



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:07 am GMT

PDB ID : 5FJI  
Title : Three-dimensional structures of two heavily N-glycosylated *Aspergillus* sp. Family GH3 beta-D-glucosidases  
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Deposited on : 2015-10-09  
Resolution : 1.95 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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

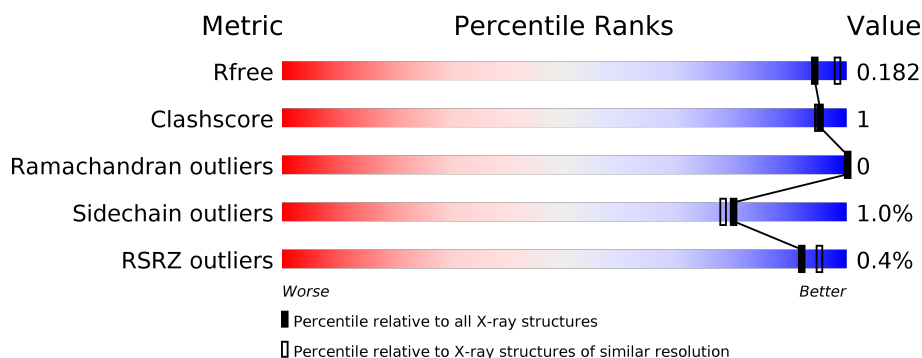
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

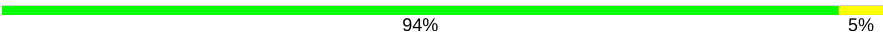

The reported resolution of this entry is 1.95 Å.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	844	 94% 5%
1	B	844	 95%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	IMD	A	1884	-	-	-	X
10	IMD	B	1882	-	-	-	X
10	IMD	B	1883	-	-	-	X
10	IMD	B	1884	-	-	-	X
11	NAG	B	1401	-	-	-	X
5	MAN	B	1311	-	-	-	X
6	NAG	A	1401	-	-	-	X
7	MAN	A	1509	-	-	-	X
7	MAN	B	1510	-	-	-	X
8	NAG	A	1801	-	-	-	X
8	NAG	B	1801	-	-	-	X
9	EDO	A	1865	-	-	-	X
9	EDO	A	1866	-	-	X	-
9	EDO	A	1868	-	-	-	X
9	EDO	A	1870	-	-	-	X
9	EDO	A	1871	-	-	-	X
9	EDO	A	1872	-	-	-	X
9	EDO	A	1874	-	-	-	X
9	EDO	A	1875	-	-	-	X
9	EDO	A	1876	-	-	-	X
9	EDO	A	1877	-	-	-	X
9	EDO	A	1878	-	-	-	X
9	EDO	A	1880	-	-	-	X
9	EDO	A	1881	-	-	-	X
9	EDO	B	1864	-	-	-	X
9	EDO	B	1867	-	-	-	X
9	EDO	B	1868	-	-	-	X
9	EDO	B	1870	-	-	-	X
9	EDO	B	1871	-	-	-	X
9	EDO	B	1872	-	-	-	X
9	EDO	B	1873	-	-	-	X
9	EDO	B	1876	-	-	-	X
9	EDO	B	1877	-	-	-	X
9	EDO	B	1879	-	-	-	X
9	EDO	B	1881	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 15929 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	840	Total	C	N	O	S	0	15	0
			6576	4147	1140	1270	19			
1	B	840	Total	C	N	O	S	0	10	0
			6513	4116	1120	1257	20			

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			72	40	2	30		
3	B	6	Total	C	N	O	0	1
			83	46	2	35		

- 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 (11-MER).

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

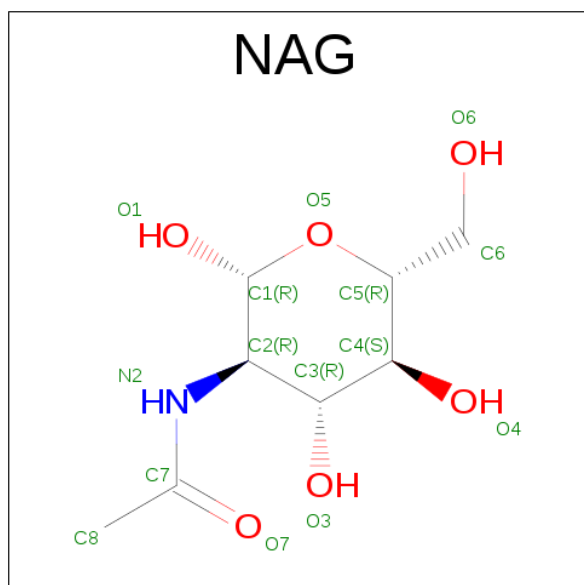
- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	9	Total	C	N	O	0	1
			119	66	3	50		
7	B	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



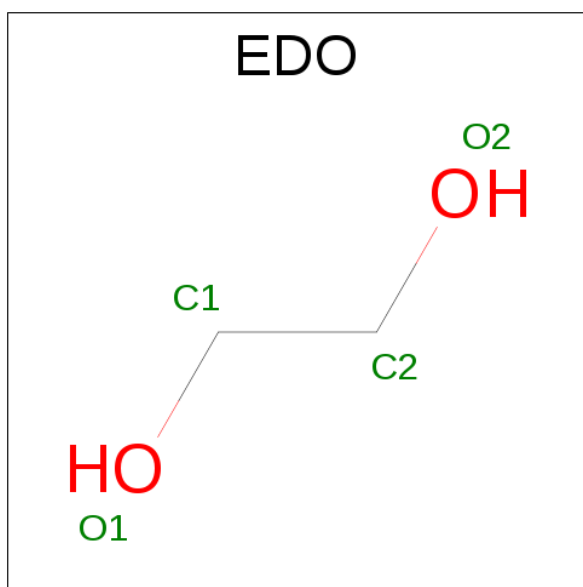
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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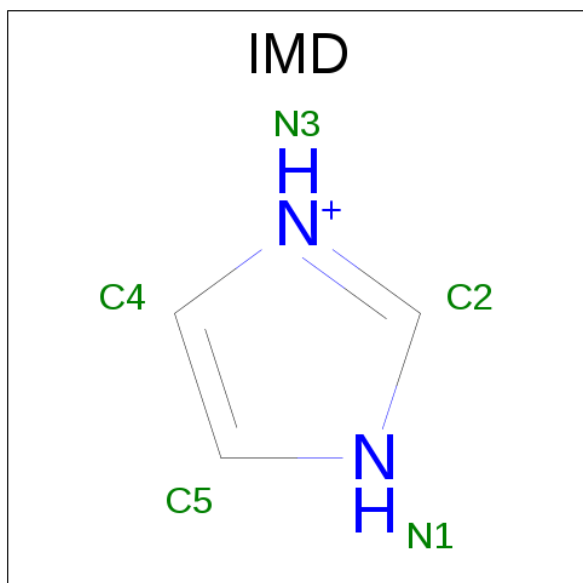
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total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

