



Full wwPDB X-ray Structure Validation Report

Dec 13, 2024 – 03:46 AM EST

PDB ID : 7G6X
Title : Crystal Structure of rat Autotaxin in complex with N-[(3,4-dichlorophenyl)methyl]-2-[4-oxo-6-[4-(4-sulfamoylbutanoyl)piperazin-1-yl]quinazolin-3-yl]acetamide, i.e. SMILES NS(=O)(=O)CCCC(=O)N1CCN(c2ccc3c(c2)C(=O)N(C=N3)CC(=O)NCc2ccc(c(c2)Cl)Cl)CC1 with IC50=0.00464057 microM
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Deposited on : 2023-06-05
Resolution : 1.54 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

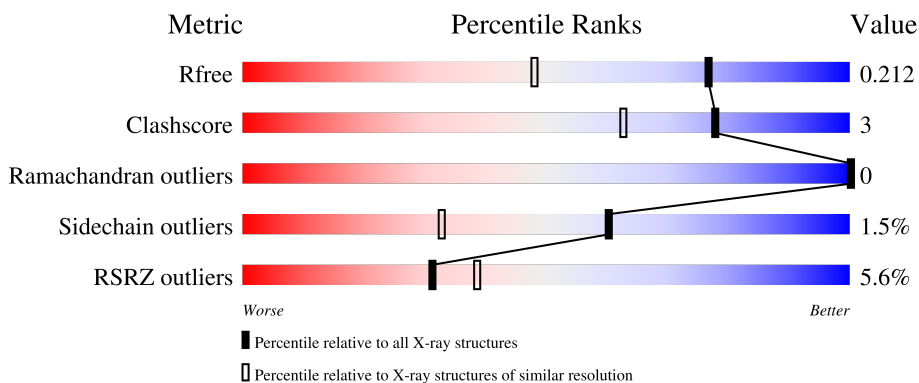
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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}	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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	
2	B	8	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 7506 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	805	6665	4237	1144	1232	52	0	27	0

There are 14 discrepancies between the modelled and reference sequences:

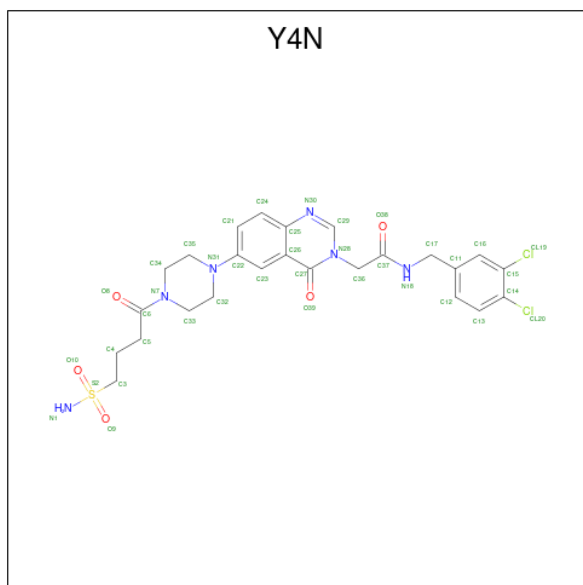
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	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)]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
			Total	C	N	O			
2	B	8	94	52	2	40	0	0	0

- Molecule 3 is N-[(3,4-dichlorophenyl)methyl]-2-[4-oxo-6-[4-(4-sulfamoylbutanoyl)piperazin-1-yl]quinazolin-3(4H)-yl}acetamide (three-letter code: Y4N) (formula: C₂₅H₂₈Cl₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



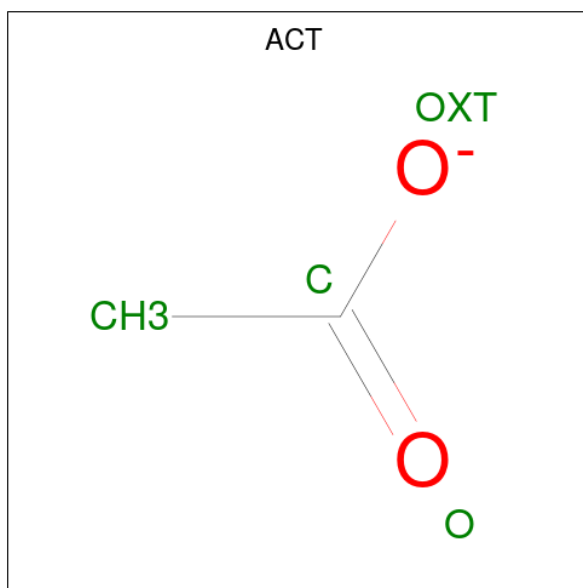
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	39	25	2	6	5	1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

