



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:22 am GMT

PDB ID : 5FJJ
Title : Three-dimensional structures of two heavily N-glycosylated *Aspergillus* sp. Family GH3 beta-D-glucosidases
Authors : Agirre, J.; Ariza, A.; Offen, W.A.; Turkenburg, J.P.; Roberts, S.M.; McNicholas, S.; Harris, P.V.; McBrayer, B.; Dohnalek, J.; Cowtan, K.D.; Davies, G.J.; Wilson, K.S.
Deposited on : 2015-10-09
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

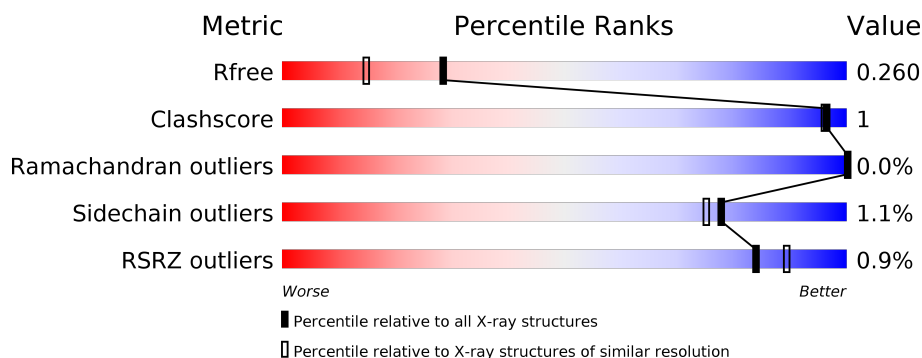
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
1	B	842	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
1	C	842	<div> <div></div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
1	D	842	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>.</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PO4	A	5001	-	-	-	X
13	MAN	B	1704	-	-	-	X
14	NAG	C	1301	-	-	-	X
5	NAG	A	1401	-	-	-	X
5	NAG	D	1102	-	-	-	X
8	MAN	A	1704	-	-	-	X
8	NAG	B	1501	-	-	-	X
8	MAN	B	1507	-	-	-	X
8	MAN	C	1507	-	-	-	X
8	MAN	D	1507	-	-	-	X
9	PEG	A	3001	-	-	-	X
9	PEG	C	6001	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 30056 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	9	0
			6506	4094	1118	1275	19			
1	B	838	Total	C	N	O	S	0	7	0
			6471	4073	1110	1269	19			
1	C	839	Total	C	N	O	S	0	8	0
			6489	4083	1114	1273	19			
1	D	838	Total	C	N	O	S	0	6	0
			6477	4079	1113	1266	19			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (11-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	11	Total	C	N	O	0	0
			127	70	2	55		
4	B	11	Total	C	N	O	0	0
			127	70	2	55		

- 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		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

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

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

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

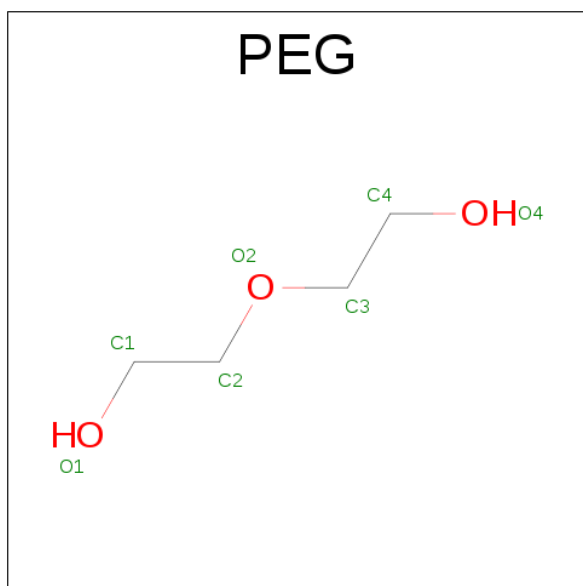
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	7	Total	C	N	O	0	0
			83	46	2	35		
8	B	7	Total	C	N	O	0	0
			83	46	2	35		
8	C	7	Total	C	N	O	0	0
			83	46	2	35		
8	C	7	Total	C	N	O	0	0
			83	46	2	35		
8	D	7	Total	C	N	O	0	0
			83	46	2	35		

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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

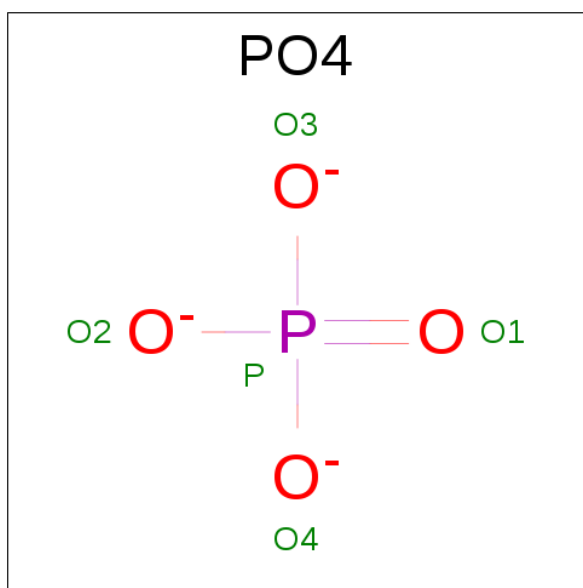


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Mg	0	0
			2	2		
10	D	1	Total	Mg	0	0
			1	1		
10	C	1	Total	Mg	0	0
			1	1		

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	Cl	0	0
			1	1		
12	A	1	Total	Cl	0	0
			1	1		
12	D	1	Total	Cl	0	0
			1	1		
12	C	1	Total	Cl	0	0
			1	1		

- Molecule 13 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	5	Total	C	N	O	0	0
			61	34	2	25		
13	C	5	Total	C	N	O	0	1
			75	42	3	30		

- Molecule 14 is a polymer of unknown type called SUGAR (9-MER).

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

- Molecule 15 is a polymer of unknown type called SUGAR (8-MER).

