



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:09 PM UTC

PDB ID : 7G54 / pdb_00007g54
Title : Crystal Structure of rat Autotaxin in complex with tert-butyl (4aR)-9-(4-chloro-2-fluorophenyl)-5,11-dioxo-2,4,4a,6-tetrahydro-1H-pyrazino[2,1-c][1,4]benzodiazepine-3-carboxylate, i.e. SMILES c1cc(cc(c1c1cc2c(cc1)NC(=O)[C@@H]1N(C2=O)CCN(C1)C(=O)OC(C)(C)C)F)Cl with IC₅₀=0.506839 microM
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Mattei, P.; Rudolph, M.G.
Deposited on : 2023-06-05
Resolution : 2.38 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](#) ①) 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

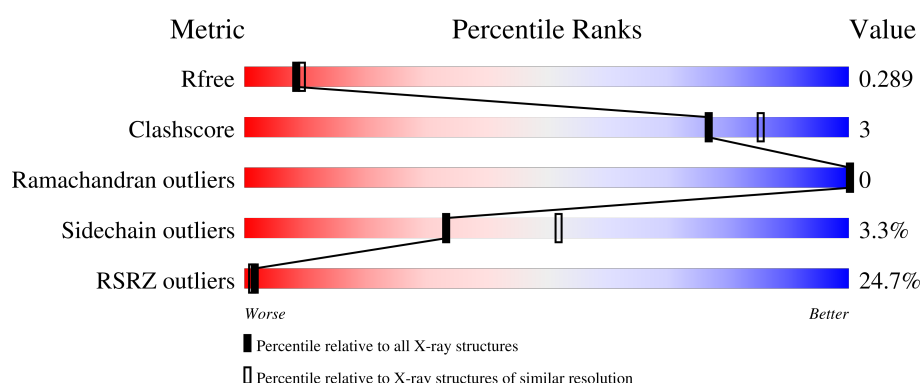
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	24% 85% 11% 5%
2	B	8	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7001 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.

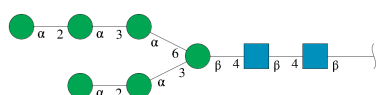
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	806	Total	C	N	O	S	0	0	0
			6508	4126	1122	1211	49			

There are 14 discrepancies between the modelled and reference sequences:

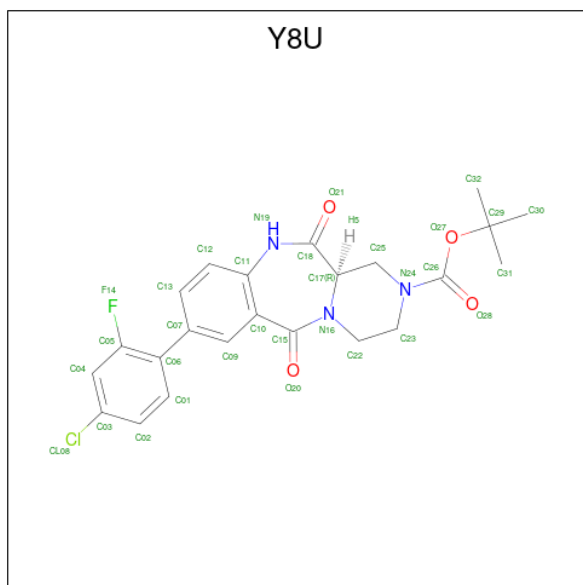
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	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 tert-butyl (5S,8M,12aR)-8-(4-chloro-2-fluorophenyl)-6,12-dioxo-3,4,6,11,12,12a-hexahydropyrazino[2,1-c][1,4]benzodiazepine-2(1H)-carboxylate (CCD ID: Y8U) (formula: $C_{23}H_{23}ClFN_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			32	23	1	1	3	4		

