wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 11:08 PM GMT

PDB ID	:	5FJI
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

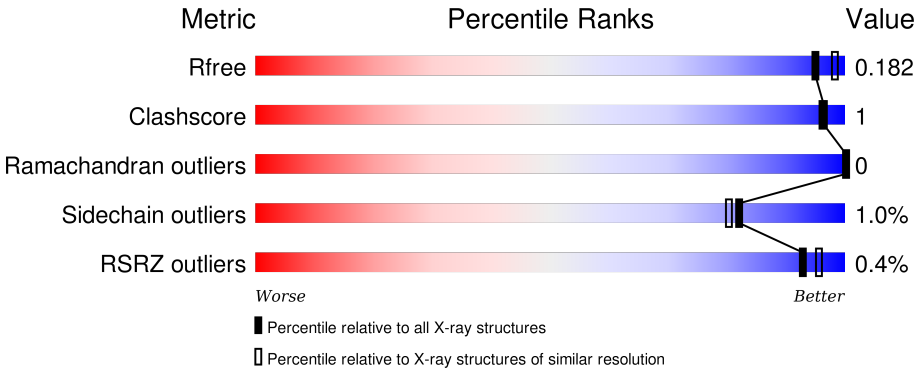
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 <=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

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		

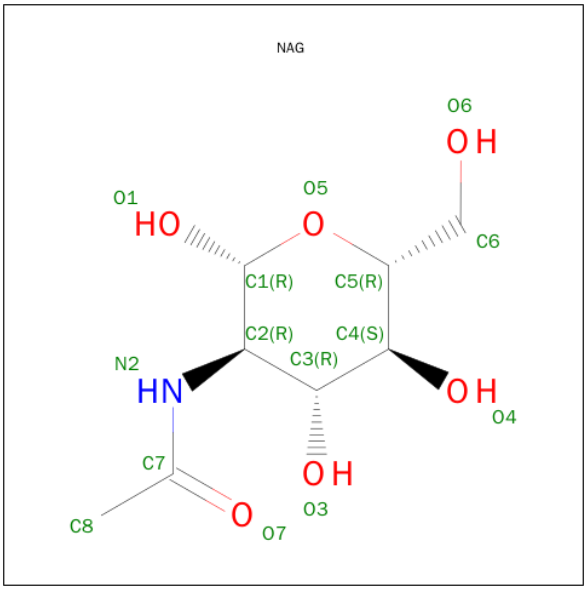
- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

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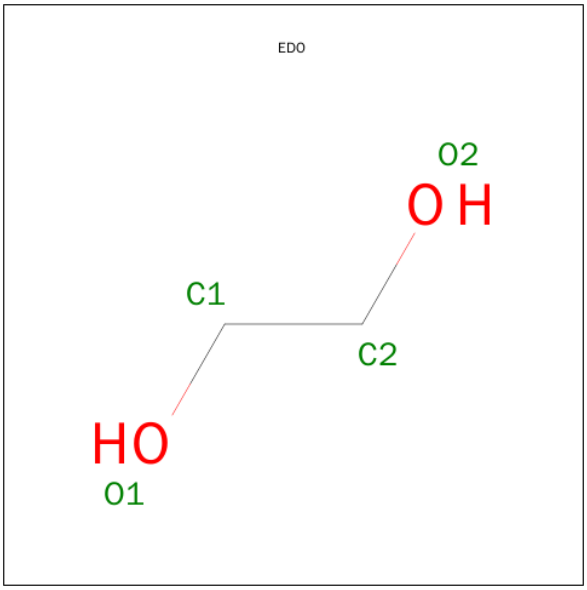
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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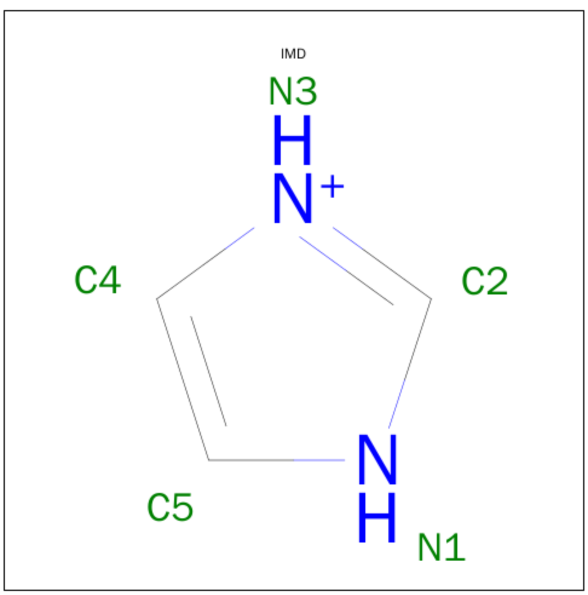
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

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

- 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 61 34 2 25	0	0

- Molecule 12 is water.

