Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:52 PM BST

PDB ID	:	4IOP
Title	:	Crystal structure of NKp65 bound to its ligand KACL
Authors	:	Li, Y.
Deposited on	:	2013-01-08
Resolution	:	3.20 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 ⓘ symbol.

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

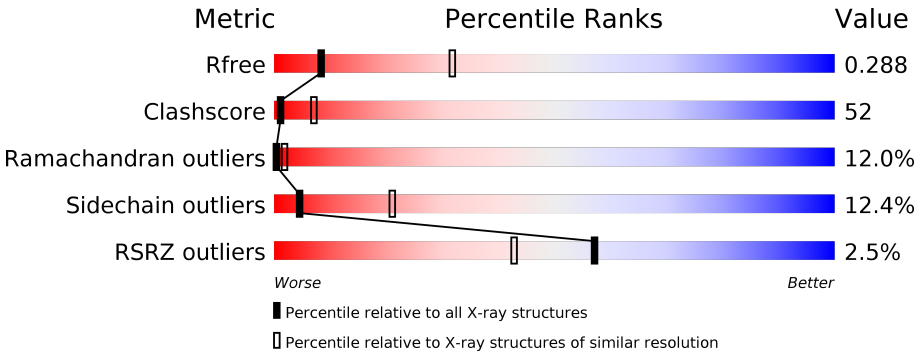
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	142	4% 31% 39% 13% 18%
2	B	158	% 26% 38% 12% 23%
3	C	3	67% 33%
3	D	3	33% 67%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1957 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 C-type lectin domain family 2 member A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			920	587	158	169	6			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	-	expression tag	UNP Q6UVW9
A	43	LEU	-	expression tag	UNP Q6UVW9
A	44	GLY	-	expression tag	UNP Q6UVW9
A	45	SER	-	expression tag	UNP Q6UVW9
A	175	ALA	-	expression tag	UNP Q6UVW9
A	176	ALA	-	expression tag	UNP Q6UVW9
A	177	ALA	-	expression tag	UNP Q6UVW9
A	178	HIS	-	expression tag	UNP Q6UVW9
A	179	HIS	-	expression tag	UNP Q6UVW9
A	180	HIS	-	expression tag	UNP Q6UVW9
A	181	HIS	-	expression tag	UNP Q6UVW9
A	182	HIS	-	expression tag	UNP Q6UVW9
A	183	HIS	-	expression tag	UNP Q6UVW9

- Molecule 2 is a protein called Killer cell lectin-like receptor subfamily F member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			959	617	158	177	7			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	59	ASP	-	expression tag	UNP D3W0D1
B	60	LEU	-	expression tag	UNP D3W0D1
B	61	GLY	-	expression tag	UNP D3W0D1

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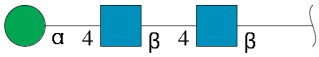
Chain	Residue	Modelled	Actual	Comment	Reference
B	62	SER	-	expression tag	UNP D3W0D1
B	208	ALA	-	expression tag	UNP D3W0D1
B	209	ALA	-	expression tag	UNP D3W0D1
B	210	ALA	-	expression tag	UNP D3W0D1
B	211	HIS	-	expression tag	UNP D3W0D1
B	212	HIS	-	expression tag	UNP D3W0D1
B	213	HIS	-	expression tag	UNP D3W0D1
B	214	HIS	-	expression tag	UNP D3W0D1
B	215	HIS	-	expression tag	UNP D3W0D1
B	216	HIS	-	expression tag	UNP D3W0D1

