1
6	MAN	A	922	6	-	0/2/19/22	0/1/1/1
6	MAN	A	923	6	-	0/2/19/22	0/1/1/1
4	NAG	A	924	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	925	4	-	0/6/23/26	0/1/1/1
4	BMA	A	926	4	-	0/2/19/22	0/1/1/1
2	NAG	A	927	1,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	928	2	-	0/6/23/26	0/1/1/1
2	BMA	A	929	2	-	0/2/19/22	0/1/1/1
2	MAN	A	930	2	-	0/2/19/22	0/1/1/1
2	MAN	A	931	2	-	0/2/19/22	0/1/1/1
2	MAN	A	932	2	-	0/2/19/22	0/1/1/1
2	MAN	A	933	2	-	0/2/19/22	0/1/1/1
2	NAG	A	934	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	935	2	-	0/6/23/26	0/1/1/1
2	BMA	A	936	2	-	0/2/19/22	0/1/1/1
2	MAN	A	937	2	-	0/2/19/22	0/1/1/1
2	MAN	A	938	2	-	0/2/19/22	0/1/1/1
2	MAN	A	939	2	-	0/2/19/22	0/1/1/1
2	MAN	A	940	2	-	0/2/19/22	0/1/1/1
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	902	2	-	0/6/23/26	0/1/1/1
2	BMA	B	903	2	-	0/2/19/22	0/1/1/1
2	MAN	B	904	2	-	0/2/19/22	0/1/1/1
2	MAN	B	905	2	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	0/2/19/22	0/1/1/1
2	MAN	B	907	2	-	0/2/19/22	0/1/1/1
9	NAG	B	909	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	910	9	-	0/6/23/26	0/1/1/1
9	BMA	B	911	9	-	0/2/19/22	0/1/1/1
9	MAN	B	912	9	-	0/2/19/22	0/1/1/1
9	MAN	B	913	9	-	0/2/19/22	0/1/1/1
9	MAN	B	914	9	-	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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	931	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	932	2	-	0/6/23/26	0/1/1/1
2	BMA	B	933	2	-	0/2/19/22	0/1/1/1
2	MAN	B	934	2	-	0/2/19/22	0/1/1/1
2	MAN	B	935	2	-	0/2/19/22	0/1/1/1
2	MAN	B	936	2	-	0/2/19/22	0/1/1/1
2	MAN	B	937	2	-	0/2/19/22	0/1/1/1
10	NAG	B	938	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	939	10	-	0/6/23/26	0/1/1/1
10	BMA	B	940	10	-	0/2/19/22	0/1/1/1
10	MAN	B	941	10	-	0/2/19/22	0/1/1/1
10	MAN	B	942	10	-	0/2/19/22	0/1/1/1
10	MAN	B	943	10	-	0/2/19/22	0/1/1/1
10	MAN	B	944	10	-	0/2/19/22	0/1/1/1
10	MAN	B	945	10	-	0/2/19/22	0/1/1/1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	940	MAN	O5-C1	-4.90	1.35	1.43
2	A	936	BMA	O5-C1	-3.74	1.37	1.43
2	A	935	NAG	O5-C1	-2.98	1.38	1.43
2	A	927	NAG	O5-C5	-2.84	1.37	1.43
6	A	922	MAN	O3-C3	-2.71	1.36	1.43
6	A	917	MAN	C2-C3	-2.70	1.48	1.52
6	A	918	MAN	O5-C1	-2.69	1.39	1.43
4	A	910	NAG	O5-C1	-2.63	1.39	1.43
5	A	913	NAG	C8-C7	-2.63	1.45	1.50
2	B	933	BMA	O4-C4	-2.56	1.36	1.43
6	B	922	MAN	O5-C1	-2.55	1.39	1.43
9	B	910	NAG	O5-C1	-2.52	1.39	1.43
2	A	935	NAG	C2-N2	-2.42	1.42	1.46
2	B	932	NAG	C2-N2	-2.39	1.42	1.46
5	A	912	NAG	C1-C2	-2.38	1.49	1.52
10	B	938	NAG	O3-C3	-2.38	1.37	1.43
2	B	901	NAG	O5-C1	-2.32	1.39	1.43
10	B	940	BMA	O4-C4	-2.31	1.37	1.43
6	A	917	MAN	O3-C3	-2.31	1.37	1.43
10	B	940	BMA	O5-C1	-2.30	1.39	1.43
5	A	912	NAG	O5-C5	-2.28	1.38	1.43
4	A	924	NAG	O4-C4	-2.25	1.37	1.43
6	B	921	MAN	O3-C3	-2.24	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	920	BMA	O5-C5	-2.20	1.38	1.43
6	A	922	MAN	O4-C4	-2.17	1.37	1.43
6	A	917	MAN	O4-C4	-2.15	1.37	1.43
10	B	942	MAN	O3-C3	-2.14	1.37	1.43
6	A	920	MAN	O5-C1	-2.08	1.40	1.43
9	B	910	NAG	C4-C5	2.00	1.57	1.53
2	B	934	MAN	C1-C2	2.01	1.57	1.52
2	A	904	MAN	C1-C2	2.06	1.57	1.52
9	B	910	NAG	C1-C2	2.06	1.55	1.52
5	A	913	NAG	O7-C7	2.07	1.28	1.23
6	A	914	NAG	C8-C7	2.09	1.54	1.50
2	A	901	NAG	C1-C2	2.13	1.55	1.52
9	B	910	NAG	C3-C2	2.18	1.57	1.52
6	A	919	MAN	C2-C3	2.19	1.55	1.52
9	B	910	NAG	O7-C7	2.22	1.28	1.23
