



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:31 PM GMT

PDB ID : 4IIB  
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus*  
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.  
Deposited on : 2012-12-20  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

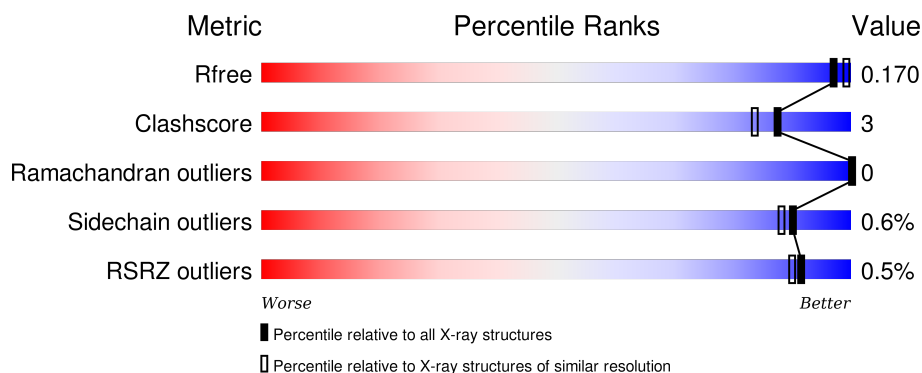
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	841	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>91%</span> <span>7% .</span> </div> </div>
1	B	841	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>90%</span> <span>8% ..</span> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MRD	A	942	-	-	-	X
10	MRD	A	943	-	-	-	X
10	MRD	B	947	-	-	-	X
10	MRD	B	948	-	-	-	X
10	MRD	B	949	-	-	-	X
14	MAN	B	942	-	-	-	X
2	MAN	A	904	-	-	X	-
2	NAG	B	910	-	-	-	X
3	NAG	B	946	-	-	-	X
4	NAG	A	909	-	-	-	X
7	MAN	B	907	-	-	-	X
8	NAG	A	926	-	-	-	X
8	MAN	A	932	-	-	-	X
8	MAN	A	936	-	-	-	X
8	MAN	B	937	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 15992 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

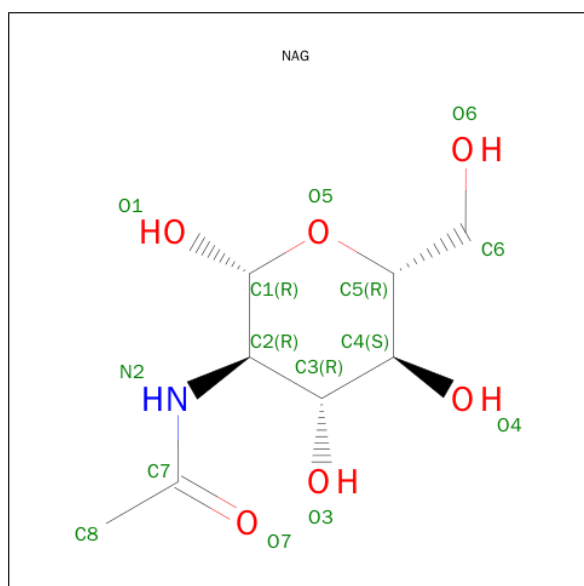
- Molecule 1 is a protein called Beta-glucosidase 1.

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

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

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

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



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

- 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		

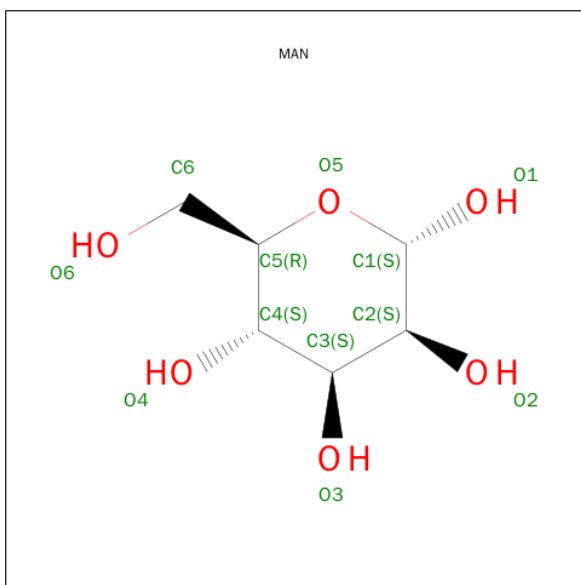
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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 (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

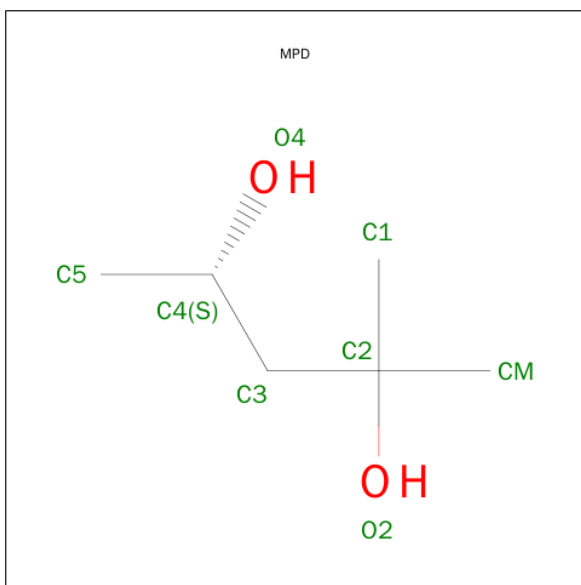


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is a polymer of unknown type called SUGAR (7-MER).

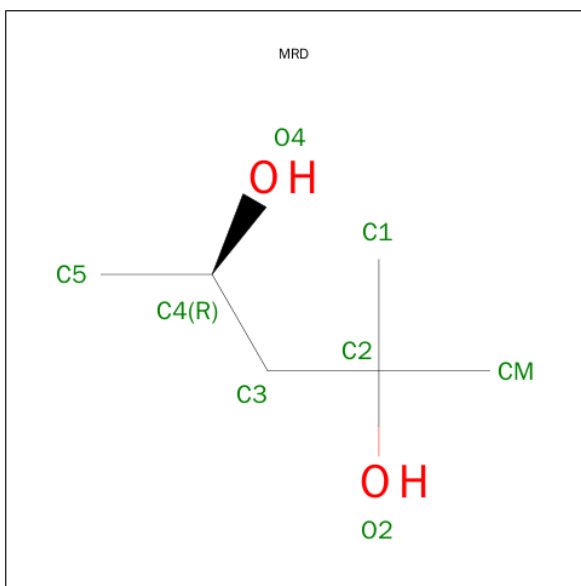
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	7	Total	C	N	O	0	0
			83	46	2	35		
8	A	7	Total	C	N	O	0	0
			83	46	2	35		
8	B	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 10 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



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

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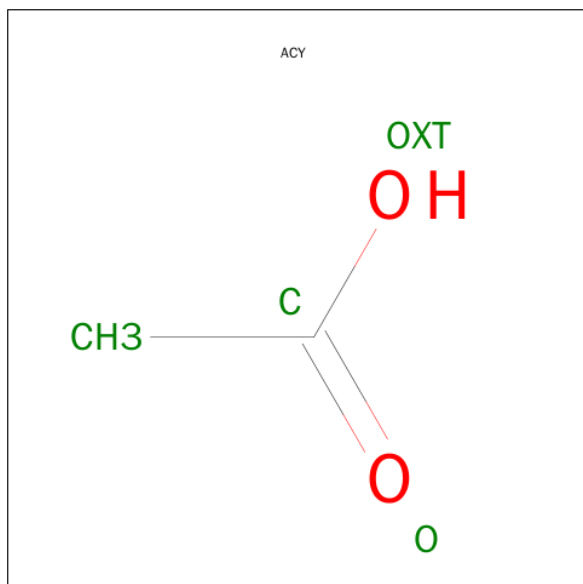
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			8	6	2		
10	B	1	Total	C	O	0	0
			8	6	2		
10	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Na	0	0
			1	1		
11	A	1	Total	Na	0	0
			1	1		

- Molecule 12 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is a polymer of unknown type called SUGAR (10-MER).



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

- Molecule 14 is a polymer of unknown type called SUGAR (8-MER).

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

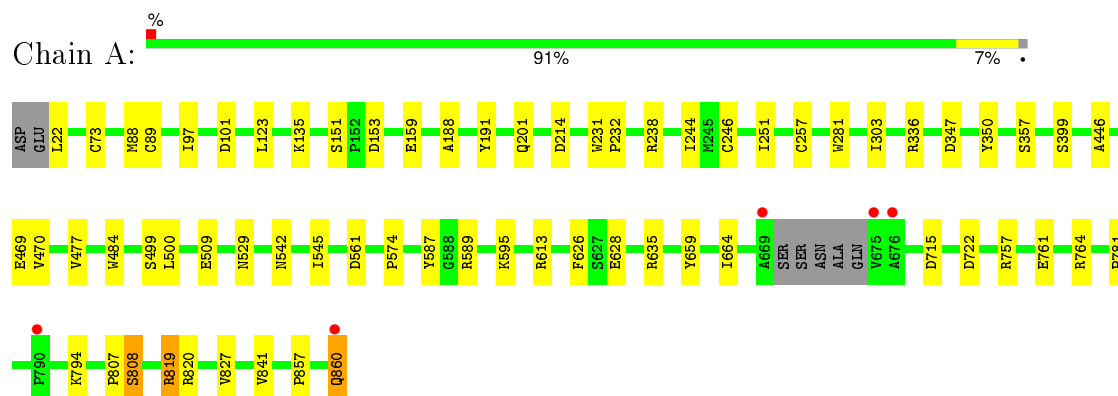
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1027	Total	O	0	0
			1027	1027		
15	B	1103	Total	O	0	0
			1103	1103		

