Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 01:19 AM EDT

PDB ID	:	6X4G
Title	:	Crystal structure of ICOS in complex with ICOS-L and an anti ICOS-L VNAR domain
Authors	:	Rujas, E.; Sicard, T.; Julien, J.P.
Deposited on	:	2020-05-22
Resolution	:	3.50 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:

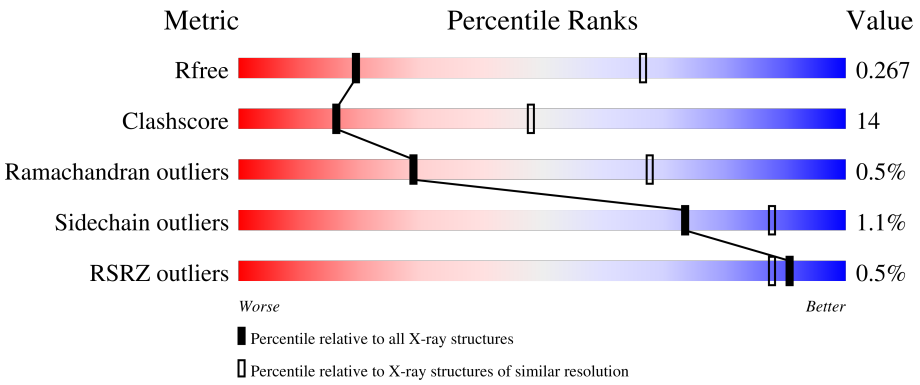
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	119	62% 20% • 17%
2	C	240	% 60% 26% • 13%
3	N	130	52% 37% • 9%
4	B	5	20% 60% 20%
4	D	5	60% 40%

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
4	MAN	D	5	-	-	-	X
5	NAG	A	201	-	-	-	X
5	NAG	C	301	-	-	-	X
5	NAG	C	305	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3513 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 Inducible T-cell costimulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	99	786	513	128	139	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	-	expression tag	UNP Q9Y6W8
A	131	THR	-	expression tag	UNP Q9Y6W8
A	132	GLU	-	expression tag	UNP Q9Y6W8
A	133	ASN	-	expression tag	UNP Q9Y6W8
A	134	LEU	-	expression tag	UNP Q9Y6W8
A	135	TYR	-	expression tag	UNP Q9Y6W8
A	136	PHE	-	expression tag	UNP Q9Y6W8
A	137	GLN	-	expression tag	UNP Q9Y6W8

- Molecule 2 is a protein called ICOS ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	209	1634	1024	282	318	10	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	THR	-	cloning artifact	UNP O75144
C	18	GLY	-	cloning artifact	UNP O75144
C	249	GLY	-	expression tag	UNP O75144
C	250	THR	-	expression tag	UNP O75144
C	251	GLU	-	expression tag	UNP O75144
C	252	ASN	-	expression tag	UNP O75144
C	253	LEU	-	expression tag	UNP O75144
C	254	TYR	-	expression tag	UNP O75144

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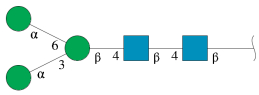
Chain	Residue	Modelled	Actual	Comment	Reference
C	255	PHE	-	expression tag	UNP O75144
C	256	GLN	-	expression tag	UNP O75144

- Molecule 3 is a protein called anti ICOS-L VHH domain VNAR.

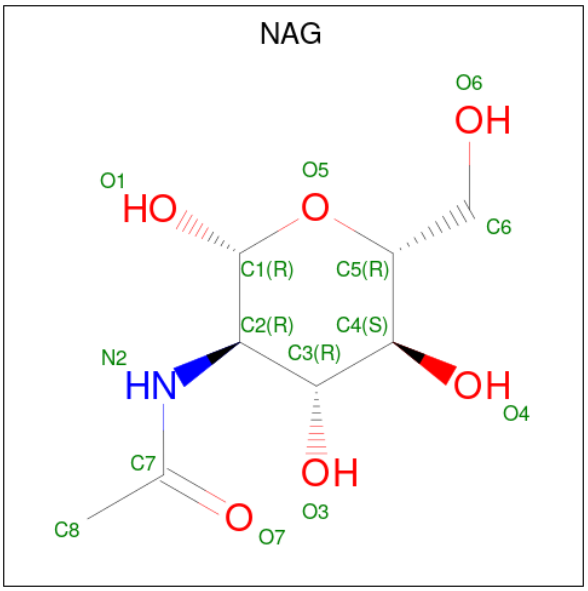
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	N	118	881	532	160	183	6	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



