



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:48 AM BST

PDB ID : 4MSL
Title : Crystal structure of the Vps10p domain of human sortilin/NTS3 in complex with AF40431
Authors : Andersen, J.L.; Strandbygaard, D.; Thirup, S.
Deposited on : 2013-09-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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
buster-report : 1.1.7 (2018)
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

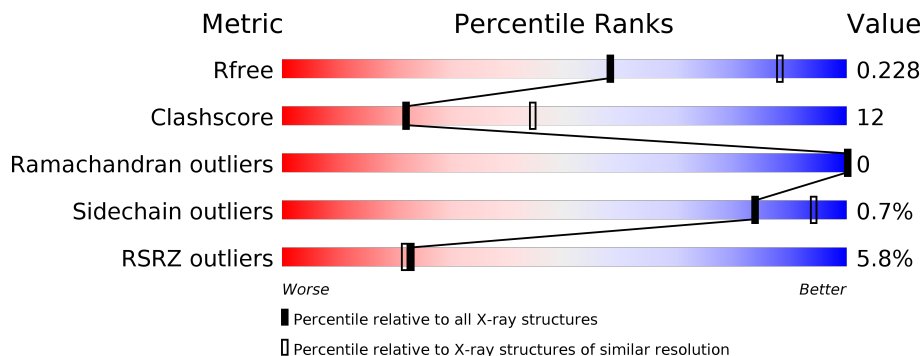
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	696	 5% 72% 22% 6%
2	B	4	 25% 25% 50%
3	C	3	 100%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5335 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	5143	3241	867	1006	29	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	MET	VAL	variant	UNP Q99523
A	724	GLY	-	expression tag	UNP Q99523
A	725	SER	-	expression tag	UNP Q99523
A	726	ALA	-	expression tag	UNP Q99523
A	727	MET	-	expression tag	UNP Q99523
A	728	ILE	-	expression tag	UNP Q99523
A	729	GLU	-	expression tag	UNP Q99523
A	730	GLY	-	expression tag	UNP Q99523
A	731	ARG	-	expression tag	UNP Q99523
A	732	GLY	-	expression tag	UNP Q99523
A	733	VAL	-	expression tag	UNP Q99523
A	734	GLY	-	expression tag	UNP Q99523
A	735	HIS	-	expression tag	UNP Q99523
A	736	HIS	-	expression tag	UNP Q99523
A	737	HIS	-	expression tag	UNP Q99523
A	738	HIS	-	expression tag	UNP Q99523
A	739	HIS	-	expression tag	UNP Q99523
A	740	HIS	-	expression tag	UNP Q99523

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



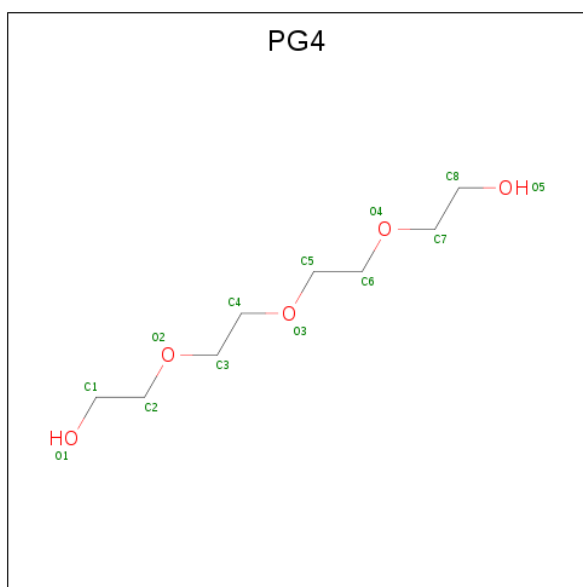
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

- 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.



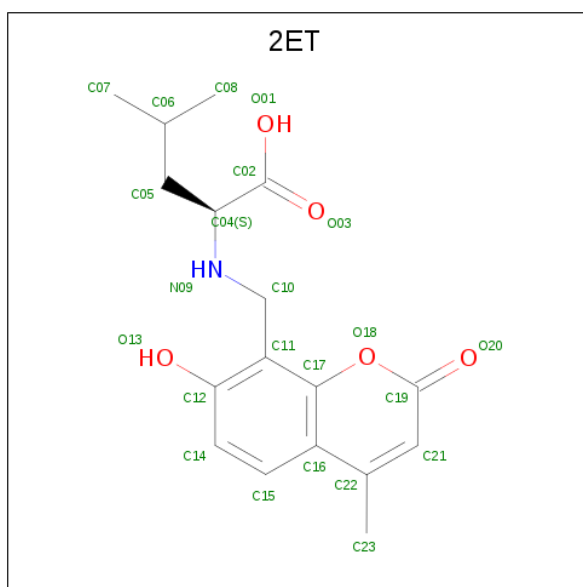
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	39	22	2	15	0	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0

- Molecule 5 is N-[(7-hydroxy-4-methyl-2-oxo-2H-chromen-8-yl)methyl]-L-leucine (three-letter code: 2ET) (formula: C₁₇H₂₁NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	23	17	1	5	0	0

