



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:26 PM UTC

PDB ID : 7Z3K / pdb_00007z3k
Title : Autotaxin in complex with orthosteric site-binder CpdA
Authors : Salgado-Polo, F.; Ford, P.; Heckmann, B.; Perrakis, A.
Deposited on : 2022-03-02
Resolution : 2.00 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

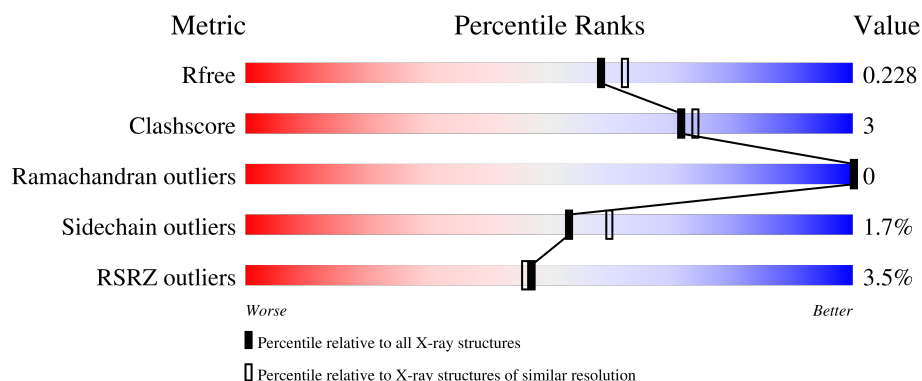
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	AAA	805	
2	AbA	2	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13509 atoms, of which 6379 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	792	Total	C	H	N	O	S	204	2	1
			12597	4062	6193	1104	1189	49			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	410	ALA	ASN	engineered mutation	UNP Q64610
AAA	591	THR	ARG	engineered mutation	UNP Q64610
AAA	806	ALA	ASN	engineered mutation	UNP Q64610

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AbA	2	Total	C	H	N	O	6	0	0
			50	14	25	1	10			

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

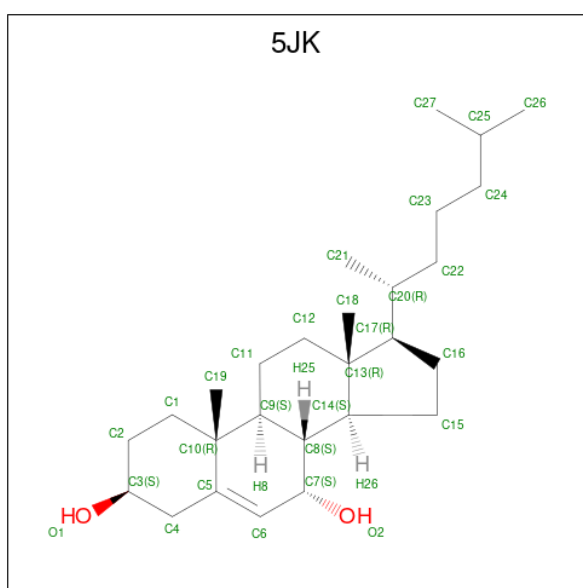


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	2	0
			28	8	14	1	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 7alpha-hydroxycholesterol (CCD ID: 5JK) (formula: C₂₇H₄₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			75	27	46	2		

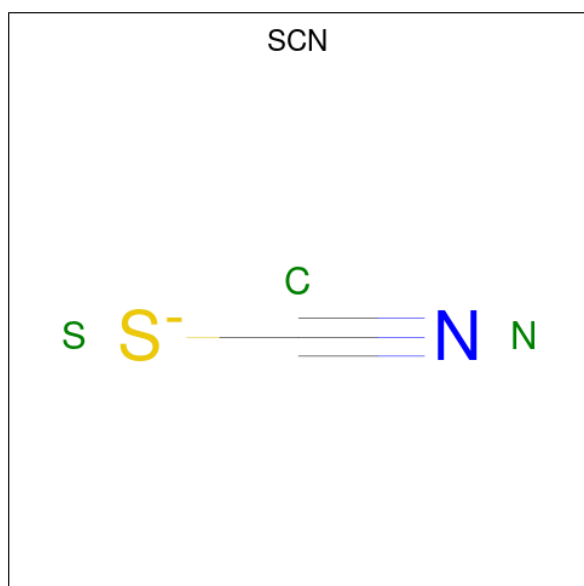
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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	17	Total	I	0	0
			17	17		

- Molecule 8 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

Continued on next page...

