



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 PM UTC

PDB ID : 7XB1 / pdb_00007xb1
Title : Crystal structure of Omicron BA.3 RBD complexed with hACE2
Authors : Li, W.; Meng, Y.; Liao, H.
Deposited on : 2022-03-19
Resolution : 2.70 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

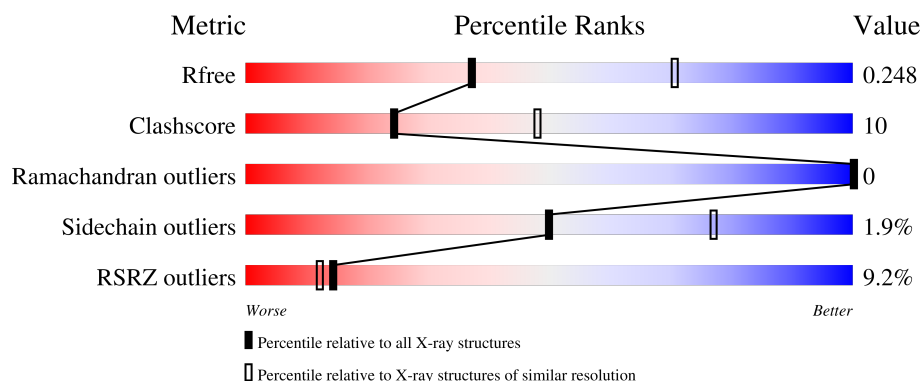
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	596	5% 74% 25% .
2	B	195	22% 73% 26% .
3	C	2	100%
4	D	4	50% 50%
5	E	3	67% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6652 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	2	0
			4877	3121	810	917	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1566	1011	265	282	8			

There are 15 discrepancies between the modelled and reference sequences:

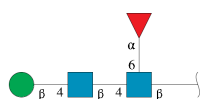
Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2

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



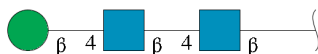
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- 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.

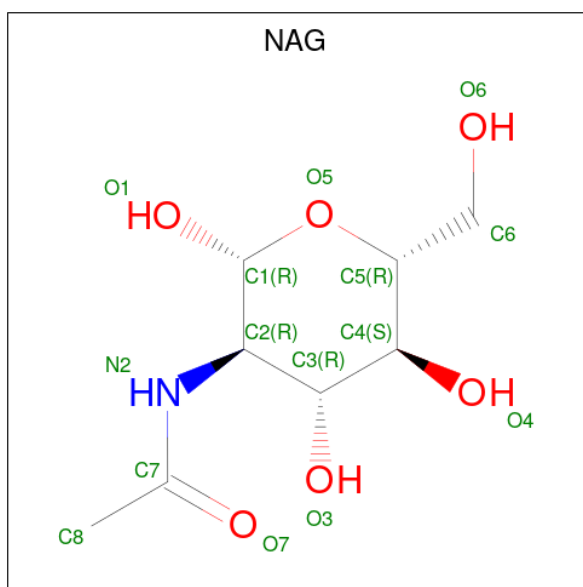


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

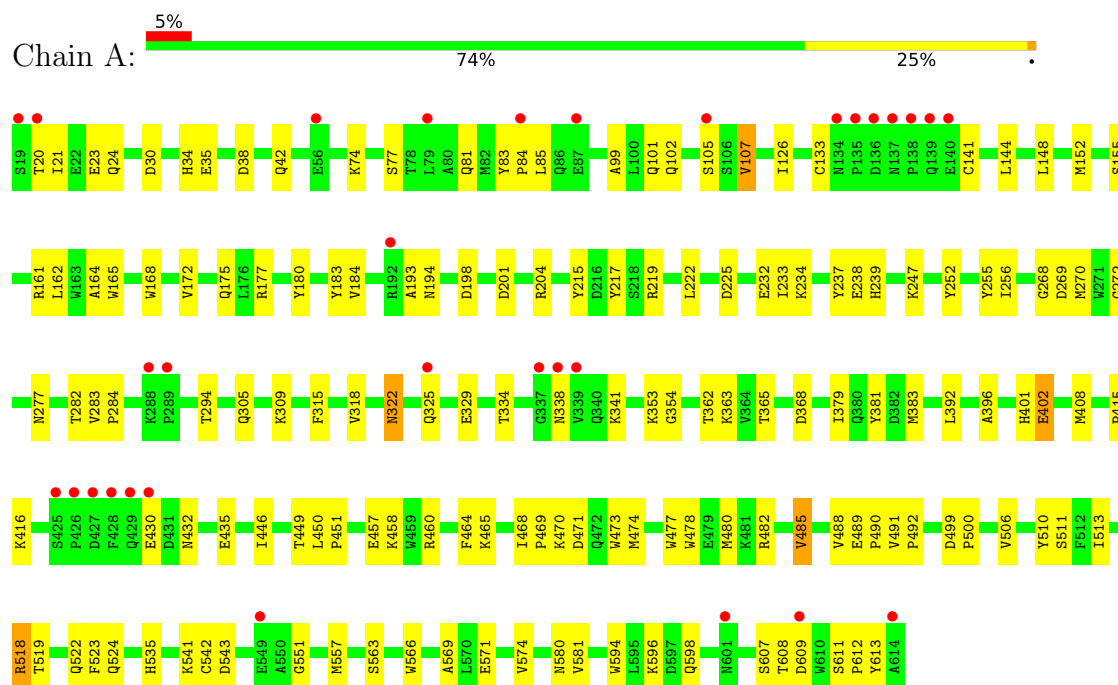
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	41	Total	O	0	0
			41	41		
8	B	9	Total	O	0	0
			9	9		

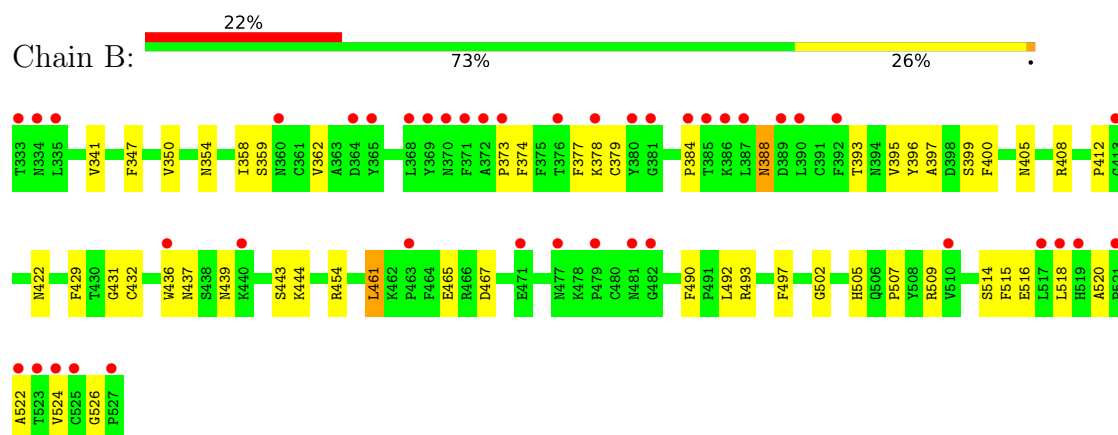
3 Residue-property plots [i](#)

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: Angiotensin-converting enzyme 2



• Molecule 2: Spike protein S1



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

Chain C:  100%

MAG1
MAG2

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

MAG1
MAG2
BMA3
FUC4

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

Chain E:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.05Å 101.05Å 222.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.70 49.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.3 (49.27-2.70) 92.5 (49.27-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.214 , 0.248 0.214 , 0.248	Depositor DCC
R_{free} test set	1514 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.0	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	0.91	EDS
Total number of atoms	6652	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: ZN, BMA, NAG, FUC

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	0.11	0/5021	0.26	0/6821
2	B	0.15	0/1614	0.34	0/2197
All	All	0.12	0/6635	0.29	0/9018

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	A	4877	0	4654	97	0
2	B	1566	0	1491	32	0
3	C	28	0	25	1	0
4	D	49	0	43	1	0
5	E	39	0	34	0	0
6	A	1	0	0	0	0
7	A	42	0	39	0	0
8	A	41	0	0	1	0
8	B	9	0	0	0	0
All	All	6652	0	6286	127	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 10.