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

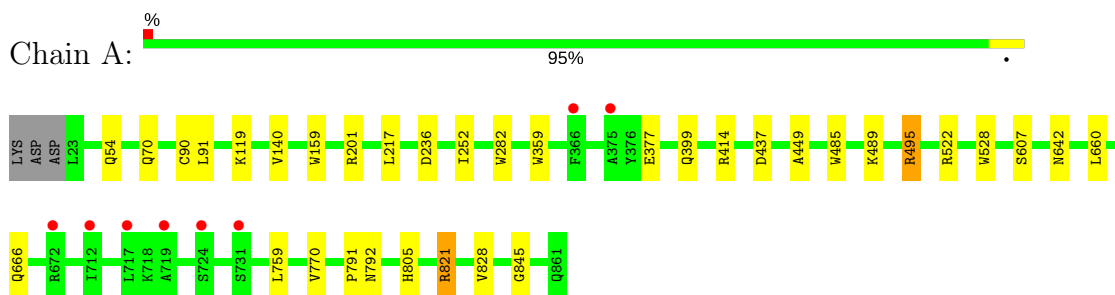
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	533	Total	O	0	4
			535	535		
16	B	501	Total	O	0	2
			503	503		
16	C	601	Total	O	0	7
			606	606		
16	D	471	Total	O	0	2
			473	473		

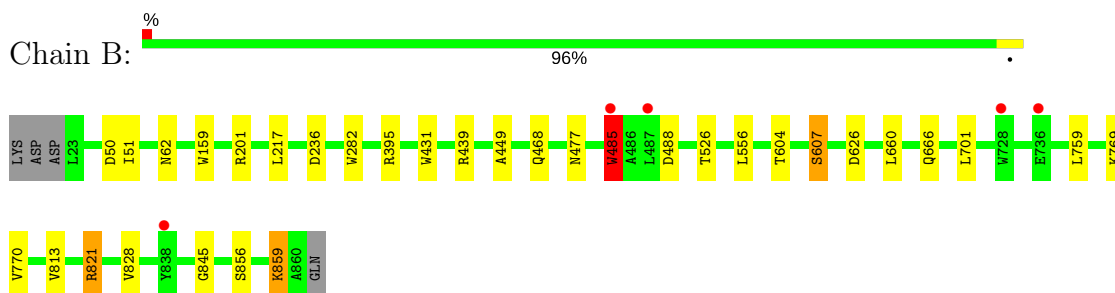
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

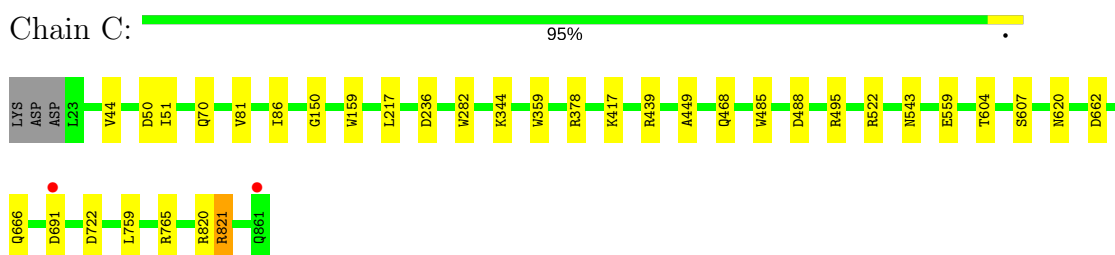
- Molecule 1: BETA-GLUCOSIDASE



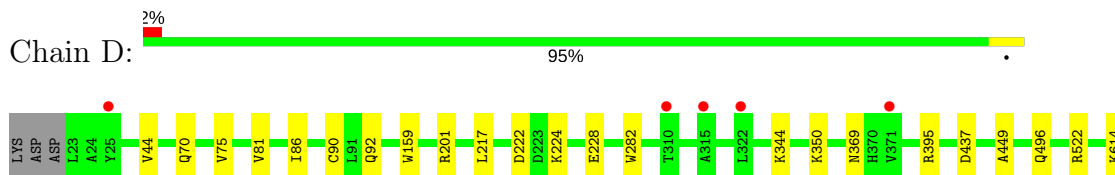
- Molecule 1: BETA-GLUCOSIDASE

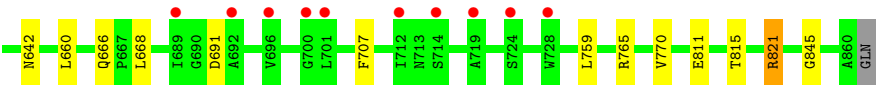


- Molecule 1: BETA-GLUCOSIDASE



- Molecule 1: BETA-GLUCOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.02Å 141.46Å 193.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.43 – 1.95 88.23 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (114.43-1.95) 97.8 (88.23-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.216 , 0.255 0.223 , 0.260	Depositor DCC
R_{free} test set	13558 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30056	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, CL, PO4, PEG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/6685	0.80	9/9111 (0.1%)
1	B	0.73	0/6651	0.80	10/9067 (0.1%)
1	C	0.71	0/6667	0.81	11/9089 (0.1%)
1	D	0.68	0/6655	0.80	11/9071 (0.1%)
All	All	0.71	0/26658	0.80	41/36338 (0.1%)

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	821	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	821	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	821	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	821	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	D	201	ARG	NE-CZ-NH1	6.95	123.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6506	0	6166	24	0
1	B	6471	0	6137	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6489	0	6151	13	0
1	D	6477	0	6151	18	0
2	A	78	0	68	0	0
2	C	39	0	34	0	0
3	A	50	0	43	3	0
3	B	100	0	86	0	0
3	C	50	0	43	0	0
3	D	50	0	43	0	0
4	A	127	0	106	0	0
4	B	127	0	106	0	0
5	A	56	0	50	0	0
5	B	56	0	50	0	0
5	C	56	0	50	1	0
5	D	84	0	75	1	0
6	A	72	0	61	3	0
6	B	72	0	61	1	0
7	A	28	0	26	0	0
7	B	14	0	13	0	0
7	C	28	0	26	2	0
7	D	28	0	26	0	0
8	A	83	0	70	0	0
8	B	83	0	70	2	0
8	C	166	0	140	3	0
8	D	166	0	140	0	0
9	A	14	0	20	0	0
9	B	7	0	10	0	0
9	C	7	0	10	0	0
9	D	7	0	10	0	0
10	A	2	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	5	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	B	61	0	52	0	0
13	C	75	0	64	0	0
14	C	105	0	88	0	0
15	D	94	0	79	0	0
16	A	535	0	0	7	0
16	B	503	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C	606	0	0	0	0
16	D	473	0	0	4	0
All	All	30056	0	26325	65	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 1.

