



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:06 AM GMT

PDB ID : 4IIC
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with isofagomine
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

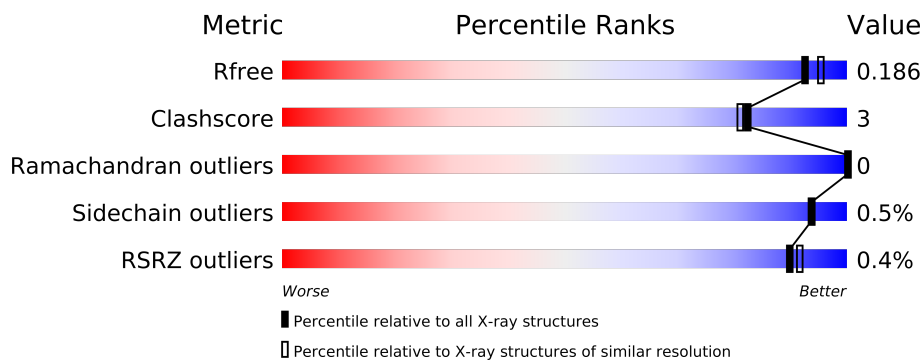
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	841	<div><div></div><div></div></div>
1	B	841	<div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	NA	B	949	-	X
3	NAG	A	906	-	X
3	NAG	B	908	-	X
3	NAG	B	944	-	X
3	NAG	B	945	-	X
8	MRD	A	941	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	MRD	B	946	-	X
8	MRD	B	947	-	X
8	MRD	B	948	-	X
9	MPD	A	942	-	X

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 15282 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

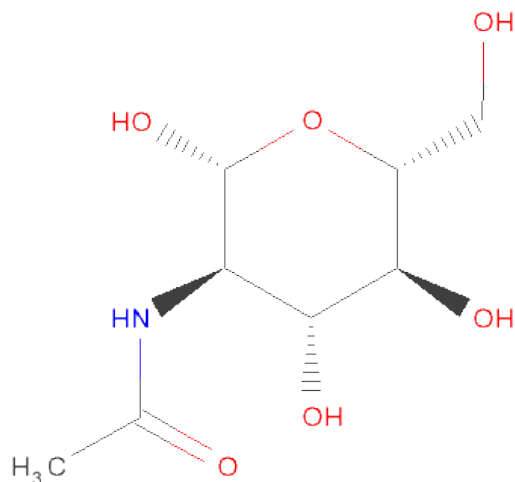
- Molecule 1 is a protein called Beta-glucosidase 1.

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 (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		

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



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

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

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

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

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

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

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

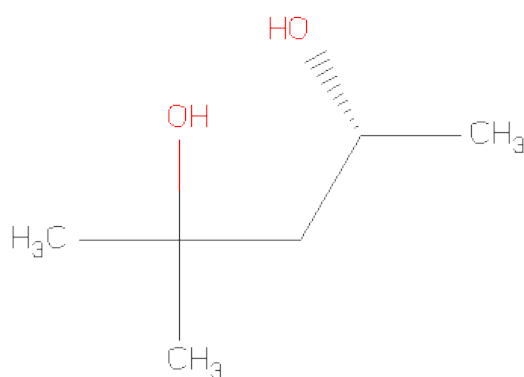
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	7	Total	C	N	O	0	0
			83	46	2	35		
7	A	7	Total	C	N	O	0	0
			83	46	2	35		

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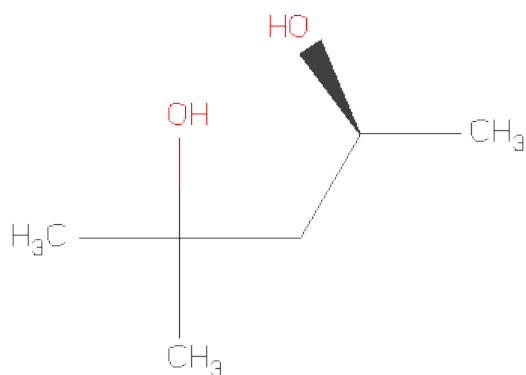
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	7	Total	C	N	O	0	0
			83	46	2	35		
7	B	7	Total	C	N	O	0	0
			83	46	2	35		

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



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

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

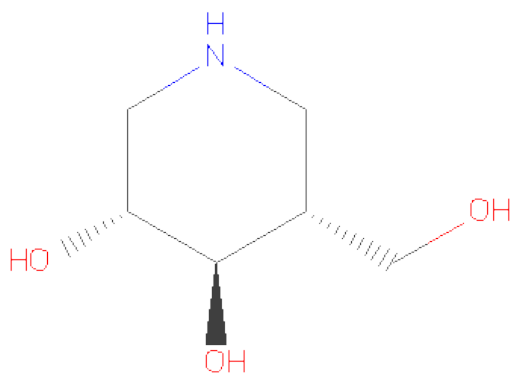


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 11 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: C₆H₁₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			10	6	1	3		
11	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 13 is a polymer of unknown type called SUGAR (8-MER).

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

- Molecule 14 is water.

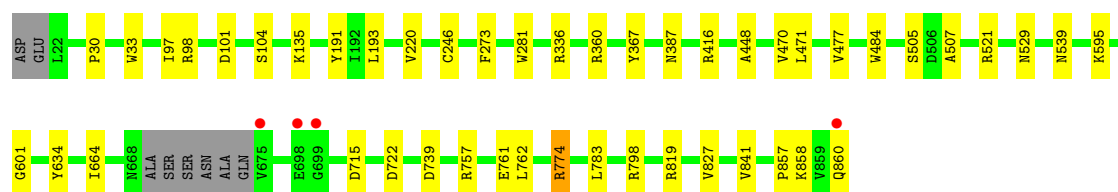
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	671	Total	O	0	0
			671	671		
14	B	761	Total	O	0	0
			761	761		

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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

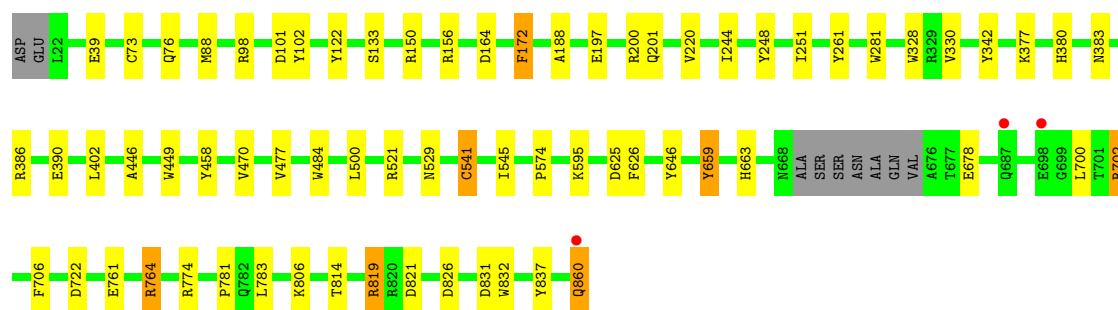
• Molecule 1: Beta-glucosidase 1

Chain A:



• Molecule 1: Beta-glucosidase 1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.14Å 122.48Å 222.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.23 – 1.90 37.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.23-1.90) 99.7 (37.23-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.145 , 0.184 0.147 , 0.186	Depositor DCC
R_{free} test set	8816 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 176093 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15282	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, IFM, 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	1.27	8/6545 (0.1%)	1.07	13/8923 (0.1%)
1	B	1.36	13/6538 (0.2%)	1.13	25/8913 (0.3%)
All	All	1.32	21/13083 (0.2%)	1.10	38/17836 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	CYS	CA-CB	9.60	1.75	1.53
1	B	122	TYR	CE1-CZ	7.42	1.48	1.38
1	B	646	TYR	CG-CD1	6.77	1.48	1.39
1	A	33	TRP	CE3-CZ3	6.75	1.50	1.38
1	B	761	GLU	CD-OE2	-5.68	1.19	1.25
1	A	761	GLU	CD-OE2	-5.65	1.19	1.25
1	B	122	TYR	CG-CD2	5.58	1.46	1.39
1	B	832	TRP	CE3-CZ3	5.51	1.47	1.38
1	B	342	TYR	CD1-CE1	5.50	1.47	1.39
1	B	197	GLU	CD-OE1	5.48	1.31	1.25
1	B	133	SER	CB-OG	5.45	1.49	1.42
1	B	328	TRP	CG-CD1	5.43	1.44	1.36
1	A	104	SER	CA-CB	5.43	1.61	1.52
1	A	601	GLY	N-CA	5.36	1.54	1.46
1	B	248	TYR	CE1-CZ	5.23	1.45	1.38
1	A	505	SER	CB-OG	5.23	1.49	1.42
1	B	458	TYR	CG-CD1	5.21	1.46	1.39
1	B	261	TYR	CE1-CZ	5.18	1.45	1.38
1	A	273	PHE	CG-CD2	5.10	1.46	1.38
1	A	471	LEU	N-CA	5.07	1.56	1.46
1	A	634	TYR	CE1-CZ	5.03	1.45	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	B	702	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	541	CYS	N-CA-CB	9.41	127.53	110.60
1	A	757	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	722	ASP	CB-CG-OD1	8.13	125.61	118.30
1	B	819	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	A	416	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	521	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	101	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	B	826	ASP	CB-CG-OD1	6.92	124.52	118.30
1	A	336	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	764	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	821	ASP	CB-CG-OD2	6.56	124.21	118.30
1	B	150	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	336	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	101	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	722	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	798	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	200	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	156	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	757	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	73	CYS	CA-CB-SG	-5.72	103.70	114.00
1	B	402	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	B	150	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	762	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	774	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	715	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	831	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	164	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	625	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	722	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	521	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	330	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	B	172	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	B	659	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	806	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	A	101	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	702	ARG	CB-CG-CD	-5.06	98.44	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6382	0	6092	24	0
1	B	6375	0	6082	34	0
2	A	61	0	52	1	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
4	A	78	0	68	1	0
4	B	78	0	68	0	0
5	A	28	0	25	0	0
6	A	116	0	96	0	0
6	B	116	0	96	0	0
7	A	166	0	139	2	0
7	B	166	0	140	2	0
8	A	16	0	28	7	0
8	B	24	0	42	8	0
9	A	8	0	14	9	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	10	0	13	0	0
11	B	10	0	13	0	0
12	B	50	0	43	1	0
13	B	94	0	77	6	0
14	A	671	0	0	6	0
14	B	761	0	0	14	0
All	All	15282	0	13153	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (84) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:541:CYS:CA	1:B:541:CYS:CB	1.75	1.64
9:A:942:MPD:C1	9:A:942:MPD:H52	1.66	1.23
9:A:942:MPD:H52	9:A:942:MPD:H11	1.08	1.05
1:B:678:GLU:HG2	14:B:1593:HOH:O	1.59	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:A:942:MPD:C1	9:A:942:MPD:C5	2.33	1.01
9:A:942:MPD:C5	9:A:942:MPD:H11	1.91	0.90
1:B:837:TYR:HE2	14:B:1541:HOH:O	1.56	0.87
8:B:947:MRD:H1C2	8:B:947:MRD:C5	2.02	0.83
1:A:819:ARG:HH12	1:A:860:GLN:C	1.81	0.83
1:A:360:ARG:HH11	8:A:941:MRD:HMC3	1.43	0.83
9:A:942:MPD:H13	9:A:942:MPD:C5	2.09	0.80
8:B:947:MRD:H1C2	8:B:947:MRD:H5C3	1.65	0.78
9:A:942:MPD:H52	9:A:942:MPD:H13	1.63	0.78
1:B:541:CYS:CB	1:B:541:CYS:C	2.55	0.74
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.70	0.72
8:A:941:MRD:HMC1	8:A:941:MRD:H5C3	1.71	0.72
8:A:941:MRD:HMC2	14:B:1147:HOH:O	1.89	0.72
1:A:98:ARG:HH22	9:A:942:MPD:H31	1.53	0.72
1:B:819:ARG:HH12	1:B:860:GLN:C	1.93	0.71
1:B:541:CYS:CB	1:B:541:CYS:HA	2.13	0.70
1:A:819:ARG:NH1	1:A:860:GLN:C	2.44	0.70
7:A:937:MAN:H3	14:A:1390:HOH:O	1.92	0.68
1:B:764:ARG:HD3	1:B:814:THR:HG21	1.78	0.66
1:B:201:GLN:HG3	14:B:1657:HOH:O	1.97	0.65
8:B:946:MRD:HMC2	14:B:1440:HOH:O	1.97	0.65
1:B:484:TRP:CE2	7:B:931:BMA:H62	2.32	0.64
8:B:948:MRD:H5C3	8:B:948:MRD:O2	2.00	0.61
1:B:764:ARG:HD3	1:B:814:THR:CG2	2.31	0.61
1:A:857:PRO:HD3	14:A:1230:HOH:O	2.01	0.60
1:A:484:TRP:CE2	7:A:927:BMA:H62	2.37	0.59
13:B:938:BMA:H62	13:B:940:MAN:H5	1.83	0.59
8:A:941:MRD:C5	8:A:941:MRD:HMC1	2.32	0.59
1:B:595:LYS:HE2	14:B:1396:HOH:O	2.02	0.59
8:B:948:MRD:O2	8:B:948:MRD:C5	2.50	0.58
1:B:98:ARG:HH12	8:B:946:MRD:HMC3	1.68	0.57
1:A:360:ARG:HH11	8:A:941:MRD:CM	2.18	0.56
13:B:938:BMA:H62	13:B:940:MAN:H3	1.89	0.54
1:B:783:LEU:HD23	1:B:783:LEU:C	2.29	0.53
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.91	0.52
8:B:947:MRD:C1	8:B:947:MRD:H5C3	2.38	0.52
1:B:390:GLU:CG	14:B:1514:HOH:O	2.57	0.52
1:B:386:ARG:NH2	14:B:1738:HOH:O	2.34	0.51
1:B:663:HIS:HB3	14:B:1652:HOH:O	2.11	0.51
8:A:940:MRD:H5C3	8:A:940:MRD:O2	2.11	0.50
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.95	0.49
1:B:172:PHE:CZ	1:B:188:ALA:HB1	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:827:VAL:HG11	4:A:908:NAG:O3	2.13	0.48
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.49	0.47
13:B:938:BMA:C6	13:B:940:MAN:H3	2.43	0.47
1:B:390:GLU:HG3	14:B:1514:HOH:O	2.15	0.47
1:A:191:TYR:O	1:A:246:CYS:HA	2.15	0.46
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.97	0.45
1:B:76:GLN:HA	1:B:88:MET:O	2.17	0.45
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.51	0.45
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.98	0.45
1:B:251:ILE:HG21	12:B:909:NAG:H82	1.99	0.45
1:A:360:ARG:HG2	8:A:941:MRD:HMC1	1.98	0.45
8:B:946:MRD:O2	8:B:946:MRD:O4	2.30	0.44
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.47	0.44
1:B:702:ARG:HD3	14:B:1082:HOH:O	2.18	0.43
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.81	0.43
13:B:938:BMA:H61	14:B:1509:HOH:O	2.18	0.43
13:B:938:BMA:H62	13:B:940:MAN:C3	2.49	0.43
9:A:942:MPD:H12	14:A:1406:HOH:O	2.19	0.43
9:A:942:MPD:H13	9:A:942:MPD:H53	1.99	0.43
1:B:172:PHE:HZ	1:B:188:ALA:HB1	1.82	0.43
1:A:387:ASN:HB2	14:A:1200:HOH:O	2.19	0.42
1:A:774:ARG:HB3	1:A:774:ARG:HE	1.45	0.42
1:A:539:ASN:HB2	14:A:1367:HOH:O	2.19	0.42
1:B:102:TYR:HB3	1:B:383:ASN:HA	2.02	0.42
13:B:938:BMA:C6	13:B:940:MAN:C3	2.98	0.42
1:A:448:ALA:HB1	1:A:507:ALA:O	2.20	0.42
1:B:595:LYS:HE3	14:B:1204:HOH:O	2.20	0.42
1:A:97:ILE:HD13	1:A:135:LYS:HG3	2.01	0.41
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.56	0.41
1:A:595:LYS:HE3	14:A:1155:HOH:O	2.19	0.41
1:A:783:LEU:C	1:A:783:LEU:HD23	2.41	0.41
1:B:39:GLU:HG2	14:B:1324:HOH:O	2.21	0.41
1:B:706:PHE:CZ	7:B:902:NAG:H82	2.56	0.41
1:B:377:LYS:HD2	1:B:380:HIS:CE1	2.56	0.40
1:A:30:PRO:HG3	1:A:739:ASP:O	2.21	0.40
1:B:500:LEU:HD23	1:B:545:ILE:HB	2.04	0.40
1:A:367:TYR:CZ	2:A:902:NAG:H83	2.57	0.40
1:B:446:ALA:HA	1:B:574:PRO:HD2	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%)	801 (97%)	28 (3%)	0	100	100
1	B	828/841 (98%)	806 (97%)	22 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	50 (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%)	95	95
1	B	670/677 (99%)	666 (99%)	4 (1%)	92	92
All	All	1341/1354 (99%)	1334 (100%)	7 (0%)	94	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	TRP
1	A	774	ARG
1	A	858	LYS
1	B	281	TRP
1	B	449	TRP
1	B	700	LEU
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 chains 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 ⓘ