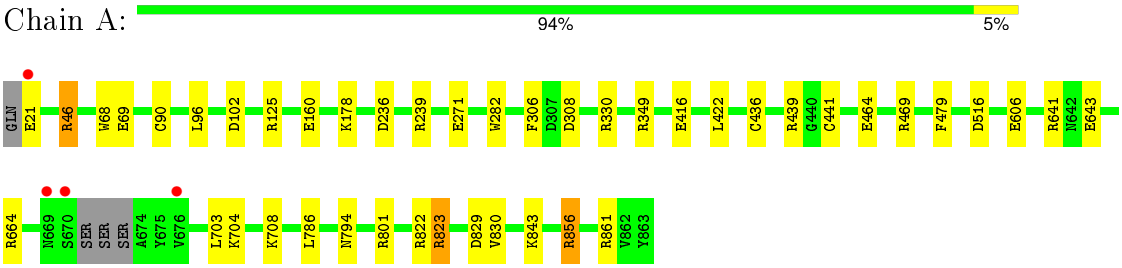
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	807	Total O 812 812	0	5
12	B	715	Total O 715 715	0	0

3 Residue-property plots (i)

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

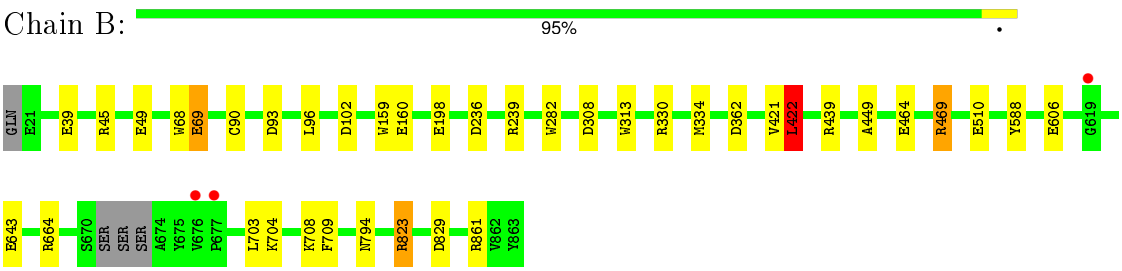
- Molecule 1: BETA-GLUCOSIDASE

Chain A:



- Molecule 1: BETA-GLUCOSIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	19.2	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 176660 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15929	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)

The worst 5 of 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

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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

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.

The worst 5 of 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

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	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 (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	698/686 (102%)	689 (99%)	9 (1%)	76	72
1	B	692/686 (101%)	687 (99%)	5 (1%)	88	88
All	All	1390/1372 (101%)	1376 (99%)	14 (1%)	82	80

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	830	VAL
1	A	856[A]	ARG
1	B	422	LEU
1	A	704	LYS
1	B	282	TRP

