



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:38 PM UTC

PDB ID : 7G4N / pdb_00007g4n

Title : Crystal Structure of rat Autotaxin in complex with [4-(trifluoromethoxy)phenyl]methyl (3aS,6aS)-2-(6-sulfamoylpyridine-3-carbonyl)-1,3,3a,4,6,6a-hexahydropsyrrolo[3,4-c]pyrrole-5-carboxylate, i.e. SMILES FC(=O)N1C[C@H]2[C@H](C1)CN(C2)C(=O)c1cnc(cc1)S(=O)(=O)N(F)F with IC50=0.0134798 microM

Authors : Stihle, M.; Benz, J.; Hunziker, D.; Mattei, P.; Rudolph, M.G.

Deposited on : 2023-06-05

Resolution : 1.67 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)

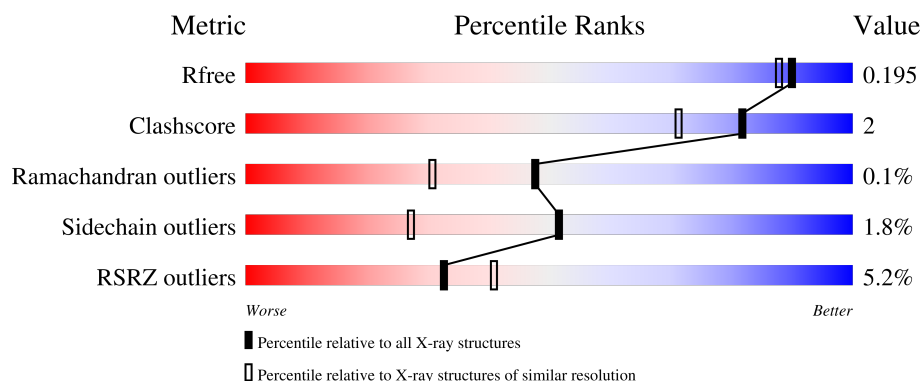
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	846	5% 88% 7% 5%
2	B	8	100%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7291 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 Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	806	Total	C	N	O	S	0	18	0
			6613	4205	1135	1222	51			

There are 14 discrepancies between the modelled and reference sequences:

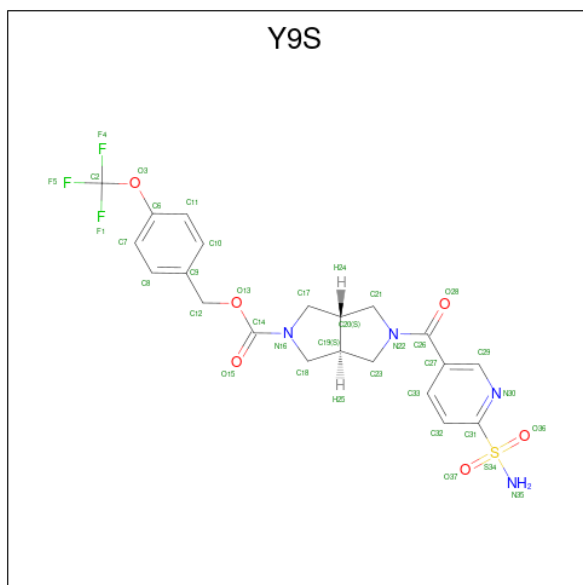
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
A	872	HIS	-	expression tag	UNP Q64610
A	873	HIS	-	expression tag	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-(1-2)-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.



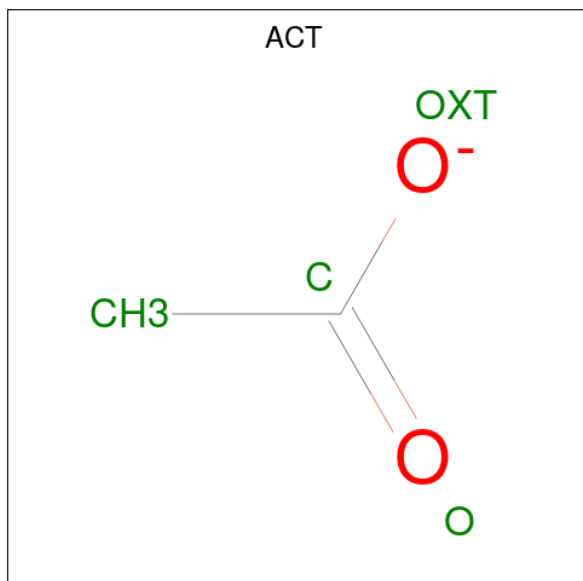
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 3 is [4-(trifluoromethoxy)phenyl]methyl (3aR,6aS)-5-(6-sulfamoylpyridine-3-carbonyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate (CCD ID: Y9S) (formula: $C_{21}H_{21}F_3N_4O_6S$) (labeled as "Ligand of Interest" by depositor).



