



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:21 AM UTC

PDB ID : 7G3V / pdb_00007g3v
Title : Crystal Structure of rat Autotaxin in complex with 5-tert-butyl-2-chloro-4-[[5-(6-methoxypyrimidin-4-yl)-1-methylimidazol-2-yl]methoxy]benzonitrile, i.e. SMILES c1c(c(cc(c1C(C)(C)C)OCC1=NC=C(N1C)c1cc(ncn1)OC)Cl)C#N with IC50=0.0417382 microM
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Deposited on : 2023-06-05
Resolution : 1.74 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

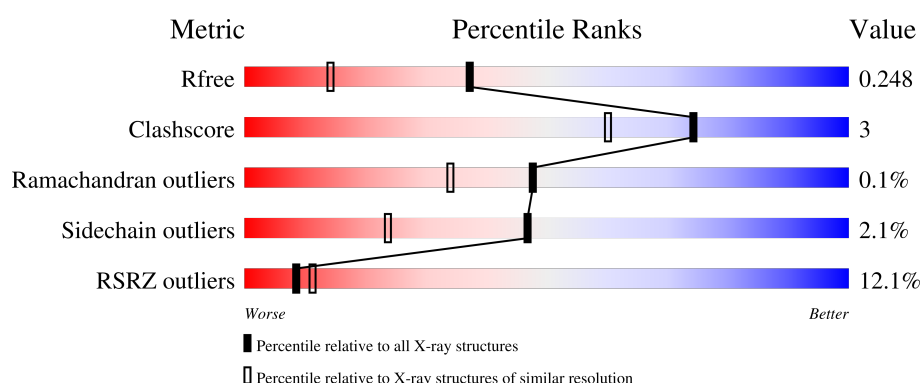
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	11% 81% 12% • 5%
2	B	8	100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7295 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.

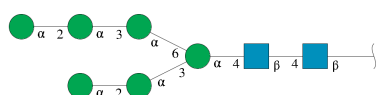
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	804	6553	4159	1126	1215	53	0	11	0

There are 14 discrepancies between the modelled and reference sequences:

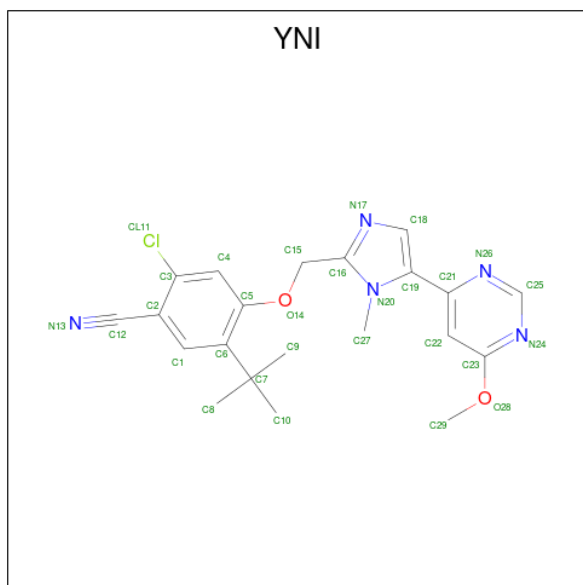
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	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)]alpha-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 5-tert-butyl-2-chloro-4-{[(5M)-5-(6-methoxypyrimidin-4-yl)-1-methyl-1H-imidazol-2-yl]methoxy}benzonitrile (CCD ID: YNI) (formula: C₂₁H₂₂ClN₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			29	21	1	5	2		

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

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

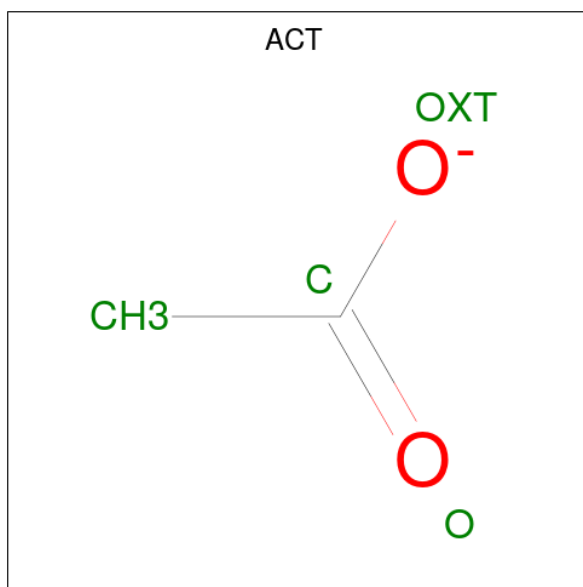
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