79 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	12,14,15	1.02	0	15,19,21	1.67	2 (13%)
2	NAG	A	902	2	12,14,15	0.84	0	15,19,21	2.31	7 (46%)
2	BMA	A	903	2	10,11,12	1.26	1 (10%)	11,15,17	2.48	5 (45%)
2	MAN	A	904	2	10,11,12	1.02	1 (10%)	11,15,17	2.41	6 (54%)
2	MAN	A	905	2	10,11,12	0.93	0	11,15,17	1.93	3 (27%)
4	NAG	A	907	1,4	12,14,15	1.10	0	15,19,21	2.04	4 (26%)
4	NAG	A	908	4	12,14,15	1.34	1 (8%)	15,19,21	1.46	3 (20%)
4	BMA	A	909	4	10,11,12	1.02	0	11,15,17	4.19	6 (54%)
5	NAG	A	910	1,5	12,14,15	0.80	0	15,19,21	1.66	3 (20%)
5	NAG	A	911	5	12,14,15	1.04	1 (8%)	15,19,21	2.44	4 (26%)
6	NAG	A	912	1,6	12,14,15	1.56	2 (16%)	15,19,21	1.32	2 (13%)
6	NAG	A	913	6	12,14,15	1.05	0	15,19,21	1.36	3 (20%)
6	BMA	A	914	6	10,11,12	0.94	0	11,15,17	1.79	2 (18%)
6	MAN	A	915	6	10,11,12	1.23	1 (10%)	11,15,17	1.75	4 (36%)
6	MAN	A	916	6	10,11,12	0.94	1 (10%)	11,15,17	1.94	4 (36%)
6	MAN	A	917	6	10,11,12	0.67	0	11,15,17	1.63	2 (18%)
6	MAN	A	918	6	10,11,12	1.16	1 (10%)	11,15,17	1.55	2 (18%)
6	MAN	A	919	6	10,11,12	0.95	1 (10%)	11,15,17	1.88	4 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	920	6	10,11,12	0.60	0	11,15,17	1.83	2 (18%)
6	MAN	A	921	6	10,11,12	0.64	0	11,15,17	2.78	2 (18%)
4	NAG	A	922	1,4	12,14,15	0.75	0	15,19,21	1.76	4 (26%)
4	NAG	A	923	4	12,14,15	0.77	0	15,19,21	1.75	2 (13%)
4	BMA	A	924	4	10,11,12	0.96	0	11,15,17	2.07	4 (36%)
7	NAG	A	925	1,7	12,14,15	1.14	1 (8%)	15,19,21	2.57	2 (13%)
7	NAG	A	926	7	12,14,15	1.03	1 (8%)	15,19,21	1.86	5 (33%)
7	BMA	A	927	7	10,11,12	0.90	0	11,15,17	1.77	2 (18%)
7	MAN	A	928	7	10,11,12	0.68	0	11,15,17	1.78	5 (45%)
7	MAN	A	929	7	10,11,12	0.75	0	11,15,17	1.82	5 (45%)
7	MAN	A	930	7	10,11,12	0.96	1 (10%)	11,15,17	1.79	4 (36%)
7	MAN	A	931	7	10,11,12	1.09	1 (10%)	11,15,17	1.63	1 (9%)
7	NAG	A	932	1,10,7	12,14,15	1.07	0	15,19,21	1.61	4 (26%)
7	NAG	A	933	7	12,14,15	0.92	1 (8%)	15,19,21	1.30	2 (13%)
7	BMA	A	934	7	10,11,12	0.98	1 (10%)	11,15,17	2.12	4 (36%)
7	MAN	A	935	7	10,11,12	0.99	0	11,15,17	3.47	2 (18%)
7	MAN	A	936	7	10,11,12	0.87	0	11,15,17	2.39	5 (45%)
7	MAN	A	937	7	10,11,12	0.55	0	11,15,17	2.49	5 (45%)
7	MAN	A	938	7	10,11,12	0.70	0	11,15,17	2.07	2 (18%)
7	NAG	B	901	1,7	12,14,15	1.06	1 (8%)	15,19,21	2.22	5 (33%)
7	NAG	B	902	7	12,14,15	1.09	1 (8%)	15,19,21	1.91	4 (26%)
7	BMA	B	903	7	10,11,12	1.23	1 (10%)	11,15,17	2.57	4 (36%)
7	MAN	B	904	7	10,11,12	0.57	0	11,15,17	2.84	6 (54%)
7	MAN	B	905	7	10,11,12	0.69	0	11,15,17	1.95	1 (9%)
7	MAN	B	906	7	10,11,12	0.69	0	11,15,17	1.67	2 (18%)
7	MAN	B	907	7	10,11,12	0.53	0	11,15,17	2.30	4 (36%)
12	NAG	B	909	1,12	12,14,15	1.25	1 (8%)	15,19,21	2.04	5 (33%)
12	NAG	B	910	12	12,14,15	1.59	3 (25%)	15,19,21	1.45	3 (20%)
12	BMA	B	911	12	10,11,12	0.67	0	11,15,17	1.64	2 (18%)
12	MAN	B	912	12	10,11,12	1.07	1 (10%)	11,15,17	3.01	5 (45%)
4	NAG	B	913	1,4	12,14,15	1.17	1 (8%)	15,19,21	2.10	5 (33%)
4	NAG	B	914	4	12,14,15	0.59	0	15,19,21	1.93	5 (33%)
4	BMA	B	915	4	10,11,12	0.75	0	11,15,17	2.30	4 (36%)
6	NAG	B	916	1,6	12,14,15	1.22	1 (8%)	15,19,21	1.97	3 (20%)
6	NAG	B	917	6	12,14,15	1.25	1 (8%)	15,19,21	1.36	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	B	918	6	10,11,12	1.21	1 (10%)	11,15,17	2.57	2 (18%)
6	MAN	B	919	6	10,11,12	1.00	0	11,15,17	1.77	3 (27%)
6	MAN	B	920	6	10,11,12	1.16	1 (10%)	11,15,17	1.95	4 (36%)
6	MAN	B	921	6	10,11,12	1.00	1 (10%)	11,15,17	2.11	5 (45%)
6	MAN	B	922	6	10,11,12	0.52	0	11,15,17	2.00	3 (27%)
6	MAN	B	923	6	10,11,12	0.77	0	11,15,17	2.41	1 (9%)
6	MAN	B	924	6	10,11,12	1.20	2 (20%)	11,15,17	2.61	6 (54%)
6	MAN	B	925	6	10,11,12	0.97	0	11,15,17	2.48	2 (18%)
4	NAG	B	926	1,4	12,14,15	0.62	0	15,19,21	1.12	2 (13%)
4	NAG	B	927	4	12,14,15	0.91	0	15,19,21	1.38	2 (13%)
4	BMA	B	928	4	10,11,12	0.70	0	11,15,17	2.88	4 (36%)
7	NAG	B	929	1,7	12,14,15	0.91	0	15,19,21	2.07	4 (26%)
7	NAG	B	930	7	12,14,15	1.36	2 (16%)	15,19,21	2.12	6 (40%)
7	BMA	B	931	7	10,11,12	0.87	0	11,15,17	1.51	2 (18%)
7	MAN	B	932	7	10,11,12	0.79	0	11,15,17	2.04	3 (27%)
7	MAN	B	933	7	10,11,12	1.11	1 (10%)	11,15,17	1.87	5 (45%)
7	MAN	B	934	7	10,11,12	0.82	0	11,15,17	2.24	4 (36%)
7	MAN	B	935	7	10,11,12	0.61	0	11,15,17	1.59	3 (27%)
13	NAG	B	936	1,10,13	12,14,15	1.27	1 (8%)	15,19,21	1.70	2 (13%)
13	NAG	B	937	13	12,14,15	0.80	0	15,19,21	1.45	3 (20%)
13	BMA	B	938	13	10,11,12	0.90	0	11,15,17	3.73	6 (54%)
13	MAN	B	939	13	10,11,12	0.87	1 (10%)	11,15,17	2.43	3 (27%)
13	MAN	B	940	13	10,11,12	0.91	0	11,15,17	1.49	2 (18%)
13	MAN	B	941	13	10,11,12	0.88	0	11,15,17	2.98	7 (63%)
