



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 AM UTC

PDB ID : 7P0K / pdb_00007p0k
Title : Crystal structure of Autotaxin (ENPP2) with 18F-labeled positron emission tomography ligand
Authors : Salgado-Polo, F.; Shao, T.; Xiao, Z.; Van, R.; Chen, J.; Rong, J.; Haider, A.; Shao, Y.; Josephson, L.; Perrakis, A.; Liang, S.H.
Deposited on : 2021-06-29
Resolution : 2.20 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

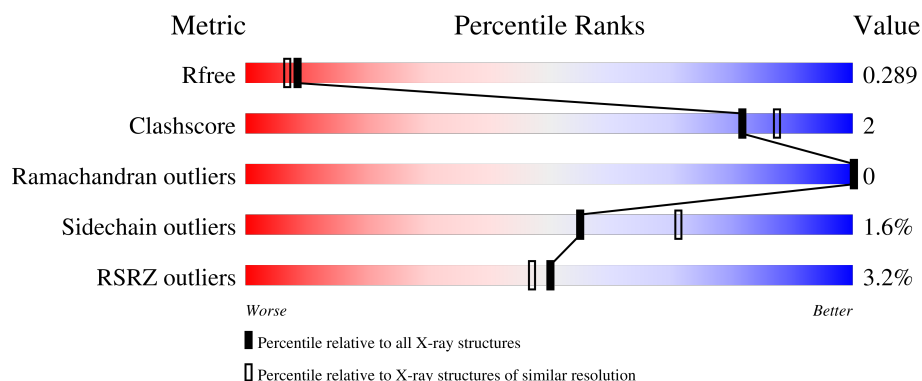
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	AAA	770	3% 92% 8%
2	AbA	7	29% 71%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	AbA	6	X	-	-	-
2	MAN	AbA	7	X	-	-	-
8	4I0	AAA	910	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12835 atoms, of which 6144 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 Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	770	Total	C	H	N	O	S	202	2	0
			12252	3955	6018	1074	1156	49			

There are 36 discrepancies between the modelled and reference sequences:

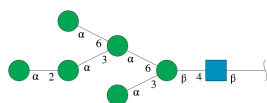
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	ASN	deletion	UNP Q64610
AAA	?	-	ASN	deletion	UNP Q64610
AAA	?	-	SER	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	410	ALA	ASN	engineered mutation	UNP Q64610
AAA	?	-	LEU	deletion	UNP Q64610
AAA	?	-	ASP	deletion	UNP Q64610
AAA	?	-	VAL	deletion	UNP Q64610
AAA	?	-	TYR	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	PRO	deletion	UNP Q64610
AAA	?	-	SER	deletion	UNP Q64610
AAA	?	-	GLY	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	GLY	deletion	UNP Q64610
AAA	?	-	ASP	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	VAL	deletion	UNP Q64610
AAA	?	-	GLU	deletion	UNP Q64610
AAA	?	-	PRO	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	ASN	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	LEU	deletion	UNP Q64610
AAA	?	-	GLU	deletion	UNP Q64610

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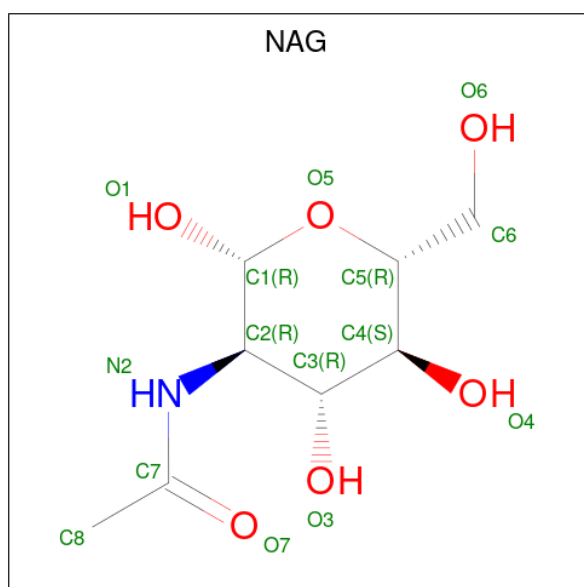
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	GLU	deletion	UNP Q64610
AAA	?	-	LEU	deletion	UNP Q64610
AAA	?	-	ASN	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	?	-	ARG	deletion	UNP Q64610
AAA	?	-	LEU	deletion	UNP Q64610
AAA	?	-	HIS	deletion	UNP Q64610
AAA	?	-	THR	deletion	UNP Q64610
AAA	?	-	LYS	deletion	UNP Q64610
AAA	591	THR	ARG	conflict	UNP Q64610

