



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:50 PM BST

PDB ID : 6QP9
Title : Drosophila Semaphorin 1a, extracellular domains 1-2
Authors : Rozbesky, D.; Robinson, R.A.; Harlos, K.; Siebold, C.; Jones, E.Y.
Deposited on : 2019-02-13
Resolution : 3.60 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

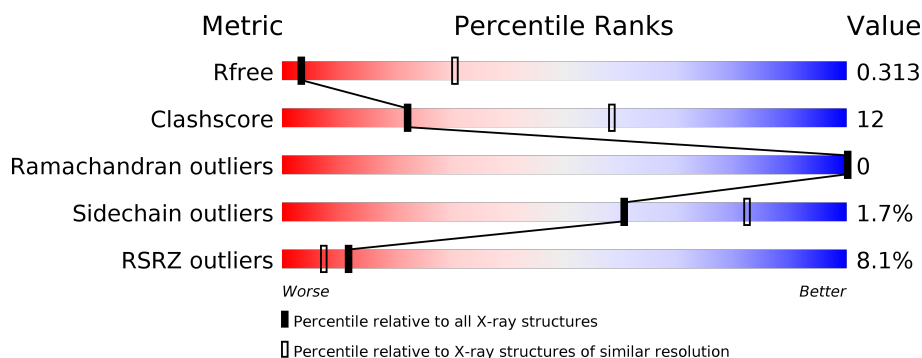
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	536	<div> <div>7%</div> <div>65%</div> <div>28%</div> <div>• 6%</div> </div>
1	B	536	<div> <div>8%</div> <div>70%</div> <div>23%</div> <div>• 6%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8000 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 Semaphorin-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3962	2499	679	763	21			
1	B	504	Total	C	N	O	S	0	0	0
			3954	2495	678	760	21			

There are 24 discrepancies between the modelled and reference sequences:

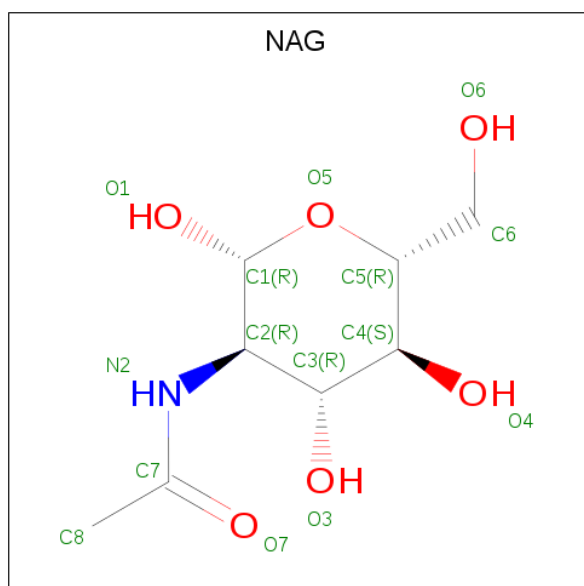
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLU	-	expression tag	UNP Q24322
A	77	THR	-	expression tag	UNP Q24322
A	78	GLY	-	expression tag	UNP Q24322
A	79	TYR	-	expression tag	UNP Q24322
A	604	THR	-	expression tag	UNP Q24322
A	605	LYS	-	expression tag	UNP Q24322
A	606	HIS	-	expression tag	UNP Q24322
A	607	HIS	-	expression tag	UNP Q24322
A	608	HIS	-	expression tag	UNP Q24322
A	609	HIS	-	expression tag	UNP Q24322
A	610	HIS	-	expression tag	UNP Q24322
A	611	HIS	-	expression tag	UNP Q24322
B	76	GLU	-	expression tag	UNP Q24322
B	77	THR	-	expression tag	UNP Q24322
B	78	GLY	-	expression tag	UNP Q24322
B	79	TYR	-	expression tag	UNP Q24322
B	604	THR	-	expression tag	UNP Q24322
B	605	LYS	-	expression tag	UNP Q24322
B	606	HIS	-	expression tag	UNP Q24322
B	607	HIS	-	expression tag	UNP Q24322
B	608	HIS	-	expression tag	UNP Q24322
B	609	HIS	-	expression tag	UNP Q24322
B	610	HIS	-	expression tag	UNP Q24322
B	611	HIS	-	expression tag	UNP Q24322

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	99.48Å 99.48Å 150.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.60 49.74 – 3.60	Depositor EDS
% Data completeness (in resolution range)	79.5 (49.74-3.60) 75.6 (49.74-3.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, R_{free}	0.287 , 0.323 0.286 , 0.313	Depositor DCC
R_{free} test set	779 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.277 for -h,-k,l 0.107 for h,-h-k,-l 0.099 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	8000	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.25	0/4055	0.45	0/5511
1	B	0.25	0/4047	0.45	0/5500
All	All	0.25	0/8102	0.45	0/11011