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

- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	N	0	0
			5	3	2		
10	A	1	Total	C	N	0	0
			5	3	2		
10	B	1	Total	C	N	0	0
			5	3	2		
10	B	1	Total	C	N	0	0
			5	3	2		
10	B	1	Total	C	N	0	0
			5	3	2		
10	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 11 is a polymer of unknown type called SUGAR (5-MER).

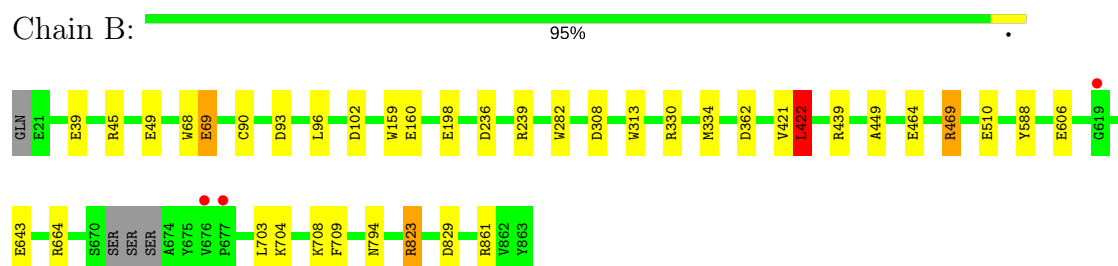
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	807	Total	O	0	5
			812	812		
12	B	715	Total	O	0	0
			715	715		



- Molecule 1: BETA-GLUCOSIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.52Å 129.67Å 217.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.41 – 1.95 69.31 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (111.41-1.95) 96.8 (69.31-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.149 , 0.174 0.159 , 0.182	Depositor DCC
$R_{free}$ test set	8876 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: MAN, BMA, NAG, IMD, EDO

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	1.04	7/6765 (0.1%)	0.97	21/9222 (0.2%)
1	B	1.02	9/6705 (0.1%)	0.98	21/9144 (0.2%)
All	All	1.03	16/13470 (0.1%)	0.97	42/18366 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	GLU	CD-OE1	8.30	1.34	1.25
1	B	823	ARG	CD-NE	-7.11	1.34	1.46
1	B	69	GLU	CD-OE1	-6.17	1.18	1.25
1	B	510	GLU	CD-OE2	6.16	1.32	1.25
1	A	464	GLU	CD-OE2	6.05	1.32	1.25
1	A	416	GLU	CD-OE2	5.65	1.31	1.25
1	B	160	GLU	CD-OE1	5.42	1.31	1.25
1	B	49	GLU	CD-OE2	5.42	1.31	1.25
1	A	606	GLU	CD-OE2	5.28	1.31	1.25
1	B	198	GLU	CD-OE2	5.23	1.31	1.25
1	A	823	ARG	CD-NE	-5.14	1.37	1.46
1	A	271	GLU	CD-OE2	5.13	1.31	1.25
1	B	464	GLU	CD-OE2	5.11	1.31	1.25
1	B	39	GLU	CG-CD	5.07	1.59	1.51
1	A	479	PHE	CG-CD2	-5.04	1.31	1.38
1	B	606	GLU	CG-CD	5.02	1.59	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	823	ARG	NE-CZ-NH2	-17.16	111.72	120.30
1	A	823	ARG	NE-CZ-NH2	-17.04	111.78	120.30
1	B	469	ARG	NE-CZ-NH1	13.52	127.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	B	823	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	A	823	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	861	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	102	ASP	CB-CG-OD1	8.17	125.66	118.30
1	A	102	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	46	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	439	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	45	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	822	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	102	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	B	439	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	125	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	330	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	861	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	664	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	236	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	236	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	829	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	308	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	861	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	239	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	102	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	708	LYS	CD-CE-NZ	-5.72	98.54	111.70
1	A	664	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	794	ASN	N-CA-C	5.69	126.37	111.00
1	A	829	ASP	CB-CG-OD1	5.61	123.34	118.30
1	B	362	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	45	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	801	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	46	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	469	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	708	LYS	CD-CE-NZ	-5.22	99.69	111.70
1	B	93	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	239	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	308	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	160	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	B	422	LEU	CA-CB-CG	-5.05	103.67	115.30
1	A	330	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6576	0	6298	23	0
1	B	6513	0	6246	12	0
2	A	83	0	70	0	0
2	B	83	0	70	1	0
3	A	72	0	61	0	0
3	B	83	0	70	0	0
4	A	78	0	68	0	0
4	B	78	0	68	0	0
5	A	127	0	106	0	0
5	B	127	0	106	0	0
6	A	50	0	43	0	0
7	A	119	0	100	1	0
7	B	105	0	88	0	0
8	A	28	0	26	0	0
8	B	28	0	26	0	0
9	A	80	0	120	5	0
9	B	76	0	114	1	0
10	A	15	0	15	0	0
10	B	20	0	20	0	0
11	B	61	0	52	0	0
12	A	812	0	0	5	0
12	B	715	0	0	3	0
All	All	15929	0	13767	36	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.