The worst 5 of 65 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791[B]:PRO:O	1:A:792[B]:ASN:HB2	1.74	0.86
1:A:791[B]:PRO:O	1:A:792[B]:ASN:CB	2.34	0.74
1:A:414:ARG:NH1	16:A:2255:HOH:O	2.21	0.72
1:A:377:GLU:OE2	16:A:2040:HOH:O	2.08	0.69
1:C:620:ASN:ND2	7:C:1901:NAG:O6	2.26	0.69

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	846/842 (100%)	818 (97%)	28 (3%)	0	100	100
1	B	843/842 (100%)	819 (97%)	24 (3%)	0	100	100
1	C	845/842 (100%)	816 (97%)	28 (3%)	1 (0%)	55	46
1	D	842/842 (100%)	816 (97%)	26 (3%)	0	100	100
All	All	3376/3368 (100%)	3269 (97%)	106 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	686/681 (101%)	679 (99%)	7 (1%)	80	78
1	B	683/681 (100%)	672 (98%)	11 (2%)	68	63
1	C	684/681 (100%)	675 (99%)	9 (1%)	73	69
1	D	683/681 (100%)	679 (99%)	4 (1%)	89	88
All	All	2736/2724 (100%)	2705 (99%)	31 (1%)	78	75

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	607[A]	SER
1	B	859	LYS
1	D	217	LEU
1	B	607[B]	SER
1	C	51	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	473	GLN
1	C	195	ASN
1	C	825	ASN
1	A	861	GLN
1	C	620	ASN

