



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:13 PM BST

PDB ID : 6KBI
Title : Crystal structure of ErbB3 N418Q mutant
Authors : Kato, K.; Yao, M.
Deposited on : 2019-06-25
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

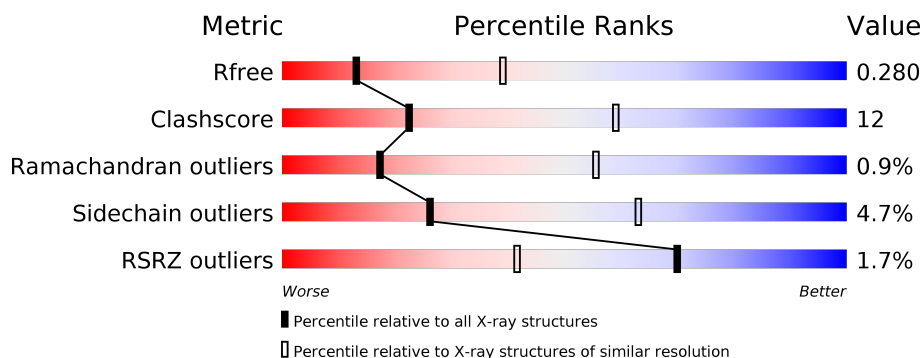
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	620	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>25%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	620	<div> <div>73%</div> <div>20%</div> <div>•</div> <div>5%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	707	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8967 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4212	2607	766	785	54			
1	B	588	Total	C	N	O	S	0	0	0
			4517	2792	818	848	59			

There are 2 discrepancies between the modelled and reference sequences:

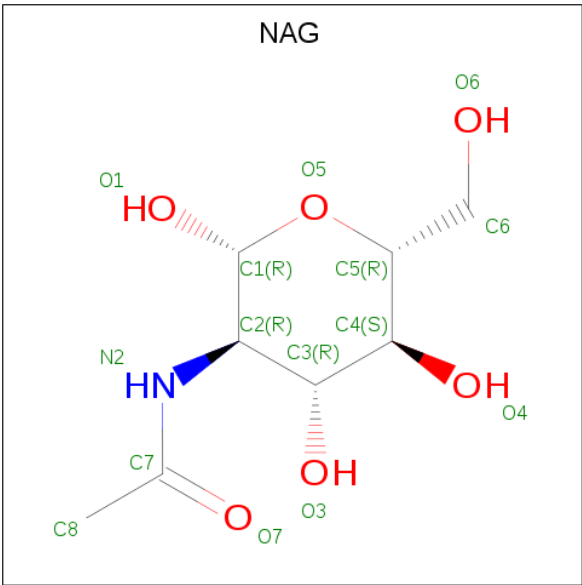
Chain	Residue	Modelled	Actual	Comment	Reference
A	418	GLN	ASN	engineered mutation	UNP P21860
B	418	GLN	ASN	engineered mutation	UNP P21860

