



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:29 PM BST

PDB ID : 6X3L
Title : Sortilin-Progranulin Interaction With Compound 2
Authors : Parthasarathy, G.; Soisson, S.M.
Deposited on : 2020-05-21
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

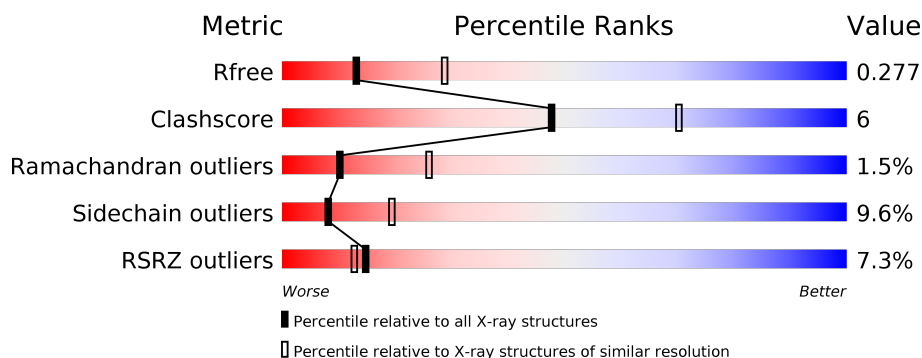
1 Overall quality at a glance

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	762	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>•</div> <div>14%</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
2	C	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5248 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 7 discrepancies between the modelled and reference sequences:

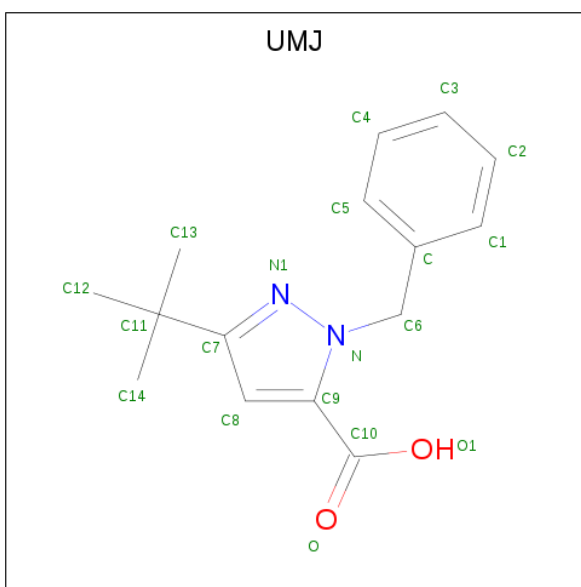
Chain	Residue	Modelled	Actual	Comment	Reference
A	617	MET	VAL	conflict	UNP Q99523
A	724	HIS	-	expression tag	UNP Q99523
A	725	HIS	-	expression tag	UNP Q99523
A	726	HIS	-	expression tag	UNP Q99523
A	727	HIS	-	expression tag	UNP Q99523
A	728	HIS	-	expression tag	UNP Q99523
A	729	HIS	-	expression tag	UNP Q99523

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



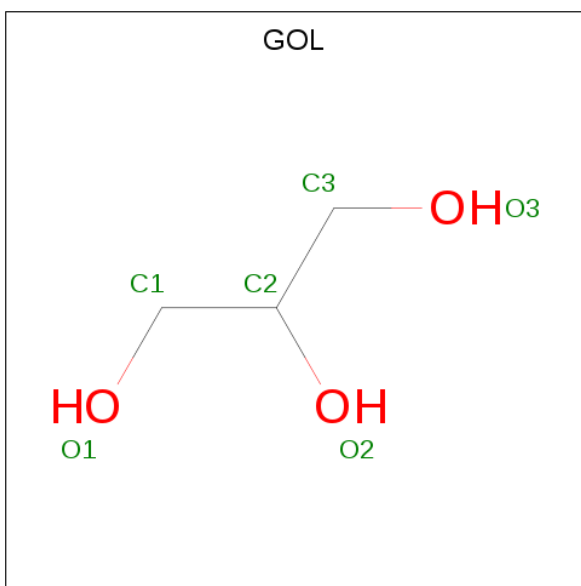
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is 1-benzyl-3-tert-butyl-1H-pyrazole-5-carboxylic acid (three-letter code: UMJ) (formula: C₁₅H₁₈N₂O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	19	15	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total 24	O 24	0	0

Chain C:

100%

RMS1
RMS2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.83Å 75.51Å 110.98Å 90.00° 127.01° 90.00°	Depositor
Resolution (Å)	46.24 – 2.70 44.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.24-2.70) 98.6 (44.31-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.217 , 0.269 0.225 , 0.277	Depositor DCC
R_{free} test set	1488 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	74.3	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: GOL, NAG, UMJ

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	0/5262	0.77	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	679	THR	C-N-CA	5.21	134.73	121.70

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	4933	59	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	A	19	0	0	0	0
4	A	6	0	8	0	0
5	A	24	0	0	1	0
All	All	5248	0	4991	59	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 6.

