Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2023 – 03:54 pm GMT

PDB ID	:	7Z3L
Title	:	Autotaxin in complex with hybrid compound ziritaxestat (GLPG1690)
Authors	:	Salgado-Polo, F.; Ford, P.; Heckmann, B.; Perrakis, A.
Deposited on	:	2022-03-02
Resolution	:	2.40 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:

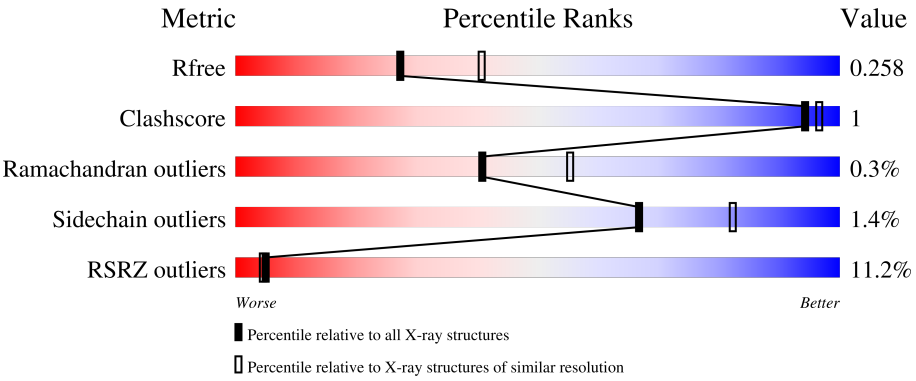
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	11% 94%
2	AcA	7	57% 43%

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
6	IOD	AAA	912	-	-	-	X
7	SCN	AAA	917	-	-	-	X
7	SCN	AAA	921	-	-	-	X
8	NA	AAA	924	-	-	-	X
9	GOL	AAA	928	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 12995 atoms, of which 6319 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.

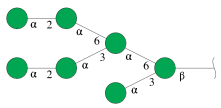
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	788	12481	4023	6133	1097	1179	49	205	0	1

There are 3 discrepancies between the modelled and reference sequences:

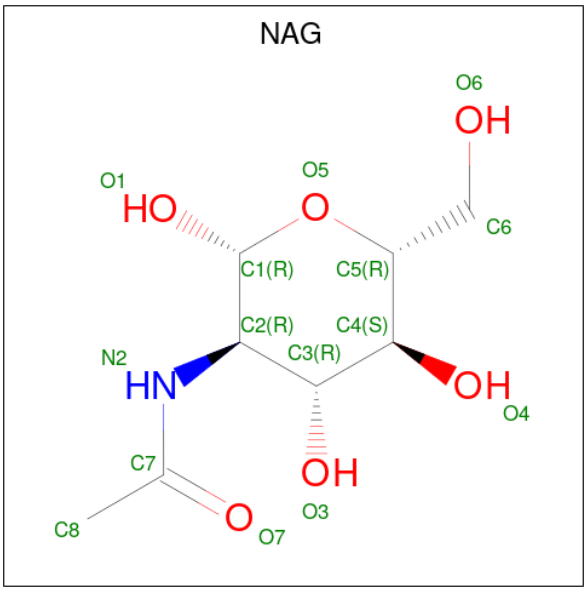
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	410	ALA	ASN	engineered mutation	UNP Q64610
AAA	591	THR	ARG	engineered mutation	UNP Q64610
AAA	806	ALA	ASN	engineered mutation	UNP Q64610

- Molecule 2 is an oligosaccharide called 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-(1-3)]beta-D-mannopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	AcA	7	154	42	77	35	23	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

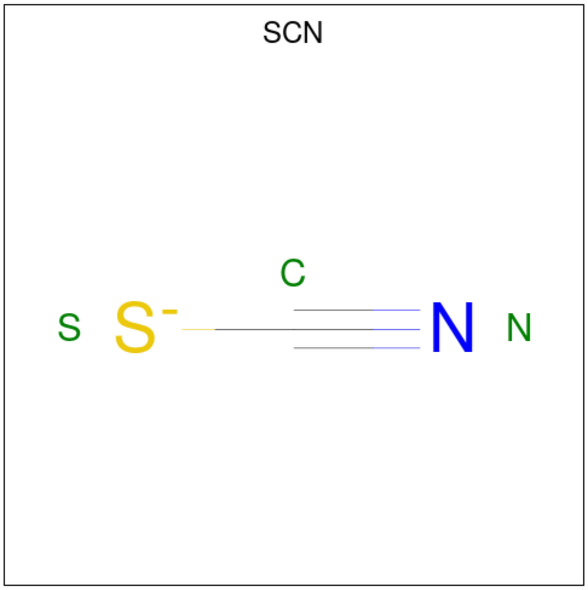
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	10	Total I 10 10	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