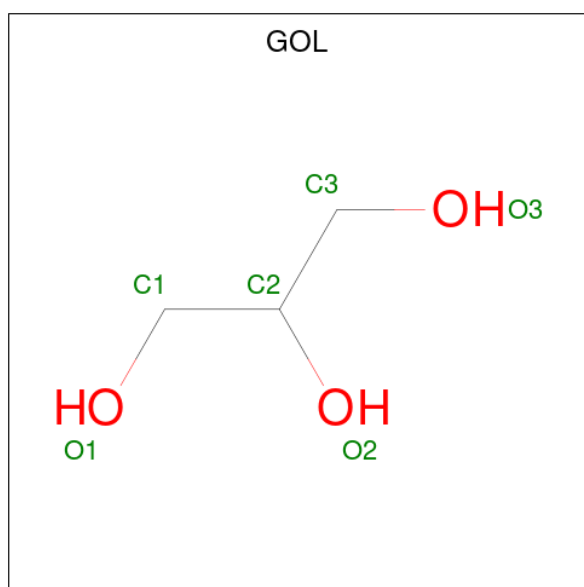
Continued from previous page...

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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	2	Total	Na	0	0
			2	2		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



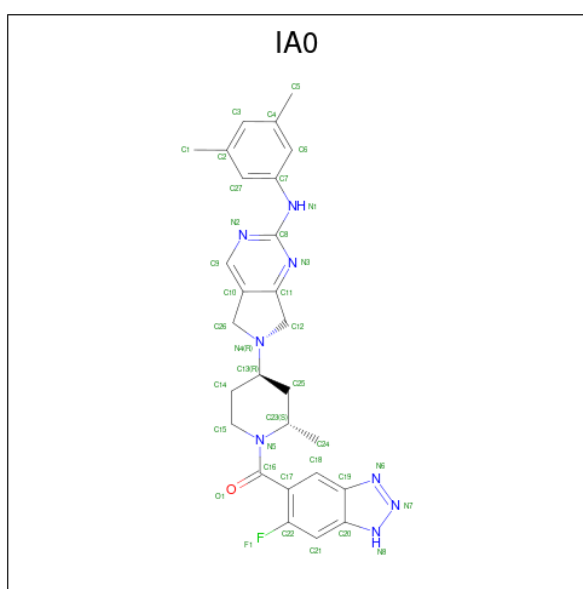
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
10	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
10	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
10	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
10	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
10	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

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

- Molecule 11 is [(2 {S},4 {R})-4-[2-[(3,5-dimethylphenyl)amino]-5,7-dihydropyrrolo[3,4-d]pyrimidin-6-yl]-2-methyl-piperidin-1-yl]-(6-fluoranyl-1 {H}-benzotriazol-5-yl)methanone (CCD ID: IA0) (formula: C₂₇H₂₉FN₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	AAA	1	Total	C	F	H	N	O	0	0
			66	27	1	29	8	1		

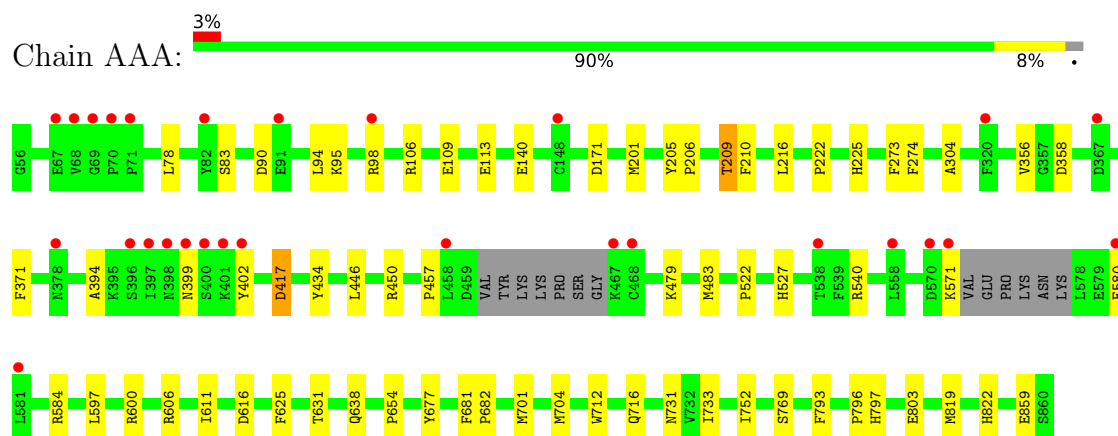
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AAA	527	Total	O	0	0
			527	527		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.66Å 62.53Å 63.64Å 104.16° 98.57° 93.15°	Depositor
Resolution (Å)	43.68 – 2.00 43.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.68-2.00) 98.0 (43.68-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.242 (Not available) , 0.228	Depositor DCC
R_{free} test set	2646 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 46.5	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	13509	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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, SCN, BMA, CA, 5JK, IA0, IOD, NA, ZN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	0.98	0/6590	1.32	0/8935

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	AAA	6404	6193	6160	40	0
2	AbA	25	25	22	0	0
3	AAA	14	14	12	0	0
4	AAA	2	0	0	0	0
5	AAA	29	46	0	0	0
6	AAA	1	0	0	0	0
7	AAA	17	0	0	3	1
8	AAA	18	0	0	0	0
9	AAA	2	0	0	0	0
10	AAA	54	72	72	1	0
11	AAA	37	29	0	2	0
12	AAA	527	0	0	2	1
All	All	7130	6379	6266	42	1

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 3.