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

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	3962	0	3819	99	0
1	B	3954	0	3815	86	0
2	C	28	0	25	0	0
2	D	28	0	25	2	0
3	A	14	0	13	0	0
3	B	14	0	13	2	0
All	All	8000	0	7710	183	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 (183) 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:355:ILE:HG12	1:B:355:ILE:HG12	1.59	0.85
1:B:288:CYS:SG	1:B:289:LYS:N	2.57	0.76
1:B:166:LEU:HB2	1:B:181:TYR:HB2	1.70	0.73
1:B:355:ILE:HD12	1:B:357:GLY:H	1.53	0.73
1:A:355:ILE:HD12	1:A:357:GLY:H	1.53	0.73
1:A:113:ASN:ND2	1:A:131:TRP:O	2.22	0.72
1:B:213:ALA:HB1	1:B:289:LYS:HE2	1.71	0.71
1:B:350:THR:OG1	1:B:357:GLY:O	2.09	0.70
1:A:112:ARG:NH1	1:A:152:GLN:OE1	2.28	0.66
1:A:506:ILE:HA	1:A:534:THR:HG22	1.78	0.65
1:B:112:ARG:NH1	1:B:152:GLN:OE1	2.29	0.65
1:A:353:ASN:HB2	1:B:320:PHE:HB2	1.78	0.65
1:A:222:VAL:HA	1:A:230:PRO:HA	1.78	0.64
1:A:143:VAL:HG23	1:A:147:ASP:HB3	1.80	0.62
1:A:482:SER:OG	1:A:488:LYS:O	2.18	0.62
1:B:566:ALA:HB3	1:B:575:ARG:HB2	1.82	0.61
1:A:534:THR:OG1	1:A:537:GLN:O	2.16	0.61
1:A:240:GLU:HB3	1:A:243:ASP:HB2	1.83	0.60
1:A:288:CYS:SG	1:A:289:LYS:N	2.74	0.60
1:A:566:ALA:O	1:A:575:ARG:N	2.35	0.59
1:B:476:LYS:HG3	1:B:494:ILE:HB	1.83	0.58
1:B:272:GLU:OE2	1:B:377:LYS:NZ	2.29	0.58
1:A:113:ASN:N	1:A:153:ASN:O	2.35	0.57
1:A:96:HIS:O	1:A:508:ASN:ND2	2.24	0.57
1:A:100:VAL:HG22	1:A:107:LEU:HD13	1.86	0.57
1:B:451:ASP:HB3	1:B:464:VAL:HB	1.87	0.57
1:A:114:THR:HG22	1:A:130:VAL:HG22	1.87	0.56
1:B:222:VAL:HA	1:B:230:PRO:HA	1.87	0.56
1:B:209:THR:HG22	1:B:252:PHE:HB3	1.87	0.56
1:A:566:ALA:HB3	1:A:575:ARG:HB2	1.88	0.56
1:B:378:GLU:HB3	1:B:388:PRO:HA	1.88	0.56
1:A:508:ASN:HB3	1:A:533:VAL:HB	1.88	0.56
1:A:97:PHE:O	1:A:110:GLY:N	2.39	0.56
1:A:166:LEU:HB2	1:A:181:TYR:HB2	1.87	0.56
1:A:294:GLY:H	1:A:299:ARG:HA	1.71	0.56
1:B:566:ALA:O	1:B:575:ARG:N	2.39	0.55
1:B:568:ASP:OD2	1:B:575:ARG:NH2	2.39	0.55
1:A:475:ILE:HG13	1:A:496:GLU:HG3	1.88	0.55
1:B:534:THR:OG1	1:B:537:GLN:O	2.18	0.55
1:A:153:ASN:HA	1:A:172:ASN:H	1.71	0.55
1:B:453:GLN:HB3	1:B:461:THR:HB	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:HD2	1:A:407:ARG:HH21	1.73	0.54
1:A:177:MET:HG3	1:A:195:ASN:HA	1.90	0.54
1:B:506:ILE:HA	1:B:534:THR:HG22	1.89	0.54
1:B:96:HIS:O	1:B:508:ASN:ND2	2.31	0.54
1:A:350:THR:OG1	1:A:357:GLY:O	2.24	0.53
1:B:218:TYR:CZ	1:B:234:ARG:HD3	2.43	0.53
1:A:117:ASN:O	1:A:126:GLN:N	2.34	0.53
1:B:234:ARG:NH2	1:B:291:ASP:O	2.40	0.53
1:B:464:VAL:HA	1:B:478:VAL:HG12	1.91	0.53
1:A:328:ALA:HA	1:A:346:GLY:HA2	1.91	0.53
1:A:216:GLU:OE1	1:A:289:LYS:NZ	2.34	0.52
1:A:97:PHE:HB3	1:A:110:GLY:HA3	1.92	0.52
1:B:411:ASP:N	1:B:412:PRO:HD2	2.23	0.52
1:B:97:PHE:O	1:B:110:GLY:N	2.42	0.52
1:A:234:ARG:NH2	1:A:291:ASP:O	2.43	0.52
1:A:411:ASP:N	1:A:412:PRO:HD2	2.25	0.52
1:A:137:ASP:OD2	1:A:172:ASN:ND2	2.43	0.51
1:B:315:PRO:HG2	1:B:432:SER:O	2.10	0.51
