



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:45 AM UTC

PDB ID : 5J68 / pdb_00005j68
Title : Structure of Astrotactin-2, a conserved vertebrate-specific and perforin-like membrane protein involved in neuronal development
Authors : Ni, T.; Harlos, K.; Gilbert, R.J.C.
Deposited on : 2016-04-04
Resolution : 5.22 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

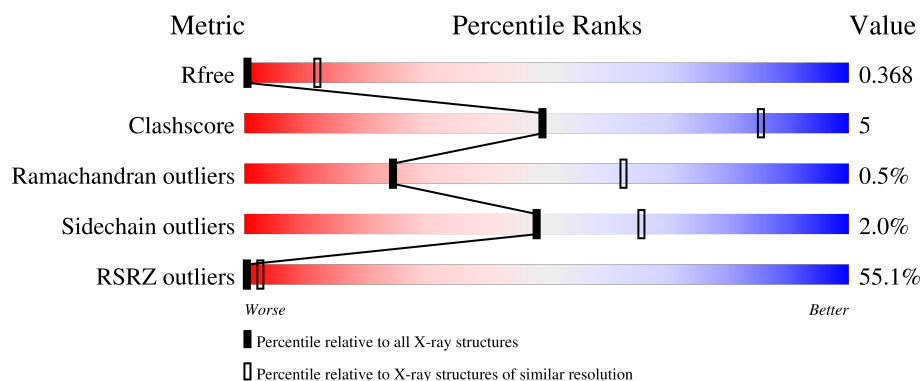
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.22 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	1012 (6.42-4.00)
Clashscore	190562	1067 (6.42-4.00)
Ramachandran outliers	187476	1023 (6.50-3.94)
Sidechain outliers	187428	1024 (6.50-3.92)
RSRZ outliers	180081	1007 (6.42-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	572	
2	B	10	

2 Entry composition [i](#)

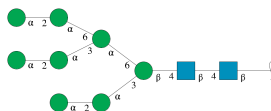
There are 4 unique types of molecules in this entry. The entry contains 4610 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Astrotactin-2.

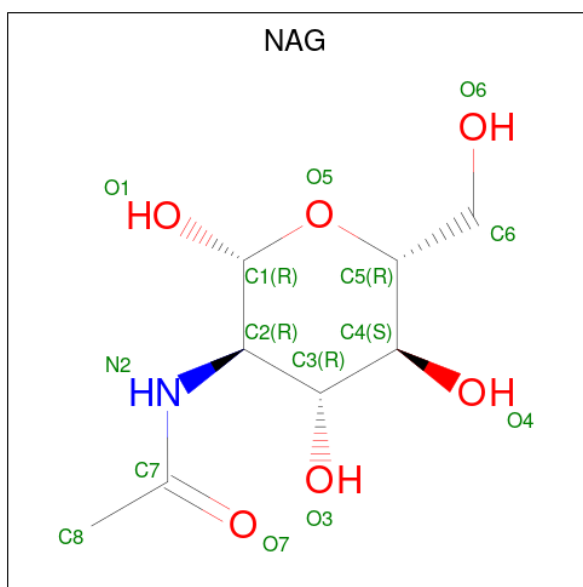
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4456	2823	758	846	29	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



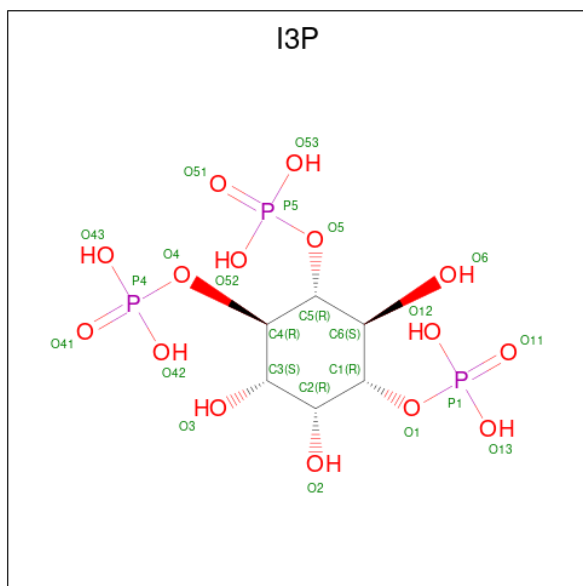
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	10	116	64	2	50	116	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: $C_6H_{15}O_{15}P_3$).