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

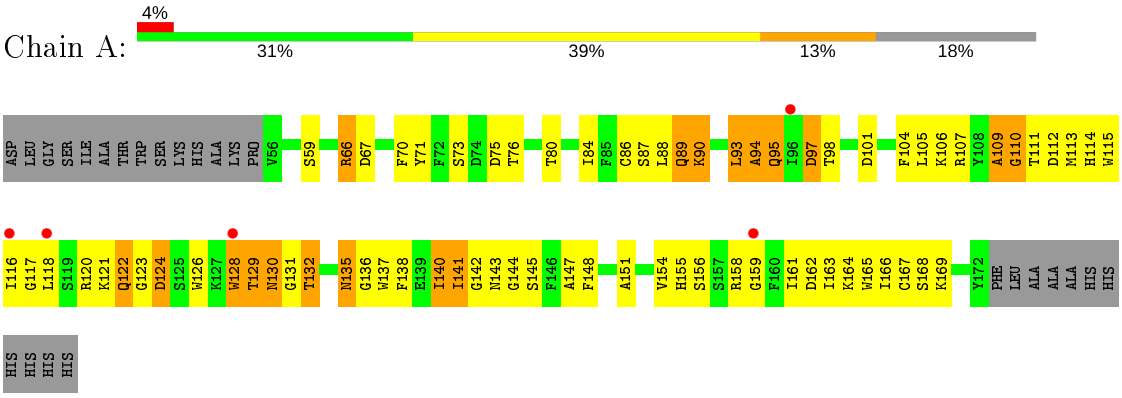


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

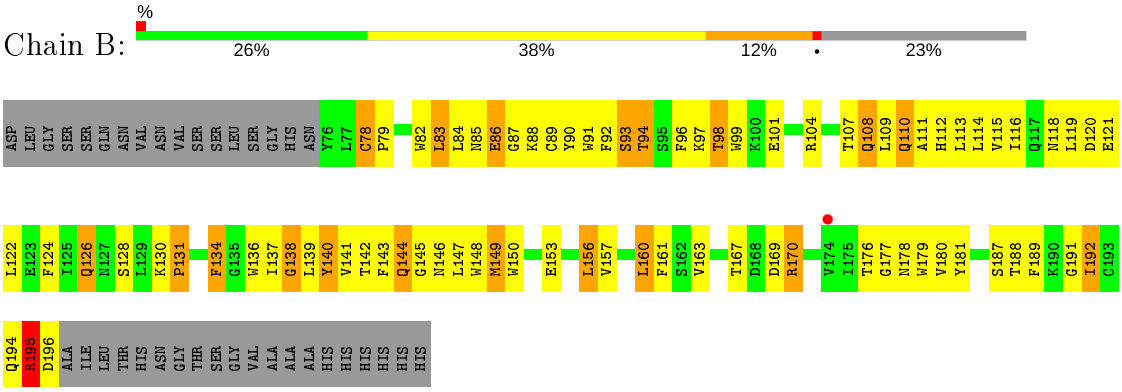
3 Residue-property plots (i)

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: C-type lectin domain family 2 member A



• Molecule 2: Killer cell lectin-like receptor subfamily F member 2



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

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


NAG1
NAG2
MAN3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	74.64Å 74.64Å 271.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 71.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.20) 99.8 (71.96-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.36 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.297 0.270 , 0.288	Depositor DCC
R_{free} test set	323 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	82.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 77.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	1957	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/947	0.69	0/1279
2	B	0.51	0/989	0.69	0/1350
All	All	0.49	0/1936	0.69	0/2629

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

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	920	0	836	89	0
2	B	959	0	863	114	0
3	C	39	0	34	5	0
3	D	39	0	34	2	0
All	All	1957	0	1767	194	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 52.