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

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

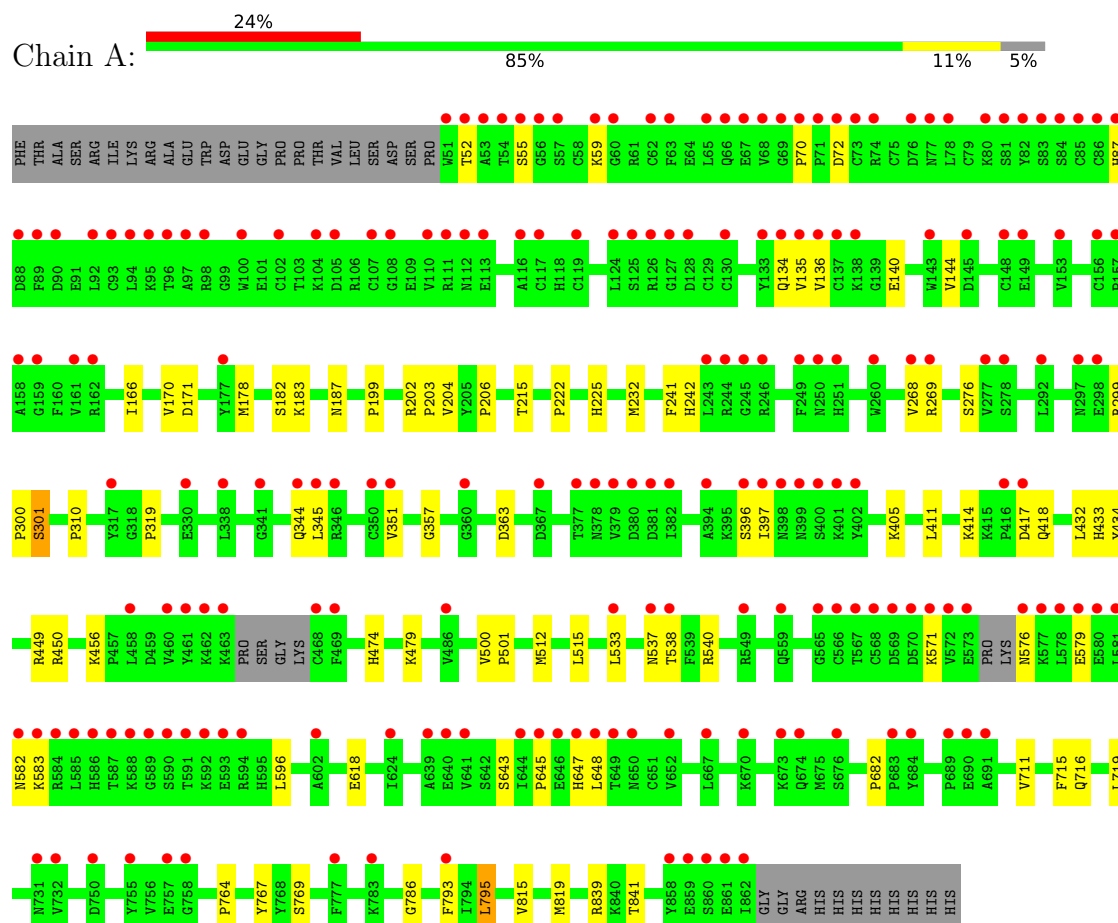
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	363	Total 363	O 363	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-(1-2)-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

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.08Å 93.06Å 121.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.49 – 2.38 43.49 – 2.38	Depositor EDS
% Data completeness (in resolution range)	90.6 (43.49-2.38) 90.6 (43.49-2.38)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.231 , 0.293 0.229 , 0.289	Depositor DCC
R_{free} test set	1976 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7001	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CA, CL, Y8U, MAN, 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	A	0.61	1/6690 (0.0%)	0.88	4/9073 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PRO	CA-C	6.02	1.55	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	795	LEU	CA-C-N	-5.81	113.95	119.76
1	A	795	LEU	C-N-CA	-5.81	113.95	119.76
1	A	786	GLY	CA-C-N	5.75	125.71	119.78
1	A	786	GLY	C-N-CA	5.75	125.71	119.78

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	A	6508	0	6254	37	0
2	B	94	0	79	0	0
3	A	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	363	0	0	5	0
All	All	7001	0	6333	38	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 3.