All (127) 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:B:373:PRO:HG2	2:B:437:ASN:HB3	1.57	0.85
1:A:325:GLN:NE2	1:A:329:GLU:OE2	2.22	0.73
2:B:393:THR:HA	2:B:522:ALA:HA	1.69	0.72
1:A:607:SER:OG	1:A:609:ASP:OD1	2.07	0.72
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.73	0.71
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.74	0.70
1:A:152:MET:HE3	1:A:164:ALA:HB3	1.77	0.67
2:B:358:ILE:HB	2:B:395:VAL:HB	1.77	0.65
1:A:500:PRO:HB2	1:A:506:VAL:HG11	1.78	0.64
2:B:388:ASN:N	2:B:388:ASN:OD1	2.30	0.64
1:A:177:ARG:NH2	1:A:470:LYS:O	2.31	0.64
2:B:379:CYS:HB2	2:B:384:PRO:HD3	1.80	0.63
2:B:362:VAL:HG23	2:B:526:GLY:HA3	1.83	0.61
2:B:461:LEU:HG	2:B:465:GLU:HB3	1.84	0.59
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.83	0.59
2:B:396:TYR:HB2	2:B:514:SER:HB2	1.83	0.58
1:A:392:LEU:HD13	1:A:563:SER:HA	1.86	0.58
1:A:252:TYR:HB2	1:A:256:ILE:HD12	1.86	0.57
1:A:557:MET:HG2	1:A:569:ALA:HB1	1.87	0.56
2:B:350:VAL:HG22	2:B:422:ASN:HB3	1.86	0.56
1:A:21:ILE:HD11	1:A:84:PRO:HD2	1.88	0.55
1:A:363:LYS:HD2	1:A:368:ASP:OD2	2.06	0.55
1:A:294:THR:HG23	1:A:365:THR:HA	1.88	0.54
2:B:431:GLY:HA2	2:B:515:PHE:CD2	2.43	0.54
1:A:252:TYR:HB3	1:A:255:TYR:HB2	1.88	0.54
1:A:474:MET:HE1	1:A:500:PRO:HD2	1.90	0.54
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.91	0.53
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.90	0.53
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.91	0.52
1:A:322:ASN:OD1	1:A:322:ASN:N	2.41	0.51
1:A:460:ARG:NH1	1:A:506:VAL:HA	2.26	0.51
1:A:24:GLN:HB3	1:A:83:TYR:HE1	1.77	0.50
1:A:237:TYR:OH	1:A:485:VAL:O	2.23	0.50
2:B:393:THR:HG21	2:B:518:LEU:HB2	1.94	0.50
1:A:482:ARG:NH1	1:A:608:THR:O	2.39	0.50
1:A:416:LYS:HD2	1:A:543:ASP:HB3	1.95	0.49
1:A:535:HIS:CD2	1:A:542:CYS:HB2	2.47	0.49
1:A:488:VAL:HG21	1:A:611:SER:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:CYS:HA	1:A:141:CYS:HA	1.95	0.48
1:A:305:GLN:OE1	1:A:309:LYS:NZ	2.47	0.48
1:A:363:LYS:NZ	8:A:804:HOH:O	2.47	0.48
1:A:396:ALA:HB1	1:A:566:TRP:HA	1.94	0.48
1:A:20:THR:HG23	1:A:23:GLU:H	1.78	0.48
1:A:477:TRP:CD2	1:A:500:PRO:HD3	2.48	0.48
1:A:269:ASP:OD1	1:A:272:GLY:N	2.47	0.48
1:A:162:LEU:HD13	1:A:490:PRO:HB2	1.96	0.47
1:A:233:ILE:HG13	1:A:581:VAL:HG21	1.97	0.47
2:B:412:PRO:HG3	2:B:429:PHE:HB3	1.96	0.47
1:A:247:LYS:HB2	1:A:282:THR:HG22	1.97	0.47
2:B:490:PHE:O	2:B:493:ARG:NH1	2.48	0.47
1:A:379:ILE:O	1:A:383:MET:HG3	2.15	0.46
1:A:268:GLY:O	1:A:277:ASN:ND2	2.35	0.46
1:A:234:LYS:O	1:A:238:GLU:HG3	2.16	0.46
1:A:524:GLN:CD	1:A:580:ASN:H	2.23	0.46
2:B:374:PHE:O	2:B:436:TRP:HA	2.16	0.46
1:A:458:LYS:HD3	1:A:480:MET:HE3	1.98	0.46
1:A:74:LYS:HZ3	1:A:105:SER:HG	1.62	0.46
2:B:393:THR:HG23	2:B:520:ALA:HB3	1.98	0.45
2:B:516:GLU:OE2	2:B:518:LEU:HD11	2.15	0.45
1:A:20:THR:OG1	1:A:21:ILE:N	2.49	0.45
1:A:381:TYR:HB3	1:A:401:HIS:CE1	2.51	0.45
1:A:152:MET:HE1	1:A:161:ARG:HA	1.98	0.45
1:A:435:GLU:OE2	1:A:541:LYS:HE3	2.16	0.45
2:B:359:SER:HA	2:B:524:VAL:HG22	1.98	0.45
1:A:38:ASP:O	1:A:42:GLN:HG3	2.17	0.45
1:A:239:HIS:CE1	1:A:596:LYS:HG2	2.51	0.45
1:A:478:TRP:NE1	1:A:499:ASP:OD2	2.47	0.45
2:B:454:ARG:NH2	2:B:467:ASP:O	2.46	0.45
1:A:237:TYR:CD1	1:A:451:PRO:HG2	2.52	0.45
1:A:478:TRP:CD2	1:A:489:GLU:HB3	2.52	0.44
1:A:594:TRP:CZ2	1:A:598:GLN:HG3	2.52	0.44
1:A:165:TRP:CH2	1:A:490:PRO:HD2	2.52	0.44
1:A:99:ALA:HA	1:A:102:GLN:HG2	2.00	0.44
1:A:126:ILE:HD13	1:A:175:GLN:HB3	1.99	0.44
2:B:341:VAL:HG11	2:B:397:ALA:HB1	2.00	0.44
1:A:284:PRO:HB3	1:A:594:TRP:CZ2	2.52	0.44
1:A:477:TRP:CZ3	1:A:500:PRO:HB3	2.52	0.44
1:A:415:PRO:HB2	1:A:430:GLU:OE2	2.18	0.43
1:A:215:TYR:OH	1:A:571:GLU:OE1	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:O	2:B:443:SER:HB2	2.18	0.43
1:A:315:PHE:HE1	1:A:408:MET:HE3	1.83	0.43
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.84	0.43
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.01	0.43
1:A:198:ASP:OD2	1:A:465:LYS:HG3	2.19	0.43
2:B:405:ASN:O	2:B:408:ARG:HG2	2.19	0.43
1:A:155:SER:O	1:A:161:ARG:HD2	2.19	0.43
1:A:354:GLY:HA3	2:B:502:GLY:HA3	2.01	0.43
1:A:460:ARG:HD3	1:A:506:VAL:HG13	2.01	0.43
2:B:497:PHE:CD2	2:B:507:PRO:HB3	2.53	0.43
1:A:30:ASP:O	1:A:34:HIS:ND1	2.43	0.42
2:B:490:PHE:CE2	2:B:492:LEU:HB2	2.53	0.42
3:C:1:NAG:H62	3:C:2:NAG:O7	2.19	0.42
1:A:81:GLN:HG3	1:A:101:GLN:HG2	2.02	0.42
2:B:347:PHE:CG	2:B:509:ARG:HG2	2.54	0.42
1:A:204:ARG:HG2	1:A:222:LEU:HD23	2.02	0.42
2:B:377:PHE:O	2:B:378:LYS:HD2	2.20	0.42
1:A:107:VAL:HG11	1:A:194:ASN:OD1	2.20	0.42
1:A:162:LEU:HD11	1:A:491:VAL:HG23	2.01	0.42
1:A:353:LYS:HA	2:B:505:HIS:CE1	2.55	0.41
1:A:510:TYR:HE1	4:D:2:NAG:H61	1.86	0.41
2:B:379:CYS:HA	2:B:432:CYS:HA	2.01	0.41
1:A:432:ASN:OD1	1:A:432:ASN:N	2.53	0.41
1:A:201:ASP:O	1:A:219:ARG:HD2	2.20	0.41
1:A:492:PRO:HD3	1:A:613:TYR:CG	2.56	0.41
1:A:519:THR:O	1:A:522:GLN:HG2	2.21	0.41
1:A:24:GLN:HB3	1:A:83:TYR:CE1	2.55	0.41
1:A:362:THR:HG23	1:A:368:ASP:HB3	2.02	0.41
2:B:347:PHE:CE2	2:B:399:SER:HB2	2.55	0.41
2:B:444:LYS:HB3	2:B:444:LYS:HE2	1.86	0.41
1:A:184:VAL:HG22	1:A:464:PHE:HE1	1.86	0.41
1:A:318:VAL:O	1:A:551:GLY:HA3	2.21	0.41
1:A:152:MET:HG3	1:A:270:MET:HA	2.02	0.41
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.56	0.41
1:A:402:GLU:HB3	1:A:518:ARG:HD2	2.02	0.41
1:A:446:ILE:O	1:A:449:THR:HG22	2.20	0.41
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.21	0.41
1:A:499:ASP:N	1:A:500:PRO:HD2	2.35	0.41
1:A:524:GLN:HB3	1:A:574:VAL:HG11	2.02	0.41
2:B:350:VAL:HA	2:B:400:PHE:HB2	2.02	0.41
1:A:35:GLU:OE2	2:B:493:ARG:NH2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:O	1:A:341:LYS:NZ	2.48	0.40
1:A:217:TYR:OH	1:A:225:ASP:OD2	2.34	0.40
1:A:74:LYS:HE3	1:A:74:LYS:HB3	1.89	0.40
1:A:107:VAL:HG13	1:A:193:ALA:HB3	2.02	0.40
1:A:237:TYR:CG	1:A:451:PRO:HG2	2.57	0.40
1:A:460:ARG:NH2	1:A:510:TYR:O	2.36	0.40
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/596 (100%)	587 (98%)	9 (2%)	0	100	100
2	B	193/195 (99%)	184 (95%)	9 (5%)	0	100	100
All	All	789/791 (100%)	771 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	528/526 (100%)	518 (98%)	10 (2%)	50	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	169/169 (100%)	166 (98%)	3 (2%)	51	78
All	All	697/695 (100%)	684 (98%)	13 (2%)	50	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	85	LEU
1	A	107	VAL
1	A	283	VAL
1	A	322	ASN
1	A	334	THR
1	A	402	GLU
1	A	485	VAL
1	A	511	SER
1	A	518	ARG
2	B	354	ASN
2	B	388	ASN
2	B	461	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	ASN
1	A	572	ASN
2	B	354	ASN
2	B	474	GLN
2	B	477	ASN
2	B	487	ASN
2	B	505	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 ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	3,1	14,14,15	0.32	0	17,19,21	0.63	0
3	NAG	C	2	3	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	D	1	4,1	14,14,15	0.20	0	17,19,21	0.36	0
4	NAG	D	2	4	14,14,15	0.16	0	17,19,21	0.44	0
4	BMA	D	3	4	11,11,12	0.52	0	15,15,17	0.95	1 (6%)
4	FUC	D	4	4	10,10,11	0.68	0	14,14,16	0.72	0
5	NAG	E	1	5,2	14,14,15	0.61	1 (7%)	17,19,21	0.65	0
5	NAG	E	2	5	14,14,15	0.21	0	17,19,21	0.64	0
5	BMA	E	3	5	11,11,12	0.64	0	15,15,17	0.76	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
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
5	NAG	E	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	O5-C1	-2.10	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-O5-C5	2.27	115.23	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

