



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2024 – 04:41 PM EST

PDB ID : 7G2T
Title : Crystal Structure of rat Autotaxin in complex with 1H-benzotriazol-5-yl-[3-[(2-tert-butyl-4-chloro-5-methylphenyl)methoxy]-4,5,7,8-tetrahydro-1H-pyrazolo[3,4-d]azepin-6-yl]methanone, i.e. SMILES c12c(cc(cc1)C(=O)N1CCC3=C(CC1)NN=C3OCc1c(cc(c(c1)C)Cl)C(C)(C)C)N=NN2 with IC50=0.295297 microM
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Rudolph, M.G.
Deposited on : 2023-06-05
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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)

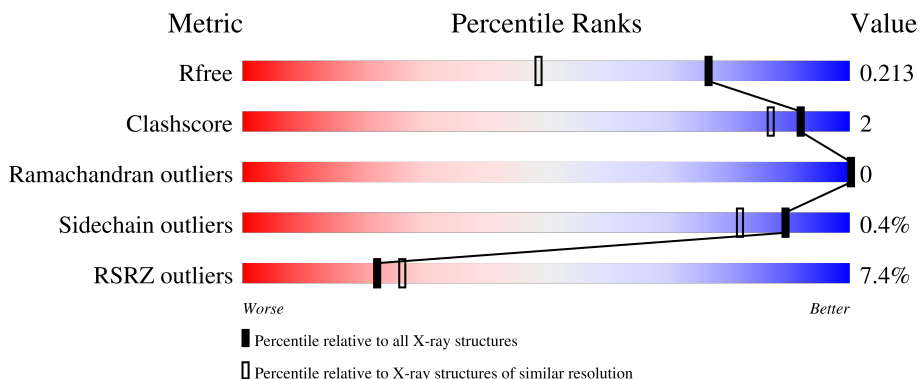
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

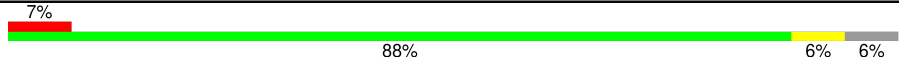
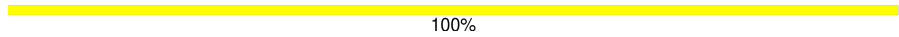
The reported resolution of this entry is 1.55 Å.

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	1935 (1.56-1.56)
Clashscore	180529	2073 (1.56-1.56)
Ramachandran outliers	177936	2037 (1.56-1.56)
Sidechain outliers	177891	2034 (1.56-1.56)
RSRZ outliers	164620	1935 (1.56-1.56)

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	 7% 88% 6% 6%
2	B	8	 100%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.40

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 7233 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	796	6522	4145	1122	1203	52	0	18	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	conflict	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.

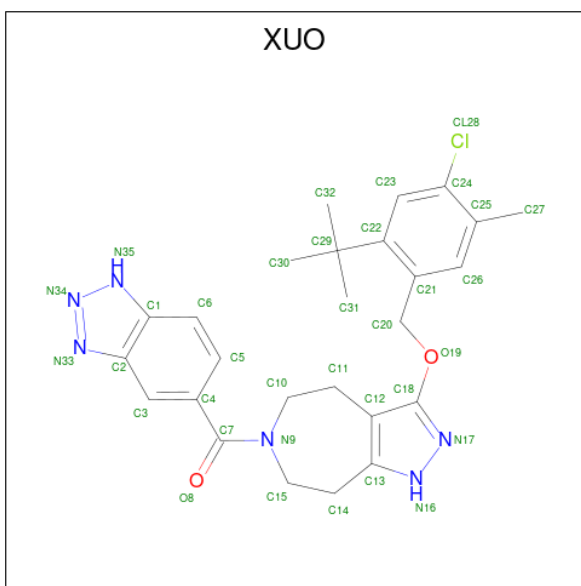


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	8	94	52	2	40	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is (1H-benzotriazol-5-yl){3-[(2-tert-butyl-4-chloro-5-methylphenyl)methoxy]-4,5,7,8-tetrahydropyrazolo[3,4-d]azepin-6(1H)-yl}methanone (three-letter code: XUO) (formula: C₂₆H₂₉ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	35	26	1	6	2	0	0
4	A	1	34	25	1	6	2	0	0