All (38) 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)
3:A:901:Y8U:C31	3:A:901:Y8U:O28	2.41	0.69
1:A:711:VAL:HG13	1:A:815:VAL:HG13	1.85	0.58
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.85	0.58
1:A:87:HIS:O	7:A:1001:HOH:O	2.17	0.58
1:A:449:ARG:O	1:A:450:ARG:HB2	2.06	0.54
1:A:841:THR:HB	7:A:1252:HOH:O	2.06	0.54
1:A:583:LYS:HB2	7:A:1244:HOH:O	2.07	0.53
1:A:764:PRO:HG2	1:A:767:TYR:CZ	2.45	0.52
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.45	0.51
1:A:134:GLN:HG3	1:A:344:GLN:HG2	1.94	0.50
1:A:268:VAL:HG13	1:A:301:SER:HB2	1.94	0.50
1:A:764:PRO:HG2	1:A:767:TYR:OH	2.12	0.49
1:A:135:VAL:HA	1:A:140:GLU:O	2.13	0.49
1:A:596:LEU:HD22	1:A:618:GLU:OE1	2.14	0.47
1:A:432:LEU:O	1:A:433:HIS:C	2.57	0.47
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.96	0.47
1:A:500:VAL:HG11	1:A:533:LEU:HD12	1.96	0.47
1:A:199:PRO:HD3	1:A:500:VAL:O	2.15	0.47
1:A:171:ASP:O	1:A:310:PRO:HD2	2.15	0.47
1:A:411:LEU:O	1:A:418:GLN:NE2	2.47	0.46
1:A:576:ASN:HD22	1:A:579:GLU:HB2	1.80	0.46
1:A:70:PRO:HA	1:A:72:ASP:H	1.81	0.45
1:A:170:VAL:O	1:A:357:GLY:HA2	2.16	0.45
1:A:643:SER:O	1:A:645:PRO:HD3	2.17	0.44
1:A:474:HIS:HE1	7:A:1222:HOH:O	1.99	0.44
1:A:715:PHE:HA	1:A:719:LEU:HD12	1.99	0.44
1:A:299:ARG:HA	1:A:300:PRO:HD3	1.85	0.44
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.53	0.44
1:A:839:ARG:HG2	7:A:1223:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HB	1:A:187:ASN:OD1	2.18	0.43
1:A:795:LEU:HD21	1:A:819:MET:HG2	2.02	0.42
1:A:769:SER:HB2	1:A:793:PHE:CZ	2.55	0.42
1:A:512:MET:HA	1:A:515:LEU:HD12	2.02	0.42
1:A:202:ARG:HA	1:A:203:PRO:HD2	1.89	0.41
1:A:647:HIS:CD2	1:A:648:LEU:HG	2.56	0.40
1:A:319:PRO:HD2	1:A:363:ASP:OD1	2.21	0.40
1:A:178:MET:O	1:A:182:SER:HB3	2.22	0.40
1:A:232:MET:HB2	1:A:241:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	800/846 (95%)	754 (94%)	46 (6%)	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	A	729/765 (95%)	705 (97%)	24 (3%)	33	52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	55	SER
1	A	59	LYS
1	A	136	VAL
1	A	183	LYS
1	A	204	VAL
1	A	215	THR
1	A	242	HIS
1	A	269	ARG
1	A	276	SER
1	A	301	SER
1	A	345	LEU
1	A	396	SER
1	A	397	ILE
1	A	405	LYS
1	A	414	LYS
1	A	417	ASP
1	A	456	LYS
1	A	479	LYS
1	A	537	ASN
1	A	538	THR
1	A	540	ARG
1	A	571	LYS
1	A	582	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	87	HIS
1	A	257	GLN
1	A	427	HIS
1	A	471	GLN
1	A	484	GLN
1	A	576	ASN
1	A	731	ASN
1	A	856	HIS

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	2,1	14,14,15	0.57	0	17,19,21	1.20	2 (11%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	1.46	1 (5%)
2	BMA	B	3	2	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
2	MAN	B	4	2	11,11,12	0.65	0	15,15,17	1.23	1 (6%)
2	MAN	B	5	2	11,11,12	0.59	0	15,15,17	0.87	1 (6%)
2	MAN	B	6	2	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
2	MAN	B	7	2	11,11,12	0.65	0	15,15,17	1.70	4 (26%)
2	MAN	B	8	2	11,11,12	0.67	0	15,15,17	1.43	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	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	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1
2	MAN	B	8	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	4.75	118.56	112.19
2	B	4	MAN	C1-O5-C5	3.60	117.01	112.19
2	B	7	MAN	C3-C4-C5	3.59	116.75	110.23
2	B	7	MAN	C1-O5-C5	3.29	116.60	112.19
2	B	3	BMA	C1-O5-C5	3.07	116.30	112.19
2	B	8	MAN	C3-C4-C5	3.04	115.75	110.23
2	B	8	MAN	C2-C3-C4	3.03	116.20	110.86
2	B	7	MAN	C2-C3-C4	2.81	115.80	110.86
2	B	5	MAN	C1-O5-C5	2.62	115.69	112.19
2	B	1	NAG	C1-O5-C5	2.41	115.41	112.19
2	B	6	MAN	C1-C2-C3	2.38	113.11	109.64
2	B	7	MAN	O5-C5-C4	2.37	116.59	110.83
2	B	1	NAG	O4-C4-C3	-2.34	104.86	110.38
2	B	3	BMA	C1-C2-C3	2.20	112.84	109.64
2	B	6	MAN	C1-O5-C5	2.18	115.10	112.19
2	B	8	MAN	C1-C2-C3	2.15	112.77	109.64

There are no chirality outliers.