4	A	926	BMA	C1-C2	2.23	1.57	1.52
9	B	911	BMA	C2-C3	2.24	1.55	1.52
4	B	928	NAG	C8-C7	2.27	1.55	1.50
2	B	905	MAN	C1-C2	2.28	1.57	1.52
4	B	929	NAG	C1-C2	2.30	1.55	1.52
6	A	914	NAG	C4-C3	2.31	1.58	1.52
2	B	931	NAG	C4-C5	2.42	1.58	1.53
4	A	910	NAG	C3-C2	2.47	1.58	1.52
10	B	941	MAN	C2-C3	2.47	1.55	1.52
6	B	927	MAN	O5-C5	2.47	1.48	1.43
6	A	920	MAN	C4-C3	2.47	1.58	1.52
2	B	936	MAN	C1-C2	2.49	1.58	1.52
4	B	929	NAG	C4-C5	2.50	1.58	1.53
2	B	933	BMA	C1-C2	2.52	1.58	1.52
6	A	920	MAN	C1-C2	2.53	1.58	1.52
4	A	926	BMA	C2-C3	2.54	1.56	1.52
6	A	917	MAN	O5-C1	2.57	1.48	1.43
2	A	901	NAG	C8-C7	2.58	1.55	1.50
2	B	901	NAG	C4-C5	2.61	1.58	1.53
2	B	903	BMA	C4-C5	2.66	1.58	1.53
2	B	901	NAG	C1-C2	2.66	1.56	1.52
2	A	939	MAN	C2-C3	2.66	1.56	1.52
4	B	929	NAG	O7-C7	2.79	1.29	1.23
9	B	910	NAG	C8-C7	2.82	1.56	1.50
6	B	919	NAG	C4-C3	2.85	1.59	1.52
10	B	945	MAN	C2-C3	2.86	1.56	1.52
4	B	930	BMA	C2-C3	3.01	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	933	MAN	C4-C5	3.13	1.59	1.53
6	A	914	NAG	C2-N2	3.15	1.51	1.46
2	A	902	NAG	C1-C2	3.21	1.56	1.52
2	B	934	MAN	C2-C3	3.23	1.56	1.52
2	A	929	BMA	C2-C3	3.32	1.57	1.52
9	B	912	MAN	C2-C3	3.37	1.57	1.52
6	B	918	NAG	C1-C2	3.65	1.57	1.52
6	B	919	NAG	C1-C2	3.75	1.57	1.52
2	A	940	MAN	C2-C3	4.15	1.58	1.52
2	B	903	BMA	C2-C3	4.77	1.59	1.52

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	929	NAG	C1-O5-C5	-8.67	101.25	112.25
10	B	940	BMA	C6-C5-C4	-7.37	94.84	113.02
2	A	904	MAN	O2-C2-C3	-5.08	99.91	110.12
4	B	930	BMA	O5-C1-C2	-5.01	102.74	110.86
10	B	942	MAN	O2-C2-C1	-4.77	99.65	109.21
2	A	903	BMA	O3-C3-C2	-4.76	101.39	110.00
2	B	902	NAG	O6-C6-C5	-4.74	95.67	111.33
9	B	914	MAN	C1-C2-C3	-4.65	104.04	109.54
4	B	917	BMA	O4-C4-C3	-4.65	99.88	110.34
2	A	938	MAN	O2-C2-C3	-4.59	100.90	110.12
4	B	929	NAG	C2-N2-C7	-4.53	117.22	123.04
6	B	924	MAN	O6-C6-C5	-4.35	96.95	111.33
4	B	916	NAG	C3-C4-C5	-4.34	102.63	110.20
2	A	905	MAN	O2-C2-C3	-4.30	101.47	110.12
4	A	925	NAG	C2-N2-C7	-4.30	117.52	123.04
2	B	901	NAG	C4-C3-C2	-4.27	104.58	111.23
2	A	927	NAG	C3-C2-N2	-4.19	100.52	110.56
2	A	904	MAN	O6-C6-C5	-4.09	97.83	111.33
2	A	905	MAN	C2-C3-C4	-3.98	104.27	111.04
5	A	912	NAG	O4-C4-C5	-3.95	98.77	109.24
2	A	906	MAN	O6-C6-C5	-3.93	98.34	111.33
6	B	922	MAN	O6-C6-C5	-3.92	98.39	111.33
10	B	945	MAN	C6-C5-C4	-3.90	103.40	113.02
6	B	921	MAN	O3-C3-C2	-3.90	102.96	110.00
2	B	907	MAN	O4-C4-C3	-3.86	101.64	110.34
6	B	922	MAN	C6-C5-C4	-3.77	103.72	113.02
4	A	910	NAG	C3-C4-C5	-3.65	103.84	110.20
10	B	940	BMA	O6-C6-C5	-3.64	99.30	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	915	NAG	O4-C4-C3	-3.61	102.20	110.34
10	B	944	MAN	C1-C2-C3	-3.57	105.31	109.54
6	B	919	NAG	C1-O5-C5	-3.56	107.73	112.25
6	B	925	MAN	O2-C2-C1	-3.54	102.12	109.21
2	B	902	NAG	O7-C7-C8	-3.52	115.61	122.06
2	A	929	BMA	O2-C2-C1	-3.48	102.23	109.21
2	A	932	MAN	O3-C3-C4	-3.48	102.50	110.34
2	B	933	BMA	O2-C2-C1	-3.46	102.27	109.21
2	B	903	BMA	C1-C2-C3	-3.43	105.48	109.54
2	A	938	MAN	C3-C4-C5	-3.40	104.27	110.20
2	A	938	MAN	O3-C3-C2	-3.39	103.86	110.00
10	B	943	MAN	O2-C2-C3	-3.38	103.31	110.12
4	A	911	BMA	O2-C2-C3	-3.36	103.36	110.12
2	A	932	MAN	C6-C5-C4	-3.32	104.82	113.02
4	B	929	NAG	O7-C7-C8	-3.32	115.97	122.06
6	B	921	MAN	O2-C2-C3	-3.31	103.45	110.12
2	B	936	MAN	C6-C5-C4	-3.30	104.86	113.02
2	A	928	NAG	C2-N2-C7	-3.28	118.83	123.04