All (194) 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:110:GLY:HA2	1:A:151:ALA:HB2	1.35	1.03
2:B:142:THR:HG22	2:B:147:LEU:H	1.24	1.02
1:A:116:ILE:HD11	1:A:147:ALA:HB3	1.44	0.98
1:A:95:GLN:HE22	3:C:1:NAG:C6	1.80	0.93
1:A:110:GLY:HA2	1:A:151:ALA:CB	2.03	0.88
2:B:176:THR:HG23	2:B:178:ASN:H	1.38	0.88
1:A:158:ARG:HH11	2:B:170:ARG:CZ	1.87	0.87
2:B:84:LEU:HD11	2:B:89:CYS:SG	2.17	0.84
2:B:126:GLN:HA	2:B:126:GLN:HE21	1.41	0.84
2:B:114:LEU:HD12	2:B:115:VAL:N	1.94	0.81
1:A:131:GLY:O	1:A:132:THR:HB	1.84	0.78
1:A:95:GLN:HE22	3:C:1:NAG:H62	1.48	0.78
2:B:176:THR:CG2	2:B:179:TRP:H	1.96	0.78
1:A:94:ALA:HA	1:A:168:SER:HB3	1.66	0.77
1:A:114:HIS:CE1	1:A:164:LYS:HE2	2.21	0.76
2:B:114:LEU:HD12	2:B:115:VAL:H	1.50	0.76
1:A:73:SER:O	1:A:164:LYS:HE3	1.87	0.74
2:B:78:CYS:SG	2:B:84:LEU:HD21	2.27	0.74
2:B:142:THR:HG22	2:B:147:LEU:N	2.01	0.73
1:A:114:HIS:HA	1:A:164:LYS:O	1.89	0.73
2:B:169:ASP:O	2:B:170:ARG:HB3	1.89	0.73
1:A:94:ALA:HA	1:A:168:SER:CB	2.18	0.72
1:A:98:THR:HG22	1:A:101:ASP:OD2	1.90	0.71
2:B:114:LEU:HB3	2:B:137:ILE:HG22	1.71	0.71
1:A:116:ILE:HD11	1:A:147:ALA:CB	2.21	0.70
1:A:115:TRP:H	1:A:165:TRP:HA	1.56	0.70
1:A:120:ARG:HD3	1:A:126:TRP:CE2	2.26	0.70
1:A:128:TRP:HE3	1:A:132:THR:HG23	1.56	0.69
1:A:141:ILE:HD11	2:B:188:THR:HG21	1.75	0.69
2:B:98:THR:OG1	2:B:101:GLU:HG3	1.93	0.69
2:B:156:LEU:HD22	2:B:157:VAL:H	1.58	0.68
1:A:162:ASP:OD1	2:B:176:THR:HG21	1.93	0.68
1:A:121:LYS:O	1:A:124:ASP:HB2	1.94	0.68
1:A:110:GLY:CA	1:A:151:ALA:HB2	2.20	0.67
2:B:83:LEU:C	2:B:84:LEU:HD22	2.14	0.67
2:B:176:THR:HG22	2:B:179:TRP:O	1.95	0.66
1:A:161:ILE:HA	2:B:181:TYR:CD2	2.29	0.66
2:B:139:LEU:HG	2:B:150:TRP:NE1	2.10	0.66
1:A:106:LYS:HD2	1:A:151:ALA:O	1.94	0.66
2:B:108:GLN:O	2:B:109:LEU:HD13	1.95	0.66
2:B:143:PHE:HA	2:B:169:ASP:HB3	1.79	0.65
2:B:176:THR:HG22	2:B:179:TRP:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:VAL:HA	2:B:147:LEU:O	1.97	0.65
2:B:142:THR:CG2	2:B:146:ASN:H	2.10	0.65
2:B:136:TRP:O	2:B:137:ILE:HG23	1.96	0.65
2:B:124:PHE:O	2:B:128:SER:HB2	1.97	0.65
1:A:86:CYS:SG	1:A:93:LEU:HD23	2.36	0.64
2:B:142:THR:O	2:B:143:PHE:HB3	1.96	0.64
1:A:95:GLN:NE2	3:C:1:NAG:H62	2.12	0.64
2:B:126:GLN:NE2	2:B:126:GLN:HA	2.12	0.64
2:B:142:THR:HG23	2:B:146:ASN:H	1.62	0.64
1:A:158:ARG:NH1	2:B:170:ARG:CZ	2.60	0.63
2:B:85:ASN:HB2	2:B:124:PHE:CE2	2.32	0.63
1:A:148:PHE:CE1	1:A:155:HIS:HB2	2.35	0.62
2:B:115:VAL:HG12	2:B:194:GLN:NE2	2.15	0.62
2:B:84:LEU:CD1	2:B:89:CYS:HA	2.29	0.62
1:A:70:PHE:HA	1:A:167:CYS:O	1.99	0.61
2:B:156:LEU:HD22	2:B:157:VAL:N	2.15	0.61
1:A:140:ILE:HG22	1:A:140:ILE:O	2.01	0.61
2:B:122:LEU:O	2:B:126:GLN:HB2	1.99	0.61
2:B:188:THR:O	2:B:189:PHE:CD2	2.54	0.61
2:B:84:LEU:HD13	2:B:89:CYS:HA	1.82	0.60
2:B:142:THR:CG2	2:B:147:LEU:H	2.07	0.60
2:B:91:TRP:CZ3	2:B:93:SER:HA	2.37	0.60
2:B:176:THR:HG23	2:B:178:ASN:N	2.13	0.59
1:A:131:GLY:O	1:A:132:THR:CB	2.50	0.59
2:B:101:GLU:O	2:B:104:ARG:HB3	2.02	0.59
1:A:115:TRP:CH2	1:A:159:GLY:HA2	2.38	0.59
