



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2026 – 05:18 PM JST

PDB ID : 9XA4 / pdb_00009xa4
Title : Structure of the Omicron BA.4/5 Spike N-terminal domain(NTD) in complex with the AC2 Fab
Authors : Zhou, J.J.; Gao, G.F.
Deposited on : 2025-10-22
Resolution : 2.52 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
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) : 2.50

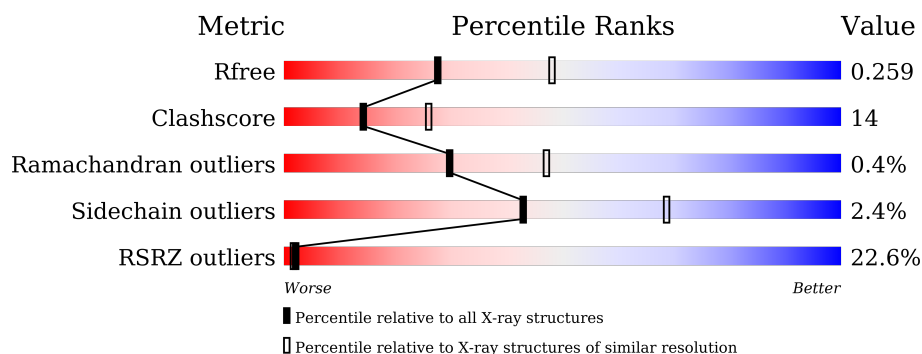
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	L	215	80%20%
2	H	240	3%75%19%••
3	A	293	51%49%39%•11%
4	B	2	100%
5	C	3	67%33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5706 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 AC2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1614	1009	263	337	5			

- Molecule 2 is a protein called AC2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	230	Total	C	N	O	S	0	0	0
			1736	1097	283	345	11			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	262	Total	C	N	O	S	0	0	0
			2101	1359	342	392	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	137	ASP	GLY	variant	UNP P0DTC2
A	208	GLY	VAL	variant	UNP P0DTC2
A	301	HIS	-	expression tag	UNP P0DTC2
A	302	HIS	-	expression tag	UNP P0DTC2
A	303	HIS	-	expression tag	UNP P0DTC2
A	304	HIS	-	expression tag	UNP P0DTC2
A	305	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	306	HIS	-	expression tag	UNP P0DTC2

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



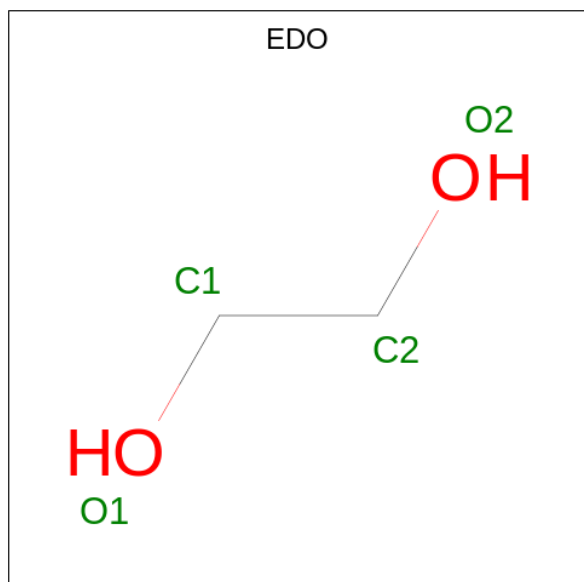
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 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
5	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

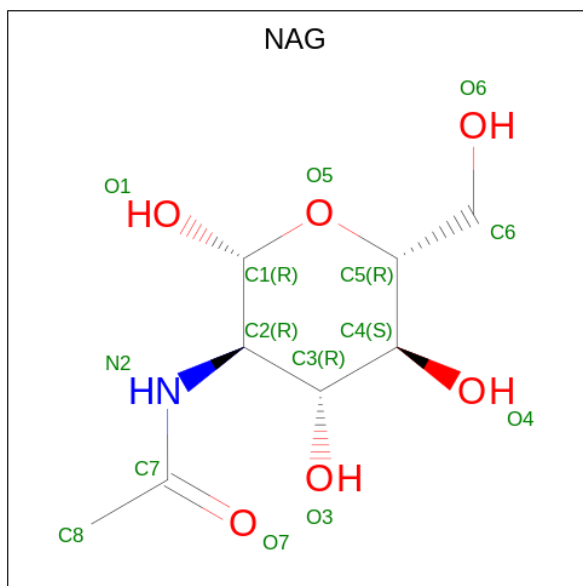
- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

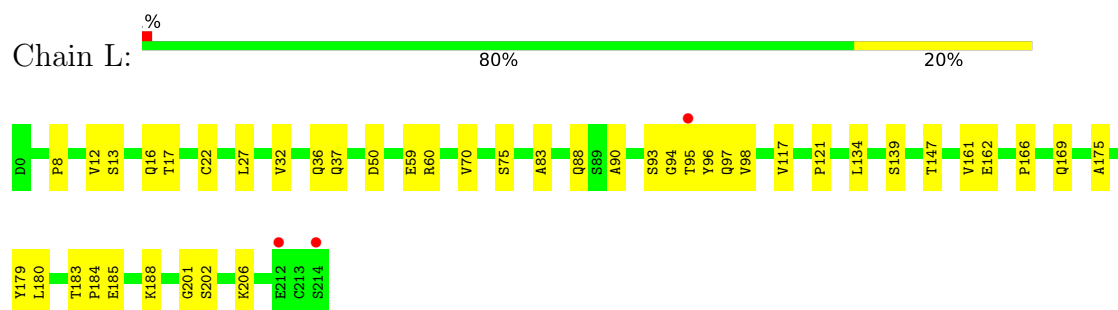
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	51	Total	O	0	0
			51	51		
8	H	38	Total	O	0	0
			38	38		
8	A	1	Total	O	0	0
			1	1		