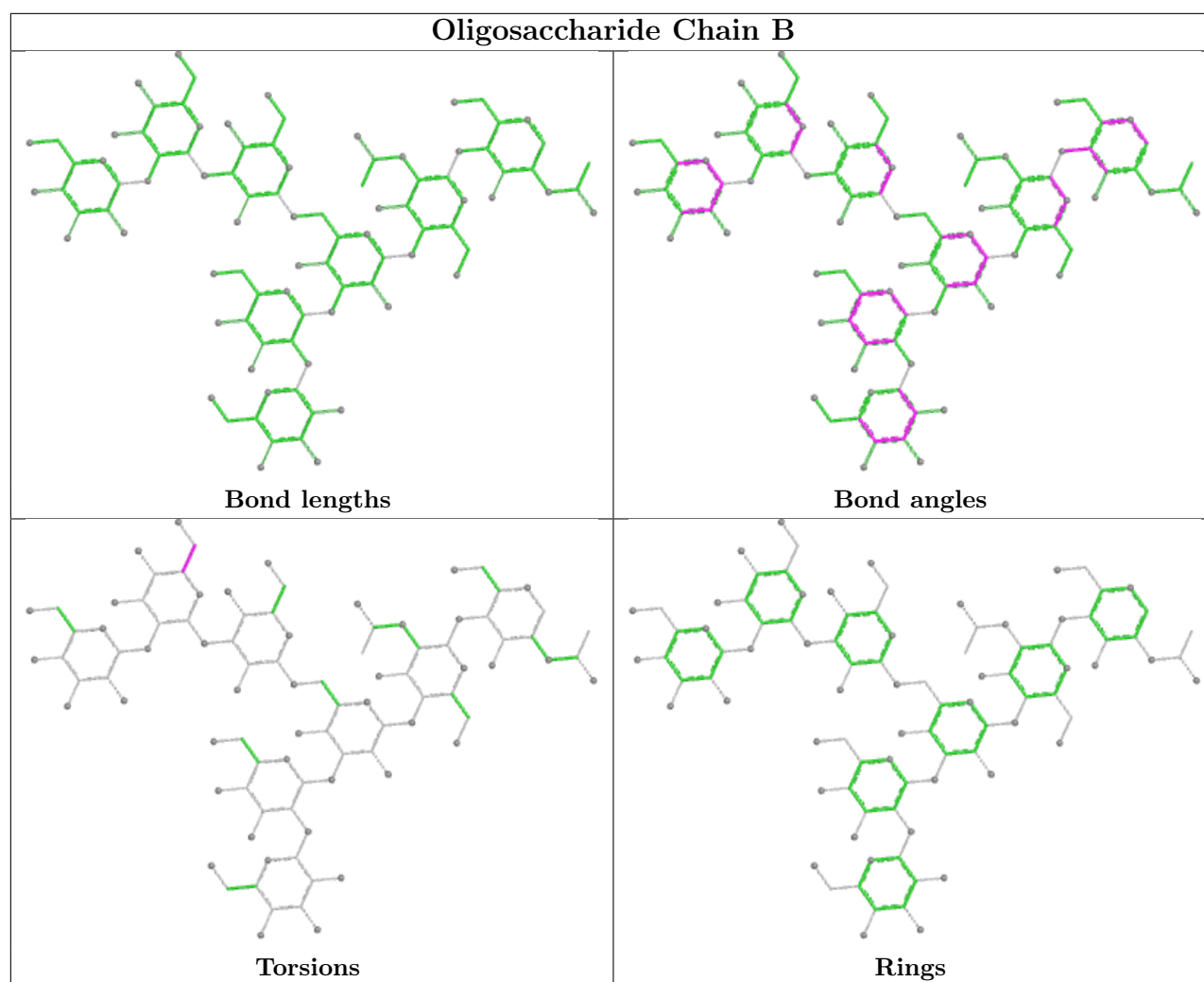
All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
3	Y8U	A	901	-	35,35,35	1.63	6 (17%)	49,53,53	1.32	6 (12%)

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	Y8U	A	901	-	-	4/13/42/42	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	Y8U	C18-N19	5.46	1.42	1.35
3	A	901	Y8U	C11-N19	3.09	1.46	1.42
3	A	901	Y8U	O27-C29	-2.75	1.43	1.48
3	A	901	Y8U	C15-N16	2.43	1.38	1.35
3	A	901	Y8U	C10-C15	-2.35	1.46	1.50
3	A	901	Y8U	O28-C26	2.19	1.24	1.21

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	Y8U	O27-C26-N24	3.54	116.15	110.78
3	A	901	Y8U	O20-C15-N16	-3.46	117.86	121.89
3	A	901	Y8U	O27-C26-O28	-3.35	121.04	126.43
3	A	901	Y8U	C23-N24-C25	3.17	119.19	113.07
3	A	901	Y8U	O21-C18-C17	2.16	125.84	122.16
3	A	901	Y8U	C22-N16-C17	2.09	120.14	115.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	Y8U	C32-C29-O27-C26
3	A	901	Y8U	C30-C29-O27-C26
3	A	901	Y8U	C31-C29-O27-C26
3	A	901	Y8U	N24-C26-O27-C29