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

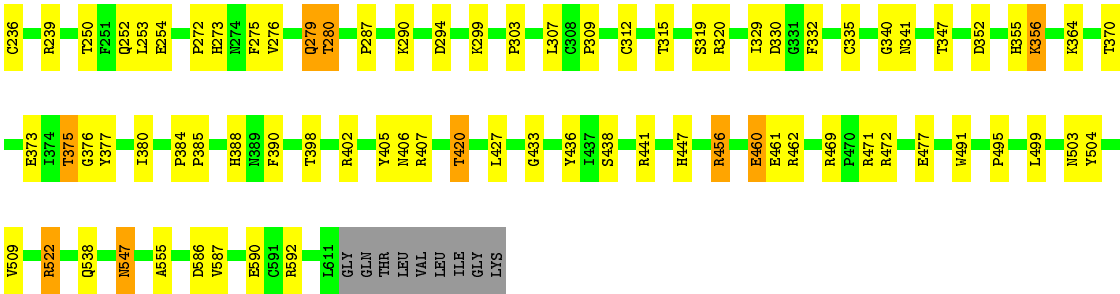


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.10 Å 49.46 Å 190.92 Å 90.00° 125.62° 90.00°	Depositor
Resolution (Å)	46.62 – 3.00 48.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.62-3.00) 99.4 (48.16-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.278 0.225 , 0.280	Depositor DCC
R_{free} test set	1832 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.956	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.53	1/4314 (0.0%)	0.85	6/5852 (0.1%)
1	B	0.50	0/4626	0.74	4/6276 (0.1%)
All	All	0.52	1/8940 (0.0%)	0.79	10/12128 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	GLU	CG-CD	-5.79	1.43	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LYS	CD-CE-NZ	-9.26	90.40	111.70
1	A	246	TYR	CA-CB-CG	6.99	126.67	113.40
1	B	441	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	557	CYS	CA-CB-SG	-5.89	103.40	114.00
1	A	457	GLY	N-CA-C	-5.74	98.74	113.10
1	A	132	LYS	CD-CE-NZ	5.73	124.88	111.70
1	B	161	GLY	N-CA-C	5.64	127.19	113.10
1	B	319	SER	N-CA-C	-5.29	96.71	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	273	HIS	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	LYS	Peptide
1	A	540	MET	Peptide
1	B	320	ARG	Peptide
1	B	355	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4212	0	4006	121	0
1	B	4517	0	4277	82	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	84	0	78	5	0
3	B	98	0	91	4	0
All	All	8967	0	8502	202	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 12.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HE3	1:A:251:PHE:HA	1.36	1.05
1:A:557:CYS:SG	1:A:561:ARG:NH1	2.36	0.97
1:A:276:VAL:HG13	1:A:299:LYS:HB2	1.49	0.95
1:A:534:HIS:CE1	1:A:551:SER:HB2	2.03	0.94
1:A:295:LYS:O	1:A:297:GLY:N	2.01	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:NH2	1:B:227:CYS:O	2.01	0.92
1:B:433:GLY:O	1:B:462:ARG:NH1	2.07	0.86
1:B:456:ARG:O	1:B:462:ARG:NH2	2.10	0.85
1:A:557:CYS:SG	1:A:561:ARG:HD2	2.19	0.82
1:A:248:LYS:HD2	1:A:248:LYS:N	1.96	0.79
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.48	0.76
1:B:250:THR:HG22	1:B:252:GLN:HG2	1.70	0.74
1:A:172:LYS:NZ	1:B:185:THR:OG1	2.20	0.74
1:A:373:GLU:HG3	1:A:398:THR:HB	1.69	0.73
1:A:9:VAL:HG23	1:A:39:VAL:HB	1.72	0.72
1:A:311:ALA:HB1	1:A:339:LEU:HD11	1.72	0.72
1:A:246:TYR:HB3	1:A:576:GLY:HA3	1.71	0.71
1:A:325:ASP:H	1:A:328:ASN:HB3	1.55	0.71
1:A:453:LYS:N	1:A:453:LYS:HD2	2.06	0.70
1:A:62:ARG:HH21	3:A:701:NAG:H82	1.56	0.70
1:B:186:LEU:O	1:B:188:LYS:N	2.23	0.70
1:A:247:ASN:C	1:A:248:LYS:HD2	2.11	0.70
1:A:512:THR:O	3:A:707:NAG:H82	1.92	0.70
1:A:77:THR:HG22	1:A:114:GLN:HB2	1.73	0.69
1:A:194:GLN:NE2	1:A:204:PRO:O	2.27	0.68
1:A:254:GLU:HG3	1:A:255:PRO:HD2	1.74	0.67
1:B:131:GLU:HG3	1:B:158:LYS:HG2	1.76	0.67
1:A:238:PRO:O	1:A:239:ARG:HG2	1.96	0.66
1:B:294:ASP:OD2	1:B:299:LYS:NZ	2.24	0.66
1:B:373:GLU:HG3	1:B:398:THR:HB	1.77	0.65
1:B:522:ARG:HH11	1:B:522:ARG:HG3	1.60	0.65
1:A:561:ARG:NH1	1:A:566:CYS:SG	2.70	0.64
1:A:158:LYS:O	1:A:160:ASN:ND2	2.31	0.64
1:A:551:SER:OG	1:A:566:CYS:N	2.30	0.64
1:B:340:GLY:H	1:B:375:THR:HG22	1.63	0.64
1:A:246:TYR:CE1	1:A:248:LYS:HE2	2.32	0.64
1:B:341:ASN:ND2	1:B:376:GLY:HA3	2.13	0.63
1:B:168:HIS:CE1	1:B:169:GLU:HG2	2.35	0.62
1:A:452:THR:HG22	1:A:459:THR:HG21	1.82	0.62
1:B:335:CYS:O	1:B:370:THR:HG23	1.99	0.62
1:A:174:ARG:HB3	1:A:184:GLN:HB3	1.80	0.62
1:A:66:GLY:HA2	1:A:90:GLN:H	1.66	0.60
1:B:7:GLN:HG2	1:B:7:GLN:O	2.02	0.59
1:A:92:TYR:HD2	1:A:93:ASP:HB2	1.67	0.59
1:A:131:GLU:OE2	1:A:132:LYS:NZ	2.20	0.59
1:A:278:ASP:OD1	1:A:290:LYS:HE3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TYR:CD2	1:A:93:ASP:HB2	2.37	0.59
1:A:190:ILE:H	1:A:190:ILE:HD12	1.68	0.59
1:A:131:GLU:O	1:A:133:ASN:ND2	2.35	0.59
1:A:287:PRO:HD2	1:A:290:LYS:HG3	1.85	0.59
1:B:279:GLN:O	1:B:280:THR:HG22	2.03	0.59
1:A:107:ASN:HD22	1:A:107:ASN:H	1.50	0.58
1:B:436:TYR:CE2	1:B:438:SER:HB2	2.39	0.58
1:A:572:HIS:CG	1:A:572:HIS:O	2.56	0.58
1:A:338:ILE:O	1:A:375:THR:HG23	2.04	0.58
1:B:250:THR:HG21	1:B:254:GLU:OE2	2.03	0.58
1:A:246:TYR:CE2	1:A:574:VAL:HB	2.39	0.58
1:A:385:PRO:HA	1:A:418:GLN:HG3	1.86	0.58
1:B:341:ASN:ND2	1:B:377:TYR:H	2.01	0.58
1:A:77:THR:O	1:A:79:PRO:HD3	2.03	0.57
1:A:150:ASP:HB3	1:A:153:ALA:HB2	1.85	0.57
1:B:100:VAL:HB	1:B:130:ILE:HG23	1.89	0.55
1:A:246:TYR:CZ	1:A:248:LYS:HE2	2.41	0.55
1:B:341:ASN:HD22	1:B:377:TYR:H	1.55	0.55
1:A:107:ASN:HD22	1:A:107:ASN:N	2.05	0.54
1:B:586:ASP:OD1	1:B:587:VAL:N	2.38	0.54
1:B:87:ARG:HG3	1:B:124:LEU:HD12	1.89	0.54
1:A:288:PRO:O	1:A:289:ASP:HB3	2.07	0.54
1:B:307:LEU:HD11	3:B:702:NAG:H61	1.89	0.54
1:A:252:GLN:HG3	1:A:254:GLU:OE1	2.08	0.54
1:A:514:CYS:HB2	1:A:516:PHE:CE1	2.43	0.53
1:B:547:ASN:OD1	3:B:708:NAG:O3	2.14	0.53
1:B:252:GLN:HG3	1:B:253:LEU:O	2.09	0.53
1:A:469:ARG:NH2	1:A:477:GLU:OE2	2.36	0.53
1:B:51:HIS:NE2	1:B:52:ASN:OD1	2.42	0.53
1:A:85:VAL:HG21	1:A:226:ALA:HB2	1.90	0.52
1:A:87:ARG:HG2	1:A:124:LEU:HD12	1.91	0.52
1:A:311:ALA:HB1	1:A:339:LEU:CD1	2.39	0.52
1:A:464:ASP:OD1	1:A:466:LYS:NZ	2.42	0.52
1:B:586:ASP:HB2	1:B:590:GLU:O	2.09	0.52
1:B:340:GLY:H	1:B:375:THR:CG2	2.21	0.52
1:A:302:GLU:HG3	1:A:303:PRO:HD2	1.92	0.52
1:A:419:VAL:HG12	1:A:443:LEU:HD13	1.91	0.52
1:A:567:VAL:HG12	1:A:568:SER:O	2.10	0.52
1:A:399:ILE:HB	1:A:430:ILE:HG12	1.92	0.52
1:B:108:SER:OG	1:B:109:SER:N	2.42	0.52