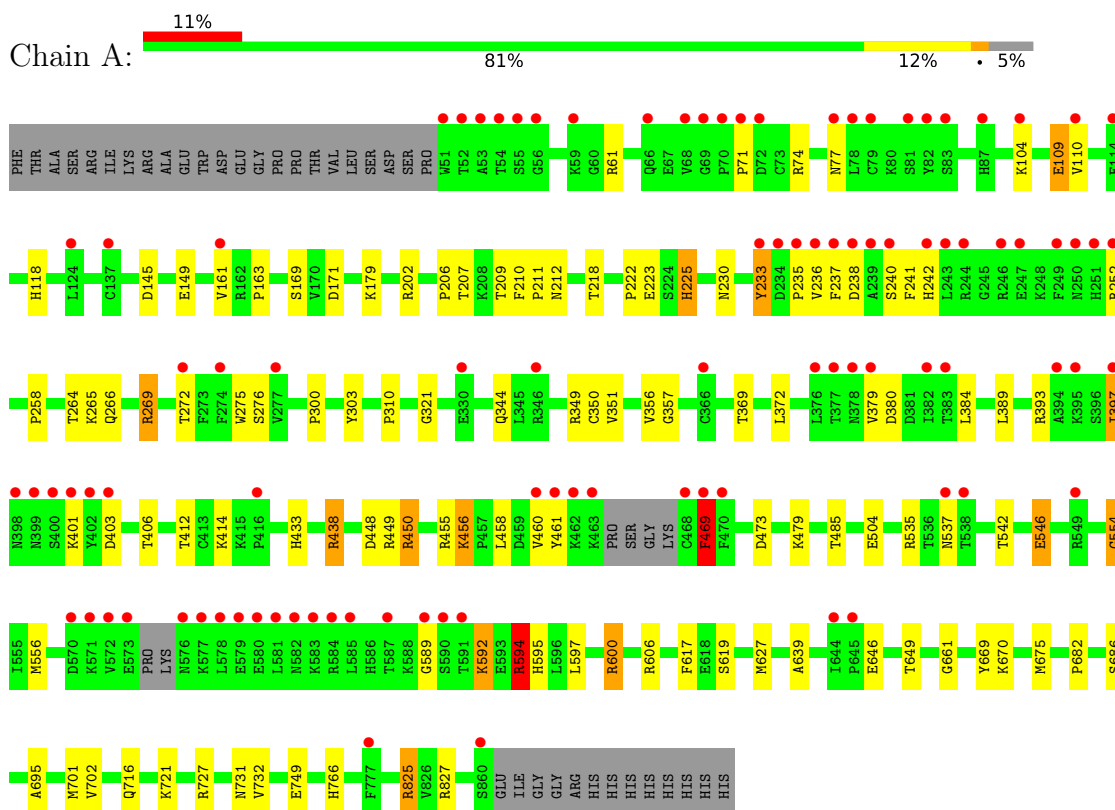
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	601	Total	O	0	0
			601	601		

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)]alpha-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	84.31Å 92.08Å 120.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.25 – 1.74 73.25 – 1.74	Depositor EDS
% Data completeness (in resolution range)	81.9 (73.25-1.74) 82.2 (73.25-1.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.194 , 0.243 0.203 , 0.248	Depositor DCC
R_{free} test set	4051 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7295	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 3.89% 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: NAG, K, YNI, ACT, NA, MAN, CA, SO4, ZN

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	1.28	37/6763 (0.5%)	1.23	22/9169 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	THR	N-CA	-7.51	1.36	1.46
1	A	627	MET	N-CA	-6.98	1.39	1.46
1	A	438	ARG	N-CA	6.83	1.55	1.46
1	A	504	GLU	C-O	6.81	1.31	1.23
1	A	272[A]	THR	C-O	6.49	1.31	1.23
1	A	272[B]	THR	C-O	6.49	1.31	1.23
1	A	554	GLY	C-O	-6.27	1.18	1.24
1	A	766	HIS	CE1-NE2	6.22	1.38	1.32
1	A	207	THR	N-CA	-5.94	1.39	1.46
1	A	218	THR	N-CA	5.89	1.53	1.45
1	A	258	PRO	C-O	5.86	1.30	1.23
1	A	473	ASP	C-O	-5.83	1.17	1.23
1	A	237	PHE	N-CA	5.81	1.53	1.46
1	A	546	GLU	CD-OE1	5.80	1.36	1.25
1	A	161	VAL	N-CA	5.76	1.54	1.46
1	A	695	ALA	N-CA	5.62	1.53	1.46
1	A	233	TYR	N-CA	-5.43	1.39	1.46
1	A	351	VAL	C-O	5.38	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	HIS	C-O	5.38	1.30	1.23
1	A	649	THR	C-O	-5.36	1.18	1.24
1	A	732	VAL	N-CA	5.36	1.52	1.46
1	A	619	SER	C-O	5.34	1.30	1.23
1	A	535	ARG	C-O	-5.29	1.17	1.24
1	A	265	LYS	C-O	-5.28	1.17	1.24
1	A	825	ARG	N-CA	-5.28	1.39	1.45
1	A	661	GLY	C-O	-5.25	1.17	1.24
1	A	118	HIS	CE1-NE2	5.22	1.37	1.32
1	A	149	GLU	C-O	-5.20	1.18	1.24
1	A	595	HIS	CE1-NE2	5.14	1.37	1.32
1	A	675	MET	N-CA	-5.11	1.39	1.46
1	A	372	LEU	C-O	5.10	1.30	1.24
1	A	321	GLY	N-CA	5.09	1.51	1.44
1	A	266	GLN	N-CA	-5.08	1.40	1.46
1	A	223	GLU	C-O	5.05	1.30	1.24
1	A	145	ASP	C-O	-5.04	1.17	1.24
1	A	670	LYS	C-O	-5.01	1.18	1.24
1	A	686	SER	N-CA	5.00	1.52	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	THR	CA-CB-OG1	-9.96	94.65	109.60
1	A	225	HIS	CA-CB-CG	8.46	122.26	113.80
1	A	749	GLU	CB-CA-C	-7.92	97.64	110.79
1	A	827	ARG	CG-CD-NE	-7.43	95.65	112.00
1	A	344	GLN	CB-CA-C	-5.96	101.28	110.81
1	A	546	GLU	CB-CG-CD	5.83	122.51	112.60
1	A	469	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	212	ASN	CA-CB-CG	-5.75	106.86	112.60
1	A	209	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	702	VAL	O-C-N	-5.55	118.19	121.69
1	A	349	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	237	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	202	ARG	CA-C-O	5.33	123.26	119.32
1	A	646	GLU	CB-CA-C	-5.32	101.63	110.68
1	A	412	THR	CA-C-N	5.25	129.58	122.07
1	A	412	THR	C-N-CA	5.25	129.58	122.07
1	A	236	VAL	O-C-N	-5.22	116.45	121.83
1	A	617	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	264	THR	CA-CB-OG1	-5.12	101.91	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	PRO	N-CA-CB	5.09	108.20	102.60
1	A	344	GLN	CB-CG-CD	5.02	121.14	112.60
1	A	537	ASN	CB-CA-C	-5.02	101.47	109.75