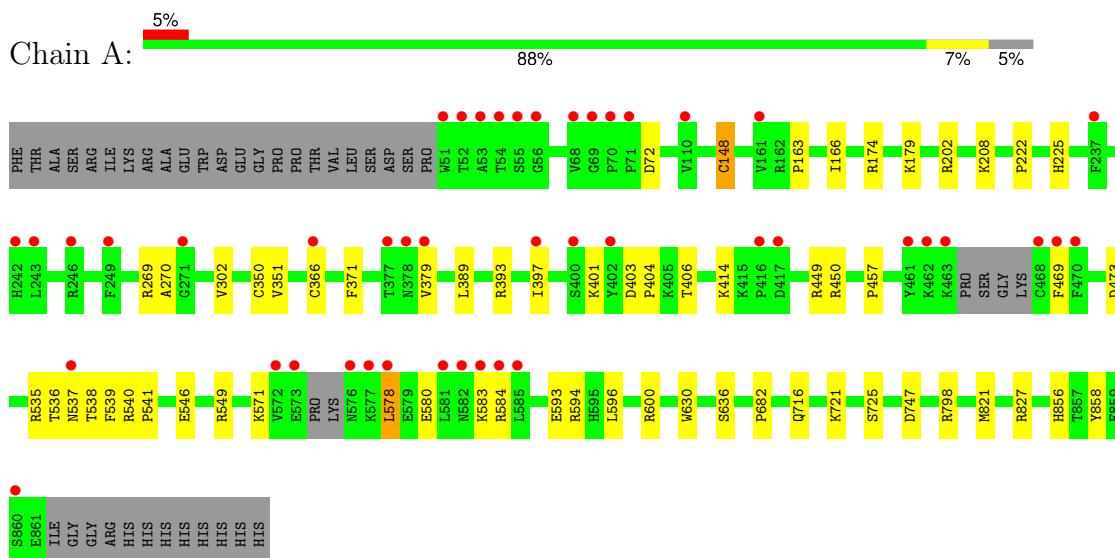
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	687	Total O 687 687	0	0

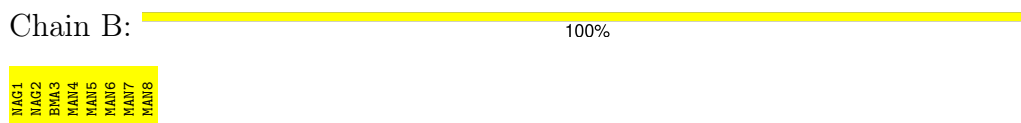
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.08Å 91.94Å 119.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.97 – 1.54 45.97 – 1.54	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.97-1.54) 95.6 (45.97-1.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.212 0.182 , 0.212	Depositor DCC
R_{free} test set	6930 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtrriage
Anisotropy	0.273	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7506	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, Y4N, BMA, MAN, NAG, MES, NA, CA, ACT