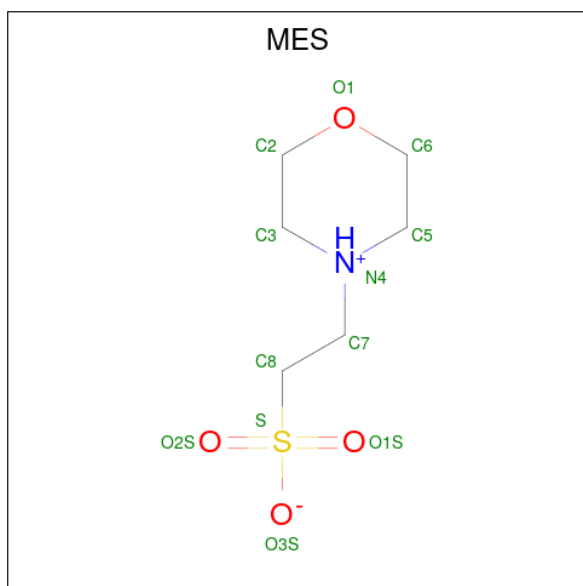
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			35	21	3	4	6	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Na	0	0
			2	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Cl 1	0	0

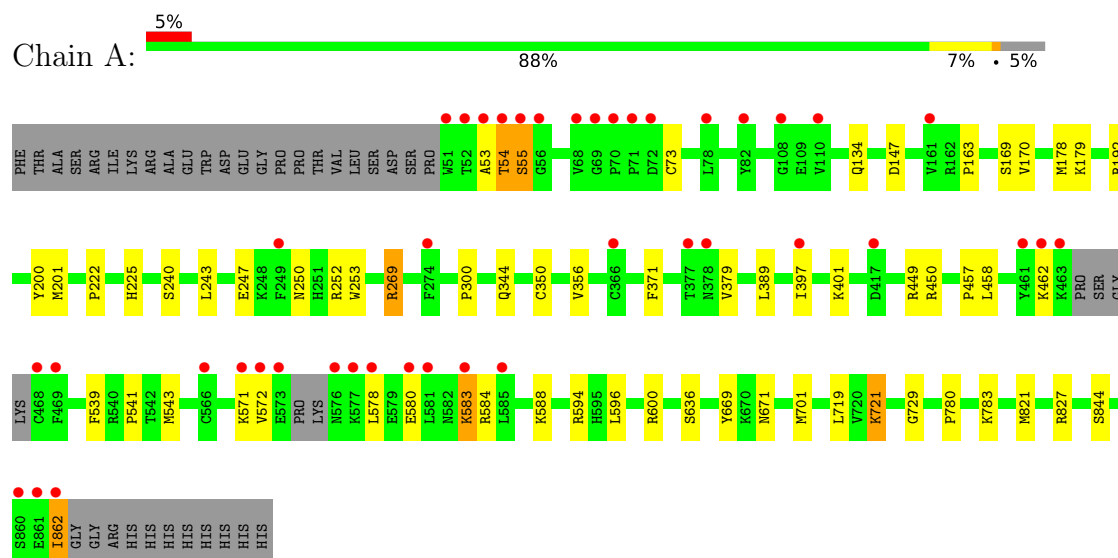
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	528	Total 528	O 528	0	0

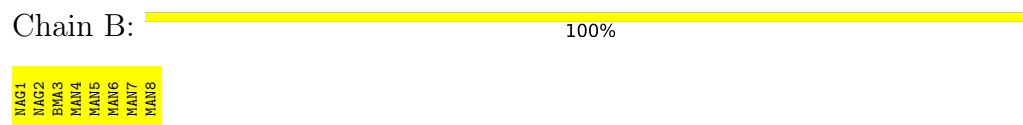
3 Residue-property plots

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: 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-(1-2)-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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.73Å 91.48Å 118.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.74 – 1.67 45.74 – 1.67	Depositor EDS
% Data completeness (in resolution range)	96.3 (45.74-1.67) 96.3 (45.74-1.67)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.215 (Not available) , 0.195	Depositor DCC
R_{free} test set	5400 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7291	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: ZN, MES, Y9S, MAN, CL, ACT, NAG, BMA, CA, NA