All (36) 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:641[A]:ARG:NE	1:A:643[A]:GLU:OE2	1.69	1.25
1:A:641[A]:ARG:NH2	1:A:643[A]:GLU:OE2	1.77	1.18
1:A:641[A]:ARG:CZ	1:A:643[A]:GLU:OE2	1.95	1.12
1:A:843:LYS:NZ	1:A:856[B]:ARG:HH22	1.76	0.83
1:A:641[A]:ARG:HE	1:A:643[A]:GLU:CD	1.87	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:CYS:HG	1:A:441:CYS:HG	0.96	0.74
1:A:349[B]:ARG:HD3	12:A:2314:HOH:O	1.91	0.71
1:A:843:LYS:HZ1	1:A:856[B]:ARG:HH22	1.37	0.71
1:A:843:LYS:NZ	1:A:856[B]:ARG:NH2	2.49	0.58
1:B:643[B]:GLU:HG3	12:B:2512:HOH:O	2.05	0.56
1:A:178:LYS:HE2	12:A:2245:HOH:O	2.11	0.51
1:B:794[A]:ASN:HB3	12:B:2621:HOH:O	2.11	0.51
1:A:436:CYS:HG	1:A:441:CYS:CB	2.23	0.50
1:A:641[A]:ARG:HH21	1:A:643[A]:GLU:CD	2.10	0.49
1:B:313:TRP:CH2	1:B:334[B]:MET:HE3	2.48	0.48
1:A:843:LYS:HZ2	1:A:856[B]:ARG:HH22	1.57	0.48
9:A:1866:EDO:H22	12:A:2805:HOH:O	2.15	0.47
1:A:306:PHE:CZ	9:A:1882:EDO:H21	2.51	0.45
1:B:588:TYR:CD2	9:B:1881:EDO:H22	2.53	0.43
1:B:313:TRP:CH2	1:B:334[B]:MET:CE	3.01	0.43
9:A:1866:EDO:H12	1:B:469:ARG:HB2	2.01	0.43
1:A:786:LEU:HD23	1:A:786:LEU:C	2.38	0.43
1:A:516:ASP:CB	7:A:1502[A]:NAG:H82	2.49	0.43
1:A:843:LYS:HZ1	1:A:856[B]:ARG:NH2	2.10	0.43
1:A:823:ARG:HD3	12:A:2719:HOH:O	2.19	0.42
1:B:159:TRP:CE2	1:B:449:ALA:HB3	2.55	0.42
1:A:469[B]:ARG:HB2	9:A:1866:EDO:H21	2.02	0.41
1:B:823:ARG:HD3	12:B:2644:HOH:O	2.20	0.41
1:A:68:TRP:CD1	1:A:69:GLU:HG3	2.56	0.41
1:B:96:LEU:C	1:B:96:LEU:HD12	2.41	0.41
1:A:469[A]:ARG:HB2	9:A:1866:EDO:H21	2.02	0.41
1:A:46:ARG:NH1	12:A:2049:HOH:O	2.47	0.41
1:A:96:LEU:C	1:A:96:LEU:HD12	2.41	0.41
1:B:68:TRP:CD1	1:B:69:GLU:HG3	2.56	0.41
1:B:421:VAL:C	1:B:422:LEU:HG	2.40	0.40
1:B:709:PHE:CZ	2:B:1002:NAG:H82	2.55	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	852/844 (101%)	828 (97%)	24 (3%)	0	100	100
1	B	846/844 (100%)	825 (98%)	21 (2%)	0	100	100
All	All	1698/1688 (101%)	1653 (97%)	45 (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	698/686 (102%)	689 (99%)	9 (1%)	73	69
1	B	692/686 (101%)	687 (99%)	5 (1%)	87	86
All	All	1390/1372 (101%)	1376 (99%)	14 (1%)	80	78

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

Mol	Chain	Res	Type
1	A	21	GLU
1	A	90	CYS
1	A	282	TRP
1	A	422	LEU
1	A	703	LEU
1	A	704	LYS
1	A	830	VAL
1	A	856[A]	ARG
1	A	856[B]	ARG
1	B	90	CYS
1	B	282	TRP
1	B	422	LEU
1	B	703	LEU
1	B	704	LYS



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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