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	0.46	0	15,19,21	0.38	0
2	NAG	A	1002	2	14,14,15	0.42	0	15,19,21	0.39	0
2	BMA	A	1003	2	11,11,12	0.27	0	15,15,17	0.54	0
2	MAN	A	1004	2	11,11,12	0.24	0	15,15,17	0.41	0
2	MAN	A	1005	2	11,11,12	0.25	0	15,15,17	0.49	0
2	MAN	A	1006	2	11,11,12	0.46	0	15,15,17	0.71	0
2	MAN	A	1007	2	11,11,12	0.27	0	15,15,17	0.44	0
3	NAG	A	1101	1,3	14,14,15	0.59	0	15,19,21	0.33	0
3	NAG	A	1102	3	14,14,15	0.68	0	15,19,21	0.44	0
3	BMA	A	1103	3	11,11,12	0.20	0	15,15,17	0.51	0
3	MAN	A	1104	3	11,11,12	0.26	0	15,15,17	0.60	0
3	MAN	A	1105	3	11,11,12	0.26	0	15,15,17	0.54	0
3	MAN	A	1106	3	11,11,12	0.22	0	15,15,17	0.44	0
4	NAG	A	1201	1,4	14,14,15	0.50	0	15,19,21	0.51	0
4	NAG	A	1202	4	14,14,15	0.55	0	15,19,21	0.50	0
4	BMA	A	1203	4	11,11,12	0.31	0	15,15,17	0.48	0
5	NAG	A	1301	1,5	14,14,15	0.83	1 (7%)	15,19,21	0.38	0
5	NAG	A	1302	5	14,14,15	0.94	1 (7%)	15,19,21	0.61	0
5	BMA	A	1303	5	11,11,12	0.15	0	15,15,17	0.48	0
5	MAN	A	1304	5	11,11,12	0.21	0	15,15,17	0.40	0
5	MAN	A	1305	5	11,11,12	0.37	0	15,15,17	0.74	1 (6%)
5	MAN	A	1306	5	11,11,12	0.30	0	15,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	A	1307	5	11,11,12	0.28	0	15,15,17	0.52	0
5	MAN	A	1308	5	11,11,12	0.35	0	15,15,17	0.73	0
5	MAN	A	1309	5	11,11,12	0.27	0	15,15,17	0.37	0
5	MAN	A	1310	5	11,11,12	0.37	0	15,15,17	0.74	0
5	MAN	A	1311	5	11,11,12	0.41	0	15,15,17	0.66	0
6	NAG	A	1401	1,6	14,14,15	0.60	0	15,19,21	0.50	0
6	NAG	A	1402	6	14,14,15	0.52	0	15,19,21	0.35	0
6	BMA	A	1403	6	11,11,12	0.30	0	15,15,17	0.49	0
6	MAN	A	1404	6	11,11,12	0.28	0	15,15,17	0.44	0
7	NAG	A	1501	1,7	14,14,15	0.54	0	15,19,21	0.63	0
7	NAG	A	1502[A]	7	14,14,15	0.51	0	15,19,21	0.44	0
7	NAG	A	1502[B]	7	14,14,15	0.48	0	15,19,21	0.56	0
7	BMA	A	1503	7	11,11,12	0.20	0	15,15,17	0.49	0
7	MAN	A	1504	7	11,11,12	0.26	0	15,15,17	0.46	0
7	MAN	A	1505	7	11,11,12	0.23	0	15,15,17	0.49	0
7	MAN	A	1506	7	11,11,12	0.27	0	15,15,17	0.44	0
7	MAN	A	1507	7	11,11,12	0.40	0	15,15,17	0.70	0
7	MAN	A	1508	7	11,11,12	0.35	0	15,15,17	0.36	0
7	MAN	A	1509	7	11,11,12	0.34	0	15,15,17	0.64	0
4	NAG	A	1701	1,4	14,14,15	0.35	0	15,19,21	0.40	0
4	NAG	A	1702	4	14,14,15	0.52	0	15,19,21	0.48	0
4	BMA	A	1703	4	11,11,12	0.34	0	15,15,17	0.39	0
2	NAG	B	1001	1,2	14,14,15	0.43	0	15,19,21	0.53	0
2	NAG	B	1002	2	14,14,15	0.50	0	15,19,21	0.33	0