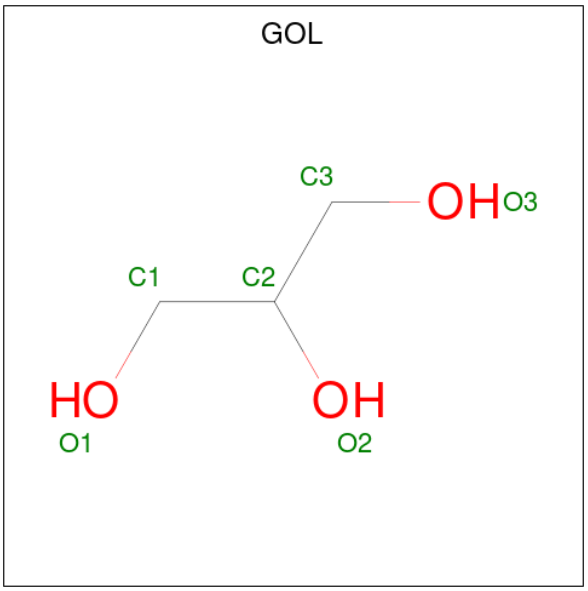
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	5	61	34	2	25	0	0	0
4	D	5	61	34	2	25	0	0	0

- Molecule 5 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		
5	A	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



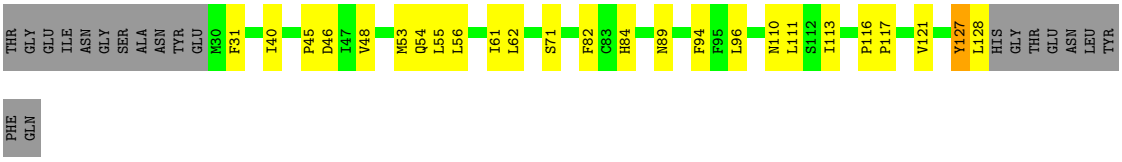
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0

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.

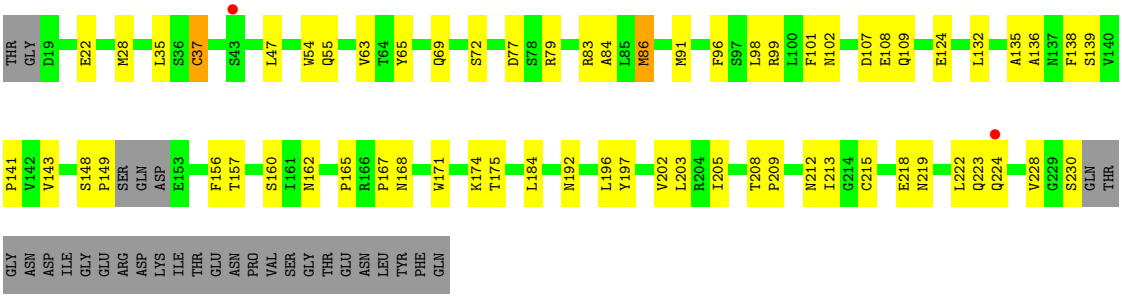
• Molecule 1: Inducible T-cell costimulator

Chain A: 62% 20% • 17%



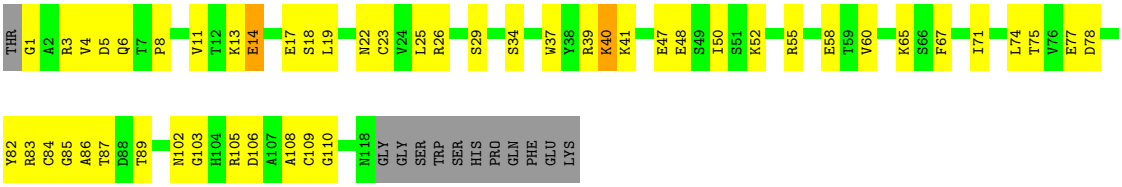
• Molecule 2: ICOS ligand

Chain C: % 60% 26% • 13%



• Molecule 3: anti ICOS-L VHH domain VNAR

Chain N: 52% 37% • 9%



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 20% 60% 20%

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.02Å 104.02Å 123.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 3.50 39.73 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.73-3.50) 88.7 (39.73-3.30)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.224 , 0.267 0.225 , 0.267	Depositor DCC
R_{free} test set	513 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	80.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3513	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 4.12% 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, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.46	0/807	0.59	0/1089
2	C	0.51	1/1665 (0.1%)	0.66	2/2268 (0.1%)
3	N	0.44	0/892	0.61	0/1206
All	All	0.48	1/3364 (0.0%)	0.63	2/4563 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	215	CYS	CB-SG	-5.09	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	86	MET	CB-CG-SD	-5.21	96.77	112.40
2	C	37	CYS	CA-CB-SG	5.06	123.11	114.00

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	786	0	775	22	0
2	C	1634	0	1588	49	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	881	0	849	34	0
4	B	61	0	52	2	0
4	D	61	0	52	0	0
5	A	14	0	13	2	0
5	C	70	0	64	2	0
6	A	6	0	8	0	0
All	All	3513	0	3401	100	1

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 14.