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



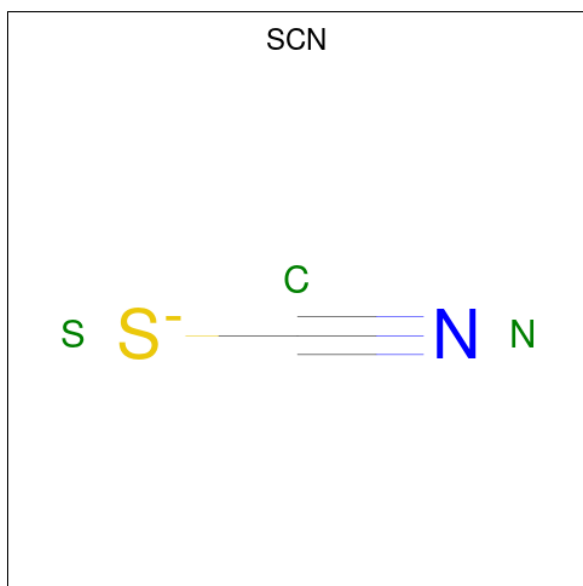
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AbA	7	Total	C	H	N	O	22	0	0
			160	44	80	1	35			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	2	0
			28	8	14	1	5		

- Molecule 4 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	N	S	0	0
			3	1	1	1		
4	AAA	1	Total	C	N	S	0	0
			3	1	1	1		
4	AAA	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	2	Total	Zn	0	0
			2	2		

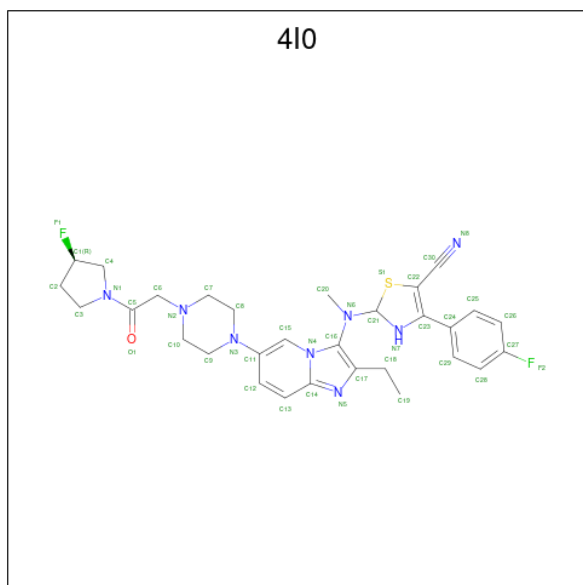
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	1	Total	Ca	0	0
			1	1		

- Molecule 7 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	5	Total I 5 5	0	0

- Molecule 8 is 2-[[2-ethyl-6-[4-[2-[(3 {R})-3-fluoranylpyrrolidin-1-yl]-2-oxidanylidene-ethyl]piperazin-1-yl]imidazo[1,2-a]pyridin-3-yl]-methyl-amino]-4-(4-fluorophenyl)-2,3-dihydro-1,3-thiazole-5-carbonitrile (CCD ID: 4I0) (formula: C₃₀H₃₄F₂N₈OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	AAA	1	Total	C	F	H	N	O	S	
			74	30	2	32	8	1	1	

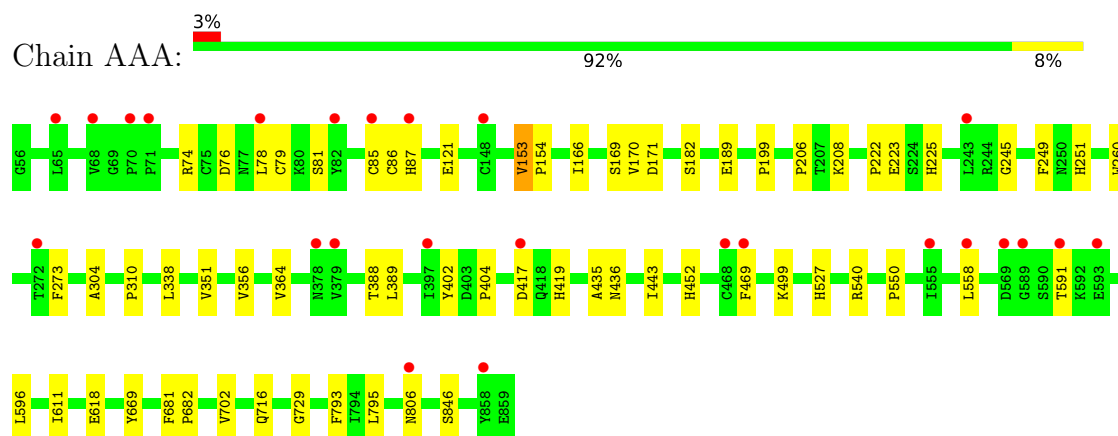
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	304	Total O 304 304	0	0