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	384	LEU	Peptide
1	A	393	ARG	Sidechain
1	A	438	ARG	Sidechain
1	A	450[A]	ARG	Sidechain
1	A	450[B]	ARG	Sidechain
1	A	455	ARG	Sidechain
1	A	469	PHE	Peptide
1	A	594	ARG	Sidechain
1	A	600	ARG	Sidechain
1	A	606	ARG	Sidechain
1	A	61	ARG	Sidechain
1	A	71	PRO	Peptide
1	A	74	ARG	Sidechain
1	A	825	ARG	Sidechain

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	6553	0	6321	38	0
2	B	94	0	79	0	0
3	A	29	0	0	1	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	5	0	0	1	0
10	A	601	0	0	10	0
All	All	7295	0	6406	40	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 (40) 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:HH21	1:A:594:ARG:HG2	1.37	0.89
1:A:230:ASN:ND2	10:A:1001:HOH:O	2.05	0.87
9:A:909:SO4:O1	10:A:1001:HOH:O	1.96	0.83
1:A:109:GLU:O	10:A:1002:HOH:O	1.99	0.79
1:A:594:ARG:HG2	1:A:594:ARG:NH2	2.01	0.71
1:A:238:ASP:HB3	10:A:1187:HOH:O	1.92	0.69
1:A:77:ASN:OD1	1:A:275:TRP:CE3	2.49	0.66
1:A:448:ASP:OD2	10:A:1004:HOH:O	2.15	0.64
1:A:479[A]:LYS:NZ	10:A:1009:HOH:O	2.32	0.62
1:A:594:ARG:NH2	1:A:594:ARG:CG	2.63	0.62
1:A:233:TYR:CE2	1:A:235:PRO:HA	2.35	0.61
1:A:163:PRO:HB3	1:A:350:CYS:O	2.01	0.59
1:A:240:SER:HB3	1:A:242:HIS:CE1	2.37	0.59
1:A:269:ARG:HB3	1:A:300:PRO:HA	1.85	0.58
1:A:171:ASP:O	1:A:310:PRO:HD2	2.06	0.55
1:A:450[A]:ARG:NH1	10:A:1003:HOH:O	2.12	0.54
1:A:546:GLU:CD	1:A:600:ARG:HH22	2.14	0.54
1:A:727:ARG:HD2	10:A:1026:HOH:O	2.08	0.53
1:A:458:LEU:HA	1:A:461:TYR:CE2	2.44	0.52
3:A:901:YNI:C27	3:A:901:YNI:N26	2.75	0.50
1:A:403:ASP:OD2	1:A:406:THR:HG23	2.12	0.50
1:A:639:ALA:HB2	10:A:1412:HOH:O	2.12	0.49
1:A:554:GLY:H	1:A:556[A]:MET:HE3	1.79	0.47
1:A:449:ARG:O	1:A:450[A]:ARG:HB2	2.14	0.47
1:A:357:GLY:HA3	1:A:485:THR:OG1	2.15	0.46
1:A:169:SER:HA	1:A:356:VAL:O	2.16	0.46
1:A:669:TYR:CE2	1:A:701[B]:MET:HE2	2.51	0.45
1:A:380:ASP:OD1	1:A:456:LYS:NZ	2.49	0.45
1:A:210:PHE:N	1:A:211:PRO:CD	2.80	0.45
1:A:449:ARG:O	1:A:450[B]:ARG:HB2	2.17	0.44
1:A:233:TYR:OH	1:A:238:ASP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PRO:HD2	1:A:303:TYR:OH	2.18	0.43
1:A:727:ARG:CD	10:A:1026:HOH:O	2.67	0.42
1:A:682:PRO:HB3	1:A:716:GLN:CD	2.45	0.42
1:A:458:LEU:HA	1:A:461:TYR:CZ	2.55	0.42
1:A:597:LEU:HD12	1:A:731:ASN:HB2	2.02	0.42
1:A:77:ASN:O	1:A:276:SER:OG	2.34	0.41
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.55	0.41
1:A:589:GLY:O	1:A:592:LYS:HB3	2.21	0.41
1:A:397:ILE:HD12	1:A:397:ILE:O	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	809/846 (96%)	775 (96%)	33 (4%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU