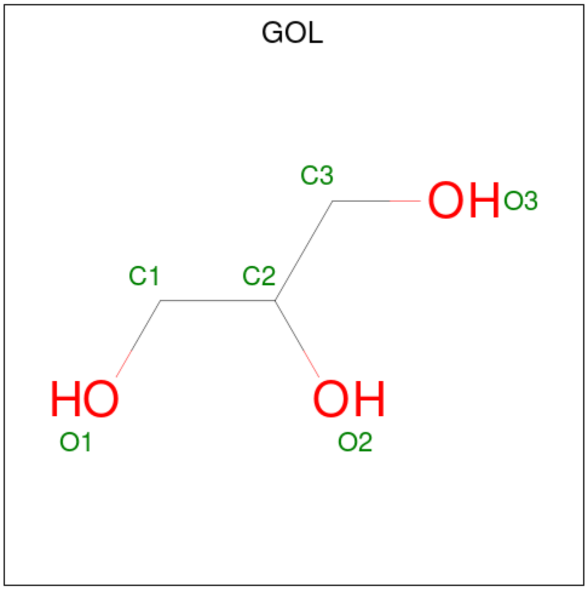


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

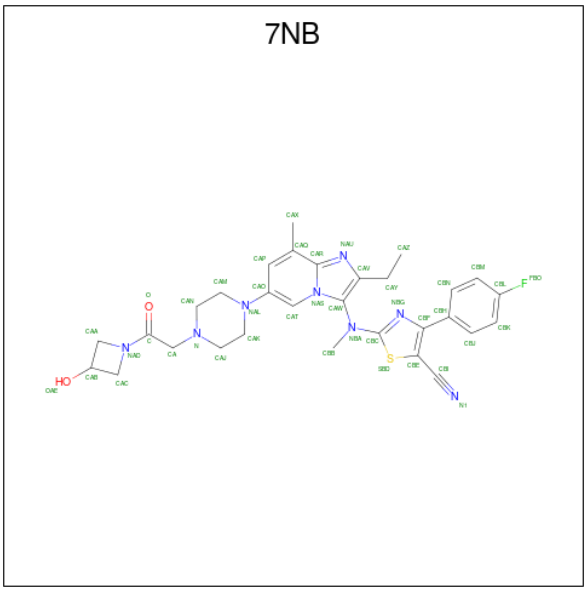
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total Na 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 is 2-[[2-ethyl-8-methyl-6-[4-[2-(3-oxidanylazetidin-1-yl)-2-oxidanylidene-ethyl]piperazin-1-yl]imidazo[1,2-a]pyridin-3-yl]-methyl-amino]-4-(4-fluorophenyl)-1,3-thiazole-5-carbonitrile (three-letter code: 7NB) (formula: $C_{30}H_{33}FN_8O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	AAA	1	Total	C	F	H	N	O	S	1	0
			75	30	1	33	8	2	1		

- Molecule 11 is water.

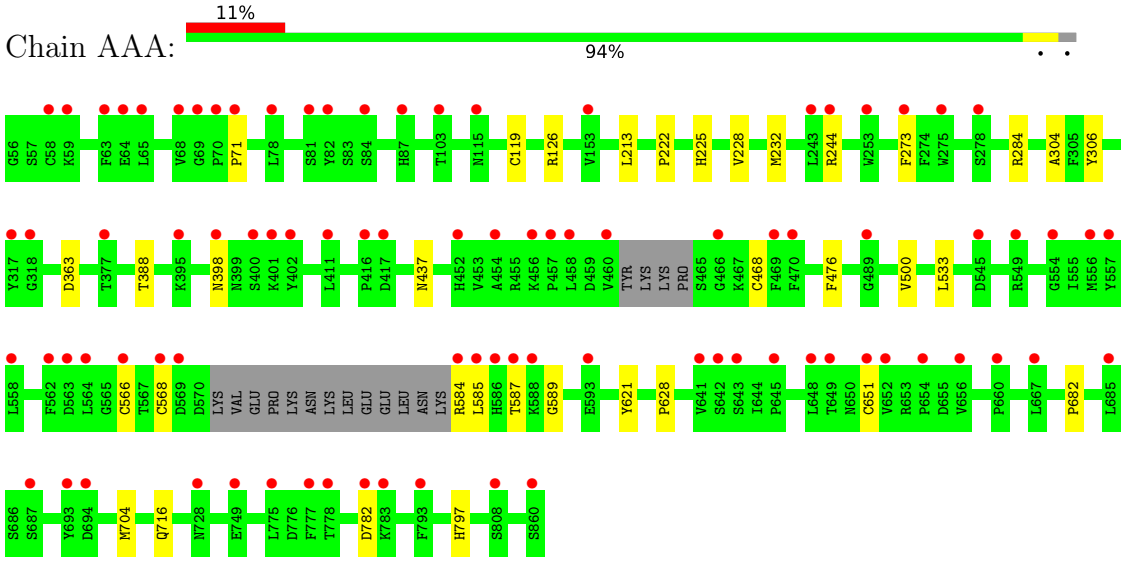
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AAA	104	Total	O	0	0
			104	104		