2	BMA	B	1003	2	11,11,12	0.27	0	15,15,17	0.56	0
2	MAN	B	1004	2	11,11,12	0.36	0	15,15,17	0.55	0
2	MAN	B	1006	2	11,11,12	0.26	0	15,15,17	0.49	0
2	MAN	B	1007	2	11,11,12	0.38	0	15,15,17	0.70	1 (6%)
2	MAN	B	1008	2	11,11,12	0.28	0	15,15,17	0.53	0
3	NAG	B	1101	1,3	14,14,15	0.44	0	15,19,21	0.34	0
3	NAG	B	1102	3	14,14,15	0.88	1 (7%)	15,19,21	0.44	0
3	BMA	B	1103[A]	3	11,11,12	0.25	0	15,15,17	0.51	0
3	BMA	B	1103[B]	3	11,11,12	0.22	0	15,15,17	0.45	0
3	MAN	B	1104	3	11,11,12	0.31	0	15,15,17	0.56	0
3	MAN	B	1105	3	11,11,12	0.27	0	15,15,17	0.65	1 (6%)
3	MAN	B	1106	3	11,11,12	0.22	0	15,15,17	0.43	0
4	NAG	B	1201	1,4	14,14,15	0.71	1 (7%)	15,19,21	0.55	0
4	NAG	B	1202	4	14,14,15	0.57	0	15,19,21	0.45	0
4	BMA	B	1203	4	11,11,12	0.29	0	15,15,17	0.41	0
5	NAG	B	1301	1,5	14,14,15	0.39	0	15,19,21	0.30	0
5	NAG	B	1302	5	14,14,15	1.01	1 (7%)	15,19,21	0.53	0
5	BMA	B	1303	5	11,11,12	0.18	0	15,15,17	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	B	1304	5	11,11,12	0.25	0	15,15,17	0.52	0
5	MAN	B	1305	5	11,11,12	0.45	0	15,15,17	0.67	0
5	MAN	B	1306	5	11,11,12	0.30	0	15,15,17	0.64	1 (6%)
5	MAN	B	1307	5	11,11,12	0.21	0	15,15,17	0.47	0
5	MAN	B	1308	5	11,11,12	0.36	0	15,15,17	0.70	0
5	MAN	B	1309	5	11,11,12	0.27	0	15,15,17	0.35	0
5	MAN	B	1310	5	11,11,12	0.37	0	15,15,17	0.63	0
5	MAN	B	1311	5	11,11,12	0.37	0	15,15,17	0.72	1 (6%)
11	NAG	B	1401	1,11	14,14,15	0.62	0	15,19,21	0.33	0
11	NAG	B	1402	11	14,14,15	0.42	0	15,19,21	0.49	0
11	BMA	B	1403	11	11,11,12	0.23	0	15,15,17	0.39	0
11	MAN	B	1404	11	11,11,12	0.31	0	15,15,17	0.63	1 (6%)
11	MAN	B	1405	11	11,11,12	0.24	0	15,15,17	0.46	0
7	NAG	B	1501	1,7	14,14,15	0.60	0	15,19,21	0.55	0
7	NAG	B	1502	7	14,14,15	0.57	0	15,19,21	0.43	0
7	BMA	B	1503	7	11,11,12	0.30	0	15,15,17	0.46	0
7	MAN	B	1504	7	11,11,12	0.23	0	15,15,17	0.45	0
7	MAN	B	1505	7	11,11,12	0.27	0	15,15,17	0.50	0
7	MAN	B	1506	7	11,11,12	0.21	0	15,15,17	0.42	0
7	MAN	B	1507	7	11,11,12	0.32	0	15,15,17	0.65	0
7	MAN	B	1509	7	11,11,12	0.32	0	15,15,17	0.40	0
7	MAN	B	1510	7	11,11,12	0.36	0	15,15,17	0.69	1 (6%)
4	NAG	B	1701	1,4	14,14,15	0.55	0	15,19,21	0.40	0
4	NAG	B	1702	4	14,14,15	0.79	1 (7%)	15,19,21	0.51	0
4	BMA	B	1703	4	11,11,12	0.29	0	15,15,17	0.35	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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

