Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2026 – 04:12 PM EDT

PDB ID	:	13EW / pdb_000013ew
Title	:	Netrin-1 with heparin oligosaccharide ligand
Authors	:	Meier, M.; Moya-Torres, A.; Gupta, M.; McDougall, M.D.; Bailey-Elkin, B.A.; Koch, M.; Stetefeld, J.
Deposited on	:	2026-05-04
Resolution	:	4.08 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:

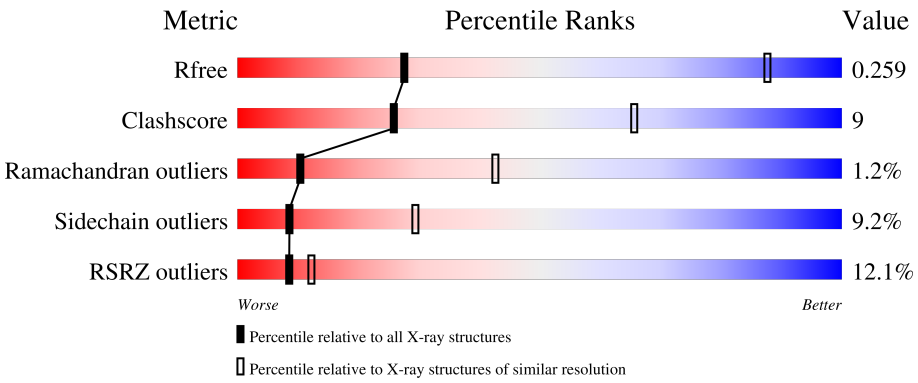
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 4.08 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}	180053	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

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	443	12%, 67%, 23%, 5%, 5%
2	N	7	100%
3	O	4	75%, 25%
4	P	6	33%, 67%
5	Q	6	17%, 83%

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Mol	Chain	Length	Quality of chain
6	H	14	79% 21%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3835 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.

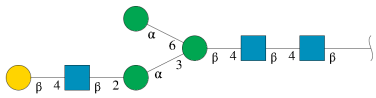
- Molecule 1 is a protein called Netrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3309	2028	619	624	38	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP Q90922
A	23	PRO	-	expression tag	UNP Q90922
A	24	LEU	-	expression tag	UNP Q90922
A	25	ALA	-	expression tag	UNP Q90922
A	459	GLY	-	expression tag	UNP Q90922
A	460	SER	-	expression tag	UNP Q90922
A	461	LEU	-	expression tag	UNP Q90922
A	462	VAL	-	expression tag	UNP Q90922
A	463	PRO	-	expression tag	UNP Q90922
A	464	ARG	-	expression tag	UNP Q90922

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



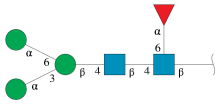
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	N	7	86	48	3	35	0	0	0

- Molecule 3 is an oligosaccharide called 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-gluco

pyranose.

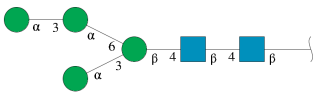
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	O	4	50	28	2	20	0	0	0

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



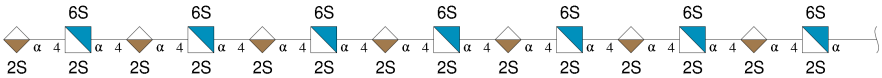
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	P	6	71	40	2	29	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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			
5	Q	6	72	40	2	30	0	0	0

- Molecule 6 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	14	246	84	7	134	21	0	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

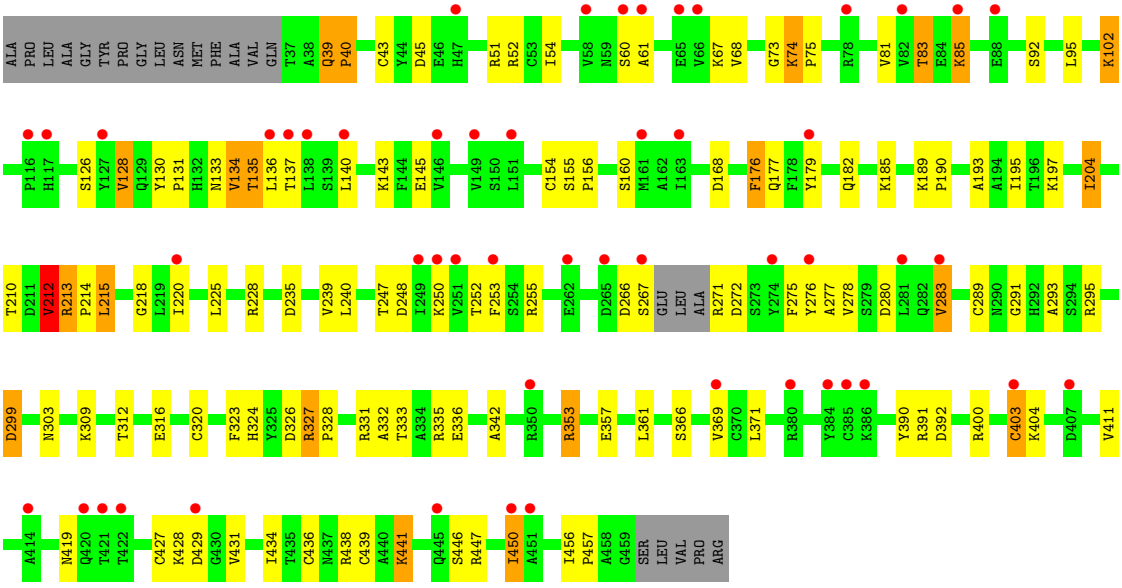
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0

3 Residue-property plots (i)

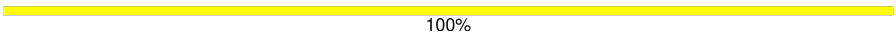
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Netrin-1

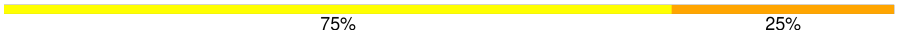
Chain A:



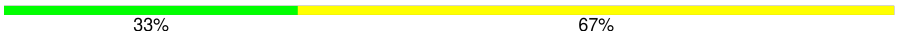
• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

• Molecule 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

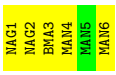
Chain O: 

• 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 6: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	204.77Å 204.77Å 99.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.23 – 4.08 49.23 – 4.08	Depositor EDS
% Data completeness (in resolution range)	76.6 (49.23-4.08) 76.6 (49.23-4.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.161 , 0.220 0.194 , 0.259	Depositor DCC
R_{free} test set	523 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	215.1	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 332.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å^2)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: CA, IDS, FUC, GAL, MAN, NAG, BMA, SGN

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	0/3390	1.15	11/4587 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	LEU	N-CA-CB	-8.32	97.68	110.65
1	A	102	LYS	CB-CA-C	6.89	121.59	110.09
1	A	135	THR	CA-CB-OG1	-6.52	99.82	109.60
1	A	145	GLU	CB-CG-CD	5.85	122.54	112.60
1	A	335	ARG	CB-CA-C	-5.57	102.10	110.90
1	A	419	ASN	CB-CA-C	5.49	118.67	109.89
1	A	323	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	299	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	176	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	248	ASP	CA-CB-CG	5.00	117.61	112.60
1	A	436	CYS	CB-CA-C	-5.00	105.16	111.86

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	ASP	Peptide
1	A	331	ARG	Sidechain
1	A	40	PRO	Peptide
1	A	73	GLY	Peptide
1	A	85	LYS	Peptide

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	3309	0	3116	67	0
2	N	86	0	73	0	0
3	O	50	0	43	1	0
4	P	71	0	61	1	0
5	Q	72	0	61	0	0
6	H	246	0	94	5	0
7	A	1	0	0	0	0
All	All	3835	0	3448	69	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 9.