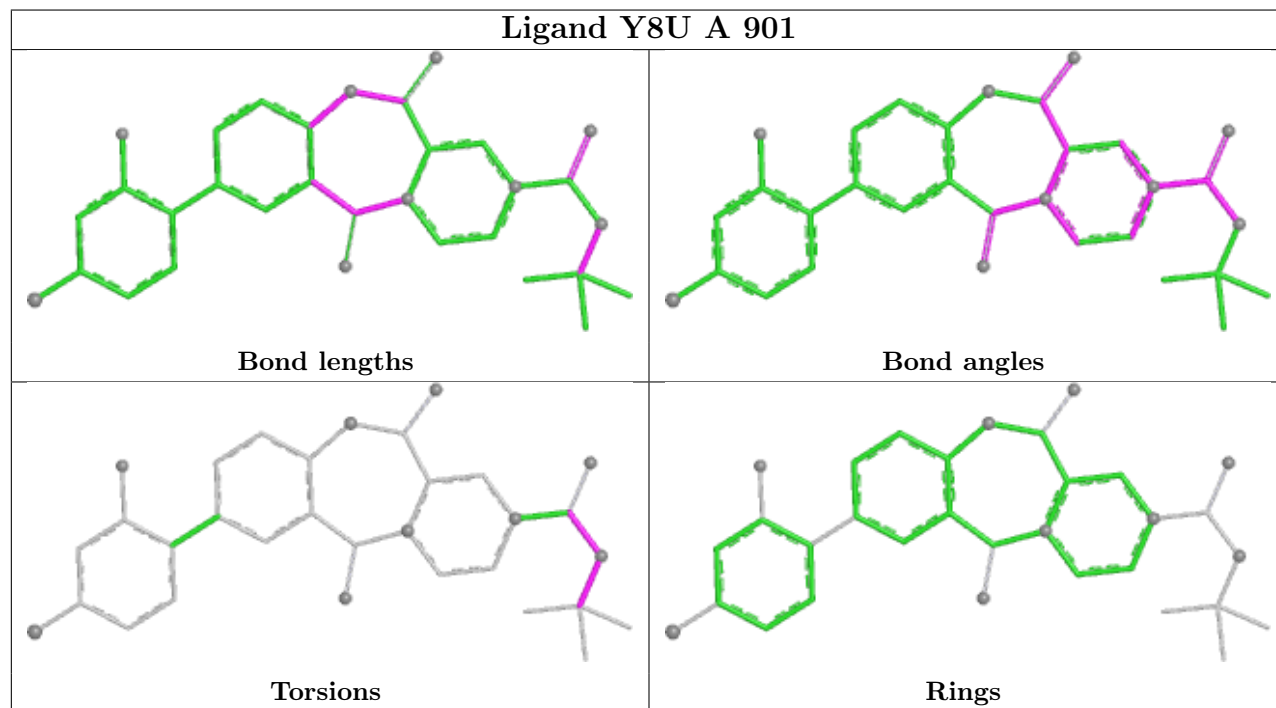
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	Y8U	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 [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%)	1.45	199 (24%) 2 1	15, 31, 76, 80	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	PHE	7.3
1	A	862	ILE	6.8
1	A	397	ILE	6.4
1	A	70	PRO	6.3
1	A	468	CYS	6.2
1	A	52	THR	5.8
1	A	572	VAL	5.7
1	A	71	PRO	5.6
1	A	461	TYR	5.5
1	A	581	LEU	5.5
1	A	463	LYS	5.5
1	A	78	LEU	5.5
1	A	68	VAL	5.4
1	A	110	VAL	5.4
1	A	585	LEU	5.3
1	A	51	TRP	5.1
1	A	578	LEU	5.0
1	A	69	GLY	5.0
1	A	573	GLU	5.0
1	A	644	ILE	4.9
1	A	587	THR	4.8
1	A	579	GLU	4.6
1	A	55	SER	4.5
1	A	860	SER	4.4
1	A	85	CYS	4.4
1	A	60	GLY	4.4
1	A	243	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	584	ARG	4.2
1	A	591	THR	4.1
1	A	590	SER	4.1
1	A	113	GLU	4.0
1	A	378	ASN	4.0
1	A	460	VAL	4.0
1	A	588	LYS	4.0
1	A	161	VAL	3.9
1	A	589	GLY	3.9
1	A	462	LYS	3.8
1	A	580	GLU	3.8
1	A	645	PRO	3.7
1	A	684	TYR	3.7
1	A	398	ASN	3.7
1	A	59	LYS	3.7
1	A	245	GLY	3.7
1	A	244	ARG	3.7
1	A	81	SER	3.6
1	A	577	LYS	3.6
1	A	94	LEU	3.6
1	A	148	CYS	3.6
1	A	582	ASN	3.6
1	A	65	LEU	3.5
1	A	54	THR	3.5
1	A	399	ASN	3.5
1	A	594	ARG	3.5
1	A	53	ALA	3.4
1	A	571	LYS	3.4
1	A	640	GLU	3.4
1	A	861	GLU	3.4
1	A	82	TYR	3.4
1	A	583	LYS	3.4
1	A	648	LEU	3.4
1	A	156	CYS	3.4
1	A	90	ASP	3.4
1	A	592	LYS	3.3
1	A	67	GLU	3.3
1	A	538	THR	3.2
1	A	379	VAL	3.2
1	A	859	GLU	3.2
1	A	458	LEU	3.2
1	A	346	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	566	CYS	3.1
1	A	87	HIS	3.1
1	A	56	GLY	3.1
1	A	858	TYR	3.1
1	A	116	ALA	3.1
1	A	107	CYS	3.1
1	A	593	GLU	3.0
1	A	86	CYS	3.0
1	A	641	VAL	3.0
1	A	586	HIS	3.0
1	A	649	THR	2.9
1	A	570	ASP	2.9
1	A	576	ASN	2.9
1	A	690	GLU	2.9
1	A	80	LYS	2.9
1	A	783	LYS	2.9
1	A	73	CYS	2.9
1	A	72	ASP	2.9
1	A	624	ILE	2.9
1	A	537	ASN	2.9
1	A	565	GLY	2.8
1	A	269	ARG	2.8
1	A	758	GLY	2.8
