



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:38 PM UTC

PDB ID : 3MJ9 / pdb_00003mj9
Title : Crystal structure of JAML in complex with the stimulatory antibody HL4E10
Authors : Verdino, P.; Wilson, I.A.
Deposited on : 2010-04-12
Resolution : 2.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

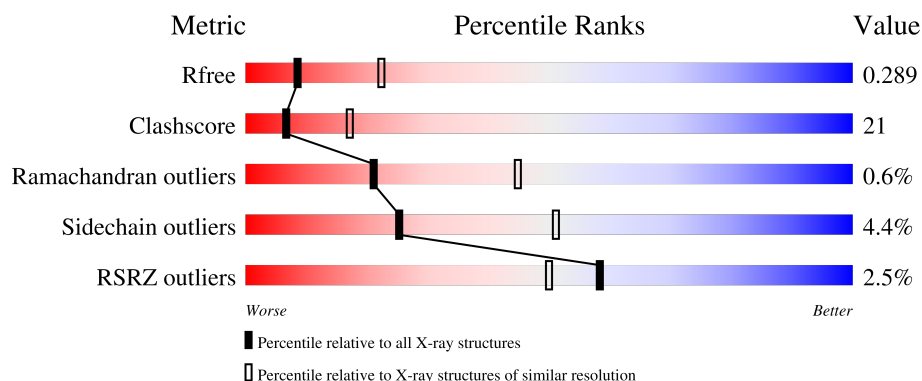
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	268	0.2% 58% 25% • 15%
2	L	213	2% 62% 33% • •
3	H	223	4% 59% 32% • 6%
4	B	6	33% 50% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5094 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 Junctional adhesion molecule-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1841	1142	328	361	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP Q80UL9
A	0	SER	-	expression tag	UNP Q80UL9
A	124	ARG	LYS	engineered mutation	UNP Q80UL9
A	211	GLN	ARG	engineered mutation	UNP Q80UL9
A	261	HIS	-	expression tag	UNP Q80UL9
A	262	HIS	-	expression tag	UNP Q80UL9
A	263	HIS	-	expression tag	UNP Q80UL9
A	264	HIS	-	expression tag	UNP Q80UL9
A	265	HIS	-	expression tag	UNP Q80UL9
A	266	HIS	-	expression tag	UNP Q80UL9

- Molecule 2 is a protein called STIMULATORY HAMSTER ANTIBODY HL4E10 FAB LIGHT CHAIN.

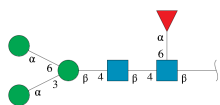
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	209	Total	C	N	O	S	0	0	0
			1575	989	261	317	8			

- Molecule 3 is a protein called STIMULATORY HAMSTER ANTIBODY HL4E10 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	210	Total	C	N	O	S	0	0	0
			1579	1002	265	306	6			

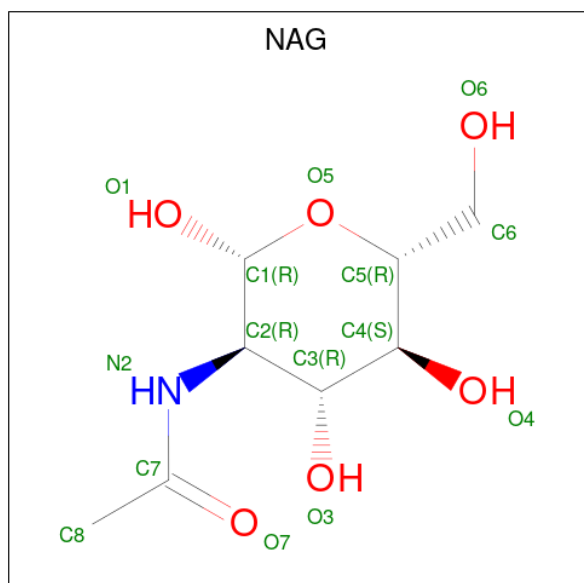
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(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
4	B	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