1:A:141:ILE:HG13	1:A:142:GLY:N	2.18	0.59
2:B:85:ASN:HB2	2:B:124:PHE:CZ	2.38	0.59
1:A:116:ILE:HD13	1:A:118:LEU:HB2	1.83	0.58
3:D:1:NAG:O3	3:D:2:NAG:H82	2.03	0.58
1:A:128:TRP:HE3	1:A:132:THR:CG2	2.16	0.58
2:B:115:VAL:HG13	2:B:115:VAL:O	2.02	0.58
1:A:161:ILE:HD13	2:B:134:PHE:HE1	1.68	0.58
2:B:130:LYS:HD3	2:B:131:PRO:HD2	1.85	0.58
1:A:120:ARG:HG2	1:A:145:SER:HA	1.86	0.58
2:B:142:THR:CG2	2:B:146:ASN:N	2.67	0.57
1:A:98:THR:HG23	1:A:101:ASP:H	1.70	0.56
2:B:138:GLY:O	2:B:150:TRP:HA	2.05	0.56
2:B:83:LEU:O	2:B:84:LEU:HD22	2.06	0.56
2:B:82:TRP:O	2:B:84:LEU:HD22	2.05	0.56
1:A:129:THR:O	1:A:130:ASN:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:H	1:A:167:CYS:HA	1.71	0.55
2:B:141:VAL:HG12	2:B:142:THR:N	2.21	0.55
2:B:78:CYS:SG	2:B:84:LEU:HD11	2.47	0.55
1:A:141:ILE:O	1:A:155:HIS:HA	2.07	0.55
1:A:87:SER:C	1:A:89:GLN:H	2.09	0.55
1:A:106:LYS:HB3	1:A:151:ALA:HA	1.89	0.55
2:B:98:THR:O	2:B:101:GLU:HB2	2.07	0.54
2:B:156:LEU:C	2:B:156:LEU:HD13	2.27	0.54
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.71	0.54
1:A:116:ILE:CD1	1:A:118:LEU:HB2	2.37	0.54
2:B:108:GLN:HA	2:B:108:GLN:NE2	2.22	0.53
2:B:170:ARG:HG2	2:B:170:ARG:O	2.07	0.53
1:A:114:HIS:HE1	1:A:164:LYS:HE2	1.69	0.53
1:A:97:ASP:N	1:A:97:ASP:OD2	2.41	0.53
2:B:108:GLN:HA	2:B:108:GLN:HE21	1.73	0.53
2:B:136:TRP:NE1	2:B:189:PHE:HB2	2.24	0.53
2:B:99:TRP:HD1	2:B:136:TRP:CE3	2.26	0.53
2:B:153:GLU:HA	2:B:153:GLU:OE1	2.09	0.52
1:A:141:ILE:CG1	1:A:142:GLY:N	2.73	0.52
2:B:140:TYR:HD2	2:B:140:TYR:H	1.55	0.52
2:B:96:PHE:O	2:B:97:LYS:HG3	2.10	0.52
2:B:141:VAL:CG1	2:B:142:THR:N	2.72	0.52
1:A:122:GLN:O	1:A:124:ASP:N	2.43	0.51
1:A:114:HIS:CE1	1:A:164:LYS:CE	2.93	0.51
2:B:115:VAL:HG12	2:B:194:GLN:HE21	1.75	0.51
1:A:158:ARG:HH11	2:B:170:ARG:NH2	2.07	0.51
2:B:82:TRP:CZ2	2:B:91:TRP:HB2	2.46	0.51
1:A:169:LYS:O	1:A:169:LYS:HG3	2.10	0.50
2:B:148:TRP:HE1	2:B:167:THR:HG22	1.75	0.50
2:B:194:GLN:O	2:B:195:ARG:HB3	2.10	0.50
2:B:115:VAL:CG1	2:B:194:GLN:NE2	2.75	0.50
1:A:84:ILE:HG22	1:A:88:LEU:HD13	1.93	0.50
1:A:71:TYR:O	1:A:166:ILE:HA	2.11	0.50
1:A:141:ILE:HD11	2:B:188:THR:CG2	2.40	0.50
1:A:76:THR:HB	1:A:162:ASP:C	2.33	0.50
1:A:115:TRP:N	1:A:165:TRP:HA	2.24	0.49
1:A:122:GLN:C	1:A:124:ASP:H	2.16	0.49
1:A:138:PHE:HE1	1:A:140:ILE:HD11	1.77	0.49
3:C:1:NAG:H61	3:C:2:NAG:C1	2.43	0.48
2:B:122:LEU:C	2:B:124:PHE:H	2.16	0.48
1:A:73:SER:HB3	1:A:165:TRP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:HG	2:B:150:TRP:CD1	2.49	0.48
2:B:149:MET:HB3	2:B:149:MET:HE3	1.74	0.48
1:A:71:TYR:HB3	1:A:167:CYS:HB2	1.96	0.47
1:A:84:ILE:O	1:A:87:SER:HB2	2.14	0.47
1:A:89:GLN:C	1:A:90:LYS:HD3	2.35	0.47
2:B:98:THR:HA	2:B:187:SER:O	2.15	0.47
2:B:134:PHE:C	2:B:134:PHE:CD2	2.87	0.47
1:A:114:HIS:HE1	1:A:164:LYS:CE	2.27	0.47
2:B:90:TYR:HE2	2:B:194:GLN:OE1	1.97	0.47
1:A:114:HIS:HB3	1:A:166:ILE:HG13	1.96	0.47
2:B:169:ASP:O	2:B:170:ARG:CB	2.62	0.47
2:B:107:THR:C	2:B:109:LEU:H	2.18	0.47
2:B:140:TYR:N	2:B:140:TYR:HD2	2.13	0.47
2:B:191:GLY:O	2:B:192:ILE:HD13	2.15	0.47
