



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2025 – 02:27 AM JST

PDB ID : 9JRC / pdb_00009jrc
Title : Crystal structure of SARS-CoV-2 receptor-binding domain complexed with squirrel ACE2
Authors : Lan, J.; Nan, X.
Deposited on : 2024-09-29
Resolution : 3.16 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

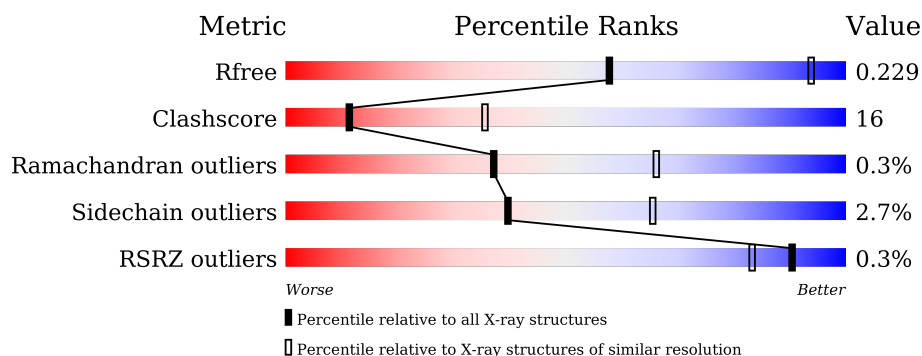
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	B	593	<div> <div>68%</div> <div>30%</div> <div>.</div> </div>
2	E	196	<div> <div>64%</div> <div>34%</div> <div>.</div> </div>
3	A	2	<div> <div>50%</div> <div>50%</div> </div>
4	C	3	<div> <div>100%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6544 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	593	Total	C	N	O	S	0	0	0
			4865	3106	819	910	30			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	PRO	-	expression tag	UNP A0A8D2KIZ1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	196	Total	C	N	O	S	0	0	0
			1555	996	260	291	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	372	THR	ALA	conflict	UNP P0DTC2
E	530	HIS	-	expression tag	UNP P0DTC2

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



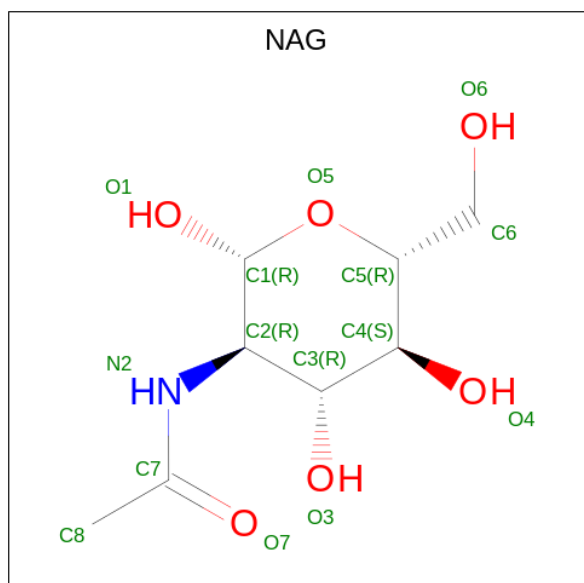
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

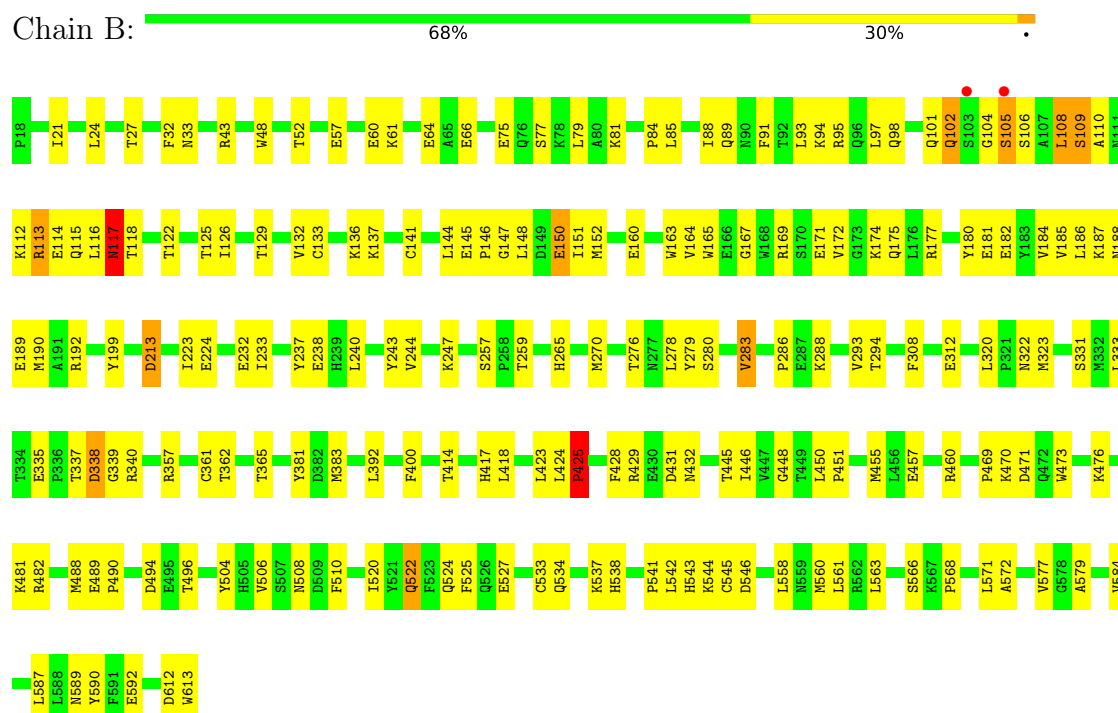
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Zn 1	0	0