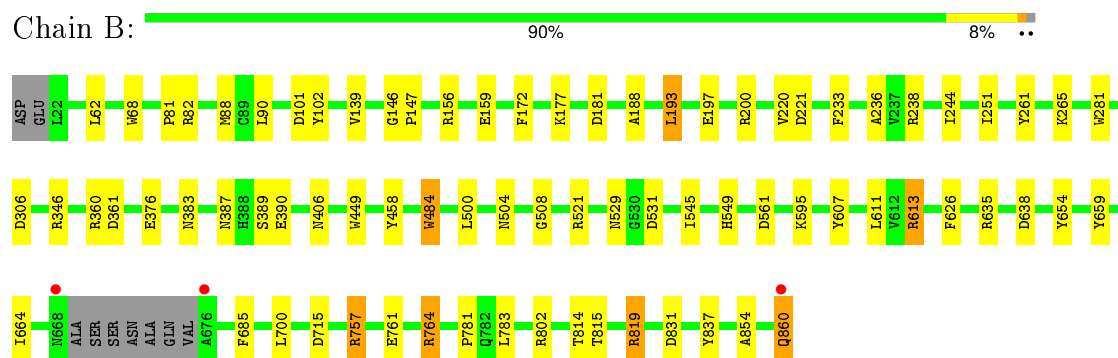
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Beta-glucosidase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.16Å 123.02Å 222.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.49 – 1.80 34.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.49-1.80) 99.9 (34.49-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.58 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.137 , 0.169 0.137 , 0.170	Depositor DCC
$R_{free}$ test set	10460 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 207752 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, NA, MRD, ACY, 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	1.48	18/6550 (0.3%)	1.22	28/8930 (0.3%)
1	B	1.48	16/6538 (0.2%)	1.25	33/8913 (0.4%)
All	All	1.48	34/13088 (0.3%)	1.23	61/17843 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	GLU	CD-OE2	-7.73	1.17	1.25
1	A	761	GLU	CD-OE2	-7.13	1.17	1.25
1	B	761	GLU	CD-OE2	-6.91	1.18	1.25
1	B	458	TYR	CG-CD2	6.30	1.47	1.39
1	A	561	ASP	CG-OD2	5.94	1.39	1.25
1	A	336	ARG	CZ-NH1	5.93	1.40	1.33
1	A	613	ARG	CZ-NH1	5.89	1.40	1.33
1	B	613	ARG	CZ-NH1	5.82	1.40	1.33
1	B	159	GLU	CD-OE1	5.80	1.32	1.25
1	B	68	TRP	CZ3-CH2	5.75	1.49	1.40
1	A	509	GLU	CD-OE1	5.68	1.31	1.25
1	B	685	PHE	CG-CD1	5.59	1.47	1.38
1	A	499	SER	CB-OG	5.59	1.49	1.42
1	A	764	ARG	CZ-NH1	5.59	1.40	1.33
1	B	837	TYR	CG-CD1	5.54	1.46	1.39
1	A	159	GLU	CD-OE1	5.47	1.31	1.25
1	A	613	ARG	CZ-NH2	5.41	1.40	1.33
1	B	197	GLU	CB-CG	5.40	1.62	1.52
1	A	22	LEU	N-CA	5.39	1.57	1.46
1	A	635	ARG	CZ-NH1	5.39	1.40	1.33
1	A	257	CYS	CB-SG	5.37	1.91	1.82
1	A	350	TYR	CG-CD1	5.34	1.46	1.39
1	B	376	GLU	CD-OE1	5.33	1.31	1.25
1	A	587	TYR	CG-CD1	5.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	654	TYR	CE1-CZ	5.28	1.45	1.38
1	B	389	SER	CB-OG	5.27	1.49	1.42
1	A	399	SER	CA-CB	5.24	1.60	1.52
1	A	357	SER	CA-CB	5.21	1.60	1.52
1	B	390	GLU	CG-CD	5.15	1.59	1.51
1	B	261	TYR	CE2-CZ	5.14	1.45	1.38
1	B	484	TRP	CE3-CZ3	5.12	1.47	1.38
1	B	607	TYR	CD2-CE2	5.03	1.46	1.39
1	A	151	SER	CA-CB	-5.02	1.45	1.52
1	B	233	PHE	CE1-CZ	5.02	1.46	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	819	ARG	NE-CZ-NH1	-12.85	113.87	120.30
1	B	764	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	336	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	764	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	589	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	819	ARG	NE-CZ-NH1	-8.47	116.06	120.30
1	B	831	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	177	LYS	CD-CE-NZ	7.85	129.76	111.70
1	A	561	ASP	CB-CG-OD2	7.58	125.13	118.30
1	B	101	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	613	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	A	820	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	715	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	521	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	A	238	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	757	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	819	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	B	238	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	820	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	764	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	200	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	626	PHE	CB-CG-CD1	6.50	125.35	120.80
1	A	101	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	561	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	B	638	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	347	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	214	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	635	ARG	NE-CZ-NH2	-6.21	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	531	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	361	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	626	PHE	CB-CG-CD2	-6.02	116.59	120.80
1	B	306	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	B	181	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	831	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	360	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	722	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	193	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	A	628	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	B	561	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	238	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	73	CYS	CA-CB-SG	-5.53	104.05	114.00
1	A	635	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	88	MET	CA-CB-CG	-5.50	103.96	113.30
1	B	221	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	88	MET	CA-CB-CG	-5.42	104.09	113.30
1	A	808	SER	CA-CB-OG	-5.41	96.60	111.20
1	B	613	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	123	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	B	757	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	626	PHE	CB-CG-CD2	-5.24	117.14	120.80
1	A	153	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	82	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	156	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	757	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	62	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	B	265	LYS	CD-CE-NZ	-5.12	99.93	111.70
1	B	406	ASN	CB-CA-C	5.10	120.61	110.40
1	B	715	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	346	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	802	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6387	0	6097	22	0
1	B	6375	0	6083	26	0
2	A	72	0	61	6	0
2	B	144	0	121	3	0
3	A	28	0	26	0	0
3	B	28	0	26	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	105	0	88	3	0
7	A	11	0	10	3	0
7	B	11	0	10	2	0
8	A	166	0	138	2	0
8	B	83	0	69	1	0
9	A	8	0	14	0	0
10	A	16	0	28	2	0
10	B	24	0	42	5	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	4	0	3	0	0
12	B	4	0	3	0	0
13	B	116	0	97	0	0
14	B	94	0	77	0	0
15	A	1027	0	0	7	0
15	B	1103	0	0	8	0
All	All	15992	0	13153	69	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 (69) 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)
2:A:903:BMA:C3	2:A:904:MAN:H5	1.82	1.09
2:A:903:BMA:H3	2:A:904:MAN:H5	1.36	1.07
2:A:903:BMA:H3	2:A:904:MAN:C5	1.84	1.07
2:A:903:BMA:C3	2:A:904:MAN:C5	2.45	0.94
1:A:819:ARG:HH12	1:A:860:GLN:C	1.71	0.92
10:A:942:MRD:C5	10:A:942:MRD:H1C2	2.00	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:907:MAN:C1	2:B:905:MAN:C2	2.52	0.86
6:A:921:MAN:C2	7:A:922:MAN:C1	2.55	0.85
1:A:857:PRO:HD3	15:A:1336:HOH:O	1.80	0.82
10:A:942:MRD:H5C3	10:A:942:MRD:H1C2	1.61	0.80
2:A:903:BMA:H3	2:A:904:MAN:C6	2.12	0.79
1:A:201:GLN:HG3	15:A:2020:HOH:O	1.86	0.75
5:A:912:NAG:H83	5:A:912:NAG:H3	1.70	0.73
10:B:948:MRD:H1C2	10:B:948:MRD:C5	2.17	0.72
6:A:921:MAN:HO2	7:A:922:MAN:C1	2.03	0.69
7:B:907:MAN:C2	2:B:905:MAN:O2	2.40	0.68
1:A:794:LYS:HG3	15:A:1747:HOH:O	1.95	0.66
1:B:815:THR:HG22	15:B:1545:HOH:O	1.95	0.65
2:A:904:MAN:H61	15:A:1834:HOH:O	1.97	0.65
10:B:948:MRD:H1C2	10:B:948:MRD:H5C3	1.79	0.64
10:B:948:MRD:H4	15:B:1369:HOH:O	2.00	0.62
1:A:542:ASN:ND2	15:A:1640:HOH:O	2.27	0.61
1:B:819:ARG:HH12	1:B:860:GLN:C	2.05	0.60
1:A:819:ARG:NH1	1:A:860:GLN:C	2.53	0.57
6:A:921:MAN:O2	7:A:922:MAN:C2	2.51	0.55
1:B:387:ASN:CG	15:B:1673:HOH:O	2.47	0.54
1:B:595:LYS:HE2	15:B:1078:HOH:O	2.07	0.53
8:A:926:NAG:H82	15:A:1150:HOH:O	2.08	0.53
1:B:764:ARG:HD3	1:B:814:THR:HG21	1.89	0.53
1:A:595:LYS:HE2	15:A:1340:HOH:O	2.09	0.53
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.91	0.51
1:B:387:ASN:ND2	15:B:1673:HOH:O	2.43	0.51
1:A:251:ILE:HG21	4:A:908:NAG:H82	1.94	0.50
1:B:860:GLN:HB3	15:B:1945:HOH:O	2.11	0.49
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.95	0.49
1:B:90:LEU:HG	1:B:139:VAL:HB	1.96	0.48
1:A:231:TRP:HB3	1:A:232:PRO:HD3	1.95	0.48
1:A:807:PRO:O	1:A:808:SER:HB2	2.13	0.48
1:B:449:TRP:CD1	1:B:508:GLY:HA3	2.49	0.47
1:A:303:ILE:HG21	5:A:912:NAG:H81	1.96	0.47
1:A:484:TRP:CE2	8:A:928:BMA:H62	2.50	0.47
1:B:613:ARG:NH1	15:B:1057:HOH:O	2.39	0.46
1:B:783:LEU:HD23	1:B:783:LEU:C	2.36	0.46
1:B:193:LEU:HD13	1:B:220:VAL:HG21	1.98	0.46
1:A:446:ALA:HA	1:A:574:PRO:HD2	1.98	0.45
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.99	0.45
1:B:172:PHE:CE2	1:B:236:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:912:NAG:C3	5:A:912:NAG:H83	2.43	0.44
1:A:97:ILE:HD13	1:A:135:LYS:HG3	1.99	0.44
1:B:251:ILE:HG21	2:B:909:NAG:H82	2.00	0.43
1:A:188:ALA:HB3	1:A:244:ILE:HD13	2.01	0.43
10:B:949:MRD:C5	10:B:949:MRD:O2	2.66	0.43
1:A:500:LEU:HD23	1:A:545:ILE:HB	2.01	0.42
1:B:500:LEU:HD23	1:B:545:ILE:HB	2.01	0.42
1:A:827:VAL:HG11	4:A:909:NAG:O3	2.20	0.42
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.85	0.42
1:B:504:ASN:HA	1:B:549:HIS:O	2.20	0.42
1:B:595:LYS:HE3	15:B:1003:HOH:O	2.20	0.41
1:B:611:LEU:HD12	1:B:613:ARG:NH2	2.35	0.41
1:B:764:ARG:HD3	1:B:814:THR:CG2	2.50	0.41
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.55	0.41
1:A:191:TYR:O	1:A:246:CYS:HA	2.20	0.41
1:B:484:TRP:CE2	8:B:933:BMA:H62	2.55	0.41
1:B:102:TYR:HB3	1:B:383:ASN:HA	2.03	0.41
1:A:659:TYR:HE1	1:A:781:PRO:HB3	1.85	0.41
10:B:948:MRD:H1C2	10:B:948:MRD:H4	1.48	0.41
1:B:664:ILE:HD11	1:B:854:ALA:HB3	2.03	0.41
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.56	0.40
1:B:146:GLY:HA2	1:B:147:PRO:C	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	830/841 (99%)	807 (97%)	23 (3%)	0	100	100
1	B	828/841 (98%)	802 (97%)	26 (3%)	0	100	100
All	All	1658/1682 (99%)	1609 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	668 (100%)	3 (0%)	93	92
1	B	670/677 (99%)	665 (99%)	5 (1%)	88	86
All	All	1341/1354 (99%)	1333 (99%)	8 (1%)	90	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	CYS
1	A	281	TRP
1	A	860	GLN
1	B	81	PRO
1	B	281	TRP
1	B	700	LEU
1	B	757	ARG
1	B	860	GLN

