Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 02:30 AM EDT

PDB ID	:	5W6G
Title	:	Human antibody 6649 in complex with influenza hemagglutinin H1 Solomon Islands
Authors	:	Raymond, D.D.; Harrison, S.C.
Deposited on	:	2017-06-16
Resolution	:	2.79 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

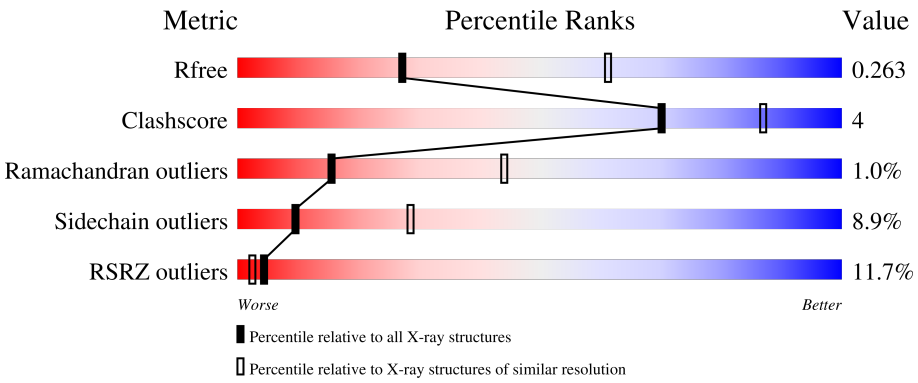
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	334	5% 85% 11% • •
2	B	178	8% 77% 15% • • 6%
3	H	230	11% 77% 19% • •
4	L	218	24% 86% 11% •
5	C	2	50% 50%

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
8	GOL	A	414	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7347 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	2563	1618	444	490	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP A7UPX0
A	-2	ASP	-	expression tag	UNP A7UPX0
A	-1	PRO	-	expression tag	UNP A7UPX0
A	0	GLY	-	expression tag	UNP A7UPX0
A	1	TYR	-	expression tag	UNP A7UPX0
A	2	LEU	-	expression tag	UNP A7UPX0
A	3	LEU	-	expression tag	UNP A7UPX0
A	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	168	1359	849	233	270	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	677	ARG	-	expression tag	UNP A7UPX0
B	678	SER	-	expression tag	UNP A7UPX0

- Molecule 3 is a protein called 6649 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	225	1708	1087	284	331	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	125	GLY	SER	conflict	UNP S6B2B6
H	148	VAL	ALA	conflict	UNP S6B2B6

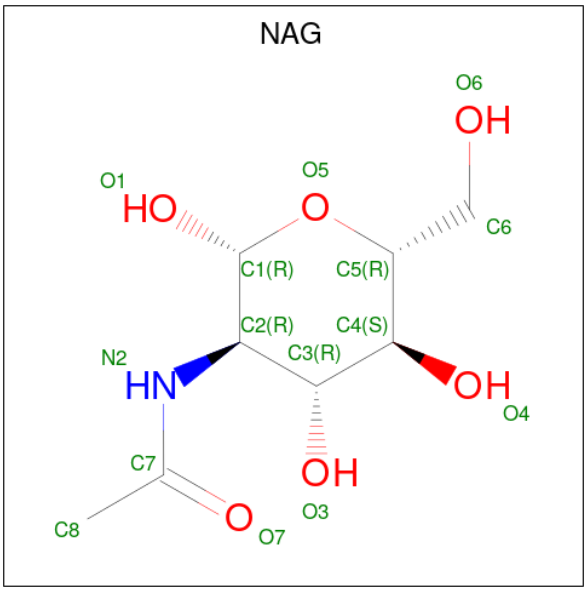
- Molecule 4 is a protein called 6649 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	214	1580	989	266	321	4	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