1:B:97:PHE:HB3	1:B:110:GLY:HA3	1.92	0.51
1:B:158:MET:HB2	1:B:168:VAL:HG12	1.93	0.51
1:A:456:THR:HG23	1:A:458:GLY:H	1.76	0.50
1:A:209:THR:HG22	1:A:252:PHE:HB3	1.92	0.50
1:A:413:THR:HA	1:A:416:PHE:HB3	1.92	0.50
1:B:551:ILE:O	1:B:552:THR:HG22	2.11	0.50
1:A:315:PRO:HG2	1:A:432:SER:O	2.12	0.50
1:B:456:THR:OG1	1:B:590:GLN:NE2	2.37	0.50
1:B:267:ARG:HB3	1:B:325:ILE:HG22	1.92	0.50
1:B:530:LEU:N	1:B:541:ILE:O	2.45	0.50
1:A:280:ILE:O	1:A:323:ASN:HB3	2.12	0.50
1:A:378:GLU:HB3	1:A:388:PRO:HA	1.94	0.50
1:B:85:LEU:HB2	1:B:540:ALA:HB3	1.94	0.50
1:B:456:THR:HG23	1:B:458:GLY:H	1.77	0.49
1:A:509:LEU:HD23	1:A:532:ILE:HA	1.94	0.49
1:B:96:HIS:HE2	1:B:507:ARG:HD2	1.77	0.49
1:B:583:LEU:HD23	1:B:583:LEU:H	1.78	0.49
1:B:380:THR:HA	1:B:386:TRP:HE3	1.78	0.49
1:A:231:ILE:HD13	1:A:238:GLN:HG3	1.94	0.49
1:B:131:TRP:HE3	1:B:153:ASN:HD21	1.61	0.49
1:A:500:LEU:HD11	1:A:539:VAL:HB	1.95	0.48
1:A:155:ILE:HA	1:A:170:GLY:HA2	1.95	0.48
1:B:103:ASP:OD1	1:B:103:ASP:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:N	1:A:103:ASP:OD1	2.45	0.48
1:A:177:MET:HA	1:A:196:GLY:H	1.79	0.48
1:B:376:PHE:HA	1:B:423:MET:HA	1.94	0.48
1:A:234:ARG:O	1:A:237:LEU:N	2.44	0.48
1:A:435:ILE:HG23	1:A:479:ASN:ND2	2.28	0.48
1:A:443:TYR:OH	1:A:496:GLU:OE2	2.23	0.48
1:B:311:ASN:ND2	3:B:703:NAG:O7	2.47	0.48
1:A:389:VAL:HG13	1:A:393:LYS:HD2	1.96	0.48
1:A:94:VAL:HG12	1:A:535:ASP:HB3	1.95	0.48
1:B:328:ALA:HA	1:B:346:GLY:HA2	1.96	0.48
1:A:339:MET:HG3	1:A:341:SER:H	1.79	0.47
1:B:231:ILE:HD13	1:B:238:GLN:HG3	1.96	0.47
1:B:530:LEU:HD23	1:B:541:ILE:HD11	1.95	0.47
1:A:83:ASP:N	1:A:83:ASP:OD1	2.47	0.47
1:B:240:GLU:HB3	1:B:243:ASP:HB2	1.96	0.47
1:A:376:PHE:HA	1:A:423:MET:HA	1.95	0.47
1:A:583:LEU:H	1:A:583:LEU:HD23	1.79	0.47
1:A:218:TYR:CZ	1:A:234:ARG:HD3	2.50	0.47
1:A:235:GLU:HA	1:A:236:PRO:HA	1.76	0.47
1:A:551:ILE:O	1:A:552:THR:HG22	2.14	0.47
1:B:113:ASN:N	1:B:153:ASN:O	2.43	0.47
1:B:131:TRP:HZ2	1:B:179:ASN:HD22	1.63	0.47
1:B:235:GLU:HA	1:B:236:PRO:HA	1.63	0.47
1:A:98:LYS:HA	1:A:109:ILE:HA	1.96	0.47
1:A:85:LEU:HB2	1:A:540:ALA:HB3	1.97	0.46
1:B:280:ILE:O	1:B:323:ASN:HB3	2.16	0.46
1:A:237:LEU:HD23	1:A:302:TRP:CD2	2.51	0.46
1:B:93:VAL:CG1	1:B:111:ALA:HB1	2.46	0.46
1:B:556:GLU:O	1:B:560:LEU:HD13	2.15	0.46
1:A:349:ASN:HA	1:A:358:SER:HA	1.97	0.45
1:A:453:GLN:HB3	1:A:461:THR:HB	1.96	0.45
2:D:1:NAG:H4	2:D:2:NAG:H2	1.72	0.45
1:A:199:VAL:HG12	1:A:219:SER:HB3	1.99	0.45
1:B:159:VAL:HG11	1:B:212:LEU:HB3	1.99	0.45
1:B:270:ALA:O	1:B:274:ILE:HG12	2.16	0.45
1:A:136:ASP:O	1:A:140:MET:HG3	2.16	0.45
1:A:222:VAL:HG12	1:A:230:PRO:HB3	1.99	0.45
1:B:443:TYR:HB3	1:B:471:HIS:HB2	1.99	0.45
1:B:93:VAL:HG13	1:B:112:ARG:O	2.17	0.45
1:A:323:ASN:HB2	1:A:351:PRO:HG3	2.00	0.44
1:B:254:SER:HB3	1:B:265:PHE:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:ALA:HB3	1:B:580:PRO:HD3	1.99	0.44
1:A:356:PRO:HA	1:A:444:ARG:CZ	2.46	0.44