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	0.85	2/6912 (0.0%)	0.91	11/9370 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE1	5.68	1.31	1.25
1	A	630	TRP	CE3-CZ3	5.08	1.47	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	148	CYS	CA-CB-SG	6.70	126.06	114.00
1	A	827	ARG	CG-CD-NE	-5.72	99.79	111.80
1	A	393	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	174	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	202	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	473	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	747	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	578	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	393	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	798	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	6665	0	6480	35	0
2	B	94	0	79	0	0
3	A	39	0	0	0	0
4	A	12	0	13	1	0
5	A	4	0	3	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	2	0	0	0	0
9	A	687	0	0	6	0
All	All	7506	0	6575	36	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 (36) 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:539[A]:PHE:O	1:A:541:PRO:HD3	1.66	0.95
1:A:856:HIS:HD2	1:A:858[A]:TYR:CZ	2.03	0.77
1:A:538[B]:THR:HB	9:A:1311:HOH:O	1.92	0.69
1:A:856:HIS:HD2	1:A:858[A]:TYR:CE1	2.19	0.59
1:A:270:ALA:HB2	1:A:302:VAL:HG12	1.83	0.59
1:A:538[B]:THR:HG22	1:A:538[B]:THR:O	2.03	0.58
1:A:535:ARG:HG2	1:A:536[A]:THR:HG23	1.88	0.56
1:A:449:ARG:O	1:A:450[A]:ARG:HB2	2.05	0.55
1:A:721[A]:LYS:HE3	1:A:725[A]:SER:OG	2.07	0.55
1:A:270:ALA:HB2	1:A:302:VAL:CG1	2.38	0.53
1:A:538[B]:THR:O	1:A:538[B]:THR:CG2	2.56	0.53
1:A:208:LYS:NZ	9:A:1002:HOH:O	2.33	0.51
1:A:856:HIS:CD2	1:A:858[A]:TYR:CE1	2.99	0.51
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.46	0.51
1:A:594:ARG:HH21	1:A:594:ARG:HG2	1.75	0.50
1:A:270:ALA:CB	1:A:302:VAL:CG1	2.89	0.50
1:A:163:PRO:HB3	1:A:350:CYS:O	2.12	0.48
1:A:540[B]:ARG:HB2	1:A:540[B]:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:O	1:A:583:LYS:HG2	2.14	0.47
4:A:902:MES:H52	9:A:1586:HOH:O	2.15	0.47
1:A:366:CYS:SG	9:A:1580:HOH:O	2.61	0.46
1:A:179:LYS:HE3	1:A:179:LYS:HB2	1.72	0.46
1:A:536[A]:THR:O	1:A:537[A]:ASN:HB2	2.15	0.46
1:A:580:GLU:HB3	1:A:584:ARG:HH21	1.81	0.46
1:A:540[A]:ARG:HA	1:A:540[A]:ARG:HD3	1.70	0.44
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.53	0.44
1:A:821:MET:HE2	9:A:1045:HOH:O	2.18	0.43
1:A:594:ARG:NH1	1:A:636:SER:HB3	2.33	0.43
1:A:596:LEU:HD21	1:A:600:ARG:HB3	2.02	0.42
1:A:414:LYS:HD3	1:A:414:LYS:HA	1.78	0.42
1:A:682:PRO:HB3	1:A:716:GLN:HB3	2.01	0.42
1:A:166:ILE:HD12	1:A:351:VAL:HG11	2.01	0.41
1:A:403:ASP:HA	1:A:404:PRO:HD2	1.86	0.41
1:A:403:ASP:OD2	1:A:406:THR:HG23	2.21	0.41
1:A:404:PRO:HG3	9:A:1275:HOH:O	2.22	0.40
1:A:580:GLU:HG2	1:A:583:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	827/846 (98%)	800 (97%)	27 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	756/765 (99%)	745 (98%)	11 (2%)	60 33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	148	CYS
1	A	379	VAL
1	A	389	LEU
1	A	397	ILE
1	A	401	LYS
1	A	469	PHE
1	A	549	ARG
1	A	571	LYS
1	A	578	LEU
1	A	593	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	586	HIS
1	A	856	HIS

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](#)