89 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	0.47	0	15,19,21	0.41	0
2	NAG	A	1002	2	14,14,15	0.43	0	15,19,21	0.63	0
2	BMA	A	1003	2	11,11,12	0.29	0	13,15,17	0.56	0
2	MAN	A	1004	2	11,11,12	0.25	0	13,15,17	0.41	0
2	MAN	A	1005	2	11,11,12	0.26	0	13,15,17	0.53	0
2	MAN	A	1006	2	11,11,12	0.48	0	13,15,17	0.76	1 (7%)
2	MAN	A	1007	2	11,11,12	0.28	0	13,15,17	0.46	0
3	NAG	A	1101	1,3	14,14,15	0.60	0	15,19,21	0.61	0
3	NAG	A	1102	3	14,14,15	0.68	0	15,19,21	1.18	1 (6%)
3	BMA	A	1103	3	11,11,12	0.21	0	13,15,17	0.51	0
3	MAN	A	1104	3	11,11,12	0.27	0	13,15,17	0.64	0
3	MAN	A	1105	3	11,11,12	0.27	0	13,15,17	0.57	0
3	MAN	A	1106	3	11,11,12	0.23	0	13,15,17	0.45	0
4	NAG	A	1201	1,4	14,14,15	0.50	0	15,19,21	0.56	0
4	NAG	A	1202	4	14,14,15	0.56	0	15,19,21	0.64	0
4	BMA	A	1203	4	11,11,12	0.33	0	13,15,17	0.50	0
5	NAG	A	1301	1,5	14,14,15	0.85	1 (7%)	15,19,21	0.65	0
5	NAG	A	1302	5	14,14,15	0.96	1 (7%)	15,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	A	1303	5	11,11,12	0.16	0	13,15,17	0.50	0
5	MAN	A	1304	5	11,11,12	0.22	0	13,15,17	0.40	0
5	MAN	A	1305	5	11,11,12	0.39	0	13,15,17	0.80	1 (7%)
5	MAN	A	1306	5	11,11,12	0.32	0	13,15,17	0.58	0
5	MAN	A	1307	5	11,11,12	0.29	0	13,15,17	0.55	0
5	MAN	A	1308	5	11,11,12	0.37	0	13,15,17	0.78	0
5	MAN	A	1309	5	11,11,12	0.27	0	13,15,17	0.36	0
5	MAN	A	1310	5	11,11,12	0.39	0	13,15,17	0.78	0
5	MAN	A	1311	5	11,11,12	0.42	0	13,15,17	0.69	0
6	NAG	A	1401	1,6	14,14,15	0.61	0	15,19,21	0.54	0
6	NAG	A	1402	6	14,14,15	0.53	0	15,19,21	0.60	0
6	BMA	A	1403	6	11,11,12	0.31	0	13,15,17	0.51	0
6	MAN	A	1404	6	11,11,12	0.29	0	13,15,17	0.47	0
7	NAG	A	1501	1,7	14,14,15	0.54	0	15,19,21	0.69	0
7	NAG	A	1502[A]	7	14,14,15	0.51	0	15,19,21	0.79	1 (6%)
7	NAG	A	1502[B]	7	14,14,15	0.48	0	15,19,21	0.63	0
7	BMA	A	1503	7	11,11,12	0.21	0	13,15,17	0.46	0
7	MAN	A	1504	7	11,11,12	0.27	0	13,15,17	0.48	0
7	MAN	A	1505	7	11,11,12	0.24	0	13,15,17	0.51	0
7	MAN	A	1506	7	11,11,12	0.28	0	13,15,17	0.43	0
7	MAN	A	1507	7	11,11,12	0.42	0	13,15,17	0.75	1 (7%)
7	MAN	A	1508	7	11,11,12	0.35	0	13,15,17	0.34	0
7	MAN	A	1509	7	11,11,12	0.35	0	13,15,17	0.70	1 (7%)
4	NAG	A	1701	1,4	14,14,15	0.35	0	15,19,21	0.41	0
4	NAG	A	1702	4	14,14,15	0.52	0	15,19,21	0.45	0
4	BMA	A	1703	4	11,11,12	0.35	0	13,15,17	0.39	0
2	NAG	B	1001	1,2	14,14,15	0.44	0	15,19,21	0.64	0
2	NAG	B	1002	2	14,14,15	0.50	0	15,19,21	0.38	0
2	BMA	B	1003	2	11,11,12	0.28	0	13,15,17	0.57	0
2	MAN	B	1004	2	11,11,12	0.38	0	13,15,17	0.59	0
2	MAN	B	1006	2	11,11,12	0.26	0	13,15,17	0.50	0
2	MAN	B	1007	2	11,11,12	0.39	0	13,15,17	0.74	1 (7%)
2	MAN	B	1008	2	11,11,12	0.29	0	13,15,17	0.56	0
3	NAG	B	1101	1,3	14,14,15	0.45	0	15,19,21	0.62	0
3	NAG	B	1102	3	14,14,15	0.89	1 (7%)	15,19,21	1.18	1 (6%)
3	BMA	B	1103[A]	3	11,11,12	0.26	0	13,15,17	0.53	0
3	BMA	B	1103[B]	3	11,11,12	0.23	0	13,15,17	0.45	0
3	MAN	B	1104	3	11,11,12	0.32	0	13,15,17	0.59	0
3	MAN	B	1105	3	11,11,12	0.28	0	13,15,17	0.71	1 (7%)
3	MAN	B	1106	3	11,11,12	0.23	0	13,15,17	0.44	0
4	NAG	B	1201	1,4	14,14,15	0.72	1 (7%)	15,19,21	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1202	4	14,14,15	0.58	0	15,19,21	0.52	0
4	BMA	B	1203	4	11,11,12	0.30	0	13,15,17	0.42	0
5	NAG	B	1301	1,5	14,14,15	0.39	0	15,19,21	0.51	0
5	NAG	B	1302	5	14,14,15	1.03	1 (7%)	15,19,21	0.64	0
5	BMA	B	1303	5	11,11,12	0.19	0	13,15,17	0.45	0
5	MAN	B	1304	5	11,11,12	0.26	0	13,15,17	0.54	0
5	MAN	B	1305	5	11,11,12	0.47	0	13,15,17	0.72	0
5	MAN	B	1306	5	11,11,12	0.31	0	13,15,17	0.67	1 (7%)
5	MAN	B	1307	5	11,11,12	0.22	0	13,15,17	0.49	0
5	MAN	B	1308	5	11,11,12	0.37	0	13,15,17	0.75	0
5	MAN	B	1309	5	11,11,12	0.27	0	13,15,17	0.35	0
5	MAN	B	1310	5	11,11,12	0.38	0	13,15,17	0.65	0
5	MAN	B	1311	5	11,11,12	0.38	0	13,15,17	0.77	1 (7%)
11	NAG	B	1401	1,11	14,14,15	0.64	0	15,19,21	0.45	0
11	NAG	B	1402	11	14,14,15	0.42	0	15,19,21	0.60	0
11	BMA	B	1403	11	11,11,12	0.24	0	13,15,17	0.39	0
11	MAN	B	1404	11	11,11,12	0.32	0	13,15,17	0.68	1 (7%)
11	MAN	B	1405	11	11,11,12	0.25	0	13,15,17	0.48	0
7	NAG	B	1501	1,7	14,14,15	0.61	0	15,19,21	0.60	0
7	NAG	B	1502	7	14,14,15	0.58	0	15,19,21	0.71	1 (6%)
7	BMA	B	1503	7	11,11,12	0.31	0	13,15,17	0.47	0
7	MAN	B	1504	7	11,11,12	0.24	0	13,15,17	0.46	0
7	MAN	B	1505	7	11,11,12	0.28	0	13,15,17	0.53	0
7	MAN	B	1506	7	11,11,12	0.22	0	13,15,17	0.41	0
7	MAN	B	1507	7	11,11,12	0.34	0	13,15,17	0.68	0
7	MAN	B	1509	7	11,11,12	0.32	0	13,15,17	0.39	0
7	MAN	B	1510	7	11,11,12	0.38	0	13,15,17	0.74	1 (7%)
4	NAG	B	1701	1,4	14,14,15	0.57	0	15,19,21	0.57	0
4	NAG	B	1702	4	14,14,15	0.80	1 (7%)	15,19,21	0.84	1 (6%)
4	BMA	B	1703	4	11,11,12	0.30	0	13,15,17	0.33	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