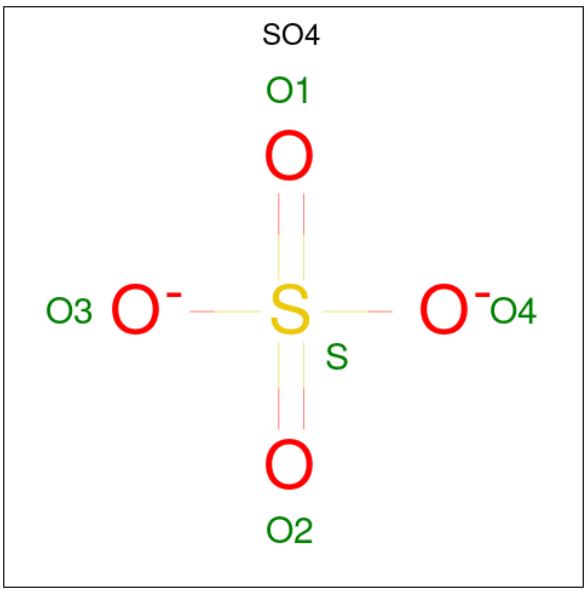
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	2	28	16	2	10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



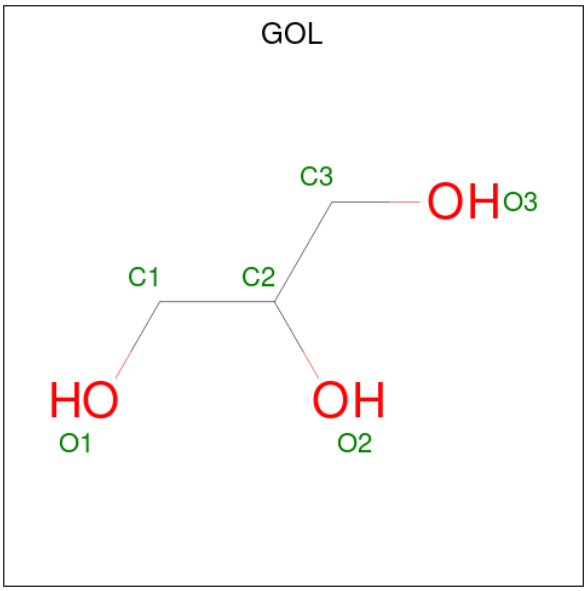
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0
			Total	C	O		
8	A	1	6	3	3	0	0

- Molecule 9 is water.

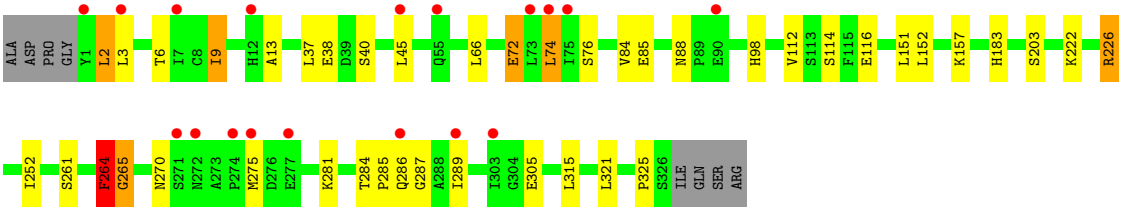
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	7	7	7	0	0
			Total	O		
9	H	2	2	2	0	0
			Total	O		
9	L	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

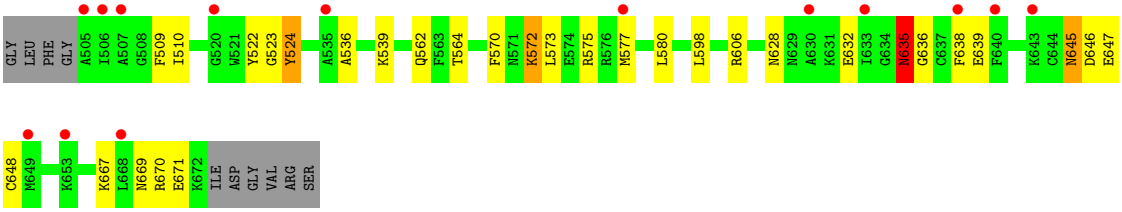
• Molecule 1: Hemagglutinin HA1

Chain A:



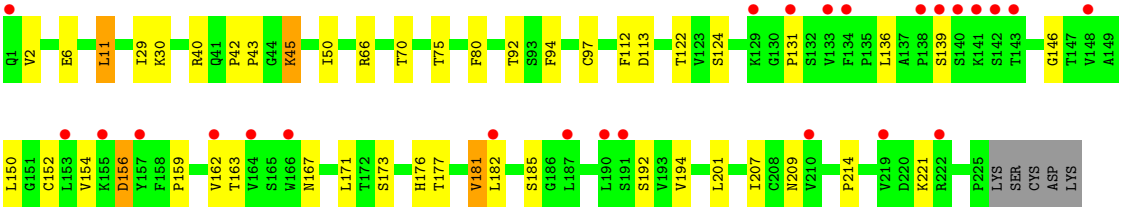
• Molecule 2: Hemagglutinin HA2

Chain B:



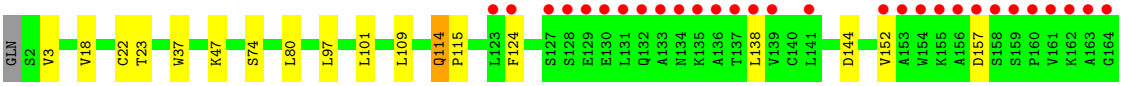
• Molecule 3: 6649 antibody heavy chain

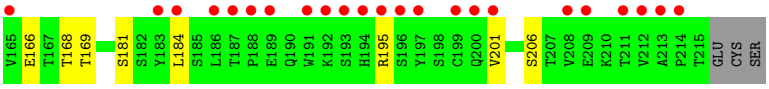
Chain H:



• Molecule 4: 6649 antibody light chain

Chain L:





• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	177.31Å 177.31Å 177.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.79 49.18 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.18-2.79) 99.6 (49.18-2.79)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.218 , 0.253 0.226 , 0.263	Depositor DCC
R_{free} test set	2291 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7347	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 0.333 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: GOL, SO4, NAG

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	0.54	0/2630	0.79	0/3580
2	B	0.51	0/1385	0.71	0/1861
3	H	0.51	0/1757	0.77	0/2400
4	L	0.49	0/1619	0.71	0/2211
All	All	0.52	0/7391	0.75	0/10052

There are no bond length outliers.

There are no bond angle outliers.

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	2563	0	2474	18	0
2	B	1359	0	1286	11	0
3	H	1708	0	1657	19	0
4	L	1580	0	1530	8	0
5	C	28	0	25	0	0
6	A	56	0	52	0	0
7	A	30	0	0	0	0
8	A	12	0	16	1	0
9	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	2	0	0	0	0
9	L	2	0	0	0	0
All	All	7347	0	7040	51	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 4.

