



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:00 PM UTC

PDB ID : 7G4Q / pdb_00007g4q

Title : Crystal Structure of rat Autotaxin in complex with (3-chloro-5-cyanophenyl)methyl rac-(3aR,6aS)-2-(1H-benzotriazole-5-carbonyl)-1,3,3a,4,6,6a-hexahydropyrrolo[3,4-c]pyrrole-5-carboxylate, i.e. SMILES C1N(C[C@@H]2[C@@H]1CN(C2)C(=O)c1ccc2c(c1)N=NN2)C(=O)OCc1cc(cc(c1)Cl)C#N with IC50=0.729656 microM

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Deposited on : 2023-06-05

Resolution : 1.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

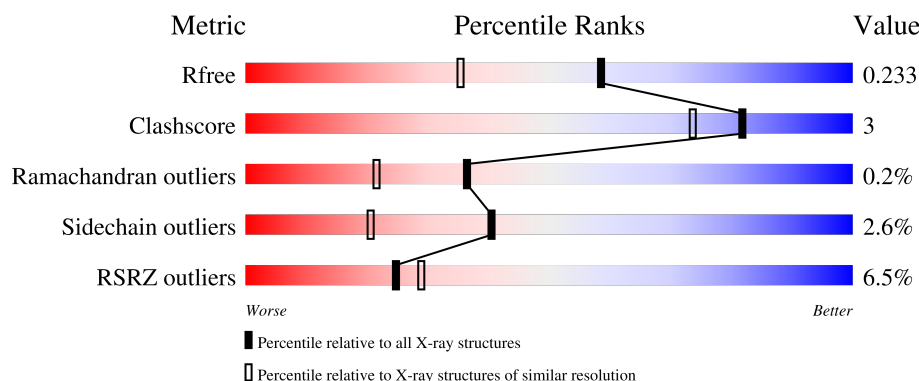
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

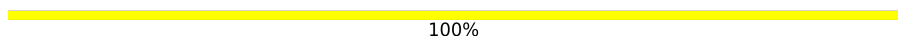
The reported resolution of this entry is 1.76 Å.

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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	 6% 82% 12% • 5%
2	B	9	 100%

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

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7154 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.

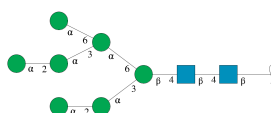
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	806	Total	C	N	O	S	0	2	0
			6522	4136	1126	1211	49			

There are 14 discrepancies between the modelled and reference sequences:

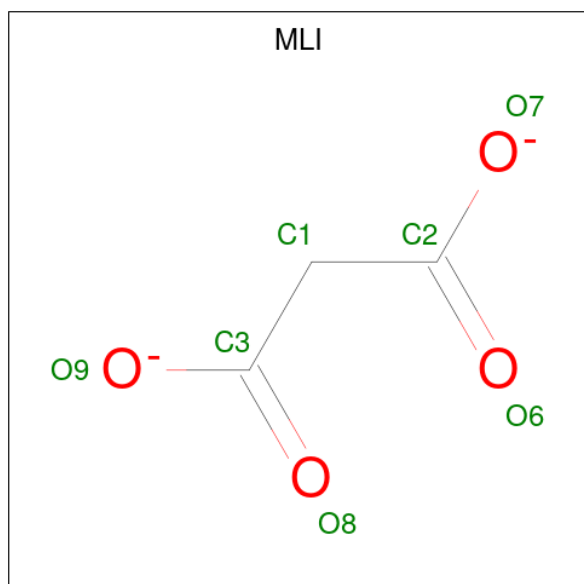
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	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-(1-6)-[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.



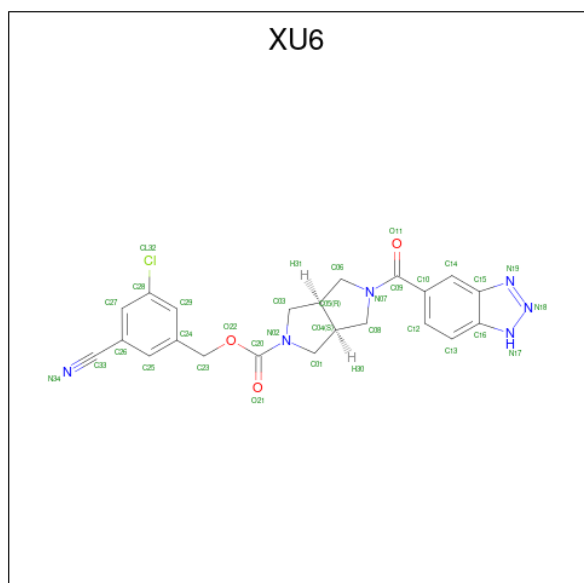
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is (3-chloro-5-cyanophenyl)methyl (3aR,6aS)-5-(1H-benzotriazole-5-carbonyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate (CCD ID: XU6) (formula: $C_{22}H_{19}ClN_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	
			64	44	2	12	6	
							0	1