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: Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.57Å 87.15Å 145.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.20 47.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.57-2.20) 97.9 (47.57-2.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.271 (Not available) , 0.289	Depositor DCC
R_{free} test set	1926 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12835	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: 4I0, BMA, SCN, NAG, ZN, IOD, CA, 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	AAA	0.98	0/6416	1.30	3/8699 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	245	GLY	CA-C-O	-5.58	118.30	122.37
1	AAA	729	GLY	CA-C-O	-5.16	117.75	122.24
1	AAA	388	THR	CA-CB-OG1	-5.12	101.91	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	436	ASN	Peptide

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	AAA	6234	6018	5985	31	0
2	AbA	80	80	67	0	0
3	AAA	14	14	12	0	0
4	AAA	9	0	0	0	0
5	AAA	2	0	0	0	0
6	AAA	1	0	0	0	0
7	AAA	5	0	0	2	0
8	AAA	42	32	0	0	0
9	AAA	304	0	0	4	0
All	All	6691	6144	6064	31	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 2.

All (31) 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:AAA:223:GLU:OE1	1:AAA:435:ALA:O	2.11	0.68
1:AAA:222:PRO:HA	1:AAA:225:HIS:CE1	2.32	0.64
1:AAA:669:TYR:O	9:AAA:1001:HOH:O	2.16	0.59
1:AAA:169:SER:HA	1:AAA:356:VAL:O	2.05	0.57
1:AAA:81:SER:HB3	1:AAA:249:PHE:CZ	2.41	0.56
1:AAA:74:ARG:NH2	1:AAA:76:ASP:OD2	2.40	0.55
1:AAA:618:GLU:HB2	9:AAA:1194:HOH:O	2.06	0.55
1:AAA:153:VAL:HG22	1:AAA:154:PRO:HD2	1.89	0.54
1:AAA:208:LYS:HD2	7:AAA:907:IOD:I	2.80	0.52
1:AAA:166:ILE:HG21	1:AAA:338:LEU:HD21	1.93	0.50
1:AAA:171:ASP:O	1:AAA:310:PRO:HD2	2.12	0.49
1:AAA:682:PRO:HB3	1:AAA:716:GLN:HB3	1.95	0.49
1:AAA:79:CYS:C	1:AAA:85:CYS:SG	2.96	0.49
1:AAA:681:PHE:CD1	1:AAA:682:PRO:HD2	2.48	0.48
1:AAA:404:PRO:HA	1:AAA:443:ILE:HD11	1.97	0.47
1:AAA:166:ILE:HD12	1:AAA:351:VAL:HG11	1.97	0.46
1:AAA:793:PHE:CD1	1:AAA:795:LEU:HG	2.51	0.45
1:AAA:199:PRO:HG3	1:AAA:499:LYS:HE2	1.99	0.45
1:AAA:206:PRO:HB3	1:AAA:389:LEU:HD13	1.99	0.45
1:AAA:364:VAL:HG11	1:AAA:452:HIS:CD2	2.52	0.44
1:AAA:417:ASP:O	1:AAA:419:HIS:CD2	2.71	0.44
1:AAA:273:PHE:CE2	1:AAA:304:ALA:HB2	2.54	0.43
1:AAA:540:ARG:NH2	9:AAA:1021:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:260:TRP:CE3	1:AAA:273:PHE:CG	3.07	0.42
1:AAA:402:TYR:N	9:AAA:1024:HOH:O	2.51	0.42
1:AAA:182:SER:HB3	1:AAA:189:GLU:HG2	2.02	0.41
1:AAA:550:PRO:HB2	1:AAA:611:ILE:HG12	2.02	0.41
1:AAA:596:LEU:CD2	1:AAA:618:GLU:HB3	2.51	0.41
1:AAA:189:GLU:HA	1:AAA:189:GLU:OE1	2.21	0.41
1:AAA:846:SER:OG	7:AAA:912:IOD:I	3.03	0.40
1:AAA:86:CYS:O	1:AAA:87:HIS:C	2.64	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	AAA	762/770 (99%)	731 (96%)	31 (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	AAA	699/697 (100%)	688 (98%)	11 (2%)	55	71