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	1005	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1006	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1007	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	1104	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1105	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1106	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1202	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1203	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1303	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1304	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1305	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1306	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1307	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1308	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1309	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1310	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1311	5	-	0/2/19/22	0/1/1/1
6	NAG	A	1401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1402	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1403	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1404	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1502[A]	7	-	0/6/23/26	0/1/1/1
7	NAG	A	1502[B]	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1503	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1504	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1505	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1506	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1507	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1508	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1509	7	-	0/2/19/22	0/1/1/1
4	NAG	A	1701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1702	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1703	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	B	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1004	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1006	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1007	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1008	2	-	0/2/19/22	0/1/1/1
3	NAG	B	1101	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1102	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1103[A]	3	-	0/2/19/22	0/1/1/1
3	BMA	B	1103[B]	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1104	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1105	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1106	3	-	0/2/19/22	0/1/1/1
4	NAG	B	1201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1202	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1203	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1303	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1304	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1305	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1306	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1307	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1308	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1309	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1310	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1311	5	-	0/2/19/22	0/1/1/1
11	NAG	B	1401	1,11	-	0/6/23/26	0/1/1/1
11	NAG	B	1402	11	-	0/6/23/26	0/1/1/1
11	BMA	B	1403	11	-	0/2/19/22	0/1/1/1
11	MAN	B	1404	11	-	0/2/19/22	0/1/1/1
11	MAN	B	1405	11	-	0/2/19/22	0/1/1/1
7	NAG	B	1501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1502	7	-	0/6/23/26	0/1/1/1
7	BMA	B	1503	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1504	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1505	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1506	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1507	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1509	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1510	7	-	0/2/19/22	0/1/1/1
4	NAG	B	1701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1702	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	B	1703	4	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	NAG	C1-C2	-2.77	1.48	1.52
4	B	1201	NAG	C1-C2	-2.11	1.49	1.52
4	B	1702	NAG	C1-C2	2.41	1.55	1.52
5	A	1301	NAG	C1-C2	2.73	1.56	1.52
5	A	1302	NAG	C1-C2	3.02	1.56	1.52
5	B	1302	NAG	C1-C2	3.19	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	NAG	O5-C1-C2	-3.96	105.96	111.47
3	A	1102	NAG	O5-C1-C2	-3.93	106.01	111.47
7	A	1502[A]	NAG	O5-C1-C2	-2.40	108.14	111.47
4	B	1201	NAG	O5-C1-C2	-2.17	108.45	111.47
7	B	1502	NAG	O5-C1-C2	-2.04	108.63	111.47
7	A	1507	MAN	C1-O5-C5	2.02	114.95	112.17
2	A	1006	MAN	C1-O5-C5	2.03	114.97	112.17
7	A	1509	MAN	C1-O5-C5	2.11	115.08	112.17
11	B	1404	MAN	C1-O5-C5	2.12	115.09	112.17
7	B	1510	MAN	C1-O5-C5	2.12	115.09	112.17
2	B	1007	MAN	C1-O5-C5	2.14	115.12	112.17
5	B	1306	MAN	C1-O5-C5	2.19	115.18	112.17
3	B	1105	MAN	C1-O5-C5	2.20	115.19	112.17
5	A	1305	MAN	C1-O5-C5	2.26	115.28	112.17
4	B	1702	NAG	O5-C1-C2	2.30	114.67	111.47
5	B	1311	MAN	C1-O5-C5	2.35	115.41	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1502[A]	NAG	1	0
2	B	1002	NAG	1	0

