



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 PM UTC

PDB ID : 5NMT / pdb_00005nmt
Title : Dimer structure of Sortilin ectodomain crystal form 1, 2.3A
Authors : Leloup, N.O.L.; Janssen, B.J.C.
Deposited on : 2017-04-07
Resolution : 2.30 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
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

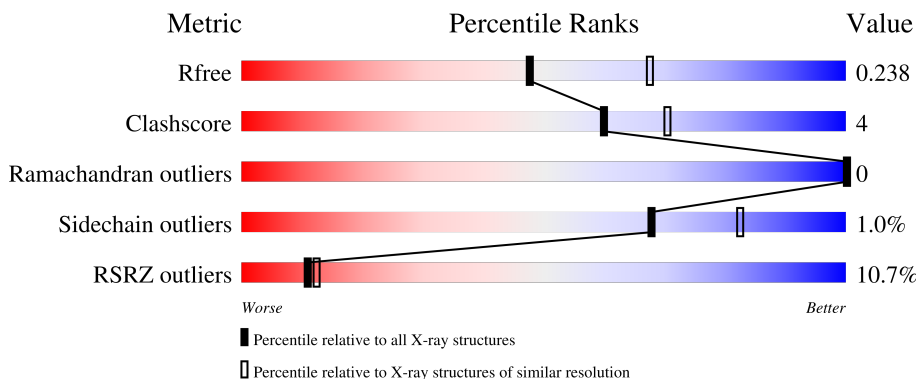
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	731	 9% 80% 9% 11%
1	B	731	 10% 79% 11% 10%
2	C	2	 100%
2	E	2	 100%
3	D	3	 33% 67%

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Mol	Chain	Length	Quality of chain
3	F	3	 33% 67%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10664 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 Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	654	5146	3250	866	1001	29	0	0	0
1	B	657	5167	3265	868	1004	30	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

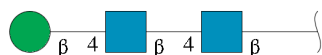
Chain	Residue	Modelled	Actual	Comment	Reference
A	723	ALA	-	expression tag	UNP Q6PHU5
A	724	ALA	-	expression tag	UNP Q6PHU5
A	725	ALA	-	expression tag	UNP Q6PHU5
A	726	HIS	-	expression tag	UNP Q6PHU5
A	727	HIS	-	expression tag	UNP Q6PHU5
A	728	HIS	-	expression tag	UNP Q6PHU5
A	729	HIS	-	expression tag	UNP Q6PHU5
A	730	HIS	-	expression tag	UNP Q6PHU5
A	731	HIS	-	expression tag	UNP Q6PHU5
B	723	ALA	-	expression tag	UNP Q6PHU5
B	724	ALA	-	expression tag	UNP Q6PHU5
B	725	ALA	-	expression tag	UNP Q6PHU5
B	726	HIS	-	expression tag	UNP Q6PHU5
B	727	HIS	-	expression tag	UNP Q6PHU5
B	728	HIS	-	expression tag	UNP Q6PHU5
B	729	HIS	-	expression tag	UNP Q6PHU5
B	730	HIS	-	expression tag	UNP Q6PHU5
B	731	HIS	-	expression tag	UNP Q6PHU5

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



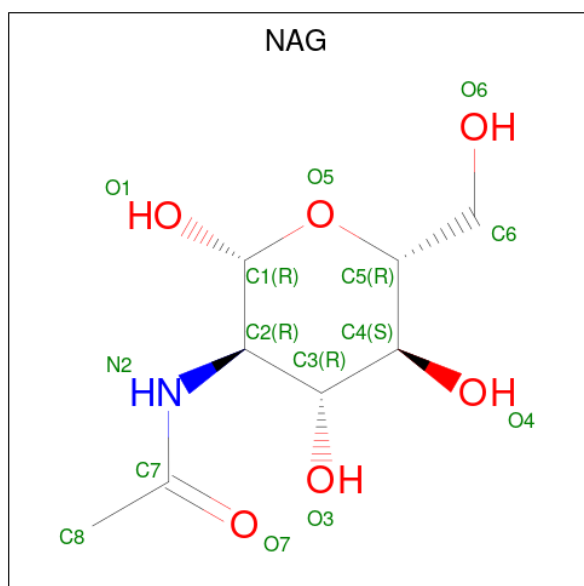
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

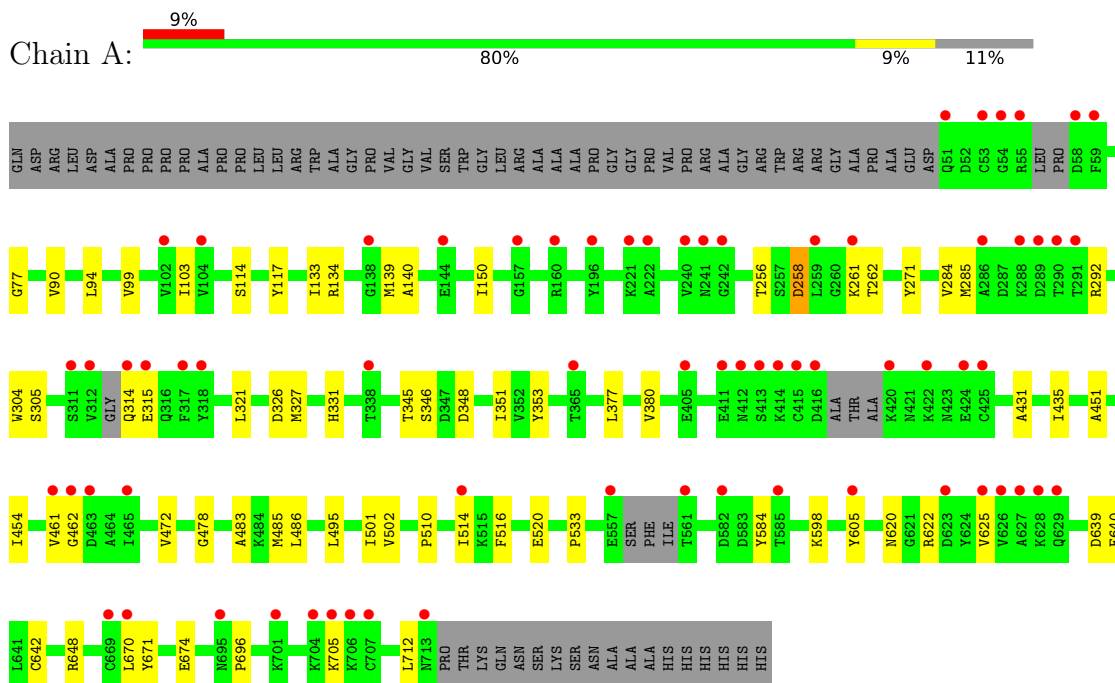
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total	O	0	0
			88	88		
6	B	71	Total	O	0	0
			71	71		