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

Mol	Chain	Res	Type
1	AAA	78	LEU
1	AAA	121	GLU
1	AAA	153	VAL
1	AAA	170	VAL
1	AAA	251	HIS
1	AAA	469	PHE
1	AAA	527	HIS
1	AAA	558	LEU
1	AAA	591	THR
1	AAA	702	VAL
1	AAA	806	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	AbA	1	2	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
2	BMA	AbA	2	2	11,11,12	0.37	0	15,15,17	1.25	3 (20%)
2	MAN	AbA	3	2	11,11,12	0.42	0	15,15,17	1.33	1 (6%)
2	MAN	AbA	4	2	11,11,12	0.63	0	15,15,17	0.74	0
2	MAN	AbA	5	2	11,11,12	0.45	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	AbA	6	2	11,11,12	0.62	0	15,15,17	1.36	3 (20%)
2	MAN	AbA	7	2	11,11,12	0.39	0	15,15,17	1.18	2 (13%)

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	AbA	1	2	-	0/6/23/26	0/1/1/1
2	BMA	AbA	2	2	-	0/2/19/22	0/1/1/1
2	MAN	AbA	3	2	-	1/2/19/22	0/1/1/1
2	MAN	AbA	4	2	-	1/2/19/22	0/1/1/1
2	MAN	AbA	5	2	-	0/2/19/22	0/1/1/1
2	MAN	AbA	6	2	1/1/5/5	1/2/19/22	0/1/1/1
2	MAN	AbA	7	2	1/1/5/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AbA	3	MAN	C1-O5-C5	4.09	117.67	112.19
2	AbA	1	NAG	C1-O5-C5	3.67	117.10	112.19
2	AbA	6	MAN	C1-O5-C5	3.49	116.87	112.19
2	AbA	7	MAN	C1-O5-C5	2.70	115.80	112.19
2	AbA	2	BMA	O5-C5-C6	2.35	112.24	107.66
2	AbA	1	NAG	O5-C1-C2	2.32	114.89	111.29
2	AbA	7	MAN	C1-C2-C3	2.26	112.94	109.64
2	AbA	6	MAN	C1-C2-C3	2.25	112.93	109.64
2	AbA	2	BMA	C1-C2-C3	2.19	112.83	109.64
2	AbA	6	MAN	C2-C3-C4	2.18	114.69	110.86
2	AbA	2	BMA	C1-O5-C5	2.10	115.00	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AbA	6	MAN	C1
2	AbA	7	MAN	C1