All (100) 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)
3:N:55:ARG:NH2	3:N:78:ASP:OD2	2.03	0.90
2:C:162:ASN:OD1	2:C:192:ASN:ND2	2.19	0.75
2:C:197:TYR:OH	3:N:106:ASP:OD2	2.07	0.72
2:C:86:MET:HE2	2:C:96:PHE:HB3	1.70	0.72
2:C:84:ALA:HB1	2:C:98:LEU:HD11	1.72	0.70
3:N:5:ASP:OD2	3:N:26:ARG:HD2	1.92	0.70
3:N:6:GLN:NE2	3:N:84:CYS:SG	2.66	0.69
4:B:1:NAG:O7	4:B:1:NAG:O3	2.10	0.68
2:C:222:LEU:HD13	2:C:224:GLN:HE21	1.60	0.67
2:C:148:SER:HB2	2:C:149:PRO:HD2	1.77	0.66
2:C:224:GLN:HB2	5:C:305:NAG:O6	1.95	0.66
1:A:127:TYR:HD1	1:A:128:LEU:N	1.94	0.66
2:C:37:CYS:HB3	2:C:96:PHE:O	1.98	0.64
1:A:48:VAL:HA	1:A:116:PRO:HD3	1.79	0.64
2:C:86:MET:CE	2:C:96:PHE:HB3	2.27	0.63
1:A:127:TYR:HD1	1:A:128:LEU:H	1.47	0.62
2:C:72:SER:N	5:C:302:NAG:O7	2.32	0.62
3:N:37:TRP:NE1	3:N:58:GLU:OE2	2.32	0.62
1:A:46:ASP:OD2	5:A:201:NAG:O6	2.18	0.61
3:N:39:ARG:HB2	3:N:50:ILE:HD11	1.83	0.61
3:N:52:LYS:NZ	3:N:58:GLU:OE1	2.34	0.60
2:C:35:LEU:HD12	2:C:98:LEU:HD23	1.83	0.60
2:C:222:LEU:HB3	2:C:224:GLN:HE21	1.67	0.59
2:C:109:GLN:HE22	3:N:103:GLY:HA3	1.69	0.58
3:N:39:ARG:HG3	3:N:82:TYR:CZ	2.39	0.57
1:A:45:PRO:O	1:A:48:VAL:HG12	2.04	0.57
2:C:162:ASN:HA	2:C:196:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:6:GLN:NE2	3:N:23:CYS:SG	2.77	0.57
3:N:8:PRO:HG2	3:N:11:VAL:HG21	1.87	0.57
2:C:86:MET:SD	2:C:91:MET:HE3	2.46	0.56
3:N:75:THR:HG22	3:N:77:GLU:H	1.69	0.56
3:N:18:SER:HA	3:N:71:ILE:O	2.06	0.55
2:C:222:LEU:HD13	2:C:224:GLN:NE2	2.20	0.55
3:N:84:CYS:O	3:N:110:GLY:N	2.40	0.55
3:N:1:GLY:HA2	3:N:105:ARG:HG2	1.88	0.55
2:C:83:ARG:O	2:C:101:PHE:HD1	1.88	0.55
2:C:156:PHE:CD2	2:C:213:ILE:HD11	2.42	0.55
1:A:54:GLN:HB2	1:A:110:ASN:HB3	1.89	0.54
2:C:184:LEU:HD13	2:C:205:ILE:HG22	1.88	0.54
3:N:47:GLU:OE2	3:N:83:ARG:NE	2.38	0.54
2:C:222:LEU:HB3	2:C:224:GLN:HG2	1.89	0.54
3:N:4:VAL:HG21	3:N:86:ALA:HB3	1.91	0.53
2:C:124:GLU:HG2	4:B:2:NAG:O3	2.08	0.52
3:N:29:SER:O	3:N:65:LYS:NZ	2.29	0.52
2:C:168:ASN:HB2	2:C:218:GLU:HB3	1.92	0.52
2:C:156:PHE:O	2:C:202:VAL:HA	2.11	0.51
3:N:77:GLU:OE2	3:N:77:GLU:HA	2.11	0.51
1:A:127:TYR:CD1	1:A:128:LEU:N	2.78	0.49
2:C:108:GLU:HG3	2:C:132:LEU:O	2.12	0.49
3:N:17:GLU:O	3:N:74:LEU:HD13	2.13	0.49
1:A:62:LEU:HD13	1:A:96:LEU:HD11	1.95	0.48