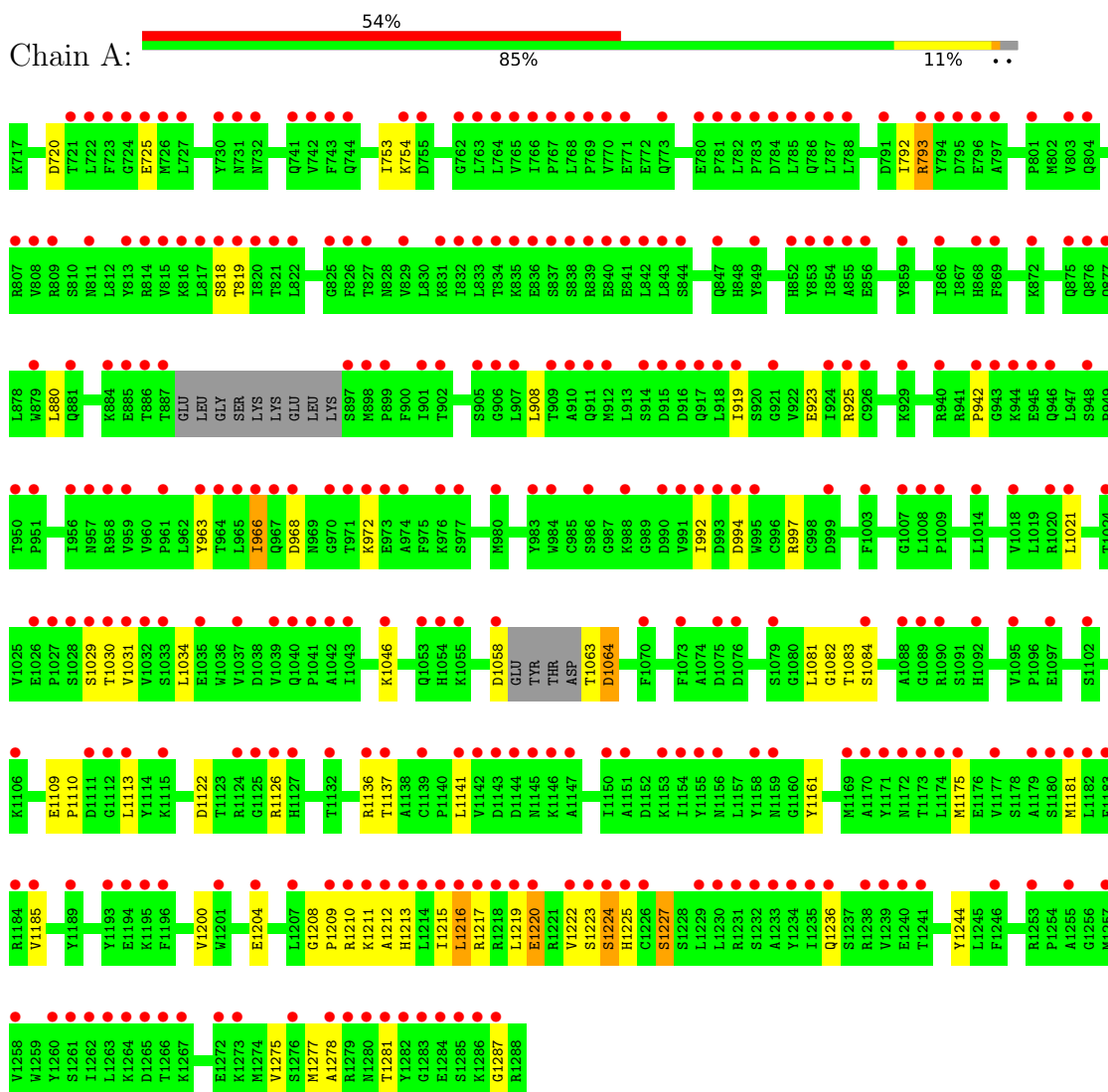


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	24	0
			24	6	15	3		

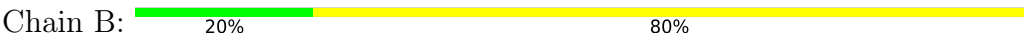
3 Residue-property plots

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: Astrotactin-2



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.90Å 103.90Å 304.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.80 – 5.22 85.80 – 5.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.80-5.22) 99.9 (85.80-5.22)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 5.12Å)	Xtriage
Refinement program	PHENIX (dev_2283: ???)	Depositor
R, R_{free}	0.348 , 0.364 0.339 , 0.368	Depositor DCC
R_{free} test set	360 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	330.4	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 716.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4610	wwPDB-VP
Average B, all atoms (Å ²)	336.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: MAN, BMA, NAG, I3P

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	0.20	0/4552	0.43	0/6166

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 [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	4456	0	4386	48	0
2	B	116	0	97	0	0
3	A	14	0	13	0	0
4	A	24	0	9	0	0
All	All	4610	0	4505	48	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 5.