All (42) 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:716:GLN:OE1	7:AAA:938:IOD:I	2.61	0.88
7:AAA:935:IOD:I	12:AAA:1454:HOH:O	2.74	0.75
1:AAA:540:ARG:NH1	12:AAA:1001:HOH:O	2.25	0.69
1:AAA:222:PRO:HA	1:AAA:225:HIS:CE1	2.32	0.65
1:AAA:399:ASN:HD21	1:AAA:402:TYR:HB2	1.68	0.58
1:AAA:654:PRO:HG3	7:AAA:910:IOD:I	2.73	0.58
1:AAA:273:PHE:HA	1:AAA:304:ALA:HB3	1.89	0.55
1:AAA:201:MET:HE1	1:AAA:356:VAL:CG2	2.40	0.52
11:AAA:928:IA0:C24	11:AAA:928:IA0:C17	2.87	0.52
1:AAA:803:GLU:OE2	1:AAA:822:HIS:HE1	1.93	0.51
1:AAA:417:ASP:OD1	1:AAA:417:ASP:N	2.42	0.51
1:AAA:522:PRO:HG2	10:AAA:922:GOL:H32	1.94	0.50
1:AAA:704:MET:HE1	1:AAA:712:TRP:CD1	2.48	0.49
1:AAA:371:PHE:CE1	1:AAA:457:PRO:HA	2.47	0.49
1:AAA:796:PRO:HD3	1:AAA:822:HIS:CD2	2.48	0.49
1:AAA:106:ARG:HD2	1:AAA:109:GLU:OE1	2.13	0.48
1:AAA:78:LEU:HD21	1:AAA:274:PHE:CB	2.44	0.47
1:AAA:682:PRO:HB3	1:AAA:716:GLN:HB3	1.97	0.46
1:AAA:479:LYS:O	1:AAA:859:GLU:HG3	2.14	0.46
1:AAA:171:ASP:OD1	1:AAA:358:ASP:OD2	2.34	0.45
1:AAA:769:SER:HB2	1:AAA:793[B]:PHE:CZ	2.51	0.45
1:AAA:600:ARG:HD2	1:AAA:611:ILE:HD11	1.98	0.45
1:AAA:793[B]:PHE:CE2	1:AAA:819:MET:HE3	2.52	0.45
1:AAA:597:LEU:HD12	1:AAA:731:ASN:HB2	1.99	0.44
1:AAA:78:LEU:HD21	1:AAA:274:PHE:HB3	2.00	0.44
1:AAA:704:MET:HA	1:AAA:797:HIS:NE2	2.33	0.44
1:AAA:90:ASP:O	1:AAA:94:LEU:HB2	2.18	0.43
1:AAA:205:TYR:CD1	1:AAA:206:PRO:HA	2.54	0.43
1:AAA:677:TYR:CD1	1:AAA:701:MET:HE3	2.54	0.43
1:AAA:446:LEU:HD23	1:AAA:446:LEU:HA	1.91	0.42
1:AAA:625:PHE:HE2	1:AAA:752:ILE:HD11	1.83	0.42
1:AAA:206:PRO:HD3	1:AAA:434:TYR:CE1	2.54	0.42
1:AAA:483:MET:HA	1:AAA:483:MET:HE2	2.02	0.42
1:AAA:95:LYS:NZ	1:AAA:113:GLU:O	2.42	0.41
1:AAA:677:TYR:CG	1:AAA:701:MET:HE3	2.56	0.41
1:AAA:681:PHE:CD1	1:AAA:682:PRO:HD2	2.55	0.41
1:AAA:606:ARG:HD2	1:AAA:606:ARG:HA	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:616:ASP:HB3	1:AAA:681:PHE:CZ	2.56	0.41
1:AAA:631:THR:O	1:AAA:733:ILE:HA	2.22	0.40
1:AAA:209:THR:HB	11:AAA:928:IA0:C24	2.51	0.40
1:AAA:394:ALA:HB2	1:AAA:402:TYR:CD1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AAA:908:IOD:I	12:AAA:1522:HOH:O[1_565]	1.83	0.37