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	0.95	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	B	2	2	14,14,15	0.98	1 (7%)	17,19,21	2.35	6 (35%)
2	BMA	B	3	2	11,11,12	0.89	1 (9%)	15,15,17	1.89	4 (26%)
2	MAN	B	4	2	11,11,12	0.92	0	15,15,17	1.74	3 (20%)
2	MAN	B	5	2	11,11,12	0.85	0	15,15,17	1.50	3 (20%)
2	MAN	B	6	2	11,11,12	0.81	0	15,15,17	1.08	2 (13%)
2	MAN	B	7	2	11,11,12	0.87	1 (9%)	15,15,17	1.79	3 (20%)
2	MAN	B	8	2	11,11,12	1.21	1 (9%)	15,15,17	1.43	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	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	-	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	MAN	C2-C3	2.87	1.56	1.52
2	B	1	NAG	O5-C1	2.27	1.47	1.43
2	B	2	NAG	C1-C2	2.14	1.55	1.52
2	B	3	BMA	C2-C3	2.12	1.55	1.52
2	B	7	MAN	C1-C2	2.08	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.52	122.26	112.19
2	B	4	MAN	C1-O5-C5	4.87	118.71	112.19
2	B	3	BMA	C1-O5-C5	4.67	118.44	112.19
2	B	8	MAN	O3-C3-C2	4.31	118.86	110.05
2	B	7	MAN	O5-C5-C6	4.26	115.95	107.66
2	B	7	MAN	C1-C2-C3	3.31	114.46	109.64
2	B	5	MAN	C1-O5-C5	3.29	116.59	112.19
2	B	2	NAG	C3-C4-C5	2.98	115.64	110.23
2	B	3	BMA	O6-C6-C5	-2.89	101.50	111.33
2	B	1	NAG	O5-C1-C2	-2.86	106.87	111.29
2	B	3	BMA	C1-C2-C3	2.72	113.61	109.64
2	B	4	MAN	O3-C3-C2	2.72	115.59	110.05
2	B	2	NAG	O7-C7-C8	-2.48	117.63	122.05
2	B	4	MAN	O2-C2-C1	2.34	114.59	109.22
2	B	5	MAN	C6-C5-C4	-2.34	107.28	113.02
2	B	6	MAN	C1-O5-C5	2.32	115.29	112.19
2	B	8	MAN	O2-C2-C3	2.27	114.84	110.15
2	B	2	NAG	C2-N2-C7	2.26	125.93	122.90
2	B	5	MAN	C3-C4-C5	2.26	114.33	110.23
2	B	7	MAN	C1-O5-C5	-2.24	109.19	112.19
2	B	3	BMA	O2-C2-C1	-2.19	104.21	109.22
2	B	2	NAG	C6-C5-C4	-2.16	107.73	113.02
2	B	6	MAN	O5-C5-C6	2.11	111.77	107.66
2	B	2	NAG	O7-C7-N2	2.11	125.71	121.98

There are no chirality outliers.

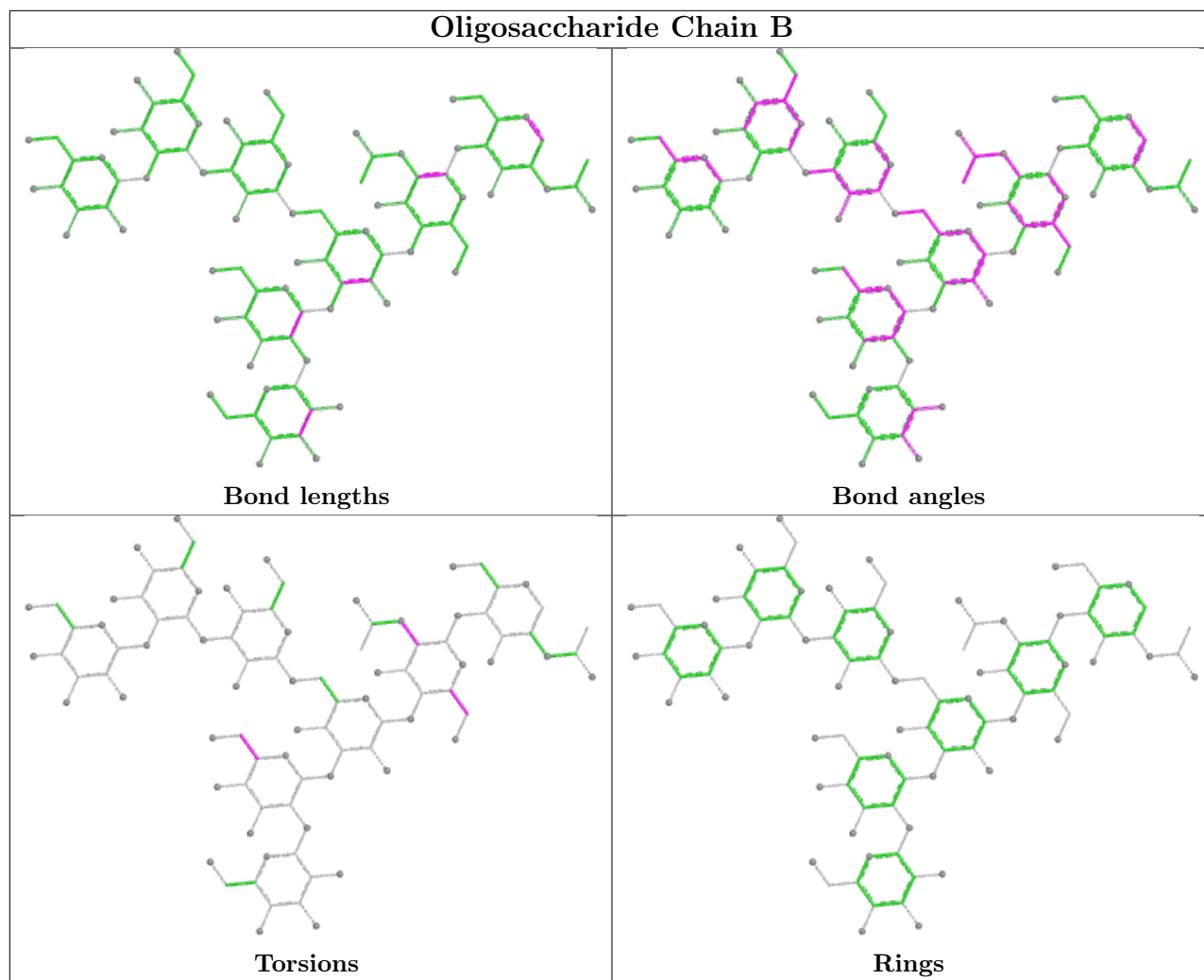
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	MAN	O5-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7