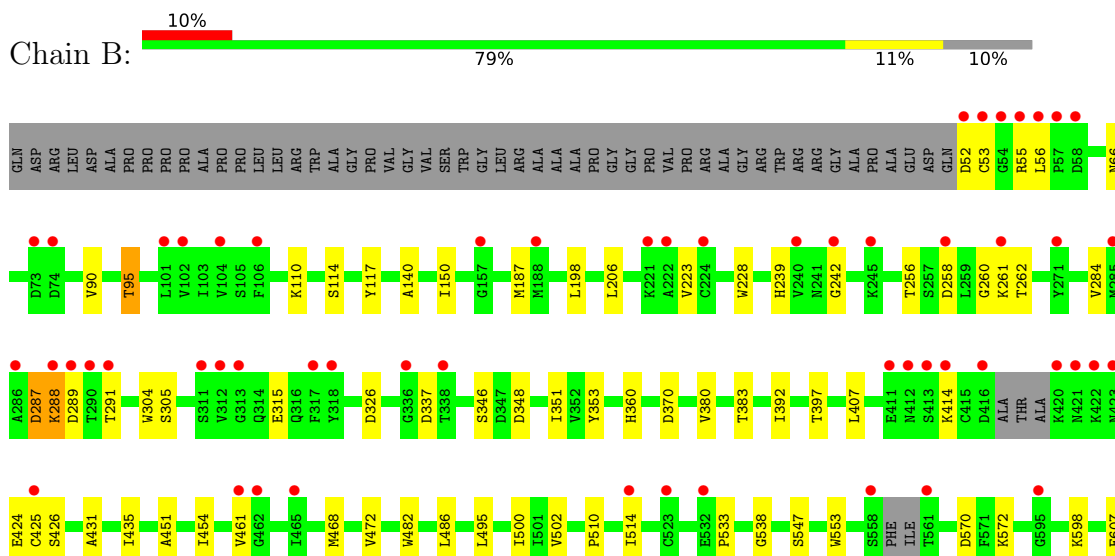
3 Residue-property plots [i](#)

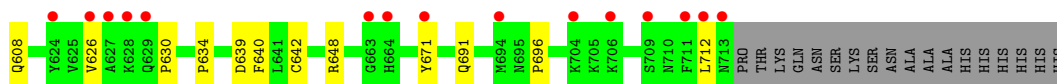
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sortilin



- Molecule 1: Sortilin





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

Chain C:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain D:  33% 67%

MAG1
MAG2
BMA3

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

Chain F:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.02Å 131.13Å 154.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.64 – 2.30 69.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (69.64-2.30) 99.1 (69.64-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.205 , 0.234 0.210 , 0.238	Depositor DCC
R_{free} test set	2650 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10664	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: BMA, CL, 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	0.14	0/5265	0.35	0/7127
1	B	0.15	0/5292	0.36	1/7167 (0.0%)
All	All	0.15	0/10557	0.36	1/14294 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	LYS	CB-CA-C	-5.75	109.92	116.54

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	5146	0	4922	40	0
1	B	5167	0	4951	51	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	39	0	34	1	0
3	F	39	0	34	1	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
6	A	88	0	0	0	0
6	B	71	0	0	0	0
All	All	10664	0	10043	89	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 4.