All (51) 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:85:GLU:O	1:A:270:ASN:HA	1.85	0.77
1:A:284:THR:HB	1:A:287:GLY:O	1.84	0.77
3:H:40:ARG:HB3	3:H:50:ILE:HD11	1.82	0.61
1:A:284:THR:HG22	1:A:286:GLN:H	1.68	0.59
3:H:167:ASN:HD22	3:H:207:ILE:HG13	1.67	0.59
3:H:167:ASN:ND2	3:H:207:ILE:H	2.00	0.58
3:H:92:THR:HG23	3:H:122:THR:HA	1.87	0.56
1:A:2:LEU:H	1:A:2:LEU:HD13	1.70	0.56
1:A:114:SER:HB3	1:A:261:SER:HB2	1.90	0.53
3:H:167:ASN:HA	3:H:207:ILE:HG13	1.91	0.52
3:H:11:LEU:HD21	3:H:124:SER:HB3	1.93	0.51
1:A:98:HIS:HA	8:A:414:GOL:H32	1.92	0.50
4:L:152:VAL:HG22	4:L:201:VAL:HG22	1.94	0.50
1:A:13:ALA:HB1	1:A:325:PRO:HB3	1.94	0.49
1:A:264:PHE:HD1	1:A:265:GLY:H	1.61	0.49
1:A:66:LEU:HD22	1:A:151:LEU:HD11	1.93	0.49
3:H:42:PRO:HB2	3:H:45:LYS:HD3	1.94	0.48
3:H:131:PRO:HB2	3:H:154:VAL:HG13	1.95	0.48
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.94	0.48
1:A:284:THR:HG23	1:A:285:PRO:HD2	1.97	0.47
2:B:510:ILE:HA	2:B:635:ASN:HB2	1.96	0.47
2:B:570:PHE:CE1	2:B:577:MET:HB3	2.50	0.47
1:A:38:GLU:HG2	1:A:289:ILE:HG23	1.95	0.47
3:H:136:LEU:HB3	4:L:124:PHE:CD2	2.50	0.47
4:L:80:LEU:HD11	4:L:109:LEU:HD21	1.96	0.46
1:A:37:LEU:HB2	1:A:315:LEU:HB2	1.97	0.46
2:B:635:ASN:HD22	2:B:636:GLY:H	1.64	0.46
2:B:523:GLY:HA3	2:B:536:ALA:HA	1.98	0.46
1:A:222:LYS:HA	1:A:226:ARG:O	2.17	0.45
1:A:6:THR:HG23	2:B:639:GLU:OE1	2.16	0.45
4:L:114:GLN:HA	4:L:115:PRO:HD2	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:159:PRO:HD2	3:H:214:PRO:CB	2.48	0.44
1:A:2:LEU:H	1:A:2:LEU:CD1	2.31	0.44
3:H:177:THR:HA	3:H:192:SER:HA	2.00	0.44
2:B:632:GLU:HG2	2:B:638:PHE:HE1	1.83	0.43
2:B:667:LYS:HG2	2:B:670:ARG:CZ	2.47	0.43
2:B:645:ASN:HD22	2:B:647:GLU:HB2	1.83	0.43
3:H:29:ILE:HD11	3:H:80:PHE:HB3	2.01	0.43
1:A:9:ILE:HG22	2:B:524:TYR:HD1	1.84	0.42
4:L:138:LEU:HD12	4:L:184:LEU:HD23	2.00	0.42
3:H:131:PRO:CB	3:H:154:VAL:HG13	2.50	0.42
2:B:509:PHE:O	2:B:635:ASN:HB3	2.20	0.41
3:H:6:GLU:HG3	3:H:97:CYS:SG	2.61	0.41
3:H:43:PRO:HG3	3:H:94:PHE:CE2	2.55	0.41
3:H:30:LYS:HD2	3:H:75:THR:HG21	2.03	0.41
2:B:572:LYS:H	2:B:572:LYS:HE2	1.85	0.41
1:A:45:LEU:HD13	1:A:84:VAL:HG11	2.03	0.40
3:H:112:PHE:CZ	4:L:101:LEU:HD13	2.56	0.40
4:L:22:CYS:HB2	4:L:37:TRP:CH2	2.57	0.40
3:H:159:PRO:HD2	3:H:214:PRO:HB3	2.02	0.40
3:H:181:VAL:CG1	4:L:168:THR:HG22	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/334 (97%)	299 (92%)	21 (6%)	4 (1%)	13	39
2	B	166/178 (93%)	154 (93%)	11 (7%)	1 (1%)	25	56
3	H	223/230 (97%)	200 (90%)	20 (9%)	3 (1%)	12	36
4	L	212/218 (97%)	200 (94%)	11 (5%)	1 (0%)	29	61
All	All	925/960 (96%)	853 (92%)	63 (7%)	9 (1%)	15	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PHE
2	B	635	ASN
3	H	146	GLY
1	A	74	LEU
3	H	156	ASP
3	H	185	SER
4	L	157	ASP
1	A	72	GLU
1	A	265	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	286/292 (98%)	267 (93%)	19 (7%)	16 44
2	B	146/153 (95%)	128 (88%)	18 (12%)	4 15
3	H	193/198 (98%)	172 (89%)	21 (11%)	6 19
4	L	177/181 (98%)	164 (93%)	13 (7%)	14 38
All	All	802/824 (97%)	731 (91%)	71 (9%)	9 28