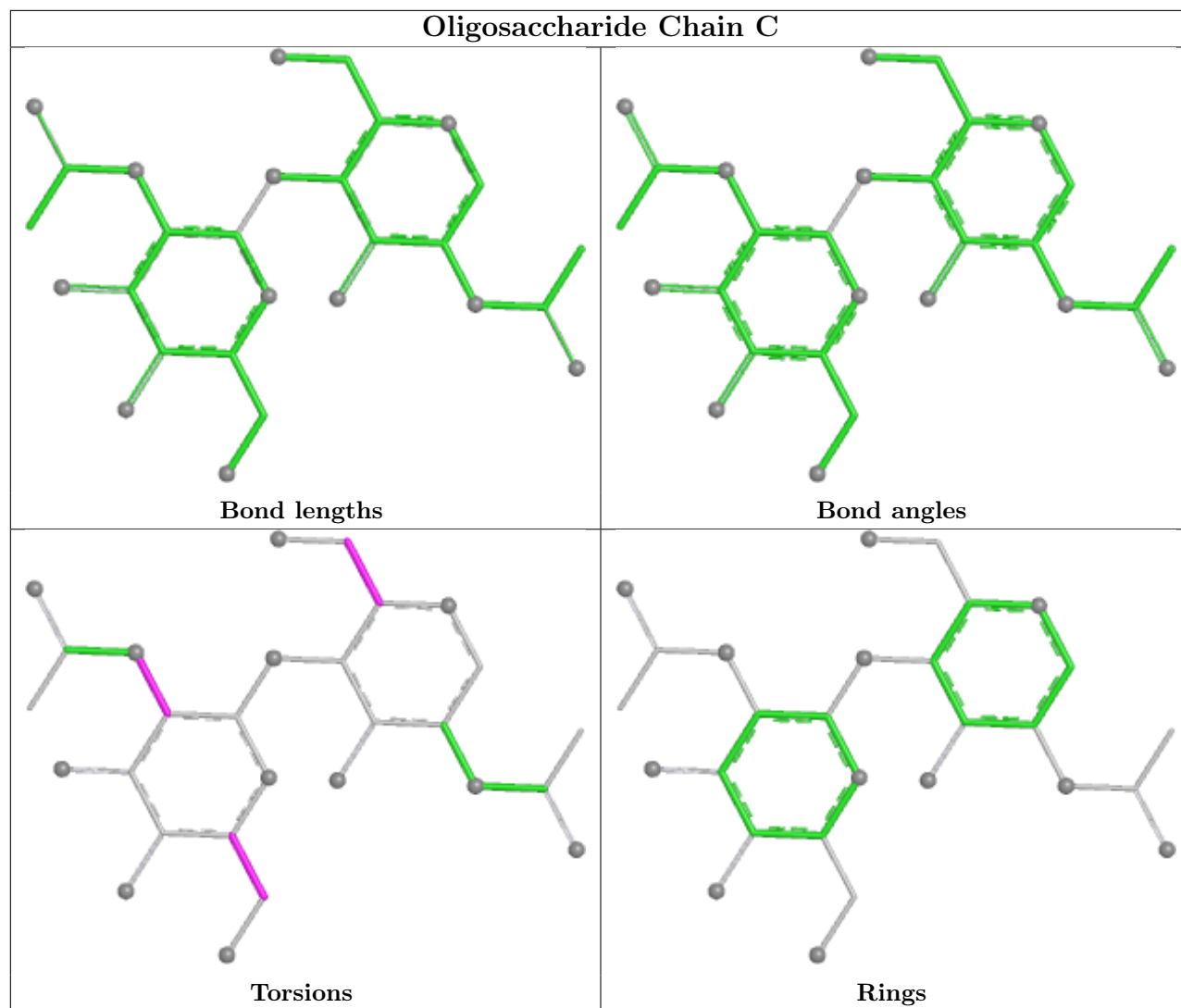
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
5	E	1	NAG	C4-C5-C6-O6