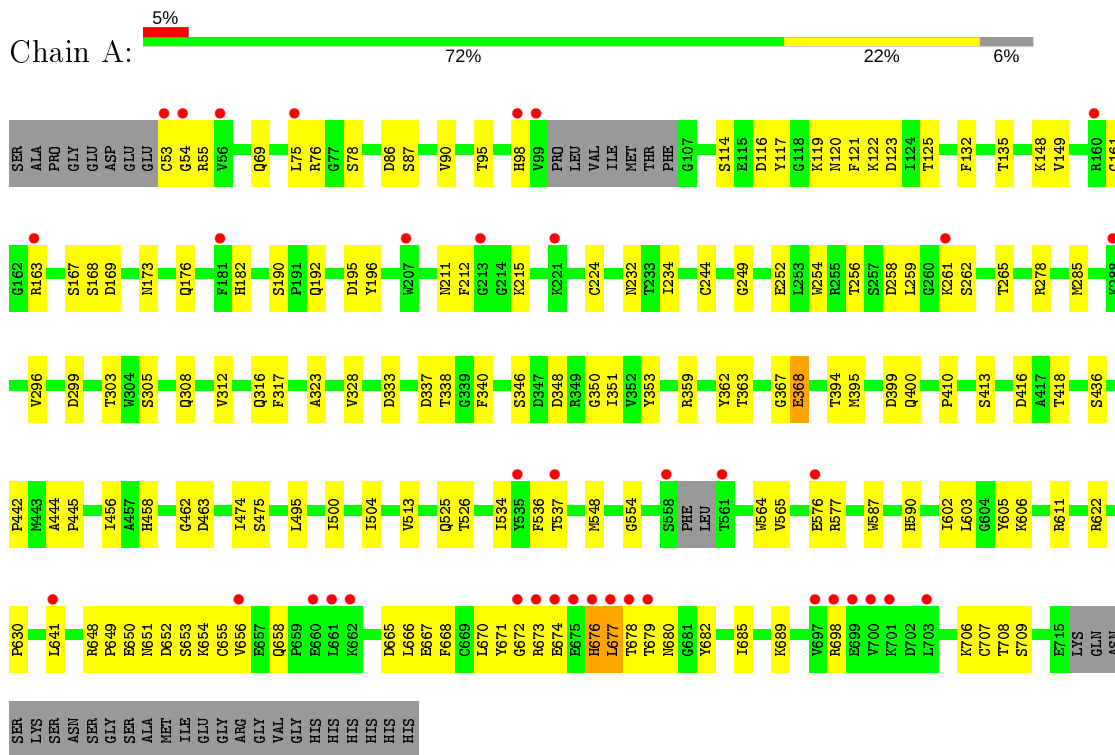
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		

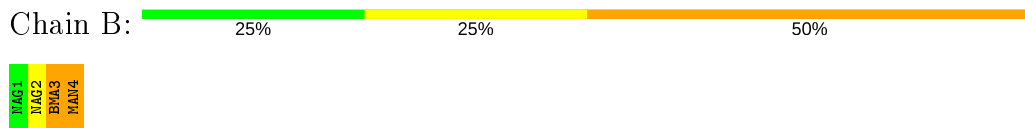
3 Residue-property plots [i](#)

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.

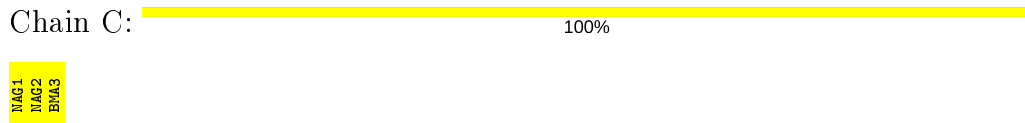
- Molecule 1: Sortilin



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



- Molecule 3: beta-D-mannopyranose-(1-4)-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	160.88Å 79.17Å 111.70Å 90.00° 127.27° 90.00°	Depositor
Resolution (Å)	46.95 – 2.70 46.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.95-2.70) 95.0 (46.95-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.227 0.207 , 0.228	Depositor DCC
R_{free} test set	1543 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtrriage
Anisotropy	0.557	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.8	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	0.94	EDS
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: PG4, BMA, NAG, 2ET, MAN

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	0.47	0/5262	0.65	1/7125 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	677	LEU	CB-CG-CD2	-5.46	101.71	111.00