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

Chain AAA:



• 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-(1-3)]beta-D-mannopyranose

Chain AcA:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.84Å 88.71Å 77.03Å 90.00° 102.83° 90.00°	Depositor
Resolution (Å)	45.92 – 2.40 45.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.92-2.40) 99.7 (45.92-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.241 , 0.255 0.247 , 0.258	Depositor DCC
R_{free} test set	1591 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	1.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12995	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 7NB, NAG, GOL, IOD, SCN, BMA, CA, ZN, 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	0.65	0/6527	0.69	0/8852

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

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	6348	6133	6099	16	0
2	AcA	77	77	64	0	0
3	AAA	28	28	24	0	0
4	AAA	2	0	0	0	0
5	AAA	1	0	0	0	0
6	AAA	10	0	0	1	0
7	AAA	27	0	0	1	0
8	AAA	1	0	0	0	0
9	AAA	36	48	48	0	0
10	AAA	42	33	0	4	0
11	AAA	104	0	0	0	0
All	All	6676	6319	6235	17	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 1.

All (17) 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:273:PHE:HB3	10:AAA:932:7NB:N1	2.03	0.73
1:AAA:273:PHE:HB3	10:AAA:932:7NB:CBI	2.26	0.66
1:AAA:568:CYS:HA	1:AAA:651:CYS:HA	1.80	0.62
1:AAA:222:PRO:HA	1:AAA:225:HIS:CE1	2.37	0.59
1:AAA:782:ASP:OD1	6:AAA:914:IOD:I	2.91	0.59
7:AAA:917:SCN:S	10:AAA:932:7NB:N1	2.76	0.58
1:AAA:273:PHE:CB	10:AAA:932:7NB:N1	2.66	0.57
1:AAA:284:ARG:NH1	1:AAA:306:TYR:O	2.45	0.50
1:AAA:704:MET:HA	1:AAA:797:HIS:NE2	2.28	0.48
1:AAA:228:VAL:HG11	1:AAA:437:ASN:HD22	1.78	0.47
1:AAA:388:THR:HG22	1:AAA:476:PHE:CZ	2.50	0.46
1:AAA:273:PHE:HA	1:AAA:304:ALA:HB3	1.98	0.45
1:AAA:500:VAL:HG11	1:AAA:533:LEU:HD23	2.01	0.43
1:AAA:682:PRO:HB3	1:AAA:716:GLN:HB3	1.99	0.43
1:AAA:621:TYR:HA	1:AAA:628:PRO:HA	1.99	0.43
1:AAA:213:LEU:HD11	1:AAA:306:TYR:CE1	2.54	0.42
1:AAA:228:VAL:HG22	1:AAA:232:MET:SD	2.60	0.41

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	782/805 (97%)	737 (94%)	43 (6%)	2 (0%)	41 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	71	PRO
1	AAA	589	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	AAA	711/729 (98%)	701 (99%)	10 (1%)	67 82

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

Mol	Chain	Res	Type
1	AAA	119	CYS
1	AAA	126	ARG
1	AAA	244	ARG
1	AAA	363	ASP
1	AAA	398	ASN
1	AAA	468	CYS
1	AAA	566	CYS
1	AAA	584	ARG
1	AAA	585	LEU
1	AAA	587	THR

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)

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	BMA	AcA	1	2	11,11,12	0.34	0	15,15,17	1.17	1 (6%)
2	MAN	AcA	2	2	11,11,12	0.30	0	15,15,17	0.67	0
2	MAN	AcA	3	2	11,11,12	0.29	0	15,15,17	0.67	0
2	MAN	AcA	4	2	11,11,12	0.29	0	15,15,17	0.68	0
2	MAN	AcA	5	2	11,11,12	0.40	0	15,15,17	1.42	2 (13%)
2	MAN	AcA	6	2	11,11,12	0.25	0	15,15,17	0.62	0
2	MAN	AcA	7	2	11,11,12	0.34	0	15,15,17	0.99	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	BMA	AcA	1	2	-	0/2/19/22	0/1/1/1
2	MAN	AcA	2	2	-	2/2/19/22	0/1/1/1
2	MAN	AcA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AcA	4	2	-	2/2/19/22	0/1/1/1
2	MAN	AcA	5	2	-	2/2/19/22	0/1/1/1
2	MAN	AcA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	AcA	7	2	-	0/2/19/22	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(^{o})	Ideal(^{o})
2	AcA	5	MAN	C3-C4-C5	3.59	116.64	110.24
2	AcA	1	BMA	C1-C2-C3	3.38	113.81	109.67
2	AcA	5	MAN	O5-C1-C2	-2.98	106.17	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AcA	7	MAN	C1-C2-C3	2.51	112.75	109.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