## 5.6 Ligand geometry

50 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
8	NAG	A	1601	1	14,14,15	0.48	0	15,19,21	0.70	1 (6%)
8	NAG	A	1801	1	14,14,15	0.79	1 (7%)	15,19,21	0.50	0
9	EDO	A	1864	-	3,3,3	0.91	0	2,2,2	0.11	0
9	EDO	A	1865	-	3,3,3	0.72	0	2,2,2	0.31	0
9	EDO	A	1866	-	3,3,3	1.01	0	2,2,2	1.65	0
9	EDO	A	1867	-	3,3,3	0.77	0	2,2,2	0.11	0
9	EDO	A	1868	-	3,3,3	0.83	0	2,2,2	0.90	0
9	EDO	A	1869	-	3,3,3	0.35	0	2,2,2	0.38	0
9	EDO	A	1870	-	3,3,3	0.41	0	2,2,2	0.15	0
9	EDO	A	1871	-	3,3,3	0.57	0	2,2,2	0.15	0
9	EDO	A	1872	-	3,3,3	0.72	0	2,2,2	0.34	0
9	EDO	A	1873	-	3,3,3	0.46	0	2,2,2	0.49	0
9	EDO	A	1874	-	3,3,3	0.29	0	2,2,2	0.43	0
9	EDO	A	1875	-	3,3,3	0.62	0	2,2,2	0.27	0
9	EDO	A	1876	-	3,3,3	0.88	0	2,2,2	0.67	0
9	EDO	A	1877	-	3,3,3	0.46	0	2,2,2	0.22	0
9	EDO	A	1878	-	3,3,3	0.39	0	2,2,2	0.65	0
9	EDO	A	1879	-	3,3,3	0.38	0	2,2,2	1.08	0
9	EDO	A	1880	-	3,3,3	0.49	0	2,2,2	0.28	0
9	EDO	A	1881	-	3,3,3	0.37	0	2,2,2	0.46	0
9	EDO	A	1882	-	3,3,3	0.16	0	2,2,2	0.88	0
10	IMD	A	1883	-	3,5,5	0.58	0	4,5,5	0.51	0
10	IMD	A	1884	-	3,5,5	0.36	0	4,5,5	0.45	0
10	IMD	A	1885	-	3,5,5	0.53	0	4,5,5	0.62	0
9	EDO	A	1900	-	3,3,3	0.46	0	2,2,2	0.32	0
8	NAG	B	1601	1	14,14,15	1.22	1 (7%)	15,19,21	1.49	1 (6%)
8	NAG	B	1801	1	14,14,15	0.41	0	15,19,21	0.55	0
9	EDO	B	1864	-	3,3,3	0.56	0	2,2,2	0.29	0
9	EDO	B	1865	-	3,3,3	0.96	0	2,2,2	0.24	0
9	EDO	B	1866	-	3,3,3	0.46	0	2,2,2	0.53	0
9	EDO	B	1867	-	3,3,3	0.77	0	2,2,2	0.24	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EDO	B	1868	-	3,3,3	0.59	0	2,2,2	0.43	0
9	EDO	B	1869	-	3,3,3	0.64	0	2,2,2	0.22	0
9	EDO	B	1870	-	3,3,3	0.74	0	2,2,2	0.17	0
9	EDO	B	1871	-	3,3,3	0.28	0	2,2,2	0.53	0
9	EDO	B	1872	-	3,3,3	0.32	0	2,2,2	0.88	0
9	EDO	B	1873	-	3,3,3	0.31	0	2,2,2	0.65	0
9	EDO	B	1874	-	3,3,3	0.30	0	2,2,2	0.26	0
9	EDO	B	1875	-	3,3,3	0.43	0	2,2,2	0.48	0
9	EDO	B	1876	-	3,3,3	0.47	0	2,2,2	0.64	0
9	EDO	B	1877	-	3,3,3	0.45	0	2,2,2	0.09	0
9	EDO	B	1878	-	3,3,3	0.22	0	2,2,2	0.67	0
9	EDO	B	1879	-	3,3,3	0.73	0	2,2,2	0.20	0
9	EDO	B	1880	-	3,3,3	0.53	0	2,2,2	0.38	0
9	EDO	B	1881	-	3,3,3	0.65	0	2,2,2	0.89	0
10	IMD	B	1882	-	3,5,5	0.34	0	4,5,5	0.89	0
10	IMD	B	1883	-	3,5,5	0.41	0	4,5,5	0.72	0
10	IMD	B	1884	-	3,5,5	0.54	0	4,5,5	0.54	0
10	IMD	B	1885	-	3,5,5	0.57	0	4,5,5	0.58	0
9	EDO	B	1900	-	3,3,3	0.49	0	2,2,2	0.32	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
8	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1801	1	-	0/6/23/26	0/1/1/1
9	EDO	A	1864	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1865	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1866	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1867	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1868	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1869	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1870	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1871	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1872	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1873	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1874	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1875	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1876	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1877	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1878	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1879	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1880	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1881	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1882	-	-	0/1/1/1	0/0/0/0
10	IMD	A	1883	-	-	0/0/0/0	0/1/1/1
10	IMD	A	1884	-	-	0/0/0/0	0/1/1/1
10	IMD	A	1885	-	-	0/0/0/0	0/1/1/1
9	EDO	A	1900	-	-	0/1/1/1	0/0/0/0
8	NAG	B	1601	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1801	1	-	0/6/23/26	0/1/1/1
9	EDO	B	1864	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1865	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1866	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1867	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1868	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1869	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1870	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1871	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1872	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1873	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1874	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1875	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1876	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1877	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1878	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1879	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1880	-	-	0/1/1/1	0/0/0/0
9	EDO	B	1881	-	-	0/1/1/1	0/0/0/0
10	IMD	B	1882	-	-	0/0/0/0	0/1/1/1
10	IMD	B	1883	-	-	0/0/0/0	0/1/1/1
10	IMD	B	1884	-	-	0/0/0/0	0/1/1/1
10	IMD	B	1885	-	-	0/0/0/0	0/1/1/1
9	EDO	B	1900	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1801	NAG	C1-C2	2.60	1.56	1.52
8	B	1601	NAG	C1-C2	4.30	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	A	1601	NAG	O5-C1-C2	2.15	114.47	111.47
8	B	1601	NAG	O5-C1-C2	5.35	118.92	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1866	EDO	4	0
9	A	1882	EDO	1	0
9	B	1881	EDO	1	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	840/844 (99%)	-0.32	4 (0%)	90 94	12, 19, 32, 44	14 (1%)
1	B	840/844 (99%)	-0.33	3 (0%)	92 95	12, 20, 35, 46	16 (1%)
All	All	1680/1688 (99%)	-0.33	7 (0%)	92 95	12, 20, 34, 46	30 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	670	SER	3.5
1	A	21	GLU	3.3
1	B	677	PRO	2.5
1	B	619	GLY	2.5
1	A	676	VAL	2.2
1	B	676	VAL	2.2
1	A	669	ASN	2.1