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 ⓘ

80 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	1.53	3 (21%)	15,19,21	1.98	5 (33%)
2	NAG	A	902	2	14,14,15	1.00	2 (14%)	15,19,21	2.32	9 (60%)
2	BMA	A	903	2	11,11,12	0.94	1 (9%)	14,15,17	2.96	5 (35%)
2	MAN	A	904	2	11,11,12	1.81	3 (27%)	14,15,17	4.18	10 (71%)
2	MAN	A	905	2	11,11,12	0.70	0	14,15,17	1.87	4 (28%)
2	MAN	A	906	2	11,11,12	0.77	0	14,15,17	2.09	6 (42%)
4	NAG	A	908	1,4	14,14,15	1.65	2 (14%)	15,19,21	1.97	4 (26%)
4	NAG	A	909	4	14,14,15	1.53	2 (14%)	15,19,21	2.71	6 (40%)
4	BMA	A	910	4	11,11,12	1.17	1 (9%)	14,15,17	3.12	6 (42%)
5	NAG	A	911	1,5	14,14,15	0.95	1 (7%)	15,19,21	1.94	4 (26%)
5	NAG	A	912	5	14,14,15	1.59	2 (14%)	15,19,21	2.26	6 (40%)
6	NAG	A	913	1,6	14,14,15	1.53	3 (21%)	15,19,21	1.57	3 (20%)
6	NAG	A	914	6	14,14,15	1.93	1 (7%)	15,19,21	1.57	2 (13%)
6	BMA	A	915	6	11,11,12	1.27	2 (18%)	14,15,17	1.73	4 (28%)
6	MAN	A	916	6	11,11,12	1.12	1 (9%)	14,15,17	2.13	5 (35%)
6	MAN	A	917	6	11,11,12	1.49	2 (18%)	14,15,17	2.59	8 (57%)
6	MAN	A	918	6	11,11,12	0.79	0	14,15,17	1.27	2 (14%)
6	MAN	A	919	6	11,11,12	1.49	2 (18%)	14,15,17	1.35	2 (14%)
6	MAN	A	920	6	11,11,12	1.27	1 (9%)	14,15,17	1.48	1 (7%)
6	MAN	A	921	7,6	11,11,12	1.28	2 (18%)	14,15,17	1.88	5 (35%)
4	NAG	A	923	1,4	14,14,15	0.95	1 (7%)	15,19,21	1.75	5 (33%)
4	NAG	A	924	4	14,14,15	1.11	2 (14%)	15,19,21	1.57	4 (26%)
4	BMA	A	925	4	11,11,12	0.92	1 (9%)	14,15,17	2.28	5 (35%)
8	NAG	A	926	1,8	14,14,15	1.45	2 (14%)	15,19,21	2.26	6 (40%)
8	NAG	A	927	8	14,14,15	0.98	0	15,19,21	2.27	5 (33%)
8	BMA	A	928	8	11,11,12	1.21	1 (9%)	14,15,17	1.20	1 (7%)
8	MAN	A	929	8	11,11,12	0.84	0	14,15,17	2.07	6 (42%)
8	MAN	A	930	8	11,11,12	0.99	1 (9%)	14,15,17	2.32	7 (50%)
8	MAN	A	931	8	11,11,12	1.07	1 (9%)	14,15,17	2.85	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	A	932	8	11,11,12	1.13	1 (9%)	14,15,17	1.27	1 (7%)
8	NAG	A	933	1,8,11	14,14,15	0.79	0	15,19,21	1.57	3 (20%)
8	NAG	A	934	8	14,14,15	1.26	2 (14%)	15,19,21	1.62	4 (26%)
8	BMA	A	935	8	11,11,12	0.96	0	14,15,17	2.21	4 (28%)
8	MAN	A	936	8	11,11,12	1.29	1 (9%)	14,15,17	1.60	2 (14%)
8	MAN	A	937	8	11,11,12	1.21	1 (9%)	14,15,17	1.44	3 (21%)
8	MAN	A	938	8	11,11,12	1.12	0	14,15,17	2.67	5 (35%)
8	MAN	A	939	8	11,11,12	1.18	2 (18%)	14,15,17	1.71	2 (14%)
2	NAG	B	901	1,2	14,14,15	1.66	3 (21%)	15,19,21	1.97	6 (40%)
2	NAG	B	902	2	14,14,15	1.06	1 (7%)	15,19,21	2.43	6 (40%)
2	BMA	B	903	2	11,11,12	1.73	3 (27%)	14,15,17	3.22	5 (35%)
2	MAN	B	904	2	11,11,12	1.14	1 (9%)	14,15,17	1.85	5 (35%)
2	MAN	B	905	2,7	11,11,12	1.09	0	14,15,17	2.25	6 (42%)
2	MAN	B	906	2	11,11,12	0.87	0	14,15,17	2.61	6 (42%)
2	NAG	B	909	1,2	14,14,15	1.03	1 (7%)	15,19,21	1.61	3 (20%)
2	NAG	B	910	2	14,14,15	1.95	6 (42%)	15,19,21	2.44	7 (46%)
2	BMA	B	911	2	11,11,12	0.96	1 (9%)	14,15,17	1.39	2 (14%)
2	MAN	B	912	2	11,11,12	1.47	1 (9%)	14,15,17	1.92	2 (14%)
2	MAN	B	913	2	11,11,12	0.77	0	14,15,17	1.95	3 (21%)
2	MAN	B	914	2	11,11,12	1.22	1 (9%)	14,15,17	1.19	1 (7%)
4	NAG	B	915	1,4	14,14,15	1.33	1 (7%)	15,19,21	1.30	1 (6%)
4	NAG	B	916	4	14,14,15	1.07	1 (7%)	15,19,21	1.74	5 (33%)
4	BMA	B	917	4	11,11,12	0.88	0	14,15,17	2.45	5 (35%)
13	NAG	B	918	1,13	14,14,15	0.97	0	15,19,21	1.91	3 (20%)
13	NAG	B	919	13	14,14,15	1.31	1 (7%)	15,19,21	1.81	2 (13%)
13	BMA	B	920	13	11,11,12	1.27	1 (9%)	14,15,17	2.29	7 (50%)
13	MAN	B	921	13	11,11,12	1.11	0	14,15,17	2.36	6 (42%)
13	MAN	B	922	13	11,11,12	0.77	0	14,15,17	2.04	4 (28%)
13	MAN	B	923	13	11,11,12	0.95	0	14,15,17	1.71	3 (21%)
13	MAN	B	924	13	11,11,12	1.41	1 (9%)	14,15,17	2.93	9 (64%)
13	MAN	B	925	13	11,11,12	1.14	0	14,15,17	1.45	4 (28%)
13	MAN	B	926	13	11,11,12	1.62	2 (18%)	14,15,17	2.59	6 (42%)
13	MAN	B	927	13	11,11,12	1.45	3 (27%)	14,15,17	1.77	4 (28%)
4	NAG	B	928	1,4	14,14,15	1.06	1 (7%)	15,19,21	2.12	3 (20%)
4	NAG	B	929	4	14,14,15	1.18	2 (14%)	15,19,21	2.08	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	B	930	4	11,11,12	1.25	1 (9%)	14,15,17	2.30	6 (42%)
8	NAG	B	931	1,8	14,14,15	1.49	4 (28%)	15,19,21	1.82	6 (40%)
8	NAG	B	932	8	14,14,15	0.88	0	15,19,21	2.04	6 (40%)
8	BMA	B	933	8	11,11,12	1.06	1 (9%)	14,15,17	2.35	4 (28%)
8	MAN	B	934	8	11,11,12	1.15	1 (9%)	14,15,17	2.46	5 (35%)
8	MAN	B	935	8	11,11,12	1.59	2 (18%)	14,15,17	2.46	7 (50%)
8	MAN	B	936	8	11,11,12	1.42	2 (18%)	14,15,17	2.34	5 (35%)
8	MAN	B	937	8	11,11,12	1.34	2 (18%)	14,15,17	2.10	7 (50%)
14	NAG	B	938	1,11,14	14,14,15	1.32	2 (14%)	15,19,21	1.95	6 (40%)
14	NAG	B	939	14	14,14,15	1.03	0	15,19,21	1.71	5 (33%)
14	BMA	B	940	14	11,11,12	1.10	2 (18%)	14,15,17	1.36	3 (21%)
14	MAN	B	941	14	11,11,12	1.18	0	14,15,17	2.56	8 (57%)
14	MAN	B	942	14	11,11,12	1.42	1 (9%)	14,15,17	2.21	7 (50%)
14	MAN	B	943	14	11,11,12	1.22	1 (9%)	14,15,17	1.56	3 (21%)
14	MAN	B	944	14	11,11,12	1.00	1 (9%)	14,15,17	1.54	4 (28%)
14	MAN	B	945	14	11,11,12	1.36	2 (18%)	14,15,17	2.48	5 (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
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
4	NAG	A	908	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	909	4	-	0/6/23/26	0/1/1/1
4	BMA	A	910	4	-	0/2/19/22	0/1/1/1
5	NAG	A	911	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	912	5	-	0/6/23/26	0/1/1/1
6	NAG	A	913	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	914	6	-	0/6/23/26	0/1/1/1
6	BMA	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	7,6	-	0/2/19/22	0/1/1/1
4	NAG	A	923	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	924	4	-	0/6/23/26	0/1/1/1
4	BMA	A	925	4	-	0/2/19/22	0/1/1/1
8	NAG	A	926	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	927	8	-	0/6/23/26	0/1/1/1
8	BMA	A	928	8	-	0/2/19/22	0/1/1/1
8	MAN	A	929	8	-	0/2/19/22	0/1/1/1
8	MAN	A	930	8	-	0/2/19/22	0/1/1/1
8	MAN	A	931	8	-	0/2/19/22	0/1/1/1
8	MAN	A	932	8	-	0/2/19/22	0/1/1/1
8	NAG	A	933	1,8,11	-	0/6/23/26	0/1/1/1
8	NAG	A	934	8	-	0/6/23/26	0/1/1/1
8	BMA	A	935	8	-	0/2/19/22	0/1/1/1
8	MAN	A	936	8	-	0/2/19/22	0/1/1/1
8	MAN	A	937	8	-	0/2/19/22	0/1/1/1
8	MAN	A	938	8	-	0/2/19/22	0/1/1/1
8	MAN	A	939	8	-	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	2,7	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	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
2	MAN	B	913	2	-	0/2/19/22	0/1/1/1
2	MAN	B	914	2	-	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
13	NAG	B	918	1,13	-	0/6/23/26	0/1/1/1
13	NAG	B	919	13	-	0/6/23/26	0/1/1/1
13	BMA	B	920	13	-	0/2/19/22	0/1/1/1
13	MAN	B	921	13	-	0/2/19/22	0/1/1/1
13	MAN	B	922	13	-	0/2/19/22	0/1/1/1
13	MAN	B	923	13	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	B	924	13	-	0/2/19/22	0/1/1/1
13	MAN	B	925	13	-	0/2/19/22	0/1/1/1
13	MAN	B	926	13	-	0/2/19/22	0/1/1/1
13	MAN	B	927	13	-	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
8	NAG	B	931	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	932	8	-	0/6/23/26	0/1/1/1
8	BMA	B	933	8	-	0/2/19/22	0/1/1/1
8	MAN	B	934	8	-	0/2/19/22	0/1/1/1
8	MAN	B	935	8	-	0/2/19/22	0/1/1/1
8	MAN	B	936	8	-	0/2/19/22	0/1/1/1
8	MAN	B	937	8	-	0/2/19/22	0/1/1/1
14	NAG	B	938	1,11,14	-	0/6/23/26	0/1/1/1
14	NAG	B	939	14	-	0/6/23/26	0/1/1/1
14	BMA	B	940	14	-	0/2/19/22	0/1/1/1
14	MAN	B	941	14	-	0/2/19/22	0/1/1/1
14	MAN	B	942	14	-	0/2/19/22	0/1/1/1
14	MAN	B	943	14	-	0/2/19/22	0/1/1/1
14	MAN	B	944	14	-	0/2/19/22	0/1/1/1
14	MAN	B	945	14	-	0/2/19/22	0/1/1/1