1	A	689	PRO	2.8
1	A	149	GLU	2.8
1	A	93	CYS	2.8
1	A	133	TYR	2.8
1	A	691	ALA	2.7
1	A	416	PRO	2.7
1	A	345	LEU	2.7
1	A	402	TYR	2.7
1	A	63	PHE	2.7
1	A	135	VAL	2.7
1	A	125	SER	2.7
1	A	350	CYS	2.7
1	A	777	PHE	2.6
1	A	298	GLU	2.6
1	A	92	LEU	2.6
1	A	344	GLN	2.6
1	A	330	GLU	2.6
1	A	652	VAL	2.6
1	A	673	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	96	THR	2.6
1	A	66	GLN	2.6
1	A	126	ARG	2.6
1	A	157	PRO	2.6
1	A	670	LYS	2.6
1	A	417	ASP	2.5
1	A	95	LYS	2.5
1	A	138	LYS	2.5
1	A	667	LEU	2.5
1	A	88	ASP	2.5
1	A	251	HIS	2.5
1	A	57	SER	2.5
1	A	351	VAL	2.5
1	A	74	ARG	2.5
1	A	162	ARG	2.5
1	A	112	ASN	2.5
1	A	341	GLY	2.5
1	A	268	VAL	2.5
1	A	277	VAL	2.5
1	A	124	LEU	2.5
1	A	533	LEU	2.5
1	A	104	LYS	2.5
1	A	77	ASN	2.5
1	A	111	ARG	2.4
1	A	117	CYS	2.4
1	A	486	VAL	2.4
1	A	292	LEU	2.4
1	A	750	ASP	2.4
1	A	97	ALA	2.4
1	A	549	ARG	2.4
1	A	136	VAL	2.4
1	A	569	ASP	2.4
1	A	127	GLY	2.4
1	A	158	ALA	2.4
1	A	89	PHE	2.4
1	A	108	GLY	2.4
1	A	602	ALA	2.4
1	A	396	SER	2.4
1	A	382	ILE	2.4
1	A	400	SER	2.3
1	A	674	GLN	2.3
1	A	381	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	84	SER	2.3
1	A	757	GLU	2.3
1	A	76	ASP	2.3
1	A	83	SER	2.3
1	A	732	VAL	2.3
1	A	128	ASP	2.2
1	A	650	ASN	2.2
1	A	102	CYS	2.2
1	A	568	CYS	2.2
1	A	647	HIS	2.2
1	A	401	LYS	2.2
1	A	177	TYR	2.2
1	A	755	TYR	2.2
1	A	246	ARG	2.2
1	A	297	ASN	2.2
1	A	159	GLY	2.2
1	A	338	LEU	2.2
1	A	105	ASP	2.1
1	A	367	ASP	2.1
1	A	380	ASP	2.1
1	A	559	GLN	2.1
1	A	62	CYS	2.1
1	A	676	SER	2.1
1	A	134	GLN	2.1
1	A	683	PRO	2.1
1	A	793	PHE	2.1
1	A	360	GLY	2.1
1	A	377	THR	2.1
1	A	567	THR	2.1
1	A	394	ALA	2.1
1	A	639	ALA	2.1
1	A	153	VAL	2.1
1	A	249	PHE	2.1
1	A	119	CYS	2.1
1	A	137	CYS	2.1
1	A	145	ASP	2.1
1	A	98	ARG	2.1
1	A	100	TRP	2.1
1	A	646	GLU	2.0
1	A	250	ASN	2.0
1	A	731	ASN	2.0
1	A	317	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	143	TRP	2.0
1	A	260	TRP	2.0
1	A	278	SER	2.0
1	A	130	CYS	2.0