13	MAN	B	942	13	10,11,12	0.96	0	11,15,17	3.26	5 (45%)
13	MAN	B	943	13	10,11,12	0.91	0	11,15,17	2.75	3 (27%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	905	2	-	0/2/19/22	0/1/1/1
4	NAG	A	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	908	4	-	0/6/23/26	0/1/1/1
4	BMA	A	909	4	-	0/2/19/22	0/1/1/1
5	NAG	A	910	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	911	5	-	0/6/23/26	0/1/1/1
6	NAG	A	912	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	913	6	-	0/6/23/26	0/1/1/1
6	BMA	A	914	6	-	0/2/19/22	0/1/1/1
6	MAN	A	915	6	-	0/2/19/22	0/1/1/1
6	MAN	A	916	6	-	0/2/19/22	0/1/1/1
6	MAN	A	917	6	-	0/2/19/22	0/1/1/1
6	MAN	A	918	6	-	0/2/19/22	0/1/1/1
6	MAN	A	919	6	-	0/2/19/22	0/1/1/1
6	MAN	A	920	6	-	0/2/19/22	0/1/1/1
6	MAN	A	921	6	-	0/2/19/22	0/1/1/1
4	NAG	A	922	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	923	4	-	0/6/23/26	0/1/1/1
4	BMA	A	924	4	-	0/2/19/22	0/1/1/1
7	NAG	A	925	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	926	7	-	0/6/23/26	0/1/1/1
7	BMA	A	927	7	-	0/2/19/22	0/1/1/1
7	MAN	A	928	7	-	0/2/19/22	0/1/1/1
7	MAN	A	929	7	-	0/2/19/22	0/1/1/1
7	MAN	A	930	7	-	0/2/19/22	0/1/1/1
7	MAN	A	931	7	-	0/2/19/22	0/1/1/1
7	NAG	A	932	1,10,7	-	0/6/23/26	0/1/1/1
7	NAG	A	933	7	-	0/6/23/26	0/1/1/1
7	BMA	A	934	7	-	0/2/19/22	0/1/1/1
7	MAN	A	935	7	-	0/2/19/22	0/1/1/1
7	MAN	A	936	7	-	0/2/19/22	0/1/1/1
7	MAN	A	937	7	-	0/2/19/22	0/1/1/1
7	MAN	A	938	7	-	0/2/19/22	0/1/1/1
7	NAG	B	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	902	7	-	0/6/23/26	0/1/1/1
7	BMA	B	903	7	-	0/2/19/22	0/1/1/1
7	MAN	B	904	7	-	0/2/19/22	0/1/1/1
7	MAN	B	905	7	-	0/2/19/22	0/1/1/1
7	MAN	B	906	7	-	0/2/19/22	0/1/1/1
7	MAN	B	907	7	-	0/2/19/22	0/1/1/1
12	NAG	B	909	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	910	12	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	B	911	12	-	0/2/19/22	0/1/1/1
12	MAN	B	912	12	-	0/2/19/22	0/1/1/1
4	NAG	B	913	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	914	4	-	0/6/23/26	0/1/1/1
4	BMA	B	915	4	-	0/2/19/22	0/1/1/1
6	NAG	B	916	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	917	6	-	0/6/23/26	0/1/1/1
6	BMA	B	918	6	-	0/2/19/22	0/1/1/1
6	MAN	B	919	6	-	0/2/19/22	0/1/1/1
6	MAN	B	920	6	-	0/2/19/22	0/1/1/1
6	MAN	B	921	6	-	0/2/19/22	0/1/1/1
6	MAN	B	922	6	-	0/2/19/22	0/1/1/1
6	MAN	B	923	6	-	0/2/19/22	0/1/1/1
6	MAN	B	924	6	-	0/2/19/22	0/1/1/1
6	MAN	B	925	6	-	0/2/19/22	0/1/1/1
4	NAG	B	926	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	927	4	-	0/6/23/26	0/1/1/1
4	BMA	B	928	4	-	0/2/19/22	0/1/1/1
7	NAG	B	929	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	930	7	-	0/6/23/26	0/1/1/1
7	BMA	B	931	7	-	0/2/19/22	0/1/1/1
7	MAN	B	932	7	-	0/2/19/22	0/1/1/1
7	MAN	B	933	7	-	0/2/19/22	0/1/1/1
7	MAN	B	934	7	-	0/2/19/22	0/1/1/1
7	MAN	B	935	7	-	0/2/19/22	0/1/1/1
13	NAG	B	936	1,10,13	-	0/6/23/26	0/1/1/1
13	NAG	B	937	13	-	0/6/23/26	0/1/1/1
13	BMA	B	938	13	-	0/2/19/22	0/1/1/1
13	MAN	B	939	13	-	0/2/19/22	0/1/1/1
13	MAN	B	940	13	-	0/2/19/22	0/1/1/1
13	MAN	B	941	13	-	0/2/19/22	0/1/1/1
13	MAN	B	942	13	-	0/2/19/22	0/1/1/1
13	MAN	B	943	13	-	0/2/19/22	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	910	NAG	C3-C2	3.27	1.59	1.52
13	B	936	NAG	O7-C7	3.11	1.30	1.23
12	B	909	NAG	O5-C5	-3.08	1.39	1.45
6	A	912	NAG	C2-N2	3.07	1.49	1.46
6	B	916	NAG	C2-N2	2.95	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	913	NAG	O5-C5	-2.85	1.40	1.45
7	B	930	NAG	O5-C5	-2.82	1.40	1.45
6	A	918	MAN	C4-C3	2.81	1.59	1.52
7	B	933	MAN	O2-C2	-2.73	1.37	1.43
6	B	918	BMA	O4-C4	-2.72	1.36	1.43
6	B	920	MAN	O5-C5	-2.71	1.40	1.45
6	A	915	MAN	O4-C4	-2.70	1.36	1.43
6	B	917	NAG	C4-C3	2.66	1.59	1.52
7	B	930	NAG	C3-C2	2.58	1.57	1.52
12	B	910	NAG	C4-C5	2.57	1.58	1.53
7	A	926	NAG	O5-C5	-2.49	1.40	1.45
5	A	911	NAG	O3-C3	-2.45	1.37	1.43
2	A	904	MAN	O5-C5	-2.40	1.41	1.45
7	B	902	NAG	C4-C5	2.38	1.58	1.53
6	A	912	NAG	C4-C3	2.36	1.58	1.52
12	B	910	NAG	O7-C7	2.30	1.28	1.23
7	A	931	MAN	C4-C5	2.26	1.58	1.53
7	A	925	NAG	C2-N2	-2.25	1.43	1.46
7	A	934	BMA	O2-C2	-2.20	1.38	1.43
7	B	901	NAG	O5-C5	-2.20	1.41	1.45
6	B	924	MAN	O3-C3	2.20	1.48	1.43
7	A	933	NAG	C2-N2	-2.17	1.43	1.46
13	B	939	MAN	O5-C5	-2.14	1.41	1.45
12	B	912	MAN	C4-C3	2.10	1.58	1.52
4	A	908	NAG	C2-N2	-2.09	1.43	1.46
6	A	916	MAN	O5-C5	-2.09	1.41	1.45
6	B	924	MAN	C4-C3	2.05	1.57	1.52
6	A	919	MAN	O2-C2	-2.04	1.39	1.43
7	A	930	MAN	O2-C2	-2.03	1.39	1.43
7	B	903	BMA	C3-C2	2.02	1.57	1.52
2	A	903	BMA	O3-C3	2.00	1.47	1.43
6	B	921	MAN	O5-C5	-2.00	1.41	1.45