2	B	904	MAN	O3-C3-C2	-3.26	104.10	110.00
2	A	931	MAN	O2-C2-C1	-3.26	102.67	109.21
5	A	913	NAG	C3-C4-C5	-3.23	104.57	110.20
5	A	913	NAG	O4-C4-C3	-3.18	103.18	110.34
2	B	901	NAG	O4-C4-C3	-3.16	103.22	110.34
2	A	905	MAN	O6-C6-C5	-3.15	100.94	111.33
9	B	910	NAG	C4-C3-C2	-3.12	106.37	111.23
6	B	926	MAN	O2-C2-C1	-3.11	102.97	109.21
6	B	922	MAN	O5-C5-C6	-3.09	100.66	107.35
6	B	925	MAN	C1-C2-C3	-3.08	105.89	109.54
10	B	943	MAN	O4-C4-C3	-3.08	103.40	110.34
2	A	902	NAG	O6-C6-C5	-3.08	101.17	111.33
2	B	936	MAN	C2-C3-C4	-3.07	105.83	111.04
6	B	920	BMA	C2-C3-C4	-3.07	105.83	111.04
2	B	902	NAG	C2-N2-C7	-3.06	119.11	123.04
6	A	917	MAN	O4-C4-C3	-3.05	103.48	110.34
10	B	941	MAN	O3-C3-C4	-3.04	103.50	110.34
9	B	911	BMA	O3-C3-C4	-3.03	103.52	110.34
6	B	921	MAN	C3-C4-C5	-3.02	104.93	110.20
6	A	920	MAN	C1-C2-C3	-2.98	106.02	109.54
9	B	909	NAG	C4-C3-C2	-2.97	106.61	111.23
2	A	930	MAN	O5-C1-C2	-2.97	106.05	110.86
2	B	904	MAN	C2-C3-C4	-2.95	106.03	111.04
10	B	942	MAN	O3-C3-C4	-2.93	103.73	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	934	MAN	C1-O5-C5	-2.91	108.56	112.25
6	A	917	MAN	C3-C4-C5	-2.88	105.18	110.20
2	B	903	BMA	C2-C3-C4	-2.87	106.16	111.04
4	B	916	NAG	O6-C6-C5	-2.87	101.84	111.33
9	B	914	MAN	O6-C6-C5	-2.83	101.97	111.33
6	A	918	MAN	O5-C5-C6	-2.83	101.22	107.35
2	B	934	MAN	O6-C6-C5	-2.82	102.01	111.33
2	A	928	NAG	O4-C4-C3	-2.82	103.99	110.34
2	A	903	BMA	C2-C3-C4	-2.81	106.27	111.04
2	A	939	MAN	C6-C5-C4	-2.78	106.16	113.02
4	B	930	BMA	C6-C5-C4	-2.76	106.20	113.02
4	B	917	BMA	C1-O5-C5	-2.76	108.75	112.25
9	B	909	NAG	C3-C2-N2	-2.73	104.03	110.56
2	A	940	MAN	O2-C2-C1	-2.71	103.78	109.21
2	A	936	BMA	O4-C4-C5	-2.69	102.11	109.24
4	A	924	NAG	O4-C4-C3	-2.68	104.30	110.34
2	A	933	MAN	C2-C3-C4	-2.67	106.50	111.04
2	B	936	MAN	C1-C2-C3	-2.66	106.40	109.54
5	A	913	NAG	O6-C6-C5	-2.65	102.57	111.33
9	B	910	NAG	O4-C4-C5	-2.65	102.22	109.24
4	A	910	NAG	C4-C3-C2	-2.65	107.12	111.23
6	B	925	MAN	O3-C3-C2	-2.63	105.24	110.00
10	B	944	MAN	O2-C2-C1	-2.61	103.97	109.21
2	B	932	NAG	O4-C4-C3	-2.61	104.46	110.34
4	A	911	BMA	O4-C4-C5	-2.61	102.33	109.24
9	B	911	BMA	C3-C4-C5	-2.61	105.65	110.20
6	B	924	MAN	C6-C5-C4	-2.60	106.61	113.02
6	A	923	MAN	O2-C2-C1	-2.60	104.00	109.21
9	B	910	NAG	O6-C6-C5	-2.58	102.79	111.33
9	B	910	NAG	C1-O5-C5	-2.58	108.97	112.25
2	B	907	MAN	C3-C4-C5	-2.58	105.70	110.20
2	A	904	MAN	C2-C3-C4	-2.57	106.67	111.04
6	A	915	NAG	C1-O5-C5	-2.56	109.00	112.25
6	A	916	BMA	O6-C6-C5	-2.55	102.92	111.33
2	B	934	MAN	O4-C4-C5	-2.54	102.51	109.24
2	B	933	BMA	O4-C4-C5	-2.53	102.55	109.24
6	A	914	NAG	C2-N2-C7	-2.52	119.80	123.04
2	B	904	MAN	O6-C6-C5	-2.51	103.03	111.33
2	B	937	MAN	C1-C2-C3	-2.51	106.57	109.54
2	A	906	MAN	C2-C3-C4	-2.51	106.78	111.04
2	A	906	MAN	O2-C2-C3	-2.50	105.08	110.12
4	B	930	BMA	O4-C4-C3	-2.50	104.71	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	929	NAG	C3-C4-C5	-2.49	105.85	110.20
10	B	942	MAN	O4-C4-C3	-2.48	104.75	110.34
4	A	910	NAG	O6-C6-C5	-2.47	103.16	111.33
10	B	938	NAG	O4-C4-C5	-2.46	102.73	109.24
4	B	928	NAG	C4-C3-C2	-2.45	107.42	111.23
2	B	937	MAN	O4-C4-C3	-2.43	104.87	110.34
2	A	904	MAN	O5-C1-C2	-2.43	106.92	110.86
6	B	918	NAG	C2-N2-C7	-2.41	119.94	123.04
6	A	922	MAN	O6-C6-C5	-2.40	103.39	111.33
4	A	910	NAG	C1-O5-C5	-2.40	109.20	112.25
6	B	923	MAN	C1-C2-C3	-2.40	106.70	109.54