1:A:95:GLN:NE2	3:C:1:NAG:O6	2.38	0.46
1:A:130:ASN:CG	1:A:131:GLY:H	2.18	0.46
1:A:80:THR:O	1:A:84:ILE:HG13	2.15	0.46
2:B:82:TRP:CE2	2:B:91:TRP:HB2	2.51	0.46
1:A:66:ARG:HB3	1:A:67:ASP:H	1.49	0.46
2:B:140:TYR:N	2:B:140:TYR:CD2	2.83	0.46
2:B:83:LEU:O	2:B:84:LEU:HD13	2.15	0.46
1:A:141:ILE:HD11	2:B:188:THR:OG1	2.16	0.46
2:B:96:PHE:HD2	2:B:189:PHE:HA	1.81	0.46
1:A:128:TRP:CE3	1:A:132:THR:HG23	2.45	0.45
2:B:188:THR:O	2:B:189:PHE:HD2	1.98	0.45
2:B:83:LEU:HD22	2:B:83:LEU:H	1.81	0.45
2:B:109:LEU:O	2:B:110:GLN:C	2.54	0.45
2:B:149:MET:HG2	2:B:150:TRP:N	2.31	0.45
2:B:112:HIS:HD2	2:B:113:LEU:O	1.98	0.45
2:B:114:LEU:O	2:B:138:GLY:N	2.38	0.45
2:B:163:VAL:HA	2:B:180:VAL:O	2.16	0.45
2:B:136:TRP:HZ2	2:B:187:SER:O	1.99	0.45
1:A:120:ARG:HD3	1:A:126:TRP:CZ2	2.51	0.45
2:B:156:LEU:HD13	2:B:157:VAL:N	2.32	0.45
1:A:135:ASN:OD1	1:A:137:TRP:HD1	2.00	0.45
2:B:118:ASN:O	2:B:120:ASP:N	2.50	0.44
1:A:73:SER:OG	1:A:75:ASP:O	2.36	0.44
3:D:1:NAG:H3	3:D:2:NAG:N2	2.33	0.44
2:B:139:LEU:HD22	2:B:148:TRP:HB3	2.00	0.44
2:B:96:PHE:HA	2:B:189:PHE:O	2.16	0.44
1:A:93:LEU:O	1:A:94:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:SER:OG	2:B:94:THR:N	2.50	0.44
1:A:144:GLY:CA	1:A:156:SER:HB3	2.48	0.44
1:A:109:ALA:O	1:A:110:GLY:C	2.56	0.43
1:A:110:GLY:O	1:A:112:ASP:N	2.52	0.43
1:A:130:ASN:CG	1:A:131:GLY:N	2.72	0.43
2:B:126:GLN:HG3	2:B:177:GLY:O	2.18	0.43
2:B:96:PHE:HB3	2:B:188:THR:HB	2.01	0.43
1:A:162:ASP:OD1	2:B:176:THR:CG2	2.65	0.43
2:B:160:LEU:HD12	2:B:161:PHE:CE2	2.54	0.43
2:B:195:ARG:C	2:B:195:ARG:HD3	2.40	0.42
2:B:86:GLU:O	2:B:88:LYS:N	2.53	0.42
1:A:93:LEU:HB2	1:A:117:GLY:CA	2.50	0.42
2:B:140:TYR:CD2	2:B:149:MET:O	2.73	0.42
1:A:161:ILE:HD12	1:A:163:ILE:HG21	2.02	0.42
2:B:142:THR:O	2:B:143:PHE:CB	2.65	0.41
2:B:83:LEU:N	2:B:83:LEU:HD22	2.35	0.41
2:B:144:GLN:HG3	2:B:145:GLY:N	2.36	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.84	0.41
1:A:114:HIS:O	1:A:148:PHE:HA	2.21	0.41
1:A:93:LEU:HB3	1:A:117:GLY:N	2.35	0.41
1:A:158:ARG:NH1	2:B:170:ARG:NH1	2.69	0.41
1:A:114:HIS:HE1	1:A:164:LYS:NZ	2.19	0.41
1:A:161:ILE:HG22	2:B:181:TYR:CD2	2.56	0.40
1:A:93:LEU:HD12	1:A:117:GLY:HA2	2.02	0.40
2:B:111:ALA:HB2	2:B:195:ARG:HG2	2.04	0.40
2:B:130:LYS:HA	2:B:131:PRO:HD2	1.78	0.40
1:A:104:PHE:CD2	1:A:105:LEU:HD23	2.57	0.40
2:B:92:PHE:CD1	2:B:192:ILE:HD12	2.56	0.40
2:B:82:TRP:CE3	2:B:89:CYS:HB3	2.56	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	115/142 (81%)	82 (71%)	17 (15%)	16 (14%)	0 1
2	B	119/158 (75%)	78 (66%)	29 (24%)	12 (10%)	0 3
All	All	234/300 (78%)	160 (68%)	46 (20%)	28 (12%)	0 2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ALA
1	A	124	ASP
1	A	130	ASN
1	A	132	THR
1	A	135	ASN
2	B	79	PRO
2	B	119	LEU
1	A	93	LEU
1	A	110	GLY
1	A	111	THR
1	A	122	GLN
1	A	128	TRP
2	B	87	GLY
2	B	93	SER
1	A	59	SER
1	A	123	GLY
1	A	136	GLY
1	A	143	ASN
2	B	94	THR
2	B	195	ARG
2	B	116	ILE
2	B	131	PRO
2	B	144	GLN
1	A	109	ALA
2	B	83	LEU
2	B	138	GLY
2	B	192	ILE
1	A	140	ILE