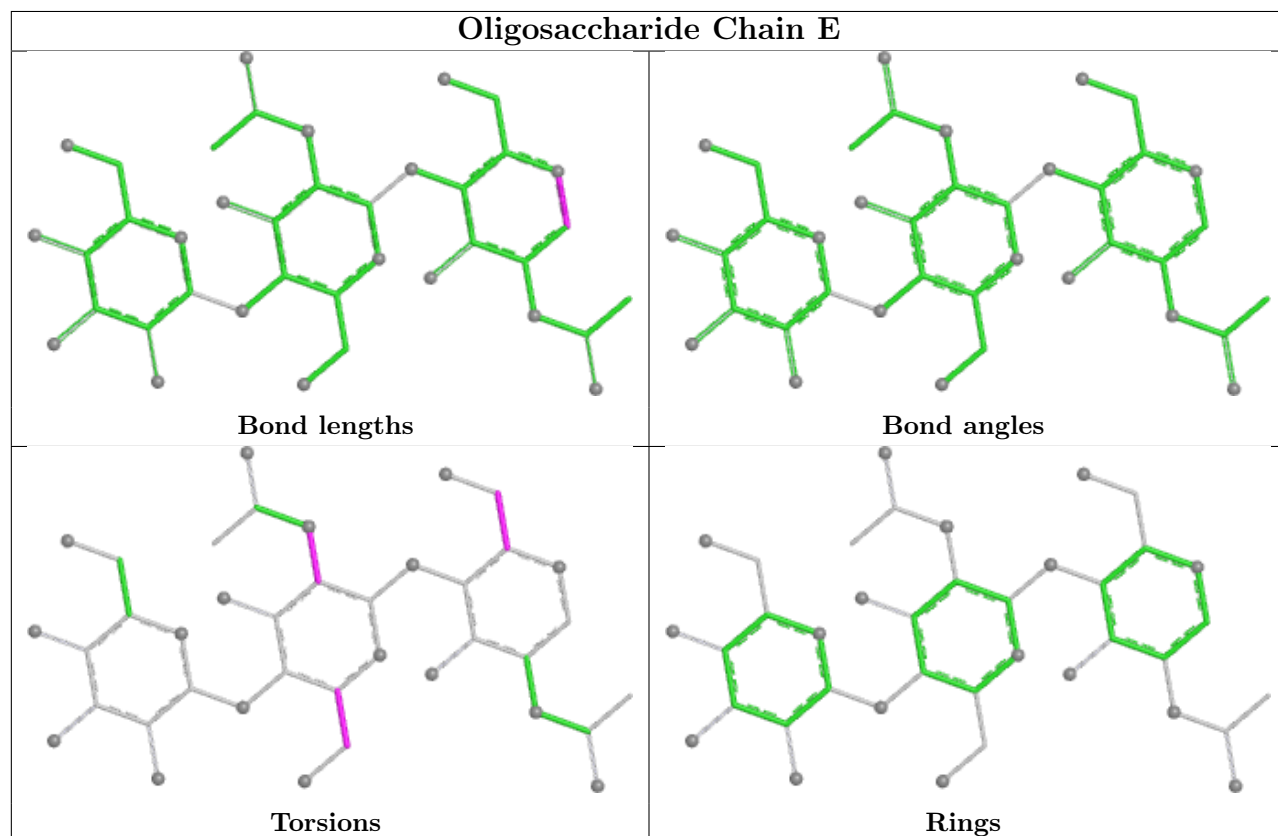
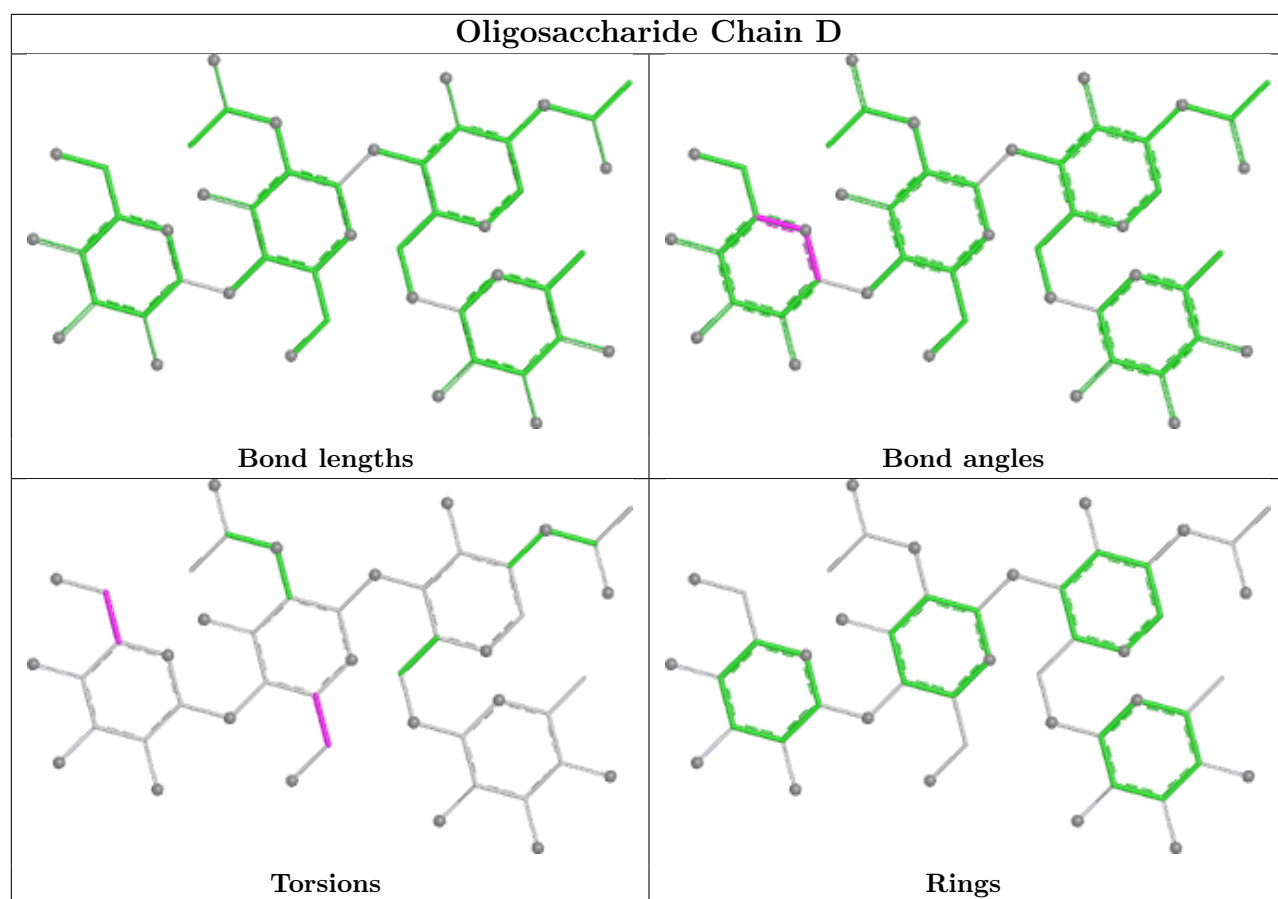
There are no ring outliers.