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	788/805 (98%)	760 (96%)	28 (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	718/729 (98%)	706 (98%)	12 (2%)	53 60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	83	SER
1	AAA	98	ARG
1	AAA	140	GLU
1	AAA	209	THR
1	AAA	210	PHE
1	AAA	216	LEU
1	AAA	417	ASP
1	AAA	527	HIS
1	AAA	571	LYS
1	AAA	580	GLU
1	AAA	584	ARG
1	AAA	638	GLN

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

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](#)

2 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	0.57	0	17,19,21	1.47	3 (17%)
2	BMA	AbA	2	2	11,11,12	0.27	0	15,15,17	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	AbA	1	2	-	0/6/23/26	0/1/1/1
2	BMA	AbA	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	AbA	1	NAG	C1-O5-C5	4.15	117.75	112.19
2	AbA	1	NAG	C4-C3-C2	2.54	114.74	111.02
2	AbA	1	NAG	O5-C1-C2	2.52	115.19	111.29

There are no chirality outliers.

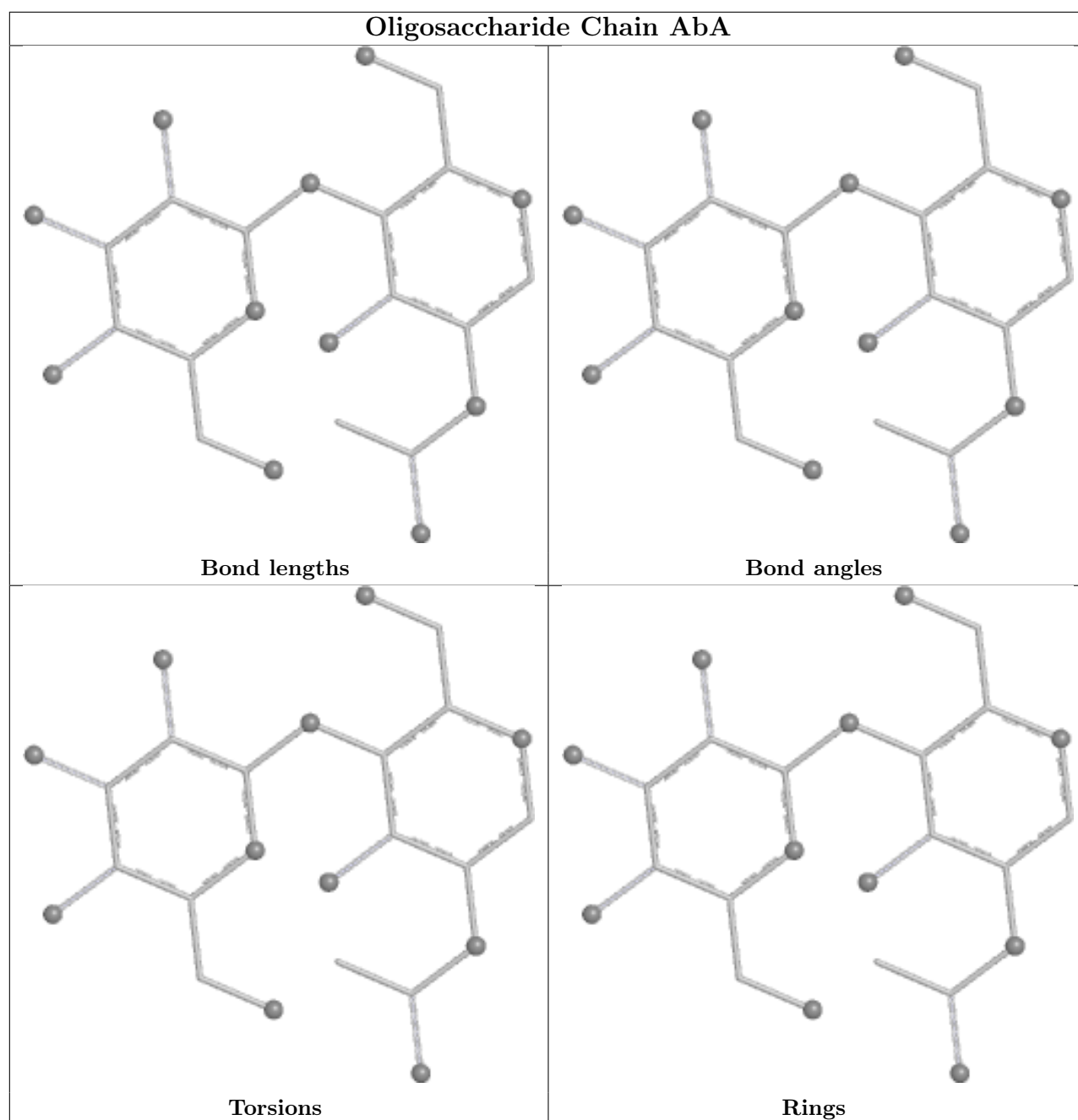
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AbA	2	BMA	O5-C5-C6-O6
2	AbA	2	BMA	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 40 ligands modelled in this entry, 22 are monoatomic - leaving 18 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
8	SCN	AAA	917	-	1,2,2	0.87	0	0,1,1	-	-
10	GOL	AAA	921	9	5,5,5	0.10	0	5,5,5	0.30	0
10	GOL	AAA	920	-	5,5,5	0.10	0	5,5,5	0.26	0
10	GOL	AAA	925	-	5,5,5	0.10	0	5,5,5	0.28	0
3	NAG	AAA	901	1	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
10	GOL	AAA	923	-	5,5,5	0.09	0	5,5,5	0.29	0
10	GOL	AAA	926	-	5,5,5	0.12	0	5,5,5	0.28	0
10	GOL	AAA	929	-	5,5,5	0.10	0	5,5,5	0.28	0