All (59) 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:416:ASP:OD1	1:A:418:THR:HG22	1.46	1.13
1:A:415:CYS:HG	1:A:425:CYS:HG	0.81	0.80
1:A:642:CYS:HG	1:A:655:CYS:HG	0.83	0.80
1:A:669:CYS:SG	1:A:707:CYS:HB3	2.24	0.77
1:A:650:GLU:HG2	1:A:651:ASN:H	1.52	0.74
1:A:540:ALA:HB3	1:A:551:SER:HB2	1.74	0.70
1:A:679:THR:HA	1:A:680:ASN:HB2	1.77	0.67
1:A:75:LEU:HD21	1:A:79:VAL:HG21	1.77	0.66
1:A:321:LEU:HD11	1:A:331:HIS:HB2	1.82	0.61
1:A:377:LEU:HD11	1:A:589:ALA:HB1	1.84	0.59
1:A:515:LYS:HG2	1:A:526:THR:HG23	1.85	0.59
1:A:75:LEU:HD22	1:A:564:TRP:CG	2.38	0.59
1:A:442:PRO:HD2	1:A:458:HIS:CE1	2.39	0.58
1:A:418:THR:HG23	1:A:463:ASP:H	1.70	0.57
1:A:206:LEU:HD23	1:A:219:ILE:HD11	1.88	0.56
1:A:519:ASP:OD2	1:A:522:GLN:HB3	2.08	0.54
1:A:75:LEU:HD22	1:A:564:TRP:CD1	2.43	0.53
1:A:75:LEU:CD2	1:A:79:VAL:HG21	2.38	0.53
1:A:410:PRO:HB2	1:A:413:SER:HB2	1.92	0.51
1:A:650:GLU:HG2	1:A:651:ASN:N	2.24	0.51
1:A:312:VAL:HB	1:A:316:GLN:HB2	1.92	0.51
1:A:323:ALA:CB	1:A:328:VAL:HG12	2.41	0.50
1:A:647:TYR:CE1	1:A:656:VAL:HG23	2.47	0.50
1:A:495:LEU:HB2	1:A:500:ILE:HB	1.94	0.50
1:A:458:HIS:CD2	1:A:472:VAL:HG22	2.47	0.49
1:A:286:ALA:HB3	1:A:289:ASP:HB3	1.94	0.49
1:A:650:GLU:CG	1:A:651:ASN:H	2.25	0.48
1:A:387:SER:HB2	1:A:393:GLN:OE1	2.12	0.48
1:A:510:PRO:HD3	1:A:535:TYR:CZ	2.50	0.47
1:A:646:TYR:CD1	1:A:681:GLY:HA2	2.50	0.47
1:A:493:THR:HG22	1:A:539:LEU:HD13	1.96	0.47
1:A:206:LEU:HB2	1:A:223:VAL:HG21	1.96	0.47
1:A:535:TYR:HE2	1:A:557:GLU:HG3	1.79	0.46
1:A:681:GLY:HA3	1:A:698:ARG:HH11	1.81	0.46
1:A:684:LYS:HE2	1:A:690:CYS:SG	2.55	0.46
1:A:96:THR:HG22	1:A:109:SER:OG	2.16	0.46
1:A:74:ASP:HB2	1:A:110:LYS:HE2	1.97	0.46
1:A:536:PHE:HZ	1:A:539:LEU:HG	1.81	0.45
1:A:606:LYS:O	1:A:630:PRO:HA	2.17	0.45
1:A:122:LYS:O	1:A:124:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:GLN:HB2	1:A:608:GLN:HE21	1.59	0.45
1:A:349:ARG:HB3	1:A:351:ILE:HD12	1.98	0.45
1:A:649:PRO:HD3	1:A:656:VAL:HG22	1.99	0.45
1:A:258:ASP:HB2	1:A:261:LYS:HD3	1.99	0.44
1:A:198:LEU:HD23	1:A:228:TRP:CE2	2.52	0.44
1:A:550:ILE:O	1:A:568:THR:HA	2.18	0.44
1:A:601:CYS:SG	1:A:633:CYS:CB	3.04	0.44
1:A:703:LEU:C	1:A:705:LYS:H	2.22	0.44
1:A:190:SER:HB3	1:A:193:ASN:O	2.18	0.43
1:A:604:GLY:CA	1:A:690:CYS:HB3	2.47	0.43
1:A:493:THR:HG21	1:A:550:ILE:HD13	2.01	0.43
1:A:539:LEU:HB3	1:A:550:ILE:HD11	2.01	0.43
1:A:293:ARG:HB2	5:A:909:HOH:O	2.18	0.42
1:A:408:ARG:HH11	1:A:408:ARG:HB3	1.85	0.42
1:A:258:ASP:CG	1:A:261:LYS:HB2	2.40	0.41
1:A:140:ALA:HB3	1:A:150:VAL:HB	2.02	0.41
1:A:435:ILE:HG13	1:A:441:VAL:HB	2.03	0.41
1:A:604:GLY:HA3	1:A:690:CYS:HB3	2.03	0.40
1:A:416:ASP:OD1	1:A:418:THR:CG2	2.40	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	648/762 (85%)	590 (91%)	48 (7%)	10 (2%)	10	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	A	222	ALA