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



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

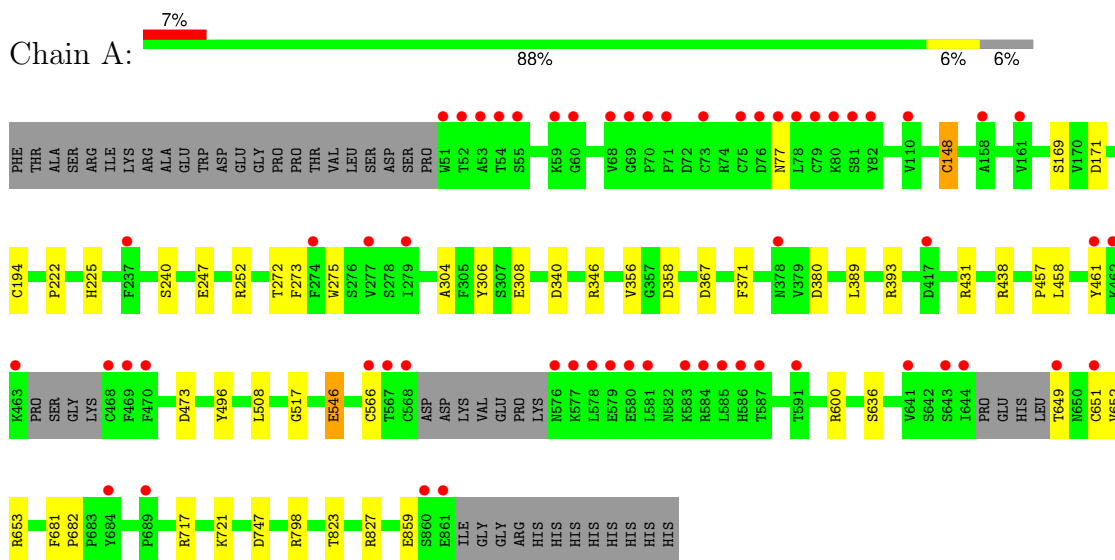
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	538	Total 538	O 538	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	82.61Å 91.02Å 117.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.51 – 1.55 45.51 – 1.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.51-1.55) 95.4 (45.51-1.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.176 , 0.206 0.186 , 0.213	Depositor DCC
R_{free} test set	6482 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: NA, NAG, BMA, MAN, CL, ZN, ACT, K, CA, XUO

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	0.91	4/6758 (0.1%)	0.96	20/9156 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE1	7.01	1.33	1.25
1	A	308	GLU	CD-OE2	6.45	1.32	1.25
1	A	308	GLU	CD-OE1	-5.96	1.19	1.25
1	A	517	GLY	N-CA	5.85	1.54	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	NE-CZ-NH2	-9.63	115.49	120.30
1	A	393	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	194[A]	CYS	CA-CB-SG	-7.09	101.23	114.00
1	A	194[B]	CYS	CA-CB-SG	-7.09	101.23	114.00
1	A	358	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	747	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	747	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	653	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	308	GLU	CG-CD-OE2	5.78	129.86	118.30
1	A	346	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	827	ARG	CG-CD-NE	-5.64	99.95	111.80
1	A	798	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	438	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	717	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	380	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	340	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	473	ASP	CB-CG-OD1	5.27	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148[A]	CYS	CA-CB-SG	-5.19	104.66	114.00
1	A	148[B]	CYS	CA-CB-SG	-5.19	104.66	114.00
1	A	308	GLU	CG-CD-OE1	-5.01	108.27	118.30

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	6522	0	6343	19	0
2	B	94	0	79	0	0
3	A	2	0	0	0	0
4	A	69	0	0	1	0
5	A	4	0	3	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	538	0	0	2	0
All	All	7233	0	6425	20	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 (20) 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:77:ASN:HD22	1:A:272:THR:HG21	1.64	0.63
1:A:367:ASP:HB3	10:A:1468:HOH:O	2.02	0.59
1:A:77:ASN:HD21	1:A:275:TRP:HA	1.70	0.57
1:A:171:ASP:OD2	1:A:306:TYR:OH	2.22	0.55
4:A:903:XUO:C21	4:A:903:XUO:O19	2.55	0.55
1:A:636:SER:O	1:A:721[A]:LYS:NZ	2.41	0.54
1:A:240:SER:O	1:A:247:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:PHE:CD1	1:A:682:PRO:HD2	2.49	0.47
1:A:566:CYS:SG	1:A:652:VAL:HB	2.56	0.46
1:A:252:ARG:NH1	10:A:1009:HOH:O	2.47	0.45
1:A:273:PHE:HA	1:A:304:ALA:HB3	1.98	0.45
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.52	0.45
1:A:148[B]:CYS:SG	1:A:496:TYR:HE1	2.41	0.44
1:A:431:ARG:HD3	1:A:823:THR:O	2.18	0.42
1:A:169:SER:HA	1:A:356:VAL:O	2.19	0.42
1:A:458:LEU:HA	1:A:461:TYR:CZ	2.55	0.41
1:A:546:GLU:OE2	1:A:600[B]:ARG:NH1	2.51	0.41
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.55	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.95	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	807/846 (95%)	786 (97%)	21 (3%)	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	738/765 (96%)	735 (100%)	3 (0%)	89 82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	LEU
1	A	649	THR
1	A	651	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	398	ASN
1	A	436	ASN