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MAN	B	1510	11/12	0.94	0.17	6.20	22,27,35,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	1401	14/15	0.96	0.13	4.13	22,24,26,26	0
7	MAN	A	1509	11/12	0.94	0.11	2.35	24,29,36,44	0
5	MAN	B	1311	11/12	0.95	0.11	2.08	25,27,30,32	0
11	NAG	B	1401	14/15	0.96	0.11	2.01	22,24,28,28	0
4	NAG	B	1701	14/15	0.96	0.09	1.68	24,29,35,36	0
7	NAG	B	1502	14/15	0.96	0.11	1.54	22,24,27,33	0
5	MAN	A	1311	11/12	0.94	0.12	1.53	20,22,23,23	0
4	NAG	A	1701	14/15	0.95	0.08	1.44	24,28,32,35	0
5	MAN	B	1310	11/12	0.95	0.11	1.37	23,25,27,29	0
3	NAG	B	1101	14/15	0.95	0.10	1.30	21,23,27,28	0
4	NAG	B	1202	14/15	0.92	0.13	0.98	34,38,41,51	0
4	NAG	A	1201	14/15	0.97	0.14	0.86	16,18,20,23	0
7	NAG	A	1502[A]	14/15	0.98	0.12	0.77	20,21,24,26	14
7	NAG	A	1502[B]	14/15	0.98	0.12	0.77	20,21,23,26	14
5	NAG	A	1302	14/15	0.97	0.11	0.53	17,18,20,21	0
2	NAG	B	1002	14/15	0.96	0.12	0.49	22,25,31,33	0
3	NAG	A	1101	14/15	0.96	0.09	0.35	21,22,23,24	0
5	MAN	A	1310	11/12	0.95	0.11	0.31	17,19,21,21	0
4	NAG	A	1202	14/15	0.95	0.14	0.26	27,30,33,43	0
5	NAG	B	1302	14/15	0.96	0.10	0.06	25,26,29,30	0
2	NAG	B	1001	14/15	0.96	0.09	-0.09	18,20,28,29	0
2	NAG	A	1001	14/15	0.98	0.08	-0.22	17,18,24,25	0
5	NAG	A	1301	14/15	0.97	0.10	-0.25	17,19,21,22	0
3	NAG	B	1102	14/15	0.96	0.09	-0.36	21,24,27,27	0
5	NAG	B	1301	14/15	0.96	0.09	-0.58	24,28,30,31	0
2	NAG	A	1002	14/15	0.97	0.08	-0.68	19,21,26,29	0
7	NAG	B	1501	14/15	0.97	0.07	-0.69	19,22,27,27	0
4	NAG	B	1201	14/15	0.97	0.09	-0.73	22,26,28,29	0
7	NAG	A	1501	14/15	0.98	0.07	-1.06	17,19,25,26	0
3	NAG	A	1102	14/15	0.97	0.07	-1.09	22,25,28,29	0
2	BMA	A	1003	11/12	0.96	0.08	-	28,33,35,42	0
4	BMA	A	1703	11/12	0.83	0.22	-	58,61,66,72	0
3	MAN	B	1105	11/12	0.93	0.14	-	40,44,46,53	0
5	MAN	A	1305	11/12	0.92	0.22	-	32,41,50,53	0
7	MAN	A	1508	11/12	0.93	0.15	-	29,36,42,47	0
4	BMA	A	1203	11/12	0.77	0.32	-	56,62,70,80	0
2	BMA	B	1003	11/12	0.96	0.09	-	31,32,40,42	0
5	BMA	A	1303	11/12	0.97	0.11	-	19,20,22,25	0
5	MAN	A	1309	11/12	0.87	0.27	-	51,54,65,67	0
7	MAN	B	1509	11/12	0.92	0.17	-	27,33,42,45	0
3	MAN	B	1106	11/12	0.74	0.22	-	40,42,46,48	11
3	MAN	A	1106	11/12	0.75	0.20	-	47,48,49,51	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1702	14/15	0.85	0.16	-	40,45,51,56	0
2	MAN	A	1005	11/12	0.94	0.12	-	36,38,43,51	0
5	MAN	A	1307	11/12	0.97	0.11	-	19,20,21,23	0
6	BMA	A	1403	11/12	0.81	0.31	-	49,60,66,67	0
11	MAN	B	1404	11/12	0.88	0.24	-	55,59,63,64	0
2	MAN	A	1006	11/12	0.90	0.15	-	45,49,55,66	0
7	MAN	B	1507	11/12	0.87	0.21	-	48,52,56,56	0
2	MAN	B	1008	11/12	0.77	0.31	-	36,37,38,40	11
11	BMA	B	1403	11/12	0.79	0.23	-	50,59,71,73	0
7	MAN	B	1506	11/12	0.96	0.11	-	26,28,32,36	0
6	NAG	A	1402	14/15	0.96	0.14	-	22,26,35,40	0
5	MAN	A	1308	11/12	0.96	0.13	-	27,29,37,39	0
6	MAN	A	1404	11/12	0.73	0.27	-	60,63,69,76	0
3	MAN	B	1104	11/12	0.95	0.09	-	29,32,33,38	0
5	BMA	B	1303	11/12	0.96	0.11	-	26,28,34,36	0
7	MAN	B	1505	11/12	0.86	0.27	-	57,65,70,71	0
4	NAG	B	1702	14/15	0.91	0.17	-	42,48,53,53	0
7	MAN	A	1507	11/12	0.79	0.24	-	48,53,58,59	0
7	MAN	A	1505	11/12	0.78	0.24	-	49,55,59,62	11
2	MAN	A	1004	11/12	0.85	0.13	-	49,57,63,66	0
11	NAG	B	1402	14/15	0.96	0.14	-	23,29,35,43	0
5	MAN	B	1306	11/12	0.90	0.19	-	51,55,60,70	0
2	MAN	B	1004	11/12	0.87	0.11	-	45,52,56,57	0
2	MAN	A	1007	11/12	0.75	0.17	-	45,50,54,55	11
3	BMA	B	1103[A]	11/12	0.95	0.10	-	27,28,30,30	11
5	MAN	B	1307	11/12	0.98	0.07	-	25,26,27,28	0
7	MAN	B	1504	11/12	0.93	0.18	-	42,46,56,60	0
7	BMA	B	1503	11/12	0.96	0.10	-	24,25,30,39	0
5	MAN	B	1305	11/12	0.90	0.19	-	47,53,57,63	0
5	MAN	B	1304	11/12	0.89	0.12	-	38,39,43,45	0
2	MAN	B	1006	11/12	0.93	0.12	-	32,37,43,52	0
4	BMA	B	1203	11/12	0.76	0.25	-	56,64,71,76	0
5	MAN	A	1306	11/12	0.92	0.17	-	37,39,43,49	0
7	MAN	A	1506	11/12	0.94	0.09	-	27,30,34,39	0
5	MAN	A	1304	11/12	0.96	0.14	-	27,32,37,38	0
3	MAN	A	1105	11/12	0.93	0.16	-	45,47,48,53	0
3	BMA	B	1103[B]	11/12	0.95	0.10	-	26,28,29,31	11
5	MAN	B	1308	11/12	0.97	0.12	-	30,34,38,42	0
2	MAN	B	1007	11/12	0.90	0.15	-	38,41,48,57	0
5	MAN	B	1309	11/12	0.88	0.25	-	51,54,59,61	0
4	BMA	B	1703	11/12	0.75	0.32	-	57,64,69,78	0
3	MAN	A	1104	11/12	0.95	0.10	-	30,32,35,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	A	1103	11/12	0.96	0.09	-	26,30,37,47	0
11	MAN	B	1405	11/12	0.87	0.21	-	45,50,52,54	11
7	BMA	A	1503	11/12	0.97	0.08	-	23,25,28,32	0
7	MAN	A	1504	11/12	0.92	0.16	-	40,46,53,54	0