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	738/765 (96%)	723 (98%)	15 (2%)	48 26

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	110	VAL
1	A	179	LYS
1	A	241	PHE
1	A	379	VAL
1	A	389	LEU
1	A	397	ILE
1	A	401	LYS
1	A	414	LYS
1	A	456	LYS
1	A	460	VAL
1	A	469	PHE
1	A	592	LYS
1	A	594	ARG
1	A	721	LYS

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	77	ASN
1	A	242	HIS
1	A	257	GLN
1	A	398	ASN
1	A	484	GLN
1	A	647	HIS
1	A	650	ASN

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	0.99	1 (7%)	17,19,21	2.02	5 (29%)
2	NAG	B	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.97	6 (35%)
2	MAN	B	3	2	11,11,12	1.09	0	15,15,17	2.34	6 (40%)
2	MAN	B	4	2	11,11,12	1.50	2 (18%)	15,15,17	2.18	6 (40%)
2	MAN	B	5	2	11,11,12	1.39	2 (18%)	15,15,17	2.10	7 (46%)
2	MAN	B	6	2	11,11,12	1.29	1 (9%)	15,15,17	2.01	2 (13%)
2	MAN	B	7	2	11,11,12	1.28	1 (9%)	15,15,17	2.57	6 (40%)
2	MAN	B	8	2	11,11,12	1.72	3 (27%)	15,15,17	2.30	5 (33%)

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	MAN	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	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	-	2/2/19/22	0/1/1/1
2	MAN	B	8	2	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	MAN	C2-C3	3.50	1.57	1.52
2	B	7	MAN	C1-C2	2.85	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C6-C5	2.50	1.60	1.51
2	B	5	MAN	C1-C2	2.49	1.58	1.52
2	B	1	NAG	C3-C2	2.44	1.57	1.52
2	B	8	MAN	O3-C3	2.40	1.48	1.43
2	B	6	MAN	O5-C5	2.40	1.48	1.43
2	B	4	MAN	O3-C3	2.25	1.48	1.43
2	B	8	MAN	C1-C2	2.17	1.57	1.52
2	B	4	MAN	C6-C5	2.14	1.59	1.51
2	B	5	MAN	O2-C2	2.11	1.47	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-6.22	101.66	111.29
2	B	8	MAN	O3-C3-C2	5.91	122.11	110.05
2	B	7	MAN	O2-C2-C3	-5.42	98.92	110.15
2	B	7	MAN	C1-C2-C3	5.21	117.24	109.64
2	B	6	MAN	C1-O5-C5	5.10	119.02	112.19
2	B	3	MAN	O2-C2-C1	-4.40	99.15	109.22
2	B	2	NAG	C1-O5-C5	4.27	117.90	112.19
2	B	3	MAN	C1-C2-C3	4.27	115.86	109.64
2	B	6	MAN	O3-C3-C2	-3.87	102.16	110.05
2	B	3	MAN	C2-C3-C4	-3.58	104.56	110.86
2	B	4	MAN	C1-O5-C5	3.57	116.98	112.19
2	B	8	MAN	O5-C5-C6	3.49	114.46	107.66
2	B	5	MAN	O2-C2-C3	-3.37	103.18	110.15
2	B	4	MAN	C3-C4-C5	3.33	116.27	110.23
2	B	5	MAN	O5-C5-C4	3.25	118.73	110.83
2	B	7	MAN	O2-C2-C1	3.22	116.60	109.22
2	B	3	MAN	O5-C5-C6	3.15	113.79	107.66
2	B	2	NAG	O7-C7-N2	3.12	127.50	121.98
2	B	4	MAN	O3-C3-C2	3.11	116.40	110.05
2	B	8	MAN	C2-C3-C4	-3.10	105.41	110.86
2	B	7	MAN	C2-C3-C4	3.07	116.27	110.86
2	B	5	MAN	C1-C2-C3	3.07	114.11	109.64
2	B	4	MAN	O6-C6-C5	2.99	121.53	111.33
2	B	2	NAG	C8-C7-N2	-2.89	111.33	116.12
2	B	4	MAN	O5-C5-C6	2.89	113.28	107.66
2	B	8	MAN	O5-C5-C4	-2.84	103.91	110.83
2	B	4	MAN	C2-C3-C4	-2.79	105.95	110.86
2	B	3	MAN	O3-C3-C2	2.77	115.70	110.05
2	B	7	MAN	O5-C5-C6	2.66	112.84	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	MAN	O2-C2-C1	2.56	115.08	109.22
2	B	5	MAN	O6-C6-C5	-2.51	102.80	111.33
2	B	1	NAG	O7-C7-N2	-2.46	117.64	121.98
2	B	5	MAN	C6-C5-C4	-2.43	107.06	113.02
2	B	2	NAG	O3-C3-C2	-2.40	104.41	109.40
2	B	3	MAN	O6-C6-C5	-2.37	103.27	111.33
2	B	5	MAN	C3-C4-C5	2.32	114.44	110.23
2	B	2	NAG	C3-C4-C5	2.28	114.37	110.23
2	B	1	NAG	O5-C5-C6	2.28	112.10	107.66
2	B	2	NAG	O4-C4-C5	-2.24	103.81	109.32
2	B	1	NAG	O3-C3-C4	-2.17	105.25	110.38
2	B	1	NAG	C2-N2-C7	2.17	125.80	122.90
2	B	8	MAN	O2-C2-C3	2.13	114.56	110.15
2	B	7	MAN	O3-C3-C4	-2.02	105.60	110.38

There are no chirality outliers.