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	1,2	14,14,15	1.16	2 (14%)	17,19,21	1.40	3 (17%)
2	NAG	B	2	2	14,14,15	1.33	3 (21%)	17,19,21	2.57	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	B	3	2	11,11,12	0.73	0	15,15,17	1.14	2 (13%)
2	MAN	B	4	2	11,11,12	1.04	0	15,15,17	1.40	1 (6%)
2	MAN	B	5	2	11,11,12	1.15	1 (9%)	15,15,17	1.54	2 (13%)
2	MAN	B	6	2	11,11,12	1.07	1 (9%)	15,15,17	1.04	2 (13%)
2	MAN	B	7	2	11,11,12	0.88	0	15,15,17	1.32	1 (6%)
2	MAN	B	8	2	11,11,12	1.16	1 (9%)	15,15,17	1.07	1 (6%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	MAN	O5-C5	2.86	1.49	1.43
2	B	2	NAG	O5-C1	-2.46	1.39	1.43
2	B	2	NAG	O6-C6	2.39	1.52	1.42
2	B	1	NAG	C4-C5	2.38	1.58	1.53
2	B	8	MAN	C2-C3	2.27	1.56	1.52
2	B	1	NAG	C1-C2	-2.19	1.49	1.52
2	B	6	MAN	O5-C5	2.09	1.47	1.43
2	B	2	NAG	C6-C5	2.01	1.58	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.45	122.17	112.19
2	B	2	NAG	C3-C4-C5	4.40	118.22	110.23
2	B	4	MAN	C1-O5-C5	3.58	116.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O7-C7-N2	3.17	127.58	121.98
2	B	5	MAN	O5-C5-C6	3.15	113.80	107.66
2	B	2	NAG	O7-C7-C8	-3.14	116.47	122.05
2	B	5	MAN	C6-C5-C4	-2.64	106.55	113.02
2	B	1	NAG	O5-C1-C2	-2.64	107.21	111.29
2	B	2	NAG	O7-C7-N2	2.47	126.35	121.98
2	B	2	NAG	O3-C3-C2	-2.31	104.61	109.40
2	B	6	MAN	O2-C2-C3	-2.27	105.46	110.15
2	B	3	BMA	O6-C6-C5	-2.26	103.63	111.33
2	B	6	MAN	C1-O5-C5	-2.22	109.21	112.19
2	B	1	NAG	O4-C4-C5	-2.20	103.91	109.32
2	B	3	BMA	O2-C2-C1	-2.10	104.42	109.22
2	B	8	MAN	C1-C2-C3	2.08	112.67	109.64
2	B	7	MAN	O5-C5-C6	2.05	111.65	107.66

There are no chirality outliers.

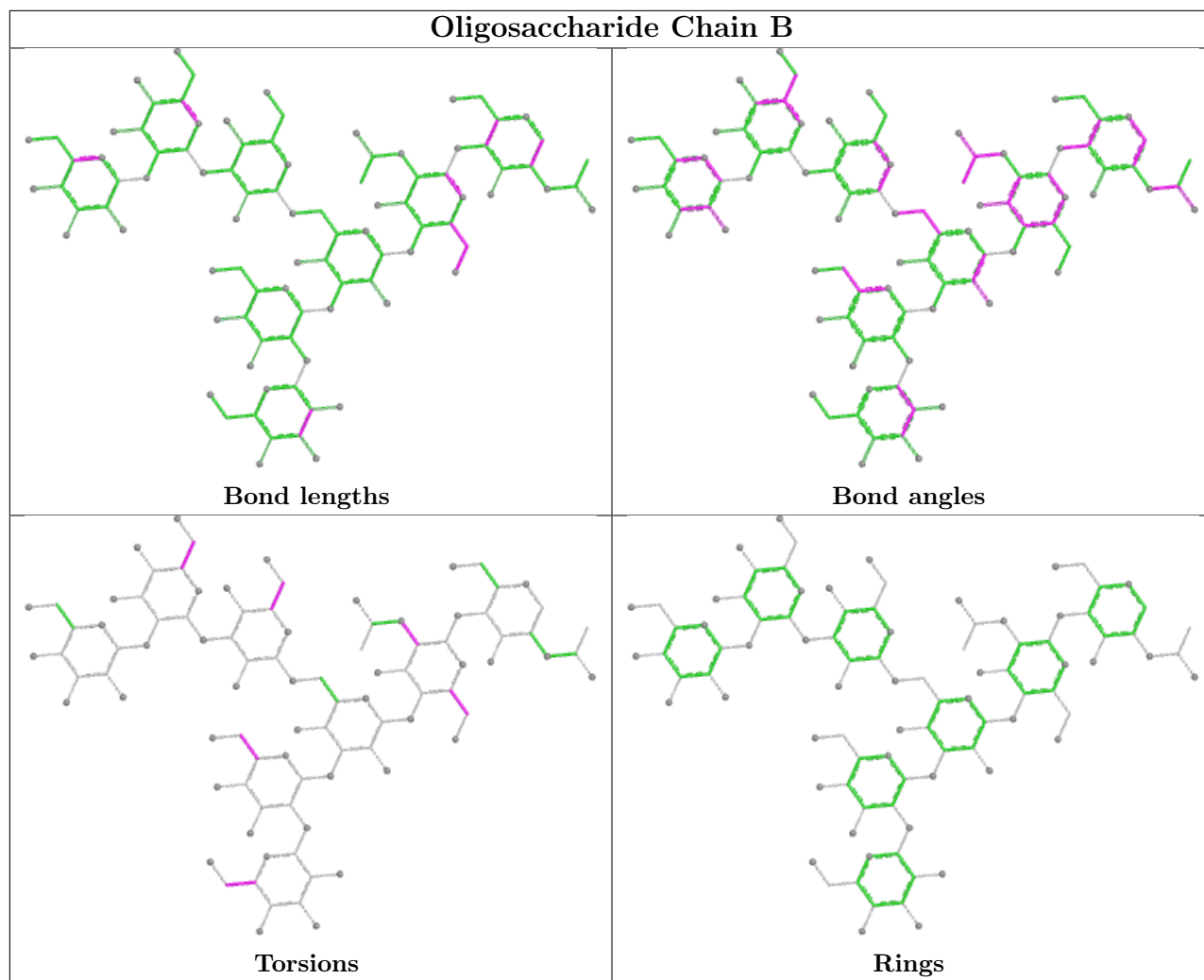
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	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, 6 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	XUO	A	903	-	32,37,39	0.90	0	39,54,58	1.24	3 (7%)
5	ACT	A	904	-	3,3,3	1.13	0	3,3,3	0.39	0
4	XUO	A	902	8	34,39,39	1.17	3 (8%)	43,58,58	1.42	7 (16%)