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	5143	0	4919	119	0
2	B	50	0	43	1	0
3	C	39	0	34	2	0
4	A	13	0	18	0	0
5	A	23	0	19	0	0
6	A	67	0	0	3	0
All	All	5335	0	5033	120	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 (120) 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:75:LEU:HB3	1:A:564:TRP:CD1	1.99	0.96
1:A:75:LEU:HB3	1:A:564:TRP:HD1	1.32	0.95
1:A:75:LEU:HD22	1:A:564:TRP:NE1	1.85	0.91
1:A:416:ASP:OD1	1:A:418:THR:HG22	1.71	0.88
1:A:168:SER:HB3	1:A:212:PHE:CE2	2.12	0.84
1:A:258:ASP:OD2	1:A:261:LYS:HB2	1.81	0.81
1:A:258:ASP:OD2	1:A:261:LYS:CB	2.33	0.77
1:A:368:GLU:OE2	1:A:436:SER:HB2	1.86	0.75
1:A:658:GLN:O	1:A:706:LYS:NZ	2.21	0.74
1:A:258:ASP:CG	1:A:261:LYS:HB2	2.07	0.73
1:A:258:ASP:OD2	1:A:262:SER:N	2.23	0.71
1:A:116:ASP:OD2	1:A:119:LYS:HB2	1.91	0.70
1:A:537:THR:O	1:A:537:THR:HG22	1.90	0.70
1:A:75:LEU:HD22	1:A:564:TRP:CD1	2.26	0.70
1:A:75:LEU:HG	1:A:95:THR:HG21	1.73	0.68
1:A:75:LEU:HD13	1:A:564:TRP:CD1	2.31	0.66
1:A:148:LYS:NZ	1:A:195:ASP:OD1	2.29	0.65
1:A:75:LEU:CB	1:A:564:TRP:HD1	2.08	0.64
1:A:224:CYS:SG	1:A:244:CYS:CB	2.86	0.63
1:A:116:ASP:OD2	1:A:120:ASN:N	2.32	0.63
1:A:650:GLU:CG	1:A:652:ASP:H	2.12	0.63
1:A:368:GLU:OE2	1:A:436:SER:CB	2.48	0.62
1:A:75:LEU:CB	1:A:564:TRP:CD1	2.79	0.62
1:A:548:MET:HG2	3:C:1:NAG:H82	1.82	0.60
1:A:211:ASN:HD21	1:A:215:LYS:HD3	1.66	0.60
1:A:234:ILE:HB	1:A:256:THR:HG22	1.84	0.60
1:A:351:ILE:HD13	1:A:676:HIS:CE1	2.38	0.59
1:A:674:GLU:O	1:A:678:THR:HG22	2.03	0.59
1:A:116:ASP:CG	1:A:119:LYS:HB2	2.24	0.58
1:A:337:ASP:HA	6:A:953:HOH:O	2.04	0.58
1:A:53:CYS:SG	1:A:54:GLY:N	2.76	0.58
1:A:650:GLU:HG2	1:A:652:ASP:H	1.69	0.58
1:A:312:VAL:HB	1:A:316:GLN:HB3	1.87	0.57
1:A:495:LEU:HB2	1:A:500:ILE:HB	1.87	0.57
1:A:410:PRO:HB2	1:A:413:SER:OG	2.05	0.55
1:A:537:THR:O	1:A:537:THR:CG2	2.53	0.55
1:A:652:ASP:OD1	1:A:653:SER:N	2.39	0.55
1:A:418:THR:HG23	1:A:463:ASP:H	1.72	0.55
1:A:305:SER:OG	1:A:673:ARG:HD3	2.08	0.54
1:A:78:SER:OG	1:A:135:THR:HG21	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD12	1:A:554:GLY:HA3	1.89	0.53
1:A:363:THR:O	1:A:367:GLY:HA2	2.09	0.53
1:A:399:ASP:O	1:A:400:GLN:HB3	2.09	0.53
1:A:278:ARG:NH2	1:A:348:ASP:O	2.41	0.53
1:A:338:THR:HB	1:A:340:PHE:CE2	2.44	0.52
1:A:299:ASP:OD2	1:A:303:THR:N	2.43	0.52
1:A:90:VAL:HA	1:A:114:SER:O	2.10	0.52
1:A:312:VAL:HB	1:A:316:GLN:CB	2.40	0.52
1:A:650:GLU:CG	1:A:651:ASN:N	2.73	0.52
1:A:655:CYS:HB2	1:A:682:TYR:CZ	2.45	0.51
1:A:169:ASP:OD2	1:A:173:ASN:N	2.43	0.51
1:A:234:ILE:HB	1:A:256:THR:CG2	2.41	0.51
1:A:668:PHE:O	1:A:672:GLY:N	2.41	0.51
1:A:399:ASP:O	1:A:400:GLN:CB	2.58	0.51
1:A:299:ASP:CG	1:A:303:THR:H	2.15	0.50
1:A:55:ARG:HB3	1:A:525:GLN:NE2	2.26	0.50
1:A:706:LYS:O	1:A:709:SER:HB3	2.11	0.50
1:A:149:VAL:HB	1:A:167:SER:OG	2.12	0.50
1:A:652:ASP:OD2	1:A:654:LYS:CB	2.60	0.50
1:A:456:ILE:HG12	1:A:474:ILE:HG13	1.93	0.50
1:A:513:VAL:HG11	1:A:526:THR:HG23	1.94	0.49
1:A:605:TYR:CD1	1:A:689:LYS:HB2	2.47	0.49
1:A:652:ASP:OD2	1:A:654:LYS:HB2	2.12	0.49
1:A:416:ASP:CG	1:A:418:THR:HG22	2.32	0.49
1:A:648:ARG:HD3	1:A:653:SER:HA	1.95	0.49
1:A:641:LEU:HD23	1:A:685:ILE:HA	1.94	0.49
1:A:116:ASP:O	1:A:117:TYR:HB2	2.12	0.49
1:A:649:PRO:O	1:A:650:GLU:HG2	2.12	0.49
1:A:394:THR:O	1:A:395:MET:HE2	2.13	0.48
1:A:114:SER:OG	1:A:116:ASP:OD1	2.32	0.48
1:A:513:VAL:CG1	1:A:526:THR:HG23	2.43	0.48
1:A:652:ASP:CG	1:A:654:LYS:H	2.17	0.48
1:A:666:LEU:O	1:A:670:LEU:HG	2.14	0.48
1:A:98:HIS:NE2	1:A:132:PHE:HZ	2.12	0.47
1:A:504:ILE:HG21	1:A:536:PHE:CD2	2.50	0.47
1:A:86:ASP:O	1:A:87:SER:HB2	2.13	0.47
1:A:116:ASP:OD1	1:A:119:LYS:N	2.48	0.47
1:A:69:GLN:HE21	1:A:565:VAL:HG21	1.80	0.46
1:A:296:VAL:HG21	1:A:350:GLY:O	2.16	0.46
1:A:442:PRO:HD2	1:A:458:HIS:CE1	2.49	0.46
1:A:75:LEU:HD13	1:A:564:TRP:CG	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLU:O	1:A:671:TYR:HD2	1.99	0.46
1:A:323:ALA:CB	1:A:328:VAL:HG12	2.46	0.46
1:A:650:GLU:HG3	1:A:652:ASP:H	1.81	0.46
1:A:346:SER:HB3	1:A:353:TYR:CE2	2.52	0.45
1:A:76:ARG:HH11	1:A:76:ARG:HG2	1.82	0.45
1:A:606:LYS:O	1:A:630:PRO:HA	2.16	0.45
1:A:161:GLY:C	1:A:182:HIS:CE1	2.90	0.44
1:A:308:GLN:NE2	1:A:665:ASP:OD1	2.50	0.44
1:A:323:ALA:O	6:A:908:HOH:O	2.21	0.44
1:A:252:GLU:HB3	1:A:254:TRP:HE1	1.81	0.44
1:A:680:ASN:OD1	1:A:698:ARG:HG3	2.17	0.44
1:A:123:ASP:OD1	1:A:125:THR:OG1	2.28	0.44
1:A:442:PRO:HD2	1:A:458:HIS:NE2	2.33	0.44
1:A:416:ASP:OD1	1:A:462:GLY:HA3	2.17	0.44
1:A:340:PHE:CD1	1:A:359:ARG:HA	2.53	0.44
1:A:622:ARG:NH1	3:C:1:NAG:O7	2.49	0.43
1:A:254:TRP:CE2	1:A:265:THR:HG22	2.53	0.43
1:A:192:GLN:HB3	1:A:232:ASN:OD1	2.19	0.43
1:A:444:ALA:HB1	1:A:445:PRO:HD2	2.00	0.43
1:A:474:ILE:HG12	1:A:475:SER:N	2.34	0.43
1:A:590:HIS:CG	1:A:602:ILE:HG13	2.54	0.43
1:A:670:LEU:HB2	1:A:671:TYR:CD2	2.54	0.42
1:A:163:ARG:HD3	1:A:176:GLN:HG3	2.02	0.42
1:A:299:ASP:OD2	1:A:303:THR:OG1	2.27	0.42
1:A:649:PRO:HG3	1:A:656:VAL:HG21	2.01	0.42
1:A:116:ASP:CG	1:A:120:ASN:H	2.22	0.42
1:A:190:SER:HB3	1:A:196:TYR:HB2	2.00	0.42
1:A:677:LEU:HD12	1:A:678:THR:N	2.35	0.42
1:A:121:PHE:O	1:A:122:LYS:HD2	2.18	0.42
1:A:148:LYS:HD2	1:A:212:PHE:CE1	2.55	0.42
2:B:3:BMA:H62	2:B:4:MAN:H2	1.65	0.42
1:A:576:GLU:HG3	1:A:577:ARG:N	2.34	0.41
1:A:708:THR:O	6:A:919:HOH:O	2.22	0.41
1:A:399:ASP:O	1:A:603:LEU:HD11	2.20	0.41
1:A:249:GLY:HA3	1:A:285:MET:HE3	2.01	0.41
1:A:317:PHE:H	1:A:333:ASP:HB3	1.86	0.40
1:A:258:ASP:O	1:A:259:LEU:HB2	2.21	0.40
1:A:587:TRP:CE3	1:A:611:ARG:HD2	2.55	0.40
1:A:679:THR:OG1	1:A:680:ASN:N	2.55	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	648/696 (93%)	634 (98%)	14 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	570/605 (94%)	566 (99%)	4 (1%)	84 94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	TYR
1	A	368	GLU
1	A	676	HIS
1	A	707	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN

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](#)

7 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	B	1	1,2	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	B	2	2	14,14,15	1.11	1 (7%)	17,19,21	0.72	1 (5%)
2	BMA	B	3	2	11,11,12	0.82	1 (9%)	15,15,17	1.02	0
2	MAN	B	4	2	11,11,12	1.26	2 (18%)	15,15,17	1.22	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.52	0	17,19,21	0.73	0
3	NAG	C	2	3	14,14,15	0.65	1 (7%)	17,19,21	0.51	0
3	BMA	C	3	3	11,11,12	1.35	2 (18%)	15,15,17	1.49	3 (20%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-4.04	1.37	1.43
3	C	3	BMA	C2-C3	2.87	1.56	1.52
2	B	4	MAN	C4-C3	2.11	1.57	1.52
3	C	2	NAG	O5-C1	-2.10	1.40	1.43
3	C	3	BMA	C4-C3	2.09	1.57	1.52
2	B	4	MAN	C4-C5	2.09	1.57	1.53
2	B	3	BMA	C4-C5	2.06	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	3.09	116.38	112.19
2	B	4	MAN	C1-O5-C5	2.61	115.72	112.19
3	C	3	BMA	C2-C3-C4	2.55	115.31	110.89
3	C	3	BMA	O2-C2-C3	-2.33	105.47	110.14
2	B	2	NAG	O4-C4-C5	-2.01	104.30	109.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