All (69) 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:182:GLN:HB3	1:A:185:LYS:HD3	1.61	0.81
1:A:353:ARG:HG2	1:A:371:LEU:HD21	1.65	0.79
1:A:177:GLN:HE22	1:A:204:ILE:HG22	1.47	0.78
1:A:215:LEU:HD13	1:A:215:LEU:H	1.48	0.77
1:A:438:ARG:NH2	6:H:5:SGN:O2S	2.26	0.69
1:A:130:TYR:HB2	1:A:255:ARG:HG3	1.78	0.65
1:A:400[B]:ARG:HG2	6:H:13:SGN:O6S	1.97	0.64
1:A:68:VAL:HG12	1:A:136:LEU:HD22	1.78	0.64
1:A:74:LYS:H	1:A:74:LYS:HD2	1.63	0.64
1:A:168:ASP:O	1:A:247:THR:OG1	2.17	0.63
1:A:189:LYS:HD3	1:A:190:PRO:HD2	1.79	0.63
1:A:390:TYR:O	1:A:403:CYS:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:H	1:A:74:LYS:CD	2.14	0.60
1:A:326:ASP:OD1	1:A:366:SER:HA	2.01	0.60
1:A:299:ASP:HB3	1:A:303:ASN:H	1.67	0.59
1:A:177:GLN:NE2	1:A:204:ILE:HG22	2.17	0.59
1:A:213:ARG:HD2	1:A:213:ARG:H	1.66	0.59
1:A:61:ALA:HB2	1:A:283:VAL:HG12	1.85	0.58
1:A:43:CYS:SG	1:A:309:LYS:HG3	2.43	0.57
1:A:324:HIS:HA	1:A:342:ALA:HA	1.86	0.56
1:A:128:VAL:HG21	1:A:134:VAL:HG23	1.89	0.55
1:A:333:THR:HG23	1:A:336:GLU:H	1.72	0.55
1:A:130:TYR:CD1	1:A:131:PRO:HA	2.43	0.53
1:A:45:ASP:HA	1:A:51:ARG:NH1	2.22	0.53
1:A:289:CYS:CB	1:A:293:ALA:HB3	2.39	0.53
1:A:155:SER:HB2	1:A:156:PRO:HD2	1.90	0.52
1:A:438:ARG:HD2	1:A:439:CYS:O	2.10	0.52
1:A:225:LEU:HA	1:A:228:ARG:HG3	1.92	0.51
6:H:9:SGN:N2	6:H:9:SGN:H5	2.25	0.51
1:A:126:SER:HA	1:A:275:PHE:HB3	1.93	0.51
1:A:67:LYS:O	1:A:136:LEU:HA	2.11	0.51
1:A:411:VAL:O	1:A:428:LYS:HD3	2.12	0.50
1:A:193:ALA:H	1:A:204:ILE:HG12	1.76	0.49
6:H:13:SGN:H3	6:H:13:SGN:O2S	2.12	0.49
1:A:214:PRO:HG2	1:A:218:GLY:HA2	1.94	0.48
1:A:312:THR:HA	1:A:320:CYS:HA	1.96	0.48
1:A:213:ARG:HA	1:A:214:PRO:C	2.38	0.47
1:A:137:THR:HG22	1:A:250:LYS:HG3	1.95	0.47
1:A:213:ARG:H	1:A:213:ARG:CD	2.25	0.47
1:A:130:TYR:CB	1:A:255:ARG:HG3	2.45	0.47
1:A:400[B]:ARG:HD3	6:H:13:SGN:O4S	2.15	0.47
1:A:450:ILE:HD13	1:A:450:ILE:H	1.79	0.47
1:A:215:LEU:H	1:A:215:LEU:CD1	2.17	0.47
1:A:428:LYS:O	1:A:431:VAL:HG23	2.15	0.47
1:A:327:ARG:HG3	1:A:328:PRO:HD2	1.97	0.45
1:A:446:SER:OG	1:A:447:ARG:N	2.49	0.45
1:A:155:SER:HB3	1:A:277:ALA:HB3	1.97	0.45
1:A:291:GLY:HA3	1:A:332:ALA:HB3	1.98	0.45
1:A:54:ILE:HG12	1:A:291:GLY:HA2	1.99	0.45
1:A:357:GLU:O	1:A:361:LEU:HG	2.16	0.44
1:A:441:LYS:HD3	1:A:441:LYS:H	1.82	0.44
1:A:52:ARG:HG3	1:A:332:ALA:HB1	2.00	0.44
1:A:212:VAL:HG23	1:A:213:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG12	1:A:83:THR:HG22	2.00	0.43
1:A:130:TYR:CG	1:A:131:PRO:HA	2.54	0.43
1:A:133:ASN:OD1	4:P:1:NAG:O5	2.35	0.43
1:A:60:SER:HB2	1:A:140:LEU:HD22	2.00	0.43
1:A:102:LYS:NZ	3:O:1:NAG:H61	2.34	0.43
1:A:39:GLN:HB3	1:A:40:PRO:HD3	2.01	0.42
1:A:160:SER:HA	1:A:179:TYR:O	2.19	0.42
1:A:428:LYS:O	1:A:429:ASP:C	2.63	0.42
1:A:391:ARG:NH2	1:A:392:ASP:O	2.52	0.42
1:A:143:LYS:HD2	1:A:316:GLU:HG2	2.03	0.41
1:A:253:PHE:HB3	1:A:276:TYR:CE1	2.54	0.41
1:A:133:ASN:HD22	1:A:252:THR:CG2	2.34	0.41
1:A:74:LYS:HA	1:A:75:PRO:HA	1.89	0.41
1:A:177:GLN:HE22	1:A:204:ILE:CG2	2.23	0.40
1:A:299:ASP:HB2	1:A:303:ASN:O	2.22	0.40
1:A:427:CYS:HB3	1:A:431:VAL:HB	2.04	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	418/443 (94%)	386 (92%)	27 (6%)	5 (1%)	10 43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	PRO
1	A	212	VAL
1	A	403	CYS
1	A	39	GLN
1	A	327	ARG

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	370/385 (96%)	335 (90%)	35 (10%)	8 28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	83	THR
1	A	85	LYS
1	A	92	SER
1	A	128	VAL
1	A	134	VAL
1	A	135	THR
1	A	154	CYS
1	A	176	PHE
1	A	195	ILE
1	A	197	LYS
1	A	204	ILE
1	A	210	THR
1	A	212	VAL
1	A	213	ARG
1	A	215	LEU
1	A	220	ILE
1	A	235	ASP
1	A	239	VAL
1	A	240	LEU
1	A	267	SER
1	A	271	ARG
1	A	272	ASP
1	A	278	VAL
1	A	280	ASP
1	A	283	VAL
1	A	295[A]	ARG
1	A	295[B]	ARG
1	A	353	ARG
1	A	369	VAL

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Mol	Chain	Res	Type
1	A	404	LYS
1	A	434	ILE
1	A	441	LYS
1	A	450	ILE
1	A	456	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	376	ASN

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)