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	93/118 (79%)	84 (90%)	9 (10%)	8 31
2	B	101/140 (72%)	86 (85%)	15 (15%)	3 14
All	All	194/258 (75%)	170 (88%)	24 (12%)	4 21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	89	GLN
1	A	90	LYS
1	A	95	GLN
1	A	97	ASP
1	A	113	MET
1	A	129	THR
1	A	141	ILE
1	A	154	VAL
2	B	78	CYS
2	B	86	GLU
2	B	98	THR
2	B	108	GLN
2	B	110	GLN
2	B	121	GLU
2	B	126	GLN
2	B	134	PHE
2	B	140	TYR
2	B	149	MET
2	B	156	LEU
2	B	160	LEU
2	B	170	ARG
2	B	195	ARG
2	B	196	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	95	GLN
1	A	114	HIS

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Mol	Chain	Res	Type
2	B	108	GLN
2	B	110	GLN
2	B	112	HIS
2	B	126	GLN
2	B	127	ASN
2	B	194	GLN

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

6 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.82	0	17,19,21	0.87	1 (5%)
3	NAG	C	2	3	14,14,15	0.77	0	17,19,21	0.78	0
3	MAN	C	3	3	11,11,12	0.85	0	15,15,17	0.88	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.94	0	17,19,21	1.76	4 (23%)
3	NAG	D	2	3	14,14,15	1.43	3 (21%)	17,19,21	1.93	5 (29%)
3	MAN	D	3	3	11,11,12	0.61	0	15,15,17	1.47	1 (6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	3.04	1.56	1.52
3	D	2	NAG	O5-C5	2.82	1.49	1.43
3	D	2	NAG	O5-C1	2.45	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	C1-O5-C5	4.76	118.64	112.19
3	D	3	MAN	C1-C2-C3	4.60	115.32	109.67
3	D	1	NAG	C4-C3-C2	-4.14	104.95	111.02
3	D	2	NAG	C4-C3-C2	-3.44	105.97	111.02
3	D	1	NAG	C3-C4-C5	-3.33	104.31	110.24
3	D	2	NAG	O5-C1-C2	3.28	116.46	111.29
3	D	1	NAG	C1-O5-C5	2.85	116.06	112.19
3	C	3	MAN	C1-C2-C3	2.75	113.04	109.67
3	D	2	NAG	O5-C5-C6	2.52	111.16	107.20
3	D	1	NAG	O4-C4-C5	2.20	114.76	109.30
3	C	1	NAG	C2-N2-C7	-2.17	119.82	122.90
3	D	2	NAG	O5-C5-C4	2.08	115.89	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

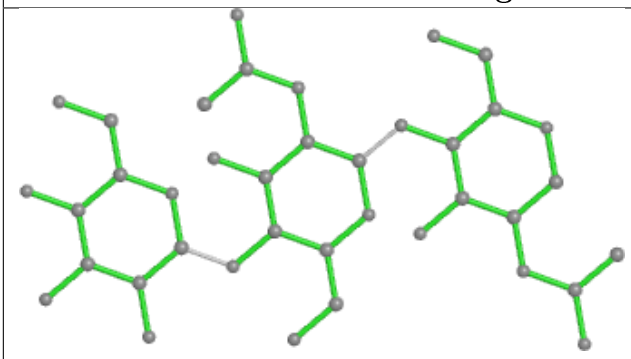
There are no ring outliers.

4 monomers are involved in 7 short contacts:

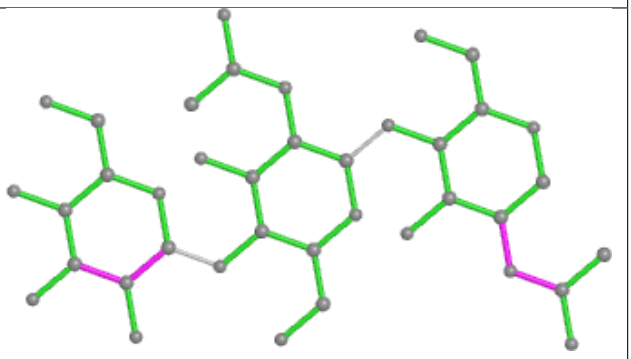
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	2	0
3	C	2	NAG	1	0
3	C	1	NAG	5	0
3	D	2	NAG	2	0