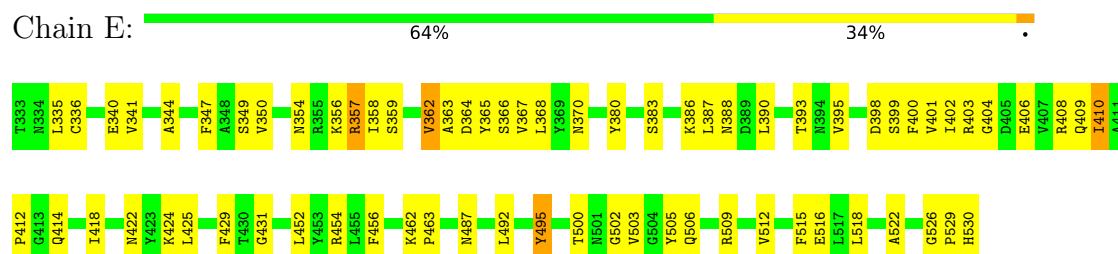
3 Residue-property plots

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: Angiotensin-converting enzyme



• Molecule 2: Spike protein S1



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



MAG1
MAG2

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

Chain C:

100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	194.13Å 194.13Å 148.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.65 – 3.16 29.65 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.65-3.16) 98.8 (29.65-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.197 , 0.229 0.204 , 0.229	Depositor DCC
R_{free} test set	1263 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6544	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: NAG, ZN, 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	B	0.57	0/4999	0.89	2/6780 (0.0%)
2	E	0.51	0/1600	0.76	2/2179 (0.1%)
All	All	0.55	0/6599	0.86	4/8959 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASN	N-CA-C	-9.31	102.42	113.88
2	E	495	TYR	CA-C-N	-6.83	116.21	122.29
2	E	495	TYR	C-N-CA	-6.83	116.21	122.29
1	B	278	LEU	N-CA-C	-5.15	106.23	112.88

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	B	4865	0	4673	162	3
2	E	1555	0	1468	45	0
3	A	28	0	25	0	0
4	C	39	0	34	0	0
5	B	42	0	39	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	14	0	13	0	0
6	B	1	0	0	0	0
All	All	6544	0	6252	204	3

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 16.