37 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	$\#\|Z\| > 2$
6	SGN	H	1	6	20,20,20	1.40	3 (15%)	25,31,31	1.16	1 (4%)
6	IDS	H	10	6	16,16,17	1.30	2 (12%)	16,24,26	1.03	1 (6%)
6	SGN	H	11	6	19,19,20	1.42	3 (15%)	23,29,31	1.27	1 (4%)
6	IDS	H	12	6	16,16,17	1.38	3 (18%)	16,24,26	0.79	0
6	SGN	H	13	6	19,19,20	2.61	5 (26%)	23,29,31	1.45	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	IDS	H	14	6	16,16,17	1.49	3 (18%)	16,24,26	1.15	1 (6%)
6	IDS	H	2	6	16,16,17	1.21	1 (6%)	16,24,26	0.96	1 (6%)
6	SGN	H	3	6	19,19,20	1.35	3 (15%)	23,29,31	1.25	1 (4%)
6	IDS	H	4	6	16,16,17	1.13	2 (12%)	16,24,26	1.00	1 (6%)
6	SGN	H	5	6	19,19,20	1.58	5 (26%)	23,29,31	1.35	2 (8%)
6	IDS	H	6	6	16,16,17	1.21	2 (12%)	16,24,26	0.98	1 (6%)
6	SGN	H	7	6	19,19,20	1.62	7 (36%)	23,29,31	1.32	1 (4%)
6	IDS	H	8	6	16,16,17	1.30	2 (12%)	16,24,26	1.13	1 (6%)
6	SGN	H	9	6	19,19,20	1.50	3 (15%)	23,29,31	1.21	1 (4%)
2	NAG	N	1	2,1	14,14,15	0.36	0	17,19,21	1.40	2 (11%)
2	NAG	N	2	2	14,14,15	1.05	1 (7%)	17,19,21	2.76	4 (23%)
2	BMA	N	3	2	11,11,12	0.82	0	15,15,17	0.92	1 (6%)
2	MAN	N	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.62	3 (20%)
2	NAG	N	5	2	14,14,15	0.78	0	17,19,21	1.01	1 (5%)
2	GAL	N	6	2	11,11,12	0.97	1 (9%)	15,15,17	0.75	0
2	MAN	N	7	2	11,11,12	0.98	0	15,15,17	1.04	2 (13%)
3	NAG	O	1	3,1	14,14,15	0.97	1 (7%)	17,19,21	2.08	5 (29%)
3	NAG	O	2	3	14,14,15	0.81	0	17,19,21	0.96	1 (5%)
3	BMA	O	3	3	11,11,12	0.68	0	15,15,17	0.83	1 (6%)
3	MAN	O	4	3	11,11,12	0.76	0	15,15,17	2.05	3 (20%)
4	NAG	P	1	4,1	14,14,15	0.72	0	17,19,21	1.05	0
4	NAG	P	2	4	14,14,15	0.62	0	17,19,21	1.68	3 (17%)
4	BMA	P	3	4	11,11,12	0.71	0	15,15,17	0.84	0
4	MAN	P	4	4	11,11,12	0.81	0	15,15,17	0.76	0
4	MAN	P	5	4	11,11,12	0.65	0	15,15,17	1.61	2 (13%)
4	FUC	P	6	4	10,10,11	1.37	1 (10%)	14,14,16	1.23	1 (7%)
5	NAG	Q	1	5,1	14,14,15	1.48	2 (14%)	17,19,21	3.07	9 (52%)
5	NAG	Q	2	5	14,14,15	1.48	3 (21%)	17,19,21	2.33	5 (29%)
5	BMA	Q	3	5	11,11,12	0.82	0	15,15,17	1.58	3 (20%)
5	MAN	Q	4	5	11,11,12	0.77	0	15,15,17	1.66	2 (13%)
5	MAN	Q	5	5	11,11,12	0.57	0	15,15,17	0.97	0
5	MAN	Q	6	5	11,11,12	0.94	1 (9%)	15,15,17	1.25	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
6	SGN	H	1	6	-	1/11/31/31	0/1/1/1
6	IDS	H	10	6	-	0/9/26/29	0/1/1/1
6	SGN	H	11	6	-	4/11/28/31	0/1/1/1
6	IDS	H	12	6	-	2/9/26/29	0/1/1/1
6	SGN	H	13	6	-	4/11/28/31	0/1/1/1
6	IDS	H	14	6	-	0/9/26/29	0/1/1/1
6	IDS	H	2	6	-	0/9/26/29	0/1/1/1
6	SGN	H	3	6	-	5/11/28/31	0/1/1/1
6	IDS	H	4	6	-	0/9/26/29	0/1/1/1
6	SGN	H	5	6	-	5/11/28/31	0/1/1/1
6	IDS	H	6	6	-	0/9/26/29	0/1/1/1
6	SGN	H	7	6	-	5/11/28/31	0/1/1/1
6	IDS	H	8	6	-	0/9/26/29	0/1/1/1
6	SGN	H	9	6	-	4/11/28/31	0/1/1/1
2	NAG	N	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	BMA	N	3	2	-	2/2/19/22	0/1/1/1
2	MAN	N	4	2	-	0/2/19/22	0/1/1/1
2	NAG	N	5	2	-	2/6/23/26	0/1/1/1
2	GAL	N	6	2	-	2/2/19/22	0/1/1/1
2	MAN	N	7	2	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	MAN	P	4	4	-	0/2/19/22	0/1/1/1
4	MAN	P	5	4	-	0/2/19/22	0/1/1/1
4	FUC	P	6	4	-	-	0/1/1/1
5	NAG	Q	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	5/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	5	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	6	5	-	0/2/19/22	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	13	SGN	O2S-S1	-7.21	1.33	1.42
6	H	13	SGN	O1S-S1	-6.53	1.34	1.42
6	H	11	SGN	O3S-S1	3.67	1.65	1.47
5	Q	1	NAG	C2-N2	3.63	1.52	1.46
6	H	1	SGN	O3S-S1	3.58	1.64	1.47
6	H	5	SGN	O3S-S1	3.57	1.64	1.47
6	H	13	SGN	O3S-S1	3.56	1.64	1.47
6	H	7	SGN	O3S-S1	3.45	1.64	1.47
6	H	9	SGN	O3S-S1	3.36	1.63	1.47
5	Q	2	NAG	C2-N2	3.27	1.51	1.46
6	H	14	IDS	O2-C2	-3.08	1.42	1.47
6	H	3	SGN	O3S-S1	3.05	1.62	1.47
2	N	2	NAG	C2-N2	2.97	1.51	1.46
6	H	5	SGN	C3-C2	2.81	1.58	1.52
6	H	14	IDS	O5-C1	2.77	1.48	1.43
6	H	8	IDS	C3-C2	2.66	1.58	1.53
6	H	9	SGN	C3-C2	2.54	1.57	1.52
5	Q	1	NAG	C1-C2	2.52	1.55	1.52
6	H	12	IDS	O1S-S	-2.51	1.34	1.45
6	H	7	SGN	C4-C5	2.51	1.58	1.53
6	H	7	SGN	S1-N2	2.51	1.62	1.59
6	H	13	SGN	C1-C2	2.50	1.55	1.52
6	H	7	SGN	O2S-S1	2.42	1.44	1.42
6	H	5	SGN	C1-C2	2.42	1.55	1.52
6	H	10	IDS	O2-C2	-2.42	1.43	1.47
6	H	5	SGN	O1S-S1	2.40	1.44	1.42
3	O	1	NAG	O4-C4	2.37	1.48	1.43
6	H	12	IDS	O3S-S	2.36	1.65	1.50
6	H	14	IDS	C3-C2	2.36	1.58	1.53
5	Q	6	MAN	C2-C3	2.34	1.56	1.52
6	H	11	SGN	O1S-S1	2.34	1.44	1.42
6	H	12	IDS	O2-S	-2.29	1.50	1.57
6	H	5	SGN	O6S-S2	2.25	1.64	1.50
6	H	8	IDS	O3S-S	2.24	1.64	1.50
6	H	6	IDS	O2-C2	-2.24	1.44	1.47
6	H	11	SGN	O6S-S2	2.24	1.64	1.50
6	H	3	SGN	C1-C2	2.23	1.55	1.52
6	H	9	SGN	O6S-S2	2.21	1.64	1.50
6	H	7	SGN	O6S-S2	2.20	1.64	1.50
6	H	2	IDS	O3S-S	2.20	1.64	1.50
6	H	10	IDS	O3S-S	2.20	1.64	1.50
6	H	3	SGN	O6S-S2	2.19	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	7	SGN	O5-C5	2.19	1.47	1.43
6	H	4	IDS	O2-C2	-2.18	1.44	1.47
6	H	4	IDS	O3S-S	2.18	1.64	1.50
6	H	1	SGN	O6S-S2	2.18	1.64	1.50
5	Q	2	NAG	C1-C2	2.15	1.55	1.52
6	H	7	SGN	O1S-S1	2.15	1.44	1.42
6	H	13	SGN	O6S-S2	2.14	1.63	1.50
6	H	6	IDS	O3S-S	2.11	1.63	1.50
6	H	1	SGN	O2S-S1	2.08	1.44	1.42
4	P	6	FUC	O5-C1	2.07	1.47	1.43
2	N	6	GAL	O5-C5	2.05	1.47	1.43
2	N	4	MAN	C2-C3	2.04	1.55	1.52
5	Q	2	NAG	O4-C4	2.02	1.48	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	2	NAG	C2-N2-C7	8.22	133.91	122.90
5	Q	2	NAG	C2-N2-C7	7.34	132.74	122.90
5	Q	1	NAG	C2-N2-C7	5.82	130.70	122.90
3	O	1	NAG	C1-O5-C5	5.74	119.87	112.19
5	Q	1	NAG	C1-O5-C5	5.36	119.36	112.19
3	O	4	MAN	C1-O5-C5	5.24	119.22	112.19
2	N	2	NAG	C1-O5-C5	5.15	119.09	112.19
6	H	9	SGN	O1S-S1-O2S	-4.93	109.40	120.36
5	Q	1	NAG	C4-C3-C2	4.91	118.22	111.02
6	H	11	SGN	O1S-S1-O2S	-4.91	109.44	120.36
6	H	7	SGN	O1S-S1-O2S	-4.89	109.47	120.36
6	H	1	SGN	O1S-S1-O2S	-4.89	109.49	120.36
6	H	3	SGN	O1S-S1-O2S	-4.86	109.55	120.36
6	H	5	SGN	O1S-S1-O2S	-4.83	109.62	120.36
5	Q	4	MAN	C1-O5-C5	4.56	118.30	112.19
5	Q	1	NAG	O7-C7-N2	4.30	129.58	121.98
5	Q	1	NAG	O7-C7-C8	-4.27	114.45	122.05
4	P	2	NAG	C2-N2-C7	4.26	128.61	122.90
3	O	4	MAN	C1-C2-C3	4.26	115.85	109.64
2	N	1	NAG	C1-O5-C5	4.23	117.86	112.19
2	N	2	NAG	C1-C2-N2	4.19	117.04	110.43
6	H	13	SGN	O1S-S1-O2S	-4.17	111.09	120.36
2	N	4	MAN	C1-O5-C5	4.09	117.67	112.19
4	P	5	MAN	C1-O5-C5	3.92	117.44	112.19
5	Q	3	BMA	C1-C2-C3	3.71	115.05	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	5	MAN	C1-C2-C3	3.55	114.81	109.64
5	Q	3	BMA	C1-O5-C5	3.49	116.86	112.19
3	O	1	NAG	C2-N2-C7	3.41	127.47	122.90
6	H	13	SGN	O5-C1-C2	3.33	116.44	111.29
4	P	2	NAG	C1-O5-C5	3.32	116.64	112.19
6	H	14	IDS	O2-C2-C3	3.28	111.53	106.95
5	Q	1	NAG	C1-C2-N2	3.26	115.57	110.43
5	Q	2	NAG	C1-C2-N2	3.13	115.36	110.43
5	Q	2	NAG	O5-C5-C6	-3.11	101.61	107.66
5	Q	1	NAG	O4-C4-C3	-2.99	103.32	110.38
6	H	5	SGN	O5-C1-C2	2.97	115.89	111.29
6	H	10	IDS	O5-C1-C2	2.88	115.34	109.51
4	P	6	FUC	O5-C5-C6	2.76	113.39	107.40
3	O	1	NAG	O4-C4-C3	2.74	116.84	110.38
6	H	4	IDS	O5-C1-C2	2.66	114.89	109.51
6	H	8	IDS	O2-C2-C3	2.53	110.49	106.95
5	Q	3	BMA	C3-C4-C5	2.53	114.82	110.23
4	P	2	NAG	C1-C2-N2	-2.50	106.49	110.43
5	Q	6	MAN	C1-O5-C5	2.46	115.48	112.19
5	Q	2	NAG	C6-C5-C4	-2.41	107.11	113.02
6	H	2	IDS	O5-C1-C2	2.40	114.36	109.51
2	N	4	MAN	C3-C4-C5	-2.37	105.94	110.23
3	O	1	NAG	C4-C3-C2	2.29	114.38	111.02
2	N	4	MAN	C1-C2-C3	2.28	112.97	109.64
5	Q	1	NAG	O4-C4-C5	-2.27	103.75	109.32
3	O	4	MAN	C3-C4-C5	-2.26	106.14	110.23
6	H	6	IDS	O5-C1-C2	2.23	114.03	109.51
2	N	1	NAG	O3-C3-C2	-2.23	104.76	109.40
2	N	7	MAN	C1-O5-C5	2.23	115.18	112.19
5	Q	4	MAN	C1-C2-C3	2.21	112.87	109.64
3	O	3	BMA	C1-O5-C5	2.21	115.15	112.19
3	O	2	NAG	C2-N2-C7	2.19	125.84	122.90
2	N	2	NAG	O7-C7-N2	2.15	125.78	121.98
5	Q	1	NAG	C6-C5-C4	2.14	118.27	113.02
2	N	5	NAG	C2-N2-C7	2.11	125.73	122.90
2	N	3	BMA	O6-C6-C5	2.06	118.35	111.33
5	Q	2	NAG	O4-C4-C5	2.05	114.36	109.32
3	O	1	NAG	C3-C4-C5	-2.02	106.57	110.23
2	N	7	MAN	O5-C5-C4	-2.02	105.91	110.83