All (48) 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:1200:VAL:HG22	1:A:1216:LEU:HD11	1.72	0.71
1:A:792:ILE:HG21	1:A:1021:LEU:HD12	1.78	0.66
1:A:1029:SER:HA	1:A:1137:THR:HB	1.78	0.66
1:A:966:ILE:HD12	1:A:972:LYS:HA	1.80	0.64
1:A:1212:ALA:O	1:A:1216:LEU:HD22	1.99	0.62
1:A:1216:LEU:HD12	1:A:1219:LEU:HD12	1.82	0.61
1:A:1083:THR:HB	1:A:1084:SER:HA	1.84	0.60
1:A:1063:THR:OG1	1:A:1064:ASP:N	2.30	0.59
1:A:1224:SER:HA	1:A:1227:SER:HB3	1.85	0.59
1:A:1200:VAL:HG13	1:A:1216:LEU:HD21	1.83	0.59
1:A:1217:ARG:HA	1:A:1220:GLU:HG3	1.83	0.59
1:A:1209:PRO:O	1:A:1213:HIS:ND1	2.25	0.58
1:A:1122:ASP:OD1	1:A:1126:ARG:N	2.38	0.55
1:A:753:ILE:HG22	1:A:754:LYS:HG3	1.89	0.55
1:A:963:TYR:HA	1:A:966:ILE:HG13	1.90	0.54
1:A:1029:SER:HB2	1:A:1110:PRO:HB3	1.90	0.54
1:A:1209:PRO:HA	1:A:1212:ALA:HB3	1.90	0.53
1:A:1224:SER:HA	1:A:1227:SER:CB	2.40	0.51
1:A:1204:GLU:HG3	1:A:1209:PRO:HG3	1.92	0.50
1:A:1031:VAL:HG11	1:A:1277:MET:HE2	1.94	0.50
1:A:1222:VAL:HG12	1:A:1223:SER:O	2.13	0.48
1:A:793:ARG:HH21	1:A:1136:ARG:NH2	2.13	0.47
1:A:1021:LEU:HD23	1:A:1034:LEU:HD23	1.96	0.46
1:A:1210:ARG:HG3	1:A:1211:LYS:N	2.30	0.46
1:A:818:SER:HA	1:A:819:THR:HA	1.59	0.46
1:A:1212:ALA:C	1:A:1216:LEU:HD22	2.40	0.46
1:A:1236:GLN:O	1:A:1281:THR:N	2.45	0.45
1:A:1113:LEU:HD13	1:A:1136:ARG:HG2	2.00	0.44
1:A:1113:LEU:HD22	1:A:1136:ARG:NH2	2.32	0.44
1:A:1181:MET:O	1:A:1185:VAL:HG13	2.19	0.43
1:A:1030:THR:HG22	1:A:1110:PRO:HD3	1.99	0.43
1:A:1208:GLY:HA2	1:A:1209:PRO:HD3	1.59	0.43
1:A:725:GLU:OE1	1:A:725:GLU:N	2.49	0.43
1:A:992:ILE:HD13	1:A:997:ARG:HB2	2.00	0.43
1:A:1058:ASP:N	1:A:1058:ASP:OD1	2.52	0.43
1:A:1113:LEU:HD22	1:A:1136:ARG:HH21	1.84	0.42
1:A:1141:LEU:HD21	1:A:1278:ALA:HB1	2.00	0.42
1:A:923:GLU:OE1	1:A:925:ARG:NH2	2.53	0.42
1:A:919:ILE:HG22	1:A:919:ILE:O	2.20	0.42
1:A:793:ARG:HH21	1:A:1136:ARG:HH22	1.68	0.41
1:A:968:ASP:O	1:A:972:LYS:HE3	2.21	0.41
1:A:1081:LEU:HA	1:A:1082:GLY:HA3	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ILE:HG22	1:A:1216:LEU:HD13	2.03	0.41
1:A:1244:TYR:CD1	1:A:1275:VAL:HG23	2.56	0.41
1:A:1175:MET:HA	1:A:1175:MET:HE2	2.02	0.40
1:A:1225:HIS:ND1	1:A:1225:HIS:N	2.69	0.40
1:A:994:ASP:O	1:A:1046:LYS:HE2	2.21	0.40
1:A:1109:GLU:HG2	1:A:1110:PRO:HD2	2.03	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	553/572 (97%)	522 (94%)	28 (5%)	3 (0%)	24 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1161	TYR
1	A	942	PRO
1	A	1287	GLY

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	501/513 (98%)	491 (98%)	10 (2%)	48 66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	ASP
1	A	793	ARG
1	A	880	LEU
1	A	908	LEU
1	A	966	ILE
1	A	1064	ASP
1	A	1216	LEU
1	A	1220	GLU
1	A	1224	SER
1	A	1227	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	736	HIS
1	A	750	ASN
1	A	828	ASN
1	A	848	HIS
1	A	875	GLN
1	A	881	GLN
1	A	883	GLN
1	A	946	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 ⓘ

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	B	1	2,1	14,14,15	1.49	1 (7%)	17,19,21	2.53	1 (5%)
2	MAN	B	10	2	11,11,12	0.58	0	15,15,17	1.01	2 (13%)
2	NAG	B	2	2	14,14,15	0.42	0	17,19,21	0.50	0
2	BMA	B	3	2	11,11,12	0.46	0	15,15,17	0.73	0
2	MAN	B	4	2	11,11,12	0.99	1 (9%)	15,15,17	1.13	2 (13%)
2	MAN	B	5	2	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
2	MAN	B	6	2	11,11,12	0.84	1 (9%)	15,15,17	1.54	2 (13%)
2	MAN	B	7	2	11,11,12	1.95	1 (9%)	15,15,17	1.60	3 (20%)
2	MAN	B	8	2	11,11,12	1.70	4 (36%)	15,15,17	1.09	1 (6%)
2	MAN	B	9	2	11,11,12	0.61	0	15,15,17	0.96	1 (6%)

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	2,1	-	3/6/23/26	0/1/1/1
2	MAN	B	10	2	-	0/2/19/22	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	2/2/19/22	0/1/1/1
2	MAN	B	8	2	-	0/2/19/22	0/1/1/1
2	MAN	B	9	2	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	MAN	C2-C3	5.45	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	5.41	1.52	1.43
2	B	8	MAN	C4-C5	3.13	1.59	1.53
2	B	8	MAN	O5-C5	3.04	1.49	1.43
2	B	4	MAN	O5-C1	-2.49	1.39	1.43
2	B	6	MAN	O5-C5	2.12	1.47	1.43
2	B	8	MAN	O5-C1	-2.11	1.40	1.43
2	B	8	MAN	C4-C3	2.10	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	10.08	125.70	112.19
2	B	6	MAN	C1-O5-C5	5.26	119.24	112.19
2	B	7	MAN	O2-C2-C3	3.05	116.48	110.15
2	B	7	MAN	C2-C3-C4	2.95	116.05	110.86
2	B	7	MAN	O3-C3-C2	2.92	116.00	110.05
2	B	10	MAN	C1-O5-C5	2.85	116.00	112.19
2	B	9	MAN	C1-O5-C5	2.69	115.79	112.19
2	B	5	MAN	C1-O5-C5	2.68	115.77	112.19
2	B	8	MAN	C1-C2-C3	-2.39	106.16	109.64
2	B	4	MAN	C3-C4-C5	2.18	114.18	110.23
2	B	10	MAN	O2-C2-C3	-2.15	105.69	110.15
2	B	4	MAN	O2-C2-C3	-2.13	105.74	110.15
2	B	6	MAN	O2-C2-C3	-2.11	105.79	110.15

There are no chirality outliers.