1:A:452:THR:OG1	1:A:453:LYS:NZ	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASP:OD2	1:B:592:ARG:NH2	2.42	0.51
1:A:325:ASP:OD1	1:A:328:ASN:HB2	2.10	0.51
1:B:329:ILE:HD13	1:B:364:LYS:HB3	1.93	0.51
1:A:434:ARG:HG2	1:A:462:ARG:HA	1.91	0.51
1:B:276:VAL:HG23	1:B:299:LYS:HB3	1.93	0.51
1:B:472:ARG:HD3	1:B:472:ARG:N	2.26	0.51
1:B:352:ASP:O	1:B:356:LYS:HA	2.11	0.50
1:A:400:GLY:O	1:A:431:SER:HB2	2.11	0.50
1:B:330:ASP:C	1:B:332:PHE:H	2.14	0.50
1:B:447:HIS:HB3	1:B:471:ARG:HE	1.75	0.50
1:B:460:GLU:O	1:B:461:GLU:HB3	2.12	0.50
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.76	0.50
1:A:368:PHE:HB2	1:A:392:VAL:HG13	1.94	0.50
1:A:244:LEU:HA	1:A:254:GLU:O	2.12	0.49
1:A:248:LYS:CE	1:A:251:PHE:HA	2.26	0.49
1:A:515:ASN:HB3	1:A:518:ASN:O	2.12	0.49
1:A:453:LYS:HE2	3:A:706:NAG:O6	2.12	0.49
1:A:569:SER:O	1:A:569:SER:OG	2.25	0.49
1:A:112:LEU:HD21	1:A:115:LEU:HD21	1.95	0.49
1:B:211:GLU:HB3	1:B:236:CYS:HB3	1.95	0.49
1:A:460:GLU:OE1	1:A:461:GLU:HG2	2.13	0.49
1:A:452:THR:HG22	1:A:459:THR:CG2	2.43	0.48
1:B:47:VAL:HA	1:B:71:ALA:O	2.13	0.48
1:B:116:ARG:NH1	1:B:116:ARG:HG3	2.19	0.47
1:B:377:TYR:CE2	1:B:405:TYR:HB2	2.48	0.47
1:A:196:ASN:N	1:A:196:ASN:OD1	2.45	0.47
1:A:203:ASN:HB2	1:A:206:GLN:HG3	1.95	0.47
1:A:201:GLY:HA3	1:A:206:GLN:OE1	2.15	0.47
1:A:534:HIS:ND1	1:A:536:GLU:OE2	2.48	0.47
1:A:330:ASP:O	1:A:333:VAL:HG23	2.15	0.47
1:A:483:PRO:O	1:A:502:ARG:HD2	2.15	0.47
1:A:62:ARG:NH2	3:A:701:NAG:H2	2.29	0.47
3:B:709:NAG:N2	3:B:709:NAG:H5	2.29	0.47
1:B:8:ALA:HB1	1:B:38:GLU:HB2	1.98	0.46
1:A:337:LYS:NZ	1:A:375:THR:HG22	2.31	0.46
1:A:186:LEU:HB2	1:B:186:LEU:HB2	1.97	0.46
1:A:384:PRO:HA	1:A:385:PRO:HD3	1.70	0.46
1:B:161:GLY:O	1:B:162:ARG:HB2	2.15	0.46
1:B:472:ARG:H	1:B:472:ARG:HD3	1.79	0.46
1:B:586:ASP:OD2	1:B:592:ARG:NE	2.46	0.46
1:A:296:ASN:OD1	1:A:298:LEU:N	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:NH2	1:A:227:CYS:O	2.37	0.45
1:A:436:TYR:CE2	1:A:438:SER:HB2	2.52	0.45
1:A:441:ARG:NH2	1:A:467:HIS:HB3	2.31	0.45
1:B:469:ARG:HH22	1:B:477:GLU:CD	2.20	0.45
1:B:101:MET:HG3	1:B:132:LYS:HZ3	1.82	0.45
1:B:329:ILE:HD11	1:B:364:LYS:O	2.17	0.45
1:A:116:ARG:HH22	1:A:182:ASP:CG	2.19	0.45
1:A:246:TYR:CD2	1:A:248:LYS:HD3	2.51	0.45
1:B:76:SER:HA	1:B:111:ALA:O	2.17	0.45
1:A:209:HIS:CD2	1:A:221:ASP:OD1	2.70	0.44
1:B:290:LYS:HG2	1:B:303:PRO:HA	2.00	0.44
1:B:427:LEU:HD23	1:B:491:TRP:CH2	2.53	0.44
1:B:82:ASN:O	1:B:84:ARG:HG3	2.17	0.44
1:B:120:LEU:HG	1:B:147:ILE:HG21	1.99	0.44
1:B:198:HIS:HB3	1:B:208:CYS:HB2	1.99	0.44
1:A:452:THR:O	1:A:456:ARG:HG2	2.17	0.44
1:B:34:TYR:HA	1:B:57:PHE:HD1	1.83	0.44
1:A:146:ASP:O	1:A:188:LYS:NZ	2.51	0.44
1:A:307:LEU:HG	1:A:308:CYS:H	1.82	0.43
1:A:315:THR:O	1:A:341:ASN:HB2	2.18	0.43
1:B:113:ARG:HA	1:B:135:LYS:O	2.18	0.43
1:B:80:LEU:HD13	1:B:83:LEU:HD22	2.00	0.43
1:B:447:HIS:HB3	1:B:471:ARG:NE	2.32	0.43
1:B:472:ARG:H	1:B:472:ARG:CD	2.30	0.43
1:A:168:HIS:CD2	1:A:180:SER:HB3	2.53	0.43
1:B:522:ARG:HH11	1:B:522:ARG:CG	2.29	0.43
1:B:96:PHE:CE2	1:B:129:TYR:HB2	2.54	0.43
1:B:150:ASP:HB3	1:B:153:ALA:HB2	2.00	0.43
1:B:555:ALA:HA	3:B:708:NAG:H81	2.00	0.43
1:A:503:ASN:HB2	1:A:504:TYR:H	1.25	0.43
1:A:552:ASP:HA	1:A:564:PRO:O	2.18	0.43
1:B:503:ASN:HB2	1:B:504:TYR:H	1.57	0.43
1:A:453:LYS:N	1:A:453:LYS:CD	2.79	0.43
1:A:76:SER:HA	1:A:111:ALA:O	2.19	0.43
1:A:337:LYS:HZ2	1:A:375:THR:HG22	1.83	0.43
1:B:272:PRO:HB2	1:B:275:PHE:CD1	2.54	0.43
1:A:189:THR:HG22	1:A:190:ILE:O	2.19	0.42
1:A:453:LYS:HD3	3:A:706:NAG:O5	2.18	0.42
1:A:140:ASP:N	1:A:140:ASP:OD1	2.40	0.42
1:B:495:PRO:HB2	1:B:509:VAL:HG13	2.00	0.42
1:B:586:ASP:OD1	1:B:587:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:C	1:A:297:GLY:H	2.13	0.42
1:A:438:SER:HA	1:A:466:LYS:O	2.20	0.42
1:A:290:LYS:HA	1:A:304:CYS:SG	2.59	0.42
1:B:148:VAL:HG21	1:B:155:ILE:HD11	2.02	0.42
1:B:380:ILE:HG21	1:B:390:PHE:CE2	2.55	0.42
1:A:421:SER:HB3	1:A:445:TYR:CD1	2.55	0.42
1:B:388:HIS:HB3	1:B:420:THR:OG1	2.20	0.42
1:B:315:THR:O	1:B:341:ASN:HB2	2.20	0.42
1:B:384:PRO:HA	1:B:385:PRO:HD3	1.73	0.42
1:A:251:PHE:HB3	1:A:562:ASP:OD2	2.20	0.41
1:A:132:LYS:HE3	1:A:132:LYS:HB2	1.84	0.41
1:A:453:LYS:HE3	1:A:453:LYS:HA	2.01	0.41
1:A:471:ARG:O	1:A:475:VAL:HG23	2.20	0.41
1:A:525:ALA:HA	1:A:529:GLU:O	2.20	0.41
1:A:39:VAL:HG22	1:A:63:GLU:HB3	2.03	0.41
1:A:96:PHE:CD2	1:A:129:TYR:HB2	2.56	0.41
1:B:168:HIS:CE1	1:B:170:VAL:HG23	2.55	0.41
1:B:56:SER:O	1:B:59:GLN:HB2	2.21	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.79	0.41
1:A:295:LYS:HG2	1:A:295:LYS:HZ2	1.72	0.41
1:B:330:ASP:C	1:B:332:PHE:N	2.74	0.41
1:A:420:THR:HA	1:A:442:GLN:O	2.20	0.41
1:A:415:LYS:HA	1:A:439:ALA:O	2.20	0.40
1:B:132:LYS:HE2	1:B:132:LYS:HB3	1.85	0.40
1:A:406:ASN:OD1	1:A:407:ARG:HG3	2.22	0.40
1:B:287:PRO:HD2	1:B:290:LYS:HB2	2.03	0.40
1:A:421:SER:HB3	1:A:445:TYR:HD1	1.85	0.40
1:A:449:LEU:HD21	1:A:491:TRP:CH2	2.57	0.40
1:A:47:VAL:HA	1:A:71:ALA:O	2.21	0.40
1:A:254:GLU:CG	1:A:255:PRO:HD2	2.48	0.40
1:B:312:CYS:N	1:B:335:CYS:SG	2.95	0.40
1:B:406:ASN:OD1	1:B:407:ARG:HG3	2.21	0.40
1:A:192:ALA:HA	1:A:193:PRO:HD3	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	546/620 (88%)	497 (91%)	44 (8%)	5 (1%)	17	55
1	B	584/620 (94%)	534 (91%)	45 (8%)	5 (1%)	17	55
All	All	1130/1240 (91%)	1031 (91%)	89 (8%)	10 (1%)	17	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	552	ASP
1	B	35	GLU
1	B	187	THR
1	A	577	ALA
1	B	279	GLN
1	B	356	LYS
1	A	306	GLY
1	A	309	PRO
1	B	309	PRO