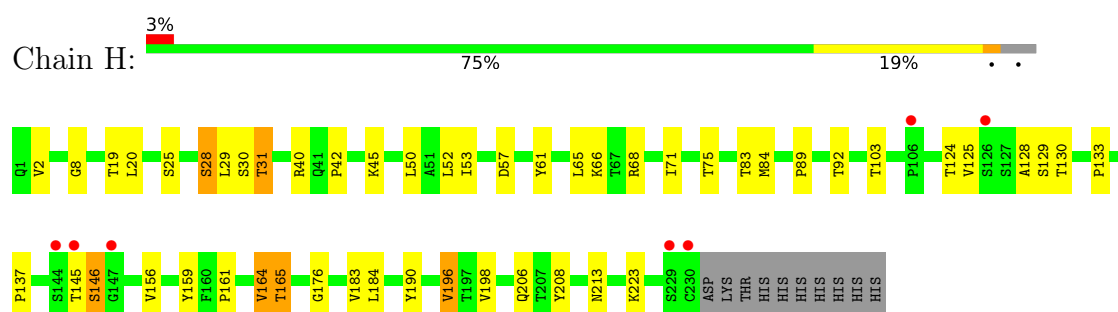
3 Residue-property plots [i](#)

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.

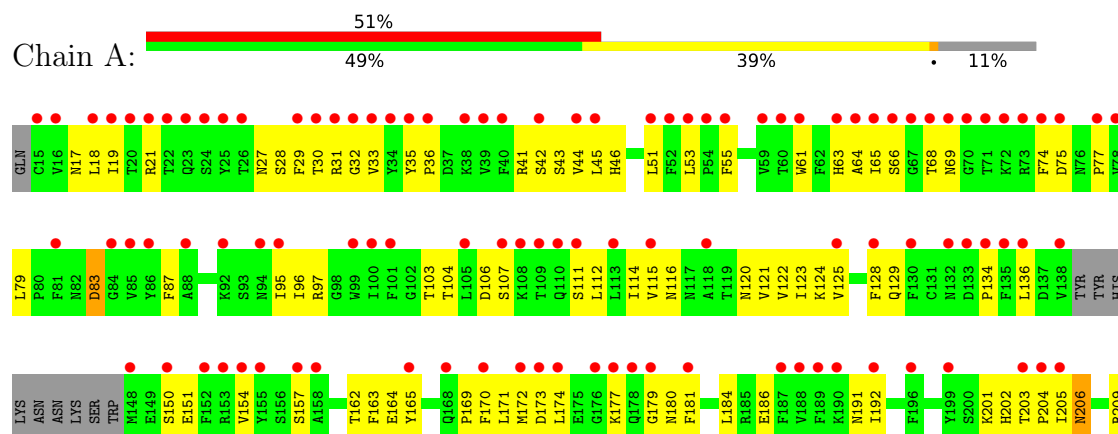
• Molecule 1: AC2 light chain

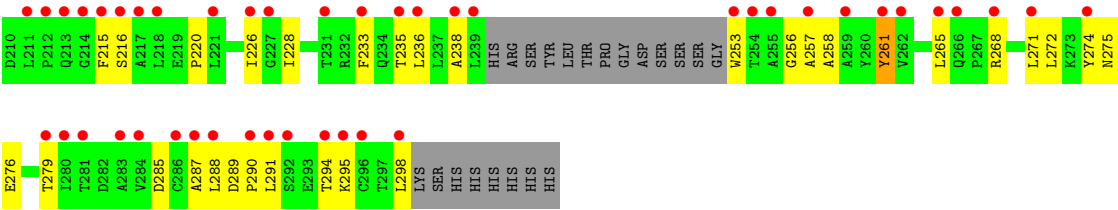


• Molecule 2: AC2 heavy chain



• Molecule 3: Spike protein S1





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

Chain B:

100%



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

Chain C:

67%33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.57Å 71.35Å 155.59Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	52.87 – 2.52 52.87 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.2 (52.87-2.52) 99.2 (52.87-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.222 , 0.257 0.228 , 0.259	Depositor DCC
R_{free} test set	1985 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5706	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG, BMA

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	L	0.47	0/1654	0.69	0/2260
2	H	0.46	0/1778	0.65	0/2433
3	A	0.29	0/2154	0.55	0/2928
All	All	0.41	0/5586	0.62	0/7621