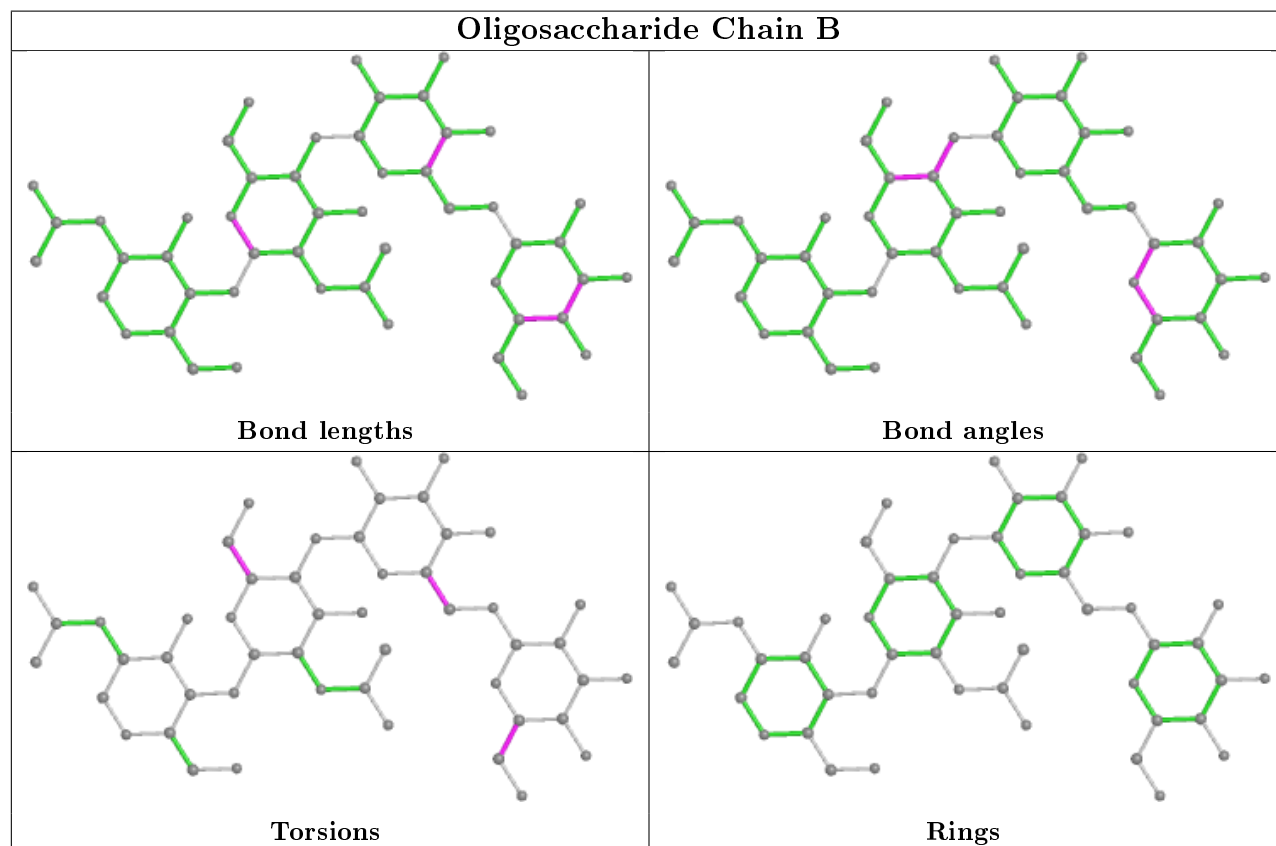
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