All (89) 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:258:ASP:OD2	1:A:262:THR:OG1	2.13	0.67
1:B:305:SER:HB3	1:B:351:ILE:HD12	1.83	0.60
1:B:607:GLU:HG3	1:B:630:PRO:HB3	1.84	0.59
1:B:95:THR:HB	1:B:110:LYS:H	1.68	0.57
1:B:258:ASP:OD2	1:B:262:THR:OG1	2.16	0.57
1:B:598:LYS:NZ	1:B:639:ASP:OD2	2.38	0.56
1:A:77:GLY:HA2	1:B:468:MET:HE2	1.88	0.56
1:B:495:LEU:HD12	1:B:500:ILE:HB	1.88	0.55
1:B:642:CYS:SG	1:B:648:ARG:HG3	2.47	0.55
1:B:304:TRP:CD1	1:B:712:LEU:HD11	2.41	0.55
1:B:407:LEU:HD11	1:B:482:TRP:HE1	1.71	0.55
1:A:431:ALA:O	1:A:435:ILE:HG12	2.07	0.54
1:B:256:THR:HG21	1:B:260:GLY:H	1.72	0.54
1:A:103:ILE:HD12	1:B:392:ILE:HB	1.89	0.53
1:A:584:TYR:CZ	1:A:622:ARG:HD3	2.44	0.53
1:B:256:THR:HG22	1:B:258:ASP:H	1.74	0.52
1:B:140:ALA:HB3	1:B:150:ILE:HB	1.92	0.52
1:A:451:ALA:HB1	1:A:454:ILE:HD12	1.92	0.51
1:A:670:LEU:HD23	1:A:671:TYR:HD2	1.76	0.51
1:A:304:TRP:CD1	1:A:712:LEU:HD11	2.46	0.51
1:A:305:SER:HB3	1:A:351:ILE:HD12	1.92	0.51
1:A:314:GLN:HG3	1:A:315:GLU:HG3	1.93	0.51
1:B:424:GLU:C	1:B:426:SER:H	2.19	0.51
1:B:431:ALA:O	1:B:435:ILE:HG12	2.11	0.51
1:A:502:VAL:HG13	1:A:514:ILE:HG23	1.92	0.50
1:A:642:CYS:SG	1:A:648:ARG:HG3	2.51	0.50
1:A:346:SER:HB3	1:A:353:TYR:CE2	2.46	0.50
1:A:510:PRO:HB2	1:A:533:PRO:HB2	1.94	0.49
1:A:461:VAL:HG12	1:A:462:GLY:H	1.78	0.48
1:B:472:VAL:HB	1:B:486:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ASN:OD1	1:A:622:ARG:HG2	2.13	0.48
1:B:256:THR:HG23	1:B:262:THR:O	2.14	0.47
1:B:284:VAL:HG21	1:B:712:LEU:HD23	1.96	0.47
1:A:326:ASP:O	1:A:348:ASP:HA	2.13	0.47
1:B:608:GLN:HB3	1:B:626:VAL:HB	1.97	0.47
1:B:451:ALA:HB1	1:B:454:ILE:HD12	1.96	0.47
1:B:326:ASP:O	1:B:348:ASP:HA	2.15	0.46
1:A:472:VAL:HB	1:A:486:LEU:HB2	1.97	0.46
1:A:140:ALA:HB3	1:A:150:ILE:HB	1.98	0.46
1:B:256:THR:HG21	1:B:260:GLY:N	2.30	0.46
1:B:634:PRO:HA	1:B:691:GLN:O	2.15	0.46
1:A:640:PHE:CZ	1:A:696:PRO:HD2	2.51	0.46
1:B:198:LEU:HD23	1:B:228:TRP:CE2	2.51	0.46
1:A:483:ALA:HB3	1:A:485:MET:HE2	1.97	0.46
1:B:239:HIS:NE2	1:B:242:GLY:O	2.44	0.46
1:A:674:GLU:HG3	1:A:705:LYS:HB3	1.98	0.45
1:B:287:ASP:N	1:B:287:ASP:OD1	2.49	0.45
1:A:454:ILE:HD11	1:A:520:GLU:HG2	1.97	0.45
1:B:502:VAL:HG13	1:B:514:ILE:HG23	1.98	0.45
1:B:55:ARG:NE	1:B:55:ARG:HA	2.32	0.45
1:B:90:VAL:HA	1:B:114:SER:O	2.17	0.45
1:B:414:LYS:HD2	1:B:461:VAL:HG21	1.98	0.45
1:A:598:LYS:NZ	1:A:639:ASP:OD2	2.50	0.44
1:B:572:LYS:HE2	1:B:572:LYS:HB3	1.79	0.44
1:B:187:MET:HE2	1:B:187:MET:HB3	1.80	0.44
1:A:284:VAL:HG21	1:A:712:LEU:HD23	1.99	0.44
1:A:285:MET:HE3	1:A:285:MET:HB2	1.94	0.44
1:B:288:LYS:O	1:B:289:ASP:C	2.60	0.44
1:B:510:PRO:HB2	1:B:533:PRO:HB2	2.00	0.44
1:B:291:THR:HG22	1:B:315:GLU:HG3	2.00	0.43
1:B:346:SER:HB3	1:B:353:TYR:CE2	2.53	0.43
1:B:538:GLY:HA3	1:B:553:TRP:CZ2	2.54	0.43
1:A:90:VAL:HA	1:A:114:SER:O	2.18	0.43
1:A:377:LEU:HD12	1:A:377:LEU:HA	1.89	0.43
1:A:99:VAL:HB	1:A:134:ARG:NH1	2.33	0.43
1:B:66:ASN:HB3	1:B:570:ASP:HB3	2.00	0.43
1:B:380:VAL:HA	1:B:397:THR:O	2.18	0.42
1:A:271:TYR:CG	1:A:292:ARG:HD3	2.54	0.42
1:B:370:ASP:HA	1:B:431:ALA:HB3	2.01	0.42
1:A:304:TRP:CG	1:A:712:LEU:HD11	2.54	0.42
1:B:206:LEU:HB2	1:B:223:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:GLY:HA3	1:B:553:TRP:CH2	2.54	0.42
1:A:117:TYR:HB2	3:D:1:NAG:H61	2.01	0.41
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.86	0.41
1:A:94:LEU:HB3	1:A:139:MET:HE2	2.01	0.41
1:A:327:MET:HE1	1:A:345:THR:HG22	2.02	0.41
1:B:261:LYS:HA	1:B:261:LYS:HD3	1.92	0.41
1:A:256:THR:HG23	1:A:262:THR:O	2.21	0.41
1:B:360:HIS:NE2	1:B:383:THR:OG1	2.46	0.41
1:A:461:VAL:HG12	1:A:462:GLY:N	2.36	0.41
1:A:501:ILE:O	1:A:516:PHE:HA	2.21	0.41
1:B:117:TYR:HB2	3:F:1:NAG:H61	2.02	0.41
1:B:305:SER:HB2	1:B:671:TYR:CE1	2.55	0.41
1:B:425:CYS:H	1:B:461:VAL:HG13	1.84	0.41
1:A:321:LEU:HD11	1:A:331:HIS:HB2	2.02	0.40
1:B:640:PHE:CZ	1:B:696:PRO:HD2	2.55	0.40
1:B:495:LEU:CD1	1:B:500:ILE:HB	2.50	0.40
1:B:495:LEU:HB2	1:B:547:SER:OG	2.21	0.40
1:A:380:VAL:HG11	1:A:478:GLY:O	2.22	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	644/731 (88%)	621 (96%)	23 (4%)	0	100	100
1	B	652/731 (89%)	628 (96%)	24 (4%)	0	100	100
All	All	1296/1462 (89%)	1249 (96%)	47 (4%)	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	571/626 (91%)	566 (99%)	5 (1%)	70 84
1	B	574/626 (92%)	568 (99%)	6 (1%)	68 82
All	All	1145/1252 (92%)	1134 (99%)	11 (1%)	68 82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ILE
1	A	258	ASP
1	A	495	LEU
1	A	605	TYR
1	A	625	VAL
1	B	52	ASP
1	B	53	CYS
1	B	56	LEU
1	B	95	THR
1	B	287	ASP
1	B	337	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	69	GLN
1	A	145	ASN
1	A	220	HIS
1	A	400	GLN
1	A	406	HIS
1	A	506	HIS
1	A	713	ASN
1	B	70	HIS
1	B	220	HIS
1	B	300	GLN

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Mol	Chain	Res	Type
1	B	440	ASN
1	B	506	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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	2,1	14,14,15	0.27	0	17,19,21	0.72	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.67	0
3	NAG	D	1	3,1	14,14,15	0.35	0	17,19,21	0.81	0
3	NAG	D	2	3	14,14,15	0.35	0	17,19,21	1.40	2 (11%)
3	BMA	D	3	3	11,11,12	0.32	0	15,15,17	0.63	0
2	NAG	E	1	2,1	14,14,15	0.34	0	17,19,21	1.23	3 (17%)
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.86	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.33	0	17,19,21	0.72	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
3	BMA	F	3	3	11,11,12	0.31	0	15,15,17	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O4-C4-C3	3.44	118.48	110.38
3	D	2	NAG	O4-C4-C5	-2.80	102.42	109.32
2	E	1	NAG	O4-C4-C3	-2.54	104.39	110.38
2	E	2	NAG	C4-C3-C2	-2.21	107.78	111.02
2	E	1	NAG	C2-N2-C7	-2.20	119.95	122.90
3	F	2	NAG	O4-C4-C5	-2.20	103.92	109.32
2	E	1	NAG	C6-C5-C4	-2.11	107.85	113.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