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	363	THR
1	A	242	GLY
1	A	336	GLY
1	A	337	ASP
1	A	367	GLY
1	A	221	LYS
1	A	700	VAL

5.3.2 Protein sidechains ⓘ

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	570/655 (87%)	515 (90%)	55 (10%)	8 19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	71	VAL
1	A	73	ASP
1	A	74	ASP
1	A	76	ARG
1	A	95	THR
1	A	109	SER
1	A	122	LYS
1	A	126	ASP
1	A	127	LEU
1	A	135	THR
1	A	156	SER
1	A	176	GLN
1	A	195	ASP
1	A	200	LEU
1	A	224	CYS
1	A	238	THR
1	A	257	SER

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Mol	Chain	Res	Type
1	A	269	LYS
1	A	283	SER
1	A	287	ASP
1	A	298	THR
1	A	305	SER
1	A	308	GLN
1	A	325	ASP
1	A	334	GLU
1	A	361	LEU
1	A	362	TYR
1	A	382	ILE
1	A	403	ARG
1	A	405	THR
1	A	408	ARG
1	A	413	SER
1	A	423	ASN
1	A	432	SER
1	A	438	LYS
1	A	450	ASN
1	A	460	SER
1	A	493	THR
1	A	513	VAL
1	A	526	THR
1	A	537	THR
1	A	541	SER
1	A	576	GLU
1	A	592	THR
1	A	608	GLN
1	A	628	LYS
1	A	631	SER
1	A	650	GLU
1	A	661	LEU
1	A	665	ASP
1	A	673	ARG
1	A	683	ARG
1	A	685	ILE
1	A	713	SER

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	440	ASN

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Mol	Chain	Res	Type
1	A	506	HIS
1	A	608	GLN

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	B	1	1,2	14,14,15	0.34	0	17,19,21	0.67	0
2	NAG	B	2	2	14,14,15	0.36	0	17,19,21	0.73	0
2	NAG	C	1	1,2	14,14,15	0.27	0	17,19,21	0.71	1 (5%)
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	1.16	3 (17%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C1-C2	-2.74	106.95	111.29
2	C	2	NAG	C1-O5-C5	2.63	115.76	112.19
2	C	1	NAG	C1-O5-C5	2.54	115.63	112.19
2	C	2	NAG	C1-C2-N2	2.38	114.56	110.49

There are no chirality outliers.