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
4	XUO	A	903	-	-	0/14/24/29	0/5/5/5
4	XUO	A	902	8	-	2/17/29/29	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	XUO	C11-C12	-3.99	1.47	1.51
4	A	902	XUO	C6-C1	-2.87	1.37	1.41
4	A	902	XUO	C18-N17	-2.04	1.31	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	XUO	C13-N16-N17	4.21	115.12	106.98
4	A	902	XUO	C13-N16-N17	3.98	114.69	106.98
4	A	902	XUO	C20-C21-C26	-3.69	112.75	120.48
4	A	903	XUO	C5-C6-C1	-2.90	117.34	120.80
4	A	902	XUO	C20-C21-C22	2.87	127.58	121.39
4	A	902	XUO	C11-C10-N9	2.30	115.52	112.41
4	A	903	XUO	C6-C1-N35	2.21	133.79	130.19
4	A	902	XUO	C6-C1-N35	2.21	133.78	130.19
4	A	902	XUO	C5-C6-C1	-2.04	118.36	120.80
4	A	902	XUO	N35-N34-N33	-2.03	108.62	111.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

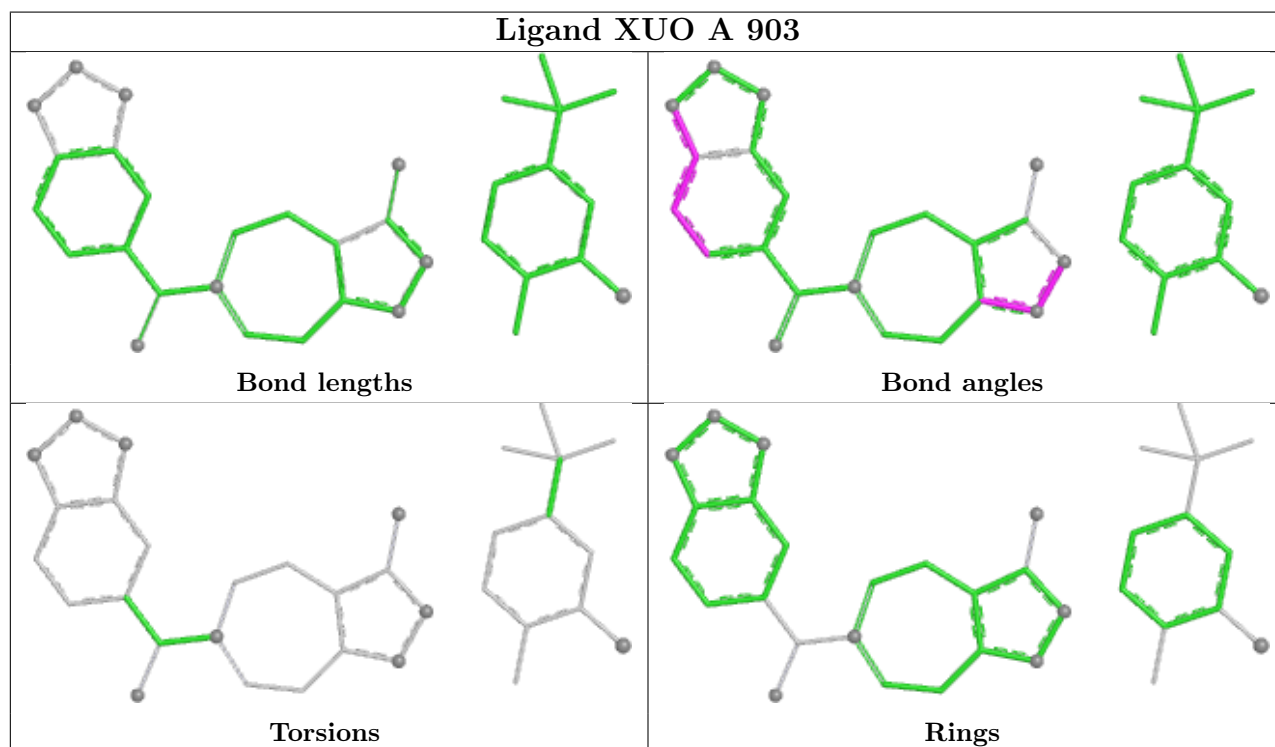
Mol	Chain	Res	Type	Atoms
4	A	902	XUO	C4-C7-N9-C15
4	A	902	XUO	O8-C7-N9-C15