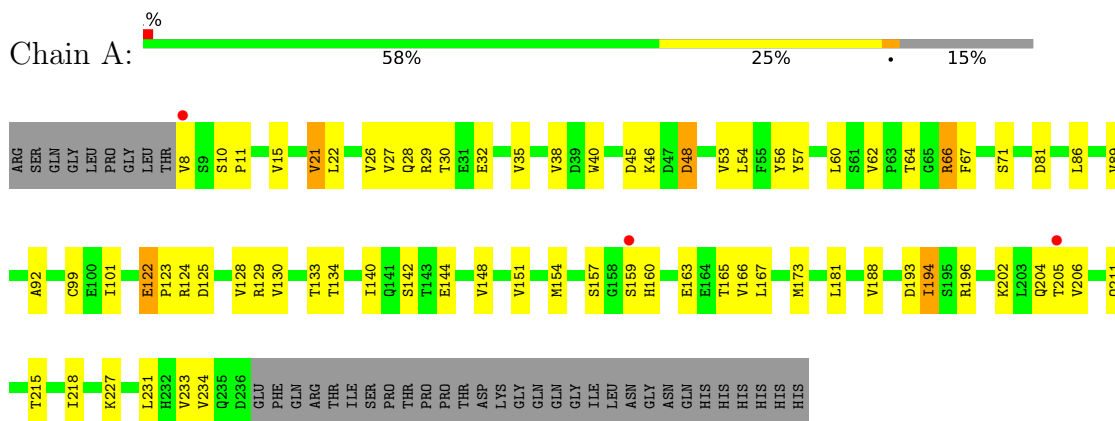


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

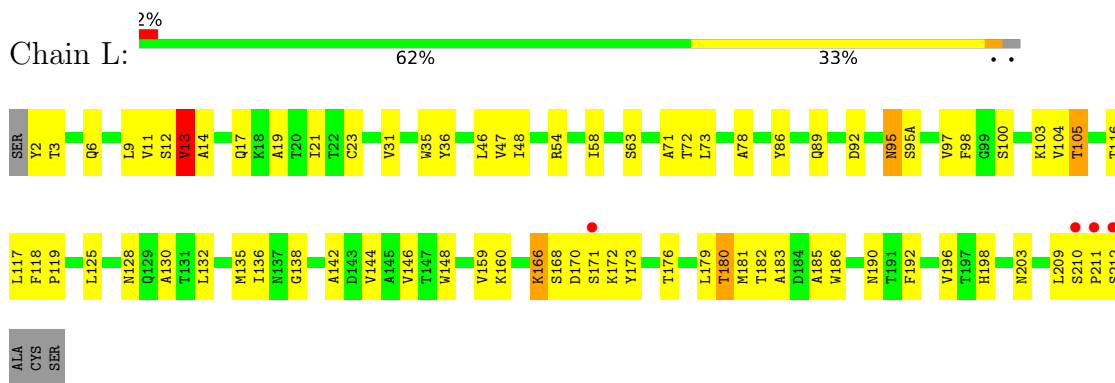
3 Residue-property plots [i](#)

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.

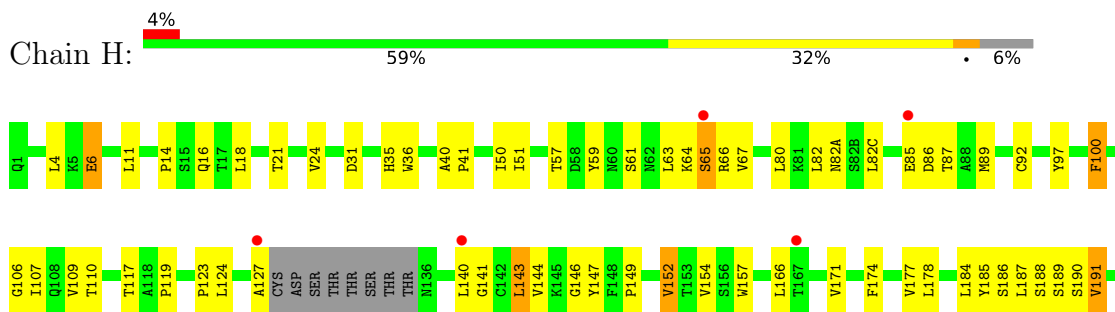
- Molecule 1: Junctional adhesion molecule-like

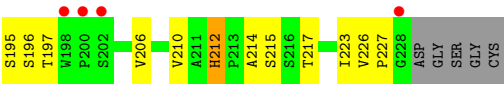


- Molecule 2: STIMULATORY HAMSTER ANTIBODY HL4E10 FAB LIGHT CHAIN



- Molecule 3: STIMULATORY HAMSTER ANTIBODY HL4E10 FAB HEAVY CHAIN





● 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 125.02Å 107.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.95 30.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.95) 97.6 (30.00-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.222 , 0.287 0.223 , 0.289	Depositor DCC
R_{free} test set	927 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, BMA, FUC, 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	0.48	0/1871	0.83	0/2522
2	L	0.45	0/1614	0.79	0/2206
3	H	0.46	0/1620	0.83	3/2215 (0.1%)
All	All	0.47	0/5105	0.82	3/6943 (0.0%)

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
2	L	0	1
3	H	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	86	ASP	N-CA-C	-9.08	102.21	113.28
3	H	212	HIS	CA-C-N	5.58	125.04	119.24
3	H	212	HIS	C-N-CA	5.58	125.04	119.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	85	GLU	Peptide
2	L	166	LYS	Peptide

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	1841	0	1809	70	0
2	L	1575	0	1518	81	0
3	H	1579	0	1553	71	0
4	B	71	0	61	1	0
5	A	28	0	26	0	0
All	All	5094	0	4967	216	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 21.