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1614	0	1552	30	0
2	H	1736	0	1723	34	0
3	A	2101	0	2038	98	0
4	B	28	0	25	0	0
5	C	39	0	34	2	0
6	H	40	0	60	3	0
6	L	44	0	66	4	0
7	A	14	0	13	0	0
8	A	1	0	0	0	0
8	H	38	0	0	4	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	51	0	0	3	1
All	All	5706	0	5511	158	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:115:VAL:HG22	3:A:122:VAL:HG22	1.55	0.87
2:H:57:ASP:OD1	8:H:401:HOH:O	1.91	0.86
3:A:30:THR:HA	3:A:55:PHE:HE1	1.41	0.84
2:H:30:SER:HB3	2:H:75:THR:HG21	1.70	0.74
3:A:30:THR:HA	3:A:55:PHE:CE1	2.23	0.74
2:H:92:THR:HG23	2:H:124:THR:HA	1.69	0.74
1:L:17:THR:H	6:L:308:EDO:H21	1.53	0.73
1:L:162:GLU:HB3	2:H:183:VAL:HG21	1.70	0.72
1:L:59:GLU:O	8:L:401:HOH:O	2.07	0.70
3:A:201:LYS:HA	3:A:201:LYS:HE2	1.74	0.70
3:A:121:VAL:HG11	3:A:170:PHE:HE1	1.57	0.68
3:A:174:LEU:HA	3:A:177:LYS:HD3	1.75	0.68
1:L:8:PRO:O	8:L:402:HOH:O	2.12	0.67
2:H:19:THR:O	8:H:402:HOH:O	2.11	0.66
2:H:42:PRO:HG2	2:H:45:LYS:HD2	1.79	0.65
3:A:171:LEU:HD22	3:A:202:HIS:HB2	1.79	0.64
3:A:116:ASN:HD21	3:A:170:PHE:HB2	1.64	0.63
2:H:89:PRO:HA	2:H:125:VAL:HB	1.81	0.62
2:H:161:PRO:HB2	6:H:303:EDO:H21	1.80	0.62
1:L:184:PRO:O	1:L:188:LYS:HG3	1.99	0.62
2:H:145:THR:O	2:H:146:SER:OG	2.16	0.61
3:A:136:LEU:HD21	3:A:150:SER:HB2	1.83	0.61
3:A:184:LEU:HB2	3:A:205:ILE:HD11	1.82	0.61
2:H:223:LYS:NZ	8:H:405:HOH:O	2.35	0.60
1:L:94:GLY:HA3	3:A:180:ASN:HB3	1.84	0.60
3:A:163:PHE:HE1	3:A:165:TYR:HB2	1.66	0.60
3:A:107:SER:HB3	3:A:129:GLN:HB2	1.85	0.59
2:H:165:THR:HG22	2:H:213:ASN:HB3	1.84	0.59
2:H:65:LEU:HD12	2:H:84:MET:HE2	1.86	0.58
2:H:128:ALA:HA	6:H:306:EDO:H11	1.86	0.57
3:A:290:PRO:O	3:A:294:THR:HG23	2.04	0.57
3:A:95:ILE:HD12	3:A:96:ILE:H	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:PRO:HD3	2:H:223:LYS:HE3	1.87	0.57
1:L:93:SER:OG	1:L:95:THR:HG22	2.05	0.57
1:L:50:ASP:OD2	3:A:209:ARG:NH2	2.20	0.56
3:A:95:ILE:HD12	3:A:96:ILE:N	2.20	0.56
3:A:295:LYS:HD2	3:A:298:LEU:HD12	1.87	0.56
3:A:134:PRO:HB2	3:A:154:VAL:HG23	1.87	0.56
3:A:226:ILE:HG22	3:A:228:ILE:H	1.70	0.56
2:H:133:PRO:HB3	2:H:159:TYR:HB3	1.87	0.56
3:A:97:ARG:HG3	3:A:238:ALA:HB2	1.87	0.55
3:A:114:ILE:HG12	3:A:123:ILE:HG12	1.89	0.55
3:A:41:ARG:HH12	3:A:46:HIS:CD2	2.23	0.55
1:L:36:GLN:OE1	6:L:301:EDO:H21	2.07	0.55
3:A:45:LEU:HB3	3:A:271:LEU:HD11	1.88	0.55
3:A:121:VAL:HG11	3:A:170:PHE:CE1	2.41	0.54
3:A:33:VAL:HG21	3:A:215:PHE:HZ	1.71	0.54
3:A:66:SER:HB3	3:A:256:GLY:H	1.72	0.54
3:A:134:PRO:HB2	3:A:154:VAL:CG2	2.37	0.53
3:A:275:ASN:OD1	3:A:276:GLU:N	2.42	0.53
3:A:17:ASN:HB3	3:A:74:PHE:HB2	1.91	0.53
2:H:206:GLN:O	8:H:403:HOH:O	2.19	0.53
2:H:28:SER:O	2:H:31:THR:HG23	2.09	0.52
3:A:121:VAL:HG21	3:A:170:PHE:CE1	2.45	0.52
3:A:154:VAL:HG21	3:A:236:LEU:HD11	1.91	0.52
3:A:17:ASN:HD22	3:A:74:PHE:HB2	1.76	0.51
3:A:103:THR:OG1	3:A:104:THR:N	2.37	0.51
3:A:33:VAL:HG21	3:A:215:PHE:CZ	2.46	0.51
3:A:122:VAL:CG1	5:C:1:NAG:H61	2.42	0.50
1:L:139:SER:HB2	1:L:169:GLN:OE1	2.11	0.50
3:A:63:HIS:CE1	3:A:65:ILE:HG13	2.47	0.50
2:H:68:ARG:O	2:H:84:MET:HA	2.11	0.50
3:A:116:ASN:ND2	3:A:170:PHE:HB2	2.27	0.50
3:A:51:LEU:H	3:A:51:LEU:HD12	1.77	0.50
3:A:21:ARG:CZ	3:A:77:PRO:HA	2.41	0.50
3:A:285:ASP:HB3	3:A:288:LEU:HD22	1.94	0.50
3:A:27:ASN:HB3	3:A:29:PHE:CZ	2.47	0.49
3:A:68:THR:HG22	3:A:69:ASN:CG	2.37	0.49
1:L:12:VAL:HG22	1:L:16:GLN:HB2	1.94	0.49
3:A:28:SER:HB2	3:A:53:LEU:HD21	1.94	0.49
3:A:64:ALA:HB3	3:A:258:ALA:HB3	1.95	0.49
3:A:201:LYS:HD3	3:A:202:HIS:N	2.27	0.49
3:A:289:ASP:HB3	3:A:291:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:191:ASN:O	3:A:192:ILE:HD13	2.13	0.49
1:L:27:LEU:HD13	1:L:70:VAL:HG13	1.94	0.49