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	LEU
1	A	9	ILE
1	A	40	SER
1	A	72	GLU
1	A	74	LEU
1	A	76	SER
1	A	88	ASN
1	A	112	VAL
1	A	116	GLU
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	157	LYS
1	A	203	SER
1	A	226	ARG
1	A	264	PHE
1	A	275	MET
1	A	281	LYS
1	A	305	GLU
1	A	321	LEU
2	B	522	TYR
2	B	524	TYR
2	B	539	LYS
2	B	562	GLN
2	B	564	THR
2	B	572	LYS
2	B	573	LEU
2	B	575	ARG
2	B	580	LEU
2	B	598	LEU
2	B	606	ARG
2	B	628	ASN
2	B	635	ASN
2	B	645	ASN
2	B	646	ASP
2	B	648	CYS
2	B	669	ASN
2	B	671	GLU
3	H	2	VAL
3	H	11	LEU
3	H	45	LYS
3	H	66	ARG
3	H	70	THR
3	H	113	ASP
3	H	139	SER
3	H	150	LEU
3	H	152	CYS
3	H	156	ASP
3	H	162	VAL
3	H	163	THR
3	H	171	LEU
3	H	173	SER
3	H	176	HIS
3	H	181	VAL

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Mol	Chain	Res	Type
3	H	182	LEU
3	H	194	VAL
3	H	201	LEU
3	H	209	ASN
3	H	221	LYS
4	L	3	VAL
4	L	18	VAL
4	L	23	THR
4	L	47	LYS
4	L	74	SER
4	L	97	LEU
4	L	114	GLN
4	L	144	ASP
4	L	166	GLU
4	L	169	THR
4	L	181	SER
4	L	195	ARG
4	L	206	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
2	B	614	ASN
2	B	625	GLN
2	B	628	ASN
2	B	635	ASN
3	H	167	ASN
4	L	114	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides 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	$\#\|Z\| > 2$
5	NAG	C	1	1,5	14,14,15	0.33	0	17,19,21	0.91	1 (5%)
5	NAG	C	2	5	14,14,15	0.31	0	17,19,21	0.66	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
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1	NAG	O5-C1-C2	-2.21	107.79	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