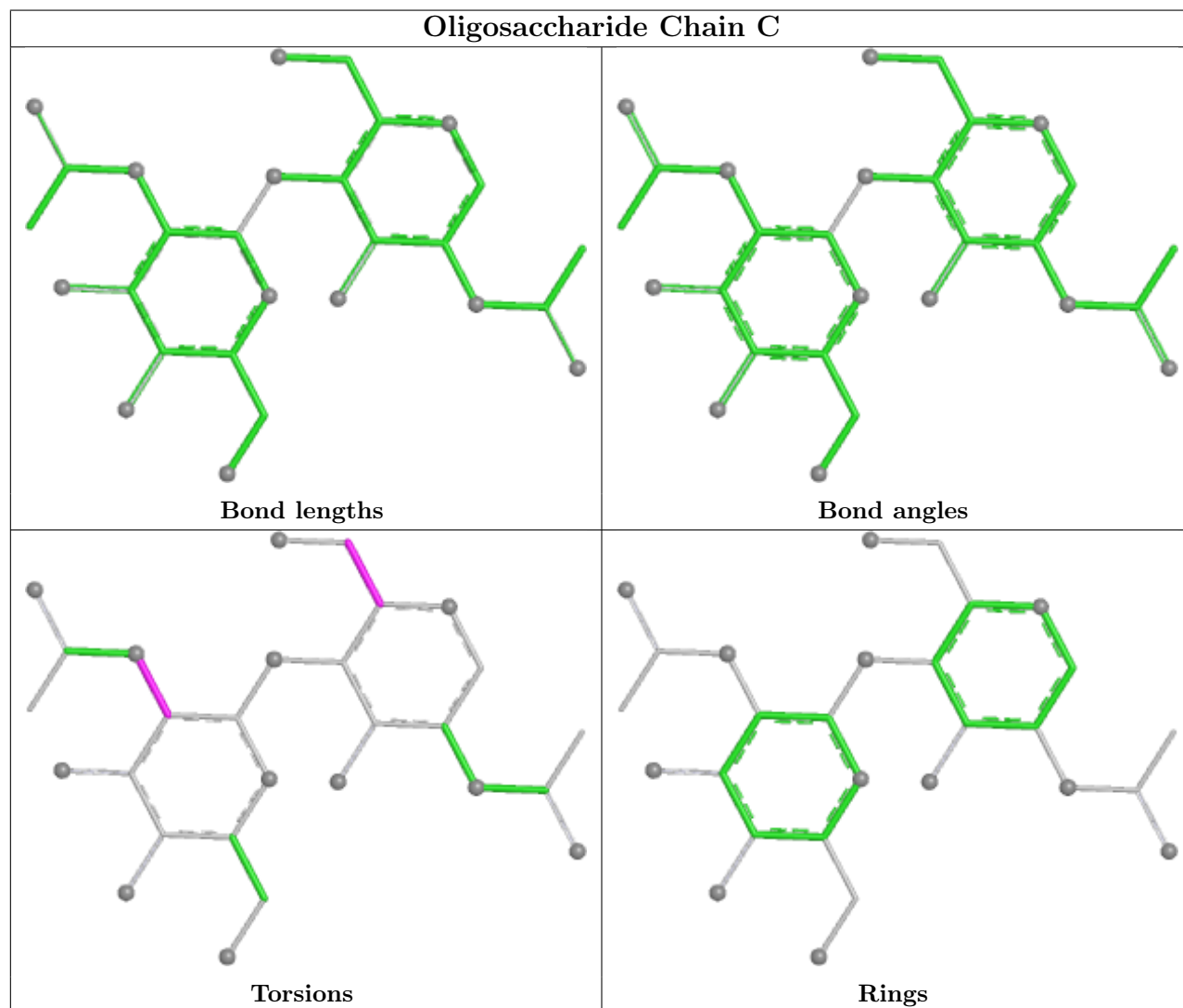
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
3	D	1	NAG	C4-C5-C6-O6