3:A:75:ASP:O	3:A:77:PRO:HD3	2.13	0.49
3:A:123:ILE:HD11	3:A:170:PHE:HZ	1.78	0.48
3:A:129:GLN:HB3	3:A:157:SER:OG	2.13	0.48
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.95	0.48
3:A:271:LEU:C	3:A:272:LEU:HD23	2.37	0.48
3:A:66:SER:HB3	3:A:256:GLY:N	2.28	0.48
3:A:268:ARG:HD2	3:A:287:ALA:HB3	1.94	0.48
3:A:61:TRP:CZ3	3:A:63:HIS:HB2	2.49	0.48
3:A:294:THR:O	3:A:298:LEU:HG	2.14	0.47
1:L:183:THR:OG1	1:L:185:GLU:HG2	2.13	0.47
3:A:35:TYR:OH	3:A:279:THR:HA	2.15	0.47
3:A:120:ASN:HA	3:A:169:PRO:HD3	1.97	0.47
2:H:198:VAL:HG11	2:H:208:TYR:CE1	2.49	0.47
3:A:79:LEU:HB2	3:A:233:PHE:CE1	2.49	0.47
3:A:61:TRP:HD1	3:A:261:TYR:CE2	2.33	0.47
1:L:117:VAL:O	1:L:206:LYS:HE3	2.15	0.47
3:A:43:SER:HA	3:A:274:TYR:O	2.15	0.46
3:A:285:ASP:HB3	3:A:288:LEU:HB2	1.95	0.46
2:H:66:LYS:O	2:H:66:LYS:HD2	2.15	0.46
3:A:31:ARG:HD3	3:A:31:ARG:HA	1.77	0.46
3:A:19:ILE:HD11	3:A:77:PRO:HG3	1.98	0.46
2:H:2:VAL:HA	2:H:25:SER:O	2.15	0.46
3:A:18:LEU:HD11	3:A:253:TRP:HD1	1.80	0.46
3:A:112:LEU:HD11	3:A:123:ILE:HG23	1.99	0.45
1:L:201:GLY:N	8:L:403:HOH:O	2.14	0.45
1:L:134:LEU:HD12	1:L:180:LEU:HD23	1.99	0.45
2:H:156:VAL:HG11	2:H:164:VAL:HG11	1.98	0.45
3:A:31:ARG:CZ	3:A:216:SER:H	2.29	0.45
1:L:147:THR:HG23	6:L:302:EDO:C1	2.46	0.45
1:L:147:THR:HG23	6:L:302:EDO:H12	1.98	0.45
2:H:29:LEU:HD23	2:H:29:LEU:HA	1.88	0.44
3:A:191:ASN:C	3:A:192:ILE:HD13	2.42	0.44
3:A:95:ILE:HD12	3:A:96:ILE:HG13	1.98	0.44
3:A:116:ASN:HD21	3:A:170:PHE:CB	2.28	0.44
2:H:129:SER:O	2:H:130:THR:C	2.59	0.44
3:A:35:TYR:HB2	3:A:220:PRO:HD3	1.98	0.44
1:L:22:CYS:HB3	1:L:70:VAL:CG2	2.48	0.44
1:L:90:ALA:HB2	1:L:97:GLN:NE2	2.33	0.44
3:A:236:LEU:HD23	3:A:236:LEU:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:61:TRP:CH2	3:A:63:HIS:HB2	2.53	0.43
3:A:21:ARG:CD	3:A:77:PRO:HB3	2.49	0.43
3:A:129:GLN:HB3	3:A:157:SER:HG	1.82	0.43
2:H:184:LEU:HD13	2:H:190:TYR:CE1	2.53	0.43
3:A:136:LEU:HD23	3:A:151:GLU:O	2.18	0.43
1:L:32:VAL:HG21	1:L:70:VAL:HG21	2.01	0.43
1:L:13:SER:HB2	1:L:16:GLN:NE2	2.34	0.42
3:A:42:SER:O	3:A:44:VAL:HG23	2.19	0.42
3:A:95:ILE:CD1	3:A:96:ILE:HG13	2.49	0.42
3:A:295:LYS:HD2	3:A:295:LYS:HA	1.92	0.42
2:H:184:LEU:HD13	2:H:190:TYR:CZ	2.55	0.42
3:A:265:LEU:H	3:A:265:LEU:HD12	1.84	0.42
1:L:95:THR:HG23	1:L:96:TYR:HD1	1.84	0.42
2:H:40:ARG:HB3	2:H:50:LEU:HD11	2.01	0.42
3:A:32:GLY:HA3	3:A:53:LEU:HB3	2.01	0.42
3:A:275:ASN:HB3	3:A:279:THR:O	2.20	0.42
1:L:60:ARG:HB2	1:L:75:SER:O	2.19	0.42
1:L:88:GLN:HA	1:L:98:VAL:O	2.20	0.42
2:H:66:LYS:HD2	2:H:66:LYS:C	2.45	0.42
1:L:166:PRO:HA	1:L:175:ALA:O	2.19	0.41
2:H:52:LEU:HD23	2:H:53:ILE:N	2.35	0.41
2:H:103:THR:HA	6:H:309:EDO:H21	2.02	0.41
3:A:83:ASP:N	3:A:83:ASP:OD1	2.52	0.41
3:A:97:ARG:O	3:A:116:ASN:HB2	2.20	0.41
3:A:128:PHE:HA	3:A:157:SER:O	2.20	0.41
2:H:61:TYR:CZ	2:H:71:ILE:HG22	2.55	0.41
2:H:176:GLY:O	2:H:196:VAL:HA	2.20	0.41
3:A:184:LEU:HB3	3:A:203:THR:O	2.20	0.41
1:L:161:VAL:HA	1:L:179:TYR:O	2.20	0.41
3:A:163:PHE:HD1	3:A:164:GLU:N	2.19	0.41
3:A:181:PHE:HA	3:A:206:ASN:HA	2.02	0.41
1:L:37:GLN:O	1:L:83:ALA:HB1	2.21	0.41
2:H:61:TYR:OH	2:H:71:ILE:HG22	2.21	0.41
3:A:122:VAL:HG11	5:C:1:NAG:H61	2.02	0.41
3:A:64:ALA:O	3:A:257:ALA:HA	2.21	0.41
3:A:173:ASP:N	3:A:173:ASP:OD1	2.54	0.41
3:A:203:THR:HA	3:A:204:PRO:HD3	1.92	0.41
1:L:94:GLY:CA	3:A:180:ASN:HB3	2.49	0.41
3:A:125:VAL:HG21	3:A:226:ILE:HG13	2.02	0.41
3:A:42:SER:HA	3:A:275:ASN:O	2.21	0.40
1:L:121:PRO:HA	1:L:134:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:87:PHE:CE2	3:A:235:THR:HG22	2.56	0.40
3:A:206:ASN:OD1	3:A:206:ASN:N	2.45	0.40
3:A:124:LYS:HG2	3:A:164:GLU:HG3	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:440:HOH:O	8:H:436:HOH:O[4_546]	2.15	0.05