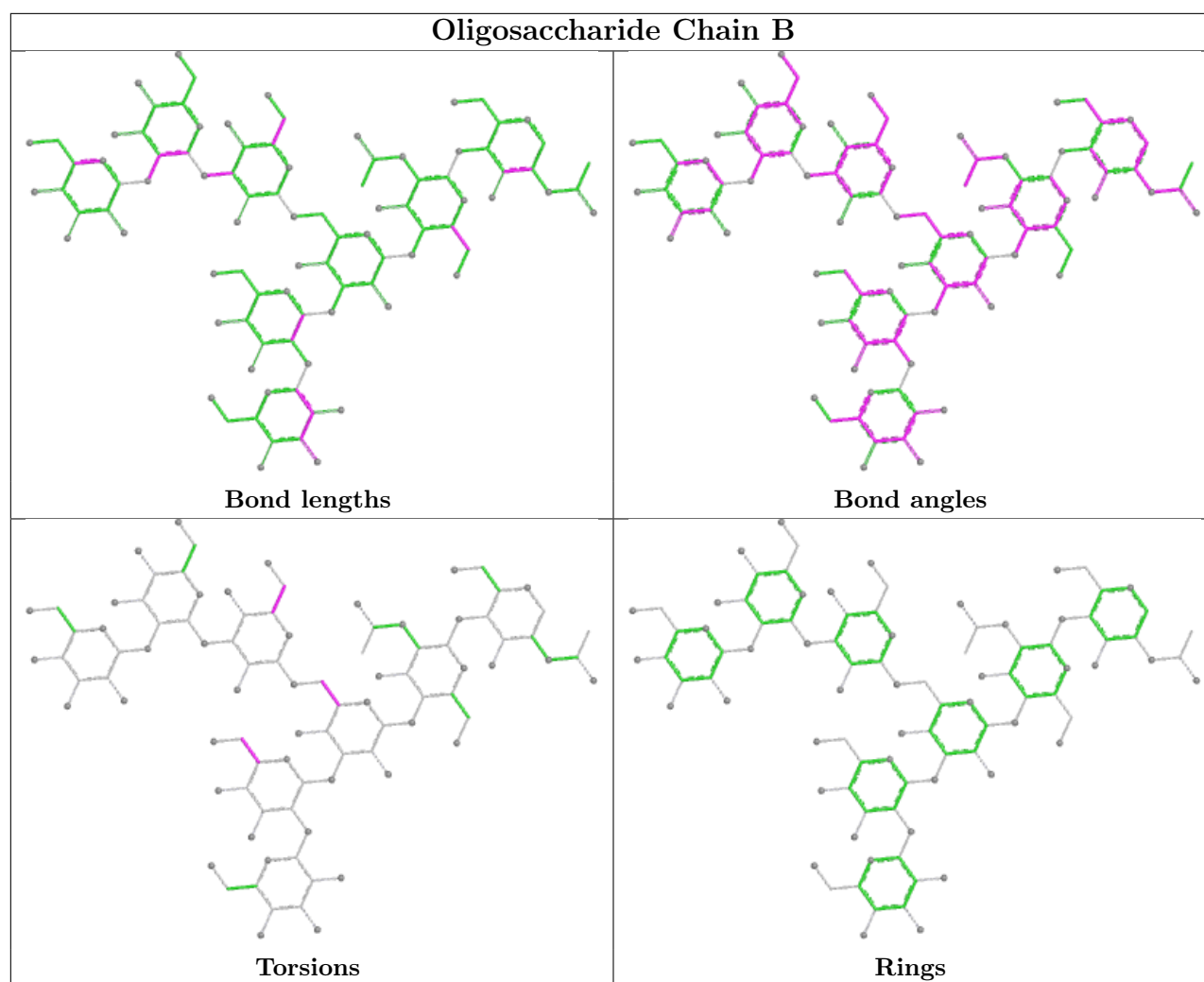
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	MAN	O5-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6
2	B	4	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 [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	ACT	A	908	-	3,3,3	1.00	0	3,3,3	1.46	0
3	YNI	A	901	-	31,31,31	2.53	14 (45%)	39,45,45	1.74	9 (23%)
9	SO4	A	909	4	4,4,4	0.51	0	6,6,6	1.19	1 (16%)
8	ACT	A	907	-	3,3,3	1.27	0	3,3,3	0.76	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
3	YNI	A	901	-	-	1/19/19/19	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	YNI	C16-N17	5.43	1.38	1.32
3	A	901	YNI	C1-C6	-5.39	1.31	1.39
3	A	901	YNI	C18-C19	4.63	1.41	1.37
3	A	901	YNI	C16-N20	3.93	1.43	1.36
3	A	901	YNI	C12-N13	3.39	1.22	1.14
3	A	901	YNI	C27-N20	-3.38	1.41	1.47
3	A	901	YNI	C23-N24	3.16	1.37	1.32
3	A	901	YNI	C7-C6	-3.03	1.49	1.54
3	A	901	YNI	C21-N26	2.81	1.39	1.34
3	A	901	YNI	C9-C7	2.73	1.61	1.53
3	A	901	YNI	C15-C16	-2.44	1.45	1.49
3	A	901	YNI	C19-N20	-2.37	1.36	1.39
3	A	901	YNI	C4-C3	-2.14	1.35	1.38
3	A	901	YNI	C22-C21	-2.07	1.34	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	YNI	C21-C22-C23	-5.12	113.42	116.73
3	A	901	YNI	C3-C2-C12	3.22	124.52	121.18
3	A	901	YNI	C10-C7-C6	2.60	115.82	110.87
3	A	901	YNI	C9-C7-C6	-2.58	105.95	110.87
3	A	901	YNI	N26-C25-N24	-2.49	124.81	128.58
3	A	901	YNI	C2-C3-CL11	2.31	121.41	119.45
3	A	901	YNI	C29-O28-C23	2.30	120.75	117.33
3	A	901	YNI	C15-C16-N20	2.27	125.95	123.32
9	A	909	SO4	O3-S-O2	2.26	121.37	109.56
3	A	901	YNI	C25-N26-C21	2.18	117.04	115.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