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	1.04	0/6854	1.04	9/9288 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	MET	CA-C-N	-6.43	113.36	119.85
1	A	543	MET	C-N-CA	-6.43	113.36	119.85
1	A	729	GLY	N-CA-C	-6.03	105.18	112.48
1	A	55	SER	N-CA-C	5.48	118.18	111.82
1	A	147	ASP	CA-C-N	-5.14	112.86	121.39
1	A	147	ASP	C-N-CA	-5.14	112.86	121.39
1	A	671	ASN	N-CA-C	5.13	117.77	111.82
1	A	719	LEU	N-CA-C	5.09	116.91	111.36
1	A	827	ARG	CG-CD-NE	-5.01	100.97	112.00

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	6613	0	6421	33	0
2	B	94	0	79	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	35	0	0	0	0
4	A	4	0	3	0	0
5	A	12	0	13	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	528	0	0	0	0
All	All	7291	0	6516	33	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 (33) 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:594:ARG:HH12	1:A:636:SER:HB3	1.51	0.73
1:A:580:GLU:HA	1:A:583:LYS:HD2	1.74	0.67
1:A:269:ARG:HB3	1:A:300:PRO:HA	1.80	0.62
1:A:580:GLU:HB3	1:A:584:ARG:HH21	1.67	0.60
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.87	0.56
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.40	0.56
1:A:539:PHE:O	1:A:541:PRO:HD3	2.08	0.53
1:A:247:GLU:HG3	1:A:253:TRP:HE1	1.74	0.53
1:A:596:LEU:HD21	1:A:600:ARG:HB3	1.93	0.51
1:A:53:ALA:C	1:A:55:SER:H	2.19	0.50
1:A:821:MET:HA	1:A:821:MET:HE2	1.94	0.50
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.46	0.49
1:A:458:LEU:O	1:A:462:LYS:HB2	2.12	0.49
1:A:594:ARG:NH1	1:A:636:SER:HB3	2.24	0.49
1:A:780:PRO:HG2	1:A:783:LYS:HB2	1.96	0.48
1:A:54:THR:HA	1:A:73:CYS:HB3	1.96	0.48
1:A:240:SER:O	1:A:247:GLU:HG2	2.14	0.47
1:A:163:PRO:HB3	1:A:350:CYS:O	2.16	0.46
1:A:669:TYR:CE2	1:A:701[A]:MET:HE3	2.52	0.45
1:A:721[A]:LYS:HA	1:A:721[A]:LYS:HD2	1.86	0.44
1:A:584:ARG:O	1:A:588:LYS:HG2	2.18	0.44
1:A:178:MET:CE	1:A:192:ARG:HD3	2.47	0.43
1:A:669:TYR:CE2	1:A:701[B]:MET:HE2	2.54	0.43
1:A:134[B]:GLN:NE2	1:A:344:GLN:HA	2.33	0.43
1:A:179:LYS:HB2	1:A:179:LYS:HE3	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LYS:HE2	1:A:583:LYS:HB3	1.82	0.42
1:A:580:GLU:O	1:A:583:LYS:HG2	2.20	0.42
1:A:449:ARG:O	1:A:450[A]:ARG:HB2	2.19	0.42
1:A:169:SER:HA	1:A:356:VAL:O	2.20	0.41
1:A:201:MET:HE1	1:A:356:VAL:CG2	2.50	0.41
1:A:200:TYR:CD1	1:A:862:ILE:HG13	2.56	0.41
1:A:243:LEU:HA	1:A:243:LEU:HD23	1.82	0.41
1:A:250:ASN:OD1	1:A:252:ARG:HG2	2.21	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	819/846 (97%)	789 (96%)	29 (4%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	THR