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	L	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	H	228/240 (95%)	218 (96%)	9 (4%)	1 (0%)	30	47
3	A	256/293 (87%)	241 (94%)	13 (5%)	2 (1%)	16	29
All	All	697/748 (93%)	664 (95%)	30 (4%)	3 (0%)	30	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	179	GLY
2	H	146	SER
3	A	36	PRO

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	L	183/183 (100%)	182 (100%)	1 (0%)	81	91
2	H	203/213 (95%)	197 (97%)	6 (3%)	36	62
3	A	235/264 (89%)	227 (97%)	8 (3%)	32	57
All	All	621/660 (94%)	606 (98%)	15 (2%)	43	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	202	SER
2	H	28	SER
2	H	31	THR
2	H	83	THR
2	H	164	VAL
2	H	165	THR
2	H	196	VAL
3	A	83	ASP
3	A	106	ASP
3	A	111	SER
3	A	162	THR
3	A	172	MET
3	A	186	GLU
3	A	206	ASN
3	A	261	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	GLN
1	L	37	GLN
1	L	41	GLN
1	L	97	GLN
1	L	190	HIS
1	L	196	GLN
2	H	41	GLN
3	A	191	ASN

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 ⓘ

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1	4,3	14,14,15	0.37	0	17,19,21	0.54	0
4	NAG	B	2	4	14,14,15	0.47	0	17,19,21	0.57	0
5	NAG	C	1	3,5	14,14,15	0.41	0	17,19,21	0.63	0
5	NAG	C	2	5	14,14,15	0.40	0	17,19,21	0.47	0
5	BMA	C	3	5	11,11,12	0.25	0	15,15,17	0.63	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	4,3	-	1/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
5	NAG	C	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

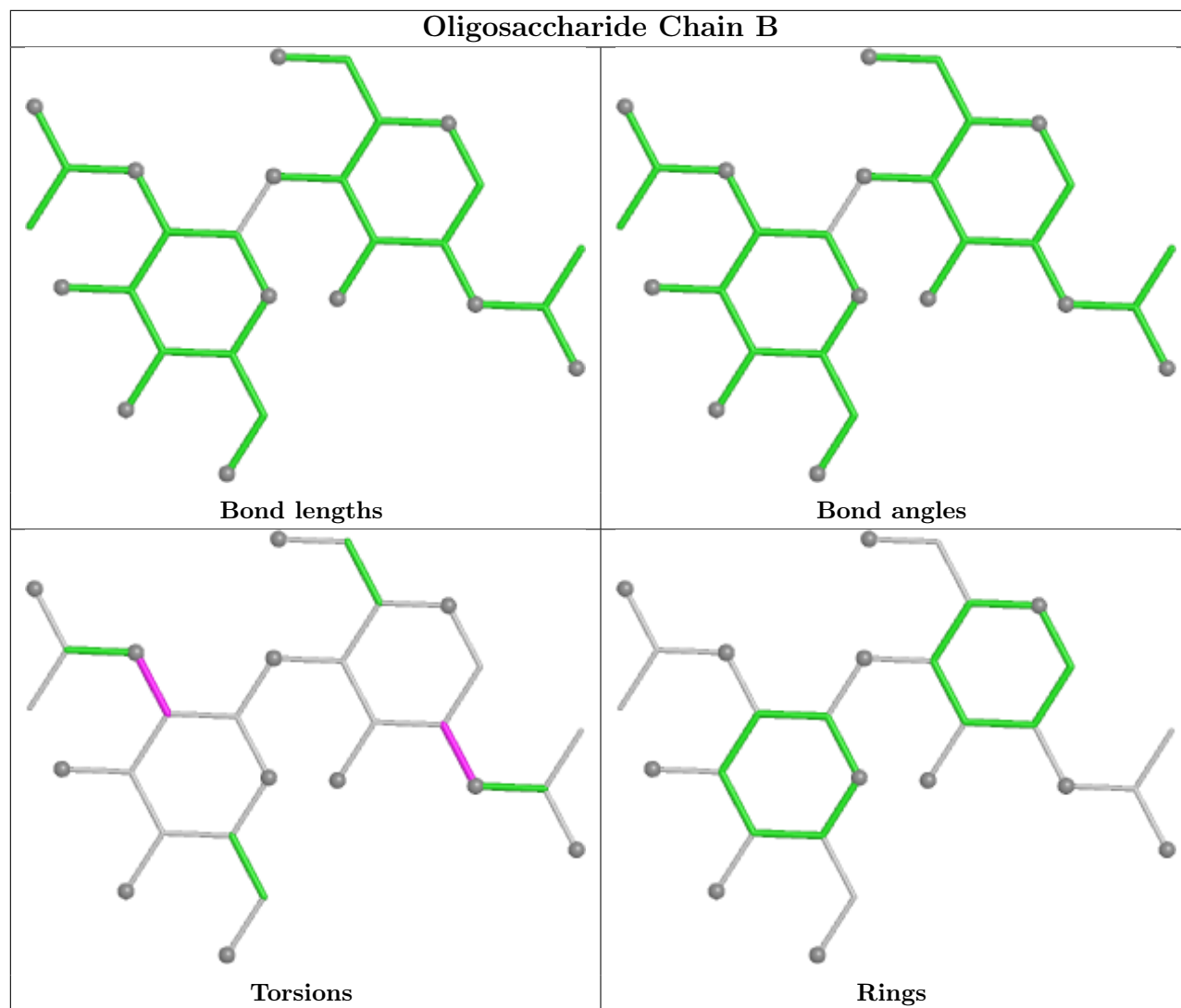
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
5	C	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7