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	474/536 (88%)	448 (94%)	26 (6%)	21	57
1	B	510/536 (95%)	490 (96%)	20 (4%)	32	69
All	All	984/1072 (92%)	938 (95%)	46 (5%)	26	63

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	107	ASN
1	A	132	LYS
1	A	181	GLU
1	A	194	GLN
1	A	196	ASN
1	A	239	ARG
1	A	248	LYS
1	A	250	THR
1	A	290	LYS
1	A	295	LYS
1	A	347	THR
1	A	367	VAL
1	A	392	VAL
1	A	410	SER
1	A	448	SER
1	A	453	LYS
1	A	456	ARG
1	A	472	ARG
1	A	503	ASN
1	A	535	PRO
1	A	536	GLU
1	A	540	MET
1	A	561	ARG
1	A	569	SER
1	A	574	VAL
1	B	10	CYS
1	B	13	THR
1	B	38	GLU
1	B	107	ASN
1	B	132	LYS
1	B	134	ASP
1	B	151	ARG
1	B	205	ASN
1	B	239	ARG
1	B	280	THR
1	B	347	THR
1	B	375	THR
1	B	402	ARG
1	B	420	THR
1	B	456	ARG
1	B	460	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	499	LEU
1	B	522	ARG
1	B	538	GLN
1	B	547	ASN