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	748/765 (98%)	734 (98%)	14 (2%)	50 25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	VAL
1	A	269	ARG
1	A	379	VAL
1	A	389	LEU
1	A	397	ILE
1	A	401	LYS
1	A	571	LYS
1	A	572	VAL
1	A	578	LEU
1	A	583	LYS
1	A	721[A]	LYS
1	A	721[B]	LYS
1	A	844	SER
1	A	862	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	242	HIS
1	A	297	ASN
1	A	398	ASN
1	A	436	ASN
1	A	471	GLN
1	A	484	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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	0.85	0	17,19,21	1.26	2 (11%)
2	NAG	B	2	2	14,14,15	1.06	0	17,19,21	2.07	5 (29%)
2	BMA	B	3	2	11,11,12	0.77	0	15,15,17	1.33	1 (6%)
2	MAN	B	4	2	11,11,12	0.87	0	15,15,17	1.57	3 (20%)
2	MAN	B	5	2	11,11,12	0.85	1 (9%)	15,15,17	2.34	5 (33%)
2	MAN	B	6	2	11,11,12	0.75	0	15,15,17	1.26	2 (13%)
2	MAN	B	7	2	11,11,12	0.70	0	15,15,17	1.16	1 (6%)
2	MAN	B	8	2	11,11,12	0.80	1 (9%)	15,15,17	1.20	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	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	-	1/2/19/22	0/1/1/1
2	MAN	B	8	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	MAN	C2-C3	2.04	1.55	1.52
2	B	5	MAN	C2-C3	2.01	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	MAN	C1-O5-C5	6.33	120.67	112.19
2	B	2	NAG	C1-O5-C5	6.26	120.57	112.19
2	B	4	MAN	C1-O5-C5	3.58	116.98	112.19
2	B	5	MAN	C3-C4-C5	3.46	116.51	110.23
2	B	5	MAN	C6-C5-C4	-3.33	104.83	113.02
2	B	6	MAN	C1-O5-C5	3.00	116.20	112.19
2	B	4	MAN	O3-C3-C2	2.85	115.87	110.05
2	B	3	BMA	C1-O5-C5	2.84	115.99	112.19
2	B	8	MAN	O3-C3-C2	2.80	115.78	110.05
2	B	2	NAG	O3-C3-C4	2.40	116.03	110.38
2	B	4	MAN	C1-C2-C3	2.39	113.13	109.64
2	B	1	NAG	O5-C1-C2	-2.36	107.64	111.29
2	B	1	NAG	O4-C4-C5	-2.36	103.51	109.32
2	B	2	NAG	C3-C4-C5	2.30	114.41	110.23
2	B	7	MAN	O5-C5-C6	2.30	112.14	107.66
2	B	8	MAN	C1-O5-C5	2.27	115.23	112.19
2	B	2	NAG	O4-C4-C5	-2.20	103.91	109.32
2	B	5	MAN	O3-C3-C4	-2.09	105.45	110.38
2	B	5	MAN	O5-C5-C4	2.09	115.90	110.83
2	B	2	NAG	O3-C3-C2	-2.01	105.23	109.40
2	B	6	MAN	O3-C3-C2	-2.00	105.96	110.05

There are no chirality outliers.

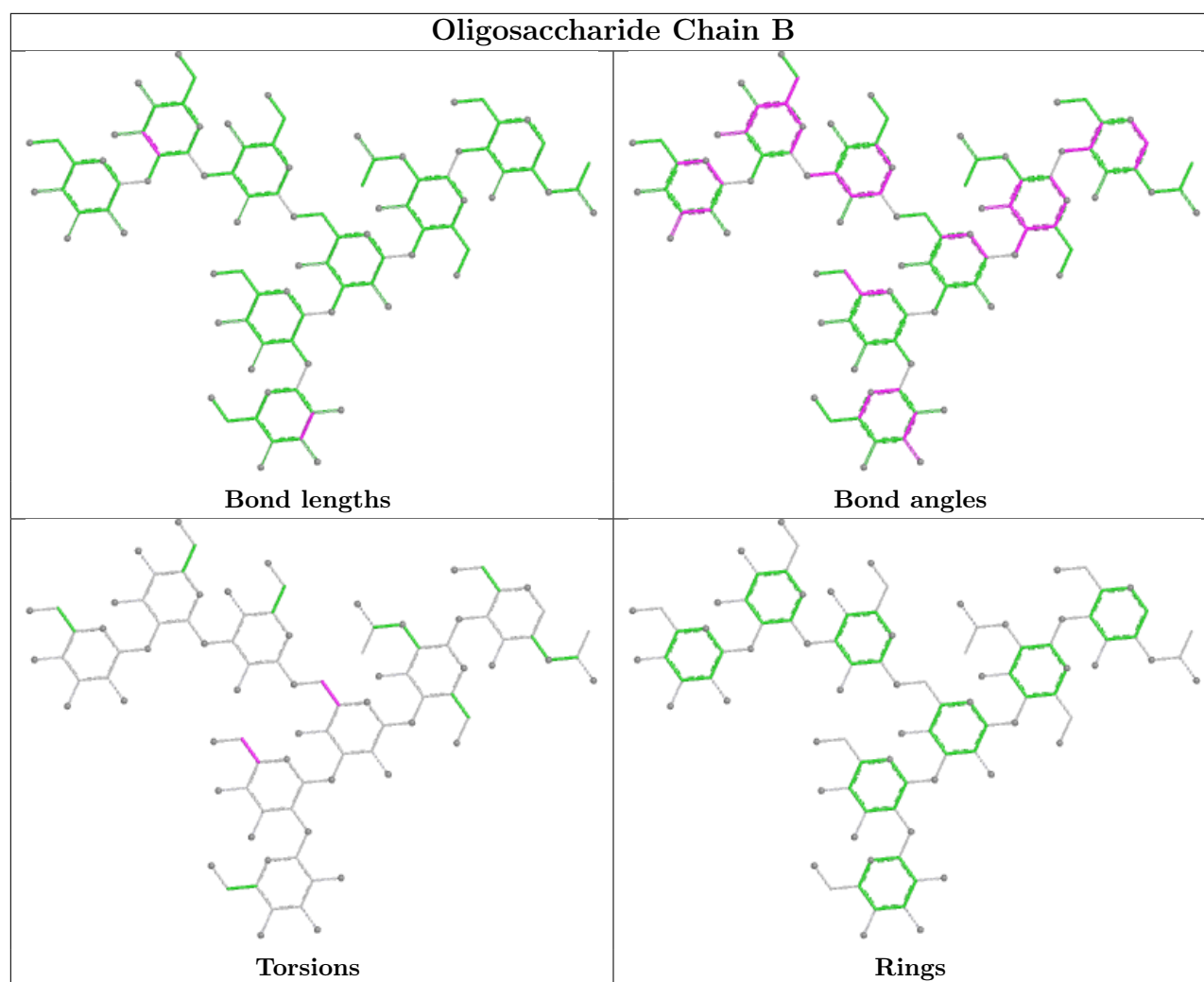
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	MAN	O5-C5-C6-O6
2	B	3	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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	ACT	A	902	-	3,3,3	1.21	0	3,3,3	0.88	0
3	Y9S	A	901	6	37,38,38	2.25	16 (43%)	52,57,57	1.81	9 (17%)
5	MES	A	903	-	12,12,12	2.43	3 (25%)	15,16,16	1.99	4 (26%)