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

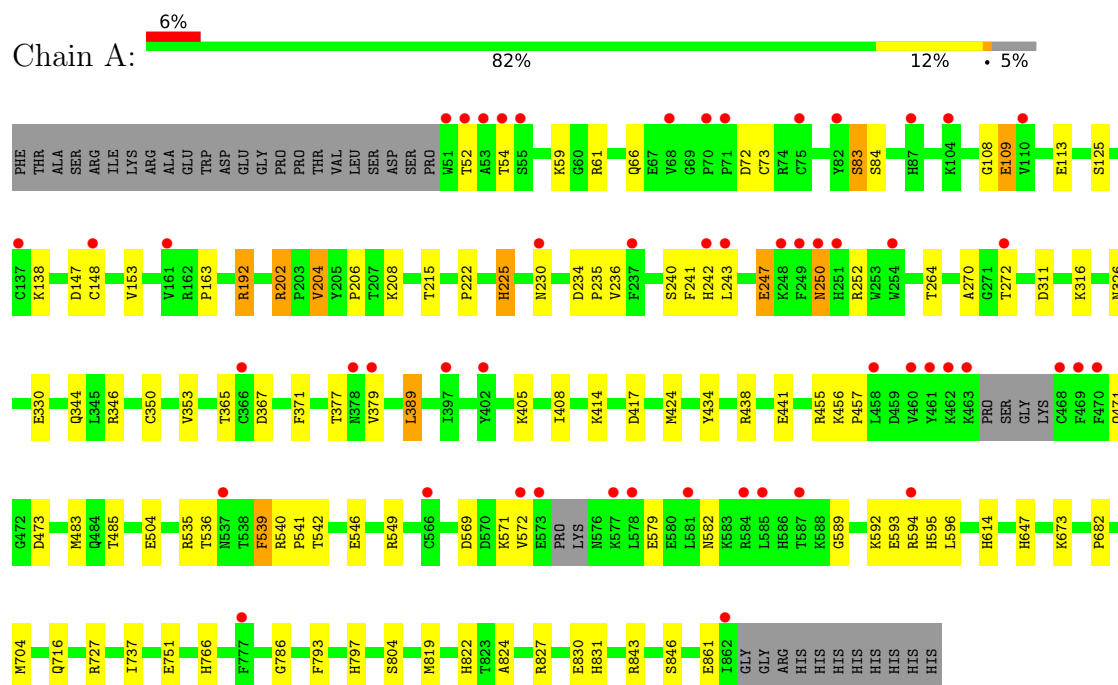
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	452	Total	O		
			452	452	0	0

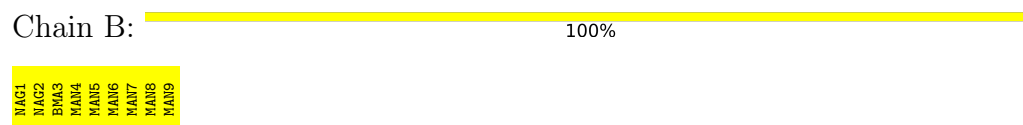
3 Residue-property plots [i](#)

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-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.95Å 91.98Å 120.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 1.76 48.82 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.82-1.76) 96.2 (48.82-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.179 , 0.224 0.189 , 0.233	Depositor DCC
R_{free} test set	4701 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	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	0.96	EDS
Total number of atoms	7154	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 3.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, MLI, NA, XU6, NAG, ZN, CA

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	1.18	11/6710 (0.2%)	1.45	38/9099 (0.4%)