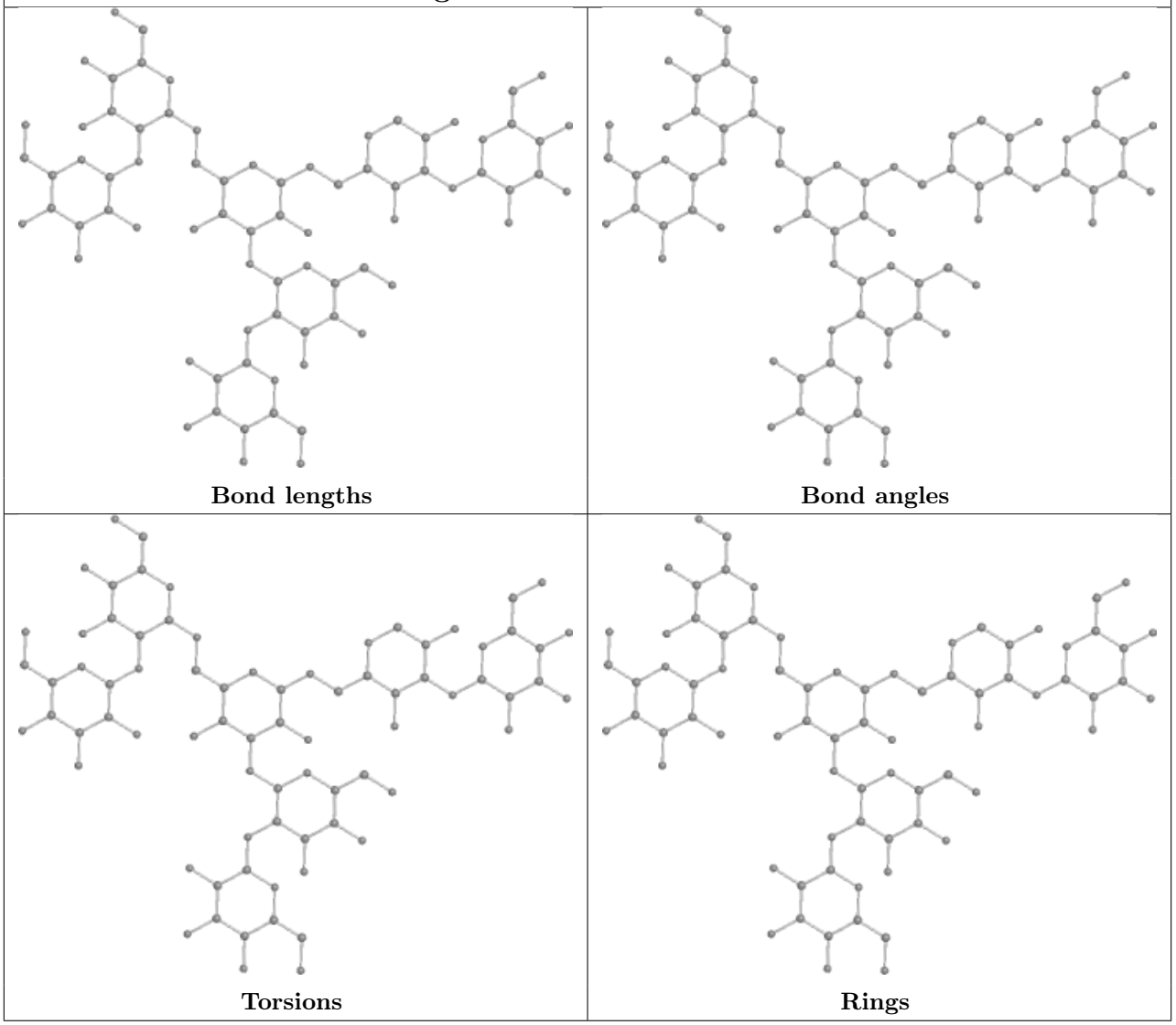
Mol	Chain	Res	Type	Atoms
2	AcA	5	MAN	O5-C5-C6-O6
2	AcA	4	MAN	C4-C5-C6-O6
2	AcA	4	MAN	O5-C5-C6-O6
2	AcA	2	MAN	O5-C5-C6-O6
2	AcA	5	MAN	C4-C5-C6-O6
2	AcA	2	MAN	C4-C5-C6-O6

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.