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	Y9S	A	901	6	-	3/27/48/48	0/4/4/4
5	MES	A	903	-	-	5/6/14/14	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	Y9S	C31-N30	6.11	1.42	1.33
5	A	903	MES	C8-S	-6.01	1.69	1.77
3	A	901	Y9S	C29-C27	4.32	1.46	1.39
3	A	901	Y9S	S34-N35	4.03	1.68	1.60
3	A	901	Y9S	C26-N22	3.64	1.42	1.34
5	A	903	MES	O1S-S	3.57	1.55	1.45
3	A	901	Y9S	O13-C14	3.29	1.41	1.34
3	A	901	Y9S	C21-N22	3.27	1.53	1.46
5	A	903	MES	O2S-S	3.20	1.54	1.45
3	A	901	Y9S	C11-C10	2.77	1.43	1.38
3	A	901	Y9S	C12-C9	2.58	1.56	1.50
3	A	901	Y9S	O36-S34	2.57	1.48	1.43
3	A	901	Y9S	C7-C6	2.52	1.43	1.38
3	A	901	Y9S	C33-C32	2.39	1.42	1.38
3	A	901	Y9S	C8-C7	2.35	1.42	1.38
3	A	901	Y9S	O15-C14	2.26	1.24	1.21
3	A	901	Y9S	C23-N22	2.19	1.50	1.46
3	A	901	Y9S	C17-N16	2.03	1.50	1.46
3	A	901	Y9S	O28-C26	2.01	1.26	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	Y9S	C31-S34-N35	-5.95	97.60	108.27
3	A	901	Y9S	O36-S34-N35	5.86	115.81	107.35
5	A	903	MES	O1S-S-C8	5.50	115.03	106.73
3	A	901	Y9S	C20-C21-N22	-3.65	97.50	103.02
3	A	901	Y9S	C21-C20-C19	-3.57	98.45	103.56
3	A	901	Y9S	C33-C27-C26	2.67	127.14	120.28
5	A	903	MES	C6-O1-C2	2.58	118.22	109.88
5	A	903	MES	O3S-S-O1S	-2.46	105.24	111.40
3	A	901	Y9S	C29-C27-C26	-2.30	114.35	121.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	Y9S	C32-C31-N30	-2.28	122.96	125.39
5	A	903	MES	O2S-S-O1S	-2.24	106.54	113.82
3	A	901	Y9S	C23-C19-C20	-2.18	100.44	103.56
3	A	901	Y9S	C32-C33-C27	-2.02	118.64	120.80

There are no chirality outliers.