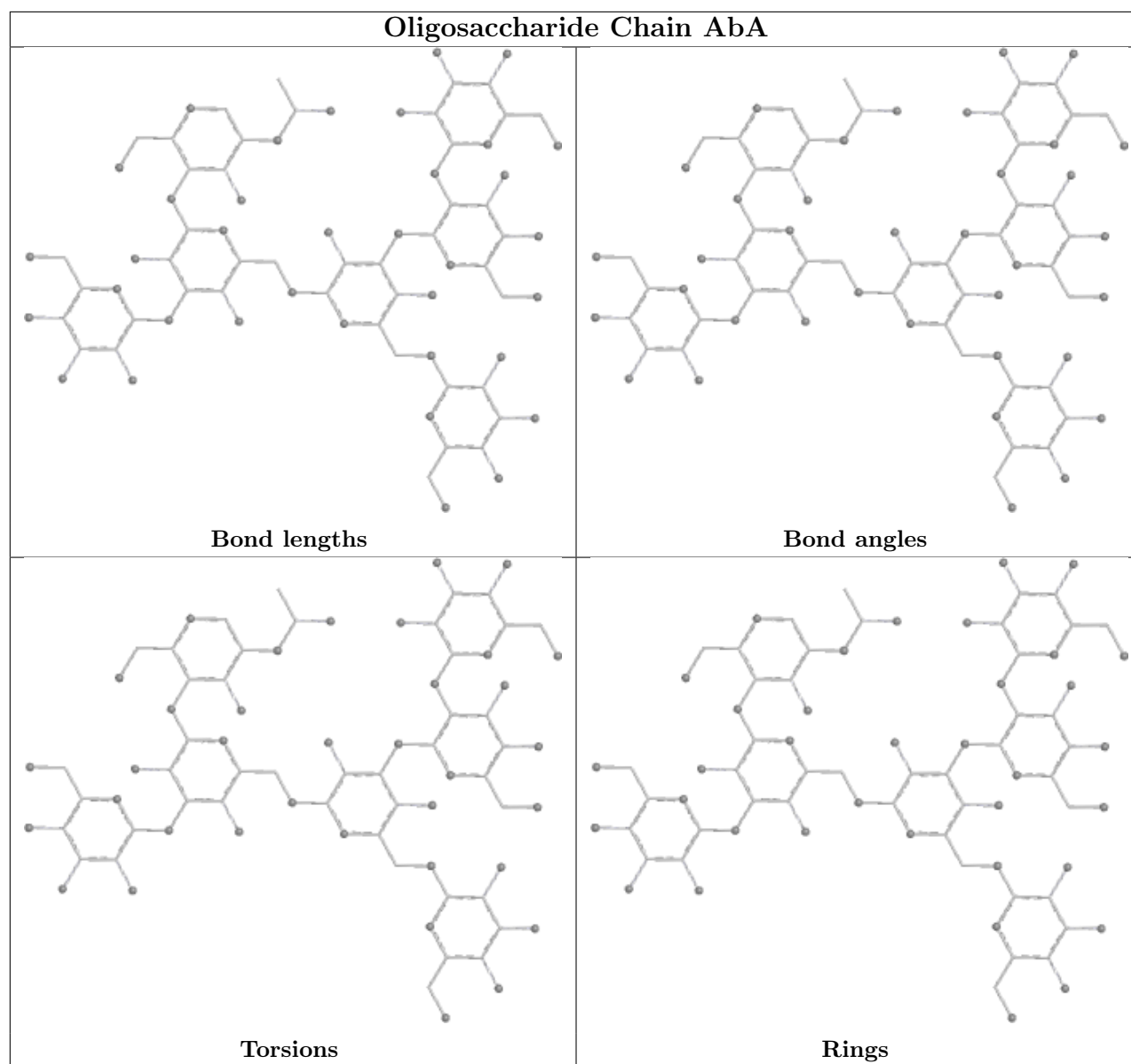
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AbA	6	MAN	O5-C5-C6-O6
2	AbA	3	MAN	O5-C5-C6-O6
2	AbA	4	MAN	C4-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](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	SCN	AAA	902	-	1,2,2	2.20	1 (100%)	0,1,1	-	-
3	NAG	AAA	901	1	14,14,15	0.40	0	17,19,21	1.08	1 (5%)
4	SCN	AAA	913	-	1,2,2	1.13	0	0,1,1	-	-
8	4I0	AAA	910	-	43,47,47	1.08	2 (4%)	48,68,68	1.36	6 (12%)
4	SCN	AAA	903	-	1,2,2	0.68	0	0,1,1	-	-

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	AAA	901	1	-	0/6/23/26	0/1/1/1
8	4I0	AAA	910	-	1/1/9/10	4/22/59/59	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AAA	910	4I0	C21-N7	-5.63	1.30	1.44
8	AAA	910	4I0	C11-N3	2.36	1.40	1.36
4	AAA	902	SCN	C-N	2.20	1.23	1.15

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AAA	910	4I0	C22-C30-N8	-5.56	168.34	177.72
8	AAA	910	4I0	C22-C23-N7	2.76	113.23	107.74
8	AAA	910	4I0	C20-N6-C16	-2.56	117.21	121.56
8	AAA	910	4I0	C9-N3-C8	2.25	117.27	112.68
8	AAA	910	4I0	C15-C11-N3	-2.20	118.81	122.22
3	AAA	901	NAG	O5-C1-C2	-2.19	107.90	111.29
8	AAA	910	4I0	C6-C5-N1	2.07	119.55	117.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	AAA	910	4I0	C21