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	EDO	A	1868	4/4	0.86	0.22	15.46	21,35,35,42	0
9	EDO	B	1879	4/4	0.70	0.31	13.16	46,50,54,63	0
9	EDO	A	1881	4/4	0.94	0.20	12.85	31,31,32,33	0
9	EDO	B	1864	4/4	0.96	0.26	11.81	39,43,43,44	0
9	EDO	A	1874	4/4	0.96	0.17	11.33	36,38,38,39	0
9	EDO	B	1870	4/4	0.89	0.14	10.40	37,39,42,43	0
9	EDO	B	1868	4/4	0.92	0.16	8.96	36,37,37,40	0
9	EDO	A	1865	4/4	0.72	0.24	7.64	34,38,38,41	4
9	EDO	B	1873	4/4	0.88	0.31	7.46	28,29,29,30	4
10	IMD	B	1883	5/5	0.93	0.13	6.17	37,39,39,41	0
10	IMD	B	1882	5/5	0.91	0.17	6.09	39,39,42,43	5
9	EDO	A	1880	4/4	0.87	0.25	5.96	64,64,67,68	0
9	EDO	B	1881	4/4	0.79	0.21	5.93	42,44,47,47	0
9	EDO	B	1872	4/4	0.93	0.16	5.78	34,36,39,41	0
9	EDO	A	1872	4/4	0.82	0.16	5.34	36,39,42,44	0
9	EDO	A	1875	4/4	0.90	0.14	5.20	35,45,46,52	0
9	EDO	A	1871	4/4	0.91	0.13	4.85	30,36,39,43	0
9	EDO	B	1877	4/4	0.90	0.18	4.72	49,56,57,58	0
9	EDO	B	1871	4/4	0.95	0.13	4.57	32,32,33,34	0
8	NAG	B	1801	14/15	0.79	0.25	4.46	52,62,64,66	0
9	EDO	A	1877	4/4	0.88	0.22	4.31	50,51,53,61	0
8	NAG	A	1801	14/15	0.78	0.31	3.98	48,54,59,59	0
9	EDO	A	1870	4/4	0.97	0.17	3.84	27,30,34,34	0
10	IMD	A	1884	5/5	0.91	0.13	3.70	33,33,36,37	0
9	EDO	A	1878	4/4	0.91	0.19	3.44	42,48,49,50	0
10	IMD	B	1884	5/5	0.88	0.19	3.35	47,47,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	EDO	B	1876	4/4	0.92	0.18	2.37	45,46,51,51	0
9	EDO	A	1876	4/4	0.78	0.19	2.18	37,42,45,48	0
9	EDO	B	1867	4/4	0.97	0.12	2.16	24,30,31,34	0
9	EDO	B	1875	4/4	0.96	0.19	2.00	25,29,31,36	0
9	EDO	B	1869	4/4	0.96	0.11	1.50	23,23,26,27	0
9	EDO	A	1879	4/4	0.96	0.14	1.06	31,33,36,42	0
9	EDO	A	1882	4/4	0.87	0.15	0.99	21,21,22,23	4
9	EDO	A	1869	4/4	0.95	0.09	0.64	36,37,39,40	0
9	EDO	A	1867	4/4	0.96	0.11	0.55	20,22,24,25	0
9	EDO	B	1874	4/4	0.94	0.10	0.13	35,35,36,39	0
9	EDO	B	1866	4/4	0.94	0.10	-0.48	26,32,32,32	0
9	EDO	A	1866	4/4	0.94	0.10	-0.74	27,28,28,29	0
9	EDO	A	1864	4/4	0.91	0.10	-	32,33,33,35	0
10	IMD	A	1883	5/5	0.89	0.39	-	40,41,42,43	5
10	IMD	B	1885	5/5	0.88	0.20	-	52,56,59,60	0
9	EDO	B	1900	4/4	0.47	0.17	-	55,56,56,60	4
8	NAG	B	1601	14/15	0.77	0.21	-	49,62,67,74	0
9	EDO	A	1873	4/4	0.85	0.17	-	50,50,52,55	0
9	EDO	B	1878	4/4	0.91	0.19	-	52,53,54,59	0
9	EDO	B	1880	4/4	0.87	0.21	-	33,34,44,49	0
10	IMD	A	1885	5/5	0.88	0.23	-	44,45,46,46	0
9	EDO	B	1865	4/4	0.90	0.13	-	27,28,30,31	0
8	NAG	A	1601	14/15	0.77	0.19	-	47,60,66,66	0
9	EDO	A	1900	4/4	0.74	0.20	-	60,60,61,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.