5.3.3 RNA [i](#)

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 ⓘ

151 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	1001	1,2	14,14,15	0.83	1 (7%)	15,19,21	0.77	0
2	NAG	A	1002	2	14,14,15	0.38	0	15,19,21	0.51	0
2	BMA	A	1003	2	11,11,12	0.27	0	13,15,17	0.46	0
3	NAG	A	1101	1,3	14,14,15	0.95	1 (7%)	15,19,21	1.06	2 (13%)
3	NAG	A	1102	3	14,14,15	0.48	0	15,19,21	0.70	0
3	BMA	A	1103	3	11,11,12	0.32	0	13,15,17	0.50	0
3	MAN	A	1106	3	11,11,12	0.26	0	13,15,17	0.49	0
2	NAG	A	1201	1,2	14,14,15	0.61	0	15,19,21	0.84	1 (6%)
2	NAG	A	1202	2	14,14,15	0.43	0	15,19,21	0.70	0
2	BMA	A	1203	2	11,11,12	0.40	0	13,15,17	0.63	0
4	NAG	A	1301	1,4	14,14,15	0.38	0	15,19,21	0.72	0
4	NAG	A	1302	4	14,14,15	0.62	0	15,19,21	0.82	1 (6%)
4	BMA	A	1303	4	11,11,12	0.25	0	13,15,17	0.57	0
4	MAN	A	1304	4	11,11,12	0.31	0	13,15,17	0.59	0
4	MAN	A	1305	4	11,11,12	0.33	0	13,15,17	0.59	0
4	MAN	A	1306	4	11,11,12	0.24	0	13,15,17	0.63	0
4	MAN	A	1307	4	11,11,12	0.19	0	13,15,17	0.44	0
4	MAN	A	1308	4	11,11,12	0.27	0	13,15,17	0.66	0
4	MAN	A	1309	4	11,11,12	0.28	0	13,15,17	0.43	0
4	MAN	A	1310	4	11,11,12	0.40	0	13,15,17	0.69	0
4	MAN	A	1311	4	11,11,12	0.32	0	13,15,17	0.74	0
5	NAG	A	1401	1,5	14,14,15	0.64	0	15,19,21	1.15	1 (6%)
5	NAG	A	1402	5	14,14,15	0.88	1 (7%)	15,19,21	1.48	2 (13%)
6	NAG	A	1501	1,6	14,14,15	0.50	0	15,19,21	0.42	0
6	NAG	A	1502	6	14,14,15	0.61	0	15,19,21	0.56	0
6	BMA	A	1503	6	11,11,12	0.25	0	13,15,17	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	1504	6	11,11,12	0.30	0	13,15,17	0.48	0
6	MAN	A	1506	6	11,11,12	0.32	0	13,15,17	0.69	0
6	MAN	A	1507	6	11,11,12	0.36	0	13,15,17	0.68	1 (7%)
8	NAG	A	1701	1,8	14,14,15	0.73	1 (7%)	15,19,21	0.34	0
8	NAG	A	1702	8	14,14,15	0.43	0	15,19,21	0.70	0
8	BMA	A	1703	8	11,11,12	0.32	0	13,15,17	0.78	0
8	MAN	A	1704	8	11,11,12	0.30	0	13,15,17	0.64	0
8	MAN	A	1705	8	11,11,12	0.34	0	13,15,17	0.65	0
8	MAN	A	1706	8	11,11,12	0.20	0	13,15,17	0.59	0
8	MAN	A	1708	8	11,11,12	0.27	0	13,15,17	0.54	0
5	NAG	A	1801	1,5	14,14,15	0.47	0	15,19,21	0.73	1 (6%)
5	NAG	A	1802	5	14,14,15	0.43	0	15,19,21	0.73	1 (6%)
3	NAG	B	1001	1,3	14,14,15	0.65	0	15,19,21	0.57	0
3	NAG	B	1002	3	14,14,15	0.52	0	15,19,21	0.47	0
3	BMA	B	1003	3	11,11,12	0.25	0	13,15,17	0.50	0
3	MAN	B	1004	3	11,11,12	0.35	0	13,15,17	0.60	0
6	NAG	B	1101	1,6	14,14,15	0.85	1 (7%)	15,19,21	1.05	1 (6%)
6	NAG	B	1102	6	14,14,15	0.52	0	15,19,21	0.62	0
6	BMA	B	1103	6	11,11,12	0.34	0	13,15,17	0.54	0
6	MAN	B	1104	6	11,11,12	0.30	0	13,15,17	0.71	0
6	MAN	B	1105	6	11,11,12	0.33	0	13,15,17	0.57	0
6	MAN	B	1106	6	11,11,12	0.27	0	13,15,17	0.54	0
3	NAG	B	1201	1,3	14,14,15	1.06	1 (7%)	15,19,21	0.74	0
3	NAG	B	1202	3	14,14,15	0.69	1 (7%)	15,19,21	0.69	0
3	BMA	B	1203	3	11,11,12	0.24	0	13,15,17	0.28	0
3	MAN	B	1204	3	11,11,12	0.26	0	13,15,17	0.59	0
4	NAG	B	1301	1,4	14,14,15	0.51	0	15,19,21	0.58	0
4	NAG	B	1302	4	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
4	BMA	B	1303	4	11,11,12	0.21	0	13,15,17	0.52	0
4	MAN	B	1304	4	11,11,12	0.25	0	13,15,17	0.55	0
4	MAN	B	1305	4	11,11,12	0.29	0	13,15,17	0.76	1 (7%)
4	MAN	B	1306	4	11,11,12	0.30	0	13,15,17	0.56	0
4	MAN	B	1307	4	11,11,12	0.29	0	13,15,17	0.56	0
4	MAN	B	1308	4	11,11,12	0.30	0	13,15,17	0.62	0
4	MAN	B	1309	4	11,11,12	0.24	0	13,15,17	0.42	0
4	MAN	B	1310	4	11,11,12	0.32	0	13,15,17	0.69	0
4	MAN	B	1311	4	11,11,12	0.34	0	13,15,17	0.69	0
5	NAG	B	1401	1,5	14,14,15	0.49	0	15,19,21	0.87	0
5	NAG	B	1402	5	14,14,15	0.46	0	15,19,21	0.94	1 (6%)
8	NAG	B	1501	1,8	14,14,15	0.65	0	15,19,21	0.69	0
8	NAG	B	1502	8	14,14,15	0.40	0	15,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	B	1503	8	11,11,12	0.28	0	13,15,17	0.47	0
8	MAN	B	1504	8	11,11,12	0.35	0	13,15,17	0.49	0
8	MAN	B	1505	8	11,11,12	0.24	0	13,15,17	0.37	0
8	MAN	B	1506	8	11,11,12	0.26	0	13,15,17	0.48	0
8	MAN	B	1507	8	11,11,12	0.29	0	13,15,17	0.69	0
13	NAG	B	1701	1,13	14,14,15	0.53	0	15,19,21	0.62	0
13	NAG	B	1702	13	14,14,15	0.43	0	15,19,21	0.99	2 (13%)
13	BMA	B	1703	13	11,11,12	0.20	0	13,15,17	0.44	0
13	MAN	B	1704	13	11,11,12	0.28	0	13,15,17	0.67	1 (7%)
13	MAN	B	1705	13	11,11,12	0.28	0	13,15,17	0.48	0
5	NAG	B	1801	1,5	14,14,15	0.46	0	15,19,21	0.58	0
5	NAG	B	1802	5	14,14,15	0.59	0	15,19,21	0.93	1 (6%)
3	NAG	C	1001	1,3	14,14,15	0.74	1 (7%)	15,19,21	0.58	0
3	NAG	C	1002	3	14,14,15	0.44	0	15,19,21	0.52	0
3	BMA	C	1003	3	11,11,12	0.43	0	13,15,17	0.66	0
3	MAN	C	1004	3	11,11,12	0.27	0	13,15,17	0.56	0
13	NAG	C	1101	1,13	14,14,15	0.39	0	15,19,21	0.57	0
13	NAG	C	1102[A]	13	14,14,15	0.46	0	15,19,21	0.91	1 (6%)
13	NAG	C	1102[B]	13	14,14,15	0.43	0	15,19,21	0.62	0
13	BMA	C	1103	13	11,11,12	0.28	0	13,15,17	0.31	0
13	MAN	C	1104	13	11,11,12	0.43	0	13,15,17	0.78	0
13	MAN	C	1105	13	11,11,12	0.27	0	13,15,17	0.64	0
2	NAG	C	1201	1,2	14,14,15	0.52	0	15,19,21	0.59	0
2	NAG	C	1202	2	14,14,15	0.51	0	15,19,21	0.61	0
2	BMA	C	1203	2	11,11,12	0.33	0	13,15,17	0.59	0
14	NAG	C	1301	1,14	14,14,15	0.80	1 (7%)	15,19,21	0.47	0
14	NAG	C	1302	14	14,14,15	0.98	1 (7%)	15,19,21	0.86	0
14	BMA	C	1303	14	11,11,12	0.23	0	13,15,17	0.52	0
14	MAN	C	1304	14	11,11,12	0.34	0	13,15,17	0.69	1 (7%)
14	MAN	C	1307	14	11,11,12	0.24	0	13,15,17	0.51	0
14	MAN	C	1308	14	11,11,12	0.25	0	13,15,17	0.51	0
14	MAN	C	1309	14	11,11,12	0.26	0	13,15,17	0.43	0
14	MAN	C	1310	14	11,11,12	0.53	0	13,15,17	0.70	1 (7%)
14	MAN	C	1311	14	11,11,12	0.37	0	13,15,17	0.74	1 (7%)
5	NAG	C	1401	1,5	14,14,15	0.63	0	15,19,21	1.12	1 (6%)
5	NAG	C	1402	5	14,14,15	0.48	0	15,19,21	0.82	1 (6%)
8	NAG	C	1501	1,8	14,14,15	0.52	0	15,19,21	0.58	0
8	NAG	C	1502	8	14,14,15	0.45	0	15,19,21	0.59	0
8	BMA	C	1503	8	11,11,12	0.22	0	13,15,17	0.47	0
8	MAN	C	1504	8	11,11,12	0.24	0	13,15,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	C	1505	8	11,11,12	0.23	0	13,15,17	0.59	0
8	MAN	C	1506	8	11,11,12	0.38	0	13,15,17	0.76	0
8	MAN	C	1507	8	11,11,12	0.41	0	13,15,17	0.95	2 (15%)
8	NAG	C	1701	1,8	14,14,15	0.57	0	15,19,21	0.81	1 (6%)
8	NAG	C	1702	8	14,14,15	0.55	0	15,19,21	0.74	0
8	BMA	C	1703	8	11,11,12	0.19	0	13,15,17	0.49	0
8	MAN	C	1704	8	11,11,12	0.30	0	13,15,17	0.63	0
8	MAN	C	1705	8	11,11,12	0.34	0	13,15,17	0.43	0
8	MAN	C	1706	8	11,11,12	0.21	0	13,15,17	0.53	0
8	MAN	C	1707	8	11,11,12	0.28	0	13,15,17	0.71	1 (7%)
5	NAG	C	1801	1,5	14,14,15	0.45	0	15,19,21	0.96	1 (6%)
5	NAG	C	1802	5	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
5	NAG	D	1001	1,5	14,14,15	0.54	0	15,19,21	0.96	1 (6%)
5	NAG	D	1002	5	14,14,15	0.79	1 (7%)	15,19,21	0.77	1 (6%)
5	NAG	D	1101	1,5	14,14,15	0.83	1 (7%)	15,19,21	0.64	0
5	NAG	D	1102	5	14,14,15	0.49	0	15,19,21	0.60	0
3	NAG	D	1201	1,3	14,14,15	0.50	0	15,19,21	0.77	1 (6%)
3	NAG	D	1202	3	14,14,15	0.66	1 (7%)	15,19,21	1.05	1 (6%)
3	BMA	D	1203	3	11,11,12	0.22	0	13,15,17	0.39	0
3	MAN	D	1204	3	11,11,12	0.32	0	13,15,17	0.73	0
15	NAG	D	1301	1,15	14,14,15	0.43	0	15,19,21	0.82	1 (6%)
15	NAG	D	1302	15	14,14,15	0.95	1 (7%)	15,19,21	0.74	0
15	BMA	D	1303	15	11,11,12	0.34	0	13,15,17	0.51	0
15	MAN	D	1307	15	11,11,12	0.36	0	13,15,17	0.45	0
15	MAN	D	1308	15	11,11,12	0.31	0	13,15,17	0.58	0
15	MAN	D	1309	15	11,11,12	0.26	0	13,15,17	0.38	0
15	MAN	D	1310	15	11,11,12	0.28	0	13,15,17	0.47	0
15	MAN	D	1311	15	11,11,12	0.39	0	13,15,17	0.74	0
5	NAG	D	1401	1,5	14,14,15	0.47	0	15,19,21	0.90	1 (6%)
5	NAG	D	1402	5	14,14,15	0.49	0	15,19,21	0.71	1 (6%)
8	NAG	D	1501	1,8	14,14,15	0.49	0	15,19,21	0.49	0
8	NAG	D	1502	8	14,14,15	0.41	0	15,19,21	0.70	0
8	BMA	D	1503	8	11,11,12	0.30	0	13,15,17	0.45	0
8	MAN	D	1504	8	11,11,12	0.28	0	13,15,17	0.49	0
8	MAN	D	1505	8	11,11,12	0.21	0	13,15,17	0.45	0
8	MAN	D	1506	8	11,11,12	0.33	0	13,15,17	0.71	1 (7%)
8	MAN	D	1507	8	11,11,12	0.24	0	13,15,17	0.59	0
8	NAG	D	1701	1,8	14,14,15	0.44	0	15,19,21	0.46	0
8	NAG	D	1702	8	14,14,15	0.69	1 (7%)	15,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	D	1703	8	11,11,12	0.23	0	13,15,17	0.58	0
8	MAN	D	1704	8	11,11,12	0.29	0	13,15,17	0.51	0
8	MAN	D	1705	8	11,11,12	0.32	0	13,15,17	0.62	0
8	MAN	D	1707	8	11,11,12	0.26	0	13,15,17	0.54	0
8	MAN	D	1708	8	11,11,12	0.21	0	13,15,17	0.54	0