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C1-C2-N2-C7
2	N	5	NAG	C8-C7-N2-C2
2	N	5	NAG	O7-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
5	Q	1	NAG	C3-C2-N2-C7
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
6	H	3	SGN	C4-C5-C6-O6
6	H	3	SGN	O5-C5-C6-O6
6	H	9	SGN	C6-O6-S2-O4S
6	H	11	SGN	C4-C5-C6-O6
6	H	11	SGN	O5-C5-C6-O6
6	H	11	SGN	C2-N2-S1-O1S
6	H	12	IDS	C1-C2-O2-S
6	H	13	SGN	C3-C2-N2-S1
6	H	13	SGN	C4-C5-C6-O6
6	H	13	SGN	O5-C5-C6-O6
3	O	1	NAG	C8-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
5	Q	3	BMA	O5-C5-C6-O6
2	N	6	GAL	O5-C5-C6-O6
2	N	6	GAL	C4-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	Q	3	BMA	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
6	H	9	SGN	C6-O6-S2-O5S
5	Q	5	MAN	O5-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
6	H	7	SGN	C6-O6-S2-O5S
6	H	7	SGN	C6-O6-S2-O6S
6	H	9	SGN	C6-O6-S2-O6S
6	H	5	SGN	C1-C2-N2-S1
3	O	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	H	5	SGN	C3-C2-N2-S1
5	Q	4	MAN	O5-C5-C6-O6
6	H	7	SGN	C2-N2-S1-O1S
4	P	1	NAG	C4-C5-C6-O6
6	H	5	SGN	C6-O6-S2-O6S
6	H	7	SGN	C6-O6-S2-O4S
5	Q	5	MAN	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
6	H	1	SGN	C2-N2-S1-O1S
2	N	1	NAG	C3-C2-N2-C7
4	P	2	NAG	C4-C5-C6-O6
6	H	5	SGN	C6-O6-S2-O4S
6	H	5	SGN	C6-O6-S2-O5S
4	P	1	NAG	O5-C5-C6-O6
6	H	3	SGN	C6-O6-S2-O5S
4	P	1	NAG	C1-C2-N2-C7
6	H	13	SGN	C2-N2-S1-O2S
4	P	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
6	H	3	SGN	C5-C6-O6-S2
6	H	11	SGN	C5-C6-O6-S2
6	H	3	SGN	C6-O6-S2-O4S
6	H	12	IDS	C2-O2-S-O2S
6	H	7	SGN	C5-C6-O6-S2
6	H	9	SGN	O5-C5-C6-O6