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	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE1	8.64	1.41	1.25
1	A	822	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	215	THR	C-O	6.77	1.31	1.24
1	A	804	SER	CA-CB	-6.17	1.45	1.53
1	A	595	HIS	CE1-NE2	5.67	1.38	1.32
1	A	614	HIS	CG-CD2	-5.51	1.29	1.35
1	A	504	GLU	CD-OE2	5.50	1.35	1.25
1	A	824	ALA	CA-CB	-5.41	1.44	1.53
1	A	504	GLU	CD-OE1	5.38	1.35	1.25
1	A	830	GLU	CD-OE1	5.21	1.35	1.25
1	A	330	GLU	CD-OE1	5.03	1.34	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	THR	CB-CA-C	7.65	122.31	109.84
1	A	148	CYS	N-CA-CB	7.63	122.85	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	GLU	CB-CG-CD	7.59	125.50	112.60
1	A	242	HIS	CA-CB-CG	7.54	121.34	113.80
1	A	424	MET	N-CA-C	-7.34	99.41	110.28
1	A	225	HIS	CA-CB-CG	7.12	120.92	113.80
1	A	250	ASN	CB-CA-C	6.72	121.14	109.65
1	A	270	ALA	CA-C-N	6.39	126.17	120.10
1	A	270	ALA	C-N-CA	6.39	126.17	120.10
1	A	247	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	540	ARG	CB-CA-C	6.08	116.97	110.65
1	A	153	VAL	O-C-N	-5.92	117.96	121.69
1	A	542	THR	CA-CB-OG1	-5.79	100.91	109.60
1	A	147	ASP	CA-C-N	-5.77	112.21	122.07
1	A	147	ASP	C-N-CA	-5.77	112.21	122.07
1	A	272	THR	N-CA-C	-5.66	100.76	109.76
1	A	326	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	831	HIS	N-CA-C	-5.55	105.23	111.28
1	A	539	PHE	CA-C-N	-5.54	113.55	123.08
1	A	539	PHE	C-N-CA	-5.54	113.55	123.08
1	A	353	VAL	O-C-N	-5.54	117.36	123.18
1	A	827	ARG	CG-CD-NE	-5.49	99.93	112.00
1	A	204	VAL	CA-CB-CG2	5.44	119.65	110.40
1	A	377	THR	CB-CA-C	5.41	118.70	109.24
1	A	549	ARG	CA-C-O	5.37	125.43	120.60
1	A	113	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	344	GLN	CB-CA-C	-5.33	101.94	110.79
1	A	751	GLU	CB-CG-CD	5.31	121.62	112.60
1	A	241	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	264	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	471	GLN	O-C-N	5.21	127.91	122.23
1	A	441	GLU	CB-CG-CD	5.17	121.38	112.60
1	A	473	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	311	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	389	LEU	CA-C-N	-5.03	118.71	122.18
1	A	389	LEU	C-N-CA	-5.03	118.71	122.18
1	A	272	THR	CA-C-O	-5.03	114.96	120.69
1	A	202	ARG	NE-CZ-NH2	-5.00	114.70	119.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	202	ARG	Sidechain
1	A	204	VAL	Mainchain
1	A	346	ARG	Sidechain
1	A	485	THR	Mainchain
1	A	727[A]	ARG	Sidechain
1	A	727[B]	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	6522	0	6279	33	0
2	B	105	0	88	0	0
3	A	7	0	2	0	0
4	A	64	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	452	0	0	5	0
All	All	7154	0	6369	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ARG:HG2	1:A:536:THR:HG23	1.74	0.67
1:A:250:ASN:OD1	1:A:252:ARG:HG2	1.94	0.66
1:A:539:PHE:O	1:A:541:PRO:HD3	1.98	0.64
1:A:108:GLY:O	1:A:109:GLU:O	2.24	0.55
1:A:786:GLY:HA2	1:A:843:ARG:NH1	2.24	0.53
1:A:54:THR:HA	1:A:73:CYS:HB3	1.91	0.53
1:A:594:ARG:NH2	8:A:1013:HOH:O	2.42	0.53
1:A:163:PRO:HB3	1:A:350:CYS:O	2.07	0.53
1:A:793:PHE:CE2	1:A:819:MET:HE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:NZ	8:A:1003:HOH:O	2.28	0.47
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.49	0.47
1:A:230:ASN:HD22	1:A:243:LEU:HD11	1.80	0.47
1:A:589:GLY:O	1:A:592:LYS:HG2	2.15	0.46
1:A:59:LYS:O	1:A:61:ARG:HG3	2.16	0.46
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.97	0.46
1:A:737:ILE:HB	1:A:766:HIS:HB2	1.97	0.45
1:A:108:GLY:O	1:A:109:GLU:C	2.61	0.44
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.53	0.44
1:A:596:LEU:O	8:A:1001:HOH:O	2.21	0.44
1:A:414:LYS:HD3	1:A:414:LYS:HA	1.75	0.43
1:A:365:THR:OG1	1:A:367:ASP:OD1	2.26	0.42
1:A:192:ARG:NH2	8:A:1026:HOH:O	2.50	0.41
1:A:234:ASP:HA	1:A:235:PRO:HD3	1.84	0.41
1:A:704:MET:HA	1:A:797:HIS:NE2	2.36	0.41
1:A:240:SER:O	1:A:247:GLU:HG2	2.21	0.41
1:A:569:ASP:OD2	1:A:647:HIS:CD2	2.74	0.41
1:A:236:VAL:HG23	1:A:438:ARG:HD2	2.02	0.41
1:A:52:THR:HG22	1:A:54:THR:HG22	2.03	0.41
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.56	0.41
1:A:455:ARG:NH2	1:A:456[A]:LYS:HE2	2.35	0.41
1:A:846:SER:HB3	8:A:1413:HOH:O	2.21	0.41
1:A:483:MET:HE2	1:A:483:MET:HA	2.03	0.40
1:A:569:ASP:OD2	1:A:647:HIS:HD2	2.05	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	802/846 (95%)	767 (96%)	33 (4%)	2 (0%)	43 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	83	SER

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	731/765 (96%)	712 (97%)	19 (3%)	40	20

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	72	ASP
1	A	83	SER
1	A	84	SER
1	A	125	SER
1	A	138	LYS
1	A	316	LYS
1	A	379	VAL
1	A	389	LEU
1	A	405	LYS
1	A	408	ILE
1	A	417	ASP
1	A	571	LYS
1	A	572	VAL
1	A	579	GLU
1	A	582	ASN
1	A	593	GLU
1	A	673	LYS
1	A	861	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	436	ASN
1	A	471	GLN
1	A	582	ASN
1	A	586	HIS
1	A	647	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 ⓘ