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	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
3	NAG	A	1101	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1102	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1103	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1106	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1201	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1202	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1203	2	-	0/2/19/22	0/1/1/1
4	NAG	A	1301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1303	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1304	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1305	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1306	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1307	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1308	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1309	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1310	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1311	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1501	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1502	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1503	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1504	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1506	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1507	6	-	0/2/19/22	0/1/1/1
8	NAG	A	1701	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1702	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	A	1703	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1704	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1705	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1706	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1708	8	-	0/2/19/22	0/1/1/1
5	NAG	A	1801	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1802	5	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1003	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1004	3	-	0/2/19/22	0/1/1/1
6	NAG	B	1101	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1102	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1103	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1104	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1105	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1106	6	-	0/2/19/22	0/1/1/1
3	NAG	B	1201	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1202	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1203	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1204	3	-	0/2/19/22	0/1/1/1
4	NAG	B	1301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1303	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1304	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1305	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1306	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1307	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1308	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1309	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1310	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1311	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	5	-	0/6/23/26	0/1/1/1
8	NAG	B	1501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1502	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1503	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1504	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1505	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1506	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1507	8	-	0/2/19/22	0/1/1/1
13	NAG	B	1701	1,13	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	B	1702	13	-	0/6/23/26	0/1/1/1
13	BMA	B	1703	13	-	0/2/19/22	0/1/1/1
13	MAN	B	1704	13	-	0/2/19/22	0/1/1/1
13	MAN	B	1705	13	-	0/2/19/22	0/1/1/1
5	NAG	B	1801	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1802	5	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1002	3	-	0/6/23/26	0/1/1/1
3	BMA	C	1003	3	-	0/2/19/22	0/1/1/1
3	MAN	C	1004	3	-	0/2/19/22	0/1/1/1
13	NAG	C	1101	1,13	-	0/6/23/26	0/1/1/1
13	NAG	C	1102[A]	13	-	0/6/23/26	0/1/1/1
13	NAG	C	1102[B]	13	-	0/6/23/26	0/1/1/1
13	BMA	C	1103	13	-	0/2/19/22	0/1/1/1
13	MAN	C	1104	13	-	0/2/19/22	0/1/1/1
13	MAN	C	1105	13	-	0/2/19/22	0/1/1/1
2	NAG	C	1201	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1202	2	-	0/6/23/26	0/1/1/1
2	BMA	C	1203	2	-	0/2/19/22	0/1/1/1
14	NAG	C	1301	1,14	-	0/6/23/26	0/1/1/1
14	NAG	C	1302	14	-	0/6/23/26	0/1/1/1
14	BMA	C	1303	14	-	0/2/19/22	0/1/1/1
14	MAN	C	1304	14	-	0/2/19/22	0/1/1/1
14	MAN	C	1307	14	-	0/2/19/22	0/1/1/1
14	MAN	C	1308	14	-	0/2/19/22	0/1/1/1
14	MAN	C	1309	14	-	0/2/19/22	0/1/1/1
14	MAN	C	1310	14	-	0/2/19/22	0/1/1/1
14	MAN	C	1311	14	-	0/2/19/22	0/1/1/1
5	NAG	C	1401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	5	-	0/6/23/26	0/1/1/1
8	NAG	C	1501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	1502	8	-	0/6/23/26	0/1/1/1
8	BMA	C	1503	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1504	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1505	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1506	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1507	8	-	0/2/19/22	0/1/1/1
8	NAG	C	1701	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	1702	8	-	0/6/23/26	0/1/1/1
8	BMA	C	1703	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1704	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1705	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	C	1706	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1707	8	-	0/2/19/22	0/1/1/1
5	NAG	C	1801	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1802	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1101	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1102	5	-	0/6/23/26	0/1/1/1
3	NAG	D	1201	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1202	3	-	0/6/23/26	0/1/1/1
3	BMA	D	1203	3	-	0/2/19/22	0/1/1/1
3	MAN	D	1204	3	-	0/2/19/22	0/1/1/1
15	NAG	D	1301	1,15	-	0/6/23/26	0/1/1/1
15	NAG	D	1302	15	-	0/6/23/26	0/1/1/1
15	BMA	D	1303	15	-	0/2/19/22	0/1/1/1
15	MAN	D	1307	15	-	0/2/19/22	0/1/1/1
15	MAN	D	1308	15	-	0/2/19/22	0/1/1/1
15	MAN	D	1309	15	-	0/2/19/22	0/1/1/1
15	MAN	D	1310	15	-	0/2/19/22	0/1/1/1
15	MAN	D	1311	15	-	0/2/19/22	0/1/1/1
5	NAG	D	1401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1402	5	-	0/6/23/26	0/1/1/1
8	NAG	D	1501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1502	8	-	0/6/23/26	0/1/1/1
8	BMA	D	1503	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1504	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1505	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1506	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1507	8	-	0/2/19/22	0/1/1/1
8	NAG	D	1701	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1702	8	-	0/6/23/26	0/1/1/1
8	BMA	D	1703	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1704	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1705	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1707	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1708	8	-	0/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	NAG	C1-C2	-3.58	1.47	1.52
8	D	1702	NAG	C1-C2	-2.00	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	NAG	C1-C2	2.03	1.55	1.52
3	B	1202	NAG	C1-C2	2.13	1.55	1.52
8	A	1701	NAG	C1-C2	2.27	1.55	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1401	NAG	C1-C2-N2	-3.01	105.34	110.49
13	C	1102[A]	NAG	O5-C1-C2	-2.97	107.34	111.47
13	B	1702	NAG	O5-C1-C2	-2.63	107.81	111.47
2	A	1201	NAG	O5-C1-C2	-2.49	108.00	111.47
15	D	1301	NAG	O5-C1-C2	-2.18	108.44	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	NAG	2	0
3	A	1102	NAG	1	0
6	A	1502	NAG	1	0
6	A	1503	BMA	2	0
6	B	1102	NAG	1	0
8	B	1503	BMA	1	0
8	B	1507	MAN	1	0
8	C	1503	BMA	1	0
8	C	1507	MAN	1	0
8	C	1701	NAG	1	0
5	C	1801	NAG	1	0
5	D	1002	NAG	1	0