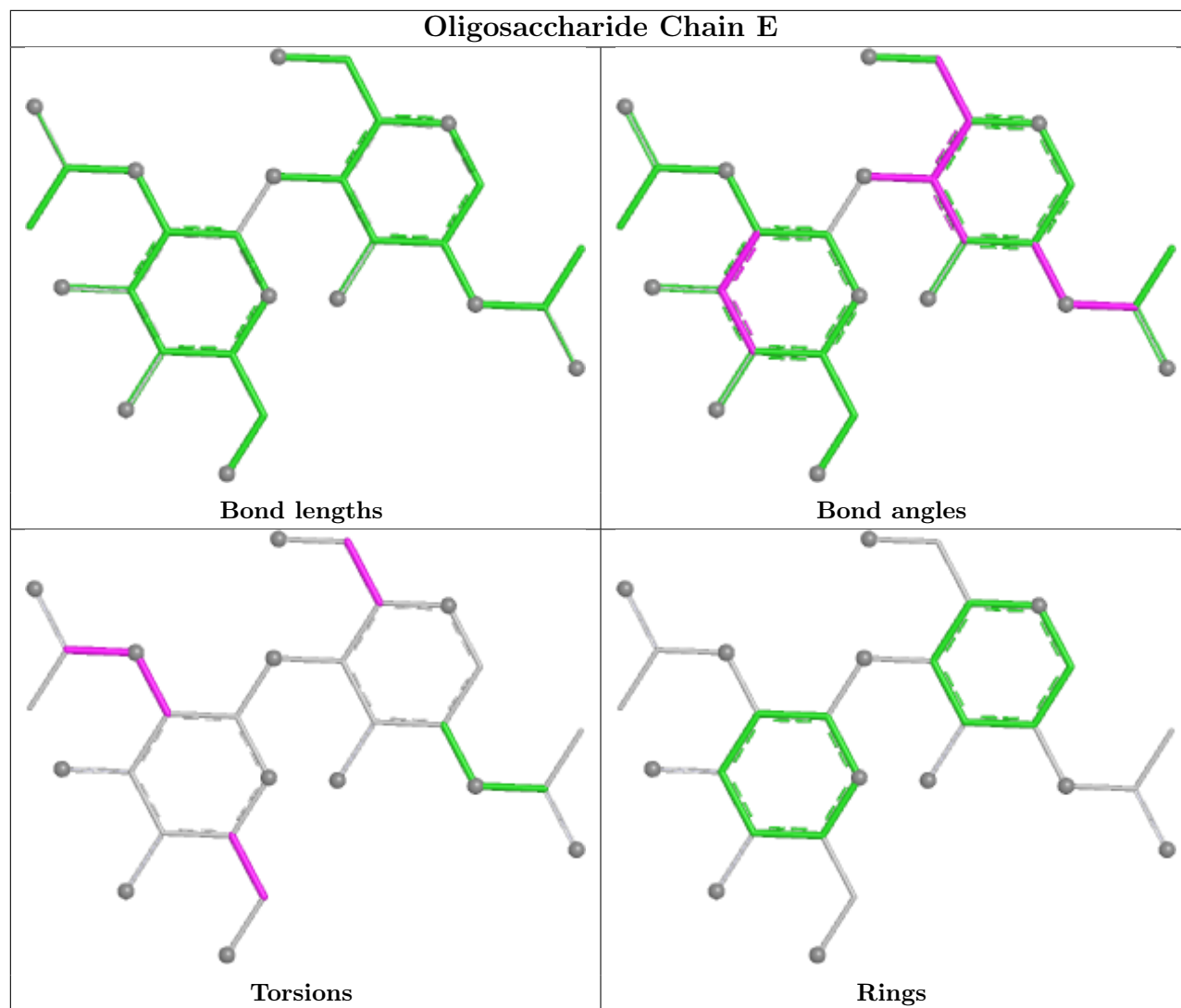
There are no ring outliers.