All (204) 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:B:112:LYS:HA	1:B:116:LEU:HD23	1.34	1.05
1:B:213:ASP:O	1:B:213:ASP:OD1	1.73	1.04
1:B:165:TRP:HA	1:B:270:MET:HE1	1.45	0.96
1:B:293:VAL:HG21	1:B:418:LEU:HD12	1.57	0.87
1:B:213:ASP:OD1	1:B:213:ASP:C	2.22	0.82
2:E:336:CYS:HB2	2:E:363:ALA:HB2	1.59	0.81
1:B:425:PRO:HD2	1:B:428:PHE:HB2	1.64	0.79
1:B:400:PHE:HE2	1:B:560:MET:HE1	1.53	0.73
1:B:152:MET:HE2	1:B:164:VAL:HB	1.71	0.71
1:B:400:PHE:CE2	1:B:560:MET:HE1	2.26	0.71
1:B:308:PHE:HE2	1:B:362:THR:HG21	1.56	0.70
1:B:81:LYS:HG2	1:B:101:GLN:HB2	1.72	0.69
1:B:132:VAL:HG21	1:B:167:GLY:HA3	1.73	0.69
1:B:455:MET:HE1	1:B:481:LYS:HE2	1.75	0.68
1:B:21:ILE:HG21	1:B:84:PRO:HD2	1.76	0.68
1:B:106:SER:HB3	1:B:113:ARG:CZ	2.24	0.67
1:B:169:ARG:NH1	1:B:270:MET:HE2	2.10	0.67
1:B:98:GLN:O	1:B:102:GLN:HB2	1.95	0.67
1:B:308:PHE:CE2	1:B:362:THR:HG21	2.29	0.67
1:B:48:TRP:CE2	1:B:52:THR:HG21	2.31	0.65
1:B:429:ARG:HE	1:B:429:ARG:HA	1.62	0.65
1:B:145:GLU:HB3	1:B:146:PRO:HD3	1.77	0.65
1:B:112:LYS:O	1:B:116:LEU:HB2	1.97	0.64
1:B:504:TYR:O	1:B:508:ASN:HB2	1.97	0.64
5:B:703:NAG:H3	5:B:703:NAG:H83	1.79	0.64
1:B:494:ASP:OD1	1:B:496:THR:HG22	1.98	0.63
2:E:383:SER:OG	2:E:386:LYS:HG2	1.97	0.63
1:B:91:PHE:O	1:B:95:ARG:HG3	1.98	0.63
2:E:341:VAL:HG22	2:E:356:LYS:HD2	1.80	0.62
1:B:577:VAL:HG23	1:B:579:ALA:H	1.65	0.62
2:E:347:PHE:CZ	2:E:399:SER:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:403:ARG:HD2	2:E:505:TYR:HA	1.83	0.60
1:B:97:LEU:O	1:B:101:GLN:HG2	2.01	0.60
1:B:293:VAL:HG21	1:B:418:LEU:CD1	2.32	0.59
1:B:538:HIS:CD2	1:B:545:CYS:HB3	2.38	0.58
2:E:366:SER:HB3	2:E:388:ASN:HD21	1.69	0.58
1:B:276:THR:OG1	1:B:445:THR:HG22	2.04	0.57
1:B:392:LEU:HD13	1:B:566:SER:HA	1.86	0.57
1:B:455:MET:SD	1:B:481:LYS:HG2	2.44	0.57
2:E:403:ARG:HG3	2:E:495:TYR:CE1	2.40	0.56
1:B:293:VAL:HG11	1:B:423:LEU:HD13	1.88	0.56
2:E:425:LEU:HD21	2:E:512:VAL:HG11	1.87	0.56
1:B:136:LYS:HG3	1:B:137:LYS:HG3	1.86	0.56
1:B:320:LEU:HD22	1:B:558:LEU:HD13	1.87	0.56
1:B:160:GLU:HA	1:B:163:TRP:CD1	2.41	0.55
1:B:43:ARG:HD2	1:B:66:GLU:OE2	2.07	0.55
1:B:112:LYS:CA	1:B:116:LEU:HD23	2.22	0.55
1:B:265:HIS:ND1	1:B:490:PRO:HG3	2.22	0.55
2:E:335:LEU:HD12	2:E:362:VAL:O	2.07	0.55
2:E:387:LEU:HD23	2:E:390:LEU:HD12	1.88	0.54
1:B:113:ARG:HA	1:B:117:ASN:OD1	2.08	0.54
1:B:108:LEU:HD12	1:B:112:LYS:HD2	1.89	0.54
2:E:516:GLU:HB3	2:E:518:LEU:HD13	1.89	0.54
1:B:113:ARG:O	1:B:117:ASN:CG	2.52	0.53
1:B:312:GLU:OE2	1:B:322:ASN:HB2	2.08	0.53
2:E:400:PHE:HZ	2:E:410:ILE:HG21	1.74	0.53
1:B:110:ALA:O	1:B:114:GLU:N	2.42	0.53
1:B:331:SER:HB3	1:B:333:LEU:HD13	1.90	0.52
1:B:560:MET:HG3	1:B:561:LEU:N	2.24	0.52
1:B:113:ARG:O	1:B:117:ASN:ND2	2.43	0.52
1:B:133:CYS:HA	1:B:141:CYS:HA	1.92	0.52
1:B:57:GLU:O	1:B:61:LYS:HG3	2.10	0.52
2:E:354:ASN:O	2:E:398:ASP:HA	2.10	0.52
2:E:431:GLY:HA2	2:E:515:PHE:HD2	1.74	0.52
1:B:116:LEU:HG	1:B:186:LEU:CD2	2.40	0.51
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.11	0.51
2:E:358:ILE:HB	2:E:395:VAL:HB	1.91	0.51
1:B:32:PHE:O	1:B:33:ASN:C	2.53	0.51
2:E:393:THR:HA	2:E:522:ALA:HA	1.91	0.51
1:B:323:MET:HA	1:B:383:MET:HE1	1.93	0.50
1:B:116:LEU:HG	1:B:186:LEU:HD22	1.94	0.50
1:B:335:GLU:HB2	1:B:361:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HD22	1:B:94:LYS:HG3	1.93	0.50
2:E:350:VAL:HG22	2:E:422:ASN:HB3	1.94	0.49
2:E:412:PRO:HG3	2:E:429:PHE:HB3	1.94	0.49
1:B:147:GLY:O	1:B:151:ILE:HD13	2.12	0.49
1:B:294:THR:HG23	1:B:365:THR:HA	1.94	0.49
1:B:533:CYS:O	1:B:538:HIS:HB3	2.13	0.49
1:B:169:ARG:HH12	1:B:270:MET:HE2	1.77	0.49
1:B:105:SER:HA	1:B:190:MET:SD	2.52	0.49
2:E:349:SER:HG	2:E:452:LEU:H	1.58	0.49
1:B:448:GLY:O	1:B:451:PRO:HD2	2.12	0.48
1:B:560:MET:HE2	1:B:572:ALA:HB1	1.95	0.48
1:B:429:ARG:HA	1:B:429:ARG:NE	2.28	0.48
2:E:414:GLN:H	2:E:424:LYS:NZ	2.12	0.48
1:B:160:GLU:HA	1:B:163:TRP:HD1	1.79	0.48
1:B:108:LEU:O	1:B:109:SER:C	2.56	0.48
1:B:115:GLN:HA	1:B:118:THR:HG23	1.95	0.48
1:B:455:MET:HE2	1:B:455:MET:HB3	1.63	0.48
1:B:24:LEU:HD13	2:E:487:ASN:ND2	2.29	0.48
1:B:125:THR:O	1:B:129:THR:HG22	2.14	0.48
1:B:445:THR:OG1	1:B:446:ILE:N	2.46	0.48
1:B:77:SER:O	1:B:81:LYS:HG3	2.14	0.48
1:B:88:ILE:HG13	1:B:97:LEU:HD12	1.95	0.48
1:B:165:TRP:CH2	1:B:490:PRO:HD2	2.48	0.47
1:B:177:ARG:O	1:B:181:GLU:HG3	2.15	0.47
1:B:381:TYR:CD1	1:B:561:LEU:HD22	2.49	0.47
1:B:237:TYR:CE1	1:B:451:PRO:HG2	2.50	0.47
2:E:357:ARG:HH12	2:E:359:SER:HA	1.80	0.47
2:E:386:LYS:O	2:E:390:LEU:HG	2.15	0.47
1:B:187:LYS:HD2	1:B:199:TYR:CZ	2.50	0.47
1:B:482:ARG:HH21	1:B:489:GLU:CD	2.23	0.46