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
3	Y4N	A	901	-	42,42,42	2.63	15 (35%)	57,60,60	2.29	14 (24%)
5	ACT	A	903	-	3,3,3	1.13	0	3,3,3	0.72	0
4	MES	A	902	-	12,12,12	1.54	1 (8%)	15,16,16	1.15	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	Y4N	A	901	-	-	1/24/34/34	0/4/4/4
4	MES	A	902	-	-	3/6/14/14	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	Y4N	O9-S2	8.69	1.49	1.44
3	A	901	Y4N	O10-S2	-6.46	1.40	1.44
3	A	901	Y4N	C29-N28	5.54	1.44	1.36
4	A	902	MES	C8-S	-4.51	1.71	1.77
3	A	901	Y4N	C29-N30	4.47	1.34	1.28
3	A	901	Y4N	S2-N1	4.22	1.67	1.61
3	A	901	Y4N	C37-N18	3.63	1.42	1.33
3	A	901	Y4N	C35-N31	3.62	1.52	1.46
3	A	901	Y4N	C32-N31	2.98	1.51	1.46
3	A	901	Y4N	C36-C37	2.87	1.57	1.52
3	A	901	Y4N	O39-C27	2.44	1.27	1.22
3	A	901	Y4N	C12-C11	2.33	1.43	1.38
3	A	901	Y4N	C27-N28	2.27	1.42	1.39
3	A	901	Y4N	C6-N7	2.24	1.39	1.35
3	A	901	Y4N	C26-C25	2.24	1.43	1.40
3	A	901	Y4N	C16-C11	2.03	1.42	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	Y4N	C15-C16-C11	-8.57	114.92	120.46
3	A	901	Y4N	N28-C29-N30	-7.06	120.43	126.31
3	A	901	Y4N	C26-C27-N28	6.96	117.89	113.76
3	A	901	Y4N	C25-N30-C29	4.62	121.39	116.69
3	A	901	Y4N	C21-C22-N31	-3.15	117.02	121.39
3	A	901	Y4N	C12-C11-C16	2.66	122.21	118.55
3	A	901	Y4N	C17-N18-C37	-2.45	118.44	122.42
3	A	901	Y4N	C23-C26-C27	2.45	123.23	118.37
3	A	901	Y4N	C24-C21-C22	-2.40	117.26	120.30
3	A	901	Y4N	C23-C26-C25	-2.12	117.82	120.14
3	A	901	Y4N	C32-C33-N7	-2.09	106.26	110.42
3	A	901	Y4N	C34-C35-N31	-2.08	106.41	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	Y4N	C26-C23-C22	2.02	123.67	120.07
3	A	901	Y4N	C12-C13-C14	-2.00	117.21	119.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