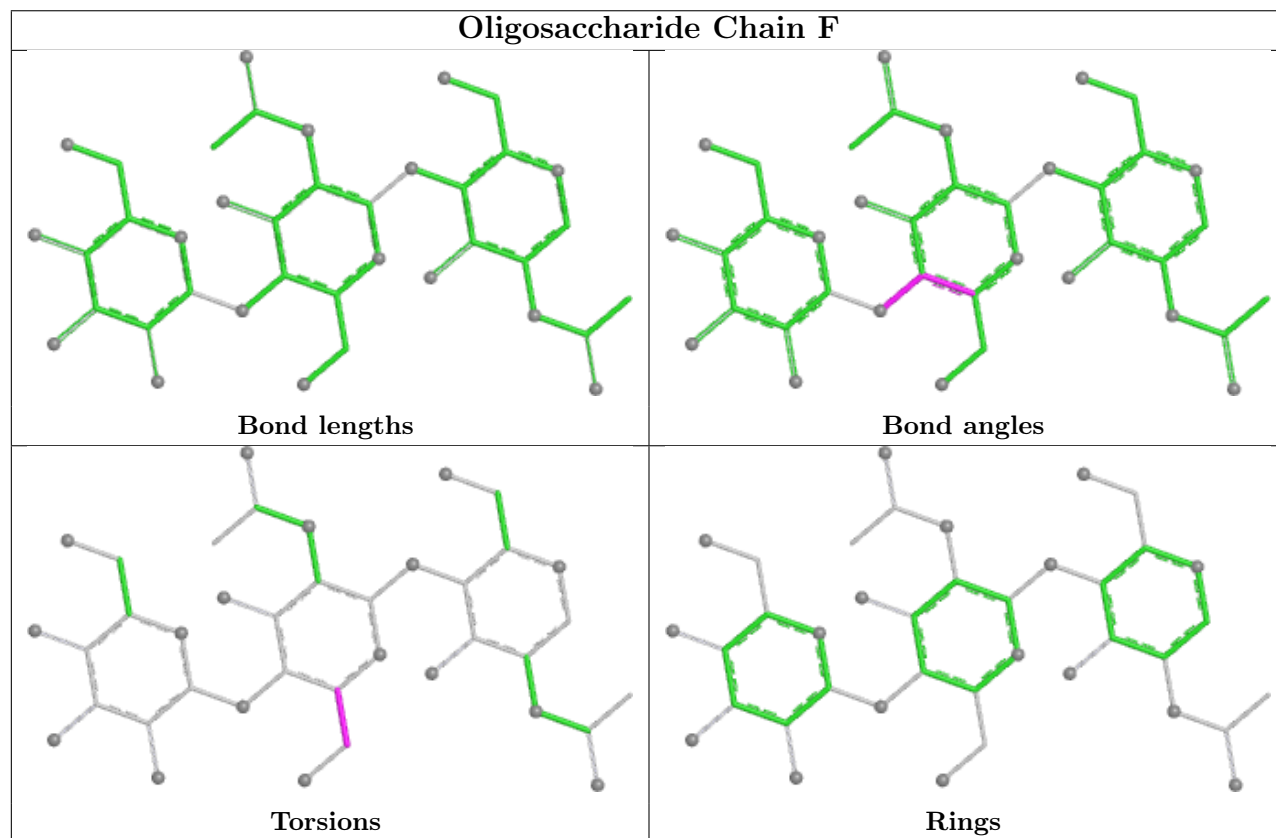
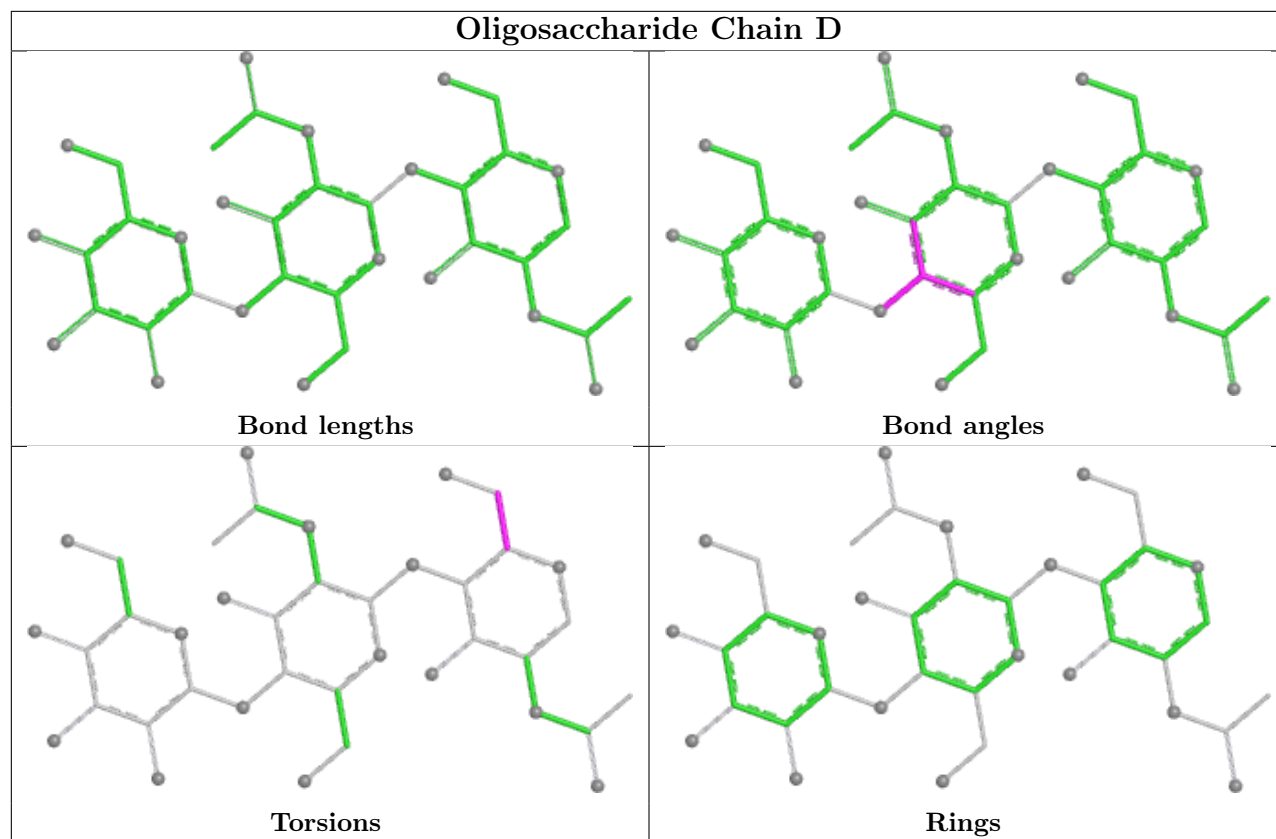
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	F	1	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	807	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	A	801	1	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	B	801	1	14,14,15	0.29	0	17,19,21	0.67	0
4	NAG	A	807	1	14,14,15	0.30	0	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	807	1	-	1/6/23/26	0/1/1/1
4	NAG	A	801	1	-	5/6/23/26	0/1/1/1
4	NAG	B	801	1	-	0/6/23/26	0/1/1/1
4	NAG	A	807	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	A	801	NAG	O5-C5-C6-O6
4	A	801	NAG	C3-C2-N2-C7
4	A	801	NAG	C4-C5-C6-O6
4	B	807	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	654/731 (89%)	0.57	69 (10%) 11 12	34, 59, 102, 141	0
1	B	657/731 (89%)	0.61	71 (10%) 11 12	36, 60, 105, 134	1 (0%)
All	All	1311/1462 (89%)	0.59	140 (10%) 11 12	34, 59, 104, 141	1 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	LEU	7.7
1	B	627	ALA	7.6
1	A	312	VAL	7.2
1	B	290	THR	6.2
1	B	312	VAL	6.1
1	B	57	PRO	5.5
1	A	415	CYS	5.4
1	A	627	ALA	5.1
1	B	561	THR	4.7
1	B	338	THR	4.6
1	A	240	VAL	4.5
1	B	240	VAL	4.5
1	A	625	VAL	4.5
1	A	290	THR	4.4
1	B	420	LYS	4.3
1	A	605	TYR	4.3
1	A	411	GLU	4.3
1	B	514	ILE	4.1
1	B	712	LEU	4.0
1	B	414	LYS	4.0
1	B	626	VAL	4.0
1	B	465	ILE	4.0
1	B	422	LYS	3.9
1	A	55	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	241	ASN	3.9
1	B	53	CYS	3.8
1	A	626	VAL	3.8
1	A	514	ILE	3.8
1	B	242	GLY	3.8
1	B	711	PHE	3.7
1	A	629	GLN	3.7
1	A	157	GLY	3.7
1	B	558	SER	3.7
1	A	461	VAL	3.6
1	B	291	THR	3.6
1	B	336	GLY	3.6
1	A	59	PHE	3.6
1	B	628	LYS	3.6
1	A	420	LYS	3.5
1	B	55	ARG	3.5
1	A	291	THR	3.5
1	A	561	THR	3.5
1	B	413	SER	3.5
1	A	628	LYS	3.4
1	B	461	VAL	3.4
1	B	425	CYS	3.4
1	A	414	LYS	3.4
1	B	713	ASN	3.4
1	B	671	TYR	3.3
1	A	422	LYS	3.3
1	A	311	SER	3.3
1	A	425	CYS	3.2
1	B	423	ASN	3.2
1	A	144	GLU	3.1
1	B	416	ASP	3.1
1	A	314	GLN	3.1
1	A	707	CYS	3.1
1	B	52	ASP	3.1
1	B	421	ASN	3.1
1	A	222	ALA	3.0
1	B	157	GLY	3.0
1	B	313	GLY	3.0
1	B	694	MET	2.8
1	B	288	LYS	2.8
1	A	424	GLU	2.8
1	A	242	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	670	LEU	2.8
1	A	701	LYS	2.8
1	B	54	GLY	2.7
1	B	462	GLY	2.7
1	A	259	LEU	2.7
1	B	317	PHE	2.7
1	A	695	ASN	2.7
1	B	289	ASP	2.7
1	A	261	LYS	2.7
1	A	288	LYS	2.7
1	B	245	LYS	2.7
1	A	58	ASP	2.6
1	B	412	ASN	2.6
1	A	53	CYS	2.6
1	A	286	ALA	2.6
1	A	317	PHE	2.6
1	B	74	ASP	2.6
1	B	258	ASP	2.6
1	B	595	GLY	2.6
1	A	413	SER	2.6
1	B	311	SER	2.6
1	B	285	MET	2.5
1	A	51	GLN	2.5
1	A	585	THR	2.5
1	B	261	LYS	2.5
1	B	58	ASP	2.5
1	A	365	THR	2.4
1	A	557	GLU	2.4
1	B	411	GLU	2.4
1	B	106	PHE	2.4
1	B	704	LYS	2.4
1	B	102	VAL	2.4
1	A	705	LYS	2.4
1	B	221	LYS	2.4
1	A	416	ASP	2.4
1	A	669	CYS	2.4
1	A	138	GLY	2.3
1	A	338	THR	2.3
1	B	629	GLN	2.3
1	B	271	TYR	2.3
1	B	224	CYS	2.3
1	A	289	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	706	LYS	2.3
1	B	624	TYR	2.3
1	B	188[A]	MET	2.3
1	B	532	GLU	2.3
1	B	104	VAL	2.3
1	B	101	LEU	2.3
1	A	462	GLY	2.3
1	A	463	ASP	2.2
1	A	196	TYR	2.2
1	B	318	TYR	2.2
1	A	221	LYS	2.2
1	B	73	ASP	2.2
1	B	663	GLY	2.2
1	A	315	GLU	2.2
1	A	704	LYS	2.2
1	B	664	HIS	2.2
1	A	318	TYR	2.2
1	A	465	ILE	2.2
1	A	405	GLU	2.2
1	B	706	LYS	2.2
1	B	286	ALA	2.2
1	A	713	ASN	2.1
1	A	54	GLY	2.1
1	B	523	CYS	2.1
1	A	412	ASN	2.1
1	A	623	ASP	2.1
1	A	104	VAL	2.1
1	A	102	VAL	2.1
1	B	222	ALA	2.1
1	A	582	ASP	2.1
1	A	160	ARG	2.0
1	B	709	SER	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.