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	935	MAN	O5-C5-C6	10.55	118.05	106.98
4	A	909	BMA	O5-C5-C6	10.24	117.72	106.98
7	A	925	NAG	C3-C2-N2	-8.27	99.16	111.76
13	B	942	MAN	O5-C5-C6	8.15	115.53	106.98
12	B	912	MAN	O5-C5-C6	8.08	115.46	106.98
13	B	943	MAN	O5-C5-C6	7.74	115.11	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	928	BMA	O5-C5-C6	7.72	115.08	106.98
6	A	921	MAN	O5-C5-C6	7.62	114.97	106.98
7	B	904	MAN	O5-C5-C6	7.54	114.89	106.98
6	B	923	MAN	O5-C5-C6	7.48	114.83	106.98
13	B	938	BMA	C6-C5-C4	-7.04	95.98	113.00
7	B	903	BMA	O5-C5-C4	-6.81	102.00	110.65
13	B	938	BMA	O5-C5-C4	6.53	118.94	110.65
7	B	929	NAG	C3-C2-N2	-6.23	102.27	111.76
13	B	939	MAN	C4-C3-C2	6.20	118.83	110.50
6	B	918	BMA	O5-C5-C4	-6.19	102.80	110.65
7	B	905	MAN	O5-C5-C6	5.98	113.25	106.98
6	B	925	MAN	O5-C5-C6	5.91	113.19	106.98
13	B	941	MAN	O5-C5-C6	5.81	113.08	106.98
4	A	907	NAG	O5-C5-C4	-5.62	103.52	110.65
7	A	937	MAN	O5-C5-C4	5.52	117.65	110.65
7	A	938	MAN	O5-C5-C6	5.28	112.52	106.98
5	A	911	NAG	O5-C5-C6	5.27	112.51	106.98
4	A	909	BMA	C3-C4-C5	5.19	119.47	110.20
7	B	934	MAN	O5-C5-C6	5.13	112.37	106.98
4	A	923	NAG	C3-C2-N2	-5.12	103.97	111.76
7	B	901	NAG	O5-C5-C4	-5.09	104.19	110.65
4	A	909	BMA	O6-C6-C5	5.01	128.62	111.36
7	B	907	MAN	O5-C5-C6	4.88	112.10	106.98
6	B	924	MAN	O5-C5-C6	4.86	112.08	106.98
7	A	936	MAN	C3-C4-C5	-4.81	101.61	110.20
2	A	901	NAG	O5-C5-C6	4.77	111.99	106.98
13	B	941	MAN	C6-C5-C4	-4.74	101.55	113.00
13	B	938	BMA	O6-C6-C5	-4.71	95.14	111.36
6	B	925	MAN	O3-C3-C4	-4.71	99.80	110.35
4	B	913	NAG	O5-C5-C6	4.70	111.92	106.98
6	B	922	MAN	O6-C6-C5	-4.70	95.19	111.36
6	B	924	MAN	O5-C5-C4	-4.70	104.69	110.65
6	B	918	BMA	C4-C3-C2	-4.65	104.27	110.50
7	A	927	BMA	O5-C5-C4	-4.58	104.83	110.65
6	A	920	MAN	O6-C6-C5	-4.53	95.76	111.36
2	A	903	BMA	C4-C3-C2	-4.53	104.43	110.50
5	A	911	NAG	C3-C4-C5	-4.53	102.12	110.20
2	A	902	NAG	O5-C5-C4	-4.51	104.92	110.65
12	B	909	NAG	C3-C2-N2	-4.48	104.95	111.76
4	B	914	NAG	C3-C4-C5	-4.45	102.25	110.20
13	B	936	NAG	O5-C5-C6	4.40	111.60	106.98
2	A	904	MAN	O5-C5-C6	-4.39	102.37	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	925	NAG	O5-C5-C4	-4.38	105.10	110.65
6	A	921	MAN	O3-C3-C2	4.36	117.91	109.94
7	A	931	MAN	O5-C5-C6	4.33	111.53	106.98
7	A	932	NAG	O5-C5-C6	4.29	111.48	106.98
4	A	909	BMA	O3-C3-C2	-4.27	102.12	109.94
4	A	922	NAG	C3-C2-N2	-4.25	105.28	111.76
6	A	914	BMA	O5-C5-C6	4.25	111.44	106.98
6	B	916	NAG	O5-C5-C6	-4.16	102.61	106.98
13	B	942	MAN	O3-C3-C4	4.16	119.68	110.35
4	B	915	BMA	O5-C5-C4	4.13	115.89	110.65
6	B	916	NAG	O5-C5-C4	-4.13	105.41	110.65
2	A	904	MAN	C3-C4-C5	4.12	117.56	110.20
7	B	907	MAN	O3-C3-C2	4.10	117.44	109.94
6	A	916	MAN	C4-C3-C2	4.06	115.95	110.50
4	A	924	BMA	O5-C5-C4	4.03	115.77	110.65
13	B	938	BMA	O2-C2-C3	4.03	118.88	110.18
7	B	902	NAG	O7-C7-C8	-4.01	114.22	122.04
5	A	910	NAG	O5-C5-C6	4.00	111.18	106.98
6	B	921	MAN	O5-C5-C4	-3.99	105.59	110.65
6	A	917	MAN	O5-C5-C6	3.93	111.11	106.98
2	A	902	NAG	O6-C6-C5	-3.90	97.94	111.36
12	B	912	MAN	O3-C3-C4	3.90	119.09	110.35
4	B	915	BMA	O4-C4-C3	-3.87	101.68	110.35
12	B	909	NAG	O5-C5-C4	-3.85	105.76	110.65
5	A	911	NAG	O5-C5-C4	-3.85	105.77	110.65
7	B	932	MAN	O4-C4-C3	-3.83	101.77	110.35
7	A	933	NAG	C3-C2-N2	-3.81	105.95	111.76
7	A	937	MAN	O3-C3-C4	3.79	118.86	110.35
7	A	934	BMA	C6-C5-C4	-3.77	103.89	113.00
7	A	934	BMA	O3-C3-C4	-3.77	101.91	110.35
2	A	903	BMA	O2-C2-C3	-3.75	102.09	110.18
5	A	911	NAG	O6-C6-C5	-3.75	98.47	111.36
7	B	906	MAN	O5-C5-C6	3.69	110.86	106.98
7	A	936	MAN	O2-C2-C3	-3.69	102.21	110.18
7	B	901	NAG	O7-C7-N2	3.63	129.48	121.90
6	A	918	MAN	C4-C3-C2	-3.62	105.64	110.50
6	B	916	NAG	O4-C4-C5	-3.61	99.78	109.28
7	A	926	NAG	O4-C4-C3	-3.59	102.31	110.35
6	B	920	MAN	O5-C5-C6	-3.59	103.22	106.98
7	B	902	NAG	O6-C6-C5	-3.55	99.14	111.36
6	B	924	MAN	O2-C2-C3	-3.55	102.51	110.18
7	B	901	NAG	C8-C7-N2	-3.51	109.24	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	924	BMA	O3-C3-C4	3.50	118.21	110.35
6	A	913	NAG	O5-C5-C4	-3.50	106.21	110.65
4	B	913	NAG	C3-C4-C5	3.44	116.34	110.20
13	B	941	MAN	O2-C2-C3	-3.40	102.83	110.18
6	B	919	MAN	O5-C5-C6	-3.40	103.41	106.98
13	B	940	MAN	O4-C4-C3	-3.39	102.74	110.35
7	B	930	NAG	O4-C4-C3	-3.39	102.75	110.35
2	A	904	MAN	C4-C3-C2	3.37	115.03	110.50
6	A	919	MAN	C3-C4-C5	3.37	116.22	110.20
13	B	939	MAN	O3-C3-C4	-3.36	102.82	110.35
7	B	931	BMA	O5-C5-C6	3.36	110.50	106.98
7	B	930	NAG	O5-C5-C4	-3.35	106.40	110.65
2	A	903	BMA	O3-C3-C4	3.31	117.76	110.35
4	B	928	BMA	C3-C4-C5	3.31	116.11	110.20
13	B	938	BMA	C3-C4-C5	3.28	116.06	110.20
7	A	927	BMA	C6-C5-C4	-3.25	105.15	113.00
13	B	941	MAN	O5-C5-C4	3.24	114.77	110.65
4	B	913	NAG	O4-C4-C5	-3.24	100.74	109.28
7	B	932	MAN	O3-C3-C2	3.23	115.85	109.94
7	B	903	BMA	O6-C6-C5	-3.23	100.26	111.36
7	B	933	MAN	O3-C3-C4	3.18	117.49	110.35
4	B	927	NAG	O7-C7-C8	-3.17	115.85	122.04
4	B	915	BMA	C3-C4-C5	3.14	115.81	110.20
5	A	910	NAG	O4-C4-C5	-3.13	101.03	109.28