3 monomers are involved in 2 short contacts:

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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
7	NAG	A	704	1	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	A	702	1	14,14,15	0.30	0	17,19,21	0.54	0
7	NAG	A	703	1	14,14,15	0.27	0	17,19,21	0.67	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
7	NAG	A	704	1	-	0/6/23/26	0/1/1/1
7	NAG	A	702	1	-	0/6/23/26	0/1/1/1
7	NAG	A	703	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

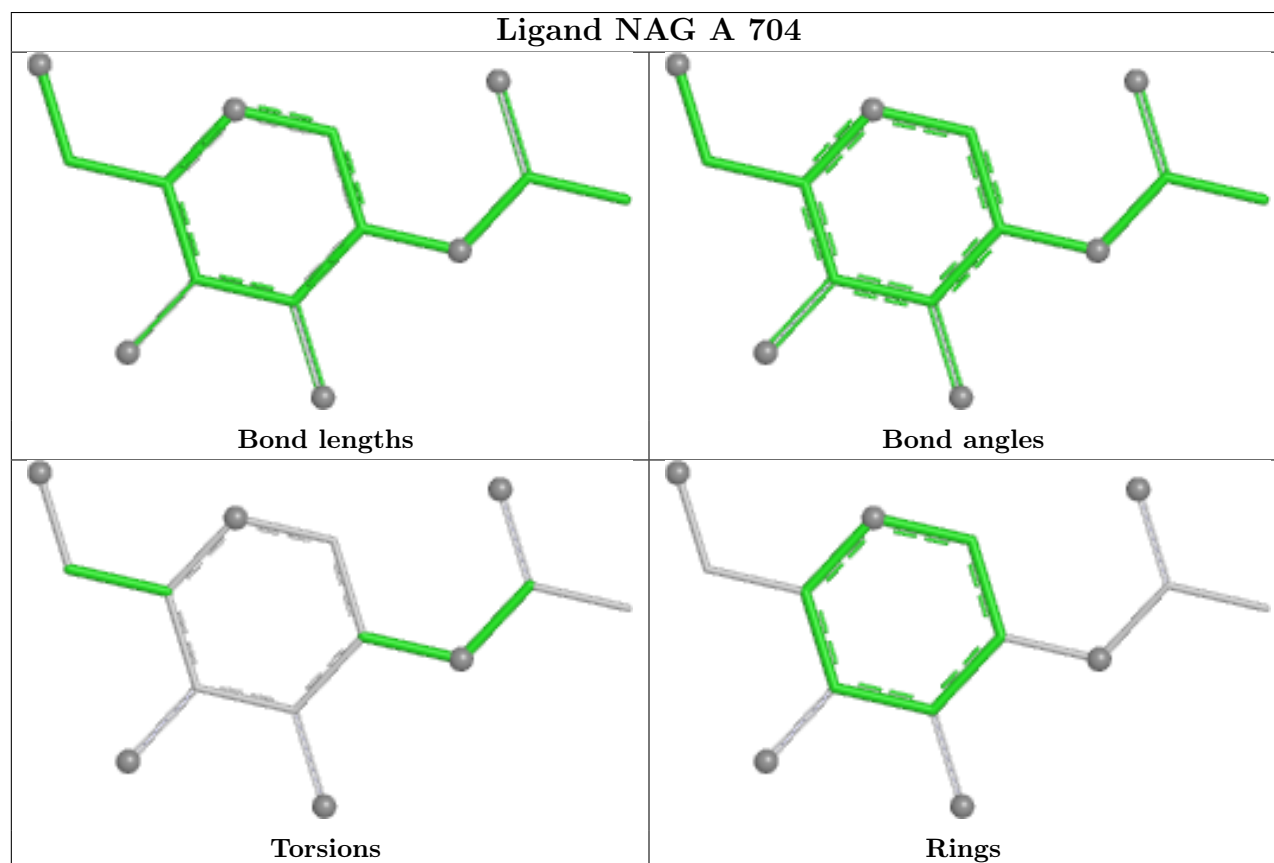
Mol	Chain	Res	Type	Atoms
7	A	703	NAG	O5-C5-C6-O6
7	A	703	NAG	C4-C5-C6-O6
7	A	703	NAG	C3-C2-N2-C7