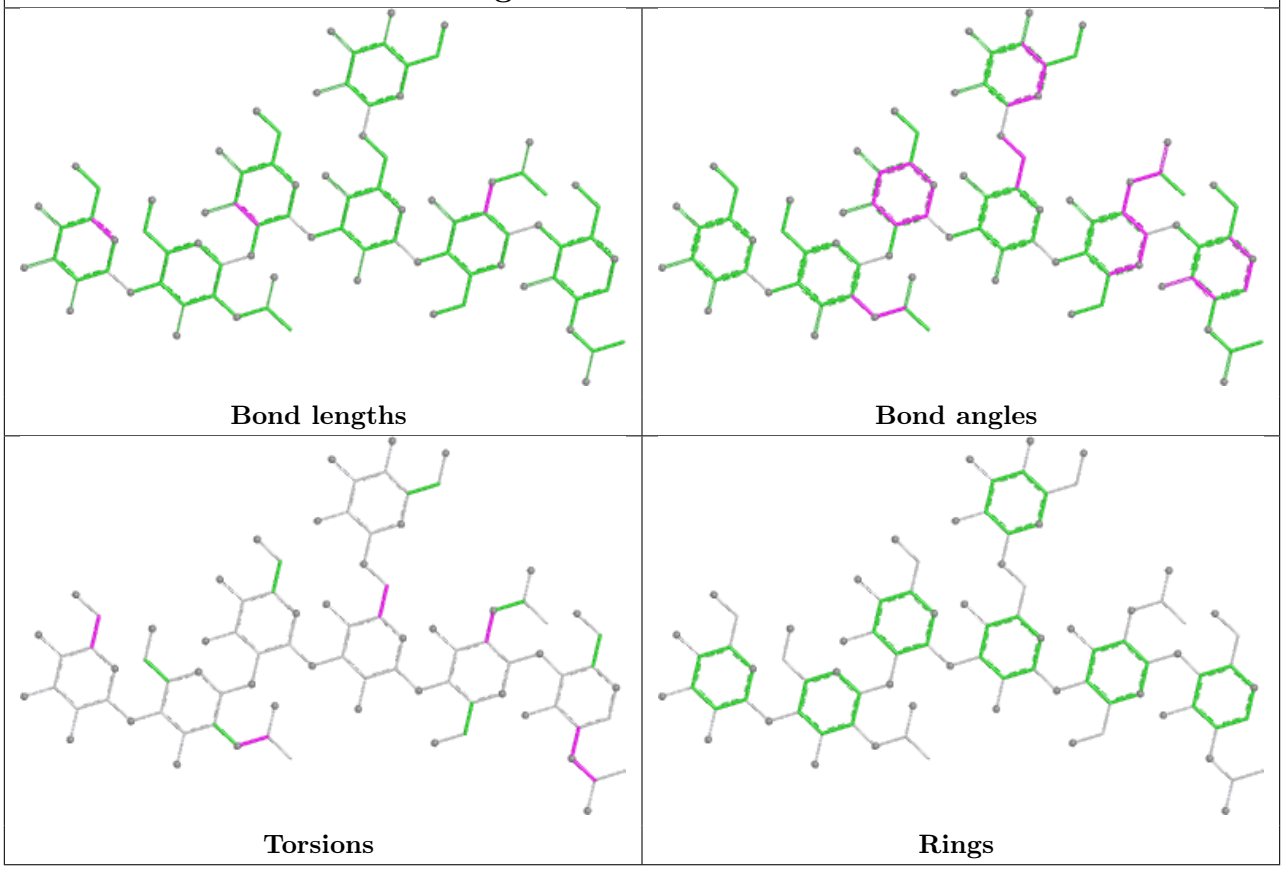
There are no ring outliers.

5 monomers are involved in 7 short contacts:

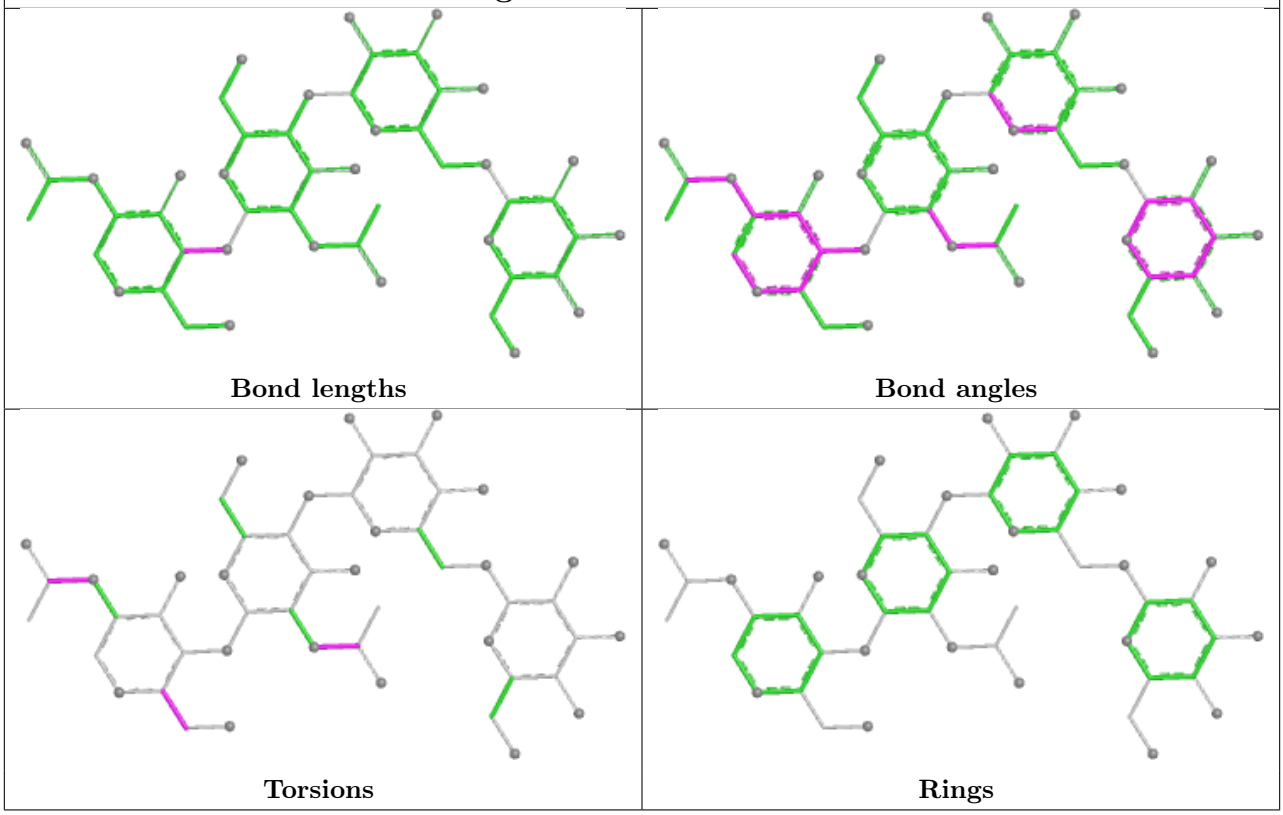
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1	NAG	1	0
6	H	5	SGN	1	0
6	H	9	SGN	1	0
6	H	13	SGN	3	0
3	O	1	NAG	1	0