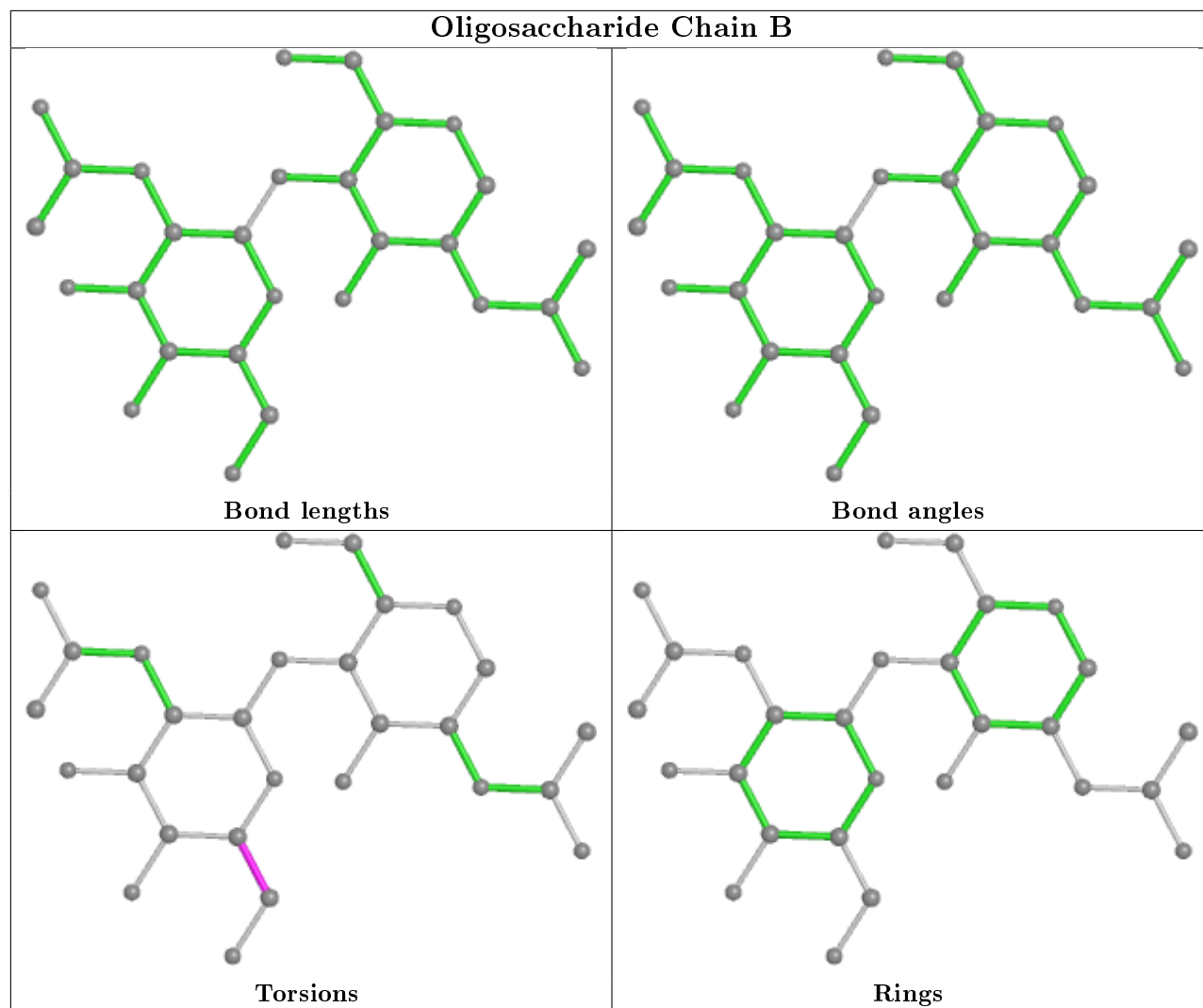
All (4) torsion outliers are listed below:

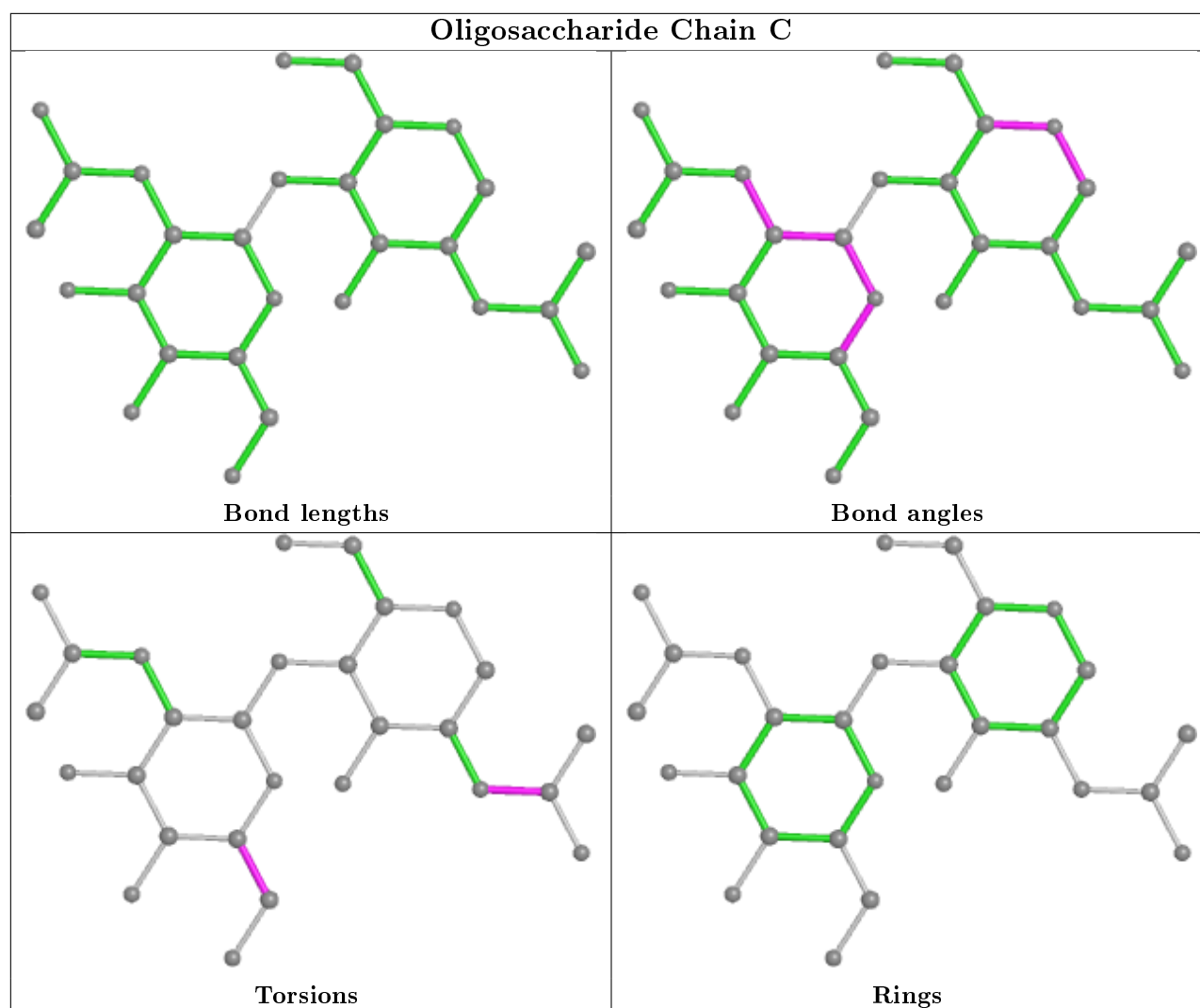
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2

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 [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	UMJ	A	805	-	16,20,20	0.40	0	21,29,29	0.33	0
4	GOL	A	806	-	5,5,5	0.27	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UMJ	A	805	-	-	0/10/14/14	0/2/2/2
4	GOL	A	806	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

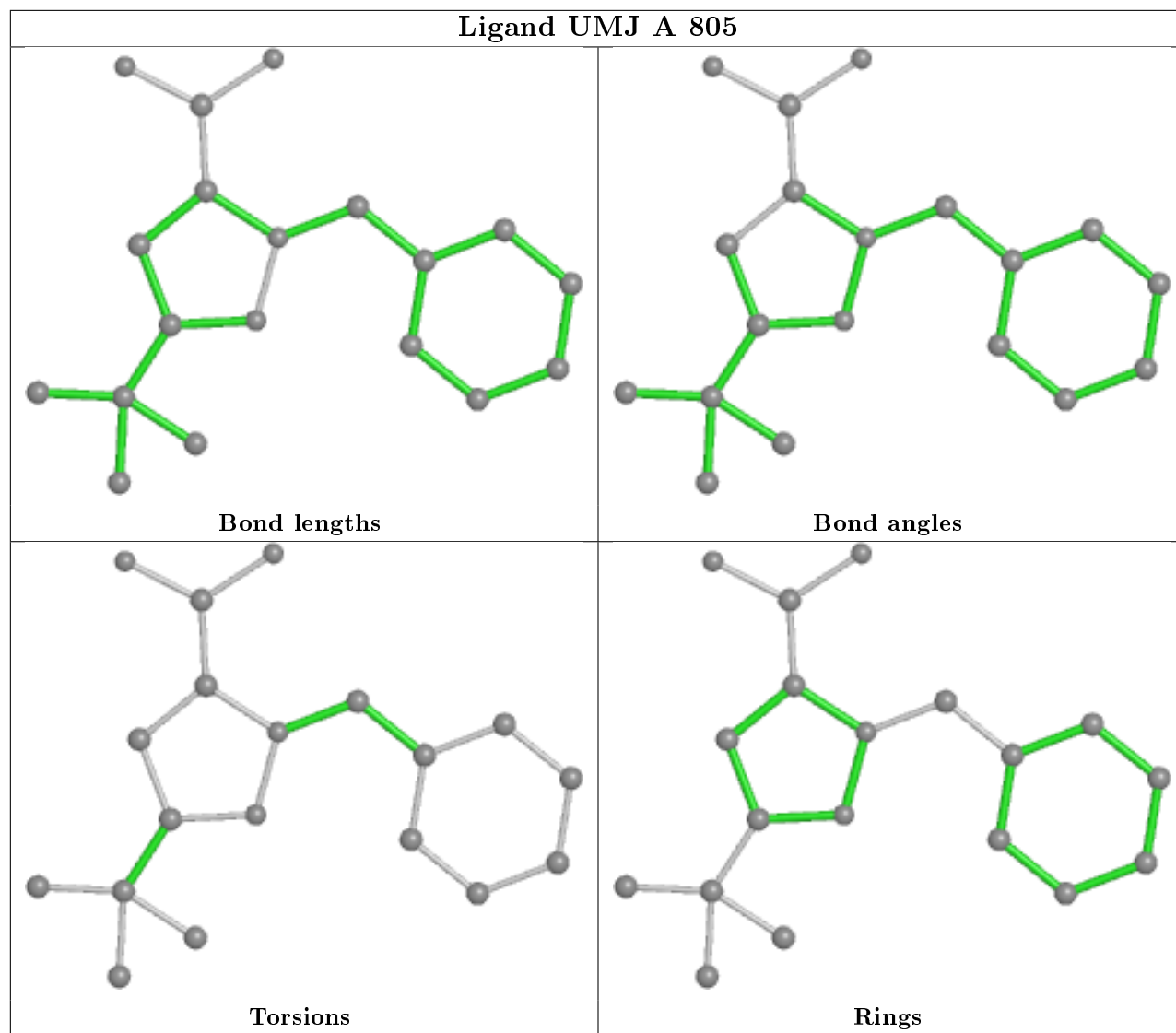
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	O1-C1-C2-C3