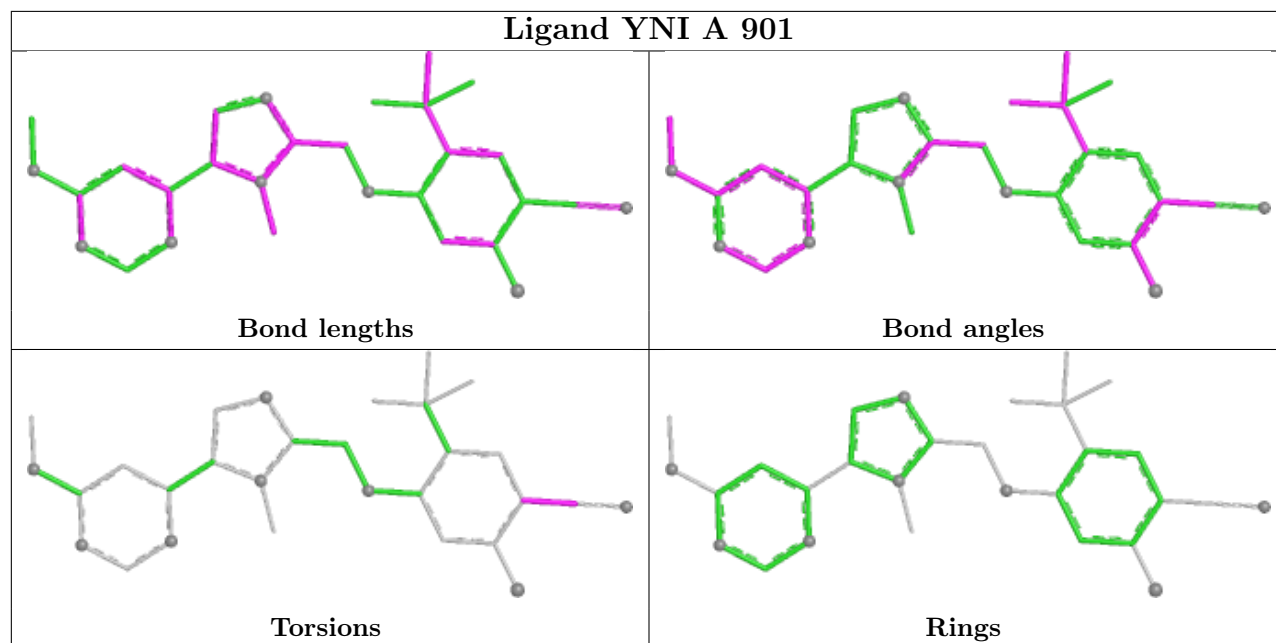
Mol	Chain	Res	Type	Atoms
3	A	901	YNI	N13-C12-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	YNI	1	0
9	A	909	SO4	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 ⓘ