2:C:77:ASP:OD2	2:C:79:ARG:HG3	2.14	0.48
3:N:85:GLY:HA2	3:N:109:CYS:HA	1.96	0.48
2:C:83:ARG:NH2	2:C:107:ASP:OD2	2.46	0.47
1:A:56:LEU:HG	1:A:61:ILE:HD13	1.96	0.47
2:C:54:TRP:HE1	2:C:86:MET:HE3	1.80	0.47
2:C:136:ALA:O	2:C:219:ASN:ND2	2.48	0.46
2:C:143:VAL:HG21	2:C:230:SER:HA	1.96	0.46
3:N:40:LYS:HD2	3:N:41:LYS:O	2.15	0.46
2:C:175:THR:HG22	2:C:212:ASN:HB2	1.98	0.46
3:N:34:SER:H	3:N:87:THR:CG2	2.28	0.46
2:C:139:SER:O	2:C:160:SER:OG	2.27	0.45
2:C:223:GLN:HA	2:C:223:GLN:OE1	2.16	0.45
3:N:3:ARG:HA	3:N:108:ALA:CB	2.46	0.45
3:N:67:PHE:HE2	3:N:84:CYS:HB2	1.82	0.45
2:C:143:VAL:HA	2:C:157:THR:O	2.16	0.45
1:A:53:MET:HE2	1:A:111:LEU:HD13	1.98	0.45
3:N:34:SER:H	3:N:87:THR:HG23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:THR:HG22	2:C:209:PRO:O	2.17	0.44
2:C:141:PRO:HG2	2:C:228:VAL:HB	1.99	0.44
3:N:4:VAL:HG22	3:N:25:LEU:HA	1.99	0.43
1:A:82:PHE:CZ	1:A:84:HIS:HA	2.53	0.43
1:A:127:TYR:O	1:A:128:LEU:HB2	2.18	0.43
3:N:39:ARG:O	3:N:48:GLU:HG2	2.18	0.43
2:C:171:TRP:CG	2:C:203:LEU:HD13	2.54	0.43
2:C:28:MET:HG3	2:C:135:ALA:O	2.19	0.43
3:N:6:GLN:HB2	3:N:22:ASN:O	2.19	0.43
3:N:60:VAL:HG22	3:N:67:PHE:HB3	2.01	0.42
1:A:117:PRO:HG2	2:C:65:TYR:CD1	2.54	0.42
1:A:111:LEU:O	1:A:121:VAL:HA	2.20	0.42
2:C:79:ARG:NH2	3:N:102:ASN:O	2.53	0.42
1:A:55:LEU:HD22	1:A:62:LEU:HD12	2.02	0.42
1:A:71:SER:HB3	2:C:69:GLN:CD	2.40	0.42
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.87	0.42
2:C:138:PHE:CE1	2:C:167:PRO:HB3	2.55	0.41
2:C:55:GLN:HA	2:C:63:VAL:HG23	2.02	0.41
3:N:13:LYS:HG3	3:N:19:LEU:HD13	2.03	0.41
2:C:138:PHE:CZ	2:C:167:PRO:HB3	2.54	0.41
2:C:174:LYS:HB2	2:C:212:ASN:C	2.41	0.41
1:A:89:ASN:CG	5:A:201:NAG:H83	2.41	0.41
1:A:117:PRO:HG2	2:C:65:TYR:CG	2.56	0.41
2:C:54:TRP:HE1	2:C:86:MET:CE	2.33	0.41
3:N:6:GLN:HB2	3:N:23:CYS:SG	2.61	0.41
1:A:48:VAL:HG23	1:A:113:ILE:HG23	2.03	0.41
1:A:55:LEU:HD12	1:A:94:PHE:CD2	2.56	0.40
2:C:222:LEU:CD1	2:C:224:GLN:HE21	2.31	0.40
1:A:31:PHE:HB3	1:A:40:ILE:HA	2.02	0.40
2:C:47:LEU:HD21	2:C:91:MET:HB3	2.02	0.40
2:C:219:ASN:ND2	2:C:222:LEU:HD12	2.37	0.40
3:N:13:LYS:HD3	3:N:14:GLU:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:GLU:OE2	2:C:102:ASN:ND2[4_544]	2.19	0.01