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

Mol	Chain	Res	Type
1	A	107	ASN
1	A	194	GLN
1	A	242	GLN
1	A	252	GLN
1	B	160	ASN
1	B	205	ASN
1	B	341	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 ⓘ

4 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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.27	0	17,19,21	1.49	3 (17%)
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	1.08	1 (7%)	17,19,21	1.23	2 (11%)
2	NAG	D	2	2	14,14,15	0.44	0	17,19,21	0.75	1 (5%)

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
2	NAG	C	1	1,2	-	6/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C2-N2	3.37	1.52	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	4.24	128.94	122.90
2	D	1	NAG	O5-C1-C2	-3.55	105.68	111.29
2	C	1	NAG	C1-C2-N2	2.93	115.49	110.49
2	D	1	NAG	C1-O5-C5	2.35	115.37	112.19
2	D	2	NAG	C3-C4-C5	2.24	114.23	110.24
2	C	1	NAG	C4-C3-C2	-2.05	108.01	111.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2

Continued on next page...

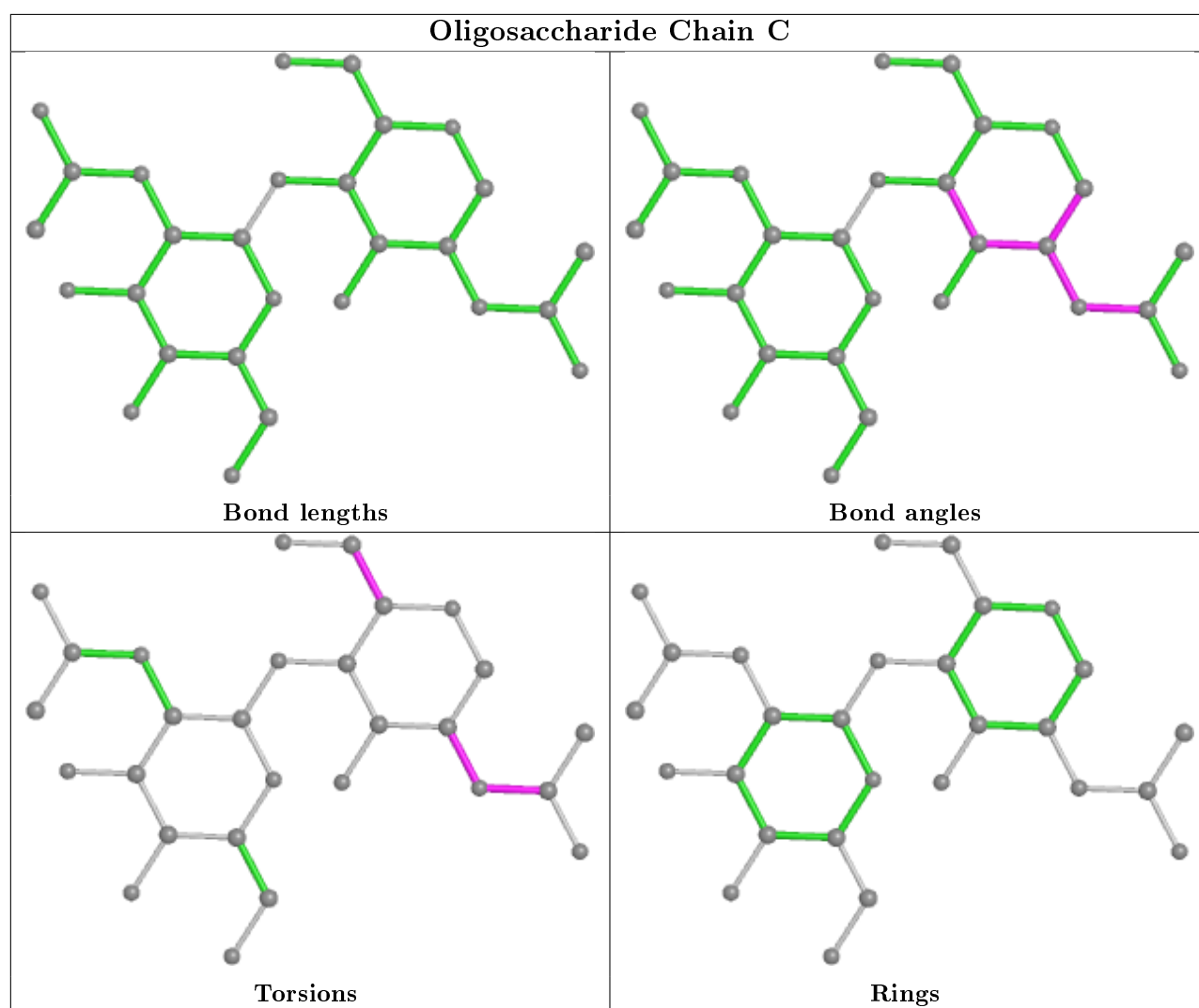
Continued from previous page...