4	A	909	NAG	C3-C2-N2	-2.40	104.82	110.56
4	B	928	NAG	O4-C4-C3	-2.40	104.94	110.34
9	B	913	MAN	O3-C3-C4	-2.38	104.99	110.34
2	B	932	NAG	O6-C6-C5	-2.37	103.50	111.33
2	B	936	MAN	O6-C6-C5	-2.34	103.60	111.33
4	A	909	NAG	C4-C3-C2	-2.33	107.61	111.23
2	B	937	MAN	C2-C3-C4	-2.31	107.11	111.04
6	B	926	MAN	O6-C6-C5	-2.30	103.72	111.33
4	A	911	BMA	O3-C3-C2	-2.29	105.86	110.00
10	B	940	BMA	O4-C4-C5	-2.29	103.17	109.24
2	A	939	MAN	O6-C6-C5	-2.29	103.77	111.33
4	A	910	NAG	O3-C3-C2	-2.29	104.59	109.11
2	B	902	NAG	O4-C4-C5	-2.28	103.18	109.24
2	B	937	MAN	O6-C6-C5	-2.28	103.79	111.33
2	A	930	MAN	C1-C2-C3	-2.28	106.84	109.54
10	B	939	NAG	O6-C6-C5	-2.28	103.80	111.33
10	B	945	MAN	O2-C2-C1	-2.27	104.65	109.21
2	A	901	NAG	C6-C5-C4	-2.27	107.42	113.02
2	A	938	MAN	O6-C6-C5	-2.26	103.87	111.33
10	B	938	NAG	C3-C4-C5	-2.26	106.26	110.20
6	B	919	NAG	O4-C4-C3	-2.26	105.26	110.34
6	A	916	BMA	O3-C3-C2	-2.24	105.95	110.00
2	B	903	BMA	O3-C3-C4	-2.24	105.30	110.34
4	B	928	NAG	O3-C3-C2	-2.24	104.68	109.11
2	A	935	NAG	O6-C6-C5	-2.23	103.95	111.33
6	B	924	MAN	O4-C4-C5	-2.22	103.35	109.24
10	B	945	MAN	O3-C3-C4	-2.22	105.34	110.34
6	A	917	MAN	O4-C4-C5	-2.21	103.39	109.24
6	A	919	MAN	C1-C2-C3	-2.20	106.94	109.54
2	A	928	NAG	O6-C6-C5	-2.20	104.08	111.33
9	B	910	NAG	C2-N2-C7	-2.19	120.22	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	913	NAG	O7-C7-C8	-2.18	118.06	122.06
4	A	911	BMA	C6-C5-C4	-2.17	107.65	113.02
2	A	927	NAG	O3-C3-C2	-2.17	104.81	109.11
2	A	929	BMA	C1-O5-C5	-2.15	109.52	112.25
2	A	929	BMA	C6-C5-C4	-2.14	107.73	113.02
4	A	926	BMA	C2-C3-C4	-2.14	107.41	111.04
9	B	911	BMA	O5-C1-C2	-2.13	107.41	110.86
4	A	924	NAG	C4-C3-C2	-2.10	107.97	111.23
6	B	921	MAN	C6-C5-C4	-2.10	107.84	113.02
4	B	916	NAG	O7-C7-C8	-2.09	118.22	122.06
10	B	941	MAN	O4-C4-C3	-2.08	105.65	110.34
2	A	904	MAN	C6-C5-C4	-2.08	107.89	113.02
6	A	917	MAN	C6-C5-C4	-2.05	107.96	113.02
2	B	935	MAN	O4-C4-C5	-2.04	103.83	109.24
2	A	932	MAN	O6-C6-C5	-2.04	104.59	111.33
10	B	944	MAN	O4-C4-C5	-2.03	103.85	109.24
2	B	906	MAN	C1-C2-C3	-2.03	107.14	109.54
2	B	903	BMA	C6-C5-C4	-2.02	108.04	113.02
2	A	932	MAN	O2-C2-C3	-2.01	106.07	110.12
2	A	934	NAG	C4-C3-C2	-2.00	108.11	111.23
2	A	907	MAN	O3-C3-C4	2.00	114.84	110.34
10	B	944	MAN	C3-C4-C5	2.01	113.70	110.20
4	B	915	NAG	C3-C4-C5	2.01	113.71	110.20
6	A	915	NAG	C3-C2-N2	2.02	115.39	110.56
2	A	937	MAN	C1-C2-C3	2.03	111.95	109.54
2	A	938	MAN	O2-C2-C1	2.06	113.34	109.21
10	B	940	BMA	O5-C1-C2	2.07	114.21	110.86
2	A	904	MAN	O2-C2-C1	2.07	113.36	109.21
6	A	923	MAN	O3-C3-C2	2.08	113.76	110.00
10	B	942	MAN	C1-O5-C5	2.09	114.90	112.25
5	A	913	NAG	O5-C5-C6	2.12	111.94	107.35
2	B	935	MAN	O3-C3-C2	2.12	113.83	110.00
2	A	932	MAN	O4-C4-C3	2.12	115.12	110.34
2	B	933	BMA	O2-C2-C3	2.13	114.40	110.12
6	A	918	MAN	O2-C2-C1	2.13	113.48	109.21
2	A	934	NAG	O5-C5-C6	2.14	111.98	107.35
4	B	917	BMA	C6-C5-C4	2.15	118.31	113.02
10	B	944	MAN	O5-C5-C6	2.17	112.04	107.35
2	B	907	MAN	O5-C5-C6	2.17	112.04	107.35
6	A	922	MAN	O5-C1-C2	2.17	114.38	110.86
6	A	921	MAN	C1-O5-C5	2.18	115.01	112.25
6	A	919	MAN	O3-C3-C2	2.18	113.94	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	936	MAN	O2-C2-C1	2.20	113.62	109.21
2	A	930	MAN	O5-C5-C6	2.21	112.13	107.35
2	B	932	NAG	O7-C7-C8	2.22	126.14	122.06
4	B	928	NAG	O7-C7-C8	2.24	126.17	122.06