9 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	0.88	1 (7%)	17,19,21	1.17	1 (5%)
2	NAG	B	2	2	14,14,15	1.43	2 (14%)	17,19,21	2.74	5 (29%)
2	BMA	B	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.78	5 (33%)
2	MAN	B	4	2	11,11,12	1.54	2 (18%)	15,15,17	1.44	3 (20%)
2	MAN	B	5	2	11,11,12	1.80	3 (27%)	15,15,17	1.02	0
2	MAN	B	6	2	11,11,12	1.71	3 (27%)	15,15,17	1.34	2 (13%)
2	MAN	B	7	2	11,11,12	1.57	2 (18%)	15,15,17	0.97	1 (6%)
2	MAN	B	8	2	11,11,12	1.31	2 (18%)	15,15,17	1.96	4 (26%)
2	MAN	B	9	2	11,11,12	1.99	2 (18%)	15,15,17	2.06	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	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	-	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	-	0/2/19/22	0/1/1/1
2	MAN	B	8	2	-	1/2/19/22	0/1/1/1
2	MAN	B	9	2	-	2/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	MAN	C2-C3	5.16	1.60	1.52
2	B	5	MAN	C2-C3	3.71	1.58	1.52
2	B	2	NAG	O6-C6	3.71	1.58	1.42
2	B	6	MAN	O5-C5	3.52	1.50	1.43
2	B	4	MAN	C2-C3	3.29	1.57	1.52
2	B	5	MAN	O5-C5	3.21	1.49	1.43
2	B	7	MAN	C2-C3	3.11	1.57	1.52
2	B	2	NAG	C6-C5	2.82	1.61	1.51
2	B	6	MAN	O5-C1	2.81	1.48	1.43
2	B	3	BMA	C2-C3	2.80	1.56	1.52
2	B	8	MAN	C2-C3	2.72	1.56	1.52
2	B	6	MAN	C2-C3	2.55	1.56	1.52
2	B	8	MAN	O5-C5	2.54	1.48	1.43
2	B	7	MAN	C4-C5	2.49	1.58	1.53
2	B	9	MAN	O5-C5	2.28	1.47	1.43
2	B	5	MAN	C4-C5	2.16	1.57	1.53
2	B	1	NAG	C2-N2	-2.13	1.42	1.46
2	B	4	MAN	O5-C5	2.06	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C2-N2-C7	7.20	132.55	122.90
2	B	2	NAG	C1-O5-C5	6.50	120.89	112.19
2	B	8	MAN	C1-C2-C3	5.12	117.10	109.64
2	B	9	MAN	O3-C3-C2	4.95	120.15	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	MAN	O2-C2-C3	3.97	118.38	110.15
2	B	4	MAN	C1-O5-C5	3.75	117.21	112.19
2	B	2	NAG	O3-C3-C2	-3.53	102.06	109.40
2	B	8	MAN	O2-C2-C3	-3.45	103.01	110.15
2	B	3	BMA	C1-O5-C5	3.31	116.63	112.19
2	B	3	BMA	C1-C2-C3	3.19	114.28	109.64
2	B	6	MAN	C1-O5-C5	2.89	116.06	112.19
2	B	2	NAG	C3-C4-C5	2.88	115.46	110.23
2	B	8	MAN	C1-O5-C5	2.81	115.96	112.19
2	B	3	BMA	O2-C2-C1	-2.72	103.01	109.22
2	B	3	BMA	O4-C4-C5	-2.64	102.82	109.32
2	B	9	MAN	C1-O5-C5	2.39	115.39	112.19
2	B	6	MAN	C2-C3-C4	2.38	115.05	110.86
2	B	3	BMA	O2-C2-C3	2.33	114.98	110.15
2	B	7	MAN	C1-O5-C5	2.33	115.30	112.19
2	B	4	MAN	C1-C2-C3	2.19	112.83	109.64
2	B	8	MAN	O2-C2-C1	2.15	114.14	109.22
2	B	1	NAG	C1-C2-N2	2.11	113.77	110.43
2	B	2	NAG	O7-C7-C8	-2.03	118.44	122.05
2	B	4	MAN	O6-C6-C5	2.00	118.16	111.33

There are no chirality outliers.

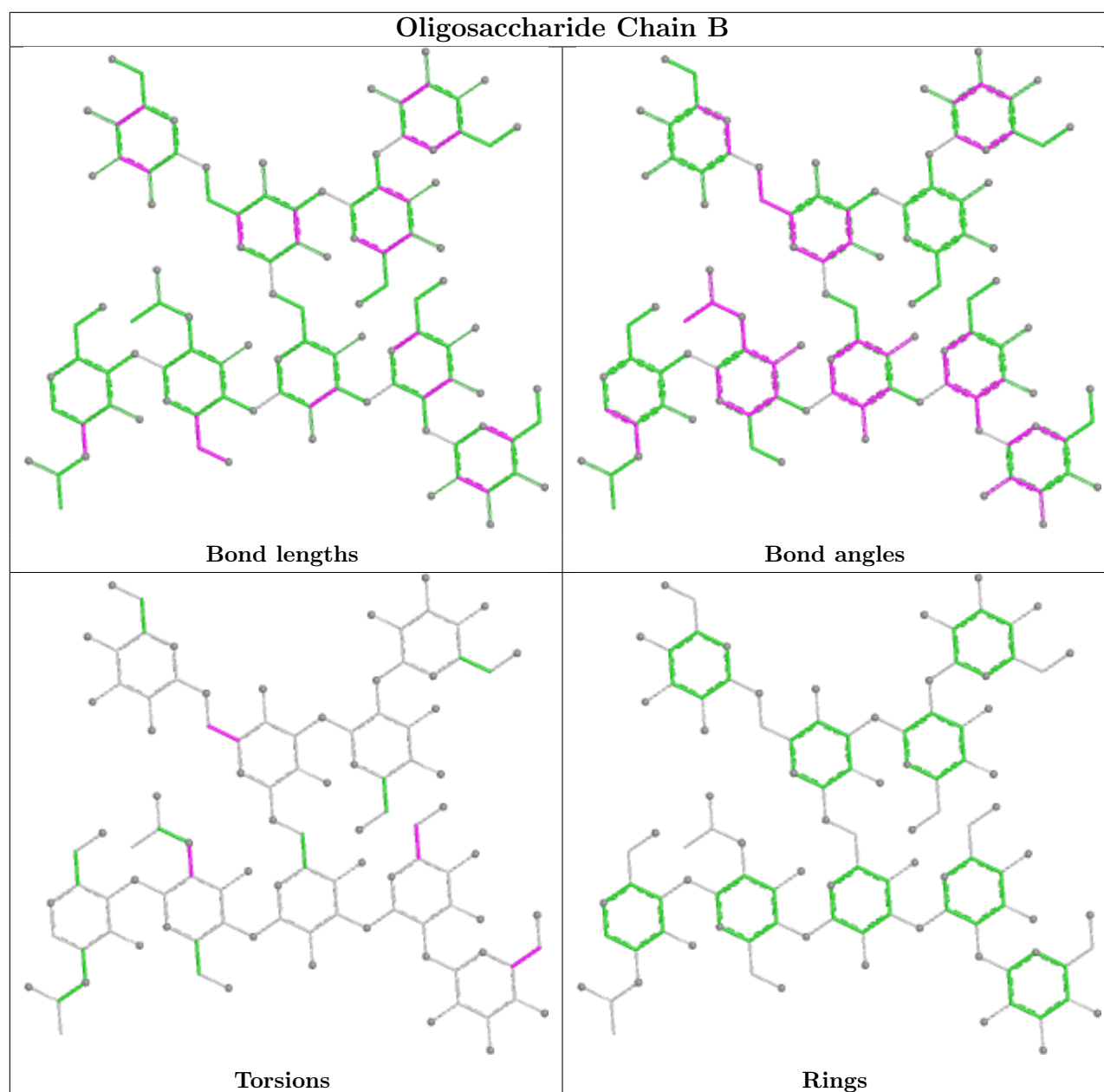
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	8	MAN	O5-C5-C6-O6
2	B	9	MAN	C4-C5-C6-O6
2	B	9	MAN	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
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 ⓘ