All (216) 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)
2:L:181:MET:HE1	2:L:186:TRP:HE3	1.03	1.14
2:L:181:MET:HE1	2:L:186:TRP:CE3	1.93	1.04
2:L:13:VAL:HG21	2:L:19:ALA:HB2	1.44	0.99
2:L:181:MET:SD	2:L:192:PHE:CZ	2.57	0.97
3:H:140:LEU:HD13	3:H:206:VAL:HG21	1.48	0.94
1:A:128:VAL:HG23	1:A:231:LEU:HD11	1.53	0.90
1:A:128:VAL:CG2	1:A:231:LEU:HD11	2.05	0.86
3:H:4:LEU:HD22	3:H:24:VAL:HG22	1.56	0.85
1:A:22:LEU:HB3	1:A:142:SER:HB3	1.59	0.82
2:L:210:SER:HB3	2:L:211:PRO:HD2	1.59	0.82
3:H:171:VAL:HG22	3:H:191:VAL:CG2	2.11	0.80
2:L:210:SER:HB3	2:L:211:PRO:CD	2.13	0.78
1:A:15:VAL:HG11	1:A:21:VAL:HG13	1.66	0.77
1:A:202:LYS:NZ	1:A:204:GLN:HE21	1.82	0.77
2:L:181:MET:SD	2:L:192:PHE:CE2	2.79	0.76
3:H:4:LEU:CD2	3:H:24:VAL:HG13	2.15	0.76
3:H:4:LEU:HD21	3:H:24:VAL:HG13	1.67	0.76
3:H:212:HIS:HB3	3:H:217:THR:CG2	2.18	0.74
1:A:124:ARG:NH1	1:A:227:LYS:HG2	2.02	0.73
3:H:178:LEU:HD12	3:H:185:TYR:CZ	2.24	0.72
2:L:159:VAL:HG22	2:L:179:LEU:CD1	2.20	0.71
2:L:9:LEU:HD12	2:L:103:LYS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG21	1:A:134:THR:HG21	1.71	0.71
1:A:130:VAL:HG22	1:A:233:VAL:HG12	1.73	0.71
1:A:166:VAL:CG1	1:A:188:VAL:HG21	2.21	0.70
1:A:62:VAL:HG12	1:A:64:THR:HG23	1.72	0.70
2:L:171:SER:O	2:L:172:LYS:HG3	1.93	0.69
1:A:60:LEU:HD12	1:A:60:LEU:O	1.94	0.68
1:A:130:VAL:HG22	1:A:233:VAL:CG1	2.24	0.68
3:H:57:THR:HG21	3:H:59:TYR:CZ	2.29	0.67
3:H:87:THR:HG23	3:H:110:THR:HA	1.77	0.67
3:H:215:SER:OG	3:H:217:THR:HG22	1.94	0.67
1:A:128:VAL:HG23	1:A:231:LEU:CD1	2.23	0.67
2:L:128:ASN:HA	2:L:183:ALA:HB2	1.77	0.67
1:A:148:VAL:HG11	1:A:194:ILE:HD11	1.77	0.66
2:L:181:MET:SD	2:L:192:PHE:HZ	2.18	0.66
2:L:159:VAL:HG22	2:L:179:LEU:HD12	1.78	0.64
1:A:26:VAL:HG11	1:A:29:ARG:HD2	1.79	0.64
1:A:167:LEU:HB2	1:A:188:VAL:HG11	1.78	0.64
2:L:47:VAL:HG12	2:L:58:ILE:HD12	1.79	0.63
3:H:154:VAL:HG11	3:H:189:SER:CB	2.28	0.63
1:A:130:VAL:CG2	1:A:233:VAL:HG12	2.27	0.63
2:L:135:MET:HE2	3:H:174:PHE:CE1	2.34	0.63
3:H:187:LEU:HD23	3:H:187:LEU:C	2.24	0.63
2:L:89:GLN:HG3	2:L:98:PHE:CE2	2.34	0.62
1:A:154:MET:HE1	1:A:163:GLU:OE1	2.00	0.62
3:H:124:LEU:HD11	3:H:143:LEU:HB2	1.80	0.62
1:A:22:LEU:HB3	1:A:142:SER:CB	2.28	0.62
1:A:202:LYS:HZ1	1:A:204:GLN:HE21	1.47	0.62
1:A:151:VAL:HG22	1:A:218:ILE:HG13	1.82	0.61
2:L:181:MET:HE3	2:L:186:TRP:HB2	1.82	0.61
2:L:181:MET:CE	2:L:186:TRP:HE3	1.96	0.60
3:H:171:VAL:HG22	3:H:191:VAL:HG22	1.81	0.60
1:A:166:VAL:HG13	1:A:188:VAL:HG21	1.84	0.60
2:L:95:ASN:ND2	2:L:95:ASN:H	1.99	0.60
2:L:166:LYS:HE2	2:L:170:ASP:O	2.02	0.60
1:A:15:VAL:HG11	1:A:21:VAL:CG1	2.32	0.60
2:L:2:TYR:CD1	2:L:97:VAL:HG11	2.37	0.59
2:L:212:SER:HB2	3:H:127:ALA:HB1	1.85	0.59
3:H:67:VAL:HG22	3:H:82:LEU:HD13	1.84	0.59
3:H:117:THR:HG21	3:H:184:LEU:HD21	1.83	0.59
3:H:63:LEU:HB3	3:H:67:VAL:HG21	1.85	0.58
3:H:51:ILE:HG23	3:H:51:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:CG1	1:A:27:VAL:O	2.52	0.57
1:A:128:VAL:HG11	1:A:206:VAL:HG21	1.86	0.57
3:H:212:HIS:HB3	3:H:217:THR:HG23	1.87	0.57
3:H:144:VAL:HG22	3:H:210:VAL:HG21	1.86	0.57
3:H:212:HIS:HB3	3:H:217:THR:HG22	1.87	0.56
1:A:166:VAL:HG12	1:A:188:VAL:HG21	1.86	0.56
2:L:117:LEU:HD23	2:L:118:PHE:N	2.21	0.56
1:A:128:VAL:HG21	1:A:231:LEU:HD11	1.85	0.56
2:L:136:ILE:HD11	2:L:146:VAL:HG22	1.88	0.55