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	935	MAN	O2-C2	-4.12	1.34	1.43
5	A	912	NAG	C8-C7	-3.59	1.43	1.50
2	B	914	MAN	O5-C1	-3.14	1.38	1.43
2	A	904	MAN	C4-C5	-3.03	1.46	1.53
6	A	921	MAN	O5-C1	-3.03	1.38	1.43
6	A	917	MAN	O5-C1	-2.90	1.38	1.43
8	A	928	BMA	O5-C5	-2.87	1.37	1.43
6	A	916	MAN	C2-C3	-2.86	1.48	1.52
4	B	930	BMA	O5-C1	-2.81	1.39	1.43
14	B	943	MAN	O5-C1	-2.76	1.39	1.43
8	A	930	MAN	O2-C2	-2.76	1.37	1.43
8	B	934	MAN	C2-C3	-2.75	1.48	1.52
2	B	904	MAN	O5-C1	-2.72	1.39	1.43
4	A	924	NAG	O5-C1	-2.63	1.39	1.43
13	B	926	MAN	O5-C1	-2.61	1.39	1.43
4	B	916	NAG	O7-C7	-2.58	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	904	MAN	O5-C1	-2.49	1.39	1.43
8	A	936	MAN	C2-C3	-2.45	1.49	1.52
4	A	924	NAG	C2-N2	-2.40	1.42	1.46
14	B	944	MAN	O5-C1	-2.39	1.39	1.43
6	A	919	MAN	C2-C3	-2.38	1.49	1.52
2	B	910	NAG	O5-C1	-2.38	1.39	1.43
2	B	911	BMA	O5-C1	-2.36	1.39	1.43
8	A	937	MAN	O5-C5	-2.29	1.38	1.43
4	B	929	NAG	O7-C7	-2.23	1.18	1.23
8	B	937	MAN	O5-C1	-2.19	1.40	1.43
4	A	925	BMA	O5-C1	-2.18	1.40	1.43
14	B	940	BMA	O2-C2	-2.14	1.38	1.43
8	B	936	MAN	O4-C4	-2.10	1.37	1.43
8	B	931	NAG	O5-C1	-2.02	1.40	1.43
4	B	929	NAG	O5-C1	-2.02	1.40	1.43
14	B	940	BMA	O5-C1	-2.01	1.40	1.43
5	A	911	NAG	O7-C7	2.03	1.27	1.23
14	B	938	NAG	C3-C2	2.05	1.57	1.52
8	A	939	MAN	C4-C5	2.05	1.57	1.53
13	B	927	MAN	C2-C3	2.06	1.55	1.52
8	A	939	MAN	C1-C2	2.06	1.57	1.52
2	B	903	BMA	C4-C5	2.06	1.57	1.53
8	B	933	BMA	C1-C2	2.09	1.57	1.52
2	B	903	BMA	C1-C2	2.09	1.57	1.52
2	A	902	NAG	C1-C2	2.10	1.55	1.52
4	B	928	NAG	O5-C5	2.11	1.48	1.43
8	A	926	NAG	O3-C3	2.12	1.48	1.43
2	A	901	NAG	C6-C5	2.14	1.59	1.51
2	B	910	NAG	C7-N2	2.17	1.42	1.34
6	A	915	BMA	C6-C5	2.19	1.59	1.51
6	A	921	MAN	O5-C5	2.20	1.48	1.43
4	A	908	NAG	C2-N2	2.21	1.50	1.46
8	A	931	MAN	O5-C1	2.21	1.47	1.43
14	B	945	MAN	O5-C1	2.22	1.47	1.43
8	A	934	NAG	C8-C7	2.23	1.55	1.50
8	A	932	MAN	O5-C5	2.27	1.48	1.43
8	B	931	NAG	C4-C5	2.28	1.57	1.53
2	B	910	NAG	C8-C7	2.29	1.55	1.50
8	B	931	NAG	O3-C3	2.32	1.48	1.43
6	A	915	BMA	C4-C3	2.33	1.58	1.52
4	A	923	NAG	C8-C7	2.36	1.55	1.50
6	A	913	NAG	O3-C3	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	920	BMA	O5-C1	2.40	1.47	1.43
14	B	945	MAN	C2-C3	2.45	1.55	1.52
2	A	903	BMA	C2-C3	2.45	1.55	1.52
2	B	901	NAG	C8-C7	2.45	1.55	1.50
2	A	902	NAG	O7-C7	2.46	1.28	1.23
13	B	927	MAN	C4-C3	2.52	1.59	1.52
6	A	920	MAN	C2-C3	2.56	1.56	1.52
8	B	931	NAG	C2-N2	2.58	1.50	1.46
4	A	909	NAG	O4-C4	2.59	1.49	1.43
4	B	915	NAG	C8-C7	2.59	1.55	1.50
6	A	919	MAN	C1-C2	2.61	1.58	1.52
4	A	909	NAG	C4-C5	2.66	1.58	1.53
14	B	938	NAG	O7-C7	2.68	1.29	1.23
13	B	927	MAN	C1-C2	2.69	1.58	1.52
8	A	934	NAG	C6-C5	2.71	1.61	1.51
8	B	935	MAN	O5-C1	2.72	1.48	1.43
6	A	913	NAG	O5-C1	2.72	1.48	1.43
2	A	901	NAG	C1-C2	2.72	1.56	1.52
2	B	902	NAG	O4-C4	2.74	1.49	1.43
8	B	936	MAN	C1-C2	2.75	1.58	1.52
13	B	924	MAN	O2-C2	2.76	1.49	1.43
4	A	910	BMA	C4-C5	2.76	1.58	1.53
2	B	910	NAG	C4-C5	2.77	1.59	1.53
2	B	901	NAG	C1-C2	2.80	1.56	1.52
2	B	909	NAG	C2-N2	2.81	1.51	1.46
6	A	917	MAN	C2-C3	2.88	1.56	1.52
2	A	901	NAG	C8-C7	2.96	1.56	1.50
13	B	926	MAN	C4-C5	3.12	1.59	1.53
13	B	919	NAG	O5-C1	3.14	1.49	1.43
8	B	937	MAN	C2-C3	3.22	1.56	1.52
2	A	904	MAN	C2-C3	3.29	1.57	1.52
2	B	910	NAG	O7-C7	3.34	1.31	1.23
2	B	910	NAG	C1-C2	3.37	1.57	1.52
6	A	913	NAG	C4-C3	3.44	1.61	1.52
2	B	912	MAN	C2-C3	3.44	1.57	1.52
2	B	901	NAG	C2-N2	3.81	1.53	1.46
8	A	926	NAG	C1-C2	3.85	1.57	1.52
5	A	912	NAG	O7-C7	3.93	1.32	1.23
2	B	903	BMA	C2-C3	3.94	1.57	1.52
14	B	942	MAN	O5-C1	3.97	1.50	1.43
4	A	908	NAG	C8-C7	5.24	1.61	1.50
6	A	914	NAG	C1-C2	6.19	1.61	1.52