Oligosaccharide Chain AcA



5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 14 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	$\#\|Z\| > 2$
7	SCN	AAA	920	-	1,2,2	0.69	0	0,1,1	-	-
9	GOL	AAA	927	-	5,5,5	0.09	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	7NB	AAA	932	-	38,47,47	0.86	2 (5%)	38,69,69	0.91	3 (7%)
7	SCN	AAA	916	-	1,2,2	0.72	0	0,1,1	-	-
3	NAG	AAA	901	1	14,14,15	0.25	0	17,19,21	0.95	2 (11%)
7	SCN	AAA	922	-	1,2,2	0.78	0	0,1,1	-	-
9	GOL	AAA	929	-	5,5,5	0.09	0	5,5,5	0.28	0
3	NAG	AAA	902	-	14,14,15	0.37	0	17,19,21	0.90	1 (5%)
7	SCN	AAA	918	-	1,2,2	0.69	0	0,1,1	-	-
7	SCN	AAA	919	-	1,2,2	0.73	0	0,1,1	-	-
7	SCN	AAA	931	-	1,2,2	0.72	0	0,1,1	-	-
9	GOL	AAA	926	-	5,5,5	0.10	0	5,5,5	0.28	0
9	GOL	AAA	925	-	5,5,5	0.10	0	5,5,5	0.26	0
9	GOL	AAA	930	-	5,5,5	0.09	0	5,5,5	0.24	0
9	GOL	AAA	928	-	5,5,5	0.08	0	5,5,5	0.27	0
7	SCN	AAA	917	-	1,2,2	0.84	0	0,1,1	-	-
7	SCN	AAA	923	-	1,2,2	0.80	0	0,1,1	-	-
7	SCN	AAA	921	-	1,2,2	0.71	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
9	GOL	AAA	927	-	-	4/4/4/4	-
10	7NB	AAA	932	-	-	3/15/46/46	0/6/6/6
3	NAG	AAA	901	1	-	0/6/23/26	0/1/1/1
9	GOL	AAA	929	-	-	0/4/4/4	-
3	NAG	AAA	902	-	-	0/6/23/26	0/1/1/1
9	GOL	AAA	926	-	-	2/4/4/4	-
9	GOL	AAA	925	-	-	2/4/4/4	-
9	GOL	AAA	930	-	-	2/4/4/4	-
9	GOL	AAA	928	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AAA	932	7NB	CAQ-CAR	-2.44	1.39	1.43
10	AAA	932	7NB	CAV-CAW	-2.36	1.38	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	901	NAG	C1-O5-C5	2.63	115.75	112.19
10	AAA	932	7NB	CAM-NAL-CAO	2.43	124.66	118.09
3	AAA	902	NAG	C1-O5-C5	2.39	115.43	112.19
10	AAA	932	7NB	CAK-NAL-CAO	2.24	124.15	118.09
3	AAA	901	NAG	O5-C1-C2	-2.23	107.77	111.29
10	AAA	932	7NB	CA-C-NAD	2.02	119.62	117.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AAA	927	GOL	C1-C2-C3-O3
10	AAA	932	7NB	NBG-CBF-CBH-CBJ
10	AAA	932	7NB	NBG-CBF-CBH-CBN
9	AAA	927	GOL	O1-C1-C2-O2
9	AAA	925	GOL	O1-C1-C2-C3
9	AAA	926	GOL	C1-C2-C3-O3
9	AAA	927	GOL	O1-C1-C2-C3
9	AAA	930	GOL	C1-C2-C3-O3
9	AAA	926	GOL	O2-C2-C3-O3
9	AAA	925	GOL	O1-C1-C2-O2
9	AAA	927	GOL	O2-C2-C3-O3
9	AAA	930	GOL	O2-C2-C3-O3
10	AAA	932	7NB	O-C-CA-N

There are no ring outliers.

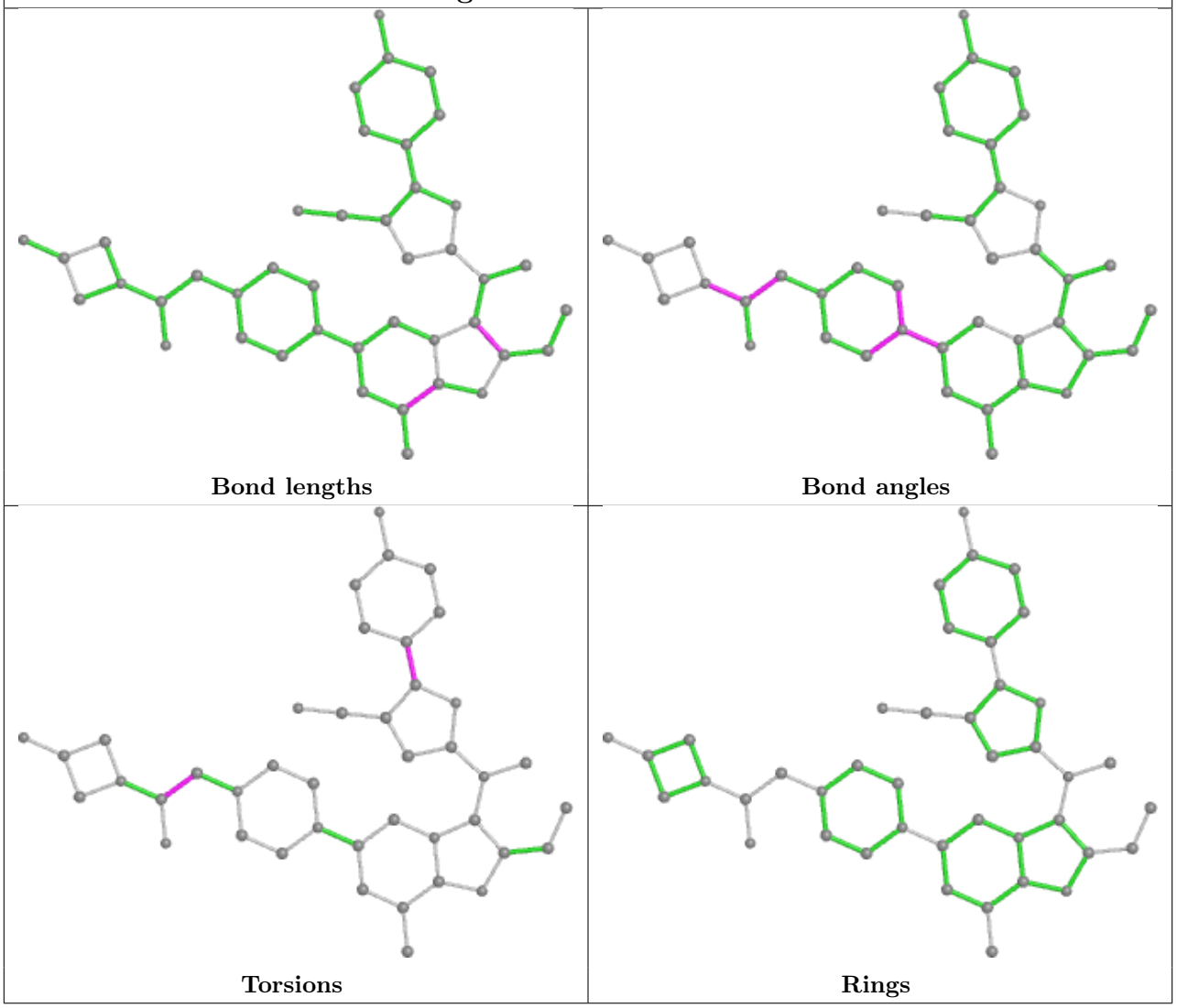
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AAA	932	7NB	4	0
7	AAA	917	SCN	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 then 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.