5	5JK	AAA	904	-	32,32,32	0.35	0	48,50,50	0.61	0
10	GOL	AAA	932	-	5,5,5	0.11	0	5,5,5	0.35	0
11	IA0	AAA	928	4	41,42,42	0.74	1 (2%)	53,62,62	1.43	11 (20%)
10	GOL	AAA	924	-	5,5,5	0.11	0	5,5,5	0.29	0
8	SCN	AAA	915	-	1,2,2	0.78	0	0,1,1	-	-
8	SCN	AAA	927	-	1,2,2	0.71	0	0,1,1	-	-
8	SCN	AAA	916	-	1,2,2	0.93	0	0,1,1	-	-
8	SCN	AAA	914	-	1,2,2	0.65	0	0,1,1	-	-
10	GOL	AAA	922	-	5,5,5	0.09	0	5,5,5	0.32	0
8	SCN	AAA	913	-	1,2,2	0.74	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
10	GOL	AAA	921	9	-	2/4/4/4	-
10	GOL	AAA	920	-	-	0/4/4/4	-
10	GOL	AAA	925	-	-	0/4/4/4	-
3	NAG	AAA	901	1	-	0/6/23/26	0/1/1/1
10	GOL	AAA	923	-	-	4/4/4/4	-
10	GOL	AAA	929	-	-	1/4/4/4	-
5	5JK	AAA	904	-	-	0/10/71/71	0/4/4/4
10	GOL	AAA	932	-	-	4/4/4/4	-
11	IA0	AAA	928	4	-	3/16/37/37	0/6/6/6
10	GOL	AAA	924	-	-	2/4/4/4	-
10	GOL	AAA	922	-	-	2/4/4/4	-
10	GOL	AAA	926	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AAA	928	IA0	C10-C11	-4.10	1.34	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AAA	928	IA0	C23-N5-C16	4.10	130.51	120.32
11	AAA	928	IA0	C25-C13-C14	3.19	114.98	110.60
11	AAA	928	IA0	C18-C17-C22	3.09	120.66	116.83
11	AAA	928	IA0	C17-C16-N5	2.79	121.67	117.85
11	AAA	928	IA0	C10-C9-N2	-2.73	119.39	123.83
11	AAA	928	IA0	C10-C11-N3	-2.73	122.40	125.35
11	AAA	928	IA0	C21-C22-C17	-2.64	120.56	123.48
3	AAA	901	NAG	C1-O5-C5	2.45	115.47	112.19
11	AAA	928	IA0	N2-C8-N3	-2.24	124.25	126.42
11	AAA	928	IA0	C15-N5-C16	-2.23	117.83	123.81
11	AAA	928	IA0	C15-N5-C23	-2.03	111.39	114.75
11	AAA	928	IA0	C24-C23-N5	2.02	114.76	111.55

There are no chirality outliers.

All (20) torsion outliers are listed below:

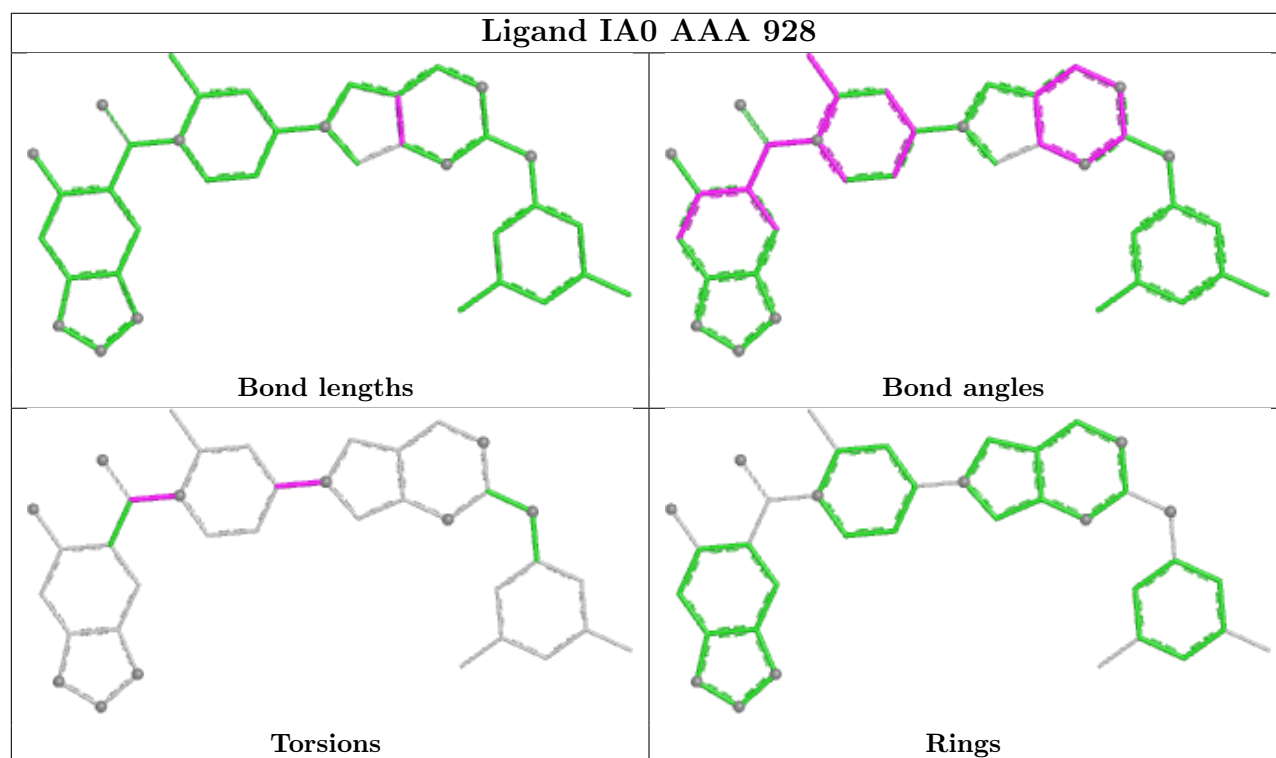
Mol	Chain	Res	Type	Atoms
10	AAA	923	GOL	C1-C2-C3-O3
10	AAA	932	GOL	C1-C2-C3-O3
10	AAA	923	GOL	O2-C2-C3-O3
10	AAA	921	GOL	C1-C2-C3-O3
10	AAA	922	GOL	O1-C1-C2-C3
10	AAA	923	GOL	O1-C1-C2-C3
10	AAA	924	GOL	C1-C2-C3-O3
10	AAA	926	GOL	C1-C2-C3-O3
10	AAA	932	GOL	O1-C1-C2-C3
10	AAA	926	GOL	O2-C2-C3-O3
10	AAA	932	GOL	O1-C1-C2-O2
10	AAA	932	GOL	O2-C2-C3-O3
11	AAA	928	IA0	O1-C16-N5-C15
10	AAA	921	GOL	O2-C2-C3-O3
11	AAA	928	IA0	C17-C16-N5-C15
10	AAA	923	GOL	O1-C1-C2-O2
10	AAA	929	GOL	C1-C2-C3-O3
10	AAA	922	GOL	O1-C1-C2-O2
10	AAA	924	GOL	O2-C2-C3-O3
11	AAA	928	IA0	C14-C13-N4-C26

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AAA	928	IA0	2	0
10	AAA	922	GOL	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 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 ⓘ

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	AAA	792/805 (98%)	0.21	28 (3%) 47 46	9, 26, 47, 78	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	397	ILE	4.8
1	AAA	399	ASN	3.6
1	AAA	398	ASN	3.5
1	AAA	581	LEU	3.4
1	AAA	400	SER	3.3
1	AAA	69	GLY	3.1
1	AAA	68	VAL	3.0
1	AAA	82	TYR	2.9
1	AAA	396	SER	2.6
1	AAA	558	LEU	2.5
1	AAA	70	PRO	2.5
1	AAA	71	PRO	2.5
1	AAA	320	PHE	2.4
1	AAA	401	LYS	2.4
1	AAA	91	GLU	2.4
1	AAA	538	THR	2.4
1	AAA	67	GLU	2.3
1	AAA	580	GLU	2.3
1	AAA	458	LEU	2.3
1	AAA	378	ASN	2.2
1	AAA	148	CYS	2.2
1	AAA	467	LYS	2.2
1	AAA	367	ASP	2.2
1	AAA	468	CYS	2.2
1	AAA	571	LYS	2.2
1	AAA	402	TYR	2.1
1	AAA	98	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	570	ASP	2.0