12	B	911	BMA	O5-C5-C4	3.13	114.62	110.65
12	B	910	NAG	C6-C5-C4	3.12	120.54	113.00
4	B	915	BMA	O3-C3-C2	3.12	115.64	109.94
6	A	912	NAG	O5-C5-C6	-3.08	103.75	106.98
2	A	905	MAN	O5-C5-C6	3.07	110.20	106.98
4	B	914	NAG	O5-C5-C4	-3.07	106.76	110.65
7	A	934	BMA	O5-C5-C6	3.06	110.19	106.98
6	B	920	MAN	O6-C6-C5	-3.06	100.84	111.36
13	B	942	MAN	C3-C4-C5	-3.05	104.75	110.20
6	A	919	MAN	O5-C5-C6	3.05	110.18	106.98
4	B	914	NAG	O6-C6-C5	-3.04	100.88	111.36
7	A	935	MAN	O4-C4-C3	-3.04	103.55	110.35
7	B	932	MAN	O2-C2-C3	3.02	116.69	110.18
4	A	907	NAG	C3-C2-N2	-3.02	107.17	111.76
7	A	930	MAN	O5-C5-C4	-3.01	106.83	110.65
6	B	921	MAN	C4-C3-C2	-3.00	106.47	110.50
6	B	919	MAN	O3-C3-C2	-3.00	104.44	109.94
7	A	928	MAN	O4-C4-C3	-2.98	103.68	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	917	NAG	O6-C6-C5	-2.97	101.13	111.36
2	A	905	MAN	O3-C3-C4	2.97	117.02	110.35
4	A	922	NAG	C2-N2-C7	2.97	128.08	123.09
13	B	943	MAN	O5-C5-C4	-2.97	106.89	110.65
13	B	942	MAN	O4-C4-C5	-2.96	101.47	109.28
12	B	909	NAG	C4-C3-C2	-2.93	104.15	111.32
13	B	942	MAN	O5-C5-C4	-2.92	106.95	110.65
2	A	905	MAN	C6-C5-C4	2.91	120.03	113.00
6	A	917	MAN	O6-C6-C5	-2.90	101.37	111.36
13	B	939	MAN	C3-C4-C5	2.86	115.31	110.20
7	B	930	NAG	C6-C5-C4	2.84	119.85	113.00
7	B	906	MAN	C6-C5-C4	-2.83	106.17	113.00
12	B	910	NAG	O6-C6-C5	-2.82	101.65	111.36
7	A	926	NAG	C2-N2-C7	-2.82	118.36	123.09
7	B	901	NAG	C4-C3-C2	-2.81	104.43	111.32
7	A	937	MAN	C4-C3-C2	-2.81	106.73	110.50
6	A	920	MAN	C6-C5-C4	-2.80	106.22	113.00
7	B	933	MAN	O2-C2-C3	-2.80	104.13	110.18
4	B	928	BMA	C6-C5-C4	-2.79	106.25	113.00
7	A	926	NAG	O5-C5-C4	-2.78	107.12	110.65
13	B	937	NAG	O5-C5-C6	2.77	109.88	106.98
4	A	908	NAG	C6-C5-C4	2.75	119.64	113.00
7	A	936	MAN	C6-C5-C4	2.72	119.57	113.00
6	A	915	MAN	O4-C4-C3	-2.69	104.32	110.35
7	B	930	NAG	C3-C4-C5	-2.69	105.40	110.20
7	B	902	NAG	O7-C7-N2	2.68	127.51	121.90
7	A	929	MAN	C6-C5-C4	2.68	119.48	113.00
6	B	921	MAN	O6-C6-C5	-2.68	102.14	111.36
7	A	937	MAN	C6-C5-C4	-2.67	106.54	113.00
4	B	926	NAG	O5-C5-C4	-2.67	107.27	110.65
4	A	924	BMA	C3-C4-C5	2.66	114.96	110.20
6	A	918	MAN	O5-C5-C6	2.66	109.77	106.98
7	B	934	MAN	C6-C5-C4	-2.66	106.58	113.00
6	B	922	MAN	O3-C3-C4	-2.65	104.41	110.35
4	B	913	NAG	O5-C5-C4	-2.64	107.30	110.65
2	A	903	BMA	C3-C4-C5	2.64	114.91	110.20
7	A	936	MAN	O4-C4-C3	-2.63	104.45	110.35
6	B	917	NAG	O4-C4-C3	-2.62	104.47	110.35
6	B	921	MAN	O2-C2-C3	2.62	115.83	110.18
7	B	904	MAN	C6-C5-C4	-2.61	106.69	113.00
13	B	940	MAN	O3-C3-C4	-2.61	104.50	110.35
7	B	907	MAN	C4-C3-C2	-2.61	107.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	914	NAG	O5-C5-C6	2.60	109.71	106.98
7	A	929	MAN	O6-C6-C5	-2.58	102.47	111.36
6	A	915	MAN	O5-C5-C4	-2.58	107.38	110.65
7	B	930	NAG	O3-C3-C2	-2.58	103.66	109.09
7	A	932	NAG	O6-C6-C5	-2.58	102.49	111.36
7	A	930	MAN	C3-C4-C5	-2.56	105.62	110.20
2	A	902	NAG	C6-C5-C4	2.56	119.18	113.00
7	A	926	NAG	O6-C6-C5	-2.55	102.58	111.36
6	A	916	MAN	O3-C3-C4	-2.53	104.68	110.35
2	A	902	NAG	O4-C4-C5	-2.52	102.65	109.28
6	A	915	MAN	O3-C3-C2	-2.52	105.33	109.94
6	B	924	MAN	O6-C6-C5	-2.51	102.73	111.36
7	A	928	MAN	O5-C5-C6	2.50	109.61	106.98
7	B	934	MAN	O6-C6-C5	-2.50	102.75	111.36
7	B	907	MAN	O4-C4-C3	-2.50	104.74	110.35
2	A	902	NAG	O3-C3-C4	2.49	115.95	110.35
2	A	902	NAG	O7-C7-C8	-2.48	117.19	122.04
7	A	930	MAN	O2-C2-C3	-2.48	104.82	110.18
7	B	934	MAN	O4-C4-C3	-2.48	104.79	110.35
13	B	941	MAN	O3-C3-C4	-2.48	104.80	110.35
4	A	909	BMA	O5-C5-C4	-2.47	107.52	110.65
4	A	922	NAG	O3-C3-C2	-2.45	103.93	109.09
6	A	916	MAN	O2-C2-C3	2.44	115.44	110.18
13	B	936	NAG	O7-C7-C8	2.44	126.80	122.04
7	A	930	MAN	O5-C5-C6	2.43	109.53	106.98
7	A	932	NAG	C6-C5-C4	-2.43	107.13	113.00
2	A	903	BMA	O3-C3-C2	-2.42	105.51	109.94
4	A	924	BMA	O4-C4-C5	-2.41	102.94	109.28
6	A	914	BMA	C4-C3-C2	-2.41	107.27	110.50
13	B	941	MAN	O6-C6-C5	-2.41	103.08	111.36
6	B	919	MAN	O2-C2-C3	-2.40	105.00	110.18
7	A	926	NAG	C3-C4-C5	-2.38	105.95	110.20
4	A	908	NAG	O3-C3-C2	-2.36	104.12	109.09
7	B	935	MAN	O6-C6-C5	-2.36	103.23	111.36
6	B	922	MAN	C6-C5-C4	-2.34	107.33	113.00
7	A	932	NAG	C2-N2-C7	-2.34	119.15	123.09
7	A	938	MAN	O2-C2-C3	2.34	115.23	110.18
12	B	911	BMA	O3-C3-C2	2.33	114.20	109.94
2	A	901	NAG	C3-C2-N2	-2.33	108.22	111.76
7	A	928	MAN	O5-C5-C4	2.32	113.59	110.65
7	A	929	MAN	O3-C3-C2	2.32	114.17	109.94
7	B	929	NAG	O5-C5-C4	-2.31	107.72	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	912	MAN	C6-C5-C4	2.30	118.56	113.00
7	B	903	BMA	O3-C3-C4	-2.28	105.23	110.35
6	B	921	MAN	O5-C5-C6	2.27	109.37	106.98
2	A	904	MAN	O3-C3-C2	2.26	114.08	109.94
7	A	929	MAN	O4-C4-C3	-2.26	105.29	110.35
6	A	915	MAN	O5-C5-C6	2.25	109.34	106.98
12	B	910	NAG	O4-C4-C5	-2.24	103.39	109.28
7	B	931	BMA	O4-C4-C5	-2.24	103.39	109.28
7	B	901	NAG	O4-C4-C3	-2.23	105.35	110.35
13	B	943	MAN	O4-C4-C5	-2.23	103.41	109.28
7	B	904	MAN	C4-C3-C2	-2.22	107.52	110.50
7	B	930	NAG	O6-C6-C5	-2.22	103.72	111.36
4	B	913	NAG	C6-C5-C4	-2.22	107.64	113.00
7	B	933	MAN	O4-C4-C5	-2.21	103.46	109.28