1:B:214:ASP:OD1	1:B:215:ASN:N	2.50	0.44
1:A:267:ARG:HB3	1:A:325:ILE:HG22	2.00	0.44
1:A:134:PRO:HD2	1:A:172:ASN:HD21	1.83	0.44
1:A:93:VAL:CG1	1:A:111:ALA:HB1	2.48	0.44
1:B:212:LEU:H	1:B:212:LEU:HD23	1.83	0.44
1:A:471:HIS:NE2	1:A:502:LYS:HG3	2.33	0.44
1:B:424:ASP:OD1	1:B:425:GLU:N	2.50	0.43
1:A:270:ALA:O	1:A:274:ILE:HG12	2.17	0.43
1:A:396:ASP:HB3	1:A:397:PRO:HD3	1.99	0.43
1:A:87:PHE:O	1:A:537:GLN:HB2	2.18	0.43
1:B:487:ASP:OD1	1:B:487:ASP:N	2.51	0.43
1:A:268:GLU:OE2	1:A:307:LYS:NZ	2.52	0.43
1:B:342:LYS:HE3	1:B:366:GLN:OE1	2.18	0.43
1:B:530:LEU:O	1:B:540:ALA:HA	2.19	0.43
1:A:449:ALA:N	1:A:466:PHE:O	2.51	0.43
1:A:563:PRO:HA	1:A:590:GLN:OE1	2.19	0.43
1:A:579:ALA:HB3	1:A:580:PRO:HD3	1.99	0.43
1:A:512:VAL:HG21	1:A:529:LYS:HB2	2.01	0.43
1:B:350:THR:HG22	1:B:354:SER:HB3	2.01	0.43
1:B:94:VAL:HG12	1:B:535:ASP:HB3	1.99	0.43
1:A:212:LEU:HD23	1:A:212:LEU:H	1.84	0.42
1:A:320:PHE:HB2	1:B:353:ASN:HB2	2.01	0.42
1:B:396:ASP:HB3	1:B:397:PRO:HD3	2.02	0.42
1:B:321:TYR:CE1	3:B:703:NAG:H82	2.54	0.42
1:A:472:GLY:HA2	1:A:506:ILE:HG13	2.01	0.42
1:B:239:THR:HG22	1:B:240:GLU:H	1.84	0.42
1:A:214:ASP:OD1	1:A:215:ASN:N	2.53	0.42
1:A:81:PRO:HD3	1:A:497:ILE:HG22	2.02	0.42
1:A:113:ASN:O	1:A:113:ASN:ND2	2.53	0.42
1:A:93:VAL:HA	1:A:112:ARG:HE	1.85	0.42
1:B:339:MET:HG2	1:B:341:SER:H	1.84	0.42
1:B:391:ASN:O	1:B:394:VAL:HG12	2.19	0.42
1:B:395:PRO:HB2	1:B:397:PRO:HD2	2.02	0.42
1:B:451:ASP:HB2	1:B:466:PHE:HE2	1.85	0.42
1:A:435:ILE:HG23	1:A:479:ASN:HD21	1.85	0.41
1:B:411:ASP:H	1:B:412:PRO:HD2	1.85	0.41
1:A:424:ASP:OD1	1:A:425:GLU:N	2.51	0.41
1:A:166:LEU:O	1:A:181:TYR:N	2.40	0.41
1:A:443:TYR:HB3	1:A:471:HIS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASP:OD1	1:B:95:ASP:N	2.53	0.41
1:B:237:LEU:HD23	1:B:302:TRP:CD2	2.55	0.41
1:B:500:LEU:HD11	1:B:539:VAL:HB	2.03	0.41
1:A:350:THR:HG22	1:A:351:PRO:HD2	2.02	0.41
1:A:376:PHE:HZ	1:A:399:PRO:HG2	1.86	0.41
1:A:377:LYS:HB2	1:A:423:MET:O	2.20	0.41
1:B:115:VAL:HG12	1:B:129:LEU:O	2.20	0.41
1:B:349:ASN:HA	1:B:358:SER:HA	2.02	0.41
1:B:108:LEU:HB2	2:D:1:NAG:H83	2.02	0.41
1:A:456:THR:HG22	1:A:460:LYS:O	2.21	0.41
1:B:237:LEU:HA	1:B:237:LEU:HD12	1.88	0.41
1:B:96:HIS:NE2	1:B:535:ASP:OD1	2.53	0.41
1:B:541:ILE:HB	1:B:545:ARG:NH2	2.36	0.41
1:A:137:ASP:OD1	1:A:137:ASP:N	2.54	0.40
1:B:158:MET:HA	1:B:167:PHE:O	2.21	0.40
1:A:530:LEU:N	1:A:541:ILE:O	2.54	0.40
1:B:122:ASP:N	1:B:122:ASP:OD1	2.54	0.40
1:A:158:MET:HA	1:A:167:PHE:O	2.21	0.40
1:A:350:THR:HG22	1:A:354:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/536 (93%)	475 (95%)	24 (5%)	0	100	100
1	B	498/536 (93%)	472 (95%)	26 (5%)	0	100	100
All	All	997/1072 (93%)	947 (95%)	50 (5%)	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	444/472 (94%)	436 (98%)	8 (2%)	59	81
1	B	443/472 (94%)	436 (98%)	7 (2%)	62	83
All	All	887/944 (94%)	872 (98%)	15 (2%)	60	82