2:L:2:TYR:CD1	2:L:2:TYR:C	2.84	0.55
2:L:92:ASP:OD2	2:L:95:ASN:ND2	2.28	0.55
3:H:11:LEU:HD13	3:H:149:PRO:HG3	1.89	0.55
3:H:195:SER:O	3:H:196:SER:OG	2.15	0.55
3:H:89:MET:HE1	3:H:106:GLY:C	2.32	0.55
3:H:119:PRO:HD2	3:H:217:THR:HG21	1.88	0.55
3:H:66:ARG:HB2	3:H:82(A):ASN:HB2	1.88	0.55
3:H:226:VAL:HG13	3:H:227:PRO:HD2	1.88	0.55
3:H:146:GLY:C	3:H:184:LEU:HD22	2.33	0.54
1:A:157:SER:O	1:A:160:HIS:N	2.38	0.54
2:L:136:ILE:HD13	2:L:196:VAL:HG13	1.90	0.54
2:L:14:ALA:HB3	2:L:17:GLN:HG3	1.90	0.54
2:L:181:MET:CE	2:L:186:TRP:CE3	2.80	0.54
3:H:123:PRO:C	3:H:124:LEU:HD12	2.33	0.53
1:A:10:SER:O	1:A:11:PRO:C	2.51	0.53
1:A:124:ARG:HH12	1:A:227:LYS:HG2	1.73	0.53
3:H:152:VAL:HG12	3:H:152:VAL:O	2.07	0.53
1:A:21:VAL:HG23	1:A:86:LEU:HB3	1.90	0.52
1:A:21:VAL:HG22	1:A:89:VAL:HG21	1.91	0.52
2:L:12:SER:HA	2:L:105:THR:HG22	1.91	0.52
2:L:117:LEU:CD2	2:L:209:LEU:HD22	2.39	0.52
1:A:26:VAL:HG12	1:A:27:VAL:O	2.09	0.52
2:L:168:SER:O	2:L:172:LYS:O	2.27	0.52
1:A:133:THR:HG21	1:A:202:LYS:HE2	1.91	0.52
2:L:116:THR:HG22	2:L:118:PHE:CE2	2.45	0.52
2:L:6:GLN:NE2	2:L:86:TYR:O	2.38	0.52
3:H:63:LEU:HB3	3:H:67:VAL:CG2	2.40	0.52
1:A:124:ARG:NH1	1:A:227:LYS:CG	2.73	0.51
3:H:212:HIS:CE1	3:H:214:ALA:HB3	2.46	0.51
1:A:8:VAL:O	1:A:8:VAL:HG12	2.11	0.51
1:A:148:VAL:CG1	1:A:194:ILE:HD11	2.40	0.51
2:L:136:ILE:HD11	2:L:146:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:187:LEU:HD23	3:H:188:SER:N	2.26	0.51
2:L:142:ALA:HB2	2:L:173:TYR:CG	2.45	0.50
1:A:28:GLN:O	1:A:28:GLN:HG3	2.10	0.50
2:L:180:THR:O	2:L:180:THR:HG22	2.11	0.50
2:L:36:TYR:CE2	2:L:46:LEU:HD13	2.47	0.50
2:L:142:ALA:HB2	2:L:173:TYR:CD2	2.46	0.50
3:H:57:THR:CG2	3:H:59:TYR:CZ	2.94	0.50
1:A:129:ARG:HA	1:A:234:VAL:HG22	1.93	0.50
2:L:48:ILE:HD12	2:L:73:LEU:CD1	2.43	0.49
1:A:26:VAL:HG22	1:A:81:ASP:HA	1.94	0.49
1:A:54:LEU:C	1:A:54:LEU:HD23	2.38	0.49
2:L:21:ILE:HD11	2:L:104:VAL:CG2	2.43	0.49
2:L:136:ILE:HD13	2:L:196:VAL:CG1	2.42	0.49
3:H:178:LEU:HD12	3:H:185:TYR:CE1	2.47	0.49
2:L:116:THR:CG2	2:L:118:PHE:CE2	2.96	0.49
3:H:89:MET:HE1	3:H:107:ILE:N	2.28	0.49
3:H:57:THR:HG21	3:H:59:TYR:OH	2.13	0.48
3:H:157:TRP:HB3	3:H:166:LEU:HD12	1.95	0.48
1:A:53:VAL:HG13	1:A:67:PHE:CG	2.47	0.48
2:L:132:LEU:CD1	2:L:181:MET:HE2	2.43	0.48
3:H:140:LEU:CD1	3:H:206:VAL:HG21	2.32	0.48
3:H:141:GLY:O	3:H:223:ILE:HD11	2.14	0.48
2:L:135:MET:HE2	3:H:174:PHE:CD1	2.49	0.48
2:L:182:THR:H	2:L:185:ALA:HB3	1.79	0.48
2:L:13:VAL:HG13	2:L:14:ALA:O	2.13	0.48
2:L:210:SER:CB	2:L:211:PRO:CD	2.82	0.48
2:L:148:TRP:CE3	2:L:179:LEU:HD22	2.49	0.48
3:H:18:LEU:HB3	3:H:82:LEU:HB3	1.96	0.48
2:L:2:TYR:C	2:L:2:TYR:HD1	2.22	0.48
1:A:27:VAL:O	1:A:28:GLN:C	2.57	0.47
2:L:181:MET:SD	2:L:186:TRP:HA	2.54	0.47
1:A:202:LYS:HZ3	1:A:204:GLN:HE21	1.60	0.47
1:A:123:PRO:O	1:A:124:ARG:HB2	2.13	0.47
3:H:67:VAL:HG22	3:H:82:LEU:CD1	2.45	0.47
1:A:211:GLN:HG3	1:A:233:VAL:HG23	1.97	0.47
3:H:16:GLN:O	3:H:82(C):LEU:HD13	2.15	0.47
1:A:46:LYS:C	1:A:48:ASP:H	2.23	0.47
3:H:14:PRO:C	3:H:16:GLN:H	2.23	0.46
3:H:35:HIS:CE1	3:H:50:ILE:HD12	2.50	0.46
2:L:13:VAL:HG11	2:L:78:ALA:CB	2.45	0.46
2:L:132:LEU:CD2	2:L:209:LEU:CD2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:4:LEU:CD2	3:H:24:VAL:HG22	2.37	0.46
3:H:61:SER:O	3:H:64:LYS:HB2	2.16	0.46
1:A:128:VAL:CG2	1:A:134:THR:HG21	2.44	0.46