7	A	936	MAN	O5-C5-C6	2.21	109.30	106.98
6	A	912	NAG	C3-C4-C5	2.21	114.15	110.20
4	A	907	NAG	O6-C6-C5	-2.21	103.77	111.36
7	B	935	MAN	O4-C4-C3	-2.20	105.41	110.35
7	A	934	BMA	O2-C2-C3	2.19	114.91	110.18
4	A	908	NAG	O6-C6-C5	-2.18	103.84	111.36
13	B	938	BMA	O4-C4-C5	-2.18	103.53	109.28
7	B	902	NAG	O4-C4-C5	-2.18	103.54	109.28
7	B	904	MAN	O5-C5-C4	2.18	113.42	110.65
7	A	928	MAN	C4-C3-C2	2.17	113.42	110.50
7	A	933	NAG	C6-C5-C4	-2.17	107.75	113.00
7	A	937	MAN	O6-C6-C5	-2.17	103.90	111.36
13	B	937	NAG	O6-C6-C5	-2.16	103.92	111.36
7	B	903	BMA	C3-C4-C5	2.15	114.04	110.20
4	A	923	NAG	O5-C5-C6	2.15	109.23	106.98
6	B	920	MAN	O2-C2-C3	2.14	114.80	110.18
2	A	902	NAG	O3-C3-C2	-2.13	104.61	109.09
13	B	937	NAG	C8-C7-N2	2.13	120.27	116.11
6	A	916	MAN	O4-C4-C3	-2.13	105.58	110.35
7	B	929	NAG	O5-C5-C6	-2.12	104.75	106.98
12	B	912	MAN	O4-C4-C3	2.12	115.10	110.35
7	A	928	MAN	O6-C6-C5	-2.10	104.12	111.36
4	B	926	NAG	C3-C2-N2	-2.09	108.58	111.76
7	B	933	MAN	O5-C5-C6	2.09	109.17	106.98
7	B	904	MAN	O6-C6-C5	-2.09	104.18	111.36
6	A	919	MAN	O4-C4-C5	2.09	114.79	109.28
5	A	910	NAG	C3-C2-N2	2.08	114.93	111.76
4	B	928	BMA	C4-C3-C2	-2.08	107.72	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	933	MAN	O6-C6-C5	-2.08	104.22	111.36
2	A	904	MAN	O4-C4-C3	-2.07	105.71	110.35
6	B	924	MAN	O3-C3-C4	-2.07	105.71	110.35
7	B	935	MAN	C6-C5-C4	-2.07	108.01	113.00
7	B	904	MAN	O2-C2-C3	-2.06	105.72	110.18
12	B	912	MAN	O4-C4-C5	-2.06	103.85	109.28
6	A	913	NAG	O4-C4-C3	-2.06	105.74	110.35
2	A	904	MAN	O5-C5-C4	2.06	113.27	110.65
6	A	919	MAN	O3-C3-C4	-2.06	105.74	110.35
12	B	909	NAG	O6-C6-C5	-2.05	104.30	111.36
4	A	907	NAG	C2-N2-C7	-2.05	119.65	123.09
13	B	941	MAN	C4-C3-C2	-2.05	107.75	110.50
6	B	920	MAN	O5-C5-C4	2.05	113.25	110.65
4	B	927	NAG	C2-N2-C7	-2.05	119.65	123.09
7	B	929	NAG	O4-C4-C3	-2.04	105.77	110.35
4	A	922	NAG	C4-C3-C2	-2.04	106.32	111.32
6	B	924	MAN	O4-C4-C3	-2.03	105.81	110.35
7	A	929	MAN	O5-C5-C6	2.02	109.10	106.98
4	A	909	BMA	O4-C4-C3	-2.01	105.84	110.35
4	B	914	NAG	C6-C5-C4	-2.01	108.15	113.00
6	A	913	NAG	O6-C6-C5	-2.01	104.45	111.36
12	B	909	NAG	O3-C3-C2	-2.01	104.88	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	906	1	12,14,15	0.74	0	15,19,21	1.52	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	939	1	12,14,15	1.15	2 (16%)	15,19,21	2.28	6 (40%)
8	MRD	A	940	-	7,7,7	1.15	0	10,10,10	0.39	0
8	MRD	A	941	-	7,7,7	1.23	0	10,10,10	1.31	3 (30%)
9	MPD	A	942	-	7,7,7	0.68	0	10,10,10	1.04	0
11	IFM	A	944	-	10,10,10	3.06	5 (50%)	13,13,13	2.24	2 (15%)
3	NAG	B	908	1	12,14,15	0.53	0	15,19,21	3.07	7 (46%)
3	NAG	B	944	1	12,14,15	0.88	0	15,19,21	2.04	5 (33%)
3	NAG	B	945	1	12,14,15	1.00	0	15,19,21	2.14	3 (20%)
8	MRD	B	946	-	7,7,7	1.15	0	10,10,10	0.50	0
8	MRD	B	947	-	7,7,7	1.02	1 (14%)	10,10,10	1.33	1 (10%)
8	MRD	B	948	-	7,7,7	0.99	1 (14%)	10,10,10	0.51	0
11	IFM	B	950	-	10,10,10	2.55	4 (40%)	13,13,13	1.57	3 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	939	1	-	0/6/23/26	0/1/1/1
8	MRD	A	940	-	-	0/5/5/5	0/0/0/0
8	MRD	A	941	-	-	0/5/5/5	0/0/0/0
9	MPD	A	942	-	-	0/5/5/5	0/0/0/0
11	IFM	A	944	-	-	0/2/16/16	0/1/1/1
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	944	1	-	0/6/23/26	0/1/1/1
3	NAG	B	945	1	-	0/6/23/26	0/1/1/1
8	MRD	B	946	-	-	0/5/5/5	0/0/0/0
8	MRD	B	947	-	-	0/5/5/5	0/0/0/0
8	MRD	B	948	-	-	0/5/5/5	0/0/0/0
11	IFM	B	950	-	-	0/2/16/16	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	944	IFM	C2-C3	5.91	1.59	1.52
11	A	944	IFM	C5-C4	5.66	1.60	1.53
11	B	950	IFM	C1-C5	4.95	1.58	1.52
11	B	950	IFM	C2-C3	4.24	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	944	IFM	C1-N	3.07	1.53	1.46
11	A	944	IFM	C6-C5	2.71	1.58	1.52
3	A	939	NAG	O3-C3	-2.29	1.37	1.43
8	B	947	MRD	C3-C2	-2.25	1.46	1.53
8	B	948	MRD	O2-C2	-2.15	1.38	1.44
11	A	944	IFM	C2-N	2.12	1.51	1.46
3	A	939	NAG	O4-C4	-2.05	1.38	1.43
11	B	950	IFM	C1-N	2.03	1.50	1.46
11	B	950	IFM	O4-C4	2.00	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	O5-C5-C6	7.51	114.86	106.98
11	A	944	IFM	C5-C4-C3	-6.14	104.99	112.80
3	B	908	NAG	C8-C7-N2	5.19	126.26	116.11
3	A	939	NAG	O5-C5-C4	-4.89	104.45	110.65
3	B	945	NAG	O5-C5-C4	-4.72	104.67	110.65
3	B	908	NAG	C2-N2-C7	4.41	130.50	123.09
3	B	945	NAG	O5-C5-C6	4.24	111.43	106.98
3	B	944	NAG	C8-C7-N2	4.13	124.18	116.11
11	B	950	IFM	C5-C4-C3	-3.94	107.79	112.80
3	B	944	NAG	O5-C5-C6	3.91	111.08	106.98
3	A	906	NAG	O5-C5-C6	3.79	110.96	106.98
3	A	939	NAG	O5-C5-C6	3.73	110.90	106.98
3	B	944	NAG	O7-C7-C8	-3.30	115.61	122.04
11	A	944	IFM	C1-C5-C6	-3.25	105.20	110.97
3	B	908	NAG	O3-C3-C4	-3.22	103.14	110.35
3	A	939	NAG	C2-N2-C7	-3.20	117.72	123.09
3	B	945	NAG	C3-C4-C5	-3.10	104.67	110.20
3	B	908	NAG	C3-C2-N2	3.04	116.40	111.76
3	B	908	NAG	O7-C7-N2	-2.71	116.24	121.90
11	B	950	IFM	C2-C3-C4	-2.68	107.02	110.23
8	B	947	MRD	O4-C4-C3	-2.62	99.05	111.04
3	A	939	NAG	O3-C3-C4	-2.58	104.58	110.35
3	A	939	NAG	C8-C7-N2	2.57	121.14	116.11
3	B	908	NAG	O7-C7-C8	-2.33	117.49	122.04