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

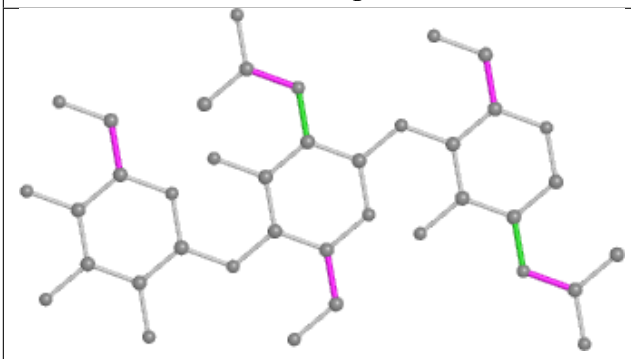
Oligosaccharide Chain C



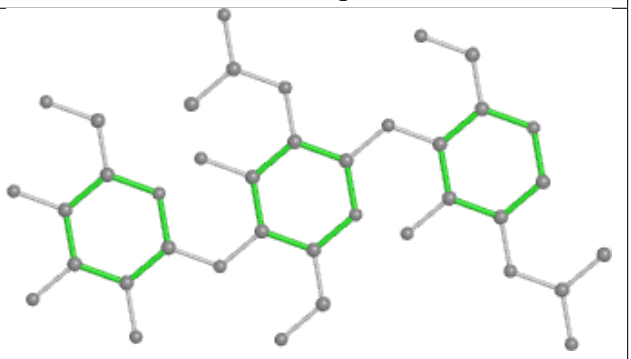
Bond lengths



Bond angles

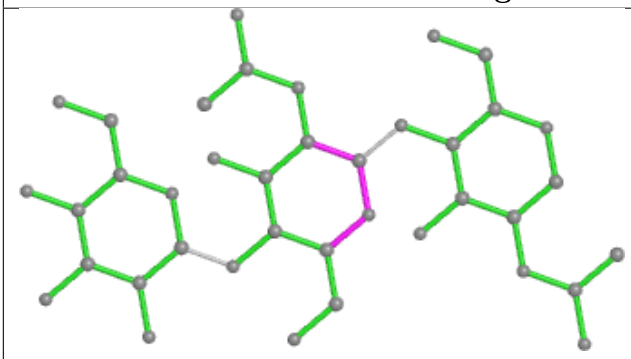


Torsions

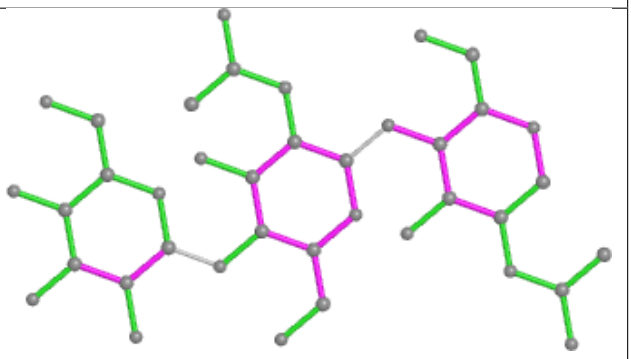


Rings

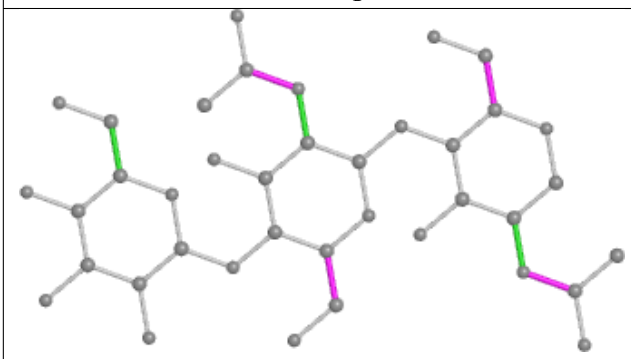
Oligosaccharide Chain D



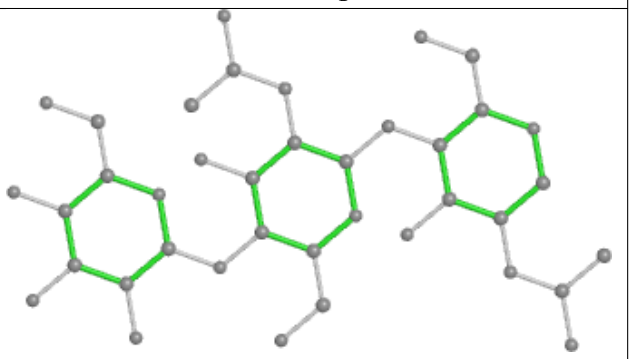
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

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	117/142 (82%)	0.10	5 (4%)	35	22	41, 96, 153, 179	0
2	B	121/158 (76%)	0.08	1 (0%)	86	78	44, 98, 133, 176	0
All	All	238/300 (79%)	0.09	6 (2%)	57	43	41, 97, 145, 179	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ILE	2.6
1	A	159	GLY	2.5
1	A	96	ILE	2.5
1	A	128	TRP	2.2
1	A	118	LEU	2.1
2	B	174	VAL	2.0

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. 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	B-factors(Å^2)	Q<0.9
3	MAN	C	3	11/12	0.76	0.23	146,146,146,146	0
3	NAG	D	1	14/15	0.85	0.18	103,103,103,103	0
3	MAN	D	3	11/12	0.85	0.19	138,138,138,138	0

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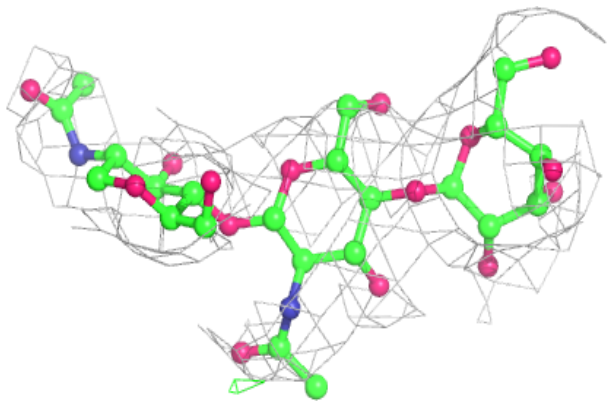
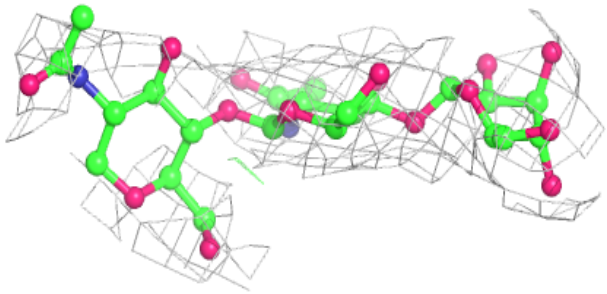
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.86	0.27	178,178,178,178	0
3	NAG	C	2	14/15	0.88	0.20	123,123,123,123	0
3	NAG	C	1	14/15	0.91	0.16	158,158,158,158	0