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	97/119 (82%)	97 (100%)	0	0	100	100
2	C	205/240 (85%)	199 (97%)	5 (2%)	1 (0%)	29	68
3	N	116/130 (89%)	114 (98%)	1 (1%)	1 (1%)	17	56
All	All	418/489 (86%)	410 (98%)	6 (1%)	2 (0%)	29	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	89	THR
2	C	165	PRO

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	90/106 (85%)	89 (99%)	1 (1%)	73	88
2	C	190/218 (87%)	189 (100%)	1 (0%)	88	94
3	N	98/108 (91%)	96 (98%)	2 (2%)	55	79
All	All	378/432 (88%)	374 (99%)	4 (1%)	73	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	TYR

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Mol	Chain	Res	Type
2	C	99	ARG
3	N	14	GLU
3	N	40	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	224	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)

10 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	$\#\|Z\| > 2$
4	NAG	B	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	B	2	4	14,14,15	0.33	0	17,19,21	0.45	0
4	BMA	B	3	4	11,11,12	0.75	0	15,15,17	0.76	0
4	MAN	B	4	4	11,11,12	0.91	1 (9%)	15,15,17	1.22	2 (13%)
4	MAN	B	5	4	11,11,12	1.78	3 (27%)	15,15,17	1.78	2 (13%)
4	NAG	D	1	4,2	14,14,15	0.50	0	17,19,21	0.56	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.70	0
4	BMA	D	3	4	11,11,12	0.86	0	15,15,17	0.91	0
4	MAN	D	4	4	11,11,12	0.87	0	15,15,17	1.04	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MAN	D	5	4	11,11,12	1.62	3 (27%)	15,15,17	2.33	4 (26%)

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
4	NAG	B	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	1/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	MAN	B	5	4	-	2/2/19/22	1/1/1/1
4	NAG	D	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5	MAN	O5-C5	3.76	1.51	1.43
4	D	5	MAN	C1-C2	3.47	1.60	1.52
4	B	5	MAN	O5-C1	2.88	1.48	1.43
4	B	1	NAG	O5-C1	-2.74	1.39	1.43
4	B	5	MAN	C2-C3	2.50	1.56	1.52
4	B	4	MAN	C1-C2	2.33	1.57	1.52
4	D	5	MAN	O5-C1	2.24	1.47	1.43
4	D	5	MAN	O5-C5	2.20	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5	MAN	C1-O5-C5	6.57	121.09	112.19
4	B	5	MAN	C1-O5-C5	5.14	119.15	112.19
4	D	5	MAN	O5-C1-C2	4.30	117.41	110.77
4	D	5	MAN	C1-C2-C3	3.30	113.72	109.67
4	D	4	MAN	O2-C2-C3	-2.77	104.59	110.14
4	B	4	MAN	O2-C2-C3	-2.73	104.67	110.14
4	B	5	MAN	O5-C5-C6	2.70	111.44	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5	MAN	O2-C2-C3	-2.29	105.54	110.14
4	B	1	NAG	C2-N2-C7	2.06	125.84	122.90
4	B	4	MAN	C1-C2-C3	2.01	112.13	109.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C3-C2-N2-C7
4	B	5	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	B	5	MAN	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	B	3	BMA	O5-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C1-C2-N2-C7
4	D	5	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

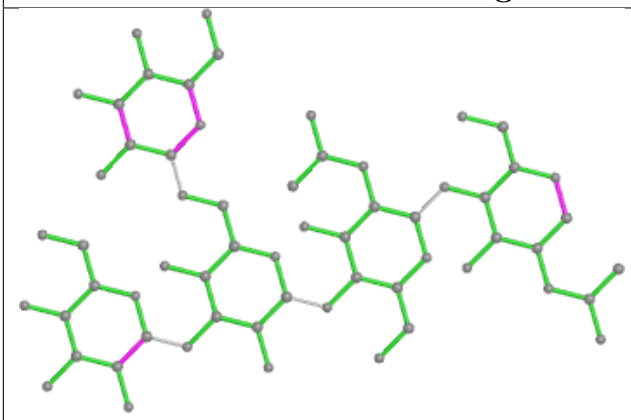
Mol	Chain	Res	Type	Atoms
4	B	5	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

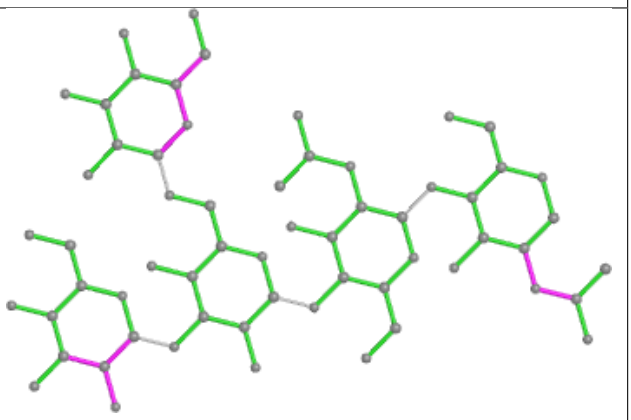
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	1	0
4	B	2	NAG	1	0