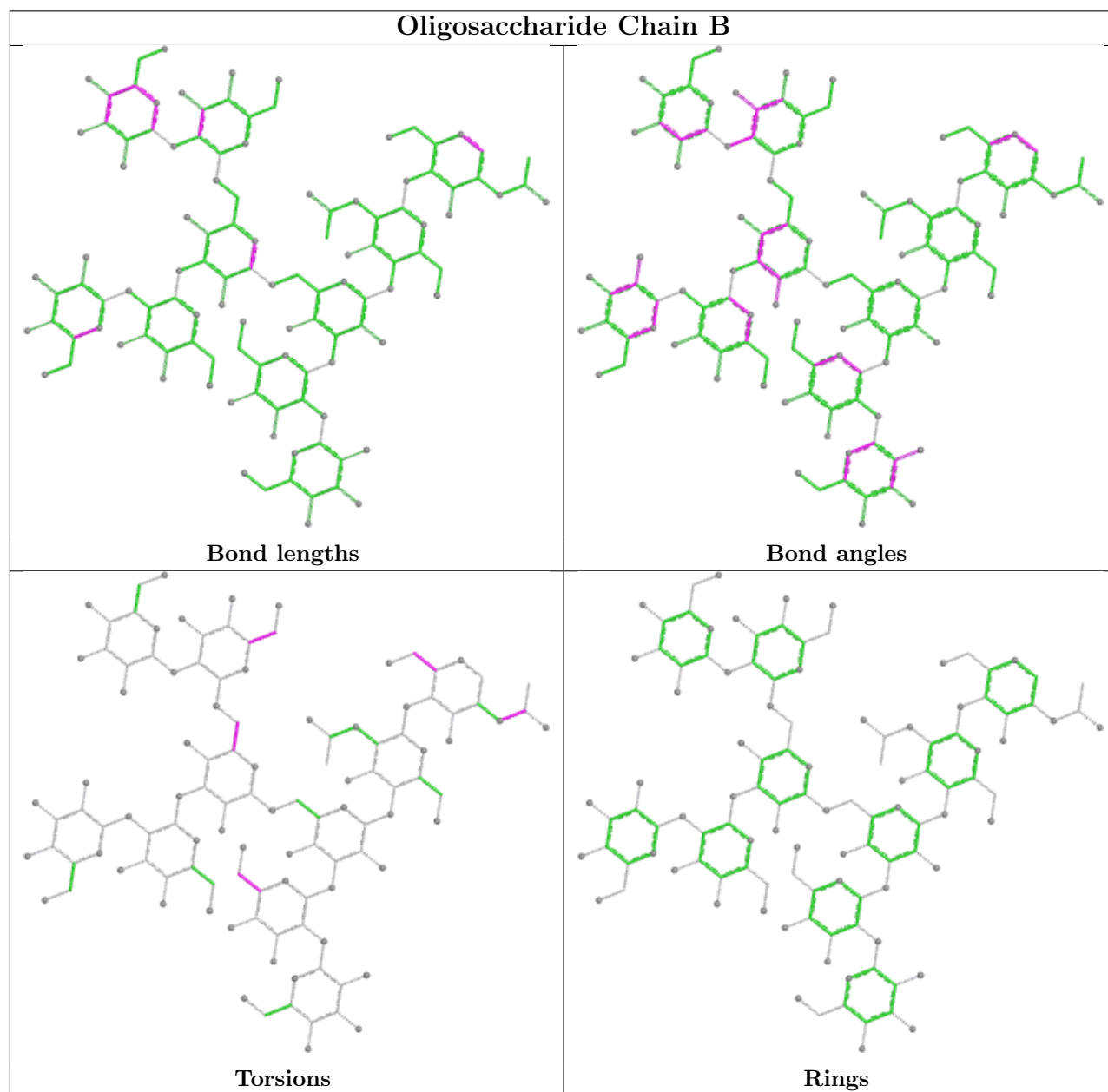
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C4-C5-C6-O6
2	B	9	MAN	C4-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
2	B	9	MAN	O5-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6

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	NAG	A	1310	1	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
4	I3P	A	1311	-	24,24,24	1.28	3 (12%)	39,39,39	0.83	1 (2%)

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	1310	1	-	2/6/23/26	0/1/1/1
4	I3P	A	1311	-	-	4/15/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1311	I3P	P4-O4	3.13	1.65	1.59
4	A	1311	I3P	P1-O1	3.11	1.65	1.59
4	A	1311	I3P	P5-O5	3.01	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1310	NAG	C1-O5-C5	2.74	115.86	112.19
4	A	1311	I3P	P5-O5-C5	-2.40	117.01	123.43

There are no chirality outliers.