Ligand 7NB AAA 932



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, 95^{th} 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	788/805 (97%)	0.91	88 (11%) 5 4	36, 69, 112, 155	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	585	LEU	7.5
1	AAA	460	VAL	6.5
1	AAA	860	SER	6.4
1	AAA	554	GLY	6.0
1	AAA	469	PHE	5.5
1	AAA	586	HIS	5.4
1	AAA	556	MET	5.3
1	AAA	587	THR	5.1
1	AAA	641	VAL	4.8
1	AAA	82	TYR	4.7
1	AAA	656	VAL	4.3
1	AAA	557	TYR	4.3
1	AAA	244	ARG	4.3
1	AAA	103	THR	4.2
1	AAA	68	VAL	4.1
1	AAA	687	SER	4.0
1	AAA	398	ASN	3.9
1	AAA	466	GLY	3.9
1	AAA	562	PHE	3.9
1	AAA	78	LEU	3.8
1	AAA	64	GLU	3.8
1	AAA	69	GLY	3.8
1	AAA	660	PRO	3.6
1	AAA	377	THR	3.3
1	AAA	569	ASP	3.3
1	AAA	693	TYR	3.1
1	AAA	416	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	648	LEU	3.0
1	AAA	71	PRO	3.0
1	AAA	643	SER	2.9
1	AAA	654	PRO	2.9
1	AAA	775	LEU	2.9
1	AAA	278	SER	2.9
1	AAA	417	ASP	2.9
1	AAA	454	ALA	2.9
1	AAA	568	CYS	2.9
1	AAA	243	LEU	2.9
1	AAA	253	TRP	2.8
1	AAA	317	TYR	2.8
1	AAA	402	TYR	2.8
1	AAA	549	ARG	2.8
1	AAA	564	LEU	2.8
1	AAA	563	ASP	2.8
1	AAA	652	VAL	2.7
1	AAA	59	LYS	2.7
1	AAA	318	GLY	2.7
1	AAA	694	ASP	2.7
1	AAA	685	LEU	2.7
1	AAA	783	LYS	2.7
1	AAA	588	LYS	2.6
1	AAA	273	PHE	2.6
1	AAA	401	LYS	2.6
1	AAA	400	SER	2.6
1	AAA	777	PHE	2.6
1	AAA	87	HIS	2.6
1	AAA	645	PRO	2.6
1	AAA	395	LYS	2.5
1	AAA	667	LEU	2.5
1	AAA	153	VAL	2.5
1	AAA	558	LEU	2.5
1	AAA	566	CYS	2.4
1	AAA	452	HIS	2.4
1	AAA	808	SER	2.4
1	AAA	275	TRP	2.4
1	AAA	470	PHE	2.4
1	AAA	584	ARG	2.3
1	AAA	58	CYS	2.3
1	AAA	489	GLY	2.3
1	AAA	649	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	545	ASP	2.3
1	AAA	456	LYS	2.3
1	AAA	793	PHE	2.3
1	AAA	749	GLU	2.3
1	AAA	782	ASP	2.2
1	AAA	115	ASN	2.2
1	AAA	651	CYS	2.2
1	AAA	728	ASN	2.2
1	AAA	778	THR	2.2
1	AAA	458	LEU	2.2
1	AAA	593	GLU	2.2
1	AAA	70	PRO	2.1
1	AAA	65	LEU	2.1
1	AAA	81	SER	2.1
1	AAA	84	SER	2.1
1	AAA	642	SER	2.0
1	AAA	411	LEU	2.0
1	AAA	63	PHE	2.0
1	AAA	457	PRO	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, 95^{th} 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.