All (372) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	904	MAN	C1-C2-C3	-8.56	99.41	109.54
2	B	903	BMA	C1-C2-C3	-7.90	100.20	109.54
2	A	903	BMA	O3-C3-C2	-7.72	96.04	110.00
4	A	909	NAG	C1-O5-C5	-6.87	103.53	112.25
8	B	934	MAN	O5-C1-C2	-6.58	100.18	110.86
13	B	924	MAN	O6-C6-C5	-6.53	89.74	111.33
8	B	933	BMA	C1-O5-C5	-6.20	104.38	112.25
2	A	904	MAN	O5-C1-C2	-6.18	100.83	110.86
8	A	938	MAN	O4-C4-C3	-6.07	96.68	110.34
4	A	910	BMA	O3-C3-C2	-6.01	99.14	110.00
8	A	927	NAG	C1-O5-C5	-5.92	104.74	112.25
2	B	903	BMA	C1-O5-C5	-5.87	104.80	112.25
13	B	919	NAG	C1-O5-C5	-5.73	104.98	112.25
2	B	905	MAN	O6-C6-C5	-5.44	93.35	111.33
2	A	904	MAN	C3-C4-C5	-5.19	101.14	110.20
8	A	926	NAG	C2-N2-C7	-5.00	116.61	123.04
2	B	902	NAG	O7-C7-C8	-5.00	112.89	122.06
8	A	931	MAN	C6-C5-C4	-4.90	100.92	113.02
2	B	910	NAG	O6-C6-C5	-4.86	95.26	111.33
4	A	908	NAG	C1-O5-C5	-4.82	106.13	112.25
13	B	918	NAG	C1-O5-C5	-4.80	106.16	112.25
4	B	928	NAG	C4-C3-C2	-4.76	103.82	111.23
6	A	914	NAG	C1-O5-C5	-4.67	106.33	112.25
14	B	941	MAN	O3-C3-C4	-4.64	99.89	110.34
4	A	910	BMA	C1-O5-C5	-4.61	106.40	112.25
2	A	901	NAG	C2-N2-C7	-4.55	117.20	123.04
2	B	906	MAN	O2-C2-C1	-4.54	100.11	109.21
4	B	928	NAG	C1-O5-C5	-4.53	106.50	112.25
14	B	945	MAN	O2-C2-C1	-4.50	100.19	109.21
5	A	912	NAG	O6-C6-C5	-4.47	96.57	111.33
6	A	916	MAN	O3-C3-C2	-4.46	101.94	110.00
13	B	922	MAN	C6-C5-C4	-4.45	102.03	113.02
13	B	924	MAN	C6-C5-C4	-4.39	102.18	113.02
2	A	903	BMA	C1-C2-C3	-4.38	104.36	109.54
13	B	920	BMA	C2-C3-C4	-4.38	103.60	111.04
4	B	929	NAG	C3-C4-C5	-4.35	102.61	110.20
2	A	903	BMA	C1-O5-C5	-4.24	106.86	112.25
8	A	931	MAN	O2-C2-C3	-3.98	102.12	110.12
13	B	920	BMA	O3-C3-C2	-3.93	102.91	110.00
4	B	930	BMA	O4-C4-C3	-3.88	101.60	110.34
14	B	942	MAN	C6-C5-C4	-3.88	103.45	113.02
8	A	926	NAG	C3-C2-N2	-3.81	101.43	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	923	NAG	C1-O5-C5	-3.81	107.42	112.25
14	B	942	MAN	O2-C2-C1	-3.74	101.70	109.21
2	A	902	NAG	O6-C6-C5	-3.73	98.99	111.33
8	B	936	MAN	C6-C5-C4	-3.71	103.86	113.02
6	A	916	MAN	O4-C4-C3	-3.70	102.01	110.34
14	B	941	MAN	O4-C4-C3	-3.69	102.03	110.34
5	A	911	NAG	C4-C3-C2	-3.69	105.50	111.23
2	B	913	MAN	C2-C3-C4	-3.68	104.78	111.04
2	B	909	NAG	C4-C3-C2	-3.65	105.56	111.23
4	B	929	NAG	C1-O5-C5	-3.63	107.64	112.25
8	A	936	MAN	O3-C3-C2	-3.62	103.46	110.00
13	B	926	MAN	O6-C6-C5	-3.62	99.39	111.33
2	B	903	BMA	O3-C3-C2	-3.57	103.55	110.00
8	A	929	MAN	C2-C3-C4	-3.56	104.99	111.04
2	B	902	NAG	O6-C6-C5	-3.54	99.62	111.33
2	A	906	MAN	O2-C2-C1	-3.52	102.15	109.21
8	B	934	MAN	C1-C2-C3	-3.51	105.38	109.54
8	A	935	BMA	O6-C6-C5	-3.50	99.77	111.33
8	B	937	MAN	O6-C6-C5	-3.50	99.78	111.33
13	B	918	NAG	C2-N2-C7	-3.49	118.56	123.04
4	B	916	NAG	C3-C4-C5	-3.49	104.12	110.20
6	A	913	NAG	C1-O5-C5	-3.47	107.84	112.25
2	B	903	BMA	O6-C6-C5	-3.46	99.89	111.33
2	B	905	MAN	O4-C4-C3	-3.45	102.57	110.34
8	B	932	NAG	C2-N2-C7	-3.43	118.64	123.04
13	B	927	MAN	C1-C2-C3	-3.42	105.49	109.54
13	B	923	MAN	O2-C2-C1	-3.42	102.36	109.21
5	A	912	NAG	C1-O5-C5	-3.42	107.91	112.25
8	B	933	BMA	O4-C4-C3	-3.42	102.65	110.34
2	A	902	NAG	C1-O5-C5	-3.40	107.93	112.25
14	B	941	MAN	C6-C5-C4	-3.40	104.64	113.02
2	B	901	NAG	C4-C3-C2	-3.39	105.96	111.23
4	B	917	BMA	O4-C4-C3	-3.38	102.72	110.34
8	A	927	NAG	C3-C4-C5	-3.37	104.33	110.20
13	B	920	BMA	O6-C6-C5	-3.35	100.26	111.33
8	A	930	MAN	O4-C4-C5	-3.35	100.36	109.24
2	B	910	NAG	C2-N2-C7	-3.35	118.74	123.04
5	A	911	NAG	O7-C7-C8	-3.33	115.94	122.06
4	B	930	BMA	C6-C5-C4	-3.33	104.79	113.02
13	B	924	MAN	O4-C4-C5	-3.33	100.42	109.24
4	B	916	NAG	C1-O5-C5	-3.31	108.04	112.25
2	A	902	NAG	O4-C4-C5	-3.28	100.54	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	915	BMA	C3-C4-C5	-3.26	104.52	110.20
6	A	921	MAN	O6-C6-C5	-3.23	100.65	111.33
8	B	931	NAG	C2-N2-C7	-3.23	118.89	123.04
8	B	937	MAN	C6-C5-C4	-3.20	105.12	113.02
13	B	927	MAN	O2-C2-C1	-3.19	102.80	109.21
14	B	942	MAN	O3-C3-C2	-3.19	104.23	110.00
2	B	912	MAN	O2-C2-C1	-3.19	102.81	109.21
5	A	911	NAG	O4-C4-C5	-3.16	100.85	109.24
14	B	941	MAN	C1-C2-C3	-3.15	105.82	109.54
6	A	913	NAG	O4-C4-C3	-3.14	103.27	110.34
2	B	910	NAG	C1-O5-C5	-3.09	108.32	112.25
2	B	902	NAG	C2-N2-C7	-3.09	119.07	123.04
6	A	919	MAN	O5-C1-C2	-3.09	105.85	110.86
13	B	924	MAN	O2-C2-C1	-3.05	103.09	109.21
8	A	926	NAG	O3-C3-C2	-3.04	103.10	109.11
8	B	932	NAG	C1-O5-C5	-3.00	108.44	112.25
8	A	927	NAG	C2-N2-C7	-2.99	119.19	123.04
4	A	909	NAG	O6-C6-C5	-2.98	101.49	111.33
8	B	935	MAN	O2-C2-C3	-2.95	104.18	110.12
8	B	934	MAN	C1-O5-C5	-2.95	108.51	112.25
14	B	938	NAG	O6-C6-C5	-2.94	101.63	111.33
14	B	943	MAN	O2-C2-C3	-2.93	104.23	110.12
8	B	931	NAG	C4-C3-C2	-2.92	106.68	111.23
13	B	924	MAN	O2-C2-C3	-2.90	104.29	110.12
8	B	937	MAN	O3-C3-C2	-2.89	104.78	110.00
4	A	923	NAG	O4-C4-C3	-2.89	103.84	110.34
8	A	929	MAN	O5-C1-C2	-2.87	106.19	110.86
4	A	909	NAG	C4-C3-C2	-2.87	106.77	111.23
2	B	904	MAN	O2-C2-C1	-2.87	103.45	109.21
8	B	932	NAG	O4-C4-C3	-2.87	103.88	110.34
2	A	902	NAG	O7-C7-C8	-2.87	116.80	122.06
6	A	913	NAG	C2-N2-C7	-2.86	119.36	123.04
4	A	923	NAG	C4-C3-C2	-2.85	106.79	111.23
14	B	938	NAG	O3-C3-C2	-2.84	103.48	109.11
8	B	932	NAG	O6-C6-C5	-2.83	101.97	111.33
13	B	926	MAN	C2-C3-C4	-2.82	106.25	111.04
4	B	916	NAG	O6-C6-C5	-2.81	102.04	111.33
8	A	931	MAN	O6-C6-C5	-2.78	102.13	111.33
4	A	924	NAG	C2-N2-C7	-2.78	119.47	123.04
4	A	908	NAG	O7-C7-C8	-2.77	116.97	122.06
8	B	936	MAN	C2-C3-C4	-2.76	106.35	111.04
8	B	934	MAN	O3-C3-C2	-2.76	105.01	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	937	MAN	C2-C3-C4	-2.76	106.36	111.04
8	B	932	NAG	C3-C4-C5	-2.75	105.41	110.20
6	A	914	NAG	O4-C4-C3	-2.74	104.16	110.34
2	B	906	MAN	C2-C3-C4	-2.73	106.40	111.04
8	B	933	BMA	C1-C2-C3	-2.73	106.32	109.54
2	A	904	MAN	C1-O5-C5	-2.71	108.81	112.25
8	A	935	BMA	O4-C4-C5	-2.68	102.13	109.24
13	B	922	MAN	O6-C6-C5	-2.68	102.48	111.33
4	A	924	NAG	C6-C5-C4	-2.68	106.41	113.02
13	B	926	MAN	C6-C5-C4	-2.68	106.41	113.02
8	B	931	NAG	O3-C3-C2	-2.67	103.82	109.11
8	A	937	MAN	C3-C4-C5	-2.67	105.54	110.20
8	A	929	MAN	C1-O5-C5	-2.64	108.90	112.25
8	A	926	NAG	O3-C3-C4	-2.63	104.42	110.34
2	B	910	NAG	C4-C3-C2	-2.61	107.17	111.23
13	B	921	MAN	C2-C3-C4	-2.60	106.62	111.04
8	B	931	NAG	O4-C4-C5	-2.60	102.35	109.24
8	A	930	MAN	O4-C4-C3	-2.59	104.50	110.34
13	B	925	MAN	O2-C2-C1	-2.57	104.05	109.21
8	A	931	MAN	O2-C2-C1	-2.57	104.05	109.21
2	A	903	BMA	O6-C6-C5	-2.57	102.84	111.33
4	A	923	NAG	O3-C3-C2	-2.56	104.04	109.11
8	A	929	MAN	O4-C4-C3	-2.55	104.60	110.34
13	B	927	MAN	O3-C3-C4	-2.55	104.60	110.34
2	B	901	NAG	C1-O5-C5	-2.55	109.02	112.25
14	B	942	MAN	O4-C4-C3	-2.54	104.62	110.34
4	B	917	BMA	C6-C5-C4	-2.53	106.76	113.02
4	A	908	NAG	C4-C3-C2	-2.53	107.30	111.23
8	B	935	MAN	O6-C6-C5	-2.52	103.00	111.33
8	A	937	MAN	C2-C3-C4	-2.52	106.76	111.04
4	B	929	NAG	O7-C7-C8	-2.52	117.44	122.06
2	B	904	MAN	O3-C3-C2	-2.52	105.45	110.00
8	A	930	MAN	O6-C6-C5	-2.51	103.03	111.33
6	A	918	MAN	O6-C6-C5	-2.51	103.05	111.33
2	A	901	NAG	C1-O5-C5	-2.50	109.07	112.25
2	B	911	BMA	C2-C3-C4	-2.50	106.79	111.04
8	B	936	MAN	O6-C6-C5	-2.50	103.08	111.33
2	B	901	NAG	C2-N2-C7	-2.50	119.83	123.04
2	A	903	BMA	C6-C5-C4	-2.50	106.86	113.02
4	A	909	NAG	O3-C3-C2	-2.49	104.17	109.11
8	A	938	MAN	C6-C5-C4	-2.49	106.88	113.02
2	B	910	NAG	O4-C4-C5	-2.48	102.68	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	929	MAN	O2-C2-C3	-2.47	105.15	110.12
4	A	925	BMA	C2-C3-C4	-2.46	106.86	111.04
4	B	928	NAG	O3-C3-C2	-2.46	104.25	109.11
8	B	937	MAN	O2-C2-C1	-2.45	104.30	109.21
14	B	944	MAN	C1-C2-C3	-2.45	106.65	109.54
2	B	905	MAN	O2-C2-C1	-2.45	104.30	109.21
13	B	920	BMA	C3-C4-C5	-2.44	105.95	110.20
6	A	921	MAN	C1-C2-C3	-2.44	106.66	109.54
6	A	915	BMA	O5-C1-C2	-2.44	106.90	110.86
6	A	919	MAN	O6-C6-C5	-2.43	103.29	111.33
14	B	938	NAG	O4-C4-C3	-2.43	104.86	110.34
8	A	926	NAG	O7-C7-C8	-2.42	117.62	122.06
13	B	919	NAG	O4-C4-C3	-2.42	104.90	110.34
6	A	917	MAN	O3-C3-C4	-2.42	104.90	110.34
6	A	921	MAN	C6-C5-C4	-2.41	107.08	113.02
8	A	936	MAN	O5-C5-C6	-2.40	102.14	107.35
13	B	918	NAG	O4-C4-C5	-2.39	102.91	109.24
2	A	902	NAG	C2-N2-C7	-2.39	119.97	123.04
2	B	913	MAN	O5-C1-C2	-2.38	106.99	110.86