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

Mol	Chain	Res	Type
1	A	95	ASP
1	A	101	THR
1	A	113	ASN
1	A	114	THR
1	A	143	VAL
1	A	373	GLU
1	A	438	ARG
1	A	552	THR
1	B	95	ASP
1	B	114	THR
1	B	131	TRP
1	B	239	THR
1	B	386	TRP
1	B	438	ARG
1	B	552	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	326	GLN
1	B	153	ASN

5.3.3 RNA [i](#)

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	0.24	0	17,19,21	0.58	0
2	NAG	C	2	2	14,14,15	0.42	0	17,19,21	0.51	0
2	NAG	D	1	1,2	14,14,15	0.44	0	17,19,21	0.78	0
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	0.56	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
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

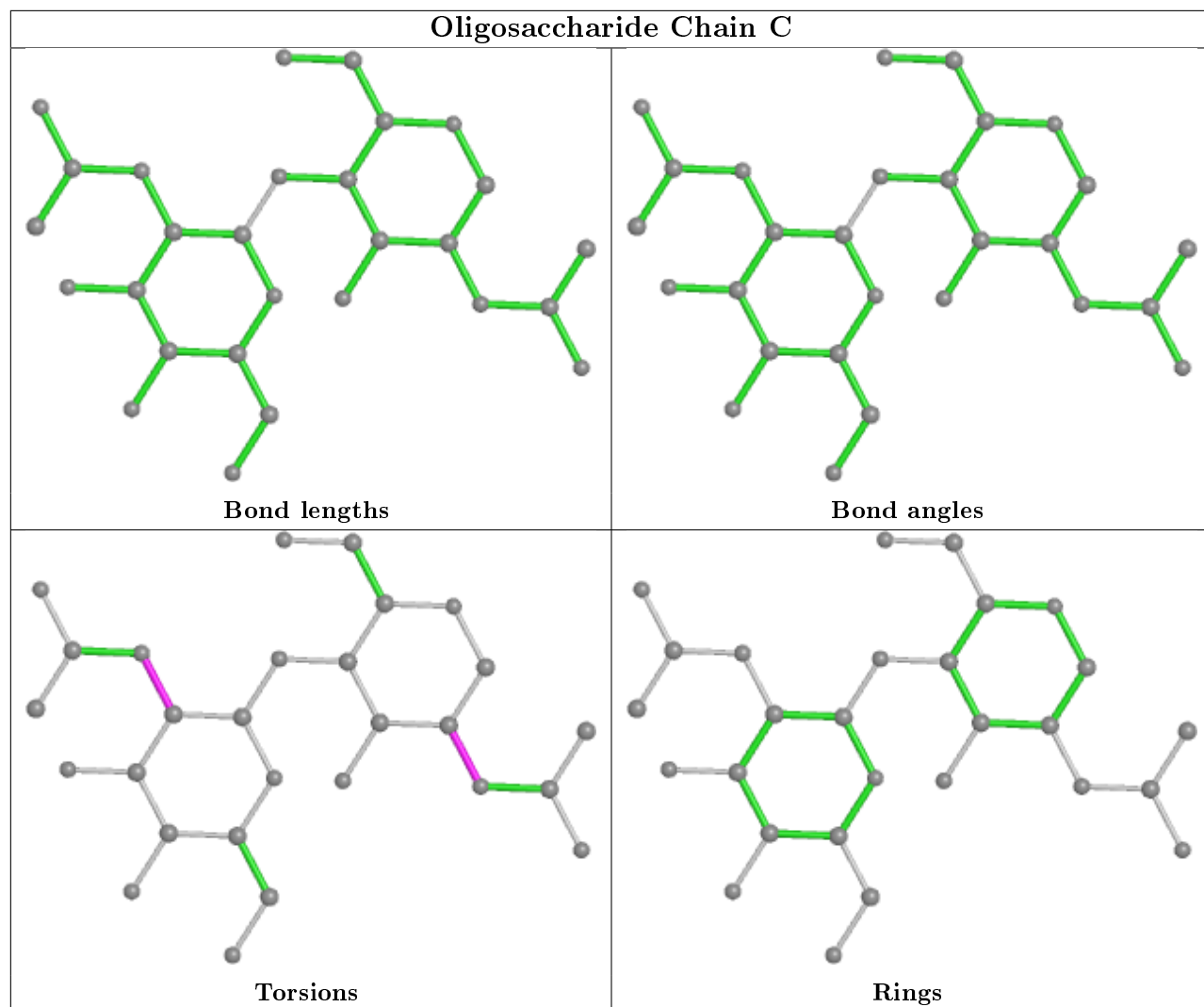
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7