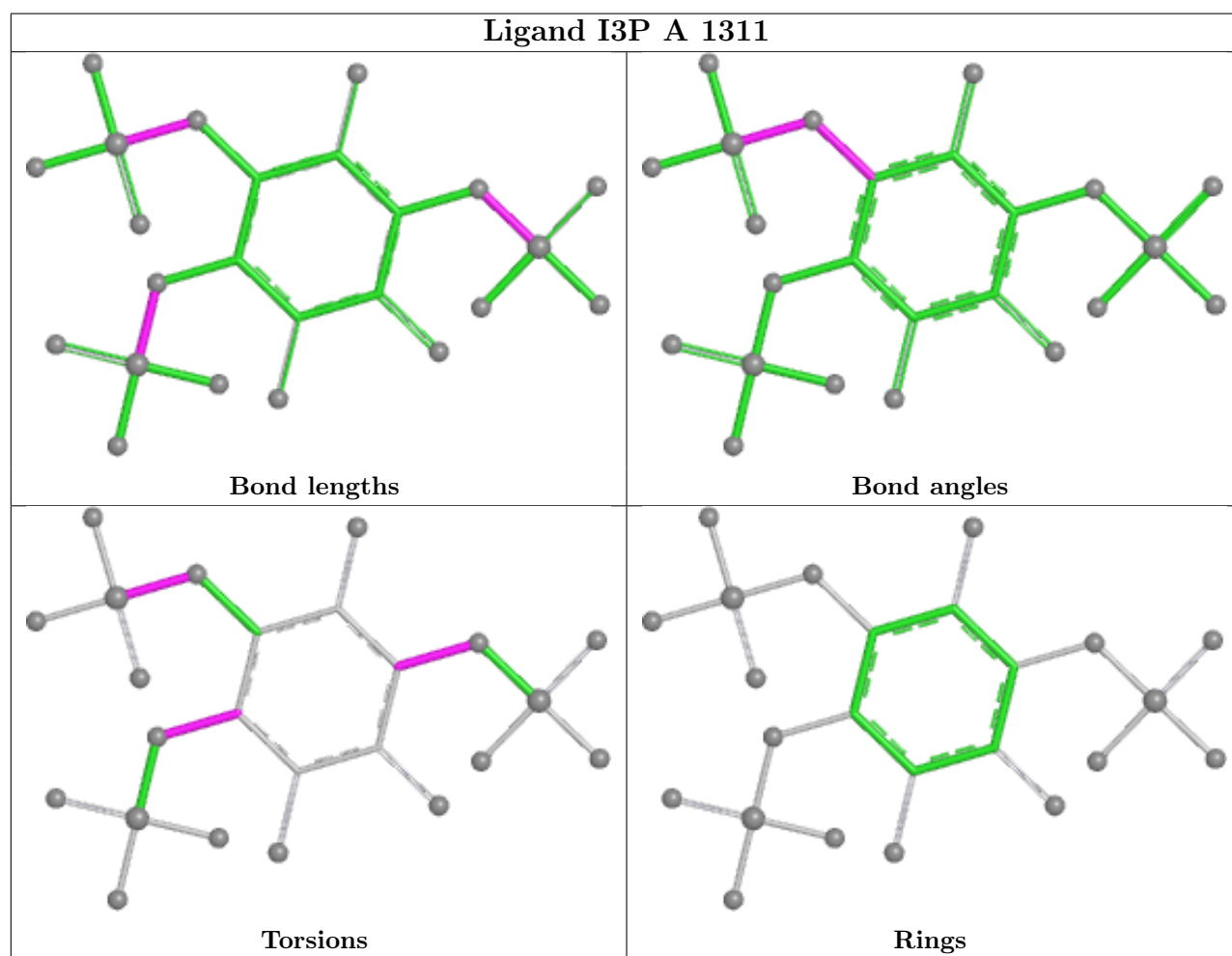
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1310	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
4	A	1311	I3P	C6-C1-O1-P1
4	A	1311	I3P	C2-C1-O1-P1
4	A	1311	I3P	C3-C4-O4-P4
4	A	1311	I3P	C5-O5-P5-O51