Of 7 ligands modelled in this entry, 4 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	XU6	A	902[B]	-	36,36,36	1.98	7 (19%)	50,52,52	1.97	10 (20%)
3	MLI	A	901	5	6,6,6	2.89	4 (66%)	7,7,7	1.21	1 (14%)
4	XU6	A	902[A]	-	36,36,36	2.30	13 (36%)	50,52,52	1.70	9 (18%)

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	XU6	A	902[B]	-	-	0/19/39/39	0/5/5/5
3	MLI	A	901	5	-	0/4/4/4	-
4	XU6	A	902[A]	-	-	1/19/39/39	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902[A]	XU6	C09-N07	7.37	1.50	1.34
4	A	902[B]	XU6	C09-N07	6.95	1.49	1.34
3	A	901	MLI	C1-C2	4.88	1.58	1.51
4	A	902[A]	XU6	O22-C20	4.08	1.42	1.34
4	A	902[B]	XU6	O22-C20	3.78	1.42	1.34
4	A	902[A]	XU6	C20-N02	3.73	1.42	1.35
4	A	902[B]	XU6	O22-C23	-3.55	1.38	1.45
3	A	901	MLI	O7-C2	-3.39	1.19	1.30
4	A	902[B]	XU6	C20-N02	3.35	1.41	1.35
4	A	902[A]	XU6	O22-C23	-3.25	1.38	1.45
4	A	902[A]	XU6	C14-C15	3.25	1.44	1.40
4	A	902[A]	XU6	C29-C24	-3.21	1.33	1.39
4	A	902[A]	XU6	C12-C10	3.20	1.44	1.39
4	A	902[A]	XU6	N19-N18	3.18	1.39	1.31
4	A	902[B]	XU6	N19-N18	2.98	1.38	1.31
4	A	902[A]	XU6	C13-C16	2.93	1.44	1.39
4	A	902[A]	XU6	C26-C33	2.80	1.50	1.44
3	A	901	MLI	O9-C3	-2.78	1.21	1.30
4	A	902[B]	XU6	C25-C24	-2.76	1.34	1.39
4	A	902[A]	XU6	C10-C09	2.76	1.54	1.50
4	A	902[A]	XU6	C05-C04	-2.35	1.47	1.54
3	A	901	MLI	C1-C3	2.24	1.54	1.51
4	A	902[A]	XU6	C16-N17	2.09	1.40	1.36
4	A	902[B]	XU6	C05-C04	-2.07	1.48	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902[B]	XU6	C03-N02-C20	5.83	141.33	123.86
4	A	902[B]	XU6	C01-N02-C20	-5.44	107.56	123.86
4	A	902[A]	XU6	C03-N02-C20	4.85	138.39	123.86
4	A	902[A]	XU6	C08-N07-C06	-4.57	104.23	112.59
4	A	902[B]	XU6	C08-N07-C06	-4.27	104.77	112.59
4	A	902[A]	XU6	C01-N02-C20	-3.99	111.91	123.86
4	A	902[B]	XU6	C27-C26-C25	3.96	125.83	119.70
4	A	902[B]	XU6	C27-C26-C33	-3.92	114.26	119.55
4	A	902[A]	XU6	C05-C06-N07	3.87	108.88	103.02
4	A	902[B]	XU6	C26-C25-C24	-3.48	116.80	120.28
4	A	902[B]	XU6	C05-C06-N07	2.97	107.51	103.02
4	A	902[B]	XU6	C29-C28-C27	-2.80	118.24	121.64
4	A	902[A]	XU6	O22-C20-O21	-2.68	120.09	124.76
4	A	902[A]	XU6	C23-O22-C20	2.45	121.68	115.51
4	A	902[A]	XU6	C04-C01-N02	2.43	106.69	103.02
4	A	902[B]	XU6	C04-C01-N02	2.35	106.57	103.02
4	A	902[A]	XU6	C13-C16-C15	-2.29	119.59	122.10
4	A	902[B]	XU6	O22-C20-O21	-2.13	121.06	124.76
3	A	901	MLI	O7-C2-O6	-2.01	118.16	123.33
4	A	902[A]	XU6	C29-C28-C27	2.01	124.08	121.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