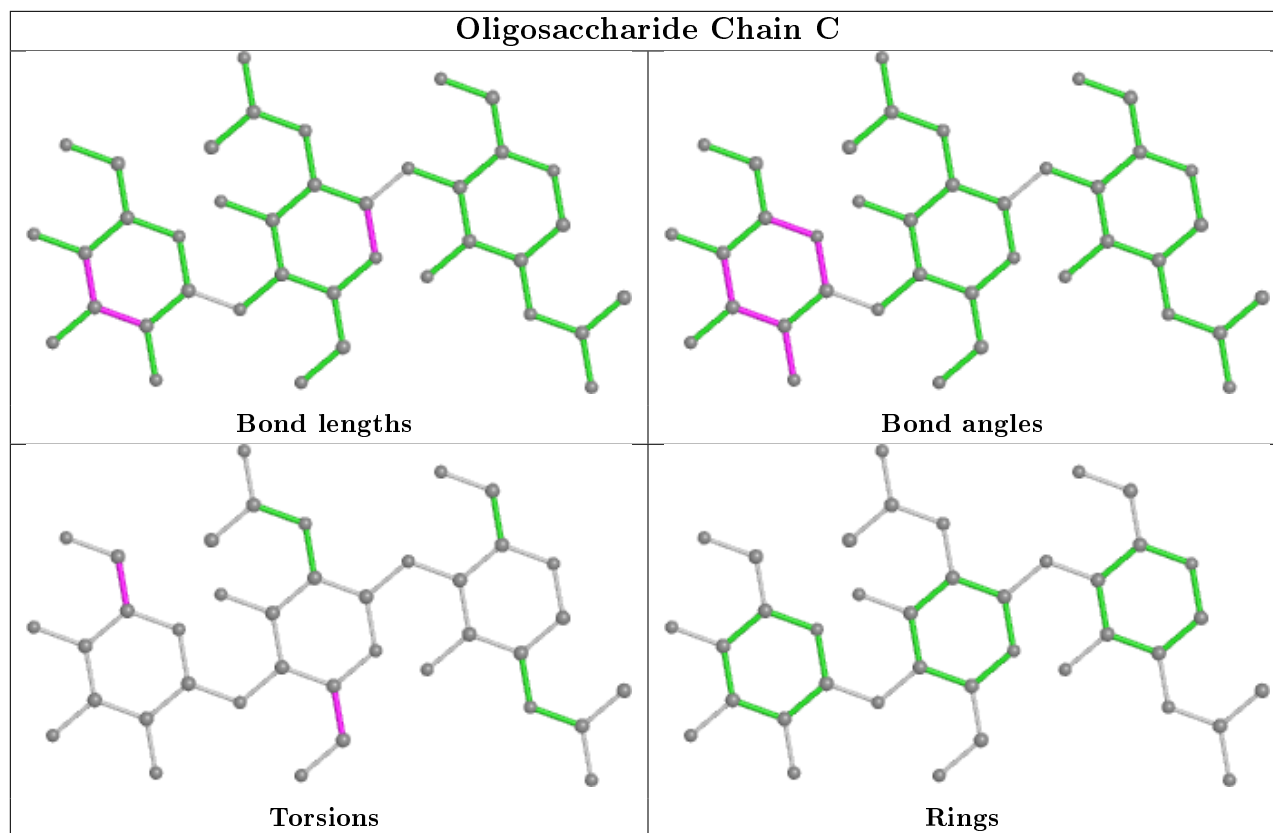
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	2	0
2	B	3	BMA	1	0
2	B	4	MAN	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	$\# Z > 2$
5	2ET	A	809	-	18,24,24	2.33	6 (33%)	23,34,34	1.32	5 (21%)
4	PG4	A	808	-	12,12,12	0.50	0	11,11,11	1.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2ET	A	809	-	-	4/9/13/13	0/2/2/2
4	PG4	A	808	-	-	5/10/10/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	809	2ET	O18-C17	6.22	1.47	1.36
5	A	809	2ET	C21-C19	4.88	1.47	1.37
5	A	809	2ET	C22-C16	2.99	1.49	1.42
5	A	809	2ET	C12-C11	2.40	1.40	1.38
5	A	809	2ET	C10-C11	2.26	1.55	1.50
5	A	809	2ET	C05-C04	-2.04	1.52	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	809	2ET	C14-C12-C11	-2.93	119.75	121.48
5	A	809	2ET	O18-C17-C11	2.53	119.18	116.17
5	A	809	2ET	C15-C16-C17	2.23	119.08	116.50
5	A	809	2ET	C21-C22-C16	2.07	119.81	117.78
5	A	809	2ET	C11-C10-N09	2.04	117.39	111.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

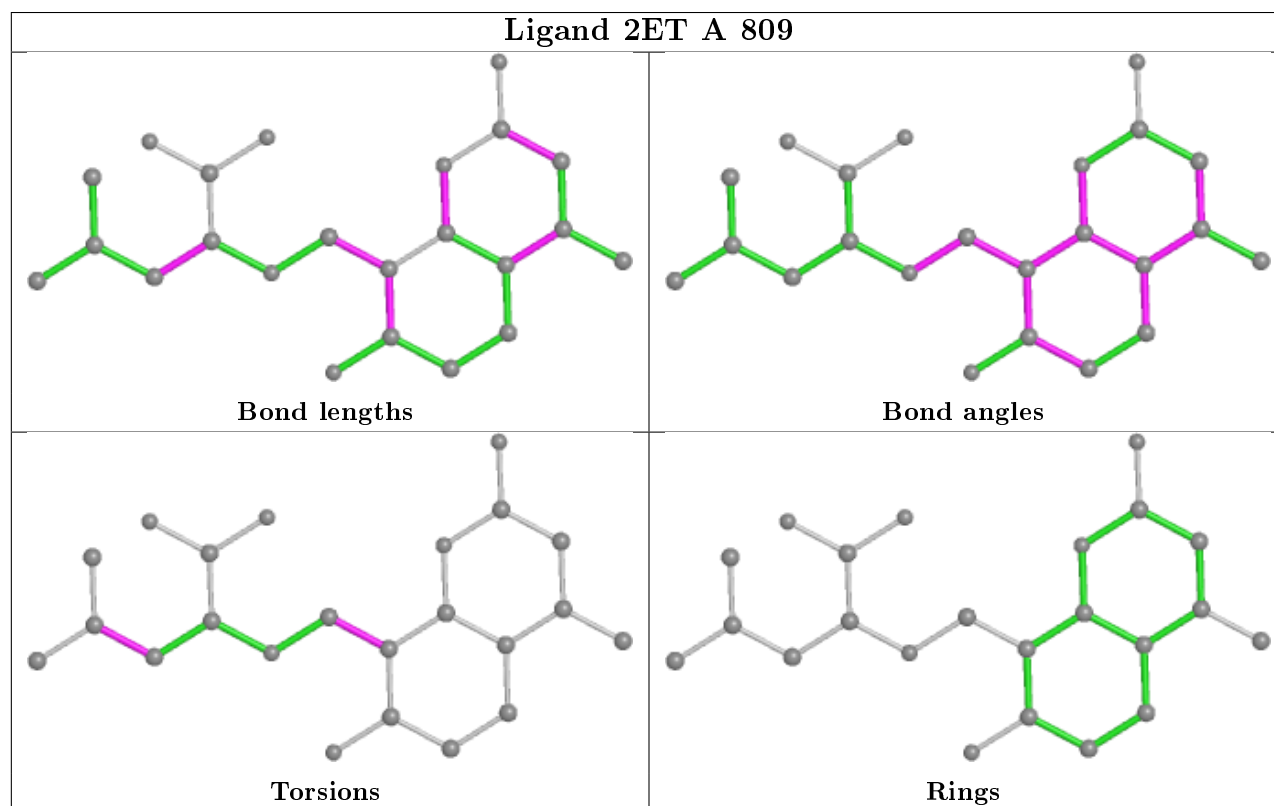
Mol	Chain	Res	Type	Atoms
5	A	809	2ET	N09-C10-C11-C17
5	A	809	2ET	N09-C10-C11-C12
4	A	808	PG4	C8-C7-O4-C6
4	A	808	PG4	O1-C1-C2-O2
4	A	808	PG4	C4-C3-O2-C2
4	A	808	PG4	O3-C5-C6-O4
5	A	809	2ET	C04-C05-C06-C08
4	A	808	PG4	O4-C7-C8-O5
5	A	809	2ET	C04-C05-C06-C07