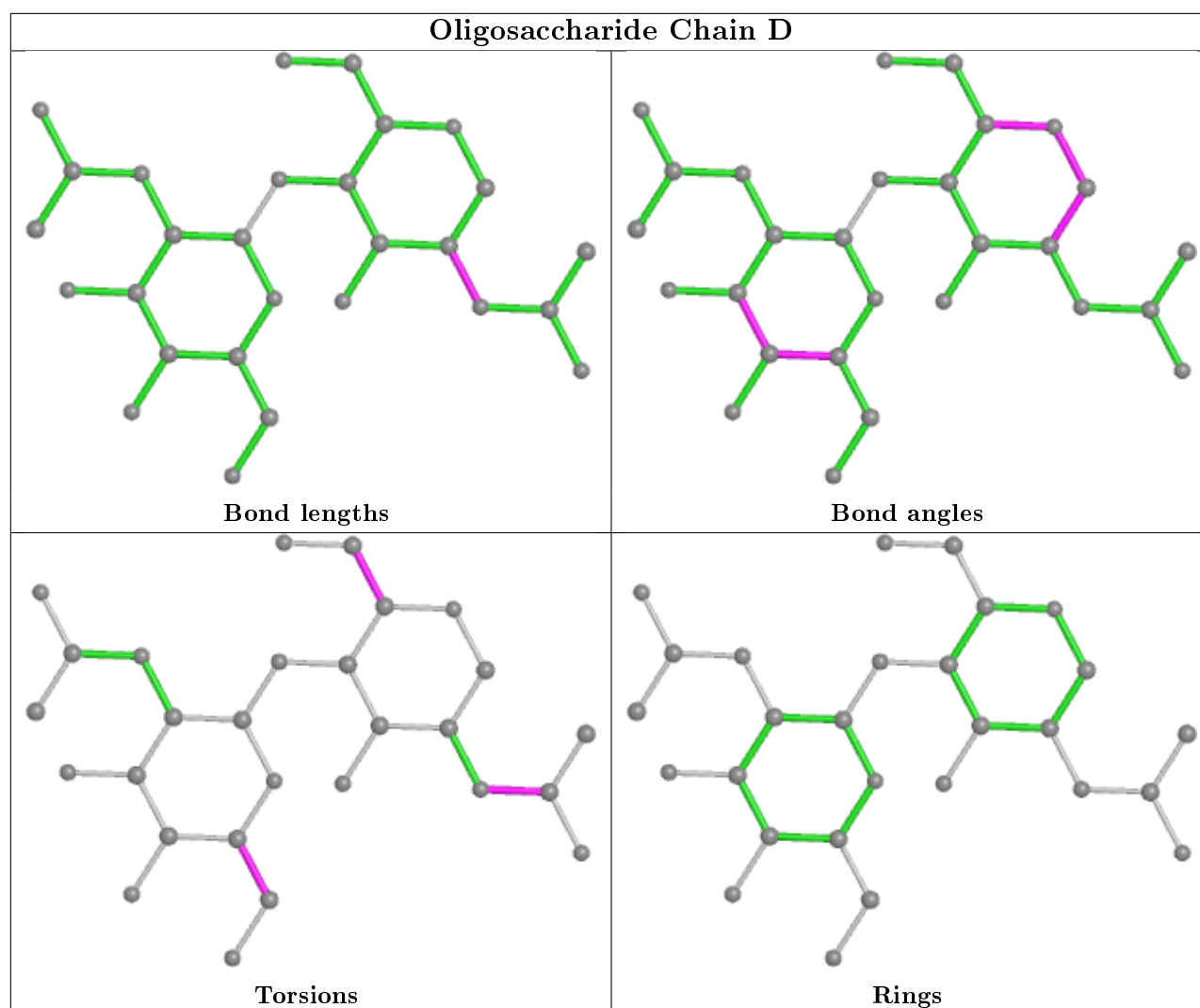
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7

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 ⓘ

13 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	$\# Z > 2$
3	NAG	B	706	1	14,14,15	0.31	0	17,19,21	0.38	0
3	NAG	B	702	1	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	B	709	1	14,14,15	0.72	1 (7%)	17,19,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	707	1	14,14,15	1.04	1 (7%)	17,19,21	0.62	0
3	NAG	A	706	1	14,14,15	0.76	1 (7%)	17,19,21	0.88	0
3	NAG	B	707	1	14,14,15	1.62	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	A	702	1	14,14,15	0.37	0	17,19,21	0.40	0
3	NAG	A	708	1	14,14,15	0.23	0	17,19,21	0.70	0
3	NAG	A	705	1	14,14,15	0.94	1 (7%)	17,19,21	0.99	2 (11%)
3	NAG	B	705	1	14,14,15	0.87	1 (7%)	17,19,21	1.11	2 (11%)
3	NAG	B	708	1	14,14,15	1.56	1 (7%)	17,19,21	0.76	0
3	NAG	A	701	1	14,14,15	0.84	1 (7%)	17,19,21	0.80	0
3	NAG	B	701	1	14,14,15	0.89	1 (7%)	17,19,21	1.07	2 (11%)

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	B	706	1	-	2/6/23/26	0/1/1/1
3	NAG	B	702	1	-	2/6/23/26	0/1/1/1
3	NAG	B	709	1	-	4/6/23/26	0/1/1/1
3	NAG	A	707	1	-	2/6/23/26	0/1/1/1
3	NAG	A	706	1	-	2/6/23/26	0/1/1/1
3	NAG	B	707	1	-	2/6/23/26	0/1/1/1
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	708	1	-	2/6/23/26	0/1/1/1
3	NAG	A	705	1	-	1/6/23/26	0/1/1/1
3	NAG	B	705	1	-	1/6/23/26	0/1/1/1
3	NAG	B	708	1	-	4/6/23/26	0/1/1/1
3	NAG	A	701	1	-	3/6/23/26	0/1/1/1
3	NAG	B	701	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	707	NAG	O5-C1	-5.95	1.34	1.43
3	B	708	NAG	C1-C2	5.11	1.60	1.52
3	B	701	NAG	O5-C1	-2.93	1.39	1.43
3	A	707	NAG	O5-C1	2.71	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	NAG	O5-C1	-2.68	1.39	1.43
3	A	701	NAG	C1-C2	2.66	1.56	1.52
3	B	705	NAG	C2-N2	2.32	1.50	1.46
3	A	706	NAG	C2-N2	-2.28	1.42	1.46
3	B	709	NAG	C1-C2	2.05	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	709	NAG	C1-O5-C5	3.85	117.40	112.19
3	B	707	NAG	C1-O5-C5	-3.33	107.68	112.19
3	B	705	NAG	O5-C1-C2	-3.06	106.46	111.29
3	B	701	NAG	C1-O5-C5	-2.94	108.21	112.19
3	B	709	NAG	C2-N2-C7	2.43	126.36	122.90
3	A	705	NAG	C3-C4-C5	2.41	114.54	110.24
3	A	705	NAG	O5-C1-C2	-2.24	107.76	111.29
3	B	701	NAG	C3-C4-C5	2.13	114.04	110.24
3	B	705	NAG	C3-C4-C5	2.04	113.88	110.24