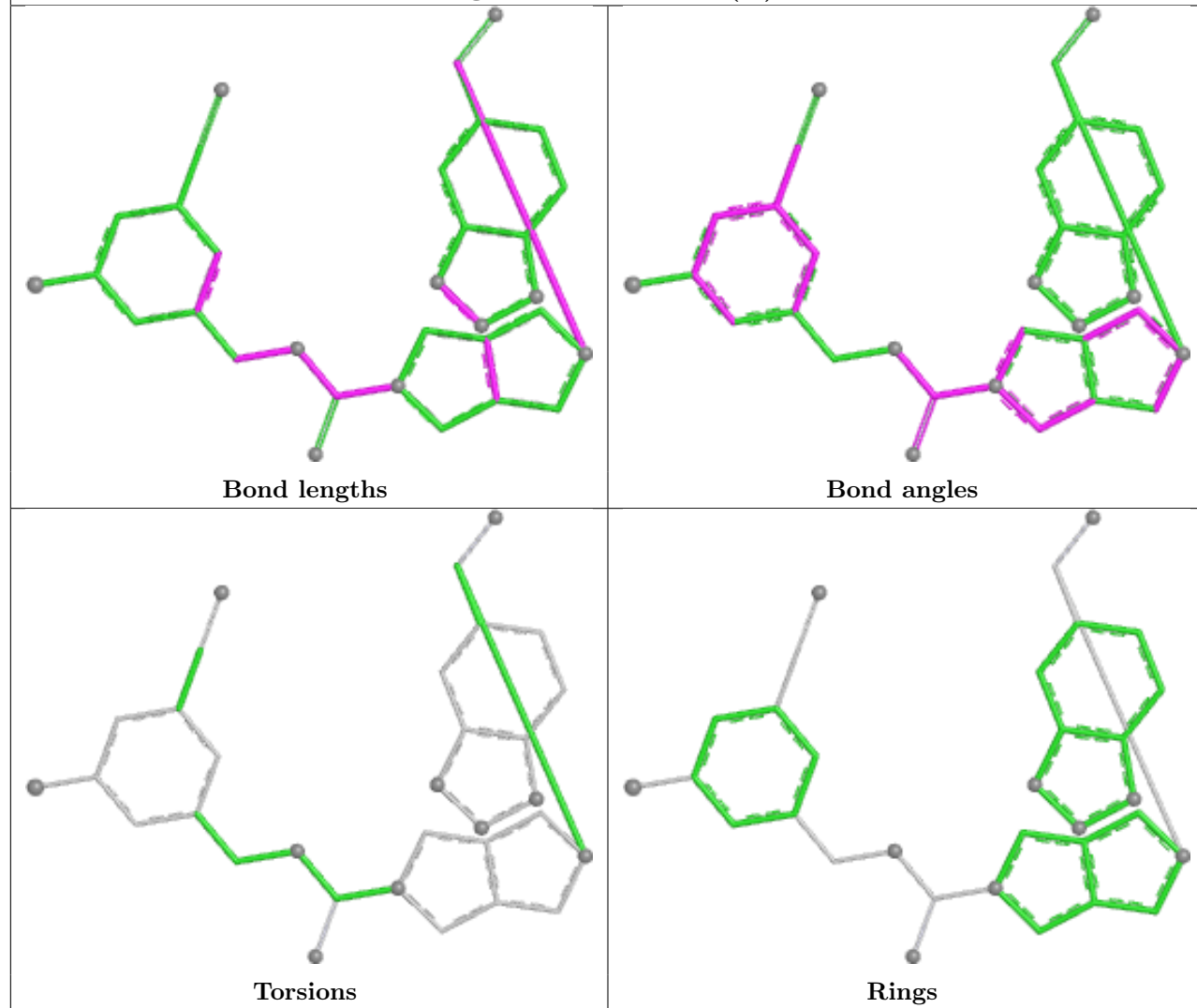
Mol	Chain	Res	Type	Atoms
4	A	902[A]	XU6	O21-C20-N02-C03