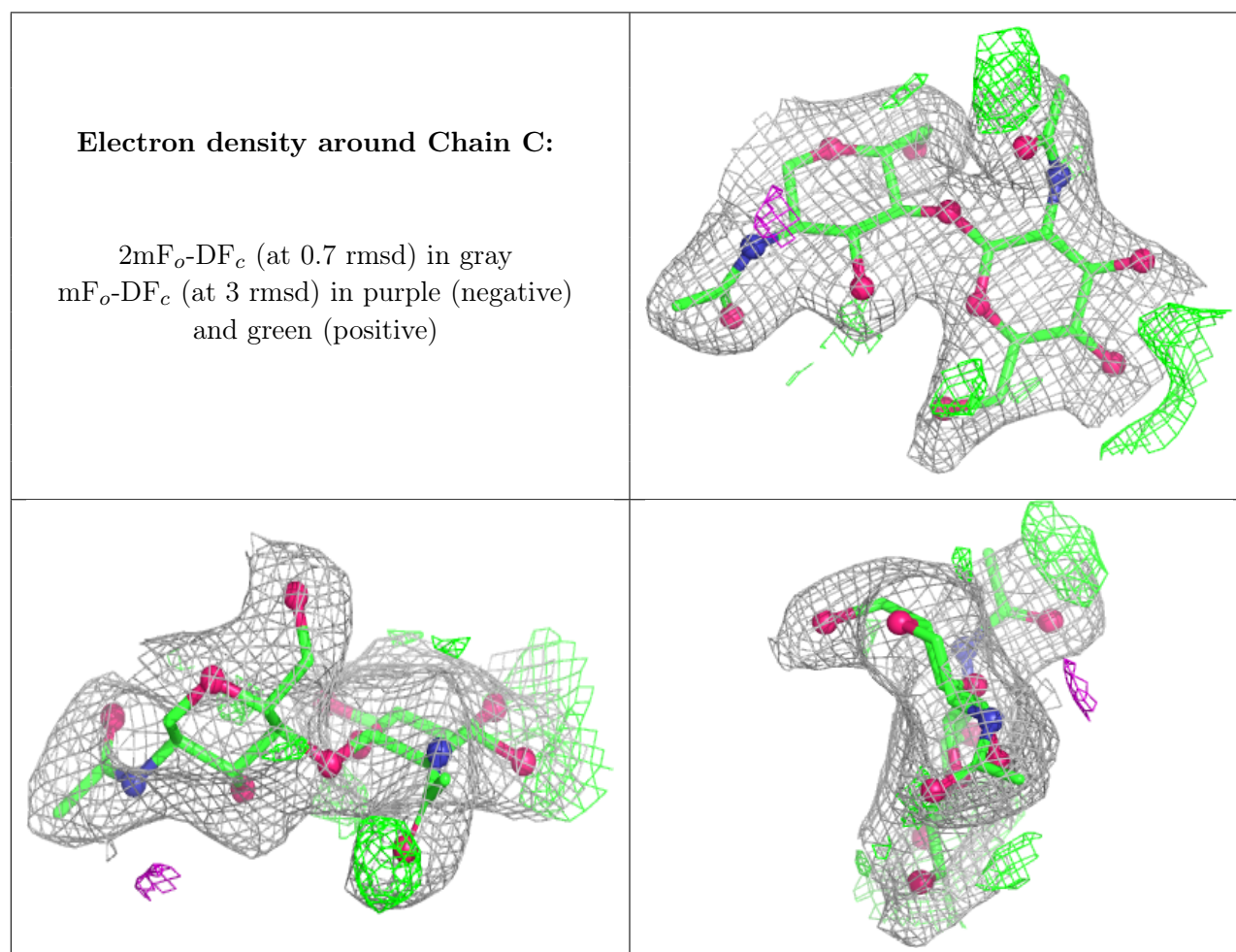
6.3 Carbohydrates [i](#)

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.