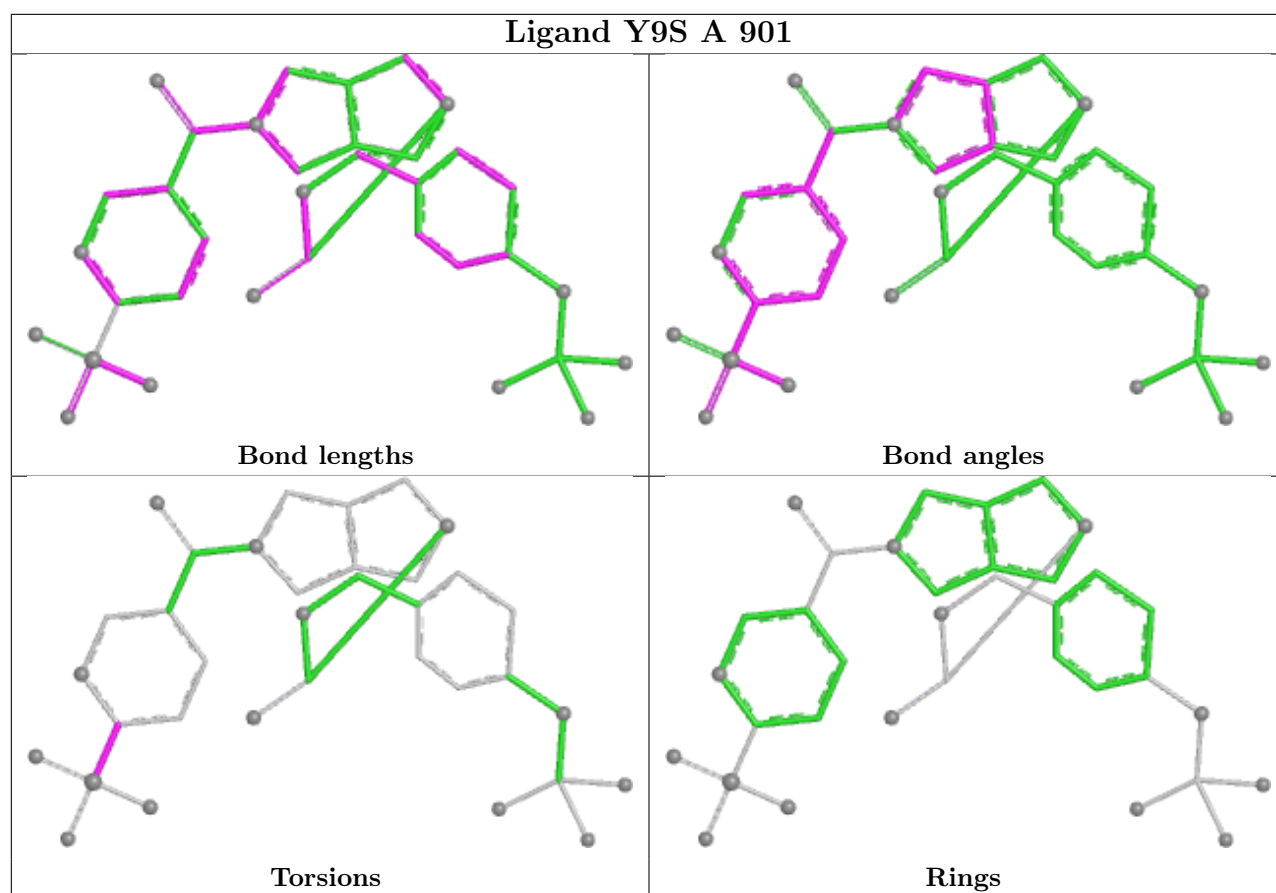
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	Y9S	C32-C31-S34-N35
5	A	903	MES	C7-C8-S-O1S
5	A	903	MES	C7-C8-S-O2S
5	A	903	MES	C8-C7-N4-C3
5	A	903	MES	C7-C8-S-O3S
5	A	903	MES	C8-C7-N4-C5
3	A	901	Y9S	N30-C31-S34-O37
3	A	901	Y9S	C32-C31-S34-O37

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	806/846 (95%)	-0.03	42 (5%)	33 41	11, 21, 48, 80	18 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	LEU	7.4
1	A	862	ILE	7.3
1	A	469	PHE	7.2
1	A	468	CYS	7.2
1	A	572	VAL	6.7
1	A	51	TRP	6.4
1	A	70	PRO	4.3
1	A	68	VAL	4.1
1	A	71	PRO	3.9
1	A	461[A]	TYR	3.4
1	A	53	ALA	3.4
1	A	366	CYS	3.4
1	A	274	PHE	3.3
1	A	56	GLY	3.2
1	A	462	LYS	3.1
1	A	463	LYS	3.0
1	A	54	THR	3.0
1	A	55	SER	3.0
1	A	82	TYR	3.0
1	A	78	LEU	3.0
1	A	581	LEU	3.0
1	A	249	PHE	3.0
1	A	861	GLU	2.9
1	A	573	GLU	2.9
1	A	72	ASP	2.8
1	A	860	SER	2.8
1	A	110	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	52	THR	2.6
1	A	378	ASN	2.6
1	A	69	GLY	2.6
1	A	397	ILE	2.6
1	A	566	CYS	2.4
1	A	576	ASN	2.4
1	A	577	LYS	2.4
1	A	583	LYS	2.3
1	A	161	VAL	2.2
1	A	377	THR	2.2
1	A	585	LEU	2.2
1	A	108	GLY	2.1
1	A	417	ASP	2.0
1	A	571	LYS	2.0
1	A	580	GLU	2.0