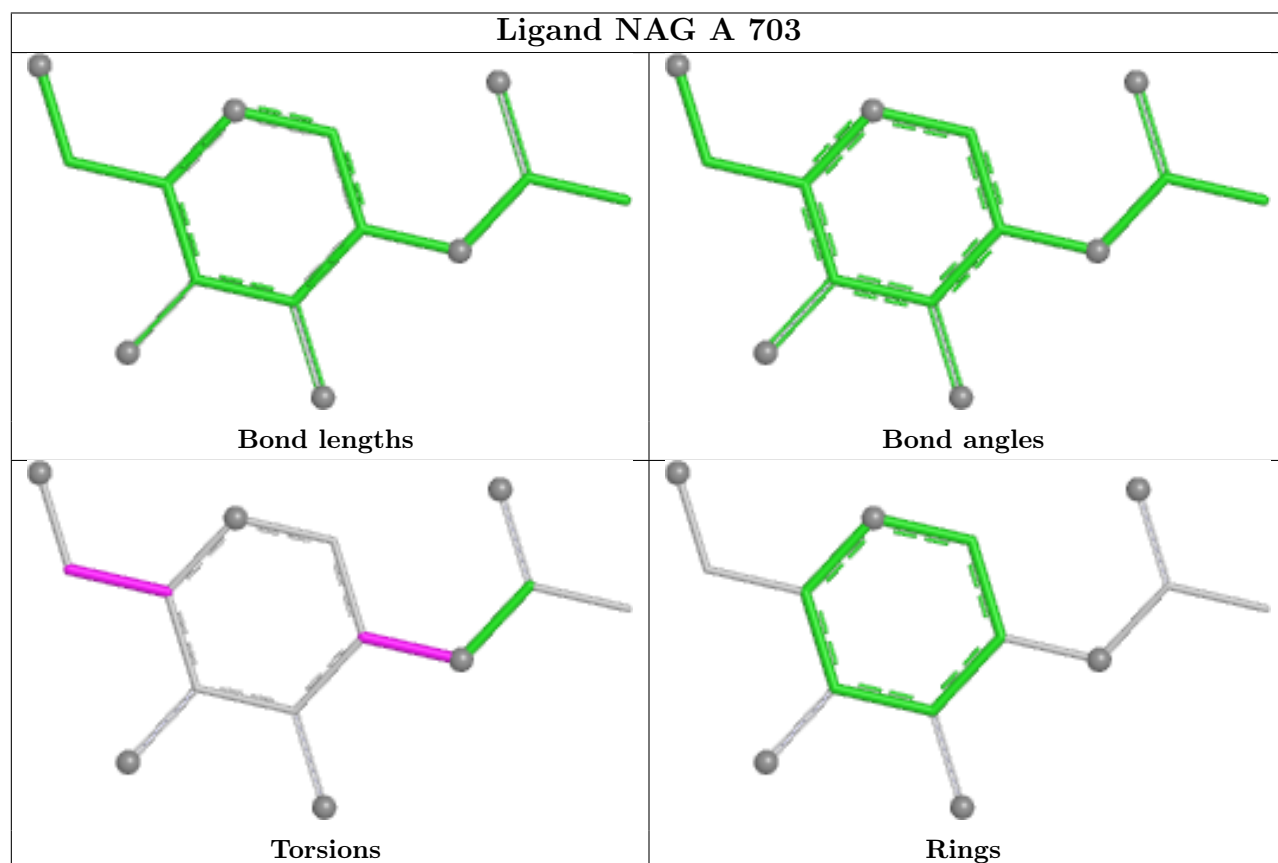
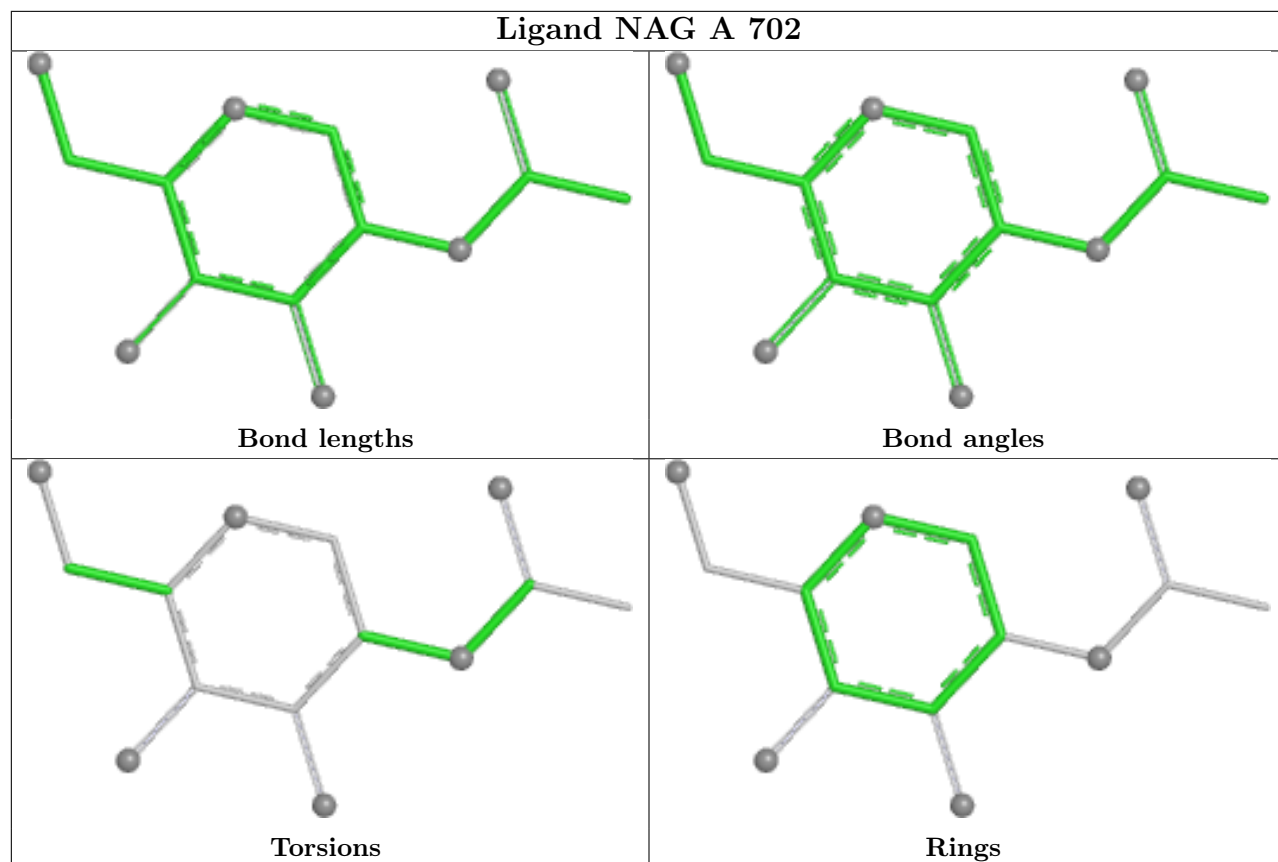
There are no ring outliers.

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	A	596/596 (100%)	0.39	31 (5%) 33 29	21, 40, 81, 130	2 (0%)
2	B	195/195 (100%)	1.15	42 (21%) 2 2	30, 58, 114, 133	0
All	All	791/791 (100%)	0.58	73 (9%) 14 12	21, 44, 95, 133	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	527	PRO	6.4
2	B	371	PHE	5.1
2	B	364	ASP	4.8
1	A	614	ALA	4.6
2	B	523	THR	4.4
2	B	517	LEU	4.4
1	A	426	PRO	4.1
2	B	390	LEU	4.1
2	B	381	GLY	3.7
2	B	368	LEU	3.6
1	A	138	PRO	3.6
2	B	525	CYS	3.6
1	A	289	PRO	3.6
1	A	339	VAL	3.3
1	A	192[A]	ARG	3.2
2	B	384	PRO	3.2
2	B	333	THR	3.2
1	A	19	SER	3.2
2	B	385	THR	3.2
1	A	135	PRO	3.1
1	A	429	GLN	3.1
1	A	288	LYS	3.1
1	A	20	THR	3.1
1	A	136	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	2.9
1	A	87	GLU	2.9
2	B	335	LEU	2.9
1	A	84	PRO	2.9
1	A	427	ASP	2.9
2	B	521	PRO	2.8
1	A	325	GLN	2.8
2	B	479	PRO	2.8
2	B	477	ASN	2.8
1	A	105	SER	2.7
2	B	386	LYS	2.7
2	B	369	TYR	2.7
2	B	334	ASN	2.6
1	A	338	ASN	2.6
2	B	481	ASN	2.6
1	A	134	ASN	2.6
2	B	524	VAL	2.5
2	B	370	ASN	2.5
2	B	373	PRO	2.5
1	A	428	PHE	2.5
2	B	519	HIS	2.5
2	B	510	VAL	2.5
1	A	601	ASN	2.4
1	A	425	SER	2.4
1	A	609	ASP	2.4
1	A	140	GLU	2.4
2	B	372	ALA	2.4
2	B	378	LYS	2.3
2	B	518	LEU	2.3
1	A	139	GLN	2.3
2	B	387	LEU	2.3
2	B	392	PHE	2.3
2	B	380	TYR	2.3
2	B	471	GLU	2.3
2	B	436	TRP	2.3
2	B	482	GLY	2.3
1	A	337	GLY	2.3
2	B	413	GLY	2.2
2	B	440	LYS	2.2
2	B	360	ASN	2.2
2	B	522	ALA	2.2
1	A	56	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	ASN	2.2
2	B	463	PRO	2.2
2	B	376	THR	2.1
2	B	365	TYR	2.1
2	B	389	ASP	2.1
1	A	549	GLU	2.0
1	A	430	GLU	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](#)