1:B:541:PRO:HB2	1:B:543:HIS:CD2	2.51	0.46
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.97	0.46
1:B:116:LEU:HB3	1:B:186:LEU:HD13	1.97	0.46
1:B:522:GLN:O	1:B:525:PHE:HB2	2.15	0.46
1:B:587:LEU:C	1:B:587:LEU:HD23	2.41	0.46
1:B:132:VAL:HG12	1:B:148:LEU:HD11	1.97	0.46
1:B:185:VAL:O	1:B:189:GLU:HG3	2.15	0.46
1:B:283:VAL:HG13	1:B:286:PRO:HG3	1.97	0.46
1:B:288:LYS:NZ	1:B:431:ASP:OD2	2.42	0.46
1:B:180:TYR:O	1:B:184:VAL:HG23	2.15	0.46
1:B:338:ASP:OD2	1:B:340:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:GLU:O	2:E:409:GLN:HB2	2.16	0.45
1:B:414:THR:HG21	1:B:545:CYS:O	2.17	0.45
1:B:233:ILE:CG1	1:B:584:VAL:HG21	2.47	0.45
1:B:470:LYS:HA	1:B:473:TRP:CD1	2.51	0.45
2:E:503:VAL:O	2:E:506:GLN:HB2	2.16	0.45
1:B:81:LYS:HE2	1:B:101:GLN:O	2.17	0.45
1:B:93:LEU:HD23	1:B:93:LEU:O	2.17	0.45
1:B:460:ARG:NH2	1:B:510:PHE:O	2.42	0.45
1:B:488:MET:HE1	1:B:613:TRP:HB2	1.98	0.45
1:B:457:GLU:HA	1:B:457:GLU:OE1	2.17	0.44
1:B:27:THR:HG23	2:E:456:PHE:CE1	2.52	0.44
1:B:520:ILE:N	1:B:520:ILE:HD12	2.33	0.44
1:B:331:SER:CB	1:B:333:LEU:HD13	2.47	0.44
1:B:110:ALA:HA	1:B:113:ARG:HG3	1.99	0.44
1:B:237:TYR:CZ	1:B:451:PRO:HG2	2.52	0.44
2:E:347:PHE:CD2	2:E:401:VAL:HG23	2.52	0.44
1:B:106:SER:HB3	1:B:113:ARG:NH2	2.33	0.44
1:B:171:GLU:O	1:B:175:GLN:HG3	2.17	0.44
2:E:380:TYR:CE2	2:E:412:PRO:HD2	2.53	0.44
1:B:122:THR:O	1:B:126:ILE:HG12	2.18	0.44
1:B:589:ASN:HA	1:B:592:GLU:HG2	2.00	0.44
2:E:335:LEU:HA	2:E:362:VAL:O	2.17	0.44
1:B:527:GLU:O	1:B:534:GLN:HB2	2.17	0.44
1:B:541:PRO:HG2	1:B:544:LYS:HD3	1.99	0.44
1:B:543:HIS:CE1	1:B:544:LYS:HG3	2.53	0.44
2:E:526:GLY:O	2:E:530:HIS:N	2.50	0.44
1:B:104:GLY:C	1:B:106:SER:N	2.73	0.43
1:B:144:LEU:O	1:B:145:GLU:C	2.61	0.43
1:B:174:LYS:HE2	1:B:496:THR:HG23	2.00	0.43
1:B:243:TYR:OH	1:B:247:LYS:HE3	2.18	0.43
1:B:522:GLN:HE21	1:B:522:GLN:HB2	1.68	0.43
1:B:188:ASN:C	1:B:192:ARG:HE	2.26	0.43
1:B:232:GLU:HB2	1:B:584:VAL:HG11	2.00	0.43
1:B:522:GLN:O	1:B:525:PHE:N	2.50	0.43
1:B:105:SER:HA	1:B:190:MET:HG3	2.00	0.43
1:B:150:GLU:HA	5:B:703:NAG:HN2	1.83	0.43
1:B:542:LEU:C	1:B:544:LYS:H	2.27	0.43
1:B:116:LEU:CG	1:B:186:LEU:HD13	2.49	0.43
1:B:424:LEU:HB3	1:B:425:PRO:CD	2.48	0.43
1:B:339:GLY:O	1:B:340:ARG:C	2.62	0.43
1:B:257:SER:C	1:B:259:THR:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:MET:HE1	1:B:481:LYS:CE	2.43	0.43
1:B:136:LYS:CG	1:B:137:LYS:HG3	2.49	0.42
1:B:279:TYR:O	1:B:280:SER:C	2.60	0.42
1:B:116:LEU:HD22	1:B:116:LEU:N	2.33	0.42
1:B:417:HIS:HB2	1:B:546:ASP:CG	2.45	0.42
1:B:88:ILE:HG13	1:B:97:LEU:CD1	2.48	0.42
1:B:331:SER:HB3	1:B:333:LEU:CD1	2.49	0.42
1:B:520:ILE:O	1:B:524:GLN:HG3	2.19	0.42
1:B:542:LEU:O	1:B:542:LEU:HD23	2.19	0.42
2:E:403:ARG:O	2:E:404:GLY:C	2.63	0.42
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.66	0.42
2:E:454:ARG:HA	2:E:492:LEU:HD23	2.00	0.42
1:B:233:ILE:HG12	1:B:584:VAL:HG21	2.01	0.42
1:B:148:LEU:HD22	1:B:164:VAL:HG13	2.01	0.42
1:B:476:LYS:HD2	1:B:476:LYS:HA	1.84	0.42
2:E:366:SER:HB3	2:E:388:ASN:ND2	2.35	0.42
2:E:350:VAL:HA	2:E:400:PHE:HB2	2.02	0.42
2:E:402:ILE:HD11	2:E:418:ILE:HD12	2.02	0.42
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.78	0.42
1:B:488:MET:CE	1:B:613:TRP:HB2	2.49	0.42
2:E:347:PHE:HD2	2:E:401:VAL:HG23	1.84	0.41
2:E:340:GLU:O	2:E:344:ALA:HB2	2.20	0.41
2:E:366:SER:O	2:E:370:ASN:N	2.52	0.41
1:B:237:TYR:O	1:B:238:GLU:C	2.64	0.41
1:B:357:ARG:HH21	2:E:500:THR:HB	1.85	0.41
1:B:381:TYR:CG	1:B:561:LEU:HD22	2.55	0.41
2:E:365:TYR:HA	2:E:368:LEU:HD23	2.02	0.41
2:E:401:VAL:HG22	2:E:509:ARG:HG2	2.02	0.41
1:B:537:LYS:HA	1:B:537:LYS:HD3	1.83	0.41
1:B:24:LEU:HD13	2:E:487:ASN:HD21	1.86	0.41
1:B:240:LEU:O	1:B:244:VAL:HG23	2.21	0.41
1:B:432:ASN:OD1	1:B:432:ASN:N	2.53	0.41
2:E:502:GLY:O	2:E:503:VAL:C	2.63	0.41
1:B:522:GLN:H	1:B:522:GLN:HG3	1.61	0.41
1:B:223:ILE:O	1:B:224:GLU:C	2.62	0.41
1:B:560:MET:HE2	1:B:560:MET:HB2	1.91	0.41
2:E:364:ASP:O	2:E:367:VAL:HG22	2.21	0.41
1:B:543:HIS:HA	1:B:590:TYR:CE1	2.56	0.41
1:B:182:GLU:O	1:B:185:VAL:HG22	2.21	0.40
1:B:223:ILE:H	1:B:223:ILE:HG13	1.65	0.40
1:B:568:PRO:O	1:B:571:LEU:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:O	1:B:64:GLU:HG3	2.20	0.40
1:B:115:GLN:C	1:B:117:ASN:H	2.29	0.40
1:B:563:LEU:HA	1:B:563:LEU:HD23	1.89	0.40
1:B:75:GLU:O	1:B:79:LEU:HG	2.22	0.40
1:B:115:GLN:HA	1:B:118:THR:CG2	2.52	0.40
1:B:460:ARG:NH1	1:B:506:VAL:HA	2.36	0.40
1:B:494:ASP:OD1	1:B:494:ASP:N	2.48	0.40
1:B:524:GLN:HB3	1:B:577:VAL:HG11	2.03	0.40
2:E:462:LYS:O	2:E:463:PRO:C	2.62	0.40