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

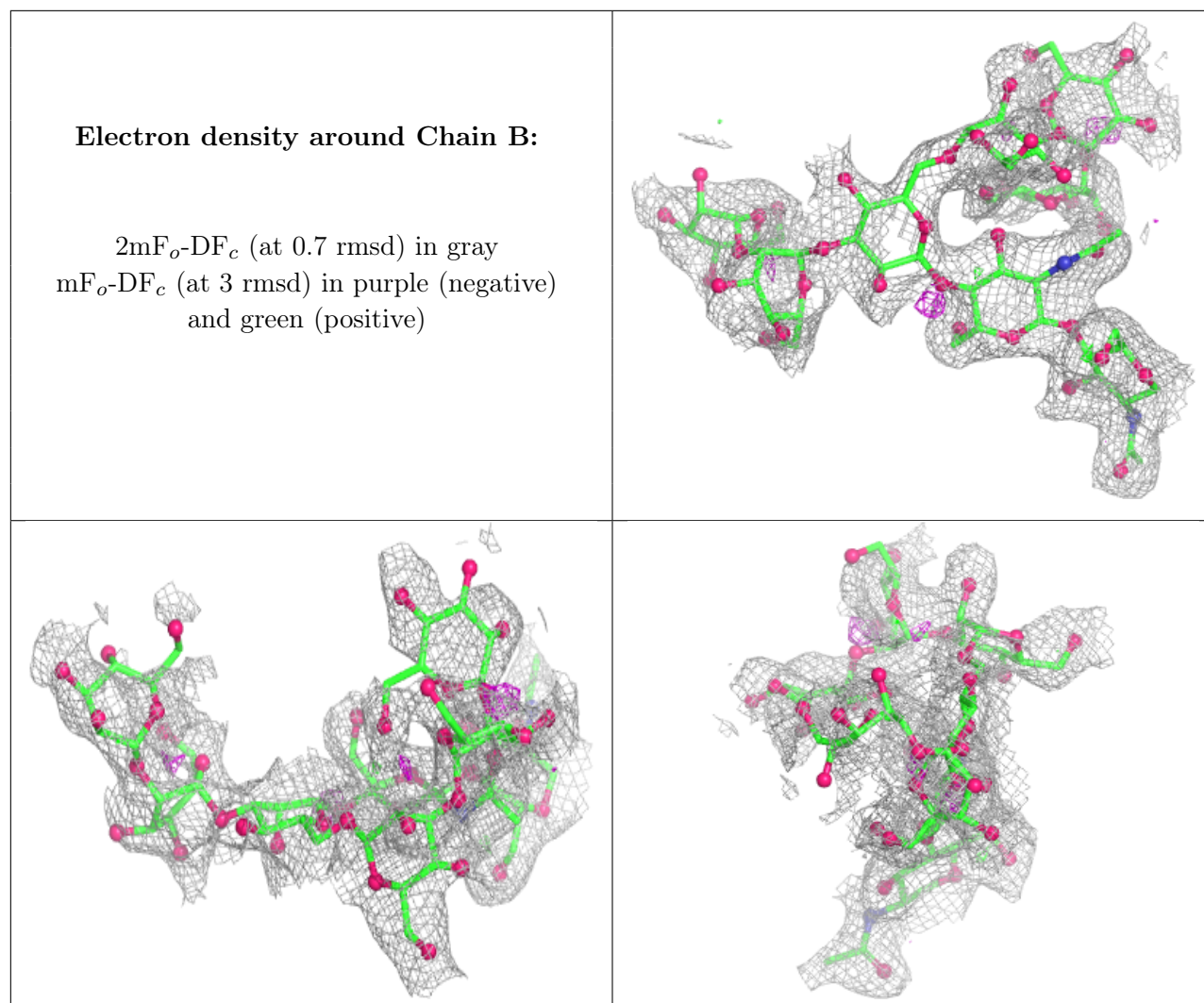
There are no non-standard protein/DNA/RNA residues in this entry.