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	654/762 (85%)	0.56	48 (7%) 15 13	53, 95, 134, 161	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	LEU	7.1
1	A	75	LEU	7.0
1	A	697	VAL	5.7
1	A	54	GLY	5.3
1	A	675	GLU	5.0
1	A	73	ASP	4.9
1	A	53	CYS	4.2
1	A	165	PHE	3.9
1	A	564	TRP	3.9
1	A	563	GLN	3.7
1	A	676	HIS	3.6
1	A	181	PHE	3.3
1	A	366	GLY	3.3
1	A	698	ARG	3.2
1	A	661	LEU	3.0
1	A	574	ILE	3.0
1	A	660	GLU	3.0
1	A	671	TYR	3.0
1	A	637	LEU	2.9
1	A	701	LYS	2.9
1	A	160	ARG	2.9
1	A	56	VAL	2.9
1	A	673	ARG	2.9
1	A	249	GLY	2.8
1	A	668	PHE	2.7
1	A	99	VAL	2.7
1	A	575	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	535	TYR	2.6
1	A	200	LEU	2.6
1	A	650	GLU	2.6
1	A	288	LYS	2.5
1	A	699	GLU	2.5
1	A	531	ARG	2.5
1	A	208	VAL	2.5
1	A	617	MET	2.4
1	A	565	VAL	2.4
1	A	694	VAL	2.4
1	A	656	VAL	2.3
1	A	213	GLY	2.3
1	A	132	PHE	2.3
1	A	576	GLU	2.2
1	A	679	THR	2.2
1	A	59	PHE	2.2
1	A	216	TRP	2.2
1	A	74	ASP	2.1
1	A	567	TYR	2.1
1	A	158	GLY	2.1
1	A	711	PHE	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 ⓘ