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	706	NAG	O5-C5-C6-O6
3	B	707	NAG	O5-C5-C6-O6
3	B	708	NAG	O5-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6
3	B	709	NAG	O5-C5-C6-O6
3	A	707	NAG	O5-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6
3	B	708	NAG	C4-C5-C6-O6
3	A	707	NAG	C4-C5-C6-O6
3	A	706	NAG	C4-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	B	709	NAG	C4-C5-C6-O6
3	B	709	NAG	C8-C7-N2-C2
3	B	709	NAG	O7-C7-N2-C2
3	B	708	NAG	C8-C7-N2-C2
3	B	708	NAG	O7-C7-N2-C2
3	A	701	NAG	C8-C7-N2-C2
3	A	701	NAG	O7-C7-N2-C2
3	B	707	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	708	NAG	O5-C5-C6-O6
3	A	708	NAG	C4-C5-C6-O6
3	B	702	NAG	C4-C5-C6-O6
3	B	705	NAG	O5-C5-C6-O6
3	A	701	NAG	O5-C5-C6-O6
3	A	705	NAG	O5-C5-C6-O6
3	B	706	NAG	O5-C5-C6-O6
3	B	706	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NAG	1	0
3	B	709	NAG	1	0
3	A	707	NAG	1	0
3	A	706	NAG	2	0
3	B	708	NAG	2	0
3	A	701	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	A	550/620 (88%)	0.08	19 (3%) 44 18	40, 70, 109, 133	0
1	B	588/620 (94%)	-0.16	0 100 100	31, 56, 87, 110	0
All	All	1138/1240 (91%)	-0.04	19 (1%) 70 41	31, 62, 102, 133	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	GLY	4.3
1	A	572	HIS	4.1
1	A	550	GLY	3.7
1	A	246	TYR	3.5
1	A	551	SER	3.2
1	A	107	ASN	3.0
1	A	574	VAL	3.0
1	A	250	THR	3.0
1	A	580	PRO	3.0
1	A	570	CYS	2.9
1	A	535	PRO	2.5
1	A	306	GLY	2.4
1	A	565	HIS	2.3
1	A	569	SER	2.2
1	A	532	SER	2.2
1	A	245	VAL	2.1
1	A	540	MET	2.1
1	A	305	GLY	2.0
1	A	556	GLN	2.0

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

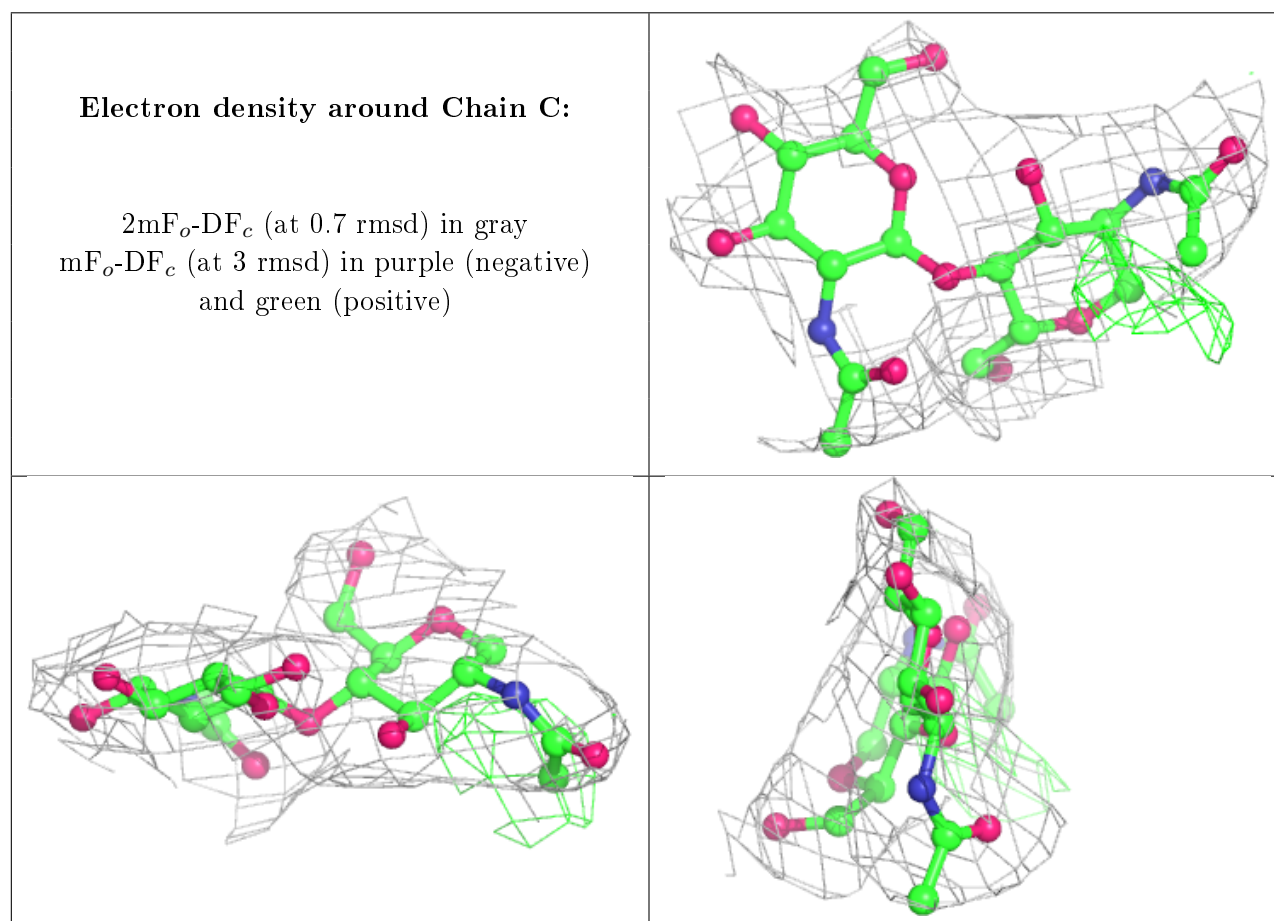
There are no non-standard protein/DNA/RNA residues in this entry.