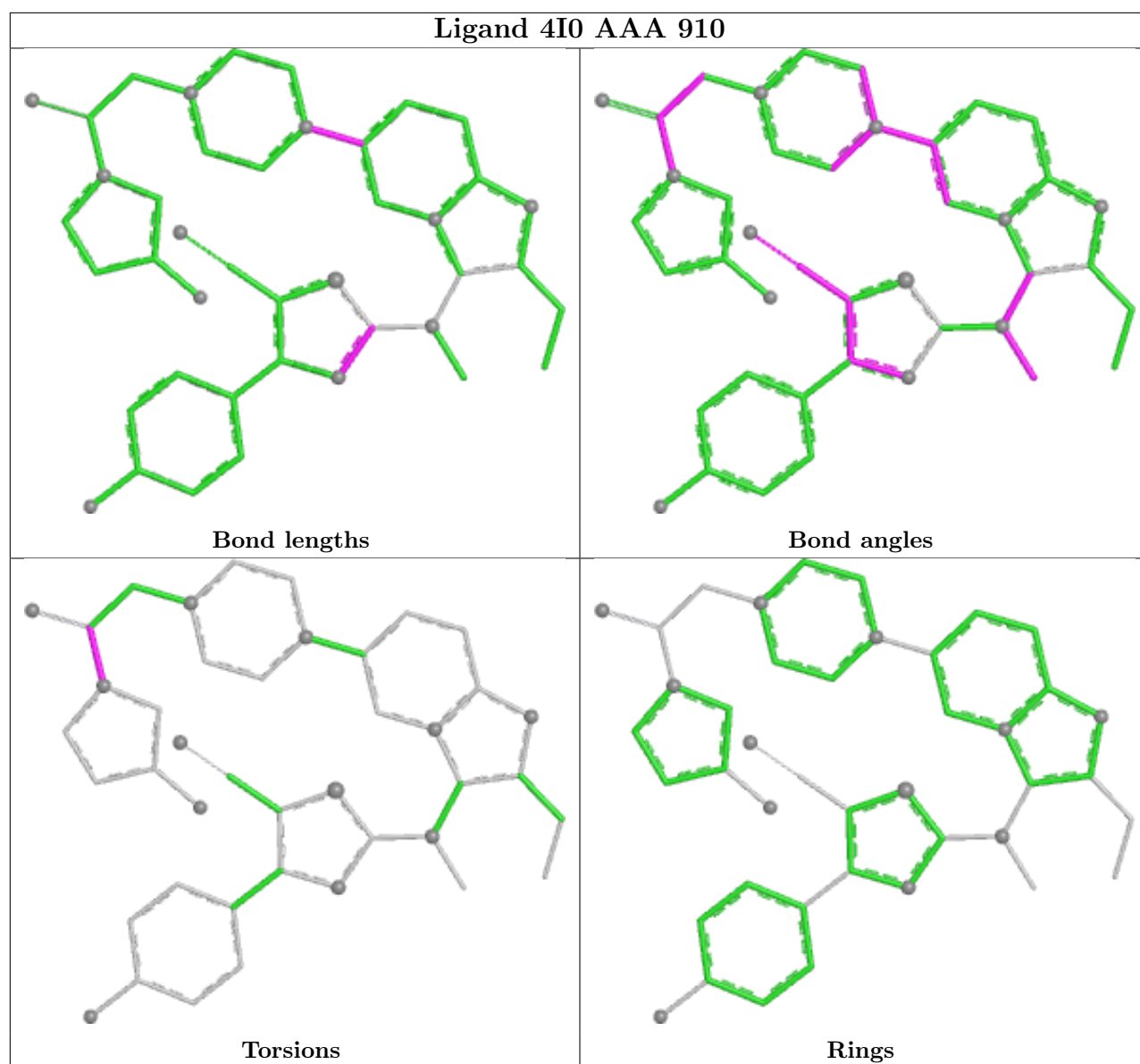
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AAA	910	4I0	C6-C5-N1-C3
8	AAA	910	4I0	O1-C5-N1-C3
8	AAA	910	4I0	C6-C5-N1-C4
8	AAA	910	4I0	O1-C5-N1-C4

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	569:ASP	C	589:GLY	N	30.60
1	AAA	457:PRO	C	468:CYS	N	13.75
1	AAA	397:ILE	C	402:TYR	N	8.68
1	AAA	553:PRO	C	555:ILE	N	3.27