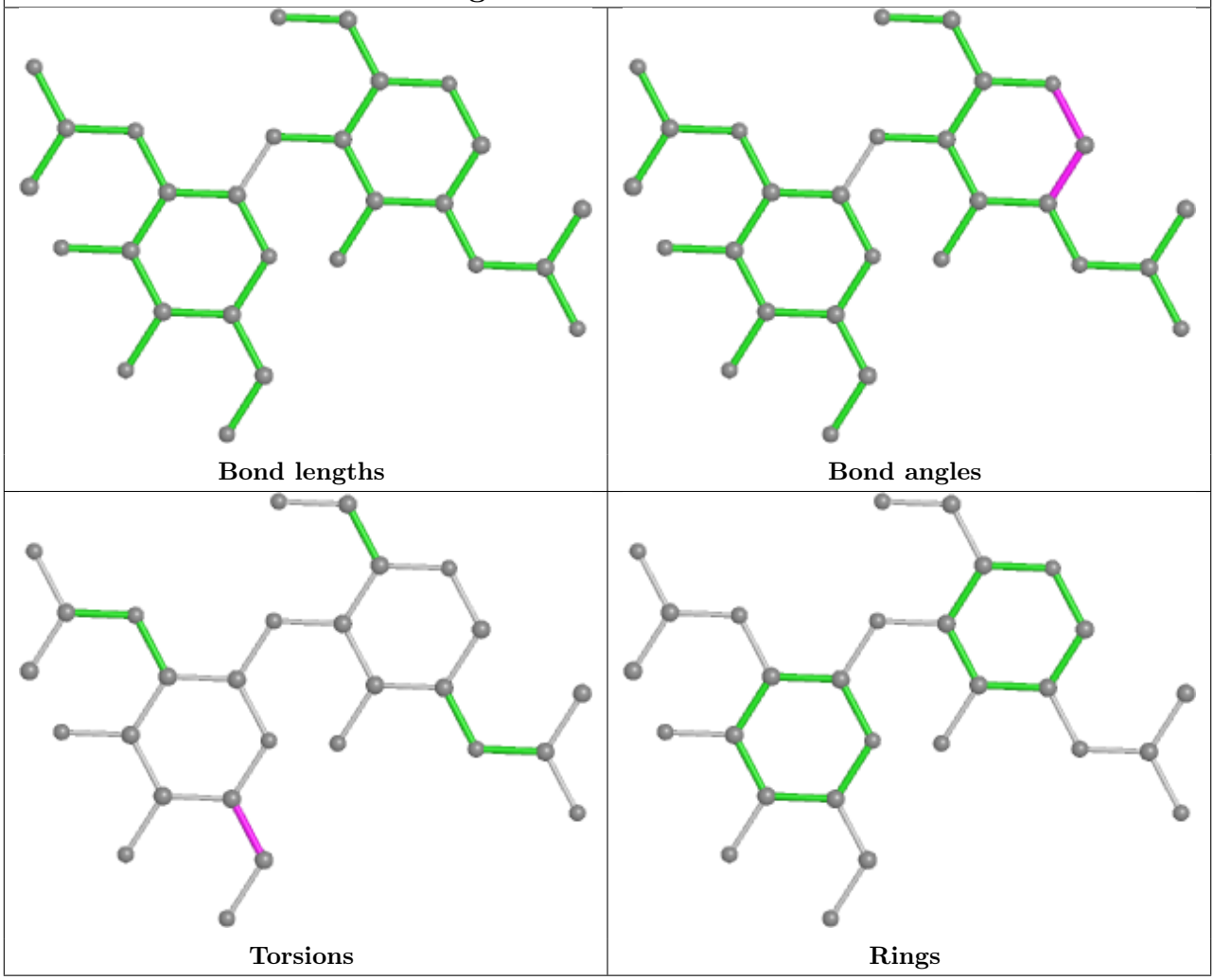
Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
7	SO4	A	407	-	4,4,4	0.22	0	6,6,6	0.24	0
7	SO4	A	409	-	4,4,4	0.22	0	6,6,6	0.24	0
7	SO4	A	410	-	4,4,4	0.15	0	6,6,6	0.20	0
7	SO4	A	412	-	4,4,4	0.23	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	404	1	14,14,15	0.31	0	17,19,21	1.19	2 (11%)
6	NAG	A	405	1	14,14,15	0.34	0	17,19,21	0.88	1 (5%)
6	NAG	A	406	1	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
7	SO4	A	411	-	4,4,4	0.19	0	6,6,6	0.76	0
8	GOL	A	413	-	5,5,5	0.14	0	5,5,5	0.44	0
8	GOL	A	414	-	5,5,5	0.09	0	5,5,5	0.27	0
7	SO4	A	408	-	4,4,4	0.18	0	6,6,6	0.27	0
6	NAG	A	403	1	14,14,15	0.36	0	17,19,21	1.31	2 (11%)