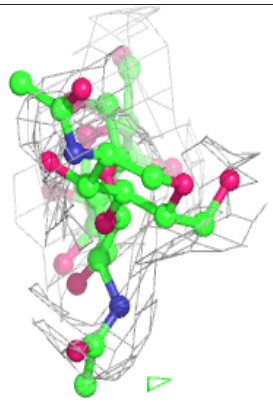
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

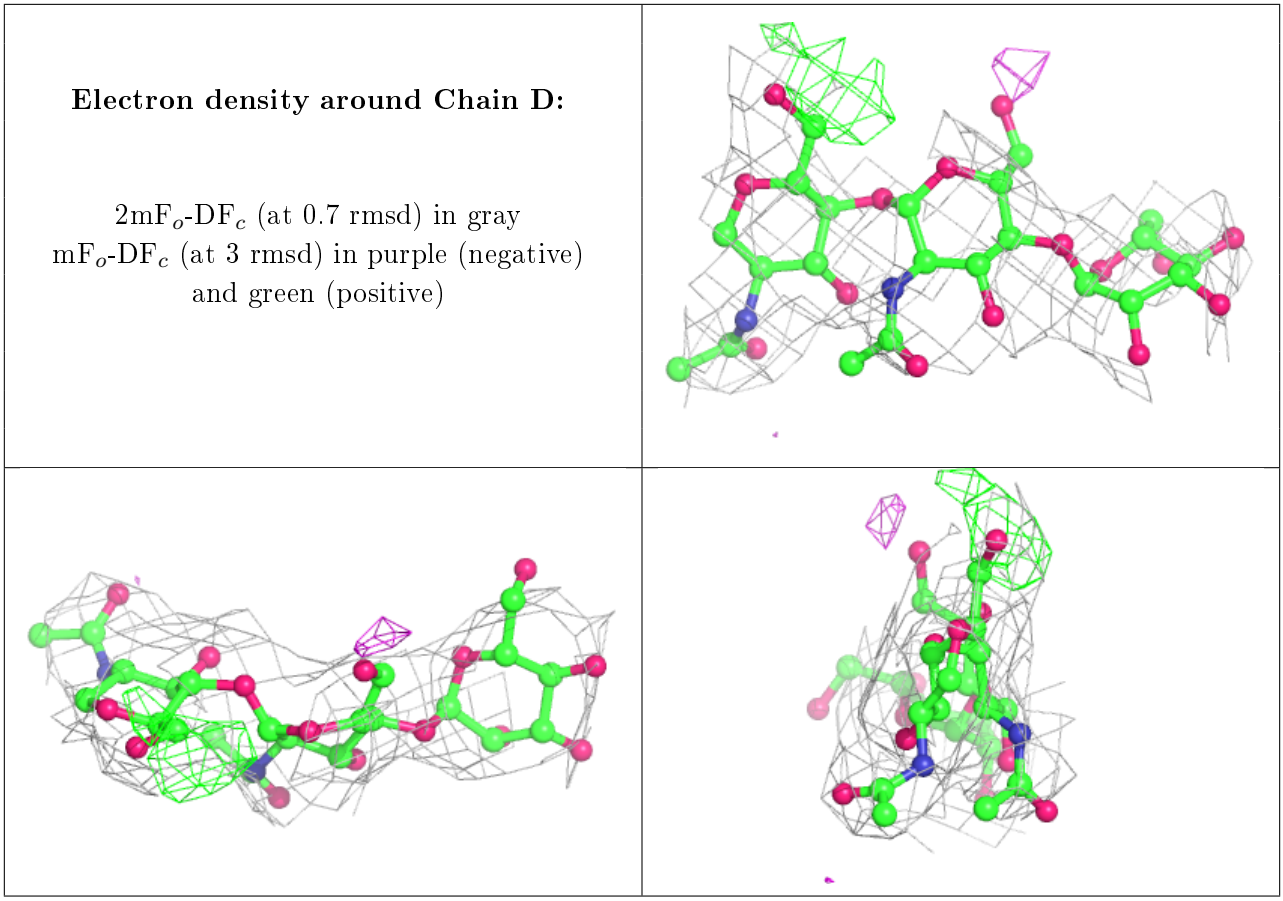






Electron density around Chain D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.