2	B	901	NAG	O7-C7-N2	2.25	126.45	121.86
2	A	906	MAN	O4-C4-C3	2.28	115.47	110.34
2	B	904	MAN	O5-C5-C6	2.29	112.31	107.35
4	B	917	BMA	O5-C5-C6	2.29	112.32	107.35
5	A	913	NAG	C2-N2-C7	2.32	126.02	123.04
4	A	926	BMA	C1-O5-C5	2.34	115.22	112.25
4	B	917	BMA	O3-C3-C2	2.36	114.26	110.00
6	A	922	MAN	C1-O5-C5	2.36	115.25	112.25
9	B	912	MAN	O4-C4-C5	2.38	115.54	109.24
2	B	935	MAN	O5-C5-C6	2.39	112.52	107.35
9	B	913	MAN	C1-C2-C3	2.41	112.39	109.54
4	B	916	NAG	O5-C5-C6	2.42	112.59	107.35
2	A	936	BMA	C1-O5-C5	2.43	115.34	112.25
10	B	942	MAN	O5-C1-C2	2.44	114.82	110.86
6	B	926	MAN	O5-C1-C2	2.45	114.83	110.86
6	A	923	MAN	O5-C5-C6	2.46	112.67	107.35
2	B	902	NAG	C1-O5-C5	2.46	115.37	112.25
10	B	941	MAN	O2-C2-C1	2.46	114.14	109.21
4	B	930	BMA	C1-C2-C3	2.46	112.46	109.54
2	B	935	MAN	O3-C3-C4	2.49	115.93	110.34
9	B	912	MAN	C1-O5-C5	2.49	115.41	112.25
4	B	929	NAG	O5-C5-C6	2.52	112.79	107.35
4	B	929	NAG	O7-C7-N2	2.54	127.04	121.86
5	A	912	NAG	C2-N2-C7	2.58	126.36	123.04
2	B	907	MAN	C6-C5-C4	2.61	119.45	113.02
2	B	937	MAN	O2-C2-C1	2.67	114.56	109.21
4	A	911	BMA	O6-C6-C5	2.68	120.18	111.33
2	A	902	NAG	C6-C5-C4	2.70	119.68	113.02
2	A	939	MAN	O3-C3-C2	2.77	115.00	110.00
2	A	906	MAN	O5-C5-C6	2.77	113.35	107.35
6	B	924	MAN	O5-C1-C2	2.78	115.36	110.86
6	B	923	MAN	C1-O5-C5	2.81	115.81	112.25
6	B	925	MAN	O5-C5-C6	2.82	113.45	107.35
9	B	911	BMA	O3-C3-C2	2.82	115.09	110.00
2	A	905	MAN	O5-C1-C2	2.82	115.44	110.86
4	B	930	BMA	O5-C5-C6	2.86	113.54	107.35
2	A	904	MAN	C1-C2-C3	2.89	112.96	109.54
2	A	906	MAN	O3-C3-C4	2.91	116.89	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	905	MAN	O2-C2-C1	2.92	115.06	109.21
4	B	929	NAG	C3-C2-N2	2.93	117.58	110.56
2	B	932	NAG	C6-C5-C4	2.95	120.30	113.02
9	B	910	NAG	C6-C5-C4	2.99	120.40	113.02
6	A	916	BMA	C1-O5-C5	3.01	116.07	112.25
2	B	935	MAN	C1-O5-C5	3.04	116.10	112.25
2	B	906	MAN	O3-C3-C2	3.04	115.50	110.00
2	A	933	MAN	C1-O5-C5	3.07	116.14	112.25
6	A	918	MAN	O2-C2-C3	3.07	116.29	110.12
10	B	945	MAN	O5-C5-C6	3.11	114.07	107.35
6	B	925	MAN	C1-O5-C5	3.11	116.19	112.25
10	B	945	MAN	C2-C3-C4	3.12	116.35	111.04
6	A	920	MAN	C1-O5-C5	3.15	116.24	112.25
4	B	929	NAG	C6-C5-C4	3.18	120.85	113.02
4	A	926	BMA	O5-C5-C6	3.20	114.28	107.35
2	A	933	MAN	C3-C4-C5	3.21	115.79	110.20
4	A	926	BMA	O2-C2-C1	3.22	115.66	109.21
10	B	941	MAN	O2-C2-C3	3.23	116.61	110.12
5	A	912	NAG	C1-O5-C5	3.26	116.38	112.25
6	A	918	MAN	O5-C1-C2	3.38	116.34	110.86
2	A	930	MAN	C2-C3-C4	3.45	116.90	111.04
6	A	918	MAN	C1-C2-C3	3.51	113.69	109.54
2	A	927	NAG	C1-O5-C5	3.55	116.75	112.25
4	A	925	NAG	C4-C3-C2	3.55	116.75	111.23
6	B	927	MAN	C1-O5-C5	3.56	116.76	112.25
2	A	904	MAN	O5-C5-C6	3.61	115.17	107.35
2	B	937	MAN	C1-O5-C5	3.66	116.89	112.25
10	B	944	MAN	O5-C1-C2	3.66	116.80	110.86
2	B	934	MAN	C2-C3-C4	3.70	117.32	111.04
4	A	910	NAG	C6-C5-C4	3.72	122.20	113.02
6	B	924	MAN	C1-O5-C5	3.73	116.98	112.25
4	B	930	BMA	O3-C3-C2	3.75	116.77	110.00
10	B	943	MAN	C6-C5-C4	3.79	122.36	113.02
9	B	911	BMA	C1-O5-C5	3.80	117.07	112.25
2	A	938	MAN	C6-C5-C4	3.81	122.42	113.02
2	B	934	MAN	O5-C5-C6	3.81	115.61	107.35
2	B	907	MAN	O3-C3-C2	3.83	116.91	110.00
4	A	926	BMA	O3-C3-C4	3.89	119.09	110.34
10	B	945	MAN	C1-C2-C3	3.89	114.14	109.54
2	B	934	MAN	C1-C2-C3	3.90	114.16	109.54
10	B	945	MAN	O2-C2-C3	3.91	117.97	110.12