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 ⓘ

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	559/572 (97%)	2.70	308 (55%) 0 2	282, 335, 369, 393	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	973	GLU	27.0
1	A	1042	ALA	19.8
1	A	1265	ASP	16.8
1	A	1282	TYR	13.5
1	A	976	LYS	12.4
1	A	993	ASP	11.9
1	A	963	TYR	10.8
1	A	1280	ASN	10.4
1	A	1196	PHE	9.7
1	A	1007	GLY	8.8
1	A	1142	VAL	8.7
1	A	1235	ILE	8.4
1	A	1043	ILE	8.1
1	A	841	GLU	8.0
1	A	942	PRO	7.9
1	A	816	LYS	7.7
1	A	1236	GLN	7.6
1	A	974	ALA	7.5
1	A	726	MET	7.0
1	A	722	LEU	7.0
1	A	1213	HIS	7.0
1	A	1180	SER	6.9
1	A	984	TRP	6.9
1	A	980	MET	6.8
1	A	964	THR	6.8
1	A	1264	LYS	6.8
1	A	1179	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	1154	ILE	6.6
1	A	723	PHE	6.5
1	A	1225	HIS	6.5
1	A	847	GLN	6.5
1	A	849	TYR	6.4
1	A	838	SER	6.4
1	A	1097	GLU	6.2
1	A	797	ALA	6.2
1	A	1267	LYS	6.2
1	A	875	GLN	6.2
1	A	822	LEU	6.1
1	A	994	ASP	6.1
1	A	1286	LYS	6.0
1	A	832	ILE	6.0
1	A	796	GLU	5.9
1	A	1234	TYR	5.8
1	A	831	LYS	5.8
1	A	837	SER	5.7
1	A	917	GLN	5.6
1	A	1181	MET	5.6
1	A	827	THR	5.6
1	A	1008	LEU	5.6
1	A	1229	LEU	5.6
1	A	1171	TYR	5.6
1	A	820	ILE	5.6
1	A	1153	LYS	5.5
1	A	967	GLN	5.5
1	A	1124	ARG	5.5
1	A	977	SER	5.5
1	A	1144	ASP	5.5
1	A	872	LYS	5.4
1	A	1284	GLU	5.4
1	A	1132	THR	5.4
1	A	1136	ARG	5.4
1	A	972	LYS	5.4
1	A	1090	ARG	5.3
1	A	721	THR	5.2
1	A	1033	SER	5.2
1	A	1141	LEU	5.2
1	A	1040	GLN	5.2
1	A	1058	ASP	5.2
1	A	992	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	876	GLN	5.1
1	A	1281	THR	5.0
1	A	1253	ARG	5.0
1	A	766	ILE	5.0
1	A	814	ARG	4.9
1	A	1170	ALA	4.9
1	A	1155	TYR	4.9
1	A	991	VAL	4.9
1	A	1285	SER	4.8
1	A	1210	ARG	4.8
1	A	821	THR	4.8
1	A	1230	LEU	4.7
1	A	916	ASP	4.7
1	A	725	GLU	4.7
1	A	1125	GLY	4.7
1	A	866	ILE	4.6
1	A	995	TRP	4.6
1	A	919	ILE	4.6
1	A	819	THR	4.6
1	A	834	THR	4.5
1	A	844	SER	4.5
1	A	901	ILE	4.5
1	A	724	GLY	4.5
1	A	764	LEU	4.4
1	A	1279	ARG	4.4
1	A	1257	MET	4.4
1	A	1204	GLU	4.3
1	A	1147	ALA	4.3
1	A	1195	LYS	4.3
1	A	1150	ILE	4.3
1	A	1174	LEU	4.3
1	A	815	VAL	4.3
1	A	1258	VAL	4.3
1	A	950	THR	4.3
1	A	1212	ALA	4.3
1	A	1184	ARG	4.2
1	A	1220	GLU	4.2
1	A	1287	GLY	4.2
1	A	781	PRO	4.2
1	A	1158	TYR	4.2
1	A	829	VAL	4.2
1	A	839	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1115	LYS	4.2
1	A	970	GLY	4.1
1	A	918	LEU	4.1
1	A	835	LYS	4.1
1	A	1145	ASN	4.1
1	A	911	GLN	4.0
1	A	1027	PRO	4.0
1	A	1266	THR	4.0
1	A	836	GLU	4.0
1	A	817	LEU	3.9
1	A	898	MET	3.9
1	A	791	ASP	3.9
1	A	879	TRP	3.9
1	A	1232	SER	3.9
1	A	881	GLN	3.9
1	A	971	THR	3.8
1	A	948	SER	3.8
1	A	1021	LEU	3.8
1	A	825	GLY	3.8
1	A	1194	GLU	3.8
1	A	769	PRO	3.7
1	A	1169	MET	3.7
1	A	818	SER	3.7
1	A	1238	ARG	3.7
1	A	914	SER	3.7
1	A	909	THR	3.7
1	A	986	SER	3.7
1	A	944	LYS	3.6
1	A	961	PRO	3.6
1	A	1222	VAL	3.6
1	A	826	PHE	3.6
1	A	1283	GLY	3.6
1	A	794	TYR	3.5
1	A	1276	SER	3.5
1	A	859	TYR	3.5
1	A	1151	ALA	3.5
1	A	990	ASP	3.5
1	A	833	LEU	3.5
1	A	1217	ARG	3.4
1	A	1020	ARG	3.4
1	A	968	ASP	3.4
1	A	782	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1143	ASP	3.4
1	A	1084	SER	3.4
1	A	768	LEU	3.4
1	A	1175	MET	3.3
1	A	1177	VAL	3.3
1	A	785	LEU	3.3
1	A	868	HIS	3.3
1	A	1262	ILE	3.3
1	A	885	GLU	3.3
1	A	803	VAL	3.3
1	A	1241	THR	3.3
1	A	1003	PHE	3.2
1	A	763	LEU	3.2
1	A	1018	VAL	3.2
1	A	1233	ALA	3.2
1	A	784	ASP	3.2
1	A	801	PRO	3.2
1	A	795	ASP	3.2
1	A	1024	THR	3.2
1	A	1028	SER	3.2
1	A	910	ALA	3.2
1	A	926	CYS	3.2
1	A	905	SER	3.2
1	A	1219	LEU	3.2
1	A	1263	LEU	3.2
1	A	1185	VAL	3.1
1	A	1278	ALA	3.1
1	A	965	LEU	3.1
1	A	1079	SER	3.1
1	A	1260	TYR	3.1
1	A	943	GLY	3.1
1	A	1054	HIS	3.1
1	A	1239	VAL	3.1
1	A	1046	LYS	3.1
1	A	907	LEU	3.1
1	A	767	PRO	3.0
1	A	853	TYR	3.0
1	A	1073	PHE	3.0
1	A	999	ASP	3.0
1	A	1014	LEU	3.0
1	A	1214	LEU	3.0
1	A	811	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	727	LEU	2.9
1	A	929	LYS	2.9
1	A	1209	PRO	2.9
1	A	912	MET	2.9
1	A	887	THR	2.9
1	A	924	ILE	2.9
1	A	741	GLN	2.9
1	A	732	ASN	2.9
1	A	1159	ASN	2.9
1	A	1031	VAL	2.9
1	A	856	GLU	2.9
1	A	1075	ASP	2.9
1	A	1026	GLU	2.8
1	A	940	ARG	2.8
1	A	754	LYS	2.8
1	A	1182	LEU	2.8
1	A	1216	LEU	2.8
1	A	988	LYS	2.8
1	A	786	GLN	2.8
1	A	945	GLU	2.8
1	A	1193	TYR	2.8
1	A	1211	LYS	2.8
1	A	813	TYR	2.8
1	A	762	GLY	2.7
1	A	1127	HIS	2.7
1	A	840	GLU	2.7
1	A	899	PRO	2.7
1	A	1183	PHE	2.7
1	A	1076	ASP	2.7
1	A	1037	VAL	2.7
1	A	1240	GLU	2.7
1	A	770	VAL	2.7
1	A	771	GLU	2.7
1	A	1261	SER	2.7
1	A	1032	VAL	2.7
1	A	743	PHE	2.7
1	A	1009	PRO	2.7
1	A	884	LYS	2.6
1	A	1231	ARG	2.6
1	A	1112	GLY	2.6
1	A	915	ASP	2.6
1	A	780	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	804	GLN	2.6
1	A	1126	ARG	2.6
1	A	902	THR	2.6
1	A	1224	SER	2.6
1	A	1089	GLY	2.6
1	A	765	VAL	2.6
1	A	787	LEU	2.6
1	A	1041	PRO	2.6
1	A	1139	CYS	2.5
1	A	1172	ASN	2.5
1	A	783	PRO	2.5
1	A	1095	VAL	2.5
1	A	1070	PHE	2.5
1	A	1246	PHE	2.5
1	A	854	ILE	2.4
1	A	1215	ILE	2.4
1	A	957	ASN	2.4
1	A	956	ILE	2.4
1	A	1102	SER	2.4
1	A	843	LEU	2.4
1	A	1111	ASP	2.4
1	A	959	VAL	2.4
1	A	983	TYR	2.4
1	A	1035	GLU	2.4
1	A	1273	LYS	2.4
1	A	966	ILE	2.4
1	A	951	PRO	2.3
1	A	807	ARG	2.3
1	A	921	GLY	2.3
1	A	1113	LEU	2.3
1	A	958	ARG	2.3
1	A	1029	SER	2.3
1	A	1088	ALA	2.3
1	A	809	ARG	2.3
1	A	842	LEU	2.3
1	A	869	PHE	2.3
1	A	852	HIS	2.3
1	A	1092	HIS	2.3
1	A	1055	LYS	2.2
1	A	742	VAL	2.2
1	A	1218	ARG	2.2
1	A	1137	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1156	ASN	2.2
1	A	1146	LYS	2.2
1	A	1272	GLU	2.2
1	A	925	ARG	2.2
1	A	1201	TRP	2.2
1	A	808	VAL	2.2
1	A	1226	CYS	2.2
1	A	773	GLN	2.1
1	A	1189	TYR	2.1
1	A	788	LEU	2.1
1	A	906	GLY	2.1
1	A	886	THR	2.1
1	A	1223	SER	2.1
1	A	1255	ALA	2.1
1	A	755	ASP	2.1
1	A	1173	THR	2.1
1	A	897	SER	2.1
1	A	1207	LEU	2.1
1	A	1039	VAL	2.1
1	A	730	TYR	2.1
1	A	1053	GLN	2.1
1	A	855	ALA	2.0
1	A	731	ASN	2.0
1	A	744	GLN	2.0
1	A	877	GLN	2.0
1	A	1106	LYS	2.0
1	A	793	ARG	2.0
1	A	946	GLN	2.0
1	A	1030	THR	2.0