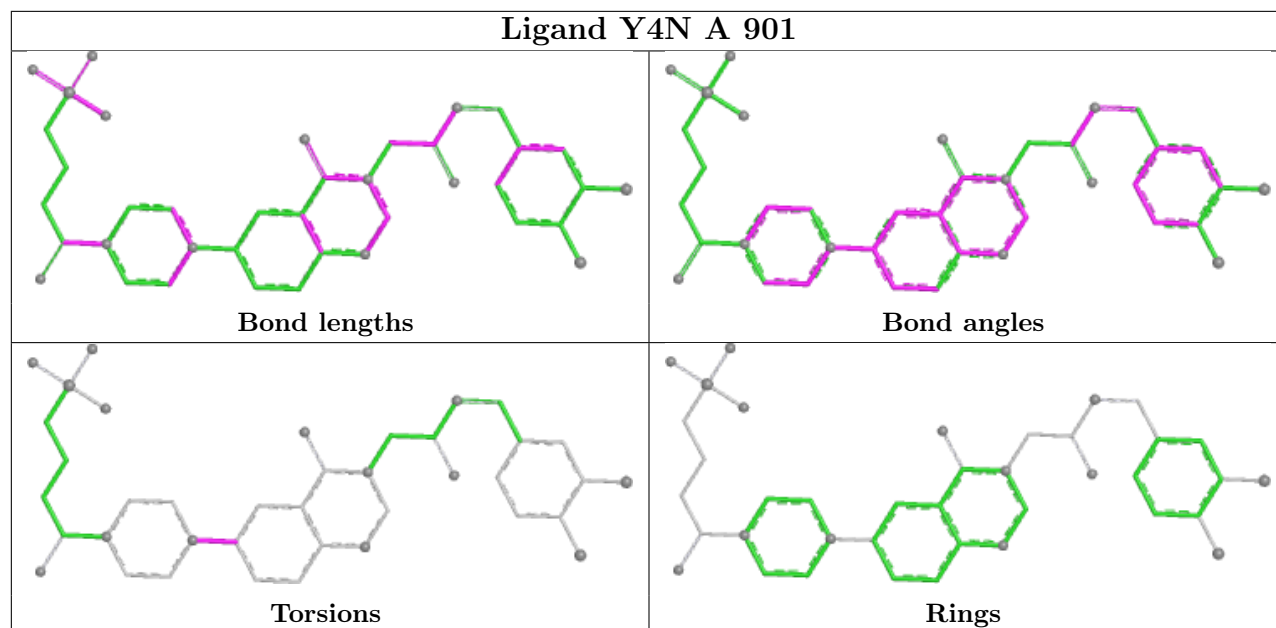
Mol	Chain	Res	Type	Atoms
4	A	902	MES	C7-C8-S-O2S
4	A	902	MES	C7-C8-S-O3S
4	A	902	MES	C7-C8-S-O1S
3	A	901	Y4N	C23-C22-N31-C32

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	MES	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	805/846 (95%)	0.13	45 (5%) 31 38	11, 24, 55, 80	27 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	LEU	7.8
1	A	469	PHE	6.9
1	A	572	VAL	6.4
1	A	468	CYS	6.0
1	A	51	TRP	5.6
1	A	581	LEU	4.8
1	A	71	PRO	4.5
1	A	366	CYS	4.3
1	A	68	VAL	4.3
1	A	397	ILE	4.0
1	A	55	SER	3.6
1	A	237	PHE	3.6
1	A	70	PRO	3.4
1	A	54	THR	3.4
1	A	463	LYS	3.1
1	A	462	LYS	3.1
1	A	585	LEU	3.0
1	A	271	GLY	2.9
1	A	161	VAL	2.8
1	A	402	TYR	2.8
1	A	243	LEU	2.8
1	A	461	TYR	2.7
1	A	52	THR	2.7
1	A	573	GLU	2.6
1	A	53	ALA	2.5
1	A	860	SER	2.5
1	A	249	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLY	2.4
1	A	69	GLY	2.4
1	A	417	ASP	2.4
1	A	577	LYS	2.3
1	A	537[A]	ASN	2.3
1	A	110	VAL	2.3
1	A	583	LYS	2.2
1	A	379	VAL	2.2
1	A	378	ASN	2.2
1	A	377	THR	2.2
1	A	242	HIS	2.2
1	A	584	ARG	2.2
1	A	576	ASN	2.2
1	A	400	SER	2.2
1	A	246	ARG	2.1
1	A	416	PRO	2.1
1	A	470	PHE	2.1
1	A	582	ASN	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.