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

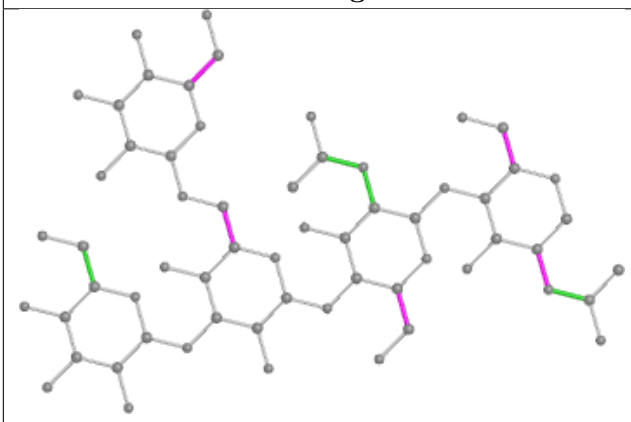
Oligosaccharide Chain B



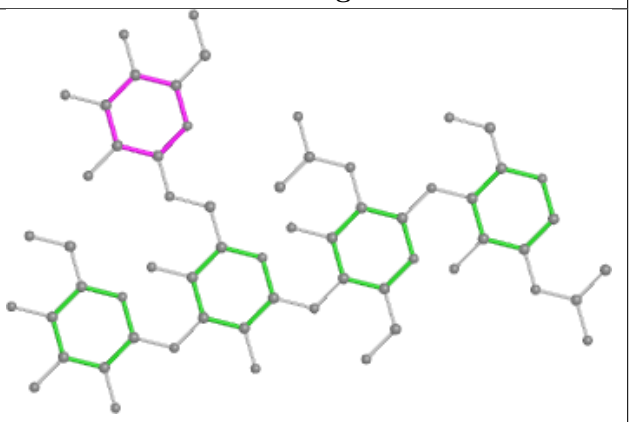
Bond lengths



Bond angles

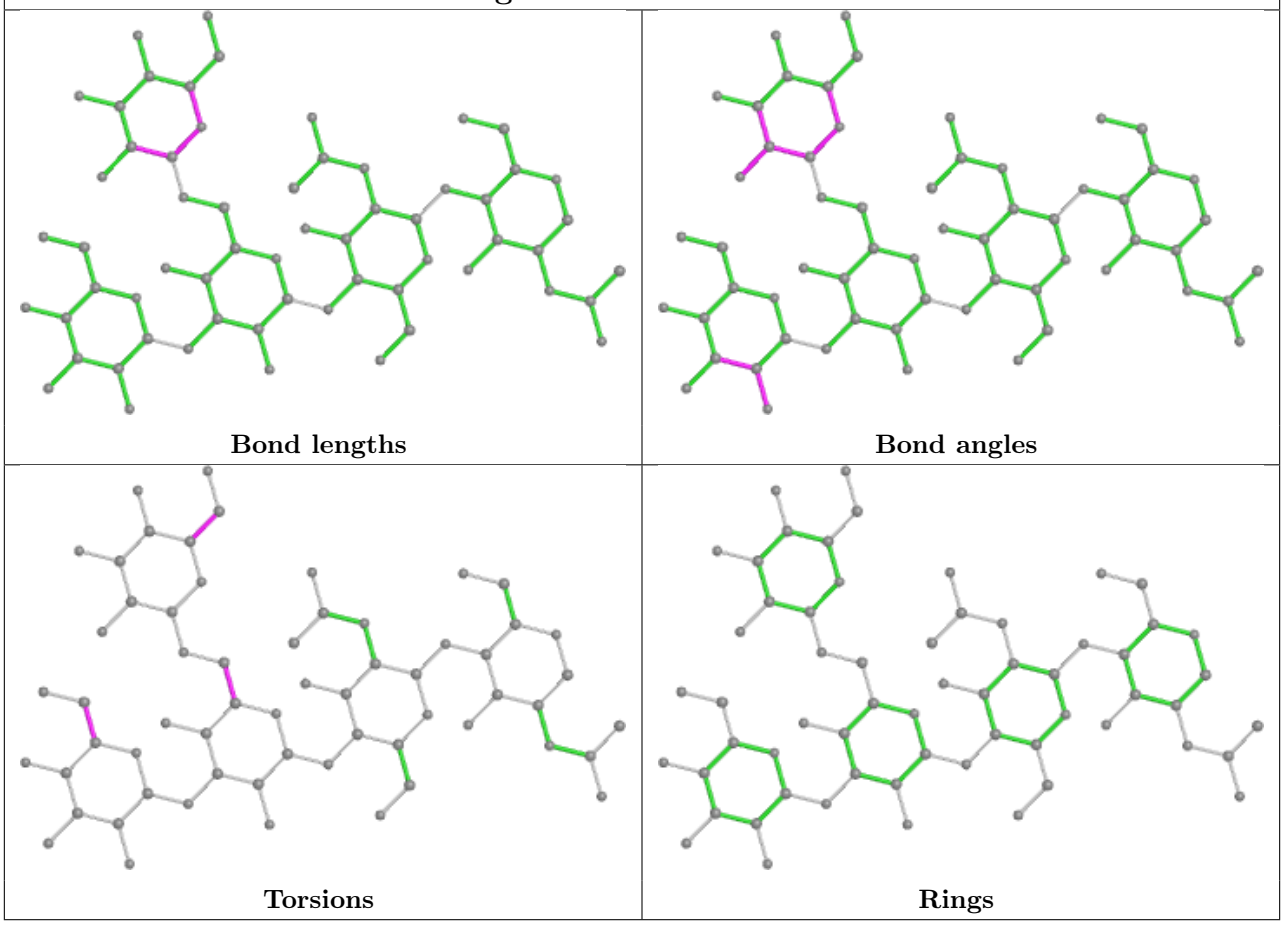


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
5	NAG	C	301	2	14,14,15	0.51	0	17,19,21	0.70	0
5	NAG	C	305	2	14,14,15	2.96	3 (21%)	17,19,21	3.66	5 (29%)
5	NAG	C	304	2	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
6	GOL	A	202	-	5,5,5	0.85	0	5,5,5	1.11	0
5	NAG	C	303	2	14,14,15	0.27	0	17,19,21	1.05	1 (5%)
5	NAG	A	201	1	14,14,15	0.55	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	302	2	14,14,15	2.00	1 (7%)	17,19,21	2.39	1 (5%)

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	301	2	-	2/6/23/26	0/1/1/1
5	NAG	C	305	2	-	5/6/23/26	0/1/1/1
5	NAG	C	304	2	-	3/6/23/26	0/1/1/1
6	GOL	A	202	-	-	0/4/4/4	-
5	NAG	C	303	2	-	0/6/23/26	0/1/1/1
5	NAG	A	201	1	-	2/6/23/26	0/1/1/1
5	NAG	C	302	2	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	305	NAG	O5-C1	7.57	1.55	1.43
5	C	305	NAG	C1-C2	7.44	1.63	1.52
5	C	302	NAG	O5-C1	7.27	1.55	1.43
5	C	305	NAG	C8-C7	2.58	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	305	NAG	C2-N2-C7	12.19	140.26	122.90
5	C	302	NAG	C1-O5-C5	9.49	125.05	112.19
5	C	305	NAG	C1-O5-C5	-6.96	102.77	112.19