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 8 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	$\# Z > 2$
7	NAG	A	1601	1	14,14,15	0.59	0	15,19,21	1.05	2 (13%)
7	NAG	A	1901	1	14,14,15	0.46	0	15,19,21	0.47	0
9	PEG	A	3001	-	6,6,6	0.50	0	5,5,5	0.76	0
11	PO4	A	5001	-	4,4,4	1.16	0	6,6,6	0.82	0
9	PEG	A	6002	-	6,6,6	0.52	0	5,5,5	0.89	0
7	NAG	B	1601	1	14,14,15	1.17	1 (7%)	15,19,21	1.75	3 (20%)
9	PEG	B	6001	-	6,6,6	0.33	0	5,5,5	0.69	0
7	NAG	C	1601	1	14,14,15	0.34	0	15,19,21	0.92	1 (6%)
7	NAG	C	1901	1	14,14,15	0.91	1 (7%)	15,19,21	1.48	1 (6%)
9	PEG	C	6001	-	6,6,6	0.83	0	5,5,5	1.15	1 (20%)
7	NAG	D	1601	1	14,14,15	0.46	0	15,19,21	0.82	1 (6%)
7	NAG	D	1801	1	14,14,15	0.59	0	15,19,21	0.96	1 (6%)
9	PEG	D	6001	-	6,6,6	0.65	0	5,5,5	0.50	0

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
7	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1901	1	-	0/6/23/26	0/1/1/1
9	PEG	A	3001	-	-	0/4/4/4	0/0/0/0
11	PO4	A	5001	-	-	0/0/0/0	0/0/0/0
9	PEG	A	6002	-	-	0/4/4/4	0/0/0/0
7	NAG	B	1601	1	-	0/6/23/26	0/1/1/1
9	PEG	B	6001	-	-	0/4/4/4	0/0/0/0
7	NAG	C	1601	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1901	1	-	0/6/23/26	0/1/1/1
9	PEG	C	6001	-	-	0/4/4/4	0/0/0/0
7	NAG	D	1601	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1801	1	-	0/6/23/26	0/1/1/1
9	PEG	D	6001	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1901	NAG	C1-C2	3.12	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1601	NAG	C1-C2	4.22	1.58	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1601	NAG	O5-C1-C2	-2.13	108.51	111.47
9	C	6001	PEG	C3-O2-C2	2.37	123.57	113.30
7	D	1601	NAG	C1-C2-N2	2.66	115.03	110.49
7	B	1601	NAG	C2-N2-C7	2.84	127.09	122.94
7	C	1601	NAG	O5-C1-C2	2.99	115.63	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1901	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	839/842 (99%)	0.23	8 (0%) 82 88	17, 30, 46, 61	12 (1%)
1	B	838/842 (99%)	0.10	5 (0%) 89 93	17, 28, 43, 58	17 (2%)
1	C	839/842 (99%)	-0.05	2 (0%) 94 97	17, 25, 39, 54	12 (1%)
1	D	838/842 (99%)	0.23	15 (1%) 69 78	18, 30, 50, 61	28 (3%)
All	All	3354/3368 (99%)	0.13	30 (0%) 84 89	17, 28, 46, 61	69 (2%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	689	ILE	3.8
1	D	719	ALA	3.6
1	A	375	ALA	3.2
1	B	728	TRP	3.0
1	D	701	LEU	2.9