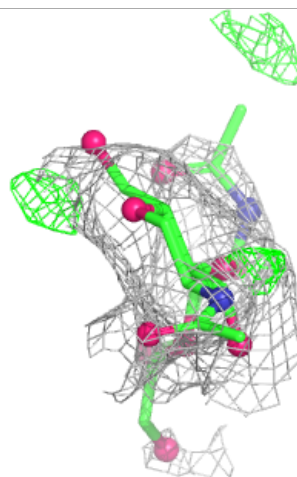
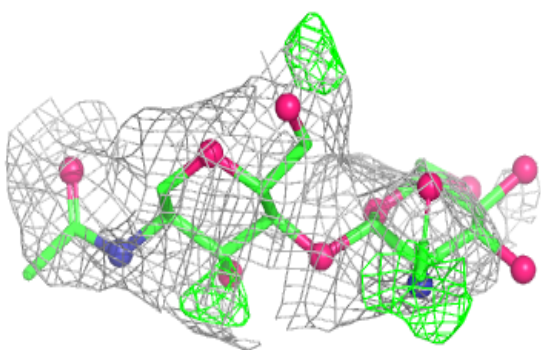
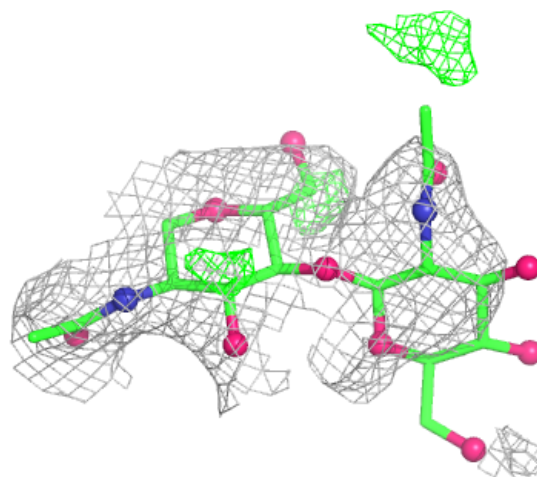
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	2	14/15	0.50	0.21	106,136,141,142	0
4	BMA	D	3	11/12	0.52	0.19	113,122,126,128	0
5	NAG	E	2	14/15	0.54	0.18	106,121,124,124	0
5	BMA	E	3	11/12	0.57	0.17	104,112,118,118	0
3	NAG	C	2	14/15	0.63	0.19	84,107,118,120	0
4	NAG	D	1	14/15	0.76	0.20	116,125,128,131	0
5	NAG	E	1	14/15	0.77	0.17	92,104,114,121	0
3	NAG	C	1	14/15	0.81	0.15	66,76,83,85	0
4	FUC	D	4	10/11	0.87	0.19	87,106,111,116	0

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

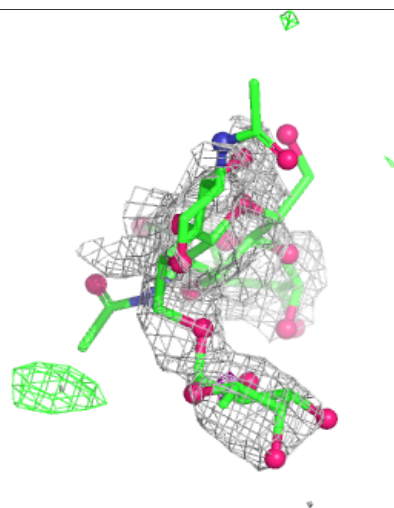
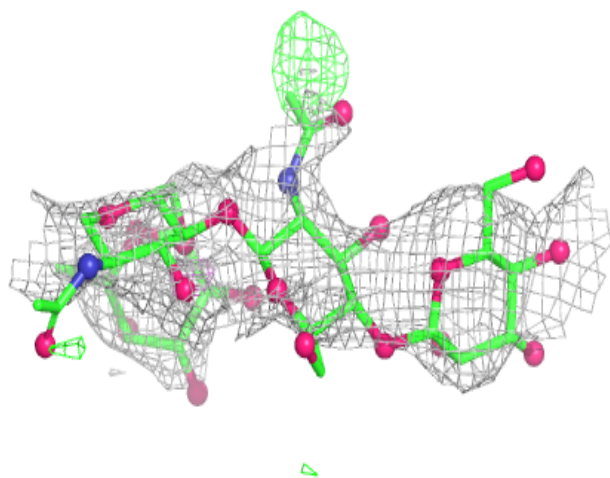
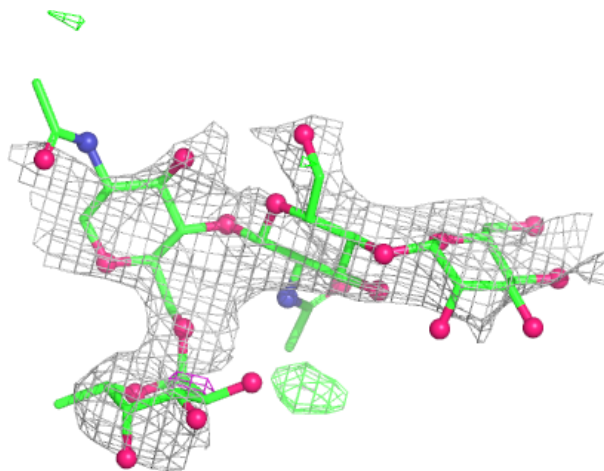
Electron density around Chain C:

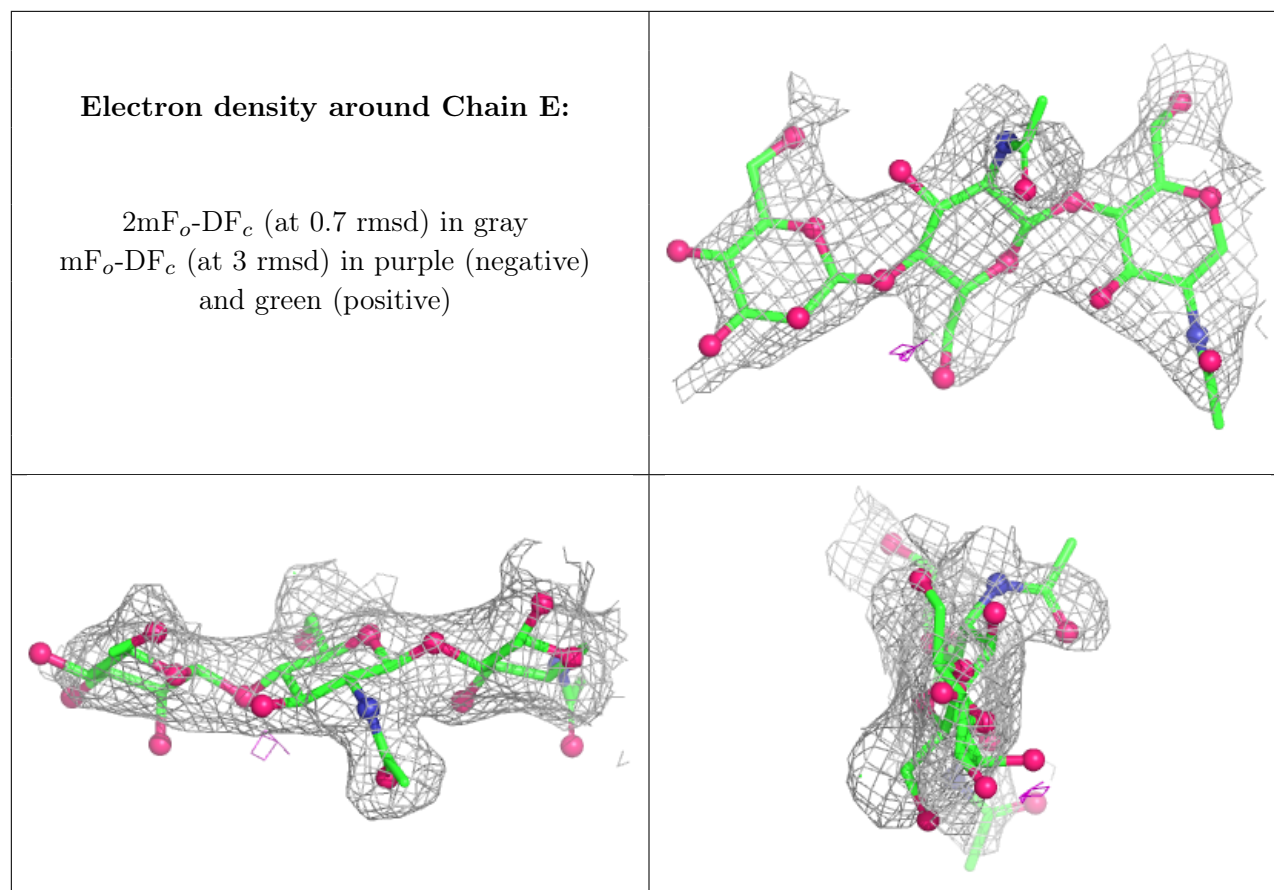
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





6.4 Ligands ⓘ

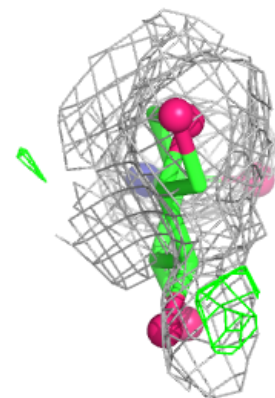
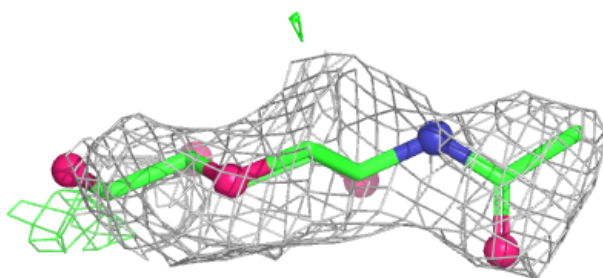
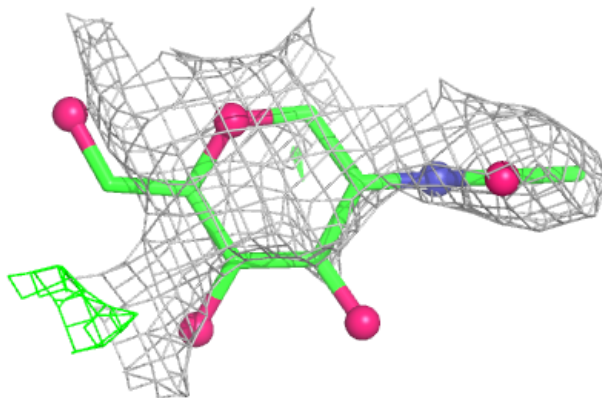
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	702	14/15	0.42	0.21	70,98,109,109	0
7	NAG	A	703	14/15	0.71	0.18	89,106,111,118	0
7	NAG	A	704	14/15	0.77	0.16	72,99,113,119	0
6	ZN	A	701	1/1	0.94	0.06	69,69,69,69	0

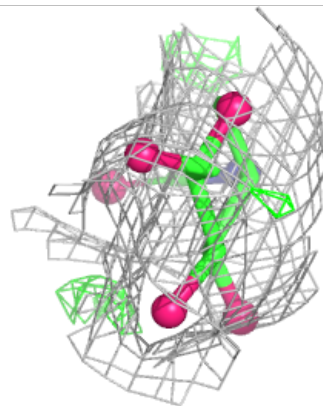
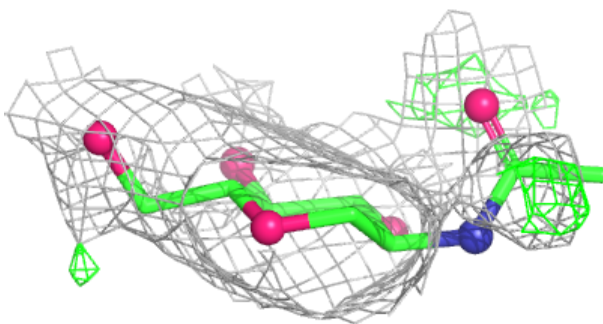
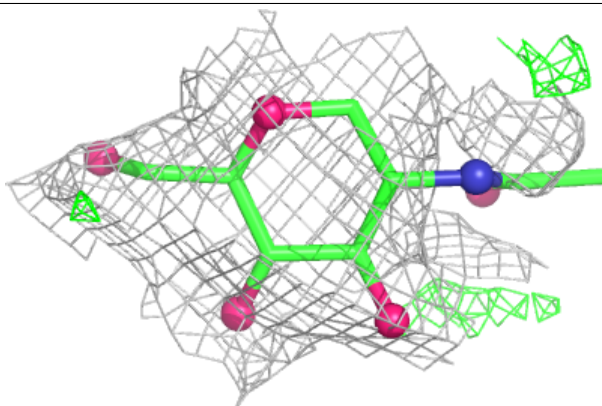
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 702:

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

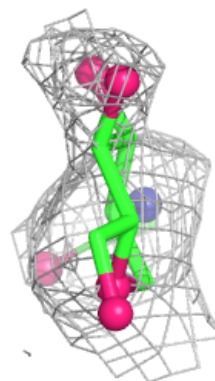
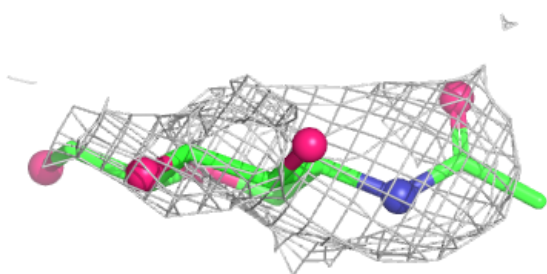
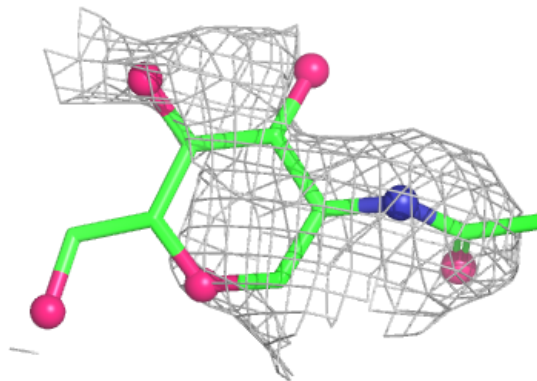
**Electron density around NAG A 703:**

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



Electron density around NAG A 704:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.