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

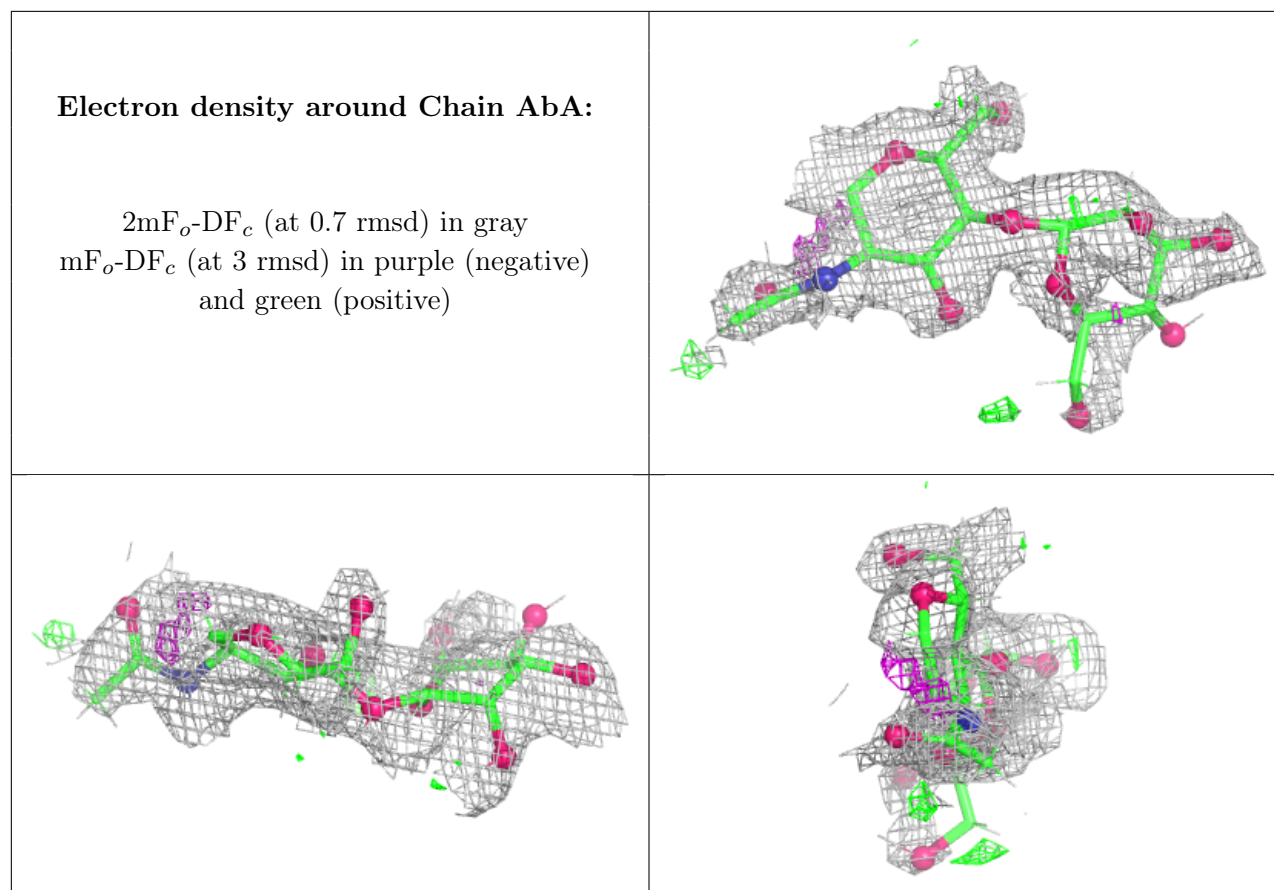
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	AbA	1	14/15	-	-	30,37,40,43	2
2	BMA	AbA	2	11/12	-	-	30,60,65,66	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.