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	654/696 (93%)	0.47	38 (5%) 23 22	48, 94, 157, 223	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	LEU	7.0
1	A	675	GLU	6.0
1	A	699	GLU	4.5
1	A	697	VAL	4.4
1	A	703	LEU	4.3
1	A	98	HIS	4.2
1	A	700	VAL	3.9
1	A	661	LEU	3.8
1	A	677	LEU	3.5
1	A	99	VAL	3.5
1	A	656	VAL	3.4
1	A	660	GLU	3.4
1	A	53	CYS	3.3
1	A	561	THR	3.3
1	A	160	ARG	3.3
1	A	181	PHE	3.0
1	A	676	HIS	2.9
1	A	672	GLY	2.9
1	A	641	LEU	2.8
1	A	698	ARG	2.8
1	A	674	GLU	2.7
1	A	662	LYS	2.7
1	A	673	ARG	2.5
1	A	679	THR	2.5
1	A	537	THR	2.5
1	A	678	THR	2.5
1	A	56	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	TRP	2.4
1	A	54	GLY	2.4
1	A	535	TYR	2.3
1	A	701	LYS	2.3
1	A	576	GLU	2.3
1	A	213	GLY	2.2
1	A	288	LYS	2.2
1	A	221	LYS	2.1
1	A	163	ARG	2.1
1	A	558	SER	2.1
1	A	261	LYS	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](#)

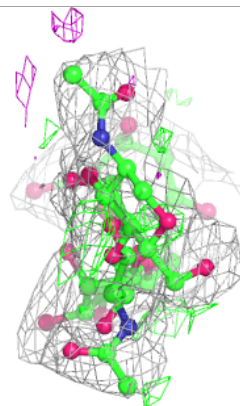
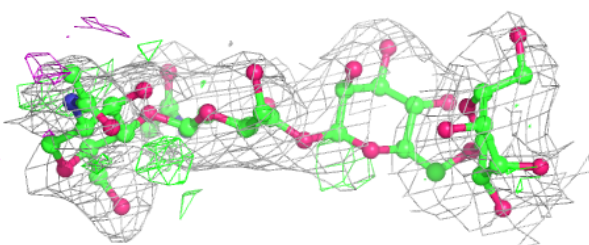
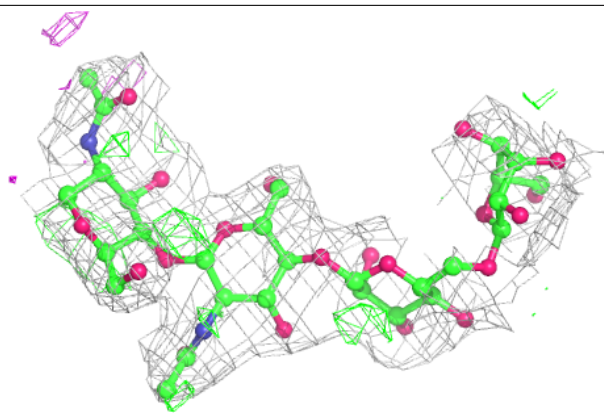
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	3	11/12	0.71	0.23	170,170,170,170	0
2	BMA	B	3	11/12	0.80	0.18	139,139,139,139	0
2	MAN	B	4	11/12	0.85	0.17	142,142,142,142	0
2	NAG	B	2	14/15	0.93	0.21	84,84,84,84	0
3	NAG	C	2	14/15	0.94	0.10	103,103,103,103	0
3	NAG	C	1	14/15	0.94	0.12	83,83,83,83	0
2	NAG	B	1	14/15	0.97	0.22	51,51,51,51	0