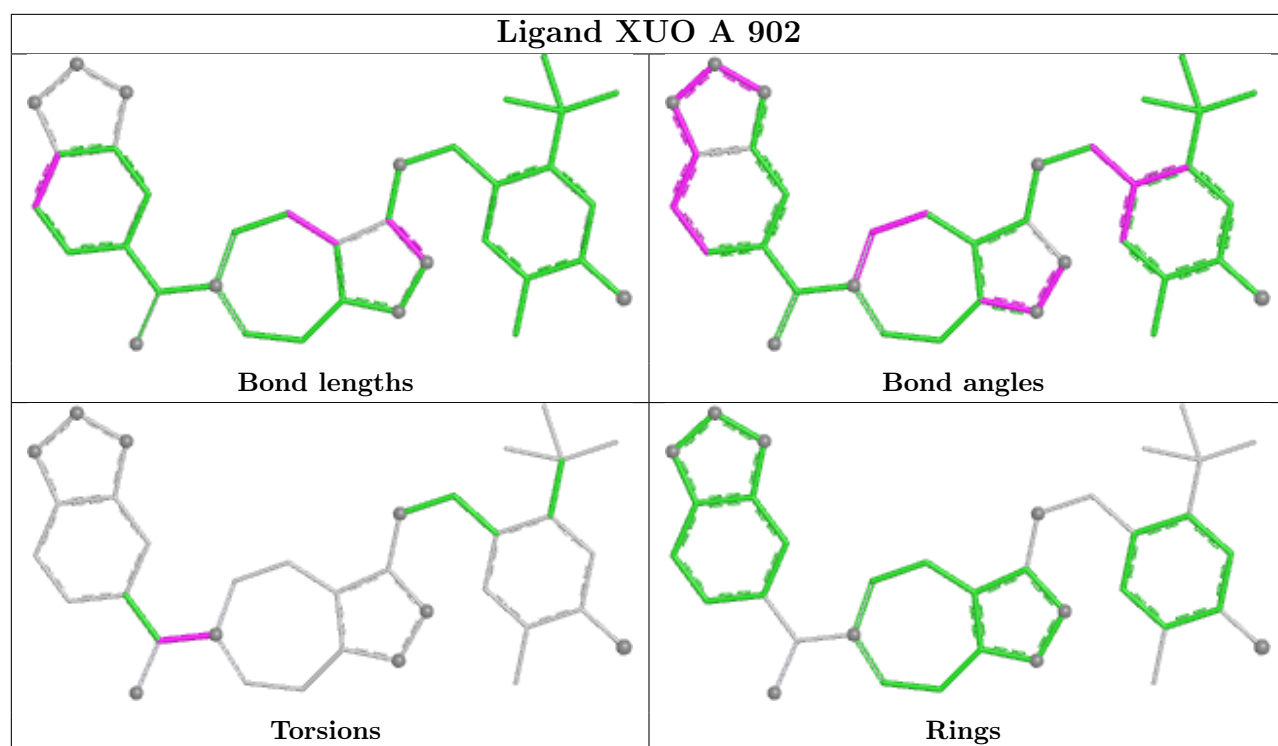
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	XUO	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	796/846 (94%)	0.31	59 (7%) 22 26	12, 25, 64, 80	18 (2%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	LEU	7.6
1	A	51	TRP	6.7
1	A	585	LEU	6.4
1	A	53	ALA	6.4
1	A	644	ILE	5.8
1	A	649	THR	5.6
1	A	469	PHE	5.6
1	A	578	LEU	5.5
1	A	468	CYS	5.3
1	A	568	CYS	5.3
1	A	461	TYR	4.8
1	A	70	PRO	4.4
1	A	651	CYS	4.2
1	A	52	THR	4.1
1	A	54	THR	4.1
1	A	567	THR	4.0
1	A	277	VAL	4.0
1	A	59	LYS	4.0
1	A	77	ASN	4.0
1	A	587	THR	3.8
1	A	463	LYS	3.8
1	A	71	PRO	3.6
1	A	462	LYS	3.5
1	A	68	VAL	3.5
1	A	577	LYS	3.4
1	A	79	CYS	3.2
1	A	689	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	110	VAL	3.0
1	A	576	ASN	3.0
1	A	579	GLU	3.0
1	A	566	CYS	3.0
1	A	378	ASN	2.9
1	A	78	LEU	2.9
1	A	584	ARG	2.9
1	A	860	SER	2.8
1	A	73	CYS	2.8
1	A	237	PHE	2.7
1	A	55	SER	2.7
1	A	60	GLY	2.7
1	A	583	LYS	2.6
1	A	684	TYR	2.6
1	A	861	GLU	2.6
1	A	81	SER	2.5
1	A	80	LYS	2.5
1	A	643	SER	2.5
1	A	82	TYR	2.5
1	A	161	VAL	2.5
1	A	75	CYS	2.4
1	A	580	GLU	2.4
1	A	417	ASP	2.4
1	A	586	HIS	2.4
1	A	158	ALA	2.3
1	A	274	PHE	2.2
1	A	69	GLY	2.2
1	A	591	THR	2.2
1	A	641	VAL	2.1
1	A	76	ASP	2.1
1	A	470	PHE	2.0
1	A	279	ILE	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.