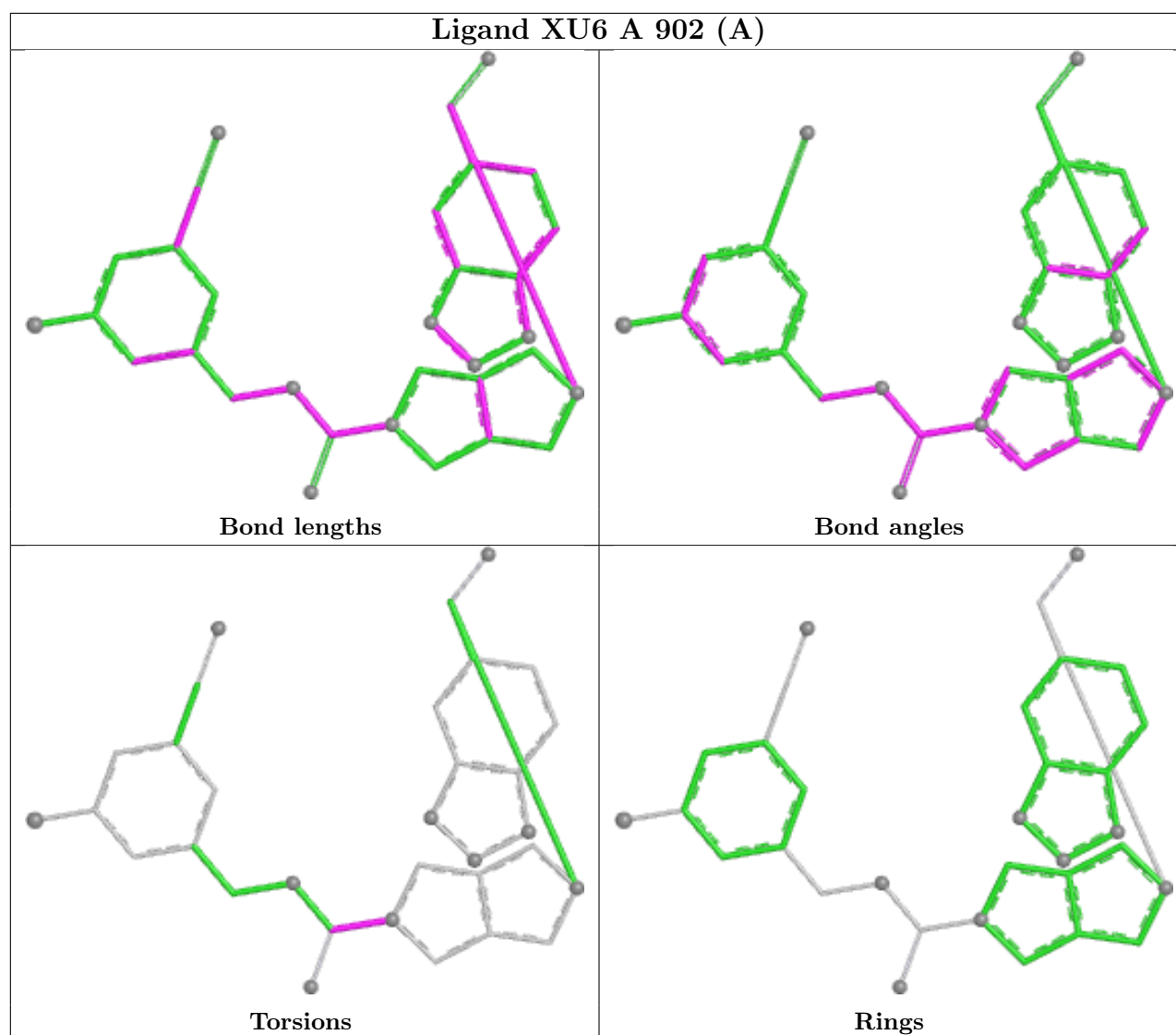
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand XU6 A 902 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	806/846 (95%)	0.27	52 (6%)	25 29	14, 29, 74, 164	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	PHE	7.2
1	A	51	TRP	6.3
1	A	578	LEU	5.7
1	A	243	LEU	5.6
1	A	572	VAL	5.6
1	A	468	CYS	5.6
1	A	68	VAL	5.5
1	A	581	LEU	5.2
1	A	71	PRO	4.9
1	A	862	ILE	4.6
1	A	461	TYR	4.5
1	A	54	THR	4.2
1	A	53	ALA	4.1
1	A	397	ILE	4.0
1	A	249	PHE	3.8
1	A	251	HIS	3.7
1	A	585	LEU	3.6
1	A	52	THR	3.5
1	A	82	TYR	3.1
1	A	237	PHE	3.0
1	A	230	ASN	3.0
1	A	272	THR	2.9
1	A	70	PRO	2.9
1	A	463	LYS	2.7
1	A	402	TYR	2.7
1	A	462	LYS	2.7
1	A	577	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	584	ARG	2.6
1	A	378	ASN	2.5
1	A	566	CYS	2.4
1	A	55	SER	2.4
1	A	148	CYS	2.4
1	A	470	PHE	2.4
1	A	777	PHE	2.4
1	A	248	LYS	2.3
1	A	242	HIS	2.3
1	A	87	HIS	2.3
1	A	587	THR	2.3
1	A	137	CYS	2.3
1	A	573	GLU	2.3
1	A	366	CYS	2.2
1	A	458	LEU	2.2
1	A	537	ASN	2.2
1	A	161	VAL	2.1
1	A	379	VAL	2.1
1	A	460	VAL	2.1
1	A	104	LYS	2.1
1	A	594	ARG	2.1
1	A	110	VAL	2.1
1	A	250	ASN	2.1
1	A	254	TRP	2.1
1	A	75	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.