2:L:181:MET:HB3	2:L:185:ALA:HB3	1.96	0.46
2:L:159:VAL:HG12	2:L:160:LYS:N	2.31	0.46
1:A:26:VAL:HG11	1:A:29:ARG:CD	2.46	0.46
1:A:26:VAL:HG13	1:A:27:VAL:O	2.15	0.46
3:H:40:ALA:O	3:H:41:PRO:C	2.59	0.45
2:L:12:SER:O	2:L:13:VAL:HG23	2.16	0.45
2:L:132:LEU:CD2	2:L:209:LEU:HD23	2.46	0.45
1:A:22:LEU:O	1:A:142:SER:HA	2.16	0.45
3:H:190:SER:O	3:H:191:VAL:HG23	2.17	0.45
1:A:66:ARG:HH22	1:A:92:ALA:C	2.25	0.45
3:H:178:LEU:HD12	3:H:185:TYR:OH	2.16	0.45
1:A:124:ARG:HH12	1:A:227:LYS:CG	2.29	0.45
3:H:177:VAL:HG12	3:H:186:SER:HB2	1.99	0.45
1:A:57:TYR:CZ	1:A:60:LEU:HD11	2.52	0.44
2:L:47:VAL:HG12	2:L:58:ILE:CD1	2.47	0.44
3:H:154:VAL:HG11	3:H:189:SER:HB3	1.98	0.44
3:H:171:VAL:HG22	3:H:191:VAL:HG21	1.95	0.44
1:A:46:LYS:C	1:A:48:ASP:N	2.74	0.44
2:L:119:PRO:HG3	3:H:127:ALA:HB3	2.00	0.44
4:B:1:NAG:O4	4:B:2:NAG:H83	2.18	0.44
2:L:21:ILE:HD11	2:L:104:VAL:HG21	1.99	0.44
2:L:135:MET:HA	2:L:176:THR:HG22	1.98	0.44
2:L:142:ALA:HB2	2:L:173:TYR:CD1	2.53	0.44
3:H:100:PHE:CD1	3:H:100:PHE:N	2.86	0.43
2:L:176:THR:HG23	3:H:174:PHE:CD2	2.53	0.43
1:A:122:GLU:HG2	1:A:123:PRO:HD2	1.99	0.43
3:H:64:LYS:O	3:H:65:SER:CB	2.66	0.43
3:H:107:ILE:O	3:H:107:ILE:HG23	2.18	0.43
3:H:124:LEU:CD1	3:H:143:LEU:HB2	2.46	0.43
1:A:148:VAL:HG11	1:A:194:ILE:CD1	2.46	0.43
1:A:30:THR:C	1:A:32:GLU:H	2.25	0.43
3:H:6:GLU:OE1	3:H:92:CYS:N	2.47	0.43
2:L:13:VAL:CG2	2:L:19:ALA:HB2	2.33	0.43
3:H:226:VAL:CG1	3:H:227:PRO:HD2	2.49	0.42
1:A:142:SER:OG	1:A:144:GLU:O	2.33	0.42
2:L:210:SER:CB	2:L:211:PRO:HD2	2.40	0.42
2:L:125:LEU:CD2	2:L:130:ALA:HB2	2.49	0.42
2:L:198:HIS:O	2:L:203:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:ILE:O	3:H:51:ILE:CG2	2.67	0.42
1:A:40:TRP:CH2	1:A:99:CYS:HB2	2.55	0.42
2:L:23:CYS:HB3	2:L:71:ALA:HB3	2.02	0.42
2:L:3:THR:HG21	2:L:100:SER:HA	2.02	0.42
2:L:138:GLY:HA2	2:L:172:LYS:HB3	2.01	0.42
2:L:168:SER:O	2:L:170:ASP:C	2.63	0.42
1:A:67:PHE:O	1:A:71:SER:OG	2.28	0.41
1:A:165:THR:HB	1:A:181:LEU:HD12	2.01	0.41
2:L:21:ILE:O	2:L:72:THR:HA	2.20	0.41
1:A:122:GLU:OE2	1:A:227:LYS:NZ	2.39	0.41
2:L:159:VAL:HG22	2:L:179:LEU:HD13	1.99	0.41
3:H:50:ILE:O	3:H:57:THR:HG23	2.21	0.41
2:L:48:ILE:HD11	2:L:63:SER:CA	2.51	0.41
2:L:132:LEU:HD21	2:L:186:TRP:CZ3	2.56	0.41
1:A:148:VAL:CG1	1:A:194:ILE:CD1	2.98	0.41
1:A:38:VAL:HB	1:A:56:TYR:HB3	2.02	0.41
1:A:122:GLU:CG	1:A:123:PRO:HD2	2.51	0.41
1:A:196:ARG:NH2	2:L:54:ARG:O	2.54	0.41
2:L:125:LEU:HD21	2:L:130:ALA:HB2	2.02	0.41
3:H:144:VAL:HG11	3:H:152:VAL:HG11	2.03	0.41
2:L:118:PHE:CD2	3:H:124:LEU:HD23	2.55	0.41
2:L:136:ILE:CD1	2:L:144:VAL:HG11	2.51	0.41
1:A:193:ASP:OD2	1:A:196:ARG:NH1	2.54	0.40
1:A:157:SER:C	1:A:159:SER:N	2.78	0.40
2:L:9:LEU:HD12	2:L:11:VAL:H	1.86	0.40
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.55	0.40
1:A:35:VAL:HG22	1:A:101:ILE:HG21	2.04	0.40
3:H:36:TRP:CE2	3:H:80:LEU:HB2	2.56	0.40
3:H:87:THR:HA	3:H:109:VAL:O	2.21	0.40
3:H:119:PRO:HB3	3:H:147:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	227/268 (85%)	209 (92%)	18 (8%)	0	100	100
2	L	207/213 (97%)	193 (93%)	12 (6%)	2 (1%)	12	32
3	H	206/223 (92%)	193 (94%)	11 (5%)	2 (1%)	12	32
All	All	640/704 (91%)	595 (93%)	41 (6%)	4 (1%)	21	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	97	TYR
2	L	190	ASN
3	H	65	SER
2	L	13	VAL