8	A	933	NAG	O7-C7-C8	-2.38	117.70	122.06
4	B	917	BMA	O5-C1-C2	-2.37	107.01	110.86
13	B	925	MAN	C1-C2-C3	-2.35	106.76	109.54
13	B	926	MAN	O3-C3-C4	-2.34	105.07	110.34
2	B	905	MAN	O2-C2-C3	-2.32	105.44	110.12
8	A	927	NAG	O7-C7-N2	-2.32	117.12	121.86
2	B	902	NAG	O4-C4-C3	-2.32	105.12	110.34
6	A	915	BMA	O6-C6-C5	-2.32	103.67	111.33
6	A	921	MAN	O2-C2-C3	-2.31	105.47	110.12
13	B	922	MAN	O3-C3-C2	-2.30	105.84	110.00
8	A	934	NAG	C6-C5-C4	-2.30	107.34	113.02
13	B	921	MAN	C6-C5-C4	-2.30	107.34	113.02
6	A	920	MAN	O2-C2-C3	-2.29	105.51	110.12
4	B	916	NAG	O7-C7-C8	-2.29	117.86	122.06
8	B	934	MAN	O4-C4-C3	-2.29	105.18	110.34
2	B	905	MAN	C1-O5-C5	-2.28	109.36	112.25
13	B	920	BMA	O5-C1-C2	-2.27	107.17	110.86
2	B	906	MAN	O4-C4-C3	-2.27	105.22	110.34
2	B	902	NAG	C1-O5-C5	-2.27	109.37	112.25
13	B	920	BMA	O3-C3-C4	-2.27	105.23	110.34
14	B	938	NAG	C4-C3-C2	-2.26	107.71	111.23
2	A	906	MAN	O4-C4-C5	-2.26	103.25	109.24
6	A	917	MAN	C6-C5-C4	-2.26	107.45	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	921	MAN	O2-C2-C1	-2.26	104.68	109.21
8	A	934	NAG	O7-C7-N2	-2.25	117.27	121.86
6	A	916	MAN	O2-C2-C1	-2.25	104.69	109.21
2	A	905	MAN	O4-C4-C3	-2.25	105.27	110.34
8	B	935	MAN	O2-C2-C1	-2.24	104.72	109.21
8	A	933	NAG	C4-C3-C2	-2.23	107.76	111.23
8	B	933	BMA	O3-C3-C2	-2.22	105.98	110.00
14	B	939	NAG	O3-C3-C4	-2.22	105.34	110.34
2	A	901	NAG	O7-C7-C8	-2.21	118.00	122.06
2	B	904	MAN	O2-C2-C3	-2.21	105.68	110.12
4	A	908	NAG	C2-N2-C7	-2.21	120.20	123.04
8	A	927	NAG	O6-C6-C5	-2.20	104.05	111.33
13	B	924	MAN	O3-C3-C2	-2.20	106.02	110.00
4	A	925	BMA	C6-C5-C4	-2.20	107.59	113.02
14	B	942	MAN	C1-O5-C5	-2.17	109.50	112.25
5	A	912	NAG	O3-C3-C2	-2.17	104.82	109.11
8	B	936	MAN	O4-C4-C3	-2.16	105.48	110.34
14	B	939	NAG	O4-C4-C5	-2.16	103.53	109.24
2	B	901	NAG	O4-C4-C3	-2.14	105.52	110.34
8	A	932	MAN	O3-C3-C4	-2.14	105.52	110.34
8	B	931	NAG	C3-C2-N2	-2.13	105.45	110.56
2	B	910	NAG	O4-C4-C3	-2.13	105.54	110.34
13	B	921	MAN	O5-C5-C6	-2.12	102.75	107.35
2	B	901	NAG	O3-C3-C2	-2.12	104.92	109.11
5	A	912	NAG	C8-C7-N2	-2.11	112.07	116.11
8	B	931	NAG	O4-C4-C3	-2.11	105.59	110.34
14	B	939	NAG	C3-C4-C5	-2.11	106.53	110.20
4	B	917	BMA	O3-C3-C4	-2.10	105.60	110.34
14	B	941	MAN	O6-C6-C5	-2.10	104.39	111.33
13	B	924	MAN	O4-C4-C3	-2.09	105.64	110.34
14	B	944	MAN	O4-C4-C3	-2.08	105.65	110.34
4	A	923	NAG	C3-C2-N2	-2.08	105.59	110.56
6	A	918	MAN	C2-C3-C4	-2.07	107.52	111.04
2	B	909	NAG	C3-C2-N2	-2.07	105.60	110.56
8	B	937	MAN	C1-C2-C3	-2.07	107.10	109.54
2	A	902	NAG	C4-C3-C2	-2.06	108.02	111.23
14	B	944	MAN	C6-C5-C4	-2.06	107.93	113.02
14	B	943	MAN	C2-C3-C4	-2.06	107.54	111.04
2	B	901	NAG	O4-C4-C5	-2.05	103.81	109.24
8	A	935	BMA	O2-C2-C1	-2.05	105.10	109.21
6	A	916	MAN	C2-C3-C4	-2.04	107.57	111.04
2	A	901	NAG	C3-C4-C5	-2.04	106.64	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	917	MAN	O6-C6-C5	-2.03	104.63	111.33
2	A	906	MAN	C1-O5-C5	2.01	114.80	112.25
13	B	927	MAN	O5-C1-C2	2.01	114.12	110.86
8	A	930	MAN	C6-C5-C4	2.02	118.00	113.02
14	B	945	MAN	O4-C4-C3	2.02	114.90	110.34
2	B	909	NAG	O7-C7-N2	2.03	126.00	121.86
2	A	902	NAG	O3-C3-C4	2.04	114.92	110.34
4	B	916	NAG	O7-C7-N2	2.04	126.02	121.86
13	B	925	MAN	O2-C2-C3	2.06	114.26	110.12
2	A	904	MAN	O6-C6-C5	2.06	118.13	111.33
14	B	940	BMA	C1-C2-C3	2.12	112.05	109.54
14	B	941	MAN	O2-C2-C3	2.15	114.45	110.12
14	B	940	BMA	O4-C4-C3	2.17	115.21	110.34
4	A	924	NAG	O5-C5-C6	2.17	112.05	107.35
4	B	930	BMA	C1-O5-C5	2.19	115.03	112.25
8	A	926	NAG	C8-C7-N2	2.21	120.33	116.11
2	B	906	MAN	O5-C1-C2	2.21	114.44	110.86
13	B	920	BMA	C1-C2-C3	2.21	112.16	109.54
8	B	937	MAN	C1-O5-C5	2.24	115.10	112.25
8	A	938	MAN	O5-C1-C2	2.32	114.62	110.86
14	B	942	MAN	O5-C1-C2	2.32	114.62	110.86
2	B	905	MAN	C6-C5-C4	2.35	118.81	113.02
14	B	938	NAG	O7-C7-N2	2.36	126.67	121.86
6	A	917	MAN	C2-C3-C4	2.36	115.05	111.04
5	A	911	NAG	C3-C4-C5	2.37	114.33	110.20
2	A	904	MAN	O2-C2-C1	2.40	114.01	109.21
2	A	905	MAN	O3-C3-C2	2.41	114.36	110.00
2	A	904	MAN	C6-C5-C4	2.42	118.98	113.02
13	B	925	MAN	C1-O5-C5	2.42	115.32	112.25
8	A	928	BMA	C1-C2-C3	2.43	112.42	109.54
8	A	934	NAG	O7-C7-C8	2.44	126.54	122.06
13	B	923	MAN	O5-C1-C2	2.47	114.86	110.86
5	A	912	NAG	C3-C2-N2	2.49	116.52	110.56
2	A	906	MAN	O3-C3-C4	2.49	115.95	110.34
8	A	937	MAN	O3-C3-C2	2.51	114.53	110.00
4	A	910	BMA	O3-C3-C4	2.53	116.02	110.34
14	B	939	NAG	C1-O5-C5	2.55	115.49	112.25
8	A	939	MAN	C1-O5-C5	2.57	115.51	112.25
6	A	916	MAN	O5-C1-C2	2.60	115.08	110.86
13	B	924	MAN	O5-C1-C2	2.62	115.11	110.86
4	A	924	NAG	C4-C3-C2	2.65	115.35	111.23
14	B	945	MAN	O5-C5-C6	2.68	113.15	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	933	NAG	O7-C7-N2	2.69	127.35	121.86
2	B	903	BMA	O2-C2-C1	2.69	114.60	109.21
4	A	910	BMA	O5-C5-C6	2.78	113.36	107.35
2	A	902	NAG	O7-C7-N2	2.79	127.55	121.86
4	B	930	BMA	C3-C4-C5	2.80	115.08	110.20
4	B	930	BMA	O5-C5-C6	2.82	113.46	107.35
14	B	942	MAN	C1-C2-C3	2.82	112.88	109.54
8	B	932	NAG	C6-C5-C4	2.84	120.02	113.02
14	B	940	BMA	C1-O5-C5	2.88	115.90	112.25
14	B	939	NAG	O5-C5-C6	2.89	113.61	107.35
6	A	915	BMA	C1-C2-C3	2.90	112.98	109.54
2	A	906	MAN	C3-C4-C5	2.90	115.26	110.20
2	B	904	MAN	C1-C2-C3	2.91	112.98	109.54
4	B	929	NAG	C4-C3-C2	2.92	115.76	111.23
2	B	911	BMA	O3-C3-C2	2.93	115.30	110.00
14	B	941	MAN	O2-C2-C1	2.96	115.14	109.21
14	B	943	MAN	O5-C5-C6	3.04	113.92	107.35
8	A	934	NAG	C1-O5-C5	3.04	116.11	112.25
14	B	945	MAN	C1-C2-C3	3.04	113.14	109.54
2	B	906	MAN	O3-C3-C2	3.04	115.49	110.00
4	A	925	BMA	O2-C2-C1	3.08	115.38	109.21
2	B	914	MAN	O5-C1-C2	3.08	115.86	110.86
8	B	935	MAN	C1-O5-C5	3.10	116.18	112.25
13	B	924	MAN	C1-O5-C5	3.14	116.23	112.25
2	A	902	NAG	C6-C5-C4	3.14	120.77	113.02
14	B	938	NAG	C1-O5-C5	3.14	116.24	112.25
2	A	901	NAG	O7-C7-N2	3.17	128.32	121.86
14	B	944	MAN	C1-O5-C5	3.19	116.30	112.25
4	A	925	BMA	O3-C3-C4	3.19	117.53	110.34
4	A	909	NAG	C8-C7-N2	3.20	122.22	116.11
6	A	917	MAN	C1-C2-C3	3.20	113.33	109.54
8	A	929	MAN	O5-C5-C6	3.32	114.53	107.35
6	A	921	MAN	C1-O5-C5	3.34	116.49	112.25
8	B	935	MAN	O3-C3-C4	3.35	117.87	110.34
8	B	935	MAN	C6-C5-C4	3.38	121.36	113.02
4	B	915	NAG	C2-N2-C7	3.41	127.42	123.04
8	A	931	MAN	C1-C2-C3	3.42	113.58	109.54
8	A	930	MAN	O3-C3-C4	3.44	118.08	110.34
6	A	917	MAN	O5-C1-C2	3.46	116.47	110.86
2	A	905	MAN	O2-C2-C1	3.52	116.25	109.21
2	A	906	MAN	O5-C1-C2	3.61	116.71	110.86
14	B	941	MAN	O3-C3-C2	3.62	116.54	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	939	MAN	C1-C2-C3	3.63	113.83	109.54
2	B	913	MAN	O5-C5-C6	3.65	115.25	107.35
2	A	905	MAN	O5-C5-C6	3.69	115.34	107.35
13	B	923	MAN	C1-O5-C5	3.73	116.99	112.25
6	A	917	MAN	O2-C2-C3	3.80	117.77	110.12
2	B	904	MAN	C1-O5-C5	3.85	117.14	112.25
13	B	926	MAN	C1-C2-C3	3.88	114.13	109.54
2	B	902	NAG	O7-C7-N2	3.92	129.86	121.86
8	A	930	MAN	C1-O5-C5	3.93	117.24	112.25
8	A	930	MAN	O5-C1-C2	3.94	117.25	110.86
13	B	921	MAN	C1-O5-C5	3.95	117.26	112.25
13	B	922	MAN	C1-O5-C5	4.07	117.41	112.25
4	A	910	BMA	O6-C6-C5	4.17	125.11	111.33
8	A	931	MAN	O3-C3-C2	4.17	117.54	110.00
4	B	930	BMA	O3-C3-C2	4.35	117.85	110.00
8	A	938	MAN	O2-C2-C1	4.36	117.95	109.21
4	A	909	NAG	C6-C5-C4	4.36	123.78	113.02
8	A	938	MAN	C1-O5-C5	4.38	117.81	112.25
2	B	910	NAG	C6-C5-C4	4.51	124.15	113.02
5	A	912	NAG	C2-N2-C7	4.53	128.85	123.04
2	A	904	MAN	O3-C3-C2	4.53	118.18	110.00
2	B	912	MAN	O2-C2-C3	4.66	119.49	110.12
2	A	904	MAN	O4-C4-C3	4.83	121.22	110.34
8	A	931	MAN	C1-O5-C5	5.20	118.85	112.25
8	A	935	BMA	C1-O5-C5	5.42	119.13	112.25
8	B	935	MAN	C1-C2-C3	5.45	115.98	109.54
13	B	921	MAN	C1-C2-C3	5.46	116.00	109.54
6	A	917	MAN	C1-O5-C5	5.48	119.20	112.25
13	B	926	MAN	C1-O5-C5	5.84	119.66	112.25
8	B	936	MAN	C1-O5-C5	5.89	119.73	112.25
4	A	925	BMA	C1-O5-C5	6.04	119.91	112.25
2	A	904	MAN	O5-C5-C6	6.04	120.43	107.35
2	B	906	MAN	C1-C2-C3	6.09	116.75	109.54
14	B	945	MAN	C1-O5-C5	6.13	120.02	112.25
4	A	910	BMA	C3-C4-C5	6.23	121.06	110.20
4	B	917	BMA	C1-O5-C5	6.59	120.61	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	BMA	5	0
2	A	904	MAN	6	0
4	A	908	NAG	1	0
4	A	909	NAG	1	0
5	A	912	NAG	3	0
6	A	921	MAN	3	0
8	A	926	NAG	1	0
8	A	928	BMA	1	0
2	B	905	MAN	2	0
2	B	909	NAG	1	0
8	B	933	BMA	1	0