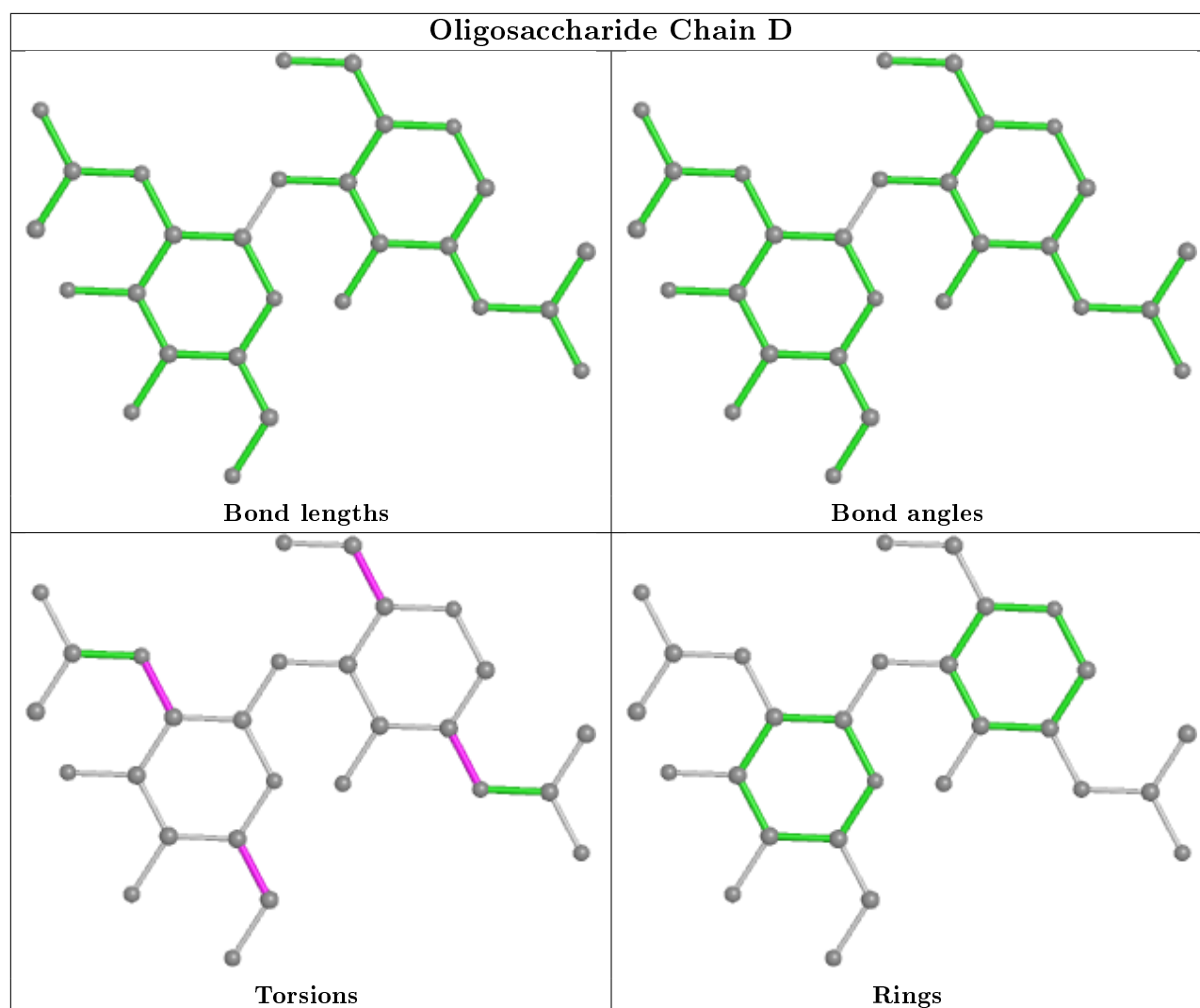
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	703	1	14,14,15	0.36	0	17,19,21	0.58	1 (5%)
3	NAG	B	703	1	14,14,15	0.39	0	17,19,21	0.69	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
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	NAG	C1-O5-C5	2.30	115.31	112.19
3	A	703	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	NAG	O5-C5-C6-O6
3	B	703	NAG	C4-C5-C6-O6
3	B	703	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
3	B	703	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	505/536 (94%)	0.49	39 (7%)	13 8	42, 102, 158, 188	0
1	B	504/536 (94%)	0.51	43 (8%)	10 6	42, 106, 162, 202	0
All	All	1009/1072 (94%)	0.50	82 (8%)	12 7	42, 103, 161, 202	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	TRP	7.7
1	B	383	ASN	7.6
1	A	385	ASN	7.2
1	A	387	LEU	7.2
1	B	552	THR	6.9
1	A	103	ASP	5.8
1	A	482	SER	5.7
1	B	387	LEU	5.4
1	A	384	SER	5.2
1	B	144	LYS	5.1
1	B	384	SER	4.9
1	B	129	LEU	4.7
1	A	162	SER	4.6
1	A	128	ARG	4.6
1	A	388	PRO	4.5
1	A	572	GLY	4.4
1	B	597	HIS	4.3
1	B	487	ASP	4.2
1	A	597	HIS	4.0
1	B	560	LEU	4.0
1	A	163	PRO	4.0
1	A	487	ASP	3.9
1	B	385	ASN	3.9
1	A	560	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	334	GLY	3.7
1	A	383	ASN	3.7
1	B	335	GLN	3.7
1	A	590	GLN	3.7
1	A	432	SER	3.6
1	A	159	VAL	3.5
1	A	583	LEU	3.5
1	B	386	TRP	3.4
1	A	552	THR	3.3
1	A	441	THR	3.2
1	B	388	PRO	3.2
1	A	166	LEU	3.1
1	B	586	ASN	3.0
1	B	206	HIS	3.0
1	A	581	ARG	2.9
1	A	415	ASN	2.9
1	B	590	GLN	2.9
1	B	133	SER	2.9
1	A	198	ALA	2.8
1	A	596	GLN	2.8
1	A	127	GLN	2.8
1	B	336	TYR	2.8
1	B	130	VAL	2.7
1	B	598	ALA	2.7
1	A	440	SER	2.6
1	B	343	LEU	2.6
1	B	588	PHE	2.6
1	B	128	ARG	2.6
1	A	586	ASN	2.6
1	B	482	SER	2.6
1	B	305	PHE	2.6
1	B	569	LYS	2.5
1	B	219	SER	2.5
1	A	393	LYS	2.5
1	B	301	ARG	2.5
1	A	575	ARG	2.5
1	B	102	LYS	2.5
1	A	181	TYR	2.5
1	A	571	ALA	2.4
1	B	488	LYS	2.4
1	A	587	TYR	2.4
1	B	587	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	90	ASN	2.3
1	A	345	TYR	2.2
1	B	435	ILE	2.2
1	B	99	LEU	2.2
1	B	98	LYS	2.2
1	A	240	GLU	2.2
1	B	264	PHE	2.1
1	A	194	LYS	2.1
1	B	153	ASN	2.1
1	A	142	LEU	2.1
1	B	441	THR	2.1
1	B	595	GLY	2.1
1	B	97	PHE	2.1
1	B	556	GLU	2.0
1	B	143	VAL	2.0
1	B	548	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