6	A	917	MAN	C1-O5-C5	3.96	117.28	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	913	MAN	O5-C5-C6	4.07	116.16	107.35
6	B	921	MAN	C1-O5-C5	4.07	117.42	112.25
10	B	941	MAN	C3-C4-C5	4.10	117.34	110.20
2	A	903	BMA	C3-C4-C5	4.12	117.39	110.20
10	B	940	BMA	C3-C4-C5	4.15	117.42	110.20
10	B	941	MAN	C2-C3-C4	4.33	118.39	111.04
2	A	936	BMA	C1-C2-C3	4.54	114.91	109.54
4	B	930	BMA	C3-C4-C5	4.63	118.27	110.20
2	A	939	MAN	C1-O5-C5	4.69	118.20	112.25
10	B	944	MAN	O2-C2-C3	4.69	119.56	110.12
2	A	929	BMA	O3-C3-C2	4.71	118.52	110.00
4	A	924	NAG	C1-O5-C5	4.79	118.33	112.25
6	B	922	MAN	C1-O5-C5	4.82	118.36	112.25
6	B	921	MAN	C1-C2-C3	4.91	115.35	109.54
9	B	914	MAN	C1-O5-C5	4.98	118.57	112.25
10	B	938	NAG	C1-O5-C5	5.08	118.70	112.25
2	A	932	MAN	C1-O5-C5	5.43	119.14	112.25
6	A	918	MAN	C1-O5-C5	5.62	119.39	112.25
4	B	930	BMA	C1-O5-C5	5.63	119.40	112.25
6	B	926	MAN	C1-O5-C5	5.65	119.42	112.25
2	B	933	BMA	O3-C3-C2	5.69	120.27	110.00
4	A	911	BMA	C3-C4-C5	5.69	120.11	110.20
10	B	945	MAN	C1-O5-C5	6.04	119.91	112.25
4	A	911	BMA	C1-C2-C3	6.28	116.97	109.54
10	B	940	BMA	C1-O5-C5	8.90	123.54	112.25
10	B	944	MAN	C1-O5-C5	11.05	126.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	BMA	1	0
2	A	907	MAN	1	0
4	A	909	NAG	2	0
5	A	913	NAG	3	0
2	A	929	BMA	1	0
2	B	902	NAG	1	0
2	B	933	BMA	3	0
2	B	935	MAN	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	940	BMA	3	0
10	B	942	MAN	2	0
10	B	945	MAN	1	0

5.6 Ligand geometry [i](#)

11 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	908	1	14,14,15	1.13	1 (7%)	15,19,21	1.02	2 (13%)
3	NAG	A	941	1	14,14,15	0.87	0	15,19,21	2.13	6 (40%)
7	MRD	A	942	-	6,7,7	1.17	1 (16%)	7,10,10	1.02	0
7	MRD	A	943	-	6,7,7	0.82	0	7,10,10	1.05	0
8	TCB	A	944	-	24,24,24	1.82	5 (20%)	28,35,35	1.75	8 (28%)
3	NAG	B	908	1	14,14,15	1.11	2 (14%)	15,19,21	3.34	8 (53%)
3	NAG	B	946	1	14,14,15	1.13	2 (14%)	15,19,21	1.62	2 (13%)
3	NAG	B	947	1	14,14,15	0.84	0	15,19,21	1.12	0
7	MRD	B	948	-	6,7,7	0.52	0	7,10,10	1.05	0
7	MRD	B	949	-	6,7,7	1.10	1 (16%)	7,10,10	0.71	0
8	TCB	B	950	-	24,24,24	2.34	6 (25%)	28,35,35	2.54	10 (35%)

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	908	1	-	0/6/23/26	0/1/1/1
3	NAG	A	941	1	-	0/6/23/26	0/1/1/1
7	MRD	A	942	-	-	0/5/5/5	0/0/0/0
7	MRD	A	943	-	-	0/5/5/5	0/0/0/0
8	TCB	A	944	-	-	0/8/48/48	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
7	MRD	B	948	-	-	0/5/5/5	0/0/0/0
7	MRD	B	949	-	-	0/5/5/5	0/0/0/0
8	TCB	B	950	-	-	0/8/48/48	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	908	NAG	O5-C1	-2.96	1.38	1.43
3	B	908	NAG	O5-C1	-2.78	1.39	1.43
8	A	944	TCB	C3'-C4'	-2.64	1.50	1.53
7	B	949	MRD	O2-C2	-2.29	1.38	1.44
3	B	908	NAG	O3-C3	-2.23	1.37	1.43
3	B	946	NAG	O5-C5	-2.20	1.38	1.43
3	B	946	NAG	O5-C1	-2.10	1.40	1.43
8	A	944	TCB	O5-C5	2.04	1.49	1.44
7	A	942	MRD	C1-C2	2.15	1.59	1.52
8	A	944	TCB	C6-C5	2.16	1.59	1.51
8	B	950	TCB	O5'-C5'	2.17	1.49	1.44
8	B	950	TCB	C6-C5	2.49	1.60	1.51
8	A	944	TCB	O5-C1	3.18	1.47	1.42
8	B	950	TCB	O5'-C1'	3.33	1.49	1.43
8	B	950	TCB	C6'-C5'	4.10	1.66	1.51
8	B	950	TCB	O5-C1	5.58	1.51	1.42
8	A	944	TCB	C5'-C4'	5.67	1.59	1.53
8	B	950	TCB	C5'-C4'	6.71	1.60	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C4-C3-C2	-7.05	100.27	111.23
8	B	950	TCB	O1'-C1'-C2'	-5.26	95.10	109.21
8	B	950	TCB	O5-C1-S4'	-4.80	97.84	110.01
3	B	908	NAG	C6-C5-C4	-3.99	103.17	113.02