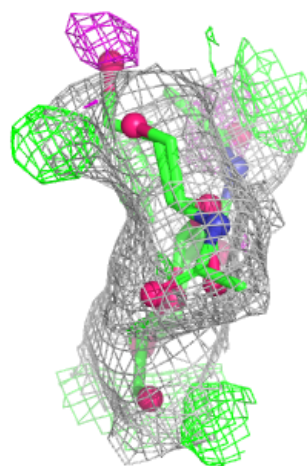
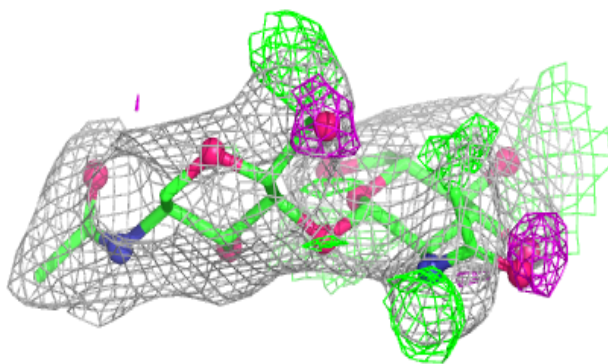
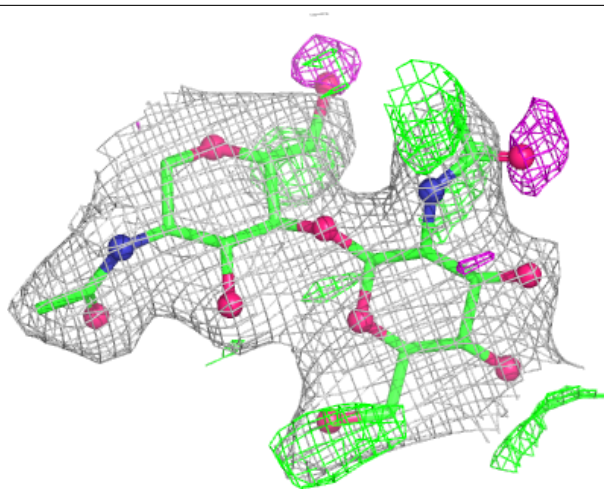
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	F	3	11/12	0.27	0.18	120,125,128,131	0
3	BMA	D	3	11/12	0.51	0.16	102,110,112,114	0
3	NAG	F	2	14/15	0.79	0.14	90,97,107,116	0
2	NAG	C	2	14/15	0.79	0.17	77,85,97,98	0
2	NAG	E	2	14/15	0.80	0.20	68,78,85,94	0
3	NAG	D	2	14/15	0.88	0.12	67,80,87,95	0
3	NAG	F	1	14/15	0.90	0.10	61,73,77,83	0
2	NAG	E	1	14/15	0.91	0.13	44,49,61,67	0
3	NAG	D	1	14/15	0.92	0.10	49,55,63,68	0
2	NAG	C	1	14/15	0.94	0.08	46,53,58,66	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.



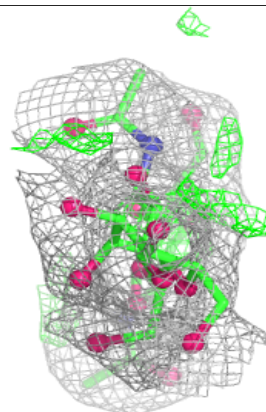
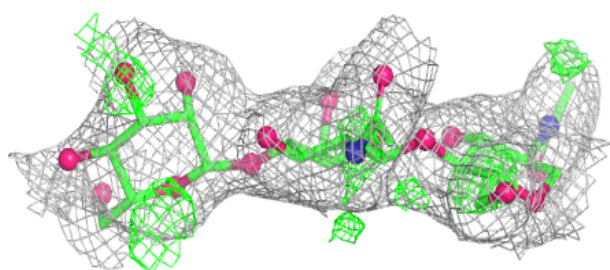
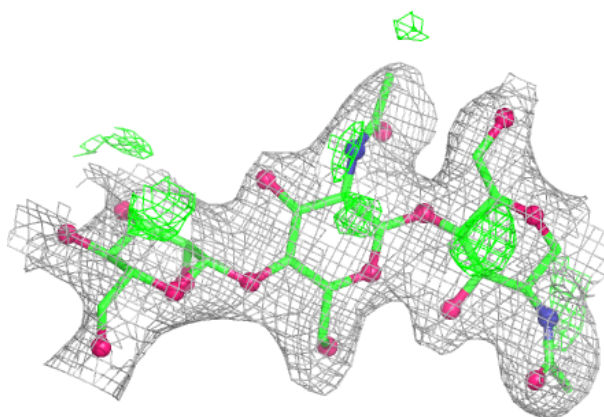
Electron density around Chain E:

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

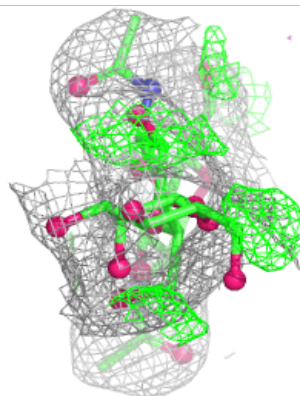
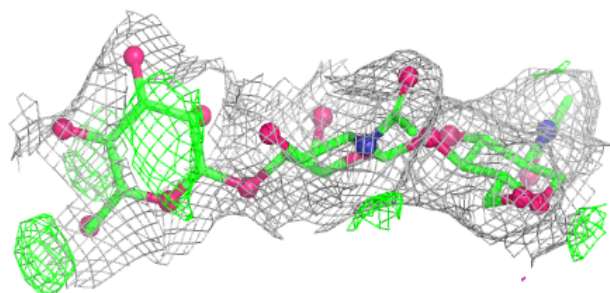
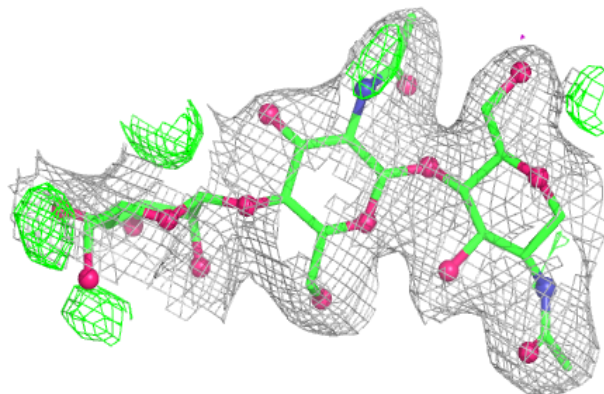


Electron density around Chain D:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	801	14/15	0.64	0.20	100,109,117,118	0
4	NAG	B	807	14/15	0.77	0.17	90,99,106,112	0
4	NAG	A	807	14/15	0.79	0.16	88,96,98,101	0
4	NAG	B	801	14/15	0.80	0.14	95,100,103,105	0
5	CL	A	808	1/1	0.85	0.17	76,76,76,76	0
5	CL	A	809	1/1	0.94	0.16	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.