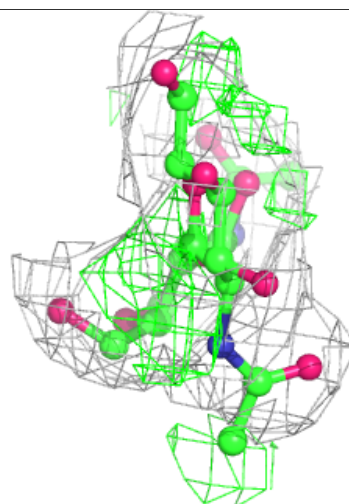
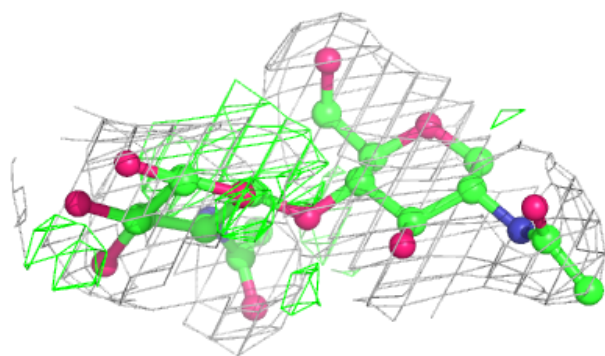
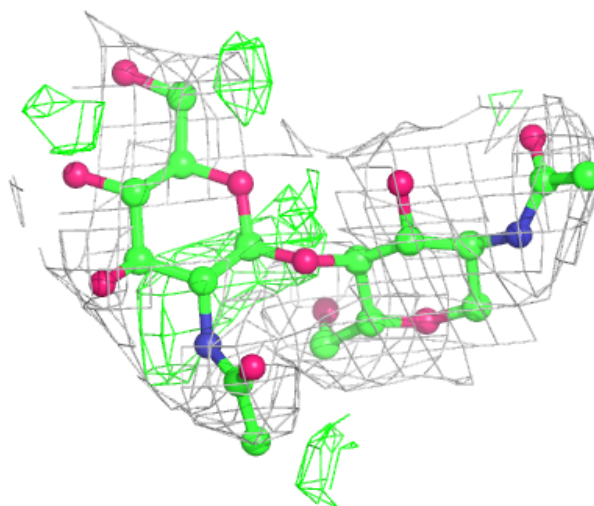
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

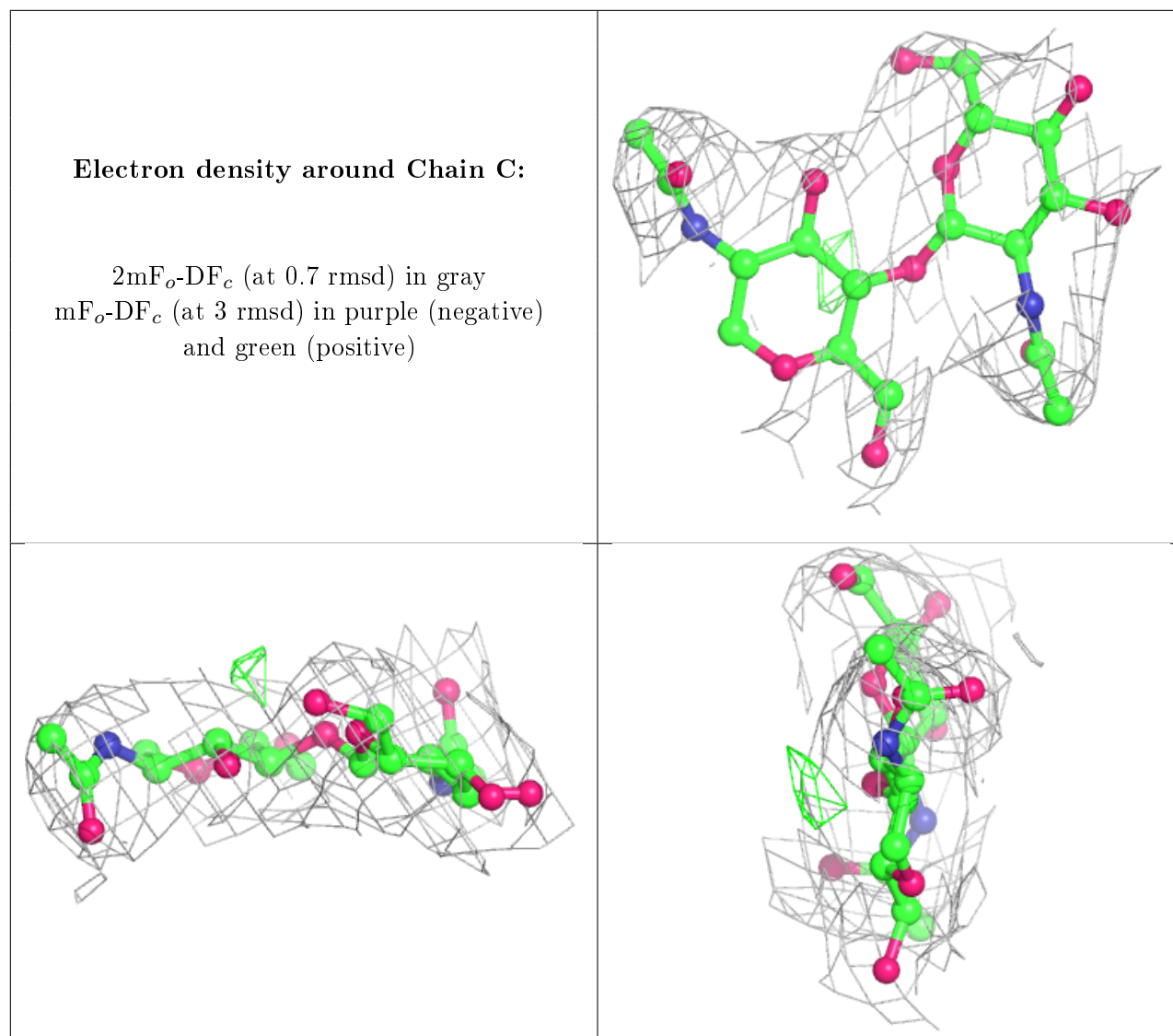
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.92	0.11	106,109,113,116	0
2	NAG	B	1	14/15	0.94	0.30	59,64,69,73	0
2	NAG	B	2	14/15	0.94	0.35	84,95,107,108	0
2	NAG	C	1	14/15	0.95	0.15	82,95,97,101	0