3	B	946	NAG	O3-C3-C4	-3.72	101.96	110.34
8	B	950	TCB	O5-C5-C4	-3.72	102.70	109.68
3	A	941	NAG	C2-N2-C7	-3.57	118.45	123.04
3	A	941	NAG	O7-C7-C8	-3.56	115.52	122.06
8	B	950	TCB	C1-C2-C3	-3.56	102.80	110.69
3	A	941	NAG	O6-C6-C5	-3.38	100.16	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C8-C7-N2	-3.30	109.79	116.11
8	A	944	TCB	O1'-C1'-C2'	-2.90	101.43	109.21
3	A	941	NAG	C3-C4-C5	-2.87	105.20	110.20
3	A	941	NAG	C4-C3-C2	-2.57	107.23	111.23
3	B	908	NAG	O4-C4-C5	-2.54	102.51	109.24
8	A	944	TCB	C1'-C2'-C3'	-2.52	106.68	110.43
3	B	946	NAG	O4-C4-C3	-2.42	104.88	110.34
8	A	944	TCB	O3'-C3'-C2'	-2.17	105.44	110.34
8	A	944	TCB	O5'-C5'-C6'	-2.17	100.86	106.36
3	A	908	NAG	O4-C4-C5	-2.15	103.53	109.24
3	A	908	NAG	O4-C4-C3	-2.07	105.68	110.34
8	A	944	TCB	C6'-C5'-C4'	2.07	119.27	113.25
3	B	908	NAG	O5-C5-C6	2.17	112.04	107.35
8	B	950	TCB	O2-C2-C1	2.29	114.89	110.43
8	A	944	TCB	O2'-C2'-C1'	2.42	115.14	109.82
8	A	944	TCB	O5-C5-C6	2.56	112.84	106.36
8	B	950	TCB	O5'-C5'-C6'	2.58	112.88	106.36
3	A	941	NAG	C8-C7-N2	2.98	121.81	116.11
3	B	908	NAG	C1-O5-C5	3.37	116.52	112.25
8	B	950	TCB	C6'-C5'-C4'	3.42	123.21	113.25
8	B	950	TCB	C3-C4-C5	3.52	116.33	110.20
3	B	908	NAG	C3-C2-N2	4.52	121.38	110.56
8	B	950	TCB	C1-O5-C5	4.70	121.71	112.74
8	A	944	TCB	O5-C1-C2	4.77	116.67	110.19
8	B	950	TCB	O5-C1-C2	5.69	117.91	110.19
3	B	908	NAG	C2-N2-C7	6.35	131.20	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	942	MRD	3	0
7	A	943	MRD	6	0
7	B	948	MRD	2	0
7	B	949	MRD	2	0
8	B	950	TCB	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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%)	-0.74	3 (0%)	93 93	5, 12, 24, 50	0
1	B	832/841 (98%)	-0.91	3 (0%)	93 93	4, 9, 20, 52	0
All	All	1665/1682 (98%)	-0.83	6 (0%)	93 93	4, 10, 23, 52	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	GLY	3.2
1	A	610	TYR	2.6
1	B	668	ASN	2.5
1	A	609	ASP	2.4
1	B	610	TYR	2.3
1	B	609	ASP	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, 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
2	MAN	A	933	11/12	0.91	0.26	16.68	23,29,41,44	0
2	MAN	B	937	11/12	0.91	0.17	9.44	23,31,39,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MAN	A	906	11/12	0.85	0.20	7.59	32,38,48,51	0
2	NAG	A	927	14/15	0.95	0.10	6.89	12,16,35,39	0
10	MAN	B	942	11/12	0.93	0.13	4.19	22,24,33,45	0
2	MAN	A	938	11/12	0.96	0.12	3.34	19,24,30,32	0
4	NAG	A	910	14/15	0.96	0.13	3.01	16,21,23,29	0
2	MAN	B	906	11/12	0.96	0.10	2.12	15,17,21,28	0
2	MAN	A	937	11/12	0.94	0.11	2.03	17,23,28,38	0
10	MAN	B	943	11/12	0.95	0.10	1.56	23,23,30,38	0
4	NAG	A	924	14/15	0.96	0.07	1.06	19,25,34,42	0
9	NAG	B	909	14/15	0.94	0.09	0.89	10,12,13,14	0
2	NAG	B	931	14/15	0.96	0.07	0.81	12,15,29,30	0
9	NAG	B	910	14/15	0.97	0.07	0.71	12,16,24,25	0
6	NAG	A	914	14/15	0.97	0.10	0.70	15,17,20,21	0
4	NAG	A	909	14/15	0.97	0.07	-0.06	13,14,16,16	0
4	NAG	B	928	14/15	0.97	0.06	-0.10	16,20,30,32	0
10	NAG	B	938	14/15	0.98	0.06	-0.34	12,14,15,16	0
6	MAN	A	922	11/12	0.96	0.06	-0.46	17,19,24,31	0
2	NAG	A	901	14/15	0.98	0.06	-0.50	13,14,15,15	0
2	NAG	A	902	14/15	0.96	0.07	-0.50	15,22,31,33	0
2	NAG	A	934	14/15	0.98	0.05	-0.52	13,15,17,18	0
6	MAN	B	926	11/12	0.98	0.06	-0.53	9,10,11,11	0
2	NAG	B	901	14/15	0.99	0.05	-0.60	8,9,10,10	0
6	NAG	B	919	14/15	0.97	0.06	-0.67	8,9,10,11	0
5	NAG	A	912	14/15	0.98	0.06	-0.75	12,13,17,18	0