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

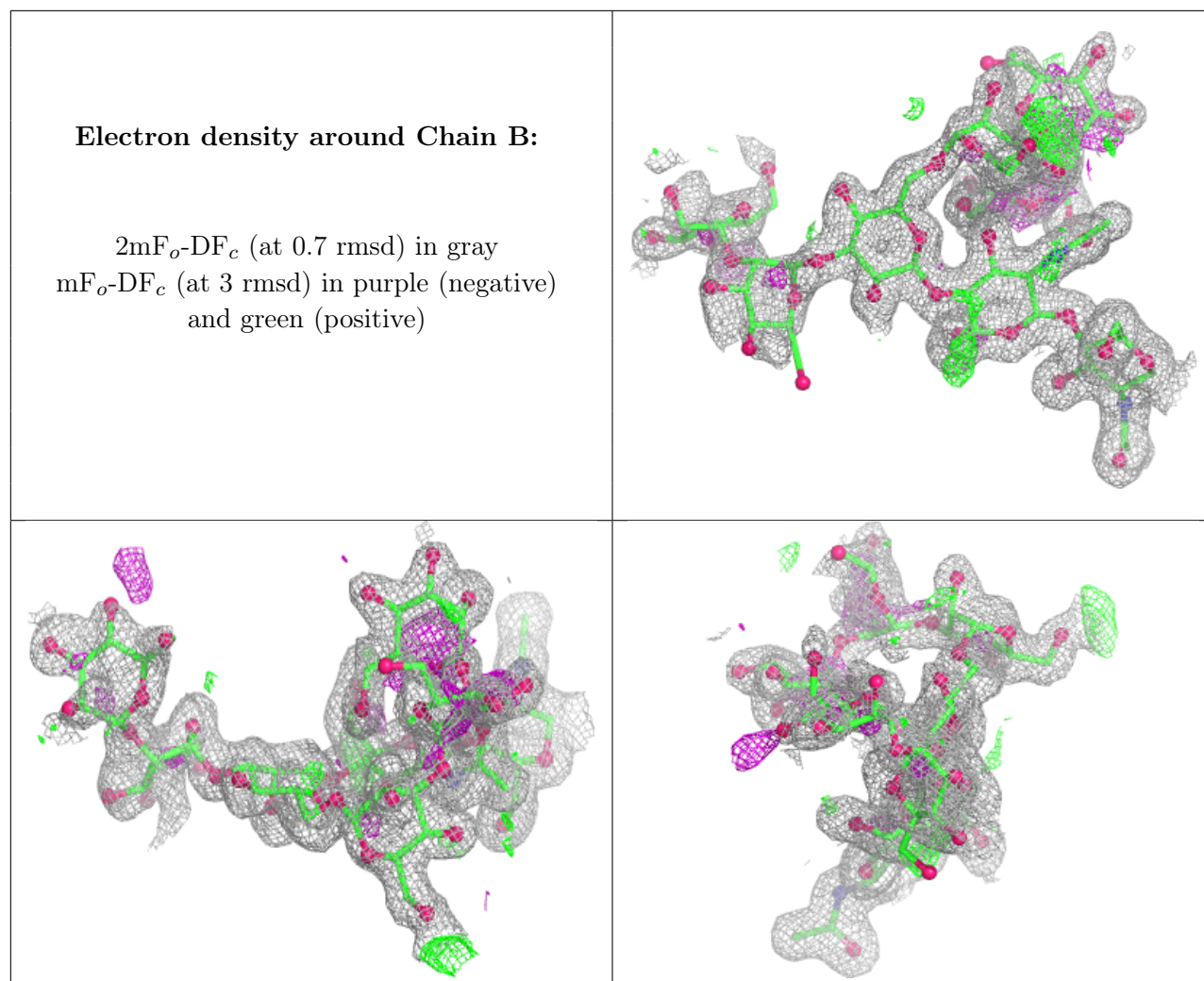
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	MAN	B	7	11/12	0.61	0.15	64,70,80,80	0
2	MAN	B	8	11/12	0.72	0.14	41,60,64,66	0
2	MAN	B	4	11/12	0.73	0.13	42,50,52,53	0
2	BMA	B	3	11/12	0.74	0.13	42,48,56,57	0
2	MAN	B	5	11/12	0.79	0.15	35,47,54,64	0
2	MAN	B	6	11/12	0.85	0.14	29,40,43,44	0
2	NAG	B	2	14/15	0.88	0.10	22,27,35,40	0
2	NAG	B	1	14/15	0.97	0.06	14,16,18,19	0