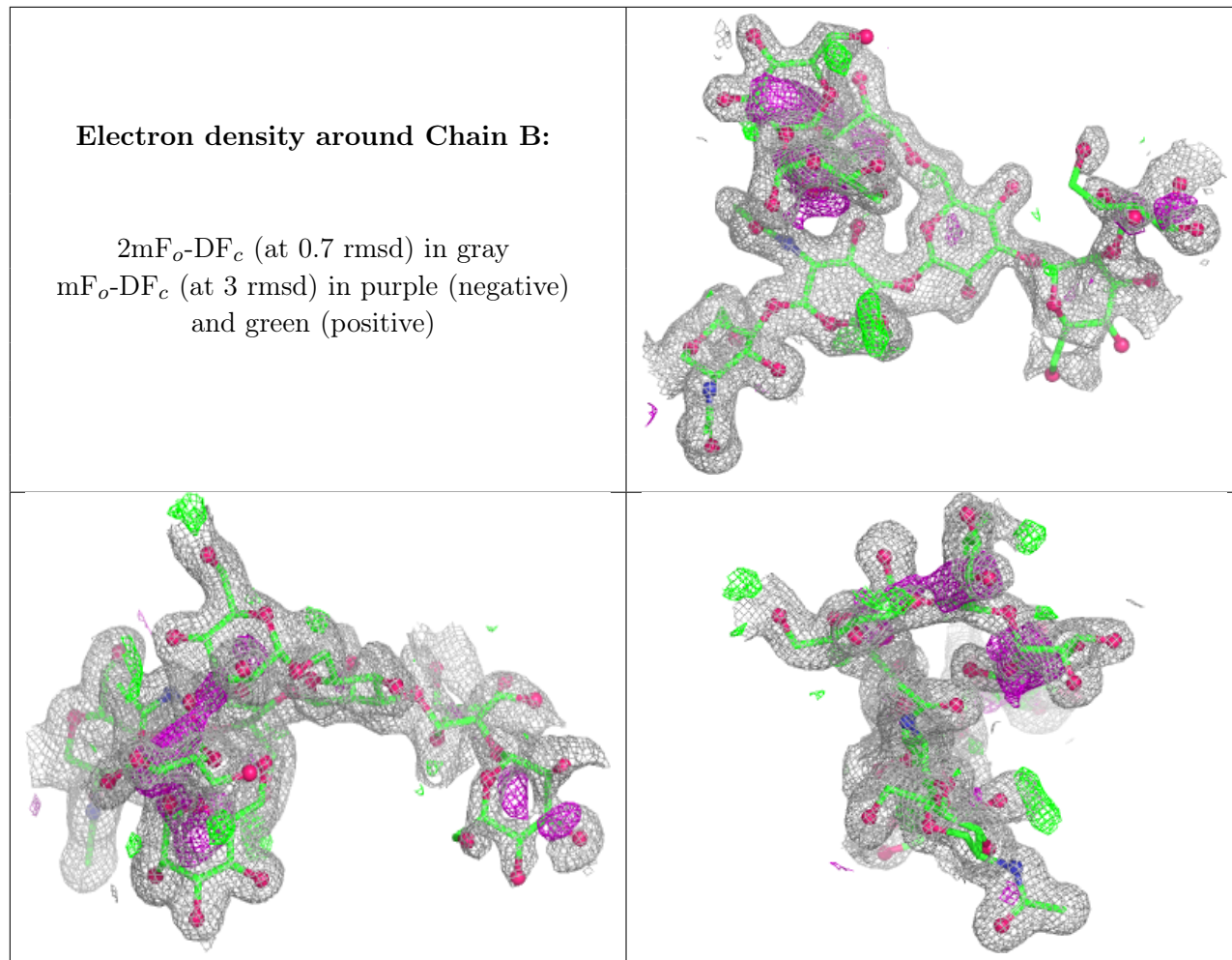
6.3 Carbohydrates [i](#)

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	0.46	0.18	72,80,80,80	0
2	BMA	B	3	11/12	0.66	0.14	53,56,64,72	0
2	MAN	B	8	11/12	0.71	0.15	38,64,70,72	0
2	MAN	B	4	11/12	0.75	0.13	46,50,53,53	0
2	MAN	B	5	11/12	0.81	0.14	38,48,51,62	0
2	MAN	B	6	11/12	0.86	0.13	31,42,46,47	0
2	NAG	B	2	14/15	0.88	0.10	26,31,41,48	0
2	NAG	B	1	14/15	0.97	0.07	16,18,22,23	0

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.