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	A	804/846 (95%)	0.54	97 (12%) 8 11	9, 22, 62, 127	11 (1%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	VAL	8.4
1	A	578	LEU	8.2
1	A	51	TRP	7.9
1	A	469	PHE	7.8
1	A	397	ILE	6.6
1	A	581	LEU	6.3
1	A	243	LEU	6.2
1	A	468	CYS	6.0
1	A	68	VAL	5.7
1	A	236	VAL	5.5
1	A	71	PRO	5.3
1	A	78	LEU	5.3
1	A	70	PRO	5.1
1	A	239	ALA	4.9
1	A	274	PHE	4.8
1	A	237	PHE	4.8
1	A	235	PRO	4.6
1	A	571	LYS	4.5
1	A	573	GLU	4.5
1	A	59	LYS	4.3
1	A	233	TYR	4.2
1	A	52	THR	4.2
1	A	244	ARG	4.1
1	A	585	LEU	4.1
1	A	378	ASN	4.0
1	A	400	SER	4.0
1	A	77	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	402	TYR	3.9
1	A	240	SER	3.8
1	A	576	ASN	3.8
1	A	82	TYR	3.7
1	A	55	SER	3.7
1	A	251	HIS	3.6
1	A	54	THR	3.6
1	A	583	LYS	3.6
1	A	238	ASP	3.6
1	A	69	GLY	3.6
1	A	462	LYS	3.5
1	A	249	PHE	3.5
1	A	463	LYS	3.5
1	A	461	TYR	3.5
1	A	401	LYS	3.4
1	A	377	THR	3.3
1	A	366	CYS	3.3
1	A	242	HIS	3.3
1	A	72	ASP	3.3
1	A	538	THR	3.2
1	A	104	LYS	3.2
1	A	582	ASN	3.2
1	A	246	ARG	3.2
1	A	53	ALA	3.2
1	A	81	SER	3.1
1	A	587	THR	3.0
1	A	580	GLU	3.0
1	A	277	VAL	3.0
1	A	591	THR	3.0
1	A	577	LYS	2.9
1	A	56	GLY	2.9
1	A	860	SER	2.9
1	A	379	VAL	2.8
1	A	579	GLU	2.8
1	A	584	ARG	2.7
1	A	470	PHE	2.7
1	A	110	VAL	2.7
1	A	398	ASN	2.7
1	A	416	PRO	2.6
1	A	395	LYS	2.6
1	A	403	ASP	2.6
1	A	87	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	394	ALA	2.5
1	A	66	GLN	2.5
1	A	570	ASP	2.5
1	A	247	GLU	2.5
1	A	537	ASN	2.4
1	A	272[A]	THR	2.4
1	A	250	ASN	2.4
1	A	124	LEU	2.4
1	A	234	ASP	2.4
1	A	83	SER	2.4
1	A	399	ASN	2.4
1	A	549	ARG	2.3
1	A	589	GLY	2.3
1	A	161	VAL	2.3
1	A	376	LEU	2.2
1	A	114	GLU	2.2
1	A	252	ARG	2.2
1	A	330	GLU	2.1
1	A	382	ILE	2.1
1	A	460	VAL	2.1
1	A	383	THR	2.1
1	A	777	PHE	2.1
1	A	644	ILE	2.1
1	A	79	CYS	2.1
1	A	137	CYS	2.0
1	A	645	PRO	2.0
1	A	346	ARG	2.0
1	A	590	SER	2.0

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

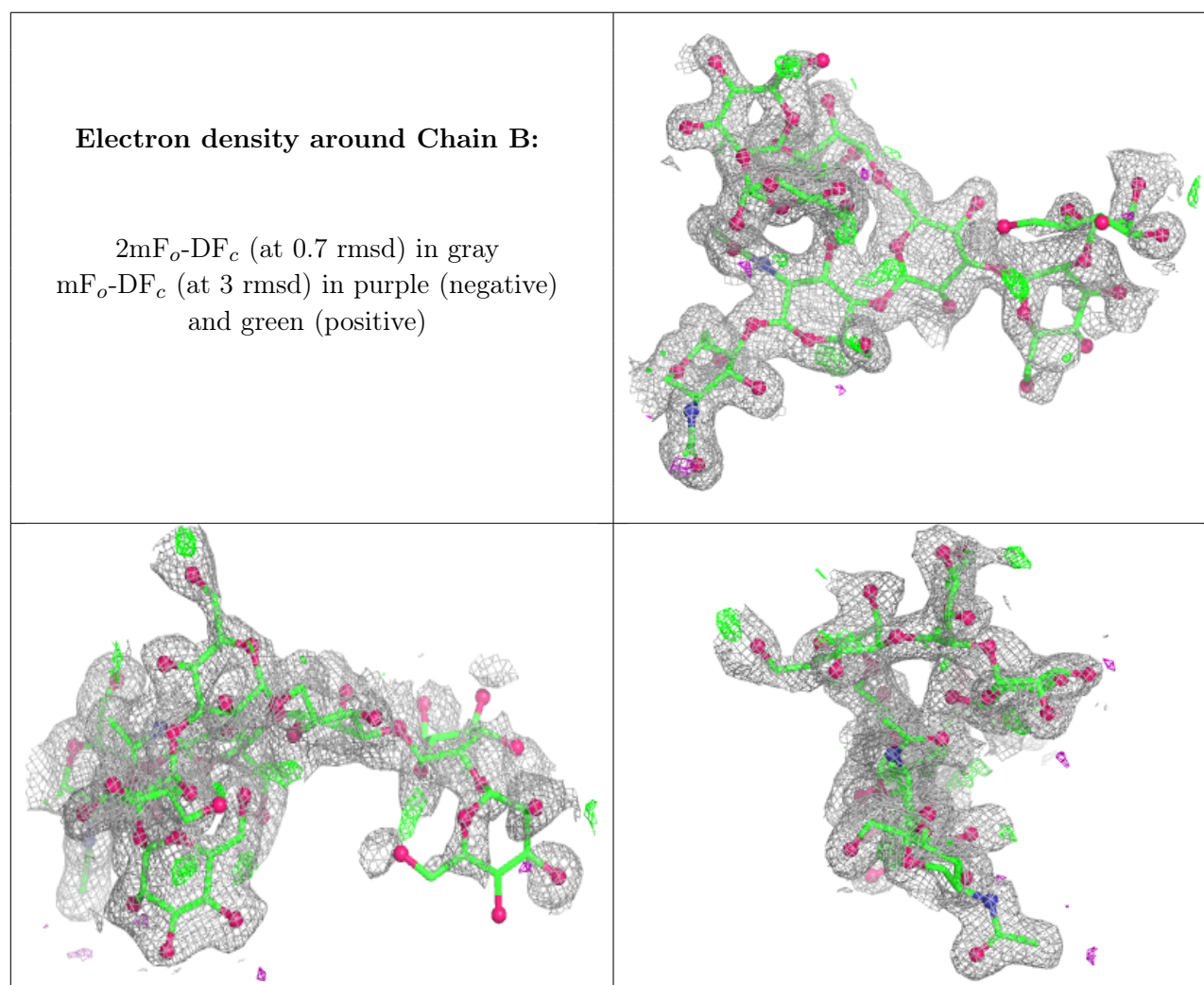
There are no non-standard protein/DNA/RNA residues in this entry.