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
6	NAG	A	404	1	-	2/6/23/26	0/1/1/1
6	NAG	A	405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	406	1	-	0/6/23/26	0/1/1/1
8	GOL	A	413	-	-	1/4/4/4	-
8	GOL	A	414	-	-	2/4/4/4	-
6	NAG	A	403	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	403	NAG	C1-C2-N2	3.84	117.06	110.49
6	A	404	NAG	C1-O5-C5	3.56	117.02	112.19
6	A	405	NAG	C1-O5-C5	3.22	116.56	112.19
6	A	403	NAG	C2-N2-C7	2.80	126.88	122.90
6	A	406	NAG	C1-O5-C5	2.12	115.07	112.19
6	A	404	NAG	C2-N2-C7	2.05	125.83	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	403	NAG	C1-C2-N2-C7
8	A	414	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	A	414	GOL	O2-C2-C3-O3
6	A	405	NAG	C4-C5-C6-O6
6	A	405	NAG	O5-C5-C6-O6
6	A	404	NAG	C1-C2-N2-C7
6	A	404	NAG	C3-C2-N2-C7
8	A	413	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	414	GOL	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, 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	326/334 (97%)	0.58	18 (5%)	25	16	54, 72, 106, 135	0
2	B	168/178 (94%)	0.69	14 (8%)	11	6	54, 99, 137, 148	0
3	H	225/230 (97%)	0.71	25 (11%)	5	3	53, 84, 121, 171	0
4	L	214/218 (98%)	1.22	52 (24%)	0	0	57, 85, 135, 152	0
All	All	933/960 (97%)	0.78	109 (11%)	4	2	53, 80, 131, 171	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	186	LEU	8.0
2	B	668	LEU	7.8
4	L	156	ALA	7.1
3	H	140	SER	6.8
4	L	154	TRP	6.3
4	L	155	LYS	6.2
3	H	141	LYS	6.0
4	L	184	LEU	6.0
4	L	165	VAL	6.0
4	L	161	VAL	6.0
4	L	197	TYR	5.9
1	A	74	LEU	5.8
4	L	160	PRO	5.1
4	L	138	LEU	5.0
4	L	162	LYS	5.0
3	H	139	SER	4.8
4	L	188	PRO	4.6
3	H	142	SER	4.6
4	L	196	SER	4.6
4	L	191	TRP	4.5
4	L	201	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
4	L	123	LEU	4.5
4	L	200	GLN	4.4
3	H	134	PHE	4.4
4	L	187	THR	4.3
4	L	132	GLN	4.3
4	L	213	ALA	4.3
4	L	135	LYS	4.2
4	L	199	CYS	4.2
4	L	136	ALA	4.1
4	L	195	ARG	4.1
4	L	163	ALA	4.0
4	L	153	ALA	3.9
3	H	148	VAL	3.9
4	L	212	VAL	3.9
1	A	73	LEU	3.8
3	H	129	LYS	3.7
4	L	192	LYS	3.7
4	L	131	LEU	3.7
4	L	194	HIS	3.6
4	L	159	SER	3.6
1	A	7	ILE	3.6
3	H	143	THR	3.4
1	A	75	ILE	3.3
4	L	183	TYR	3.3
4	L	208	VAL	3.3
3	H	1	GLN	3.3
4	L	193	SER	3.2
4	L	127	SER	3.2
2	B	535	ALA	3.2
2	B	506	ILE	3.2
1	A	45	LEU	3.1
1	A	90	GLU	3.1
1	A	55	GLN	3.0
4	L	128	SER	3.0
4	L	134	ASN	3.0
4	L	141	LEU	3.0
2	B	643	LYS	3.0
3	H	187	LEU	2.9
4	L	164	GLY	2.9
4	L	209	GLU	2.9
4	L	152	VAL	2.8
3	H	191	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	640	PHE	2.7
3	H	210	VAL	2.7
4	L	214	PRO	2.7
2	B	633	ILE	2.7
3	H	222	ARG	2.7
4	L	139	VAL	2.7
2	B	630	ALA	2.6
3	H	219	VAL	2.6
1	A	1	TYR	2.6
1	A	275	MET	2.6
3	H	131	PRO	2.5
4	L	124	PHE	2.5
3	H	162	VAL	2.5
3	H	153	LEU	2.4
4	L	157	ASP	2.4
2	B	507	ALA	2.4
2	B	653	LYS	2.4
4	L	158	SER	2.3
3	H	133	VAL	2.3
3	H	157	TYR	2.3
2	B	505	ALA	2.3
3	H	190	LEU	2.3
2	B	520	GLY	2.3
4	L	137	THR	2.3
3	H	164	VAL	2.3
1	A	271	SER	2.3
3	H	138	PRO	2.3
4	L	129	GLU	2.2
2	B	638	PHE	2.2
1	A	3	LEU	2.2
4	L	189	GLU	2.2
1	A	289	ILE	2.2
3	H	155	LYS	2.2
1	A	272	ASN	2.1
4	L	133	ALA	2.1
1	A	286	GLN	2.1
3	H	182	LEU	2.1
1	A	277	GLU	2.1
2	B	649	MET	2.1
3	H	166	TRP	2.1
1	A	274	PRO	2.0
1	A	303	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
4	L	211	THR	2.0
2	B	577	MET	2.0
1	A	12	HIS	2.0
4	L	130	GLU	2.0