5.3.2 Protein sidechains ⓘ

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	213/247 (86%)	202 (95%)	11 (5%)	21	46
2	L	175/178 (98%)	169 (97%)	6 (3%)	32	58
3	H	181/192 (94%)	173 (96%)	8 (4%)	25	51
All	All	569/617 (92%)	544 (96%)	25 (4%)	25	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	45	ASP
1	A	48	ASP
1	A	66	ARG
1	A	122	GLU
1	A	125	ASP

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Mol	Chain	Res	Type
1	A	140	ILE
1	A	173	MET
1	A	194	ILE
1	A	205	THR
1	A	215	THR
2	L	13	VAL
2	L	31	VAL
2	L	95	ASN
2	L	95(A)	SER
2	L	105	THR
2	L	180	THR
3	H	6	GLU
3	H	21	THR
3	H	31	ASP
3	H	100	PHE
3	H	143	LEU
3	H	152	VAL
3	H	191	VAL
3	H	197	THR

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

Mol	Chain	Res	Type
1	A	28	GLN
1	A	87	GLN
1	A	204	GLN
2	L	89	GLN
2	L	203	ASN
3	H	1	GLN
3	H	53	HIS
3	H	60	ASN
3	H	179	HIS

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
4	NAG	B	1	1,4	14,14,15	0.50	0	17,19,21	0.86	1 (5%)
4	NAG	B	2	4	14,14,15	0.57	0	17,19,21	0.93	0
4	BMA	B	3	4	11,11,12	0.69	0	15,15,17	1.16	2 (13%)
4	MAN	B	4	4	11,11,12	0.80	0	15,15,17	0.88	1 (6%)
4	MAN	B	5	4	11,11,12	0.58	0	15,15,17	0.77	0
4	FUC	B	6	4	10,10,11	0.63	0	14,14,16	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	3/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	2/2/19/22	0/1/1/1
4	MAN	B	5	4	-	1/2/19/22	0/1/1/1
4	FUC	B	6	4	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	MAN	C1-O5-C5	-2.81	108.42	112.19
4	B	1	NAG	O5-C1-C2	-2.28	107.76	111.29
4	B	3	BMA	C6-C5-C4	-2.15	107.75	113.02
4	B	3	BMA	C1-O5-C5	-2.05	109.44	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