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	AAA	770/770 (100%)	0.31	25 (3%)	50 47	18, 33, 59, 95	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	469	PHE	4.7
1	AAA	555	ILE	4.1
1	AAA	78	LEU	4.0
1	AAA	71	PRO	3.4
1	AAA	82	TYR	3.3
1	AAA	68	VAL	3.3
1	AAA	468	CYS	3.2
1	AAA	397	ILE	2.9
1	AAA	65	LEU	2.9
1	AAA	589	GLY	2.9
1	AAA	591	THR	2.7
1	AAA	243	LEU	2.7
1	AAA	148	CYS	2.6
1	AAA	858	TYR	2.6
1	AAA	272	THR	2.5
1	AAA	593	GLU	2.3
1	AAA	569	ASP	2.3
1	AAA	70	PRO	2.3
1	AAA	417	ASP	2.3
1	AAA	87	HIS	2.3
1	AAA	379	VAL	2.2
1	AAA	85	CYS	2.2
1	AAA	558	LEU	2.2
1	AAA	378	ASN	2.1
1	AAA	806	ASN	2.1

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 ⓘ

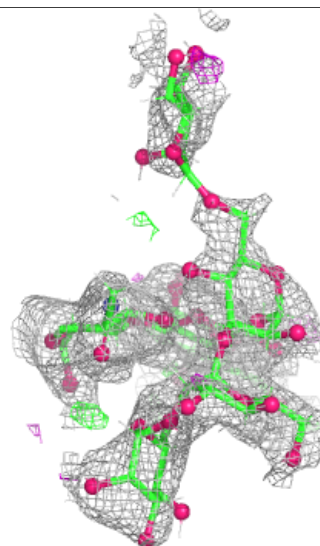
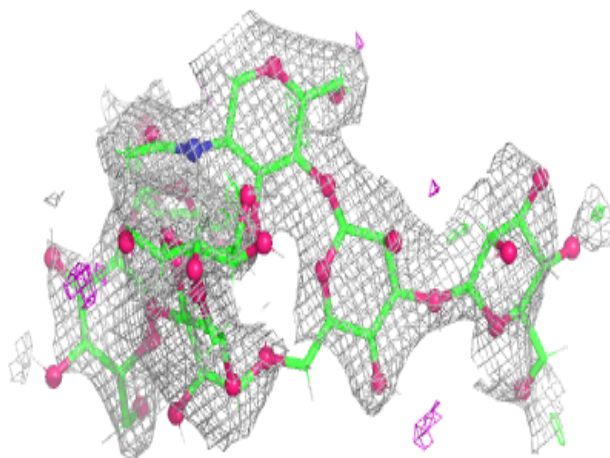
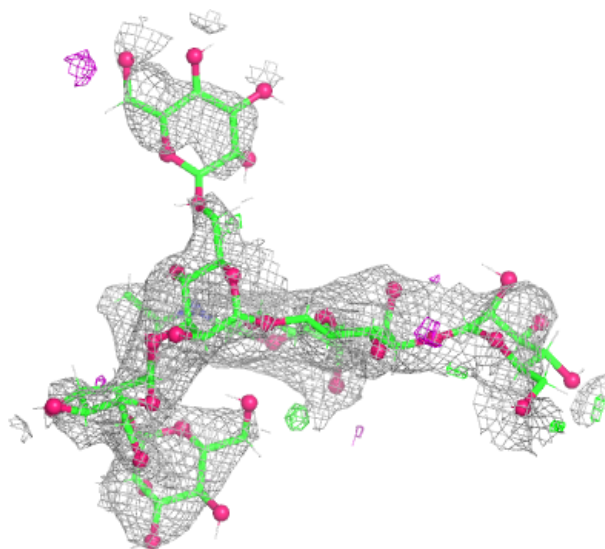
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AbA	1	14/15	-	-	30,39,44,47	2
2	BMA	AbA	2	11/12	-	-	30,63,67,67	3
2	MAN	AbA	3	11/12	-	-	30,64,72,79	2
2	MAN	AbA	4	11/12	-	-	30,59,62,64	3
2	MAN	AbA	5	11/12	-	-	30,59,62,65	4
2	MAN	AbA	6	11/12	-	-	30,82,88,91	4
2	MAN	AbA	7	11/12	-	-	30,83,87,91	4

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 AbA:

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.