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	MAN	B	7	11/12	0.52	0.20	74,88,101,101	0
2	MAN	B	3	11/12	0.70	0.16	51,56,64,71	0
2	MAN	B	8	11/12	0.73	0.21	34,74,81,86	0
2	MAN	B	4	11/12	0.74	0.15	45,54,56,56	0
2	MAN	B	5	11/12	0.79	0.16	36,47,53,54	0
2	MAN	B	6	11/12	0.84	0.15	29,40,46,46	0
2	NAG	B	2	14/15	0.89	0.10	23,28,40,47	0
2	NAG	B	1	14/15	0.96	0.05	12,13,16,18	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.



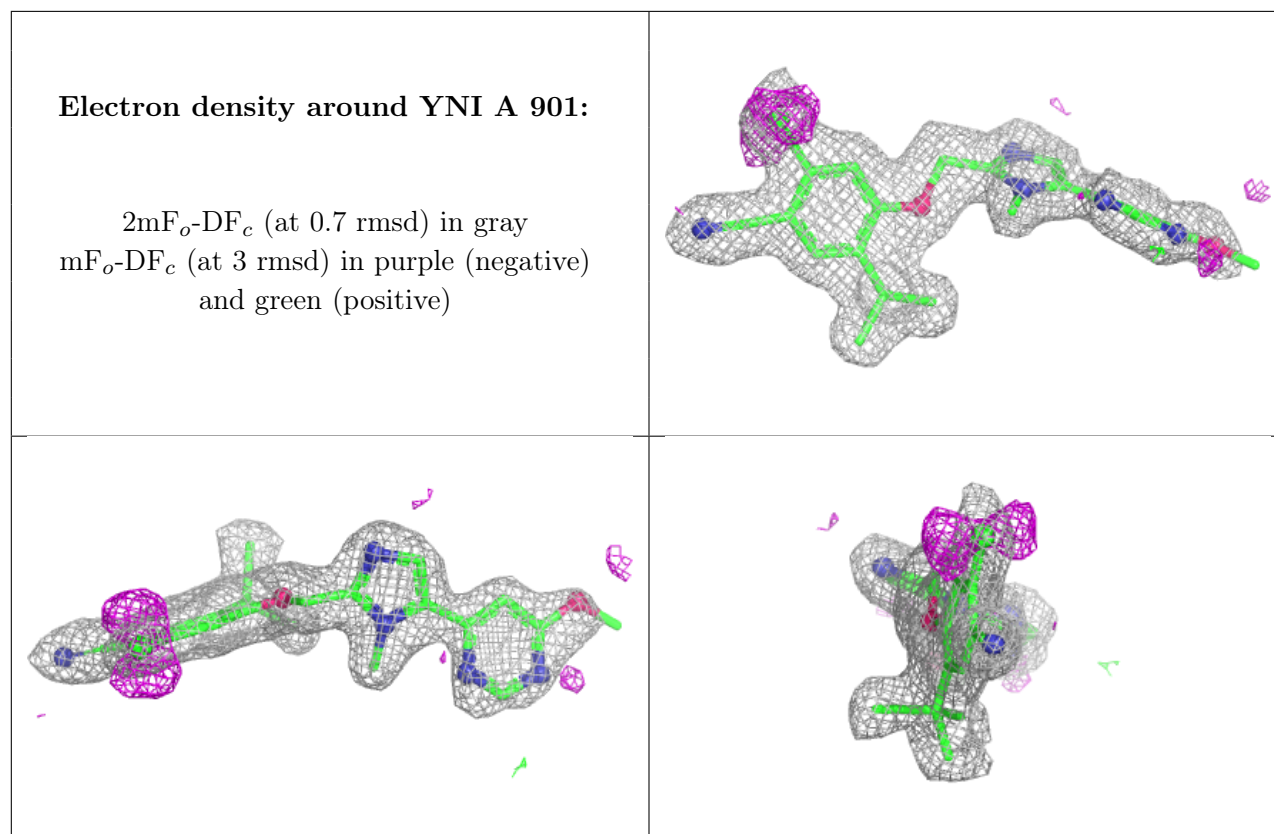
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
8	ACT	A	907	4/4	0.82	0.17	30,30,36,38	0
9	SO4	A	909	5/5	0.86	0.21	51,71,91,92	0
8	ACT	A	908	4/4	0.88	0.14	35,36,42,43	0
3	YNI	A	901	29/29	0.90	0.11	21,26,49,54	0
7	K	A	906	1/1	0.96	0.05	24,24,24,24	0
5	NA	A	903	1/1	0.96	0.06	33,33,33,33	0
6	CA	A	905	1/1	0.98	0.05	39,39,39,39	0
4	ZN	A	902	1/1	0.99	0.02	18,18,18,18	0
6	CA	A	904	1/1	1.00	0.02	13,13,13,13	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.