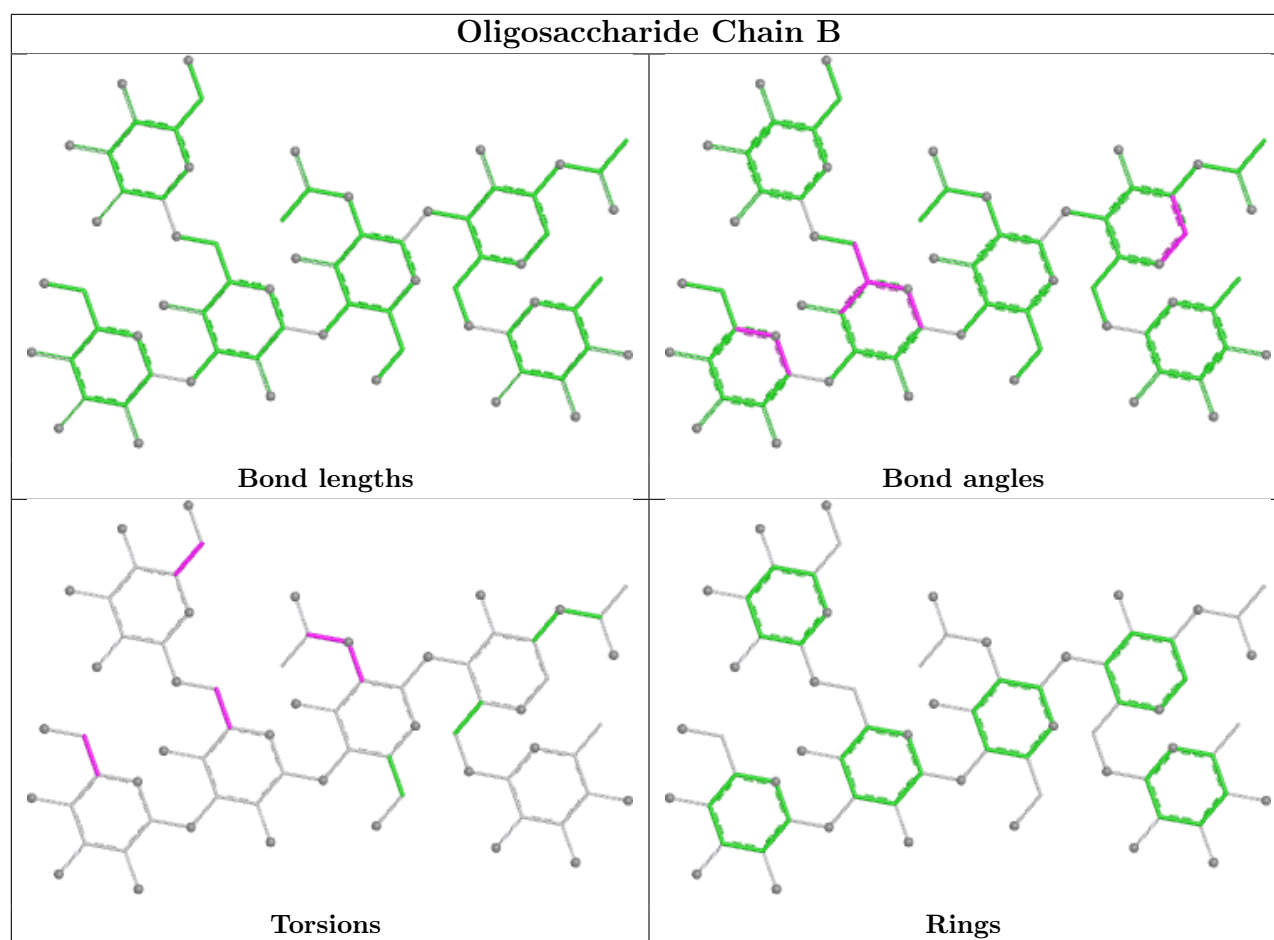
Mol	Chain	Res	Type	Atoms
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	4	MAN	C4-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
4	B	4	MAN	O5-C5-C6-O6
4	B	5	MAN	O5-C5-C6-O6
4	B	3	BMA	O5-C5-C6-O6
4	B	2	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 1 short contact:

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.



5.6 Ligand geometry [i](#)

2 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	A	301	1	14,14,15	0.57	0	17,19,21	1.37	3 (17%)
5	NAG	A	401	1	14,14,15	0.69	0	17,19,21	1.88	3 (17%)

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	A	301	1	-	4/6/23/26	0/1/1/1
5	NAG	A	401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	NAG	C1-O5-C5	-5.67	104.58	112.19
5	A	401	NAG	O5-C1-C2	-3.91	105.24	111.29
5	A	401	NAG	C1-C2-N2	2.45	114.29	110.43
5	A	301	NAG	C8-C7-N2	2.40	120.10	116.12
5	A	301	NAG	O5-C1-C2	-2.31	107.72	111.29
5	A	301	NAG	C1-C2-N2	-2.26	106.87	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	NAG	C4-C5-C6-O6
5	A	301	NAG	O5-C5-C6-O6
5	A	301	NAG	C8-C7-N2-C2
5	A	301	NAG	O7-C7-N2-C2
5	A	401	NAG	O5-C5-C6-O6