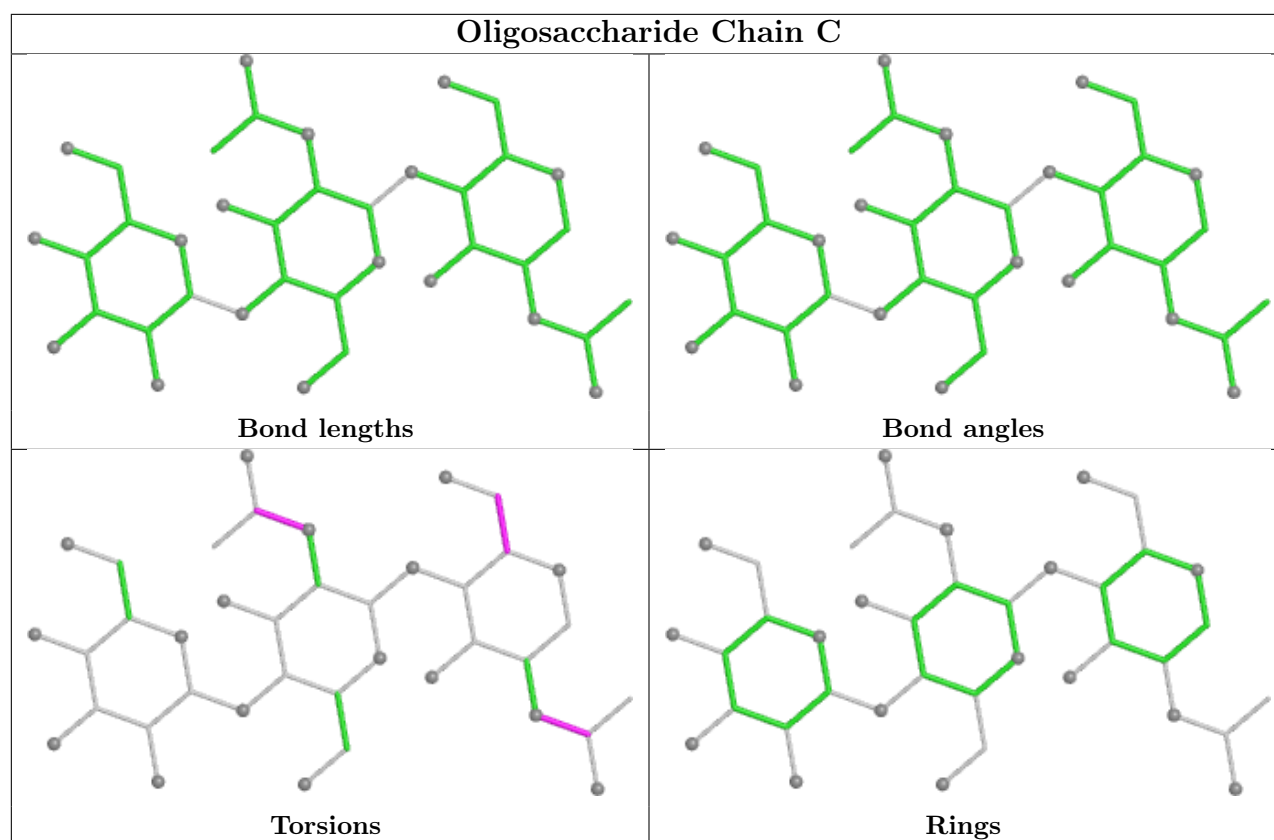
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	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.