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

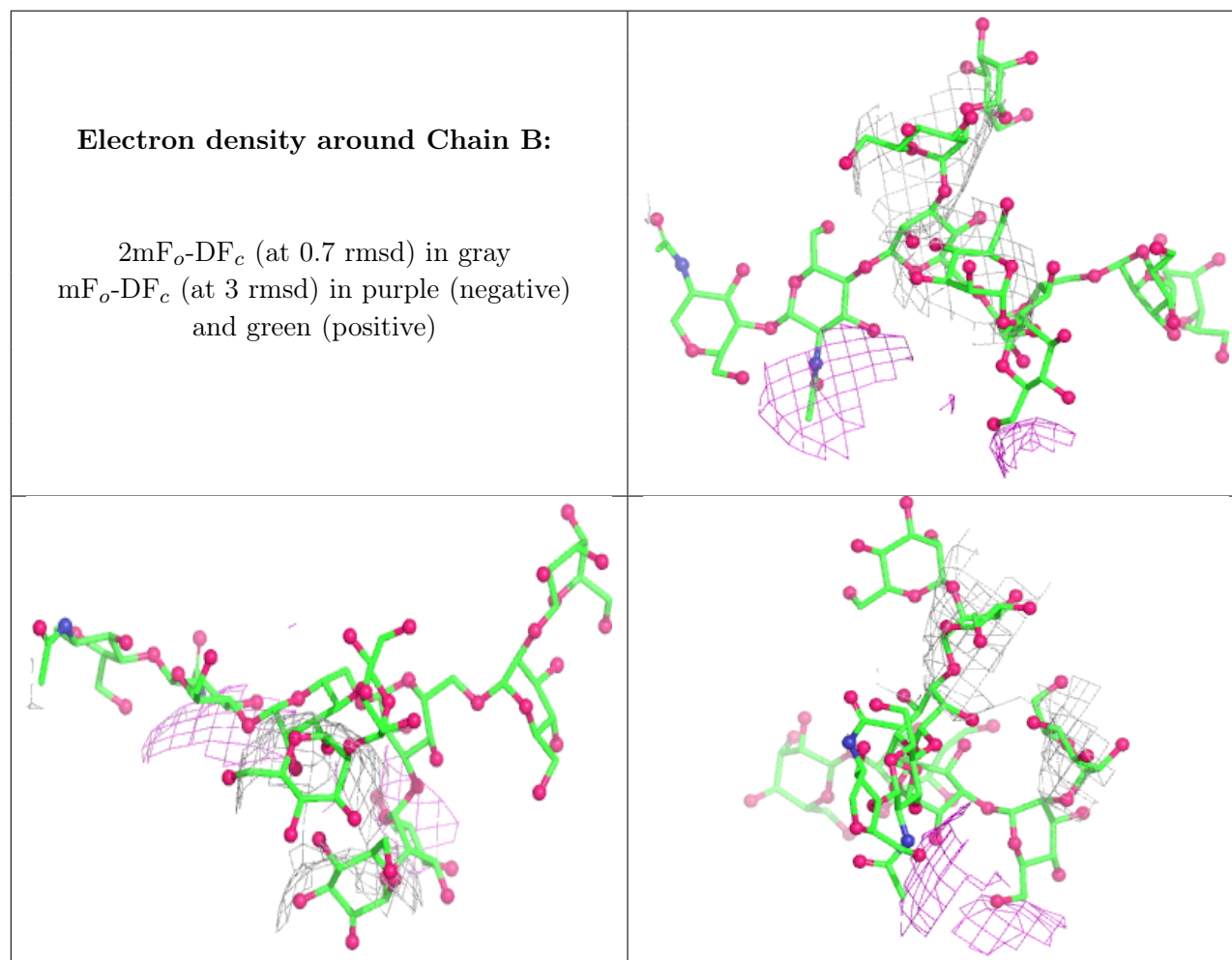
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	1	14/15	-	-	330,333,334,335	14
2	NAG	B	2	14/15	-	-	330,333,339,341	14
2	BMA	B	3	11/12	-	-	336,340,348,349	11
2	MAN	B	4	11/12	-	-	341,345,354,359	11
2	MAN	B	5	11/12	-	-	350,353,354,355	11
2	MAN	B	6	11/12	-	-	347,352,358,360	11
2	MAN	B	7	11/12	-	-	340,343,354,363	11
2	MAN	B	8	11/12	-	-	349,353,357,360	11
2	MAN	B	9	11/12	-	-	338,347,351,352	11
2	MAN	B	10	11/12	-	-	338,347,352,354	11