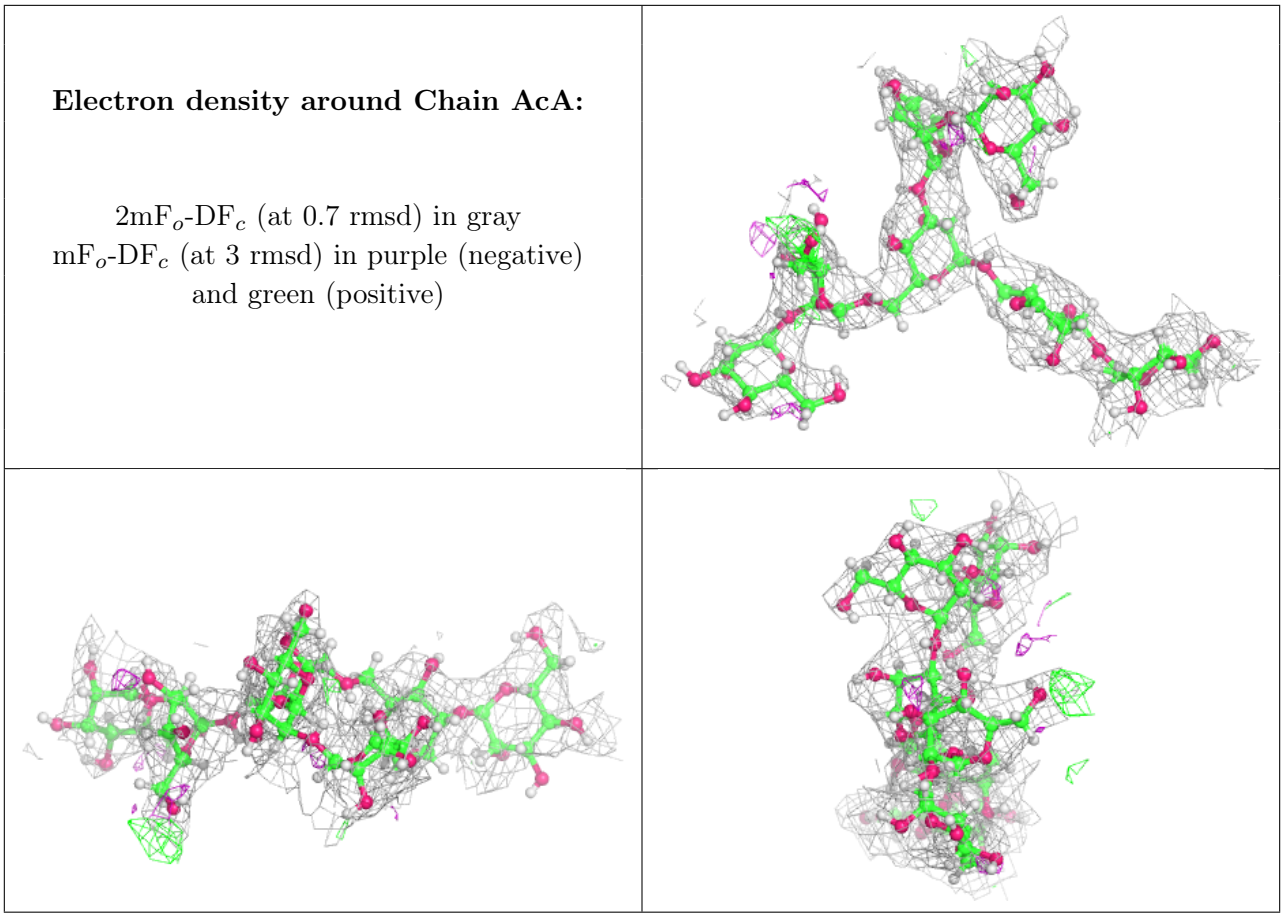
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	AcA	7	11/12	0.71	0.26	30,82,88,90	4
2	MAN	AcA	6	11/12	0.79	0.23	30,77,79,80	4
2	MAN	AcA	5	11/12	0.84	0.21	30,72,76,78	3
2	MAN	AcA	2	11/12	0.86	0.17	30,73,76,77	2
2	MAN	AcA	4	11/12	0.87	0.20	30,66,69,70	4
2	BMA	AcA	1	11/12	0.90	0.18	30,73,77,78	3
2	MAN	AcA	3	11/12	0.91	0.14	30,69,74,76	3