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	D	1507	11/12	0.82	0.24	13.11	33,37,39,40	11
8	MAN	C	1507	11/12	0.87	0.20	4.13	48,56,63,64	0
5	NAG	D	1102	14/15	0.87	0.20	3.76	27,34,41,42	14
8	MAN	A	1704	11/12	0.88	0.13	2.51	44,48,54,60	0
13	MAN	B	1704	11/12	0.83	0.23	2.47	35,36,40,41	11
5	NAG	A	1401	14/15	0.84	0.13	2.40	43,50,54,58	0
8	MAN	B	1507	11/12	0.85	0.25	2.37	52,58,63,68	0
8	NAG	B	1501	14/15	0.93	0.15	2.05	33,37,57,59	0
14	NAG	C	1301	14/15	0.95	0.17	2.05	25,29,32,32	0
6	MAN	A	1507	11/12	0.83	0.14	1.84	41,48,50,55	11
5	NAG	D	1401	14/15	0.87	0.13	1.65	34,44,55,56	0
5	NAG	C	1401	14/15	0.89	0.13	1.53	37,44,50,58	0
8	MAN	C	1705	11/12	0.89	0.16	1.43	48,51,66,68	0
4	MAN	B	1311	11/12	0.94	0.12	1.37	32,34,35,36	0
13	NAG	C	1102[B]	14/15	0.94	0.14	1.14	29,32,36,40	14
8	MAN	D	1704	11/12	0.90	0.12	1.13	36,41,43,46	0
8	NAG	A	1701	14/15	0.95	0.13	1.11	26,30,33,34	0
5	NAG	B	1401	14/15	0.88	0.15	1.11	40,48,59,65	0
15	MAN	D	1308	11/12	0.86	0.16	1.06	36,41,43,44	0
4	MAN	A	1310	11/12	0.87	0.17	0.95	29,40,47,53	0
13	NAG	C	1102[A]	14/15	0.94	0.14	0.92	31,35,37,41	14
8	NAG	D	1701	14/15	0.94	0.11	0.76	25,29,33,33	0
4	MAN	B	1310	11/12	0.94	0.13	0.76	28,31,33,36	0
15	NAG	D	1301	14/15	0.90	0.17	0.32	37,48,60,60	0
15	MAN	D	1311	11/12	0.89	0.14	0.21	37,39,45,45	0
6	NAG	A	1501	14/15	0.94	0.11	0.15	31,34,49,53	0
6	NAG	B	1101	14/15	0.94	0.12	0.15	23,30,34,34	0
13	NAG	B	1701	14/15	0.94	0.11	0.14	34,36,39,42	0
5	NAG	D	1002	14/15	0.86	0.17	0.08	48,56,58,58	0
4	NAG	B	1301	14/15	0.92	0.14	0.04	28,31,36,40	0
3	NAG	D	1202	14/15	0.89	0.19	0.01	42,45,54,60	0
3	NAG	B	1001	14/15	0.91	0.11	-0.02	27,30,31,33	0
13	NAG	C	1101	14/15	0.96	0.10	-0.03	27,29,31,33	0
14	MAN	C	1311	11/12	0.95	0.09	-0.04	28,29,31,32	0
15	NAG	D	1302	14/15	0.91	0.15	-0.04	37,41,48,48	0
15	MAN	D	1310	11/12	0.91	0.15	-0.06	35,38,40,40	0
3	NAG	A	1101	14/15	0.94	0.14	-0.07	33,36,39,41	0
2	NAG	C	1201	14/15	0.94	0.12	-0.10	22,26,30,34	0
5	NAG	B	1801	14/15	0.93	0.13	-0.16	36,40,43,43	0
4	NAG	A	1301	14/15	0.91	0.15	-0.19	35,42,46,47	0
14	NAG	C	1302	14/15	0.94	0.12	-0.25	23,26,29,30	0
3	NAG	C	1001	14/15	0.94	0.10	-0.30	25,27,30,31	0
4	NAG	B	1302	14/15	0.95	0.12	-0.42	29,32,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	1801	14/15	0.92	0.17	-0.45	36,44,57,65	0
6	NAG	A	1502	14/15	0.92	0.11	-0.45	36,39,44,47	0
4	NAG	A	1302	14/15	0.91	0.15	-0.48	34,40,42,46	0
14	MAN	C	1310	11/12	0.93	0.09	-0.54	25,26,28,29	0
5	NAG	C	1801	14/15	0.93	0.14	-0.55	33,37,46,54	0
14	MAN	C	1308	11/12	0.96	0.09	-0.55	24,25,28,31	0
3	NAG	B	1002	14/15	0.92	0.10	-0.63	28,32,39,45	0
5	NAG	D	1001	14/15	0.91	0.11	-0.69	32,43,49,52	0
5	NAG	D	1101	14/15	0.93	0.12	-0.69	33,39,44,44	0
8	MAN	C	1704	11/12	0.94	0.13	-0.70	48,54,60,63	0
8	NAG	C	1701	14/15	0.94	0.09	-0.76	28,31,34,38	0
6	NAG	B	1102	14/15	0.92	0.12	-0.79	33,38,45,51	0
3	NAG	A	1102	14/15	0.93	0.12	-0.82	41,45,55,62	0
3	NAG	D	1201	14/15	0.92	0.14	-0.85	32,37,42,46	0
2	NAG	A	1201	14/15	0.93	0.12	-0.86	26,33,39,41	0
4	MAN	A	1308	11/12	0.91	0.11	-0.89	33,34,41,43	0
4	MAN	A	1311	11/12	0.93	0.11	-0.94	31,38,41,43	0
3	NAG	C	1002	14/15	0.94	0.10	-0.97	26,31,39,39	0
2	NAG	C	1202	14/15	0.96	0.09	-1.07	27,29,34,35	0
2	NAG	A	1001	14/15	0.92	0.11	-1.11	32,35,38,39	0
2	NAG	A	1202	14/15	0.93	0.11	-1.24	30,32,36,38	0
4	MAN	B	1308	11/12	0.92	0.10	-1.63	27,33,37,42	0
2	NAG	A	1002	14/15	0.93	0.10	-1.76	40,44,48,48	0
3	NAG	B	1201	14/15	0.96	0.09	-1.76	24,27,29,29	0
3	NAG	B	1202	14/15	0.95	0.10	-1.90	29,31,33,35	0
8	NAG	B	1502	14/15	0.93	0.15	-	31,37,40,46	0
5	NAG	D	1402	14/15	0.81	0.26	-	22,33,38,43	14
8	MAN	C	1706	11/12	0.89	0.15	-	46,47,49,51	11
8	NAG	A	1702	14/15	0.87	0.13	-	34,39,52,53	0
13	NAG	B	1702	14/15	0.88	0.14	-	40,43,56,70	0
8	MAN	A	1706	11/12	0.87	0.20	-	43,44,48,56	11
2	BMA	C	1203	11/12	0.79	0.17	-	40,45,51,55	0
14	MAN	C	1307	11/12	0.94	0.10	-	24,25,27,27	0
5	NAG	C	1402	14/15	0.83	0.19	-	45,52,58,71	0
5	NAG	C	1802	14/15	0.88	0.21	-	22,28,30,30	14
2	BMA	A	1203	11/12	0.81	0.14	-	27,33,36,41	11
3	MAN	C	1004	11/12	0.67	0.29	-	31,37,43,47	11
8	BMA	C	1503	11/12	0.91	0.12	-	33,37,44,45	0
13	MAN	B	1705	11/12	0.73	0.20	-	34,37,40,48	11
8	MAN	B	1505	11/12	0.73	0.28	-	45,48,51,56	11
3	BMA	C	1003	11/12	0.86	0.11	-	39,45,50,54	0
14	BMA	C	1303	11/12	0.95	0.09	-	24,27,31,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	BMA	B	1503	11/12	0.92	0.17	-	39,42,45,52	0
4	MAN	B	1306	11/12	0.80	0.22	-	32,35,37,38	11
6	MAN	A	1506	11/12	0.85	0.16	-	45,50,56,60	11
13	MAN	C	1104	11/12	0.82	0.13	-	45,54,59,60	0
15	BMA	D	1303	11/12	0.80	0.15	-	37,44,46,49	0
8	NAG	D	1501	14/15	0.94	0.11	-	27,32,42,42	0
8	NAG	C	1502	14/15	0.96	0.12	-	25,29,31,32	0
6	BMA	B	1103	11/12	0.88	0.13	-	46,50,54,59	0
3	BMA	D	1203	11/12	0.75	0.21	-	41,45,47,48	11
4	MAN	B	1309	11/12	0.90	0.16	-	42,51,54,67	0
5	NAG	B	1802	14/15	0.84	0.16	-	46,53,60,63	0
8	MAN	D	1506	11/12	0.68	0.26	-	40,41,44,45	11
8	MAN	C	1505	11/12	0.73	0.22	-	47,49,52,53	11
13	BMA	C	1103	11/12	0.88	0.11	-	36,43,50,51	0
13	MAN	C	1105	11/12	0.78	0.17	-	38,47,51,52	11
14	MAN	C	1304	11/12	0.84	0.13	-	40,41,45,47	0
4	MAN	A	1306	11/12	0.85	0.14	-	50,51,53,55	11
4	BMA	B	1303	11/12	0.92	0.10	-	29,34,41,42	0
8	MAN	A	1708	11/12	0.76	0.23	-	54,57,59,65	0
8	MAN	A	1705	11/12	0.91	0.15	-	38,45,55,62	0
8	NAG	D	1502	14/15	0.94	0.09	-	28,31,35,38	0
6	MAN	A	1504	11/12	0.85	0.14	-	51,55,58,65	0
8	MAN	B	1504	11/12	0.90	0.11	-	51,53,57,62	0
8	BMA	D	1703	11/12	0.93	0.09	-	34,38,44,45	0
8	MAN	D	1708	11/12	0.74	0.27	-	42,44,48,50	11
3	BMA	B	1003	11/12	0.87	0.12	-	35,36,38,39	11
4	MAN	A	1309	11/12	0.85	0.15	-	46,49,55,58	0
5	NAG	A	1802	14/15	0.71	0.26	-	27,30,34,35	14
8	MAN	D	1505	11/12	0.72	0.30	-	39,44,50,51	11
8	NAG	C	1702	14/15	0.92	0.12	-	38,42,52,55	0
13	BMA	B	1703	11/12	0.80	0.18	-	37,42,44,47	11
3	BMA	B	1203	11/12	0.76	0.17	-	33,36,41,46	11
8	MAN	C	1504	11/12	0.86	0.14	-	45,49,57,58	0
4	MAN	A	1307	11/12	0.91	0.13	-	30,32,36,37	0
4	MAN	A	1304	11/12	0.89	0.17	-	40,45,52,59	0
8	BMA	A	1703	11/12	0.89	0.15	-	42,49,52,54	0
6	MAN	B	1106	11/12	0.71	0.18	-	40,47,52,54	11
8	MAN	D	1504	11/12	0.84	0.14	-	48,53,55,60	0
15	MAN	D	1309	11/12	0.82	0.17	-	30,37,41,44	11
3	MAN	B	1004	11/12	0.71	0.21	-	33,36,39,41	11
3	BMA	A	1103	11/12	0.80	0.16	-	50,53,56,56	0
15	MAN	D	1307	11/12	0.91	0.12	-	34,39,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	C	1707	11/12	0.86	0.28	-	34,38,40,41	11
5	NAG	A	1402	14/15	0.74	0.24	-	39,48,51,54	14
3	MAN	A	1106	11/12	0.70	0.26	-	42,42,46,46	11
2	BMA	A	1003	11/12	0.84	0.17	-	56,59,61,69	0
8	NAG	C	1501	14/15	0.95	0.11	-	26,29,41,46	0
6	MAN	B	1105	11/12	0.75	0.15	-	47,51,55,56	11
6	MAN	B	1104	11/12	0.89	0.15	-	47,51,52,54	11
5	NAG	B	1402	14/15	0.89	0.13	-	44,52,57,66	0
4	BMA	A	1303	11/12	0.88	0.16	-	27,36,39,39	0
4	MAN	B	1305	11/12	0.81	0.25	-	35,39,40,44	11
6	BMA	A	1503	11/12	0.87	0.12	-	40,45,49,54	0
4	MAN	A	1305	11/12	0.79	0.24	-	57,61,71,76	0
8	MAN	C	1506	11/12	0.81	0.16	-	55,61,64,68	0
3	MAN	B	1204	11/12	0.46	0.31	-	40,43,45,48	11
3	MAN	D	1204	11/12	0.76	0.16	-	43,49,53,58	11
4	MAN	B	1304	11/12	0.90	0.14	-	43,48,52,58	0
8	BMA	D	1503	11/12	0.91	0.12	-	39,41,45,49	0
8	MAN	D	1707	11/12	0.88	0.17	-	41,44,45,48	11
8	MAN	B	1506	11/12	0.88	0.22	-	50,58,67,72	0
8	MAN	D	1705	11/12	0.91	0.15	-	39,43,50,55	0
8	BMA	C	1703	11/12	0.91	0.15	-	44,56,68,71	0
14	MAN	C	1309	11/12	0.91	0.14	-	37,43,47,49	0
4	MAN	B	1307	11/12	0.93	0.10	-	28,29,32,32	0
8	NAG	D	1702	14/15	0.92	0.11	-	33,37,42,43	0