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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	907	1	14,14,15	0.94	1 (7%)	15,19,21	1.35	2 (13%)
7	MAN	A	922	6	11,11,12	0.58	0	14,15,17	2.35	4 (28%)
3	NAG	A	940	1	14,14,15	0.85	1 (7%)	15,19,21	1.40	4 (26%)
9	MPD	A	941	-	6,7,7	0.89	0	7,10,10	1.54	1 (14%)
10	MRD	A	942	-	6,7,7	1.34	1 (16%)	7,10,10	1.36	1 (14%)
10	MRD	A	943	-	6,7,7	1.05	0	7,10,10	0.27	0
12	ACY	A	945	-	1,3,3	3.88	1 (100%)	0,3,3	0.00	-
7	MAN	B	907	2	11,11,12	1.07	1 (9%)	14,15,17	2.65	6 (42%)
3	NAG	B	908	1	14,14,15	1.15	2 (14%)	15,19,21	2.67	6 (40%)
3	NAG	B	946	1	14,14,15	0.79	0	15,19,21	1.59	2 (13%)
10	MRD	B	947	-	6,7,7	1.06	1 (16%)	7,10,10	0.72	0
10	MRD	B	948	-	6,7,7	1.34	1 (16%)	7,10,10	1.27	0
10	MRD	B	949	-	6,7,7	1.08	0	7,10,10	1.56	1 (14%)
12	ACY	B	951	-	1,3,3	6.21	1 (100%)	0,3,3	0.00	-