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)

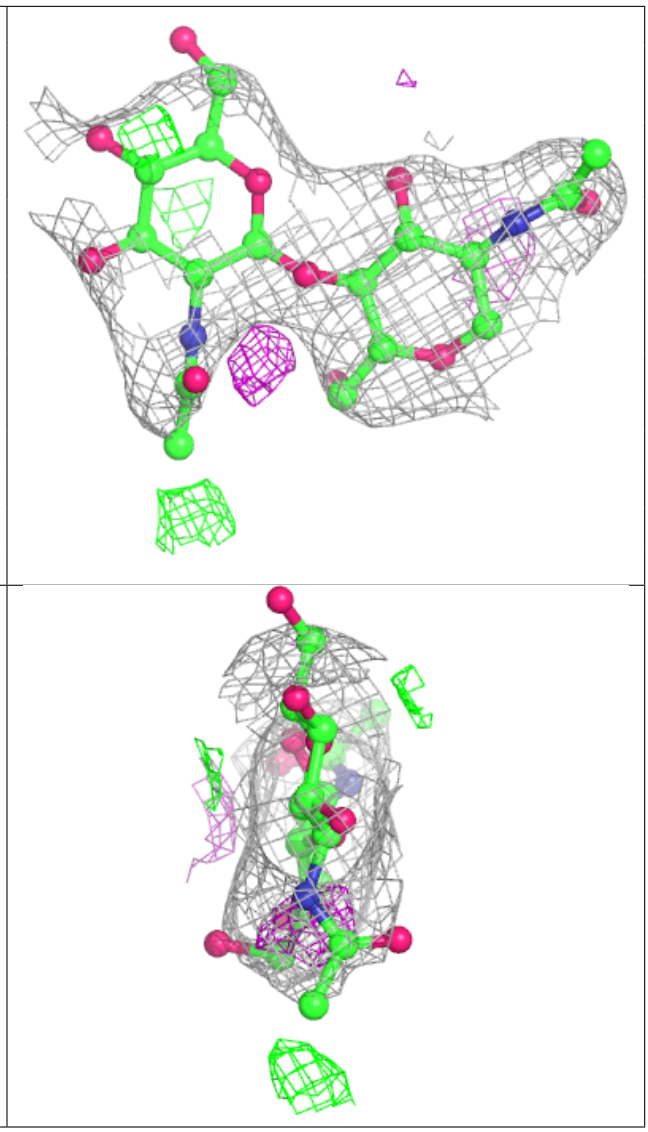
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	2	14/15	0.79	0.22	116,121,126,127	0
5	NAG	C	1	14/15	0.95	0.25	84,95,101,109	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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. 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	B-factors(Å^2)	Q<0.9
8	GOL	A	414	6/6	0.69	0.45	103,106,108,108	0
6	NAG	A	406	14/15	0.71	0.16	130,133,134,135	0
8	GOL	A	413	6/6	0.75	0.30	88,99,101,102	0
7	SO4	A	409	5/5	0.76	0.20	139,139,141,142	0
6	NAG	A	405	14/15	0.83	0.27	122,128,131,131	0
7	SO4	A	412	5/5	0.85	0.16	139,139,139,139	0
6	NAG	A	403	14/15	0.87	0.30	133,136,137,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	A	410	5/5	0.88	0.24	145,146,146,147	0
6	NAG	A	404	14/15	0.90	0.15	100,102,105,108	0
7	SO4	A	411	5/5	0.92	0.21	106,107,108,109	0
7	SO4	A	407	5/5	0.92	0.14	116,118,120,120	0
7	SO4	A	408	5/5	0.99	0.17	75,79,81,84	0

6.5 Other polymers (i)

There are no such residues in this entry.