5.6 Ligand geometry [i](#)

22 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	$\# Z > 2$
6	EDO	H	302	-	3,3,3	0.46	0	2,2,2	0.65	0
6	EDO	H	306	-	3,3,3	0.55	0	2,2,2	0.31	0
6	EDO	L	310	-	3,3,3	0.71	0	2,2,2	0.39	0
6	EDO	H	304	-	3,3,3	0.44	0	2,2,2	0.47	0
6	EDO	H	308	-	3,3,3	0.63	0	2,2,2	0.42	0
6	EDO	L	308	-	3,3,3	0.61	0	2,2,2	0.28	0
6	EDO	H	309	-	3,3,3	0.54	0	2,2,2	0.36	0
6	EDO	L	303	-	3,3,3	0.44	0	2,2,2	0.55	0
6	EDO	H	303	-	3,3,3	0.49	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	L	306	-	3,3,3	0.44	0	2,2,2	0.58	0
6	EDO	L	311	-	3,3,3	0.64	0	2,2,2	0.27	0
6	EDO	H	305	-	3,3,3	0.50	0	2,2,2	0.35	0
7	NAG	A	401	3	14,14,15	1.04	1 (7%)	17,19,21	0.84	0
6	EDO	H	301	-	3,3,3	0.50	0	2,2,2	0.42	0
6	EDO	L	301	-	3,3,3	0.43	0	2,2,2	0.33	0
6	EDO	L	307	-	3,3,3	0.58	0	2,2,2	0.19	0
6	EDO	L	304	-	3,3,3	0.62	0	2,2,2	0.16	0
6	EDO	L	305	-	3,3,3	0.51	0	2,2,2	0.32	0
6	EDO	L	302	-	3,3,3	0.57	0	2,2,2	0.31	0
6	EDO	H	310	-	3,3,3	0.51	0	2,2,2	0.50	0
6	EDO	H	307	-	3,3,3	0.54	0	2,2,2	0.57	0
6	EDO	L	309	-	3,3,3	0.62	0	2,2,2	0.73	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
6	EDO	H	302	-	-	1/1/1/1	-
6	EDO	H	306	-	-	1/1/1/1	-
6	EDO	L	310	-	-	0/1/1/1	-
6	EDO	H	304	-	-	0/1/1/1	-
6	EDO	H	308	-	-	0/1/1/1	-
6	EDO	L	308	-	-	0/1/1/1	-
6	EDO	H	309	-	-	0/1/1/1	-
6	EDO	L	303	-	-	0/1/1/1	-
6	EDO	H	303	-	-	1/1/1/1	-
6	EDO	L	306	-	-	1/1/1/1	-
6	EDO	L	311	-	-	0/1/1/1	-
6	EDO	H	305	-	-	0/1/1/1	-
7	NAG	A	401	3	-	0/6/23/26	0/1/1/1
6	EDO	H	301	-	-	0/1/1/1	-
6	EDO	L	301	-	-	0/1/1/1	-
6	EDO	L	307	-	-	0/1/1/1	-
6	EDO	L	304	-	-	1/1/1/1	-
6	EDO	L	305	-	-	1/1/1/1	-
6	EDO	L	302	-	-	1/1/1/1	-
6	EDO	H	310	-	-	0/1/1/1	-
6	EDO	H	307	-	-	1/1/1/1	-
6	EDO	L	309	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	401	NAG	C1-C2	3.62	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	305	EDO	O1-C1-C2-O2
6	H	306	EDO	O1-C1-C2-O2
6	L	304	EDO	O1-C1-C2-O2
6	L	309	EDO	O1-C1-C2-O2
6	L	302	EDO	O1-C1-C2-O2
6	L	306	EDO	O1-C1-C2-O2
6	H	302	EDO	O1-C1-C2-O2
6	H	303	EDO	O1-C1-C2-O2
6	H	307	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	306	EDO	1	0
6	L	308	EDO	1	0
6	H	309	EDO	1	0
6	H	303	EDO	1	0
6	L	301	EDO	1	0
6	L	302	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	L	215/215 (100%)	0.09	3 (1%) 73 71	28, 43, 72, 109	0
2	H	230/240 (95%)	0.47	7 (3%) 52 49	32, 53, 76, 88	0
3	A	262/293 (89%)	2.32	150 (57%) 0 0	60, 108, 140, 147	0
All	All	707/748 (94%)	1.04	160 (22%) 2 2	28, 63, 131, 147	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	32	GLY	7.3
3	A	152	PHE	6.6
3	A	53	LEU	5.4
3	A	291	LEU	5.1
3	A	284	VAL	4.9
3	A	298	LEU	4.7
3	A	138	VAL	4.6
3	A	211	LEU	4.6
3	A	178	GLN	4.5
3	A	216	SER	4.5
3	A	16	VAL	4.4
3	A	45	LEU	4.4
3	A	70	GLY	4.3
3	A	85	VAL	4.3
3	A	253	TRP	4.2
3	A	226	ILE	4.2
1	L	214	SER	4.2
3	A	290	PRO	4.1
3	A	239	LEU	4.1
3	A	148	MET	4.1
3	A	15	CYS	4.1
3	A	71	THR	4.0
3	A	29	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
3	A	213	GLN	3.9
3	A	280	ILE	3.9
3	A	86	TYR	3.8
3	A	95	ILE	3.8
3	A	19	ILE	3.8
3	A	75	ASP	3.7
3	A	261	TYR	3.7
3	A	88	ALA	3.7
3	A	255	ALA	3.7
3	A	30	THR	3.6
3	A	238	ALA	3.6
3	A	212	PRO	3.6
3	A	67	GLY	3.6
3	A	271	LEU	3.6
3	A	281	THR	3.5
3	A	77	PRO	3.5
3	A	254	THR	3.5
3	A	44	VAL	3.5
3	A	54	PRO	3.5
3	A	22	THR	3.4
3	A	51	LEU	3.4
3	A	217	ALA	3.3
3	A	31	ARG	3.3
3	A	25	TYR	3.3
3	A	172	MET	3.3
3	A	295	LYS	3.3
3	A	215	PHE	3.2
3	A	259	ALA	3.2
3	A	236	LEU	3.2
3	A	135	PHE	3.2
3	A	189	PHE	3.2
3	A	33	VAL	3.2
3	A	55	PHE	3.1
3	A	111	SER	3.1
3	A	179	GLY	3.1
3	A	214	GLY	3.1
3	A	177	LYS	3.1
3	A	204	PRO	3.1
3	A	35	TYR	3.1
3	A	231	THR	3.1
3	A	279	THR	3.0
3	A	199	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	128	PHE	2.9
3	A	154	VAL	2.9
3	A	60	THR	2.9
3	A	203	THR	2.9
3	A	235	THR	2.9
3	A	74	PHE	2.9
3	A	233	PHE	2.9
3	A	34	TYR	2.8
2	H	147	GLY	2.8
3	A	92	LYS	2.8
2	H	144	SER	2.8
3	A	257	ALA	2.8
3	A	59	VAL	2.8
3	A	294	THR	2.8
3	A	18	LEU	2.8
3	A	36	PRO	2.8
3	A	287	ALA	2.8
3	A	174	LEU	2.7
3	A	218	LEU	2.7
3	A	65	ILE	2.7
2	H	229	SER	2.7
3	A	61	TRP	2.7
3	A	130	PHE	2.6
3	A	205	ILE	2.6
3	A	262	VAL	2.6
3	A	133	ASP	2.6
3	A	21	ARG	2.6
3	A	125	VAL	2.6
3	A	283	ALA	2.6
3	A	73	ARG	2.6
3	A	40	PHE	2.6
2	H	145	THR	2.6
3	A	170	PHE	2.5
3	A	20	THR	2.5
3	A	26	THR	2.5
3	A	23	GLN	2.5
3	A	296	CYS	2.5
3	A	136	LEU	2.5
3	A	39	VAL	2.5
3	A	109	THR	2.5
3	A	176	GLY	2.5
3	A	132	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	64	ALA	2.4
2	H	230	CYS	2.4
3	A	72	LYS	2.4
3	A	84	GLY	2.4
3	A	153	ARG	2.4
3	A	115	VAL	2.4
1	L	212	GLU	2.4
3	A	118	ALA	2.4
3	A	227	GLY	2.4
3	A	52	PHE	2.4
3	A	181	PHE	2.4
3	A	266	GLN	2.3
3	A	134	PRO	2.3
3	A	150	SER	2.3
3	A	66	SER	2.3
3	A	288	LEU	2.3
3	A	190	LYS	2.3
3	A	94	ASN	2.3
3	A	113	LEU	2.3
3	A	192	ILE	2.3
3	A	108	LYS	2.3
3	A	69	ASN	2.2
3	A	221	LEU	2.2
2	H	106	PRO	2.2
2	H	126	SER	2.2
3	A	99	TRP	2.2
3	A	158	ALA	2.2
3	A	38	LYS	2.2
3	A	24	SER	2.2
3	A	292	SER	2.2
3	A	268	ARG	2.2
3	A	187	PHE	2.2
3	A	188	VAL	2.1
3	A	105	LEU	2.1
3	A	286	CYS	2.1
3	A	42	SER	2.1
3	A	81	PHE	2.1
3	A	63	HIS	2.1
3	A	265	LEU	2.1
3	A	107	SER	2.1
3	A	101	PHE	2.1
3	A	274	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	168	GLN	2.1
3	A	78	VAL	2.0
3	A	196	PHE	2.0
3	A	68	THR	2.0
3	A	100	ILE	2.0
3	A	165	TYR	2.0
3	A	157	SER	2.0
3	A	110	GLN	2.0
1	L	95	THR	2.0
3	A	173	ASP	2.0
3	A	155	TYR	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](#)