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

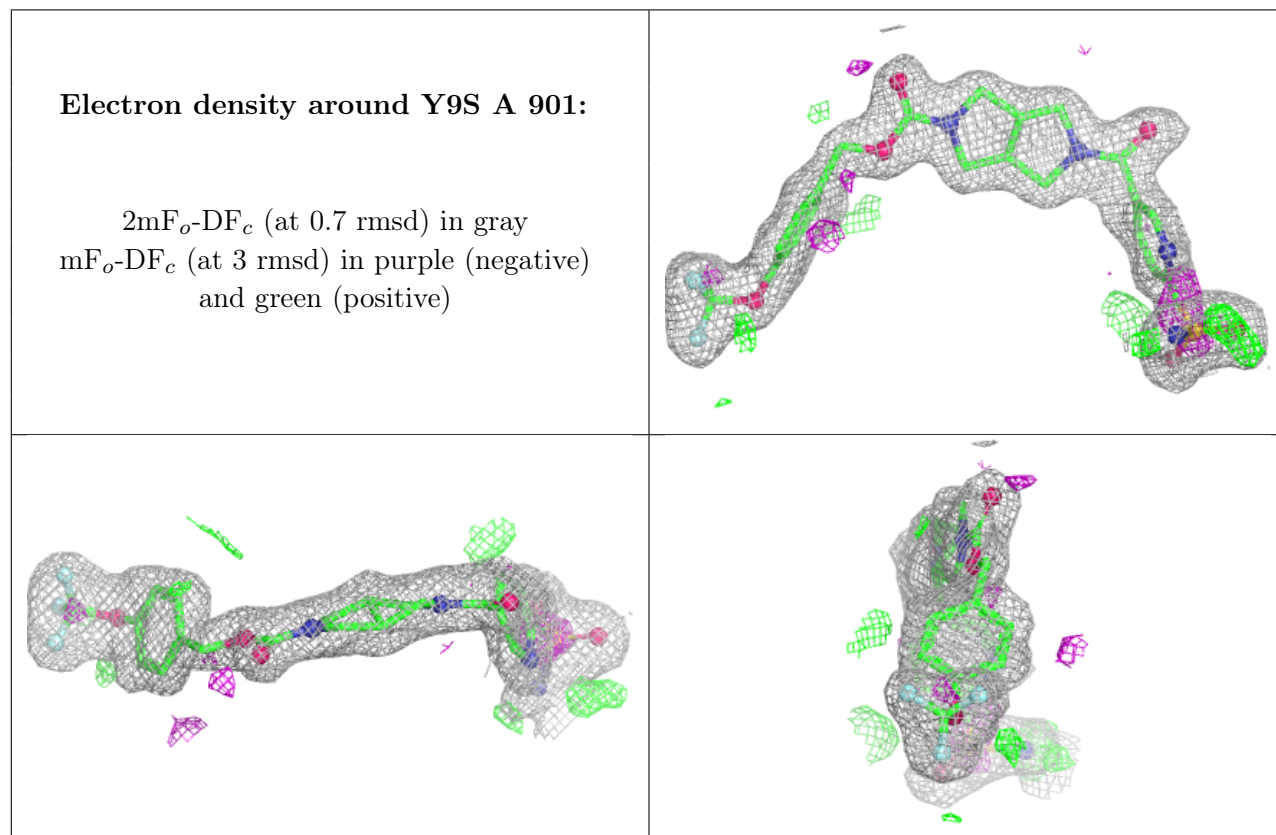


6.4 Ligands [i](#)

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
5	MES	A	903	12/12	0.79	0.21	29,39,53,55	0
9	CL	A	908	1/1	0.90	0.13	44,44,44,44	0
4	ACT	A	902	4/4	0.91	0.11	26,27,32,34	0
3	Y9S	A	901	35/35	0.94	0.08	23,29,37,37	0
7	NA	A	905	1/1	0.96	0.07	21,21,21,21	0
7	NA	A	907	1/1	0.98	0.04	22,22,22,22	0
8	CA	A	906	1/1	1.00	0.01	14,14,14,14	0
6	ZN	A	904	1/1	1.00	0.02	19,19,19,19	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.