5	C	303	NAG	C1-O5-C5	3.19	116.52	112.19
5	C	305	NAG	O5-C5-C6	3.02	111.94	107.20
5	C	305	NAG	O7-C7-N2	-2.44	117.47	121.95
5	C	305	NAG	O4-C4-C5	2.43	115.32	109.30
5	C	304	NAG	C2-N2-C7	2.28	126.15	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	305	NAG	C1-C2-N2-C7
5	C	305	NAG	C8-C7-N2-C2
5	C	305	NAG	O7-C7-N2-C2
5	C	305	NAG	O5-C5-C6-O6
5	A	201	NAG	C8-C7-N2-C2
5	A	201	NAG	O7-C7-N2-C2
5	C	305	NAG	C4-C5-C6-O6
5	C	304	NAG	O5-C5-C6-O6
5	C	302	NAG	C3-C2-N2-C7
5	C	304	NAG	C4-C5-C6-O6
5	C	304	NAG	C3-C2-N2-C7
5	C	301	NAG	C1-C2-N2-C7
5	C	301	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	305	NAG	1	0
5	A	201	NAG	2	0
5	C	302	NAG	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	99/119 (83%)	-0.17	0 100 100	50, 74, 144, 168	0
2	C	209/240 (87%)	-0.11	2 (0%) 82 77	49, 77, 125, 146	0
3	N	118/130 (90%)	-0.14	0 100 100	53, 82, 122, 138	0
All	All	426/489 (87%)	-0.13	2 (0%) 91 88	49, 78, 132, 168	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	43	SER	2.7
2	C	224	GLN	2.4

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
4	MAN	D	5	11/12	0.63	0.43	123,135,143,144	0
4	MAN	B	5	11/12	0.79	0.22	109,120,137,137	0
4	BMA	D	3	11/12	0.83	0.28	119,125,133,138	0
4	MAN	B	4	11/12	0.83	0.29	110,125,136,145	0
4	NAG	D	1	14/15	0.86	0.17	103,110,119,123	0
4	NAG	D	2	14/15	0.88	0.35	123,128,131,136	0