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

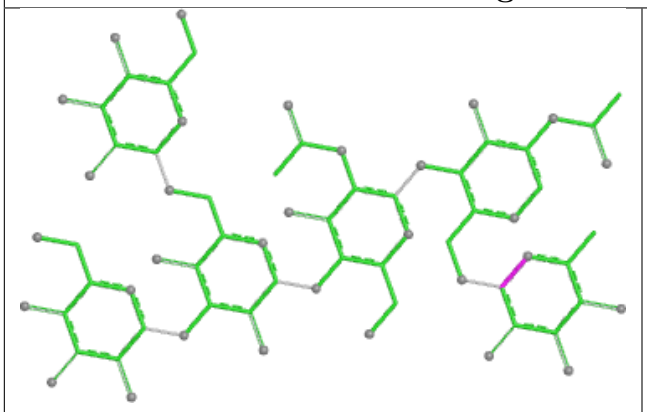
Oligosaccharide Chain N



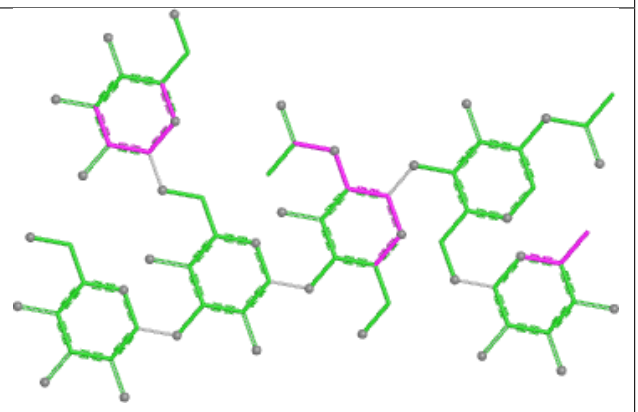
Oligosaccharide Chain O



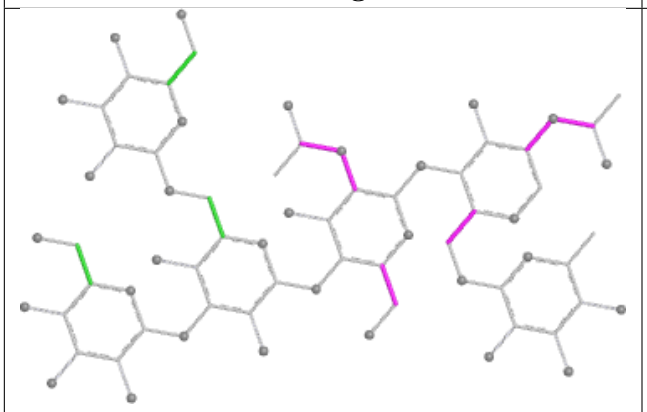
Oligosaccharide Chain P



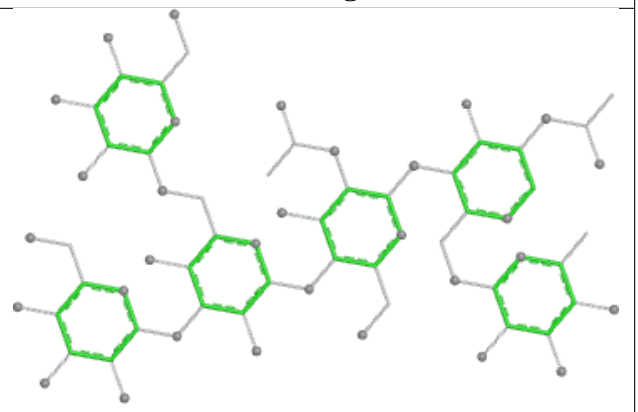
Bond lengths



Bond angles

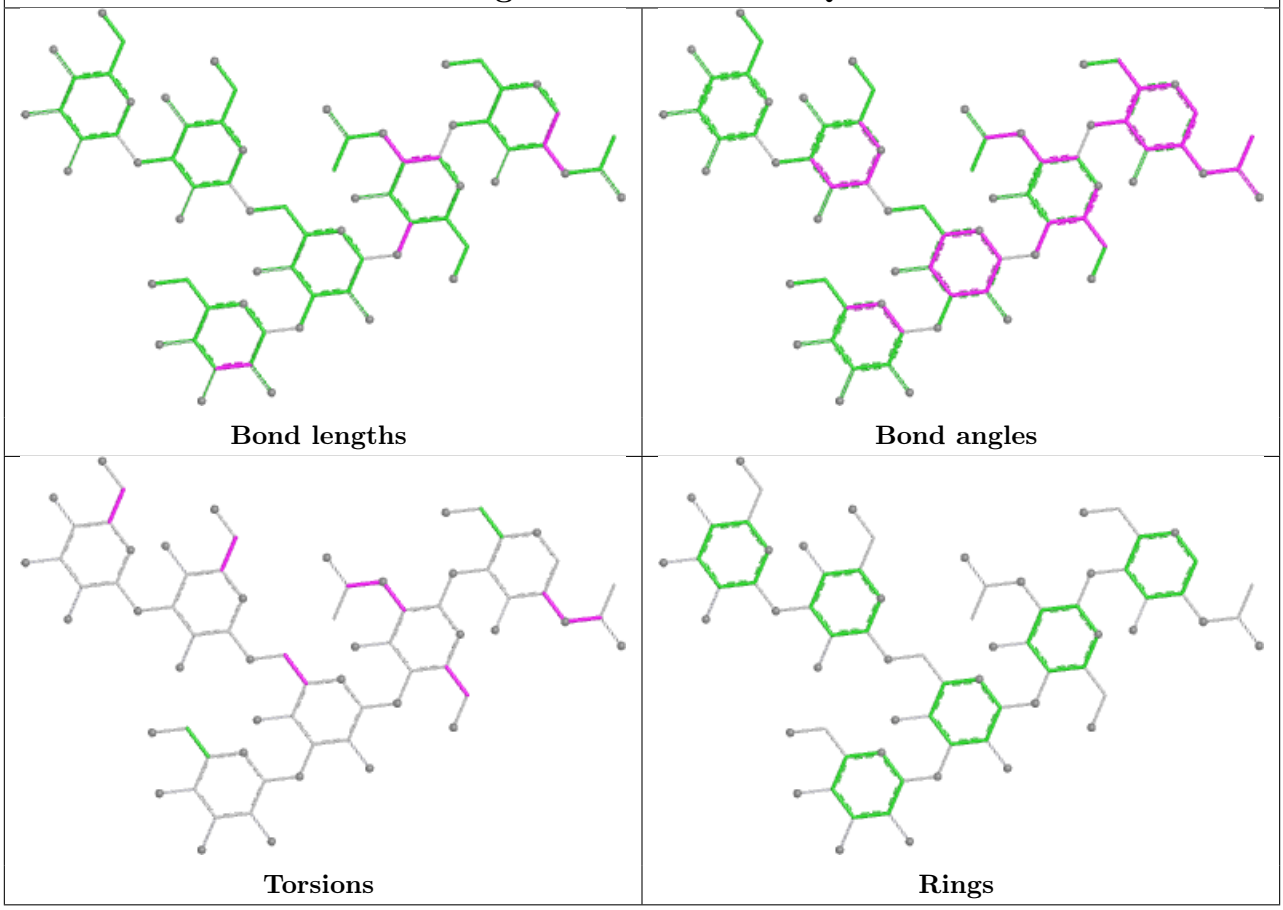


Torsions

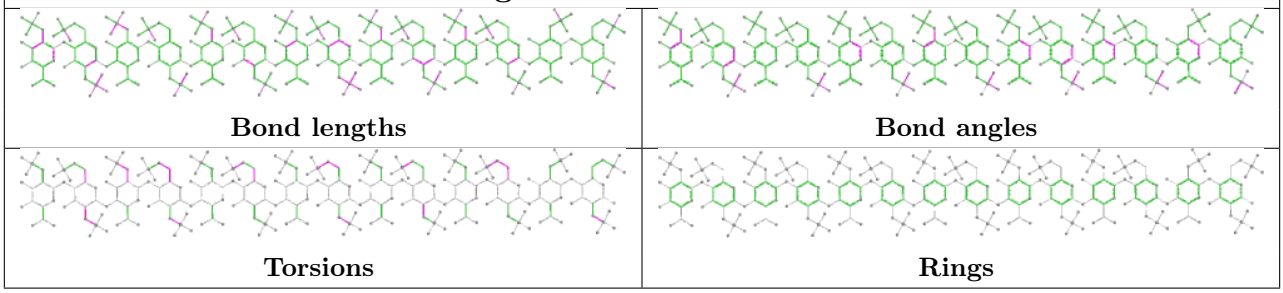


Rings

Oligosaccharide Chain Q



Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	420/443 (94%)	0.61	51 (12%)	8	12	106, 247, 337, 530	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	GLU	6.7
1	A	60	SER	6.5
1	A	117	HIS	6.3
1	A	384	TYR	5.7
1	A	450	ILE	5.4
1	A	249	ILE	5.2
1	A	281	LEU	5.1
1	A	161	MET	5.0
1	A	136	LEU	4.9
1	A	251	VAL	4.8
1	A	283	VAL	4.5
1	A	149	VAL	4.5
1	A	253	PHE	4.4
1	A	451	ALA	4.3
1	A	138	LEU	4.2
1	A	414	ALA	4.2
1	A	179	TYR	4.2
1	A	151	LEU	4.0
1	A	369	VAL	3.9
1	A	163	ILE	3.7
1	A	429	ASP	3.5
1	A	116	PRO	3.4
1	A	61	ALA	3.4
1	A	220	ILE	3.2
1	A	250	LYS	3.1
1	A	407	ASP	3.1
1	A	146	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	386	LYS	3.1
1	A	140	LEU	2.9
1	A	276	TYR	2.8
1	A	421	THR	2.8
1	A	385	CYS	2.7
1	A	65	GLU	2.7
1	A	380	ARG	2.6
1	A	350	ARG	2.6
1	A	420	GLN	2.6
1	A	66	VAL	2.5
1	A	82	VAL	2.5
1	A	85	LYS	2.5
1	A	265	ASP	2.3
1	A	445	GLN	2.2
1	A	78	ARG	2.2
1	A	422	THR	2.2
1	A	47	HIS	2.2
1	A	403	CYS	2.1
1	A	58	VAL	2.1
1	A	267	SER	2.1
1	A	127	TYR	2.0
1	A	262	GLU	2.0
1	A	274	TYR	2.0
1	A	137	THR	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
2	NAG	N	1	14/15	-	-	273,319,367,373	0
2	NAG	N	2	14/15	-	-	284,363,468,568	0
2	BMA	N	3	11/12	-	-	357,410,437,489	0