All (3) 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)
1:B:89:GLN:OE1	1:B:213:ASP:OD2[6_545]	1.17	1.03
1:B:89:GLN:CD	1:B:213:ASP:OD2[6_545]	1.67	0.53
1:B:89:GLN:CG	1:B:213:ASP:OD2[6_545]	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	B	591/593 (100%)	546 (92%)	44 (7%)	1 (0%)	44	72
2	E	194/196 (99%)	175 (90%)	18 (9%)	1 (0%)	25	57
All	All	785/789 (100%)	721 (92%)	62 (8%)	2 (0%)	37	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	529	PRO
1	B	425	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	B	523/523 (100%)	508 (97%)	15 (3%)	37	63
2	E	170/170 (100%)	166 (98%)	4 (2%)	44	68
All	All	693/693 (100%)	674 (97%)	19 (3%)	40	65

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
1	B	105	SER
1	B	108	LEU
1	B	109	SER
1	B	113	ARG
1	B	117	ASN
1	B	150	GLU
1	B	172	VAL
1	B	213	ASP
1	B	283	VAL
1	B	337	THR
1	B	338	ASP
1	B	425	PRO
1	B	522	GLN
1	B	612	ASP
2	E	357	ARG
2	E	362	VAL
2	E	408	ARG
2	E	410	ILE