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
8	SCN	AAA	927	3/3	0.69	0.22	56,56,59,62	0
10	GOL	AAA	921	6/6	0.73	0.17	30,48,49,49	2
8	SCN	AAA	913	3/3	0.75	0.23	57,57,59,61	0
10	GOL	AAA	926	6/6	0.76	0.20	30,37,41,41	2
10	GOL	AAA	929	6/6	0.76	0.17	30,58,60,60	2
10	GOL	AAA	920	6/6	0.79	0.15	30,50,51,51	2
10	GOL	AAA	932	6/6	0.79	0.23	30,43,46,46	2
10	GOL	AAA	924	6/6	0.80	0.18	30,42,43,43	2
10	GOL	AAA	922	6/6	0.80	0.13	30,36,37,39	2
8	SCN	AAA	916	3/3	0.81	0.21	40,40,41,42	0
7	IOD	AAA	940	1/1	0.82	0.24	135,135,135,135	0
8	SCN	AAA	917	3/3	0.82	0.15	39,39,40,40	0
10	GOL	AAA	925	6/6	0.84	0.14	30,39,41,42	2

Continued on next page...

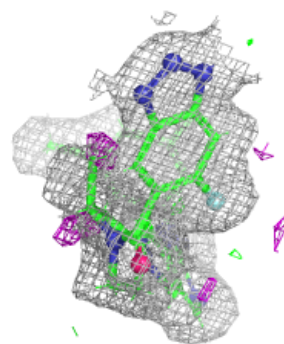
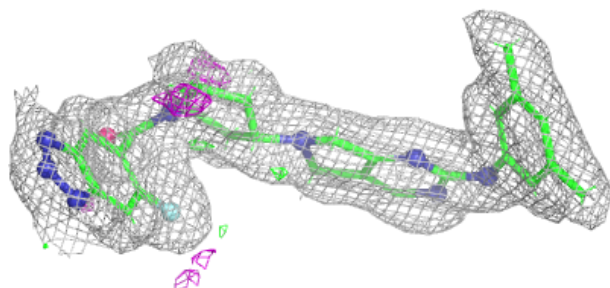
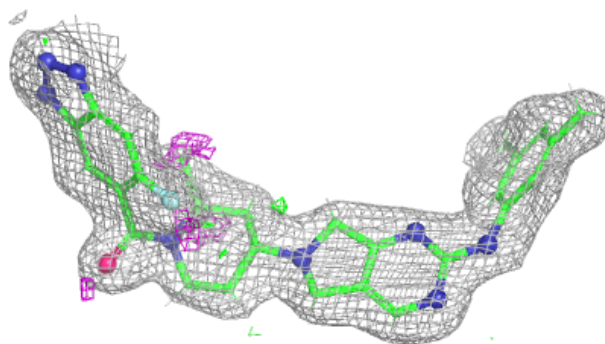
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	IOD	AAA	936	1/1	0.84	0.19	118,118,118,118	0
9	NA	AAA	918	1/1	0.86	0.14	41,41,41,41	0
5	5JK	AAA	904	29/29	0.87	0.09	22,24,25,30	1
10	GOL	AAA	923	6/6	0.88	0.15	30,40,42,43	2
7	IOD	AAA	934	1/1	0.91	0.22	103,103,103,103	0
7	IOD	AAA	937	1/1	0.91	0.21	98,98,98,98	0
7	IOD	AAA	938	1/1	0.91	0.16	86,86,86,86	0
9	NA	AAA	919	1/1	0.92	0.06	26,26,26,26	0
7	IOD	AAA	939	1/1	0.92	0.16	65,65,65,65	0
8	SCN	AAA	914	3/3	0.93	0.12	37,37,37,38	0
11	IA0	AAA	928	37/37	0.93	0.07	16,20,22,23	0
8	SCN	AAA	915	3/3	0.95	0.09	35,35,35,36	0
7	IOD	AAA	933	1/1	0.95	0.10	42,42,42,42	0
4	ZN	AAA	903	1/1	0.95	0.15	108,108,108,108	0
7	IOD	AAA	931	1/1	0.95	0.14	100,100,100,100	0
3	NAG	AAA	901	14/15	0.96	0.06	17,20,24,30	2
7	IOD	AAA	935	1/1	0.97	0.21	79,79,79,79	0
7	IOD	AAA	908	1/1	0.97	0.12	56,56,56,56	0
7	IOD	AAA	907	1/1	0.97	0.15	67,67,67,67	0
7	IOD	AAA	909	1/1	0.98	0.11	59,59,59,59	0
7	IOD	AAA	910	1/1	0.98	0.07	56,56,56,56	0
7	IOD	AAA	930	1/1	0.98	0.16	73,73,73,73	0
4	ZN	AAA	902	1/1	0.99	0.02	22,22,22,22	0
7	IOD	AAA	906	1/1	0.99	0.02	25,25,25,25	0
7	IOD	AAA	911	1/1	0.99	0.10	40,40,40,40	0
7	IOD	AAA	912	1/1	0.99	0.11	45,45,45,45	0
6	CA	AAA	905	1/1	1.00	0.01	20,20,20,20	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.

Electron density around IA0 AAA 928:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.