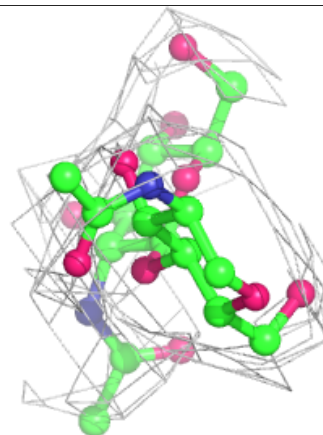
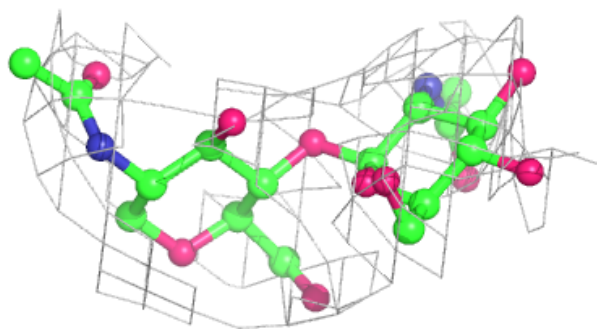
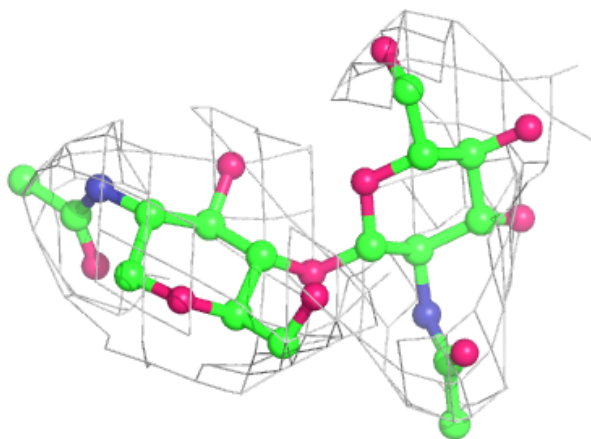
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