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

Mol	Chain	Res	Type
1	B	76	GLN
1	B	96	GLN
1	B	98	GLN

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Mol	Chain	Res	Type
1	B	102	GLN
1	B	239	HIS
1	B	522	GLN
1	B	543	HIS
1	B	602	ASN
2	E	370	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	$\# Z > 2$
3	NAG	A	1	3,1	14,14,15	0.60	0	17,19,21	0.57	0
3	NAG	A	2	3	14,14,15	0.53	0	17,19,21	1.14	2 (11%)
4	NAG	C	1	4,1	14,14,15	0.35	0	17,19,21	1.03	1 (5%)
4	NAG	C	2	4	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
4	BMA	C	3	4	11,11,12	1.60	3 (27%)	15,15,17	1.17	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	1/6/23/26	0/1/1/1
4	NAG	C	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	BMA	C1-C2	3.10	1.59	1.52
4	C	3	BMA	C4-C5	2.63	1.58	1.53
4	C	3	BMA	C4-C3	2.32	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	3.12	116.42	112.19
4	C	3	BMA	C1-O5-C5	2.73	115.89	112.19
3	A	2	NAG	C2-N2-C7	2.72	126.77	122.90
3	A	2	NAG	C3-C4-C5	2.54	114.77	110.24
4	C	2	NAG	C2-N2-C7	2.25	126.10	122.90

There are no chirality outliers.

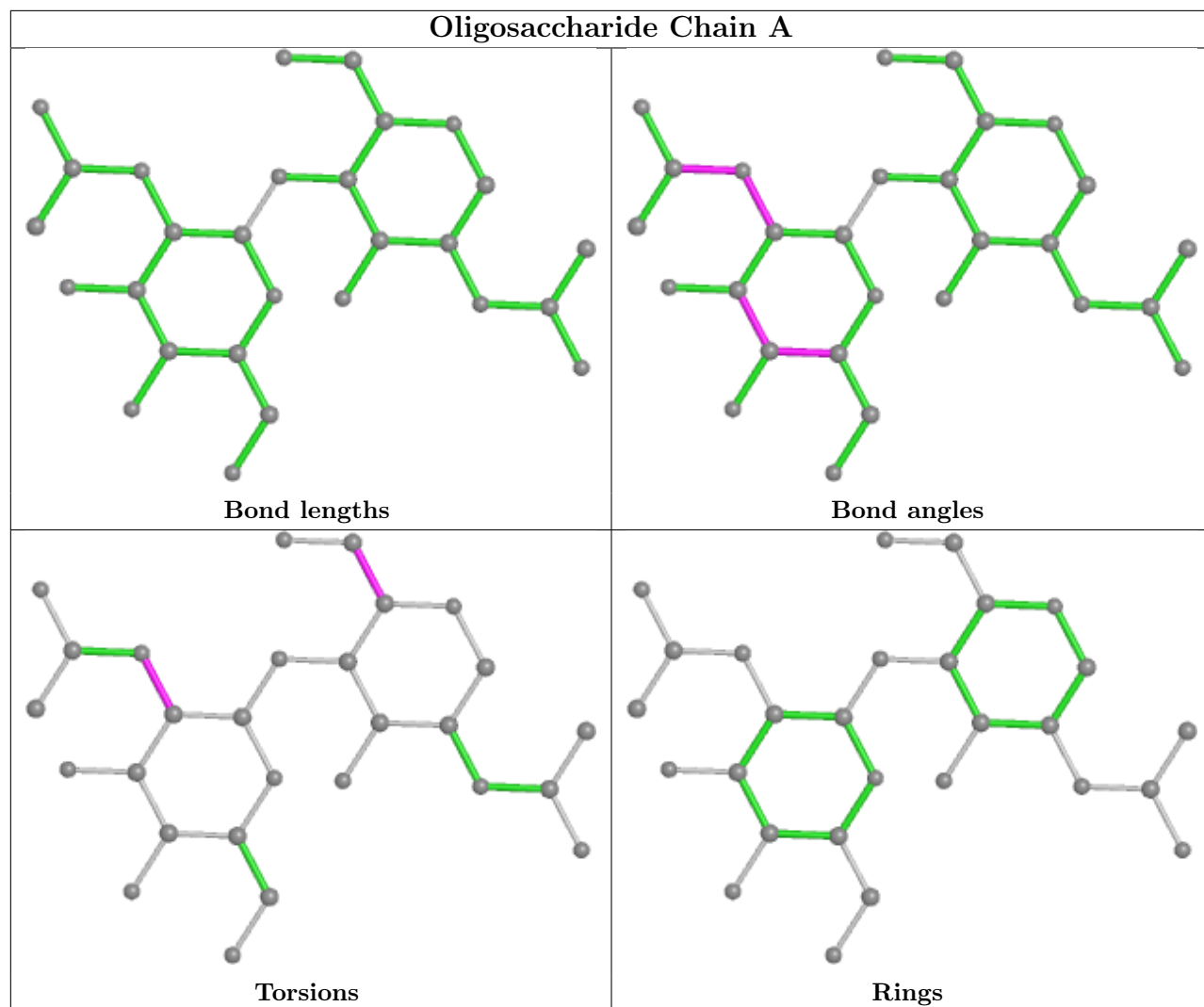
All (5) torsion outliers are listed below:

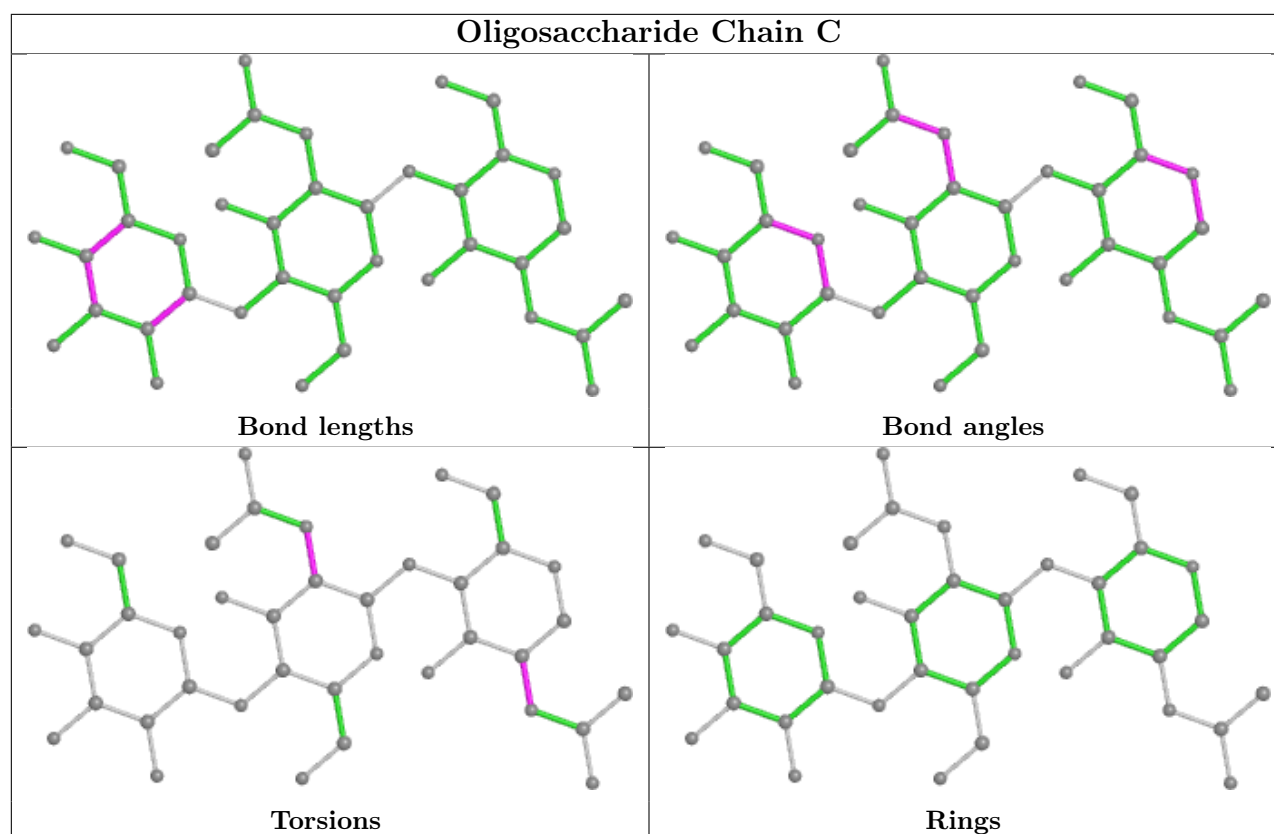
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C3-C2-N2-C7
3	A	1	NAG	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	2	NAG	C3-C2-N2-C7
4	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	B	703	1	14,14,15	1.00	2 (14%)	17,19,21	1.42	2 (11%)
5	NAG	B	701	1	14,14,15	0.44	0	17,19,21	0.58	0
5	NAG	B	702	1	14,14,15	0.31	0	17,19,21	1.36	2 (11%)
5	NAG	E	601	2	14,14,15	0.42	0	17,19,21	0.66	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
5	NAG	B	703	1	-	4/6/23/26	0/1/1/1
5	NAG	B	701	1	-	4/6/23/26	0/1/1/1
5	NAG	B	702	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	703	NAG	C1-C2	2.71	1.56	1.52
5	B	703	NAG	O5-C1	2.28	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	703	NAG	C2-N2-C7	4.42	129.20	122.90
5	B	702	NAG	C1-O5-C5	4.38	118.13	112.19
5	B	703	NAG	C1-O5-C5	2.76	115.93	112.19
5	B	702	NAG	C2-N2-C7	2.03	125.79	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	701	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	B	701	NAG	C8-C7-N2-C2
5	B	701	NAG	O7-C7-N2-C2
5	B	703	NAG	C8-C7-N2-C2
5	B	703	NAG	O7-C7-N2-C2
5	E	601	NAG	C8-C7-N2-C2
5	E	601	NAG	O7-C7-N2-C2
5	E	601	NAG	C4-C5-C6-O6
5	B	701	NAG	C4-C5-C6-O6
5	B	702	NAG	O5-C5-C6-O6
5	B	703	NAG	C3-C2-N2-C7
5	B	703	NAG	O5-C5-C6-O6
5	B	702	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	B	703	NAG	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 [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	B	593/593 (100%)	-0.42	2 (0%) 90 83	53, 76, 125, 189	0
2	E	196/196 (100%)	-0.19	0 100 100	65, 91, 165, 179	0
All	All	789/789 (100%)	-0.37	2 (0%) 90 83	53, 80, 145, 189	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	SER	3.3
1	B	103	SER	2.1