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	229/268 (85%)	0.20	3 (1%) 75 69	44, 67, 100, 149	0
2	L	209/213 (98%)	0.22	4 (1%) 66 58	43, 81, 116, 124	0
3	H	210/223 (94%)	0.29	9 (4%) 40 32	49, 79, 114, 130	0
All	All	648/704 (92%)	0.24	16 (2%) 58 50	43, 77, 112, 149	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	SER	4.1
1	A	205	THR	2.8
2	L	171	SER	2.8
3	H	167	THR	2.7
1	A	8	VAL	2.5
3	H	127	ALA	2.5
3	H	65	SER	2.4
3	H	200	PRO	2.4
2	L	210	SER	2.4
3	H	198	TRP	2.4
2	L	212	SER	2.3
2	L	211	PRO	2.3
3	H	228	GLY	2.2
3	H	85	GLU	2.1
3	H	140	LEU	2.0
3	H	202	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

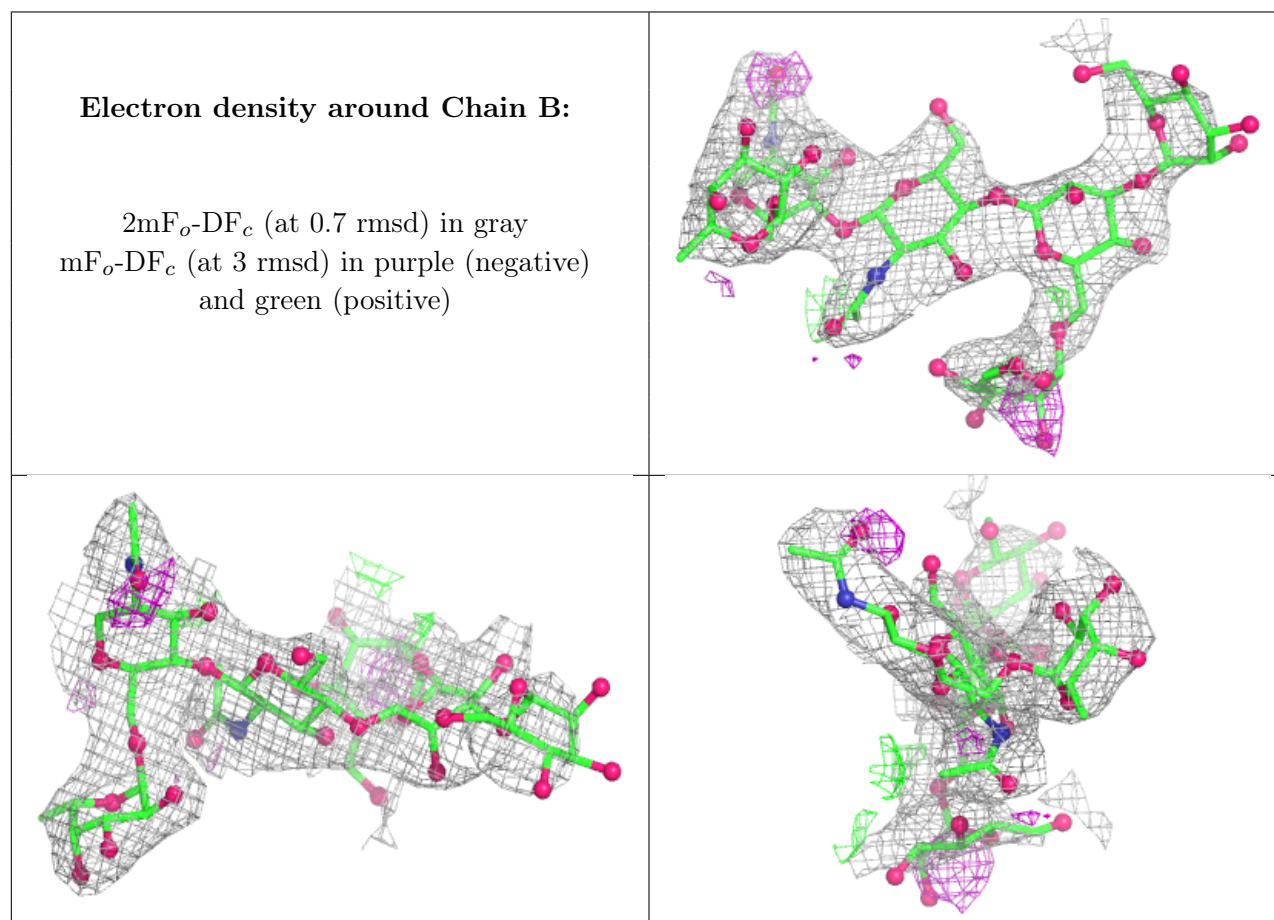
There are no non-standard protein/DNA/RNA residues in this entry.

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
4	NAG	B	1	14/15	-	-	46,51,53,58	0
4	NAG	B	2	14/15	-	-	55,62,75,88	0
4	BMA	B	3	11/12	-	-	99,110,117,123	0
4	MAN	B	4	11/12	-	-	128,134,143,149	0
4	MAN	B	5	11/12	-	-	117,121,124,125	0
4	FUC	B	6	10/11	-	-	58,62,66,66	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.



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($\text{\AA}^2$)	Q<0.9
5	NAG	A	401	14/15	0.65	0.15	110,122,135,136	0
5	NAG	A	301	14/15	0.67	0.15	104,111,119,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.