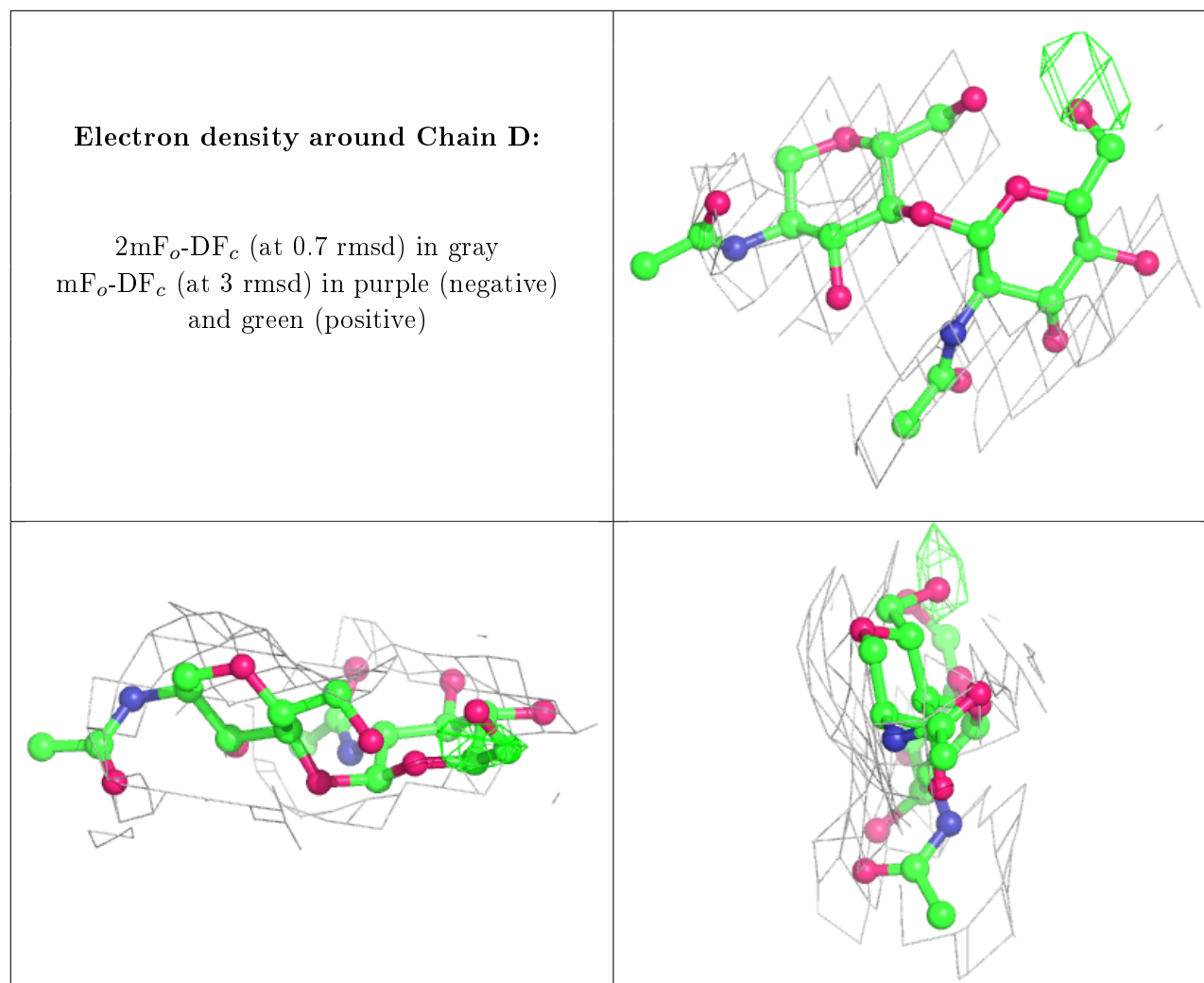
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.72	0.24	141,155,169,174	0
2	NAG	C	2	14/15	0.74	0.24	135,143,154,158	0
2	NAG	D	1	14/15	0.82	0.26	119,142,159,163	0
2	NAG	C	1	14/15	0.90	0.23	110,130,144,148	0

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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	703	14/15	0.82	0.25	75,77,79,82	0
3	NAG	B	703	14/15	0.88	0.22	69,70,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.