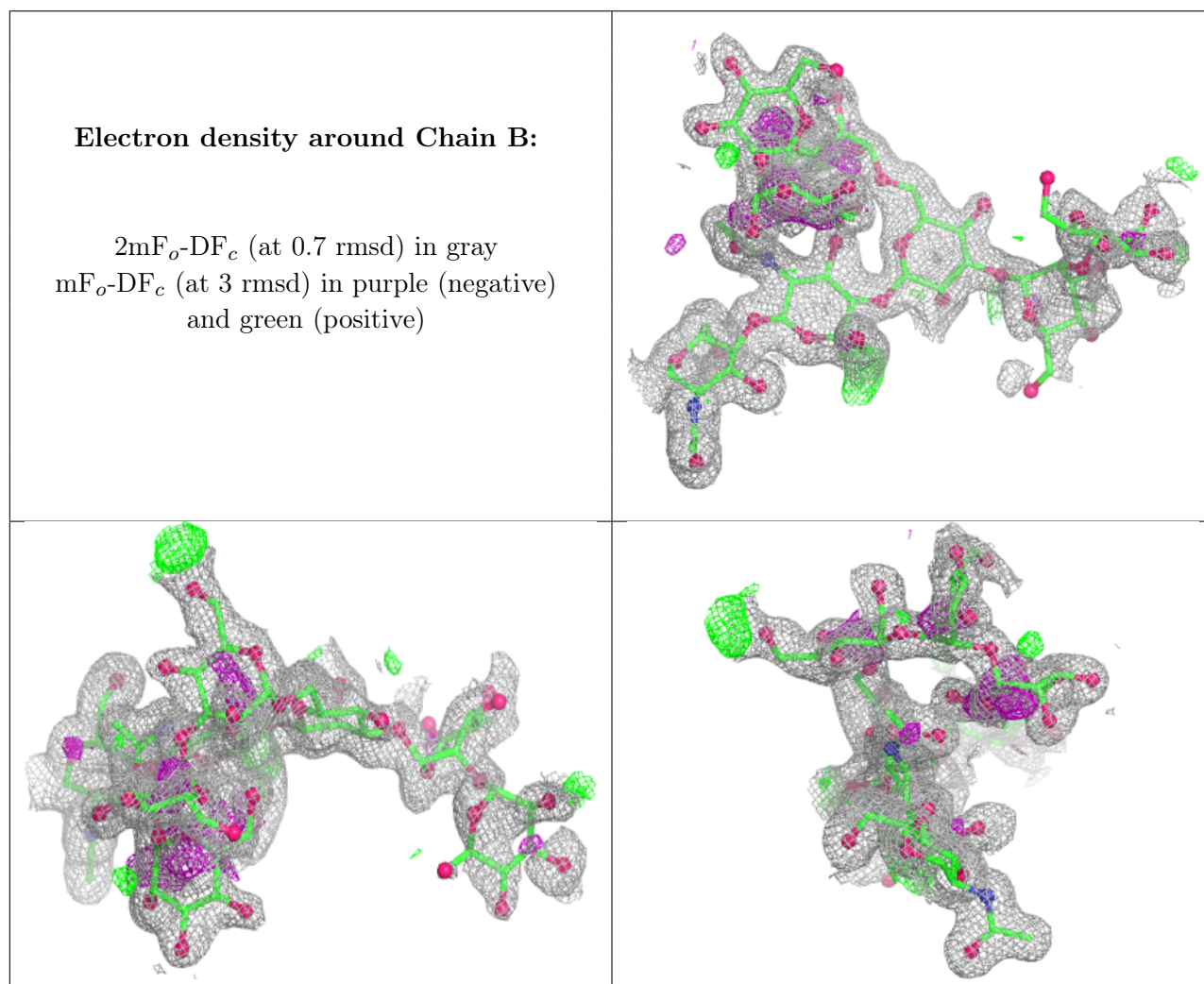
6.3 Carbohydrates [i](#)