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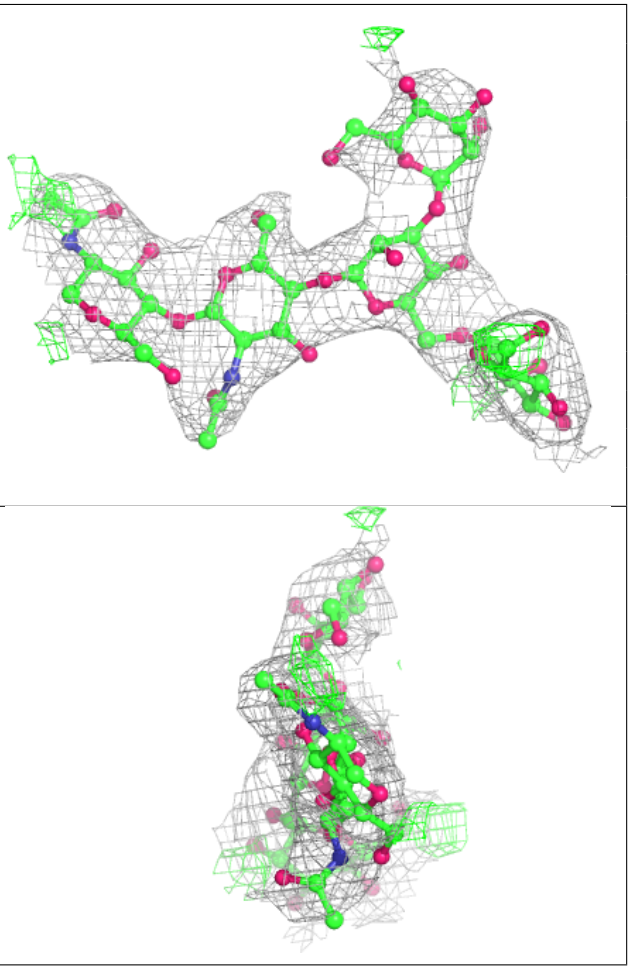
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	2	14/15	0.89	0.25	76,97,116,117	0
4	MAN	D	4	11/12	0.89	0.27	94,109,115,116	0
4	BMA	B	3	11/12	0.89	0.17	118,122,130,132	0
4	NAG	B	1	14/15	0.95	0.26	71,83,99,100	0

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.

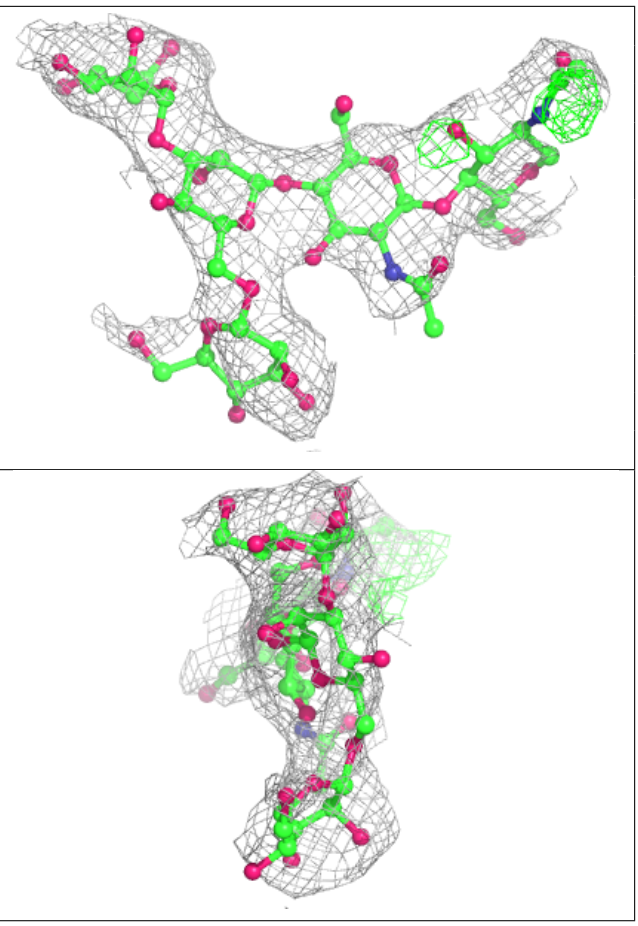
Electron density around Chain B:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain D:

$2mF_o$-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
5	NAG	C	301	14/15	0.72	0.54	111,131,136,138	0
5	NAG	A	201	14/15	0.74	0.48	129,135,144,144	0
5	NAG	C	305	14/15	0.74	0.47	86,107,119,140	0
5	NAG	C	304	14/15	0.81	0.24	105,122,133,137	0
6	GOL	A	202	6/6	0.84	0.26	62,73,79,82	0
5	NAG	C	302	14/15	0.85	0.20	106,123,134,134	0
5	NAG	C	303	14/15	0.95	0.25	76,81,87,88	0

6.5 Other polymers (i)

There are no such residues in this entry.