6	MAN	B	924	11/12	0.97	0.06	-0.76	12,14,18,24	0
6	NAG	B	918	14/15	0.98	0.05	-0.89	9,11,14,15	0
6	MAN	B	927	11/12	0.99	0.05	-0.98	11,11,14,17	0
6	NAG	A	915	14/15	0.98	0.06	-1.12	12,13,14,14	0
4	NAG	B	915	14/15	0.99	0.05	-1.16	8,10,11,12	0
6	MAN	A	921	11/12	0.98	0.05	-1.33	13,14,15,19	0
6	MAN	A	920	11/12	0.98	0.05	-1.49	12,13,15,15	0
2	NAG	B	902	14/15	0.98	0.04	-1.56	9,12,15,21	0
4	BMA	B	930	11/12	0.79	0.20	-	42,51,62,68	0
2	MAN	A	930	11/12	0.79	0.31	-	52,58,67,68	0
4	NAG	B	929	14/15	0.91	0.15	-	25,32,36,44	0
9	BMA	B	911	11/12	0.93	0.12	-	22,25,29,33	0
6	BMA	B	920	11/12	0.99	0.04	-	10,11,12,13	0
9	MAN	B	912	11/12	0.80	0.21	-	37,42,50,51	0
6	MAN	A	917	11/12	0.97	0.09	-	16,18,23,24	0
10	MAN	B	941	11/12	0.82	0.22	-	51,60,65,66	0
4	NAG	B	916	14/15	0.94	0.09	-	13,17,28,32	0
2	BMA	B	903	11/12	0.96	0.07	-	12,17,19,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	NAG	B	939	14/15	0.96	0.10	-	17,22,28,29	0
2	NAG	A	935	14/15	0.96	0.10	-	14,18,24,29	0
2	MAN	A	939	11/12	0.85	0.24	-	36,39,46,47	0
6	MAN	A	923	11/12	0.95	0.13	-	22,24,28,31	0
9	MAN	B	914	11/12	0.91	0.21	-	37,39,46,54	0
2	NAG	A	928	14/15	0.94	0.12	-	15,19,23,26	0
2	MAN	A	907	11/12	0.80	0.14	-	45,53,59,60	0
6	MAN	B	922	11/12	0.95	0.11	-	22,32,38,39	0
5	NAG	A	913	14/15	0.94	0.12	-	15,23,32,33	0
2	MAN	B	905	11/12	0.96	0.09	-	16,23,32,37	0
10	BMA	B	940	11/12	0.87	0.12	-	25,31,38,45	0
2	MAN	B	907	11/12	0.95	0.09	-	20,27,30,31	0
2	MAN	A	904	11/12	0.83	0.27	-	52,58,63,65	0
10	MAN	B	944	11/12	0.80	0.23	-	44,50,62,64	0
2	NAG	B	932	14/15	0.93	0.11	-	14,17,23,24	0
2	MAN	B	934	11/12	0.73	0.25	-	56,65,71,77	0
9	MAN	B	913	11/12	0.91	0.17	-	33,35,41,41	0
2	BMA	A	929	11/12	0.94	0.17	-	20,24,31,40	0
6	MAN	A	919	11/12	0.98	0.05	-	13,14,16,18	0
2	MAN	A	940	11/12	0.78	0.26	-	49,53,62,70	0
6	MAN	B	925	11/12	0.96	0.08	-	19,21,25,26	0
6	MAN	A	918	11/12	0.95	0.12	-	25,32,46,53	0
2	BMA	B	933	11/12	0.95	0.11	-	23,26,31,41	0
2	MAN	B	904	11/12	0.96	0.10	-	18,25,31,32	0
2	MAN	B	936	11/12	0.92	0.14	-	22,27,31,34	0
2	MAN	A	931	11/12	0.92	0.14	-	27,31,39,43	0
4	BMA	A	911	11/12	0.83	0.17	-	25,34,40,46	0
2	MAN	A	905	11/12	0.80	0.26	-	55,60,62,63	0
4	NAG	A	925	14/15	0.81	0.18	-	40,48,59,62	0
10	MAN	B	945	11/12	0.76	0.22	-	48,54,66,71	0
2	MAN	A	932	11/12	0.94	0.16	-	20,26,34,48	0
6	MAN	B	921	11/12	0.98	0.04	-	12,14,18,19	0
2	MAN	B	935	11/12	0.93	0.12	-	27,28,38,40	0
6	BMA	A	916	11/12	0.98	0.05	-	14,15,17,18	0
2	BMA	A	903	11/12	0.86	0.17	-	35,60,65,67	0
4	BMA	A	926	11/12	0.62	0.32	-	45,66,75,79	0
4	BMA	B	917	11/12	0.81	0.23	-	45,59,70,74	0
2	BMA	A	936	11/12	0.93	0.16	-	21,29,41,45	0
6	MAN	B	923	11/12	0.99	0.06	-	9,9,10,12	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, 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
7	MRD	A	943	8/8	0.82	0.20	14.84	15,26,33,39	0
7	MRD	B	949	8/8	0.92	0.17	8.19	35,39,42,43	0
7	MRD	B	948	8/8	0.94	0.13	6.47	15,19,33,35	0
3	NAG	B	947	14/15	0.96	0.13	3.36	22,24,28,31	0
8	TCB	B	950	23/23	0.87	0.15	1.72	16,41,59,60	0
3	NAG	A	941	14/15	0.94	0.15	1.34	24,32,36,36	0
7	MRD	A	942	8/8	0.94	0.09	1.11	16,17,20,27	0
8	TCB	A	944	23/23	0.88	0.14	0.76	23,44,55,57	0
3	NAG	A	908	14/15	0.83	0.38	-	39,53,62,67	0
3	NAG	B	908	14/15	0.90	0.21	-	34,39,46,46	0
3	NAG	B	946	14/15	0.90	0.20	-	34,50,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.