11	B	950	IFM	O4-C4-C3	-2.28	105.92	110.03
8	A	941	MRD	CM-C2-C1	2.21	115.01	110.11
3	A	939	NAG	C3-C4-C5	-2.16	106.35	110.20
8	A	941	MRD	O4-C4-C3	-2.13	101.33	111.04
3	B	944	NAG	O4-C4-C3	2.09	115.05	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	941	MRD	C2-C3-C4	-2.05	105.48	116.70
3	B	944	NAG	O6-C6-C5	-2.05	104.32	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.36	4 (0%) 88 90	10, 17, 30, 53	0
1	B	832/841 (98%)	-0.48	3 (0%) 90 91	9, 14, 26, 53	0
All	All	1665/1682 (98%)	-0.42	7 (0%) 90 91	9, 15, 29, 53	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	860	GLN	2.6
1	A	699	GLY	2.3
1	B	698	GLU	2.2
1	A	698	GLU	2.1
1	A	675	VAL	2.0
1	A	860	GLN	2.0
1	B	687	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	BMA	A	924	11/12	0.31	62.50	41,51,62,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MAN	A	938	11/12	0.24	47.57	50,55,60,72	0
13	MAN	B	942	11/12	0.27	18.14	47,52,60,63	0
7	MAN	A	937	11/12	0.25	14.85	40,51,55,66	0
13	MAN	B	943	11/12	0.25	13.56	42,50,57,62	0
12	BMA	B	911	11/12	0.18	12.83	32,38,48,49	0
7	MAN	A	929	11/12	0.13	10.17	24,26,38,39	0
2	MAN	A	905	11/12	0.17	9.83	41,50,56,62	0
7	MAN	A	931	11/12	0.15	9.01	18,22,33,38	0
7	MAN	A	930	11/12	0.14	8.84	19,22,34,37	0
4	BMA	B	928	11/12	0.20	5.55	35,42,55,67	0
13	MAN	B	941	11/12	0.13	5.34	24,31,35,42	0
7	NAG	A	925	14/15	0.08	4.19	15,18,39,42	0
4	BMA	A	909	11/12	0.21	4.08	34,42,51,57	0
4	NAG	A	908	14/15	0.16	3.08	23,27,34,37	0
7	NAG	A	926	14/15	0.10	3.03	17,23,28,34	0
7	MAN	A	936	11/12	0.10	2.90	24,31,40,43	0
13	MAN	B	940	11/12	0.16	2.78	27,31,39,42	0
4	NAG	B	926	14/15	0.08	2.60	18,23,32,33	0
12	NAG	B	910	14/15	0.10	2.58	17,23,31,31	0
7	MAN	B	935	11/12	0.11	2.49	18,22,29,32	0
7	NAG	B	929	14/15	0.10	2.19	16,20,39,43	0
5	NAG	A	911	14/15	0.11	2.12	25,30,47,49	0
7	NAG	B	930	14/15	0.12	2.03	18,23,32,33	0
7	MAN	B	933	11/12	0.13	1.96	23,28,38,43	0
7	MAN	B	934	11/12	0.11	1.87	21,23,29,34	0
4	NAG	B	914	14/15	0.10	1.71	18,23,42,43	0
7	MAN	B	906	11/12	0.11	1.47	22,26,29,37	0
4	NAG	A	922	14/15	0.08	1.46	19,25,35,38	0
7	MAN	B	907	11/12	0.12	1.45	22,29,34,34	0
7	MAN	A	935	11/12	0.10	1.41	22,29,39,50	0
4	NAG	A	907	14/15	0.10	0.78	17,20,22,24	0
6	MAN	B	925	11/12	0.07	0.67	16,17,19,21	0
12	NAG	B	909	14/15	0.08	0.57	16,18,20,21	0
7	MAN	B	905	11/12	0.10	0.14	23,30,37,47	0
6	MAN	A	915	11/12	0.10	-0.16	24,25,32,33	0
6	MAN	A	919	11/12	0.09	-0.19	18,20,21,22	0
7	NAG	A	932	14/15	0.06	-0.37	17,20,23,24	0
6	NAG	B	916	14/15	0.06	-0.46	12,14,19,22	0
6	NAG	B	917	14/15	0.06	-0.61	12,15,15,16	0
2	NAG	A	901	14/15	0.07	-0.63	16,19,21,23	0
13	NAG	B	936	14/15	0.06	-0.66	15,18,21,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	902	14/15	0.08	-0.75	20,28,38,42	0
6	MAN	A	920	11/12	0.07	-0.79	20,24,30,34	0
6	MAN	B	922	11/12	0.07	-0.85	18,21,22,33	0
6	MAN	B	919	11/12	0.06	-0.85	18,20,24,26	0
6	MAN	A	918	11/12	0.06	-0.90	16,18,21,22	0
6	NAG	A	912	14/15	0.07	-0.93	20,23,26,29	0
7	NAG	B	901	14/15	0.06	-0.96	12,14,17,18	0
6	NAG	A	913	14/15	0.07	-0.99	17,19,20,22	0
4	NAG	B	913	14/15	0.06	-0.99	14,16,19,19	0
7	NAG	B	902	14/15	0.06	-1.03	14,16,20,28	0
6	MAN	B	924	11/12	0.06	-1.03	13,14,16,16	0
6	BMA	B	918	11/12	0.05	-1.13	14,16,18,18	0
5	NAG	A	910	14/15	0.07	-1.18	16,19,23,25	0
6	MAN	B	921	11/12	0.05	-1.86	14,15,15,16	0
6	MAN	A	917	11/12	0.06	-1.99	17,20,22,23	0
6	BMA	A	914	11/12	0.08	-2.42	19,21,26,27	0
7	BMA	A	927	11/12	0.15	-	21,25,32,43	0
13	NAG	B	937	14/15	0.10	-	24,29,35,36	0
12	MAN	B	912	11/12	0.30	-	53,60,64,65	0
2	BMA	A	903	11/12	0.16	-	33,46,53,57	0
4	BMA	B	915	11/12	0.34	-	56,73,91,97	0
4	NAG	A	923	14/15	0.20	-	36,43,52,56	0
7	MAN	A	928	11/12	0.30	-	52,62,64,67	0
6	MAN	B	923	11/12	0.12	-	25,28,34,35	0
7	BMA	A	934	11/12	0.17	-	30,37,47,51	0
2	MAN	A	904	11/12	0.27	-	60,74,81,87	0
7	BMA	B	903	11/12	0.10	-	19,21,22,24	0
4	NAG	B	927	14/15	0.13	-	24,29,41,41	0
7	NAG	A	933	14/15	0.11	-	22,27,32,37	0
13	MAN	B	939	11/12	0.25	-	59,67,77,86	0
6	MAN	B	920	11/12	0.12	-	27,36,41,43	0
7	BMA	B	931	11/12	0.16	-	24,28,34,45	0
7	MAN	B	904	11/12	0.15	-	24,31,40,41	0
6	MAN	A	921	11/12	0.16	-	27,29,34,40	0
7	MAN	B	932	11/12	0.33	-	58,63,67,71	0
13	BMA	B	938	11/12	0.16	-	35,38,46,58	0
6	MAN	A	916	11/12	0.15	-	31,37,44,57	0

6.4 Ligands

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	908	14/15	0.31	33.73	39,48,52,53	0
8	MRD	A	941	8/8	0.17	10.96	18,30,41,43	0
3	NAG	A	906	14/15	0.35	9.81	42,52,57,58	0
8	MRD	B	948	8/8	0.16	7.34	32,41,42,43	0
3	NAG	B	944	14/15	0.26	6.56	36,50,55,59	0
8	MRD	B	946	8/8	0.20	4.57	19,32,40,43	0
9	MPD	A	942	8/8	0.21	3.96	37,39,45,48	0
10	NA	B	949	1/1	0.23	3.67	29,29,29,29	0
8	MRD	B	947	8/8	0.10	3.56	20,25,37,37	0
3	NAG	B	945	14/15	0.15	2.54	26,29,33,34	0
10	NA	A	943	1/1	0.14	1.00	26,26,26,26	0
3	NAG	A	939	14/15	0.12	0.74	35,38,42,46	0
11	IFM	A	944	10/10	0.15	0.66	12,13,14,15	0
11	IFM	B	950	10/10	0.11	0.40	10,11,11,11	0
8	MRD	A	940	8/8	0.07	0.11	20,22,25,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.