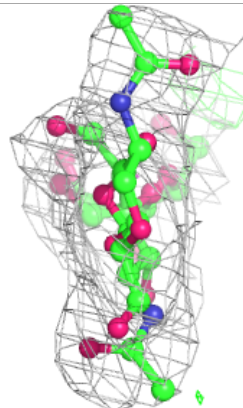
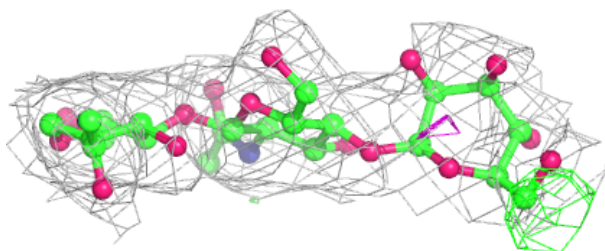
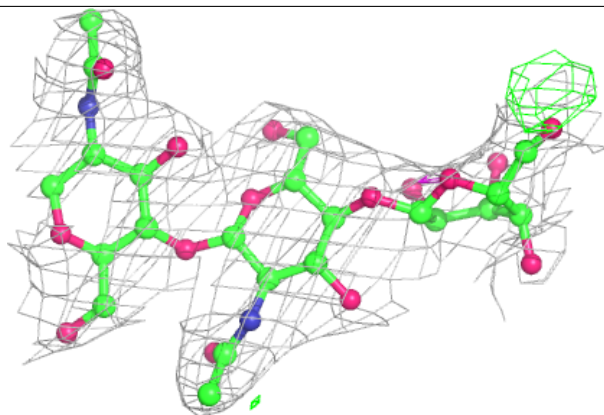
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**Electron density around Chain C:**

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

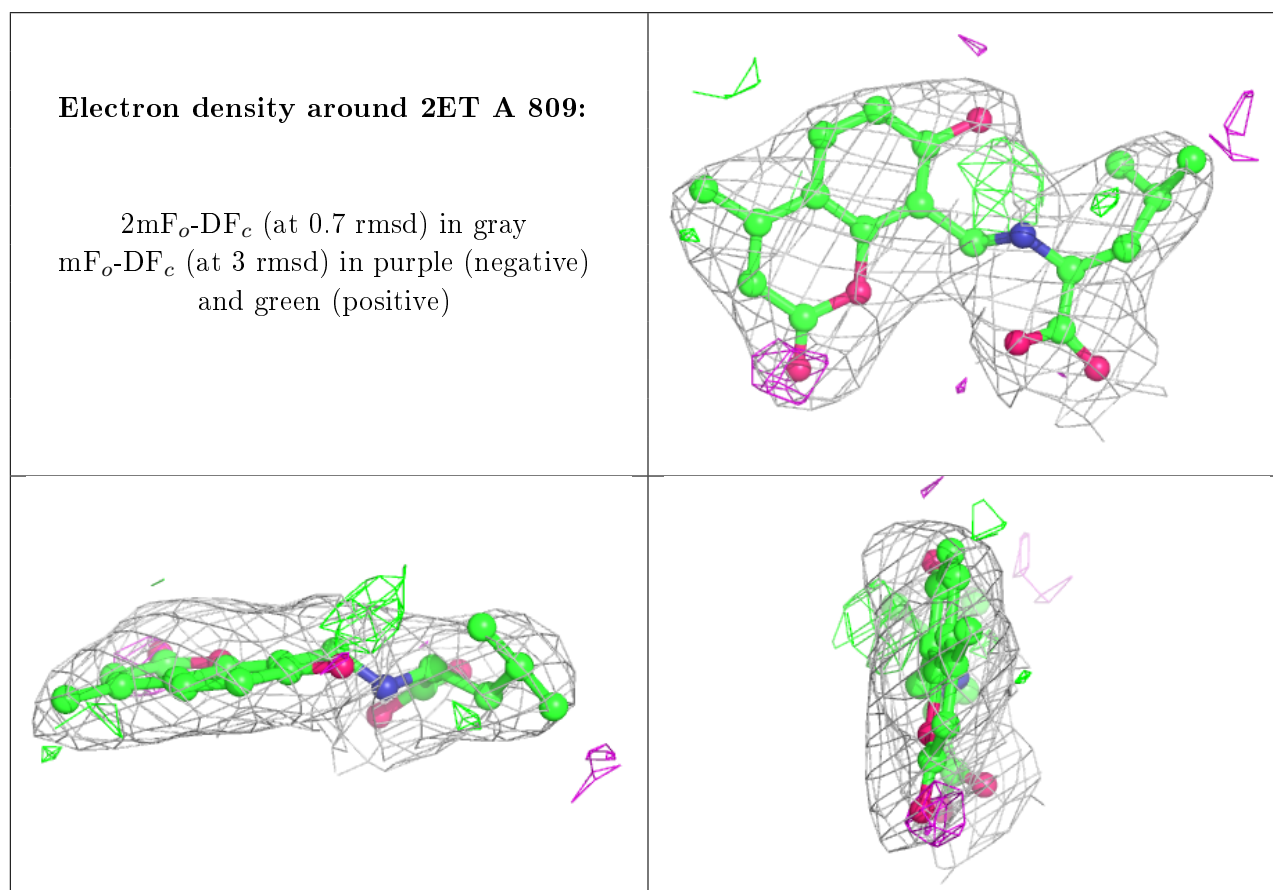


6.4 Ligands [i](#)

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	PG4	A	808	13/13	0.80	0.26	104,104,104,104	0
5	2ET	A	809	23/23	0.94	0.21	63,63,63,63	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.