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



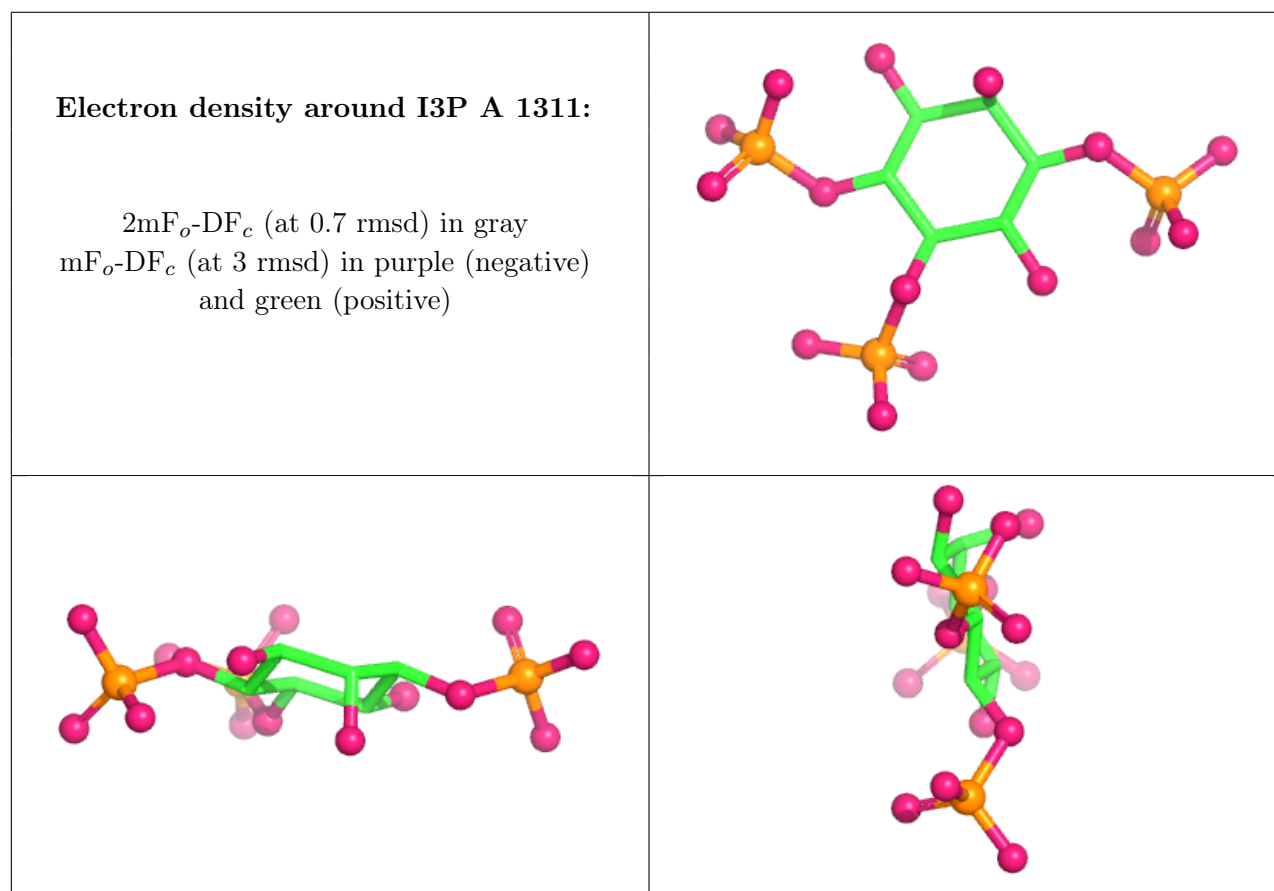
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1310	14/15	-	-	357,362,367,371	14
4	I3P	A	1311	24/24	-	-	332,350,361,362	24

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.