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)



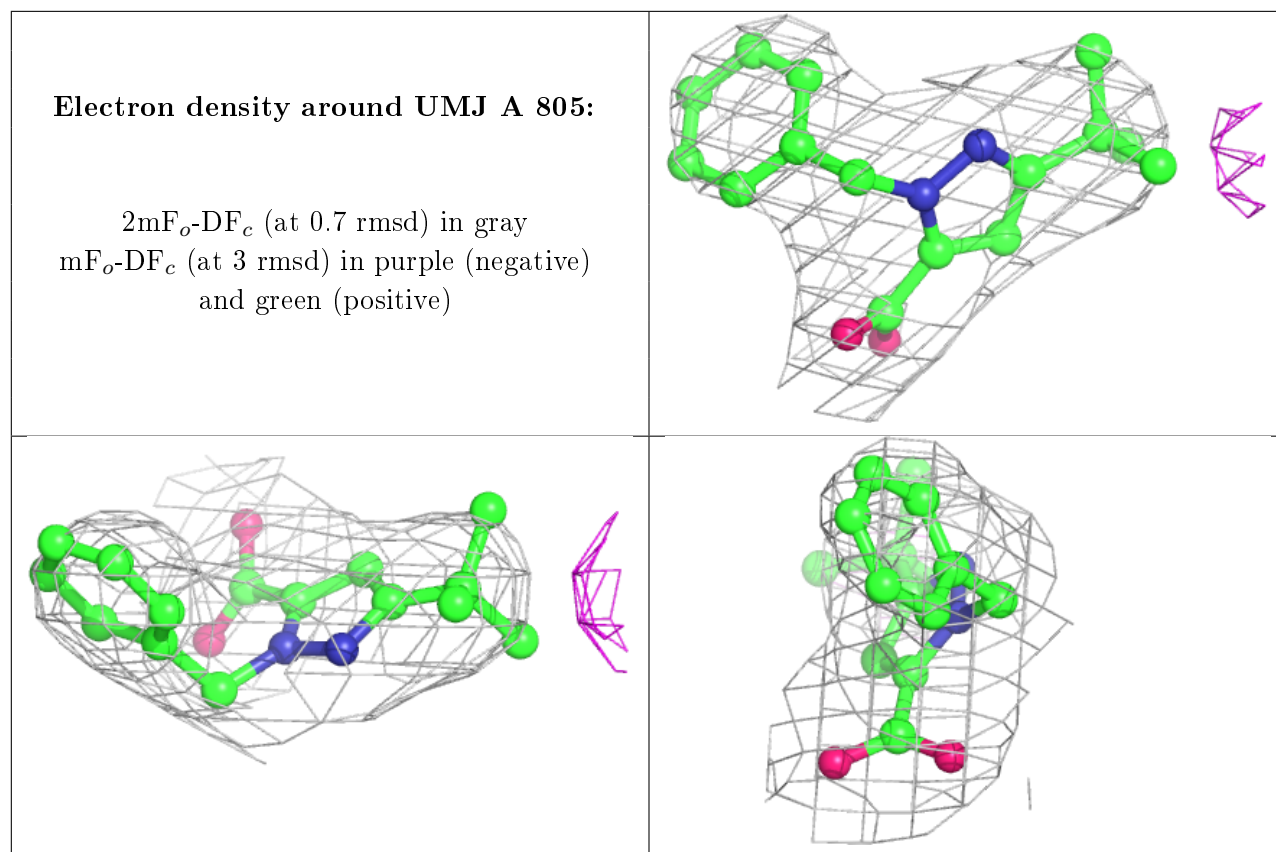


6.4 Ligands ⓘ

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
4	GOL	A	806	6/6	0.65	0.32	98,101,105,106	0
3	UMJ	A	805	19/19	0.93	0.27	81,83,94,96	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.