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	8	11/12	0.44	0.23	80,80,80,80	0
2	MAN	B	7	11/12	0.52	0.20	77,80,80,80	0
2	MAN	B	5	11/12	0.56	0.25	79,80,80,80	0
2	MAN	B	4	11/12	0.60	0.22	79,80,80,80	0
2	BMA	B	3	11/12	0.64	0.21	67,74,78,80	0
2	MAN	B	6	11/12	0.64	0.26	59,66,70,70	0
2	NAG	B	2	14/15	0.72	0.17	41,44,51,61	0
2	NAG	B	1	14/15	0.87	0.11	25,28,31,36	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.



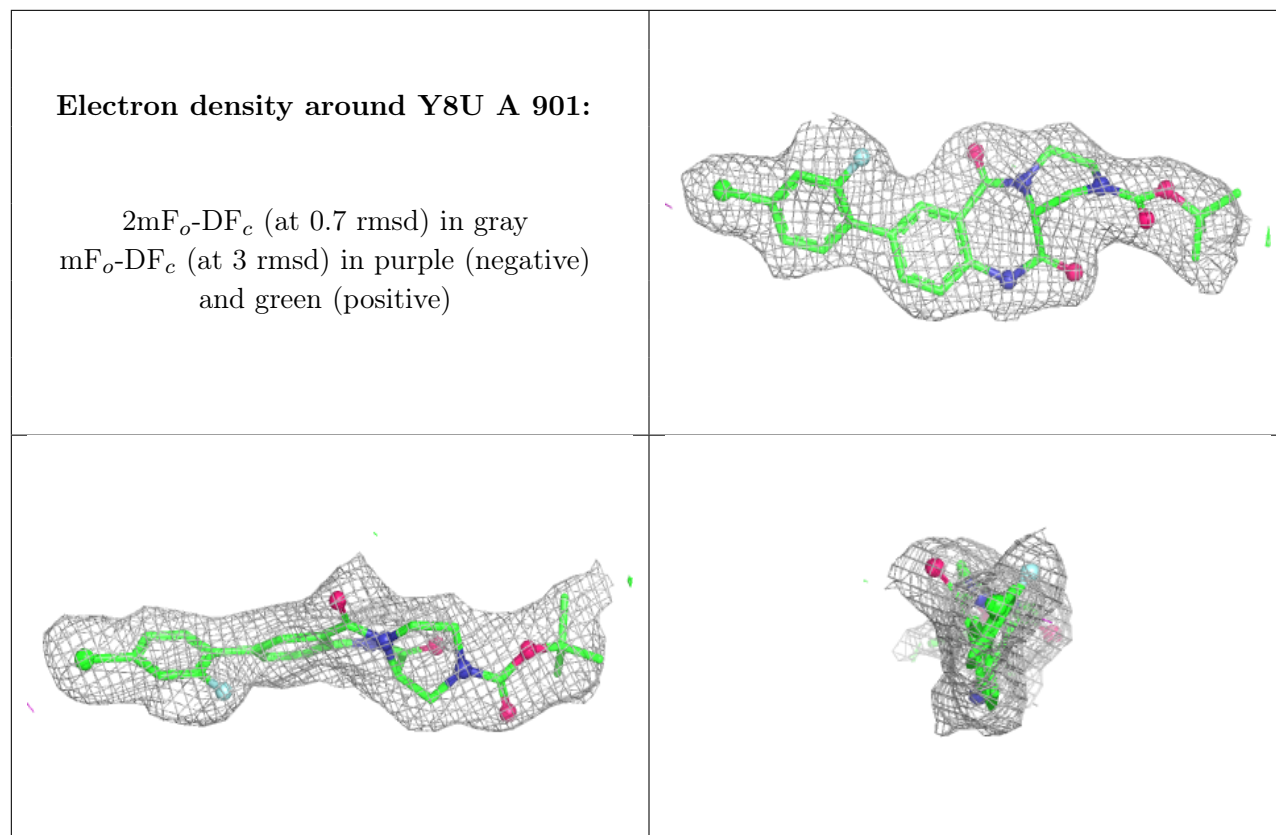
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	Y8U	A	901	32/32	0.92	0.09	21,25,32,34	0
6	CL	A	905	1/1	0.93	0.18	35,35,35,35	0
5	CA	A	904	1/1	0.98	0.03	34,34,34,34	0
4	ZN	A	902	1/1	0.98	0.03	22,22,22,22	0
4	ZN	A	903	1/1	1.00	0.02	23,23,23,23	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.