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	0.51	0.16	75,80,80,80	0
2	MAN	B	8	11/12	0.68	0.15	41,65,72,73	0
2	BMA	B	3	11/12	0.70	0.13	50,54,62,63	0
2	MAN	B	4	11/12	0.74	0.13	37,49,56,60	0
2	MAN	B	5	11/12	0.79	0.15	39,42,50,59	0
2	MAN	B	6	11/12	0.87	0.14	30,40,44,45	0
2	NAG	B	2	14/15	0.88	0.10	25,33,38,47	0
2	NAG	B	1	14/15	0.97	0.06	16,18,21,22	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.

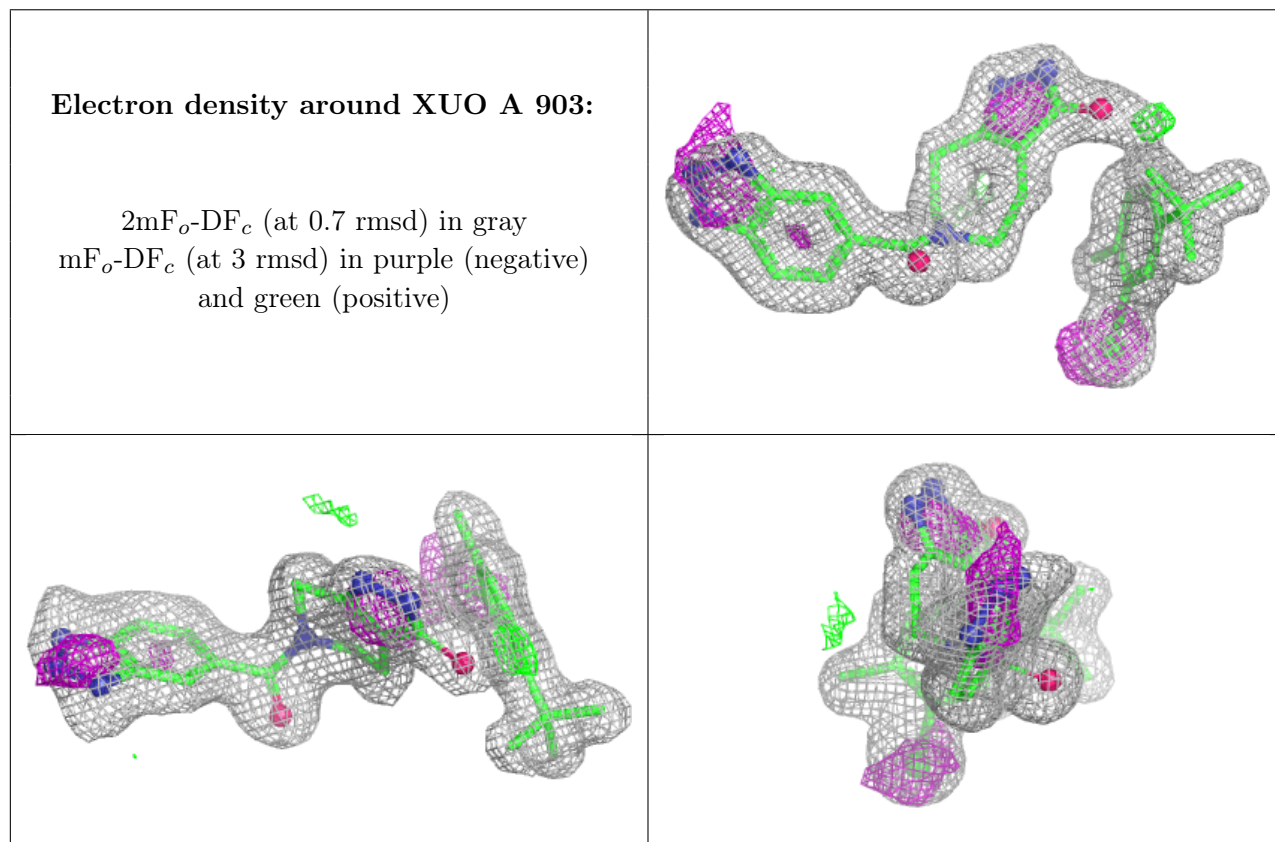


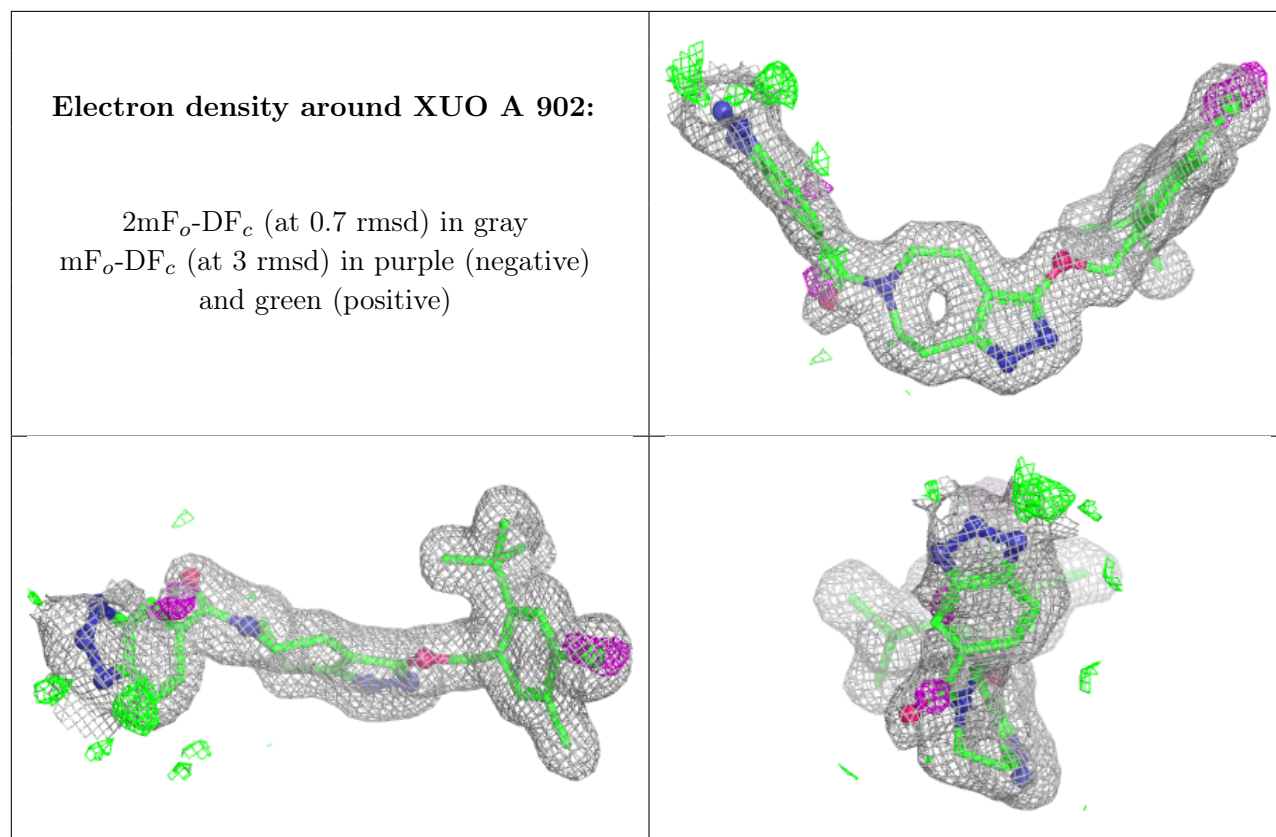
6.4 Ligands [i](#)

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
4	XUO	A	903	34/35	0.89	0.11	29,33,40,43	0
9	NA	A	908	1/1	0.93	0.09	32,32,32,32	0
4	XUO	A	902	35/35	0.94	0.09	20,26,45,55	0
6	CL	A	905	1/1	0.95	0.08	39,39,39,39	0
3	CA	A	901	1/1	0.95	0.20	38,38,38,38	0
7	K	A	906	1/1	0.96	0.07	29,29,29,29	0
5	ACT	A	904	4/4	0.96	0.08	25,31,31,34	0
8	ZN	A	907	1/1	1.00	0.02	20,20,20,20	0
3	CA	A	909	1/1	1.00	0.02	17,17,17,17	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.