The worst 5 of 6 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	NAG	C1-C2	-2.72	1.48	1.52
4	B	1201	NAG	C1-C2	-2.08	1.49	1.52
4	B	1702	NAG	C1-C2	2.33	1.55	1.52
5	A	1301	NAG	C1-C2	2.64	1.56	1.52
5	A	1302	NAG	C1-C2	2.93	1.56	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1404	MAN	C1-O5-C5	2.00	115.09	112.14
7	B	1510	MAN	C1-O5-C5	2.01	115.09	112.14
2	B	1007	MAN	C1-O5-C5	2.03	115.12	112.14
5	B	1306	MAN	C1-O5-C5	2.07	115.18	112.14
3	B	1105	MAN	C1-O5-C5	2.08	115.19	112.14

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 (i)

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	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	1801	1	14,14,15	0.77	1 (7%)	15,19,21	0.31	0
9	EDO	A	1864	-	3,3,3	0.89	0	2,2,2	0.13	0
9	EDO	A	1865	-	3,3,3	0.71	0	2,2,2	0.33	0
9	EDO	A	1866	-	3,3,3	0.99	0	2,2,2	1.71	0
9	EDO	A	1867	-	3,3,3	0.75	0	2,2,2	0.10	0
9	EDO	A	1868	-	3,3,3	0.81	0	2,2,2	0.93	0
9	EDO	A	1869	-	3,3,3	0.35	0	2,2,2	0.42	0
9	EDO	A	1870	-	3,3,3	0.41	0	2,2,2	0.16	0
9	EDO	A	1871	-	3,3,3	0.56	0	2,2,2	0.16	0
9	EDO	A	1872	-	3,3,3	0.70	0	2,2,2	0.34	0
9	EDO	A	1873	-	3,3,3	0.46	0	2,2,2	0.52	0
9	EDO	A	1874	-	3,3,3	0.29	0	2,2,2	0.47	0
9	EDO	A	1875	-	3,3,3	0.61	0	2,2,2	0.26	0
9	EDO	A	1876	-	3,3,3	0.85	0	2,2,2	0.70	0
9	EDO	A	1877	-	3,3,3	0.46	0	2,2,2	0.24	0
9	EDO	A	1878	-	3,3,3	0.39	0	2,2,2	0.70	0
9	EDO	A	1879	-	3,3,3	0.38	0	2,2,2	1.16	0
9	EDO	A	1880	-	3,3,3	0.48	0	2,2,2	0.31	0
9	EDO	A	1881	-	3,3,3	0.37	0	2,2,2	0.50	0
9	EDO	A	1882	-	3,3,3	0.17	0	2,2,2	0.94	0
10	IMD	A	1883	-	3,5,5	0.56	0	4,5,5	0.60	0
10	IMD	A	1884	-	3,5,5	0.35	0	4,5,5	0.50	0
10	IMD	A	1885	-	3,5,5	0.51	0	4,5,5	0.64	0
9	EDO	A	1900	-	3,3,3	0.45	0	2,2,2	0.36	0
8	NAG	B	1601	1	14,14,15	1.18	1 (7%)	15,19,21	0.37	0
8	NAG	B	1801	1	14,14,15	0.40	0	15,19,21	0.39	0
9	EDO	B	1864	-	3,3,3	0.54	0	2,2,2	0.32	0
9	EDO	B	1865	-	3,3,3	0.94	0	2,2,2	0.27	0
9	EDO	B	1866	-	3,3,3	0.46	0	2,2,2	0.57	0
9	EDO	B	1867	-	3,3,3	0.75	0	2,2,2	0.25	0
9	EDO	B	1868	-	3,3,3	0.58	0	2,2,2	0.45	0
9	EDO	B	1869	-	3,3,3	0.63	0	2,2,2	0.25	0
9	EDO	B	1870	-	3,3,3	0.73	0	2,2,2	0.16	0
9	EDO	B	1871	-	3,3,3	0.28	0	2,2,2	0.58	0
9	EDO	B	1872	-	3,3,3	0.32	0	2,2,2	0.95	0
9	EDO	B	1873	-	3,3,3	0.31	0	2,2,2	0.71	0
9	EDO	B	1874	-	3,3,3	0.30	0	2,2,2	0.28	0
9	EDO	B	1875	-	3,3,3	0.42	0	2,2,2	0.52	0
9	EDO	B	1876	-	3,3,3	0.46	0	2,2,2	0.69	0
9	EDO	B	1877	-	3,3,3	0.44	0	2,2,2	0.11	0
9	EDO	B	1878	-	3,3,3	0.23	0	2,2,2	0.73	0
9	EDO	B	1879	-	3,3,3	0.71	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	EDO	B	1880	-	3,3,3	0.52	0	2,2,2	0.42	0
9	EDO	B	1881	-	3,3,3	0.64	0	2,2,2	0.92	0
10	IMD	B	1882	-	3,5,5	0.32	0	4,5,5	0.88	0
10	IMD	B	1883	-	3,5,5	0.40	0	4,5,5	0.77	0
10	IMD	B	1884	-	3,5,5	0.52	0	4,5,5	0.52	0
10	IMD	B	1885	-	3,5,5	0.54	0	4,5,5	0.62	0
9	EDO	B	1900	-	3,3,3	0.48	0	2,2,2	0.36	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.52	1.56	1.52
8	B	1601	NAG	C1-C2	4.17	1.58	1.52

There are no bond angle outliers.

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

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, 95^{th} 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	840/844 (99%)	-0.32	4 (0%)	91	95	12, 19, 32, 44	14 (1%)
1	B	840/844 (99%)	-0.33	3 (0%)	93	95	12, 20, 35, 46	16 (1%)
All	All	1680/1688 (99%)	-0.33	7 (0%)	93	95	12, 20, 34, 46	30 (1%)

The worst 5 of 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

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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 (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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.