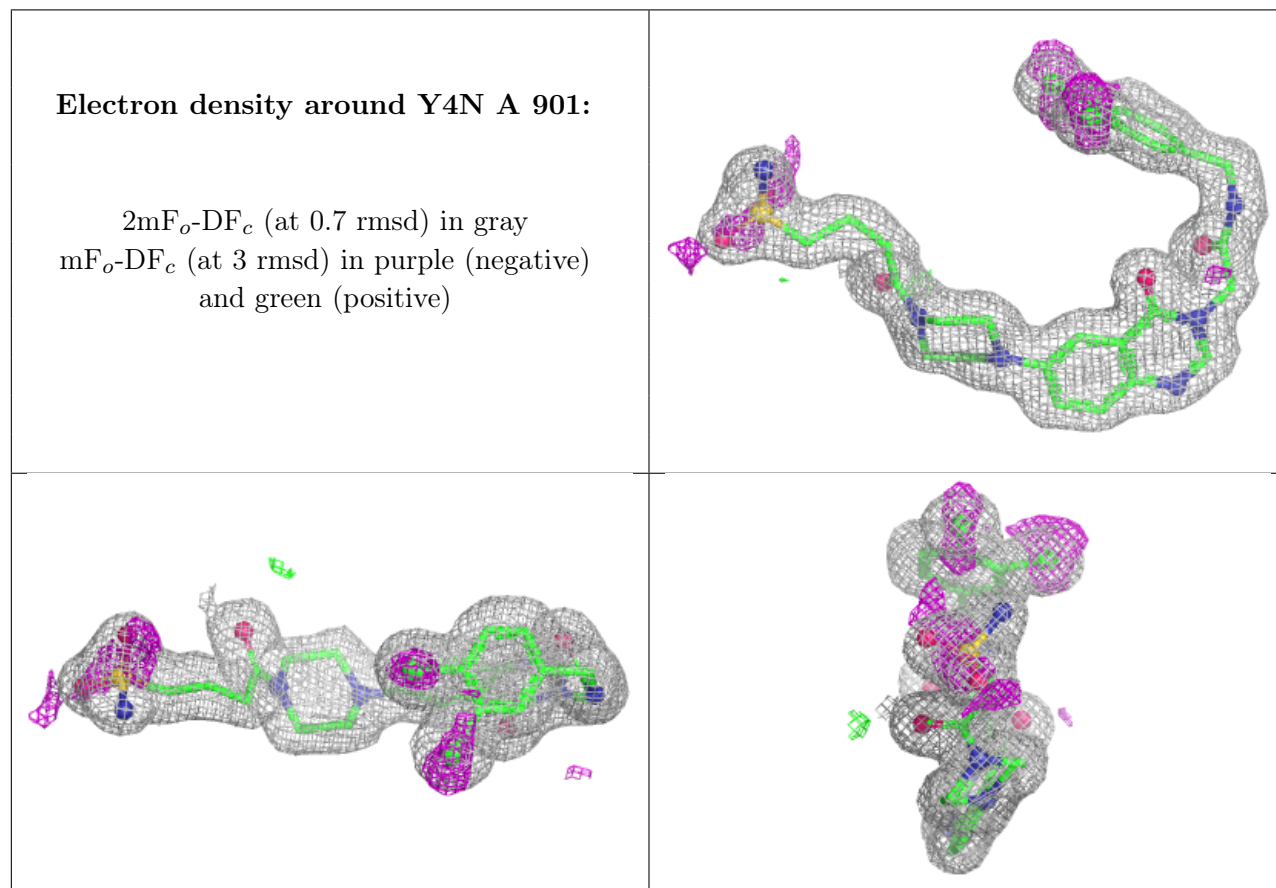


6.4 Ligands [i](#)

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
5	ACT	A	903	4/4	0.84	0.11	31,33,37,41	0
4	MES	A	902	12/12	0.89	0.19	35,56,68,71	0
8	NA	A	906	1/1	0.95	0.09	28,28,28,28	0
8	NA	A	908	1/1	0.95	0.08	29,29,29,29	0
3	Y4N	A	901	39/39	0.96	0.08	23,26,32,35	0
7	ZN	A	905	1/1	0.99	0.02	21,21,21,21	0
6	CA	A	904	1/1	0.99	0.10	25,25,25,25	0
6	CA	A	907	1/1	0.99	0.03	18,18,18,18	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.