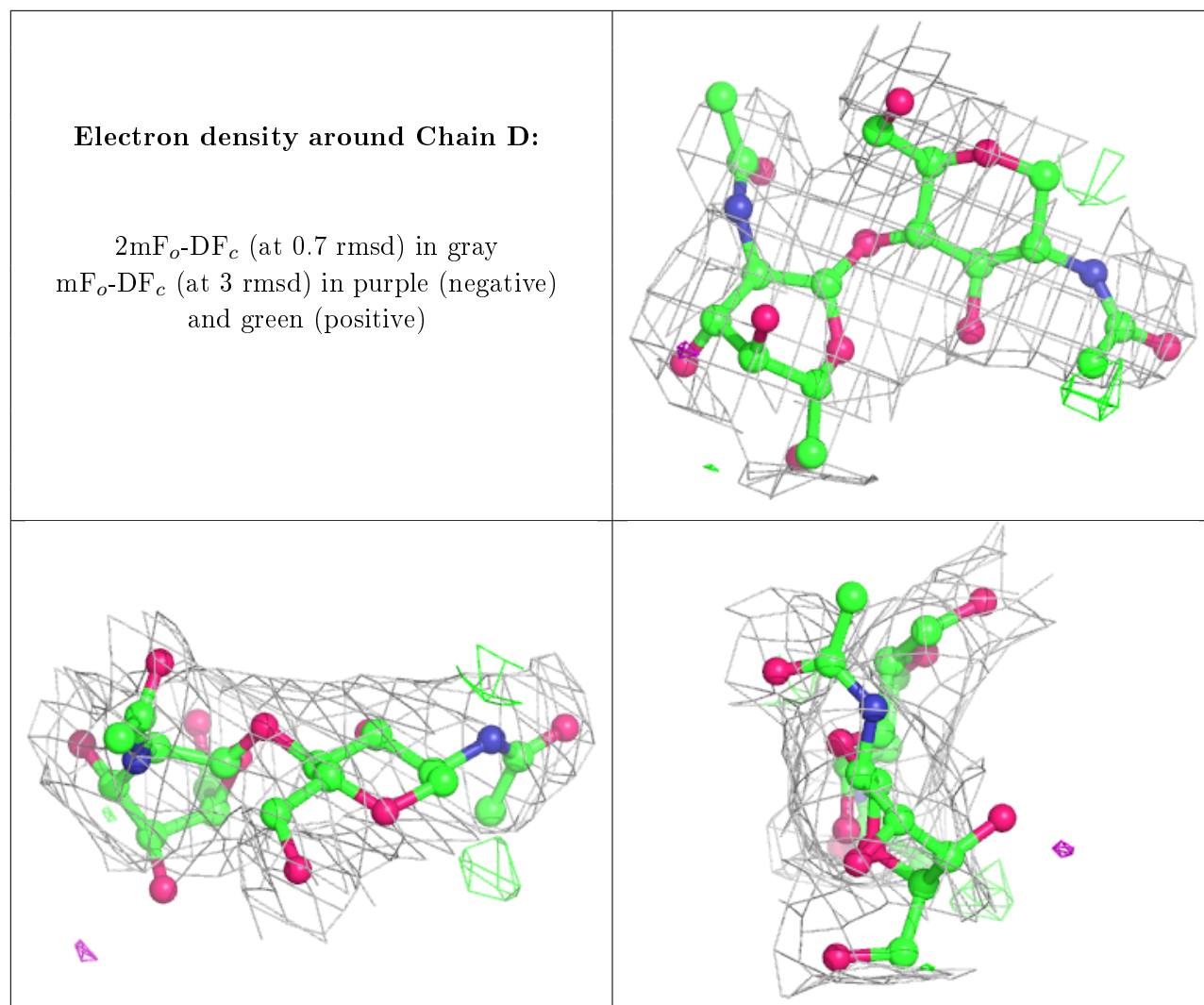
6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
2	NAG	D	2	14/15	0.85	0.20	98,112,117,123	0
2	NAG	C	2	14/15	0.86	0.16	88,104,110,112	0
2	NAG	C	1	14/15	0.94	0.17	58,72,86,93	0
2	NAG	D	1	14/15	0.95	0.14	64,73,86,94	0

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





6.4 Ligands ⓘ

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	B	709	14/15	0.68	0.24	81,95,104,107	14
3	NAG	A	707	14/15	0.68	0.69	81,109,117,122	0
3	NAG	B	705	14/15	0.69	0.37	86,106,128,132	0
3	NAG	B	708	14/15	0.77	0.34	79,87,92,95	0
3	NAG	A	708	14/15	0.82	0.34	91,110,123,125	0
3	NAG	A	706	14/15	0.84	0.24	96,110,116,120	0
3	NAG	A	705	14/15	0.85	0.40	110,120,127,132	0
3	NAG	B	701	14/15	0.85	0.22	54,79,89,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	702	14/15	0.88	0.14	84,106,114,116	0
3	NAG	B	702	14/15	0.89	0.14	86,95,102,105	0
3	NAG	A	701	14/15	0.89	0.17	56,64,72,74	0
3	NAG	B	706	14/15	0.89	0.22	75,90,101,106	0
3	NAG	B	707	14/15	0.90	0.22	66,70,85,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.