2	MAN	N	4	11/12	-	-	356,367,457,506	0

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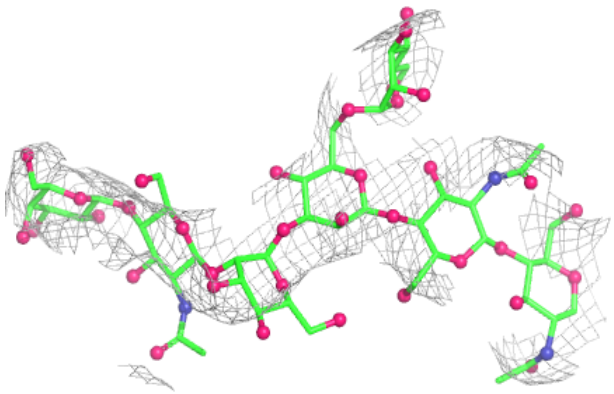
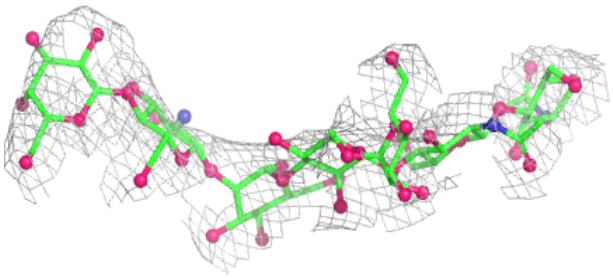
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	N	5	14/15	-	-	339,390,438,458	0
2	GAL	N	6	11/12	-	-	276,373,452,470	0
2	MAN	N	7	11/12	-	-	342,394,475,538	0
3	NAG	O	1	14/15	-	-	333,439,474,475	0
3	NAG	O	2	14/15	-	-	460,506,588,637	0
3	BMA	O	3	11/12	-	-	454,505,536,545	0
3	MAN	O	4	11/12	-	-	490,523,588,620	0
4	NAG	P	1	14/15	-	-	247,269,299,393	0
4	NAG	P	2	14/15	-	-	273,289,359,385	0
4	BMA	P	3	11/12	-	-	389,414,462,496	0
4	MAN	P	4	11/12	-	-	453,473,518,564	0
4	MAN	P	5	11/12	-	-	441,449,455,482	0
4	FUC	P	6	10/11	-	-	242,368,417,474	0
5	NAG	Q	1	14/15	-	-	197,242,273,313	0
5	NAG	Q	2	14/15	-	-	218,290,388,465	0
5	BMA	Q	3	11/12	-	-	348,379,434,454	0
5	MAN	Q	4	11/12	-	-	399,480,489,494	0
5	MAN	Q	5	11/12	-	-	426,459,482,488	0
5	MAN	Q	6	11/12	-	-	303,345,378,405	0
6	SGN	H	1	20/20	-	-	282,339,434,445	20
6	IDS	H	2	16/17	-	-	307,357,463,506	16
6	SGN	H	3	19/20	-	-	234,298,395,436	19
6	IDS	H	4	16/17	-	-	249,333,493,495	16
6	SGN	H	5	19/20	-	-	247,299,398,403	19
6	IDS	H	6	16/17	-	-	303,353,433,520	16
6	SGN	H	7	19/20	-	-	299,362,556,592	19
6	IDS	H	8	16/17	-	-	304,339,416,425	16
6	SGN	H	9	19/20	-	-	268,331,490,508	19
6	IDS	H	10	16/17	-	-	254,326,413,451	16
6	SGN	H	11	19/20	-	-	286,314,446,464	19
6	IDS	H	12	16/17	-	-	269,323,374,433	16
6	SGN	H	13	19/20	-	-	254,307,361,376	19
6	IDS	H	14	16/17	-	-	242,281,412,413	16

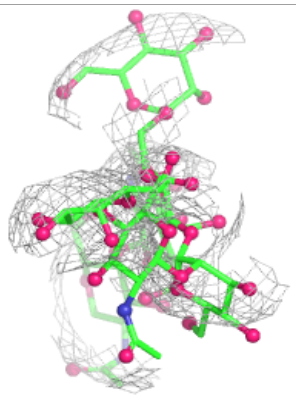
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain N:

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

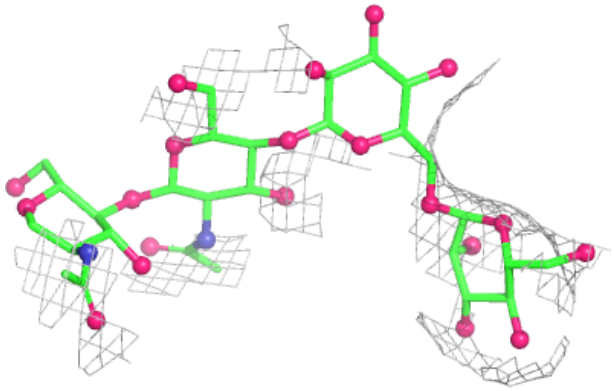


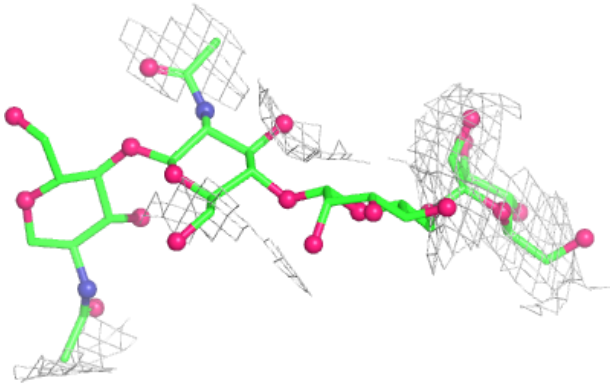


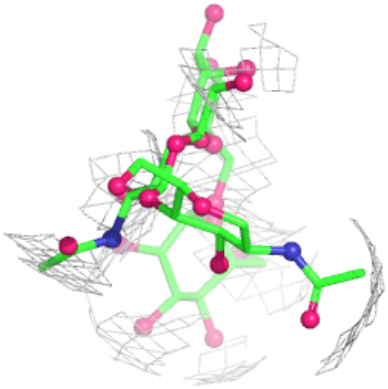


Electron density around Chain O:

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

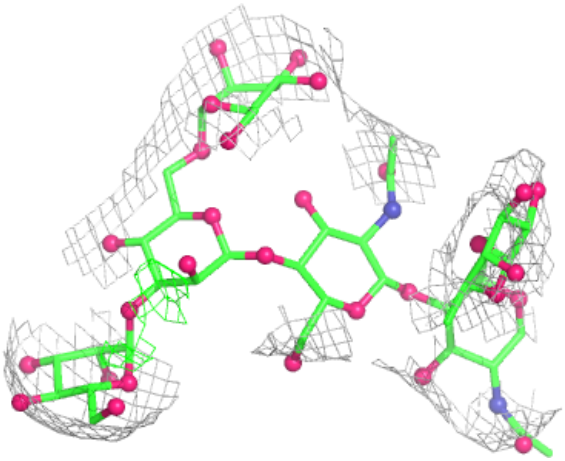


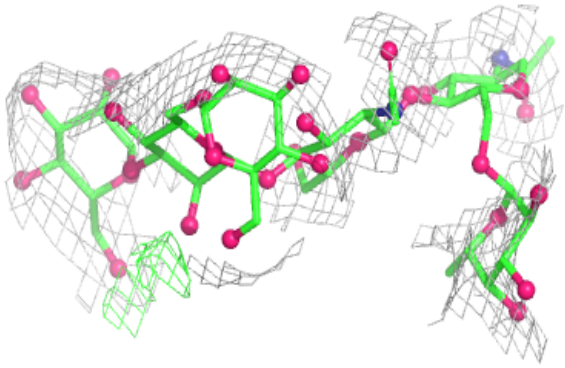


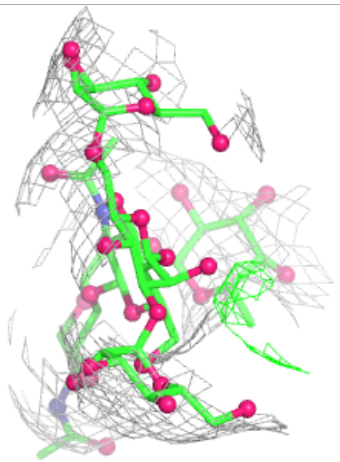


Electron density around Chain P:

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

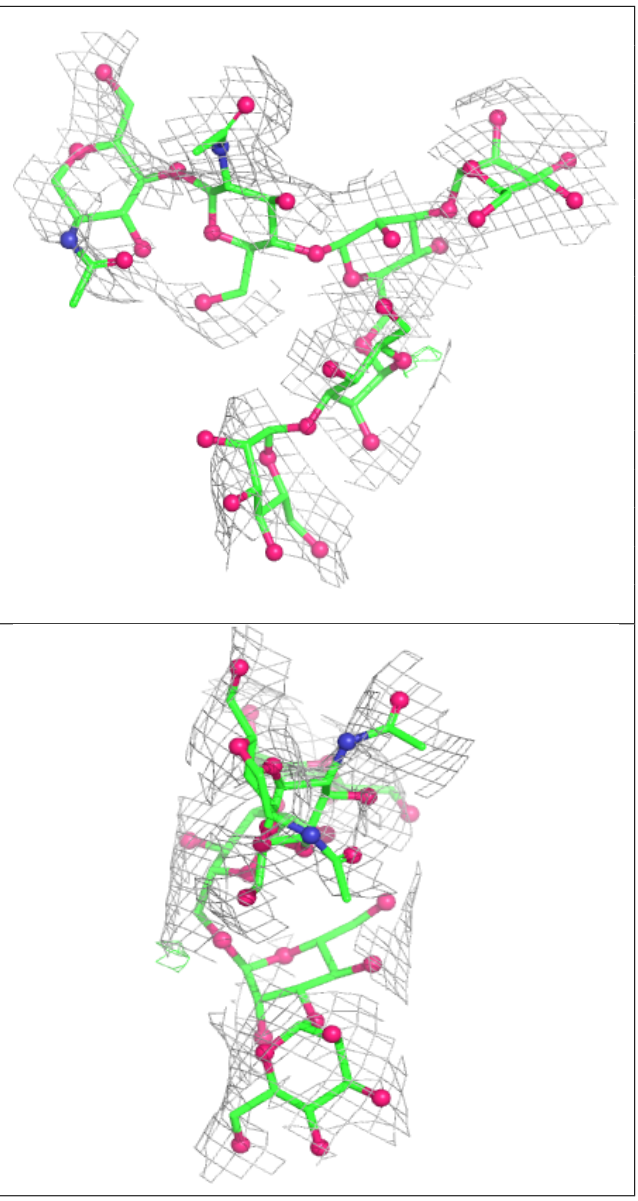






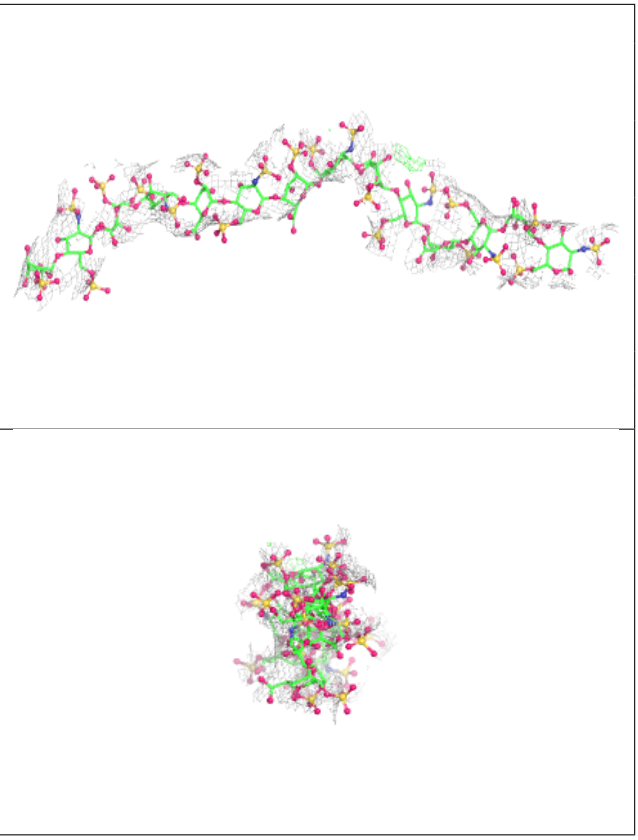
Electron density around Chain Q:

$2mF_o$-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 H:

$2mF_o$-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
7	CA	A	501	1/1	0.98	0.12	238,238,238,238	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CA A 501: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	

6.5 Other polymers (i)

There are no such residues in this entry.