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](#)

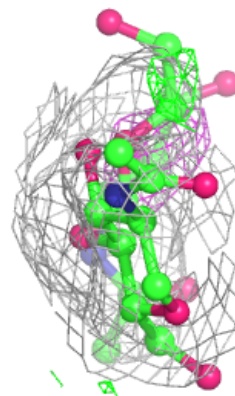
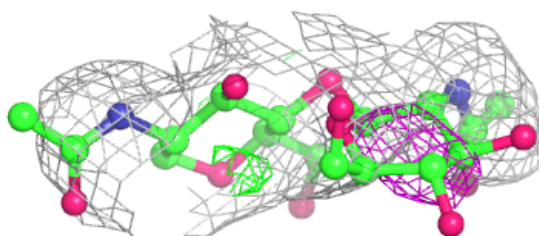
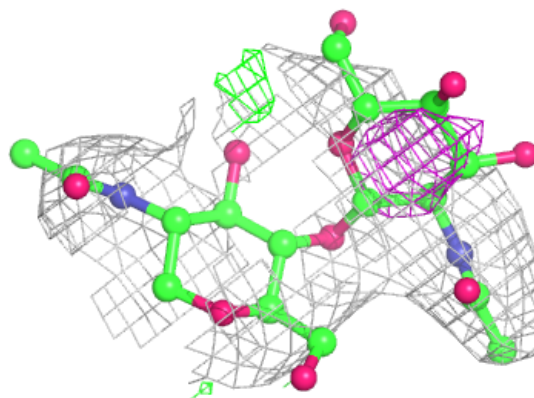
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	1	14/15	-	-	105,117,129,133	0
3	NAG	A	2	14/15	-	-	127,139,147,148	0
4	NAG	C	2	14/15	0.33	0.14	109,115,121,124	0
4	NAG	C	1	14/15	0.66	0.13	88,93,102,106	0
4	BMA	C	3	11/12	-	-	111,121,125,126	0

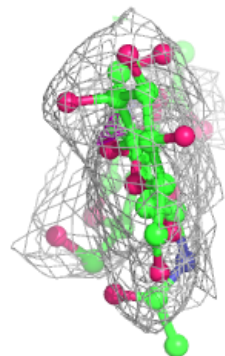
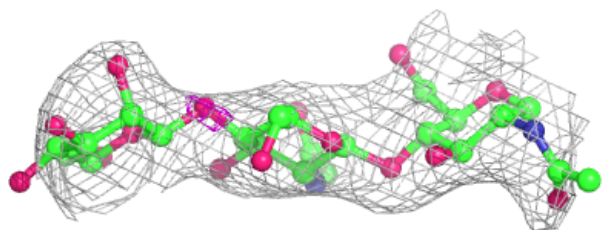
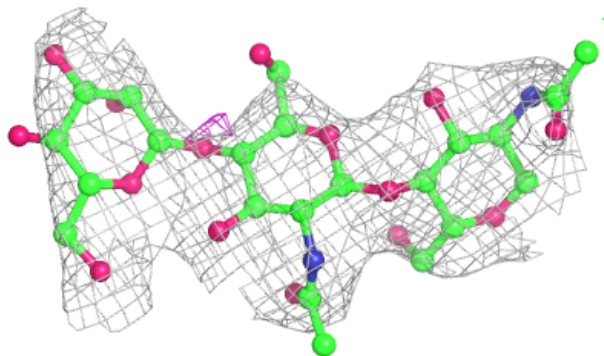
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

$2mF_o-DF_c$ (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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	703	14/15	0.56	0.14	123,129,135,138	0
6	ZN	B	704	1/1	0.63	0.18	260,260,260,260	0
5	NAG	E	601	14/15	0.71	0.14	110,127,133,134	0
5	NAG	B	702	14/15	0.71	0.11	107,110,115,117	0
5	NAG	B	701	14/15	0.86	0.09	93,104,111,114	0

6.5 Other polymers

There are no such residues in this entry.