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	PEG	A	3001	7/7	0.83	0.20	6.03	46,52,53,57	0
9	PEG	C	6001	7/7	0.86	0.17	4.87	29,30,37,39	0
11	PO4	A	5001	5/5	0.94	0.19	2.82	58,59,67,69	0
9	PEG	B	6001	7/7	0.92	0.14	1.76	32,33,38,47	0
9	PEG	A	6002	7/7	0.86	0.14	0.98	37,40,46,47	0
9	PEG	D	6001	7/7	0.83	0.12	0.17	37,40,48,48	0
7	NAG	D	1801	14/15	0.83	0.17	-0.53	54,58,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	MG	C	3001	1/1	0.87	0.10	-	42,42,42,42	0
7	NAG	C	1601	14/15	0.77	0.28	-	43,48,54,57	14
10	MG	D	4001	1/1	0.98	0.03	-	27,27,27,27	0
12	CL	D	5001	1/1	0.96	0.07	-	39,39,39,39	0
7	NAG	C	1901	14/15	0.74	0.27	-	66,72,81,84	0
12	CL	B	5001	1/1	0.95	0.13	-	35,35,35,35	0
12	CL	A	6001	1/1	0.93	0.10	-	36,36,36,36	0
10	MG	A	4001	1/1	0.98	0.06	-	31,31,31,31	0
7	NAG	B	1601	14/15	0.69	0.35	-	36,39,45,46	14
10	MG	A	3002	1/1	0.92	0.13	-	46,46,46,46	0
7	NAG	D	1601	14/15	0.80	0.17	-	47,60,67,77	0
7	NAG	A	1901	14/15	0.69	0.24	-	44,47,49,49	14
12	CL	C	5001	1/1	0.97	0.11	-	33,33,33,33	0
7	NAG	A	1601	14/15	0.89	0.13	-	38,45,51,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.