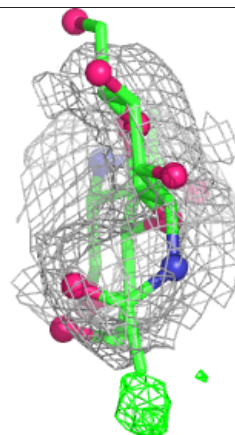
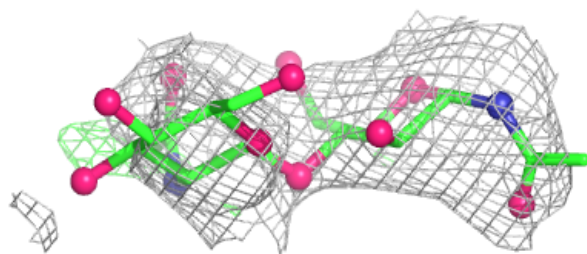
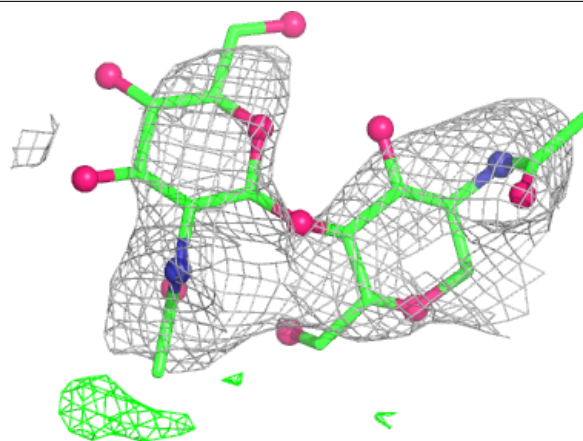
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	-	-	112,127,132,135	0
4	NAG	B	2	14/15	-	-	122,134,137,141	0
5	NAG	C	1	14/15	-	-	122,130,133,136	0
5	NAG	C	2	14/15	-	-	132,137,144,146	0
5	BMA	C	3	11/12	-	-	134,142,145,146	0

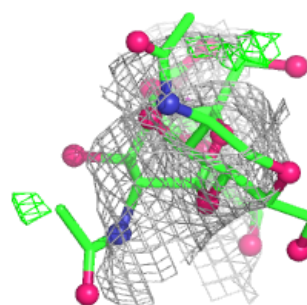
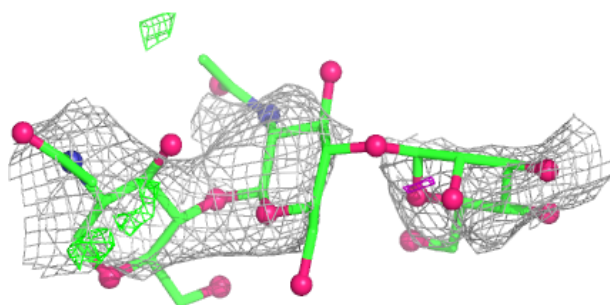
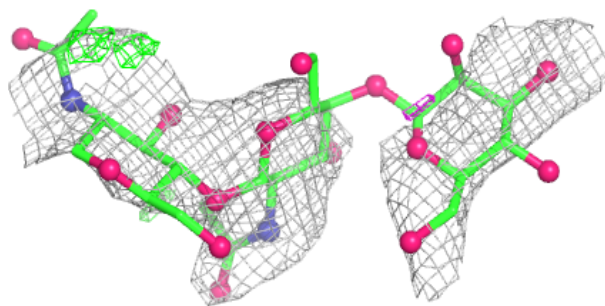
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**Electron density around Chain C:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	401	14/15	0.35	0.20	128,135,137,140	0
6	EDO	L	307	4/4	0.68	0.21	68,69,71,74	0
6	EDO	L	304	4/4	0.71	0.26	56,64,71,71	0
6	EDO	H	308	4/4	0.73	0.24	66,69,74,86	0
6	EDO	H	310	4/4	0.80	0.16	69,71,72,82	0
6	EDO	H	306	4/4	0.80	0.20	67,71,72,74	0
6	EDO	L	308	4/4	0.82	0.18	56,61,70,71	0
6	EDO	H	301	4/4	0.83	0.22	55,57,60,60	0
6	EDO	H	309	4/4	0.85	0.20	70,73,73,78	0
6	EDO	L	309	4/4	0.85	0.17	60,65,67,68	0
6	EDO	L	303	4/4	0.85	0.16	48,49,56,57	0
6	EDO	H	305	4/4	0.86	0.17	53,58,61,75	0
6	EDO	H	307	4/4	0.86	0.19	69,71,72,72	0
6	EDO	L	301	4/4	0.87	0.15	44,47,53,57	0
6	EDO	H	304	4/4	0.88	0.13	43,53,61,64	0
6	EDO	L	310	4/4	0.88	0.18	55,58,69,70	0
6	EDO	L	305	4/4	0.89	0.17	57,58,65,73	0
6	EDO	L	306	4/4	0.89	0.12	54,55,55,72	0
6	EDO	L	311	4/4	0.89	0.18	53,62,62,65	0
6	EDO	H	303	4/4	0.90	0.14	52,55,59,59	0
6	EDO	H	302	4/4	0.93	0.12	47,49,52,52	0
6	EDO	L	302	4/4	0.95	0.11	45,49,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.