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	907	1	-	0/6/23/26	0/1/1/1
7	MAN	A	922	6	-	0/2/19/22	0/1/1/1
3	NAG	A	940	1	-	0/6/23/26	0/1/1/1
9	MPD	A	941	-	-	0/5/5/5	0/0/0/0
10	MRD	A	942	-	-	0/5/5/5	0/0/0/0
10	MRD	A	943	-	-	0/5/5/5	0/0/0/0
12	ACY	A	945	-	-	0/0/0/0	0/0/0/0
7	MAN	B	907	2	-	0/2/19/22	0/1/1/1
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	946	1	-	0/6/23/26	0/1/1/1
10	MRD	B	947	-	-	0/5/5/5	0/0/0/0
10	MRD	B	948	-	-	0/5/5/5	0/0/0/0
10	MRD	B	949	-	-	0/5/5/5	0/0/0/0
12	ACY	B	951	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	907	NAG	O5-C1	-2.66	1.39	1.43
3	B	908	NAG	O5-C1	-2.17	1.40	1.43
3	A	940	NAG	C1-C2	-2.12	1.49	1.52
3	B	908	NAG	C2-N2	-2.01	1.42	1.46
10	A	942	MRD	CM-C2	2.06	1.59	1.52
7	B	907	MAN	C1-C2	2.17	1.57	1.52
10	B	947	MRD	C1-C2	2.27	1.60	1.52
10	B	948	MRD	CM-C2	2.44	1.60	1.52
12	A	945	ACY	CH3-C	3.88	1.54	1.48
12	B	951	ACY	CH3-C	6.21	1.57	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C4-C3-C2	-7.21	100.01	111.23
7	B	907	MAN	O2-C2-C1	-5.03	99.12	109.21
7	A	922	MAN	O2-C2-C1	-4.25	100.69	109.21
9	A	941	MPD	CM-C2-C1	-3.81	101.94	110.24
3	B	946	NAG	C1-O5-C5	-3.75	107.49	112.25
3	B	908	NAG	C6-C5-C4	-3.64	104.03	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	907	MAN	O6-C6-C5	-3.19	100.81	111.33
3	B	946	NAG	O6-C6-C5	-3.08	101.16	111.33
3	A	907	NAG	C2-N2-C7	-3.02	119.16	123.04
3	A	940	NAG	C2-N2-C7	-2.75	119.51	123.04
3	B	908	NAG	O7-C7-N2	-2.73	116.30	121.86
3	A	940	NAG	O7-C7-C8	-2.55	117.38	122.06
7	B	907	MAN	C6-C5-C4	-2.31	107.31	113.02
10	A	942	MRD	C2-C3-C4	-2.27	105.94	116.66
3	A	940	NAG	O6-C6-C5	-2.25	103.89	111.33
7	B	907	MAN	C3-C4-C5	-2.23	106.31	110.20
3	A	907	NAG	O4-C4-C3	-2.12	105.56	110.34
7	A	922	MAN	O3-C3-C4	-2.05	105.72	110.34
3	A	940	NAG	C8-C7-N2	2.02	119.96	116.11
3	B	908	NAG	C8-C7-N2	2.07	120.07	116.11
3	B	908	NAG	O3-C3-C4	2.20	115.29	110.34
7	A	922	MAN	O5-C5-C6	2.67	113.13	107.35
7	B	907	MAN	C1-C2-C3	2.69	112.72	109.54
10	B	949	MRD	CM-C2-C1	3.58	118.05	110.24
3	B	908	NAG	C2-N2-C7	3.78	127.90	123.04
7	B	907	MAN	C1-O5-C5	6.09	119.97	112.25
7	A	922	MAN	C1-O5-C5	6.22	120.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	922	MAN	3	0
10	A	942	MRD	2	0
7	B	907	MAN	2	0
10	B	948	MRD	4	0
10	B	949	MRD	1	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	834/841 (99%)	-0.55	5 (0%) 90 88	5, 12, 23, 55	0
1	B	832/841 (98%)	-0.59	3 (0%) 93 91	5, 9, 20, 51	0
All	All	1666/1682 (99%)	-0.57	8 (0%) 91 90	5, 10, 22, 55	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	VAL	3.8
1	B	668	ASN	3.2
1	B	860	GLN	3.0
1	A	860	GLN	2.8
1	A	669	ALA	2.7
1	B	676	ALA	2.7
1	A	676	ALA	2.3
1	A	790	PRO	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MAN	A	932	11/12	0.96	0.15	8.00	12,16,25,33	0
8	MAN	B	937	11/12	0.95	0.13	5.05	15,18,27,30	0
8	NAG	A	926	14/15	0.97	0.09	3.86	11,13,38,40	0
4	NAG	A	909	14/15	0.94	0.14	3.57	17,23,26,29	0
14	MAN	B	942	11/12	0.94	0.14	3.54	16,20,25,28	0
8	MAN	A	936	11/12	0.96	0.12	3.42	15,20,24,25	0
2	NAG	B	910	14/15	0.96	0.08	2.21	11,16,25,27	0
4	NAG	A	923	14/15	0.95	0.09	1.97	14,18,26,26	0
8	NAG	B	931	14/15	0.97	0.08	1.29	10,13,33,33	0
6	NAG	A	913	14/15	0.95	0.09	1.04	13,15,20,22	0
4	NAG	B	928	14/15	0.96	0.07	0.84	12,14,23,28	0
6	MAN	A	920	11/12	0.97	0.09	0.66	13,15,16,16	0
13	NAG	B	918	14/15	0.98	0.07	0.25	9,10,15,15	0
13	MAN	B	927	11/12	0.98	0.07	-0.05	11,13,14,15	0
2	NAG	B	909	14/15	0.97	0.07	-0.16	10,13,16,16	0
6	MAN	A	921	11/12	0.95	0.08	-0.17	12,17,19,31	0
14	NAG	B	938	14/15	0.98	0.07	-0.19	11,13,17,18	0
2	NAG	A	902	14/15	0.97	0.07	-0.29	13,18,28,33	0
2	NAG	A	901	14/15	0.97	0.07	-0.29	11,13,15,15	0
13	NAG	B	919	14/15	0.97	0.07	-0.29	8,10,11,11	0
4	NAG	A	908	14/15	0.96	0.07	-0.50	11,15,16,18	0
13	MAN	B	924	11/12	0.95	0.08	-0.53	11,13,17,24	0
13	MAN	B	926	11/12	0.98	0.07	-0.55	8,9,11,12	0
8	NAG	A	933	14/15	0.98	0.06	-0.72	11,13,16,18	0
2	NAG	B	902	14/15	0.98	0.06	-0.76	9,11,15,22	0
6	NAG	A	914	14/15	0.98	0.06	-0.79	12,13,14,15	0
5	NAG	A	911	14/15	0.97	0.06	-0.86	11,14,16,16	0
4	NAG	B	915	14/15	0.98	0.06	-0.91	9,10,12,13	0
6	MAN	A	919	11/12	0.98	0.06	-1.14	11,13,15,16	0
2	NAG	B	901	14/15	0.99	0.05	-1.21	7,9,11,11	0
2	MAN	B	904	11/12	0.96	0.13	-	20,27,33,36	0
6	BMA	A	915	11/12	0.97	0.06	-	13,15,17,18	0
14	MAN	B	943	11/12	0.94	0.11	-	18,20,25,28	0
2	BMA	B	911	11/12	0.91	0.16	-	24,27,31,31	0
2	MAN	A	905	11/12	0.85	0.24	-	25,27,32,32	0
2	MAN	B	913	11/12	0.88	0.23	-	32,36,43,44	0
8	BMA	A	928	11/12	0.93	0.16	-	15,18,25,30	0
14	NAG	B	939	14/15	0.96	0.11	-	18,22,24,29	0
8	MAN	B	935	11/12	0.96	0.12	-	17,19,28,35	0
2	MAN	B	912	11/12	0.82	0.32	-	33,37,44,45	0
14	MAN	B	945	11/12	0.89	0.22	-	26,34,37,45	0
14	MAN	B	944	11/12	0.87	0.22	-	41,49,56,61	0
4	NAG	B	916	14/15	0.93	0.12	-	13,17,26,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	B	906	11/12	0.92	0.11	-	22,26,29,36	0
14	MAN	B	941	11/12	0.76	0.23	-	48,58,65,69	0
8	NAG	A	927	14/15	0.96	0.09	-	13,16,25,27	0
14	BMA	B	940	11/12	0.93	0.14	-	20,26,29,33	0
5	NAG	A	912	14/15	0.93	0.12	-	12,22,31,38	0
6	MAN	A	917	11/12	0.93	0.17	-	31,36,46,51	0
8	MAN	A	931	11/12	0.95	0.13	-	15,16,26,34	0
8	MAN	A	929	11/12	0.80	0.30	-	52,55,61,62	0
2	BMA	B	903	11/12	0.97	0.07	-	12,14,19,19	0
8	MAN	A	939	11/12	0.90	0.23	-	25,28,34,34	0
2	MAN	B	905	11/12	0.95	0.14	-	20,29,40,58	0
13	MAN	B	923	11/12	0.99	0.06	-	9,9,12,12	0
13	MAN	B	925	11/12	0.95	0.11	-	18,21,27,32	0
2	MAN	A	904	11/12	0.73	0.31	-	28,45,54,60	0
13	BMA	B	920	11/12	0.98	0.06	-	9,10,12,12	0
4	NAG	A	924	14/15	0.85	0.21	-	26,32,39,39	0
13	MAN	B	921	11/12	0.98	0.06	-	12,14,17,18	0
4	BMA	A	925	11/12	0.79	0.29	-	30,40,51,58	0
8	MAN	A	937	11/12	0.94	0.11	-	16,21,24,26	0
4	BMA	B	917	11/12	0.75	0.29	-	53,62,81,82	0
8	MAN	A	930	11/12	0.94	0.13	-	18,23,30,30	0
4	BMA	A	910	11/12	0.85	0.21	-	31,37,46,57	0
8	BMA	B	933	11/12	0.94	0.15	-	16,18,27,28	0
2	MAN	A	906	11/12	0.92	0.15	-	26,33,39,41	0
13	MAN	B	922	11/12	0.92	0.13	-	19,25,30,32	0
4	NAG	B	929	14/15	0.92	0.16	-	20,26,42,44	0
4	BMA	B	930	11/12	0.86	0.22	-	33,40,48,56	0
2	MAN	B	914	11/12	0.86	0.26	-	34,36,43,47	0
8	MAN	B	934	11/12	0.80	0.31	-	54,63,69,71	0
6	MAN	A	916	11/12	0.97	0.07	-	17,18,22,25	0
8	MAN	B	936	11/12	0.95	0.12	-	16,19,28,34	0
6	MAN	A	918	11/12	0.99	0.05	-	11,12,14,15	0
8	NAG	A	934	14/15	0.95	0.10	-	15,20,23,25	0
8	NAG	B	932	14/15	0.94	0.12	-	12,19,25,28	0
2	BMA	A	903	11/12	0.92	0.17	-	19,24,27,30	0
8	BMA	A	935	11/12	0.92	0.14	-	20,25,30,34	0
8	MAN	A	938	11/12	0.90	0.24	-	38,49,56,67	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	MRD	A	942	8/8	0.92	0.13	17.18	13,16,31,33	0
10	MRD	B	949	8/8	0.88	0.19	8.09	28,39,42,42	0
10	MRD	A	943	8/8	0.88	0.15	6.67	19,23,27,28	0
10	MRD	B	947	8/8	0.89	0.15	6.56	17,21,24,24	0
10	MRD	B	948	8/8	0.94	0.10	5.45	13,19,32,35	0
3	NAG	B	946	14/15	0.97	0.16	3.66	19,23,28,32	0
7	MAN	B	907	11/12	0.94	0.13	2.54	18,21,29,35	0
3	NAG	A	940	14/15	0.96	0.16	1.93	21,28,36,39	0
9	MPD	A	941	8/8	0.95	0.08	1.05	16,18,20,22	0
12	ACY	B	951	4/4	0.94	0.10	0.45	13,16,16,18	0
12	ACY	A	945	4/4	0.95	0.10	0.04	18,18,20,21	0
11	NA	A	944	1/1	0.98	0.12	-	16,16,16,16	0
7	MAN	A	922	11/12	0.94	0.14	-	22,25,32,35	0
11	NA	B	950	1/1	0.97	0.11	-	20,20,20,20	0
3	NAG	B	908	14/15	0.88	0.26	-	30,40,47,51	0
3	NAG	A	907	14/15	0.83	0.33	-	37,48,55,57	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.