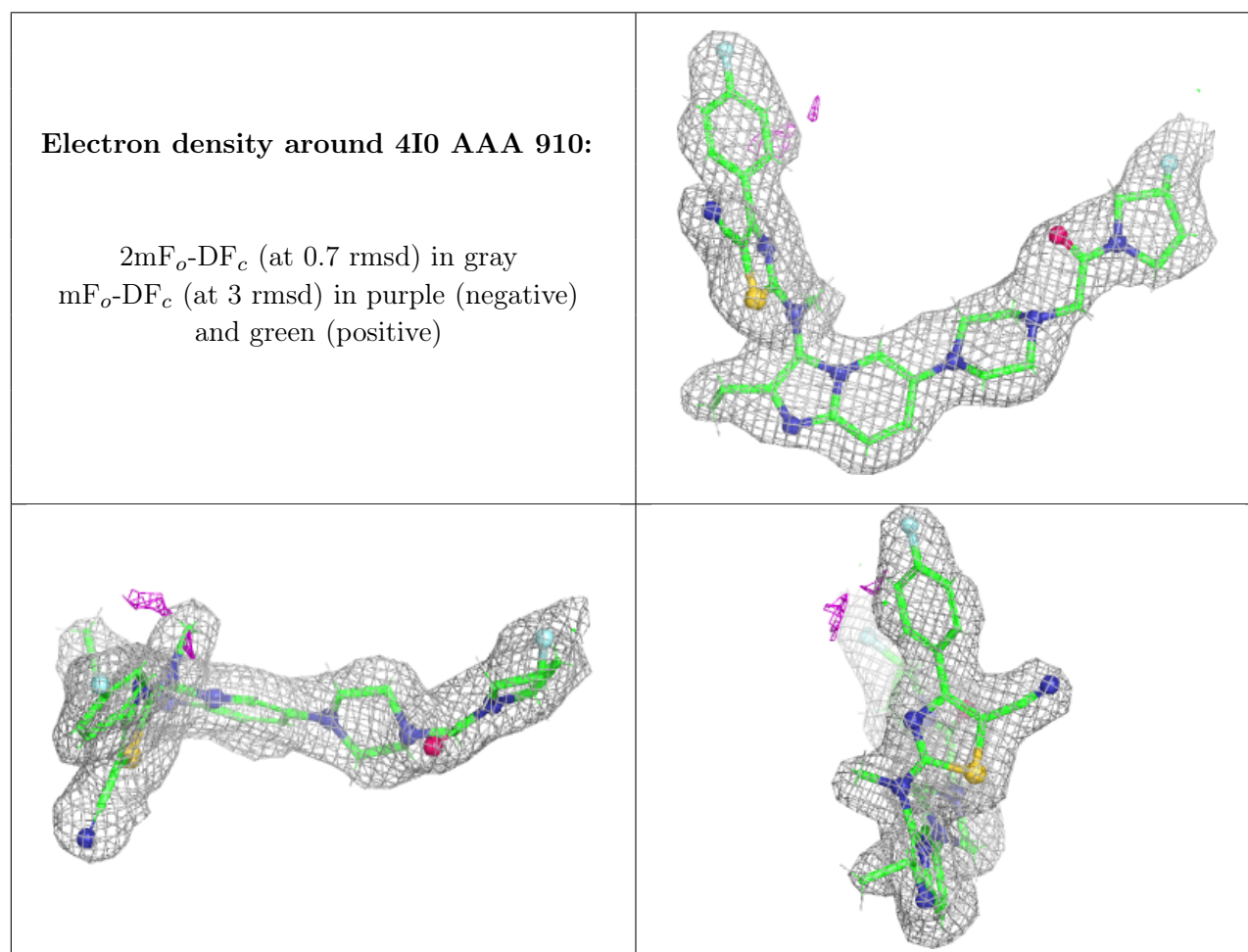
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SCN	AAA	913	3/3	0.75	0.16	52,52,56,70	0
4	SCN	AAA	902	3/3	0.78	0.19	47,47,62,63	0
4	SCN	AAA	903	3/3	0.87	0.14	50,50,51,60	0
5	ZN	AAA	905	1/1	0.92	0.15	61,61,61,61	0
8	4I0	AAA	910	42/42	0.92	0.09	26,32,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	AAA	901	14/15	0.94	0.07	23,26,30,31	2
7	IOD	AAA	908	1/1	0.96	0.26	83,83,83,83	0
7	IOD	AAA	909	1/1	0.98	0.14	80,80,80,80	0
6	CA	AAA	906	1/1	0.99	0.08	29,29,29,29	0
7	IOD	AAA	911	1/1	0.99	0.17	60,60,60,60	0
7	IOD	AAA	912	1/1	0.99	0.17	64,64,64,64	0
5	ZN	AAA	904	1/1	0.99	0.03	31,31,31,31	0
7	IOD	AAA	907	1/1	1.00	0.01	37,37,37,37	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 ⓘ

There are no such residues in this entry.