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain AcA:

$2mF_o$-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, 95^{th} 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
9	GOL	AAA	928	6/6	-0.32	1.62	30,126,128,129	2
8	NA	AAA	924	1/1	0.33	0.58	125,125,125,125	0
7	SCN	AAA	917	3/3	0.37	0.48	101,101,101,101	0
6	IOD	AAA	912	1/1	0.45	0.65	242,242,242,242	0
7	SCN	AAA	921	3/3	0.54	0.57	109,109,111,113	0
9	GOL	AAA	926	6/6	0.65	0.38	30,74,77,77	2
7	SCN	AAA	931	3/3	0.73	0.29	74,74,76,79	0
7	SCN	AAA	918	3/3	0.73	0.31	95,95,95,95	0
6	IOD	AAA	909	1/1	0.79	0.15	242,242,242,242	0
9	GOL	AAA	925	6/6	0.80	0.34	30,81,84,85	2
7	SCN	AAA	919	3/3	0.81	0.28	72,72,73,74	0

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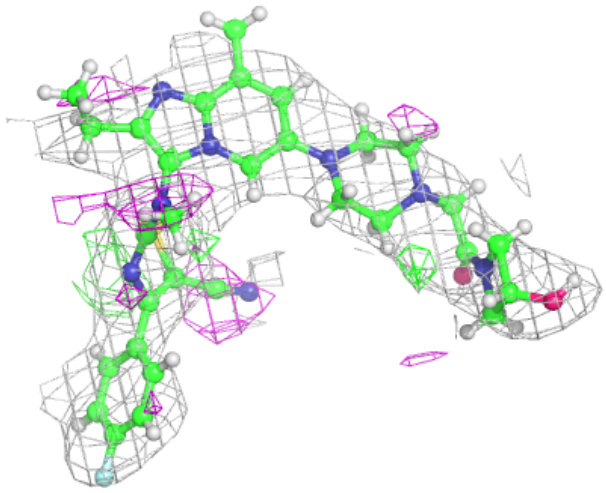
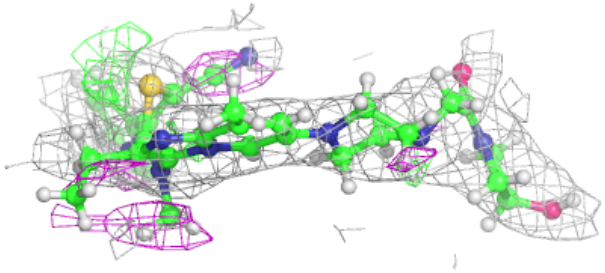
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GOL	AAA	930	6/6	0.81	0.42	30,99,103,103	2
9	GOL	AAA	927	6/6	0.83	0.70	30,71,73,75	2
6	IOD	AAA	915	1/1	0.84	0.15	136,136,136,136	0
6	IOD	AAA	910	1/1	0.84	0.18	250,250,250,250	0
9	GOL	AAA	929	6/6	0.84	0.47	30,103,106,107	2
6	IOD	AAA	913	1/1	0.84	0.07	134,134,134,134	0
7	SCN	AAA	920	3/3	0.86	0.25	81,81,82,83	0
10	7NB	AAA	932	42/42	0.86	0.28	30,64,71,72	1
4	ZN	AAA	904	1/1	0.89	0.07	87,87,87,87	0
7	SCN	AAA	922	3/3	0.93	0.31	83,83,83,84	0
3	NAG	AAA	902	14/15	0.94	0.18	30,54,59,62	2
3	NAG	AAA	901	14/15	0.95	0.21	30,42,46,47	2
7	SCN	AAA	916	3/3	0.95	0.13	100,100,101,102	0
7	SCN	AAA	923	3/3	0.95	0.16	82,82,84,86	0
6	IOD	AAA	911	1/1	0.95	0.09	127,127,127,127	0
6	IOD	AAA	908	1/1	0.97	0.06	100,100,100,100	0
6	IOD	AAA	907	1/1	0.97	0.11	112,112,112,112	0
6	IOD	AAA	914	1/1	0.98	0.10	133,133,133,133	0
6	IOD	AAA	906	1/1	0.99	0.15	55,55,55,55	0
4	ZN	AAA	903	1/1	0.99	0.12	59,59,59,59	0
5	CA	AAA	905	1/1	0.99	0.17	51,51,51,51	0

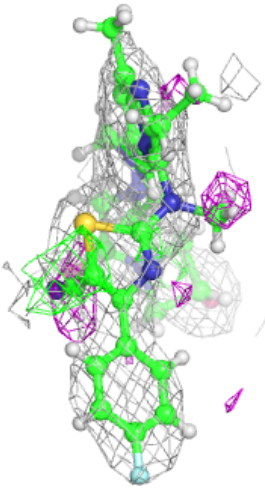
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7NB AAA 932:

$2mF_o$-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

There are no such residues in this entry.