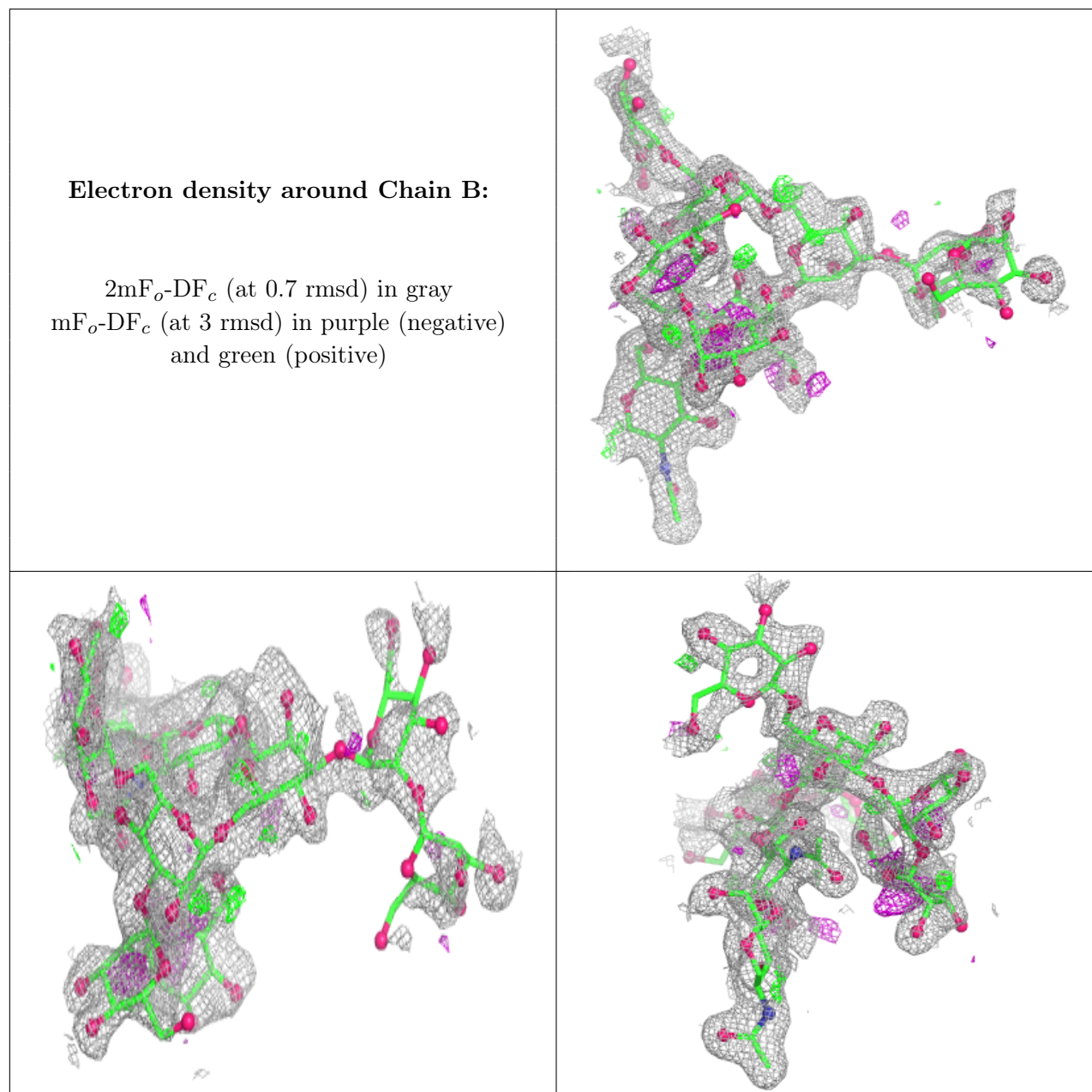
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	8	11/12	0.44	0.18	106,120,129,129	0
2	MAN	B	7	11/12	0.60	0.14	72,102,116,126	0
2	BMA	B	3	11/12	0.62	0.15	59,77,86,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	B	9	11/12	0.65	0.17	52,87,118,138	0
2	MAN	B	4	11/12	0.77	0.12	50,67,81,86	0
2	MAN	B	5	11/12	0.81	0.15	45,61,71,83	0
2	MAN	B	6	11/12	0.84	0.18	34,58,64,68	0
2	NAG	B	2	14/15	0.90	0.10	26,38,49,72	0
2	NAG	B	1	14/15	0.97	0.06	16,21,25,26	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 ⓘ

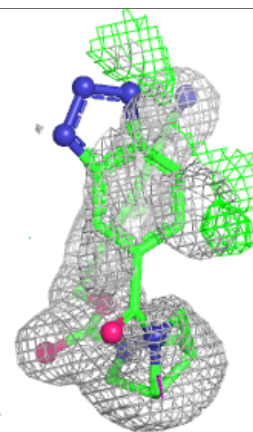
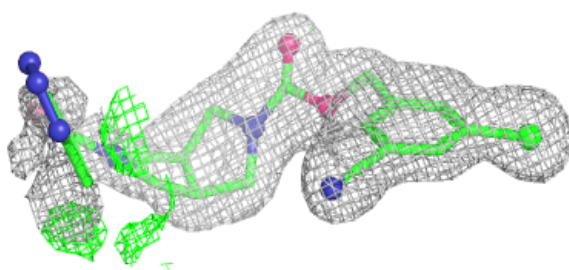
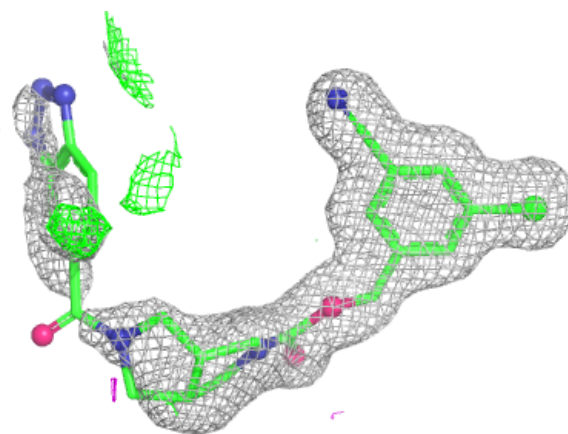
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	XU6	A	902[A]	32/32	0.91	0.14	21,38,87,89	32
4	XU6	A	902[B]	32/32	0.91	0.14	24,46,80,81	32
3	MLI	A	901	7/7	0.94	0.09	24,33,40,48	0
6	NA	A	904	1/1	0.95	0.06	30,30,30,30	0
6	NA	A	905	1/1	0.96	0.09	47,47,47,47	0
7	CA	A	906	1/1	0.99	0.02	20,20,20,20	0
5	ZN	A	903	1/1	1.00	0.03	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.

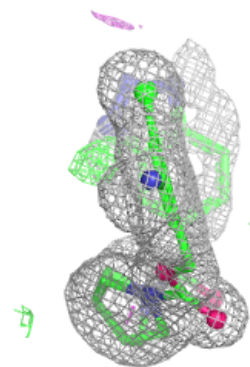
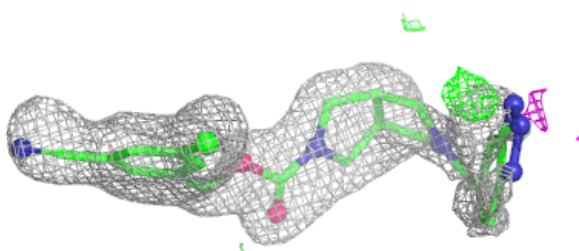
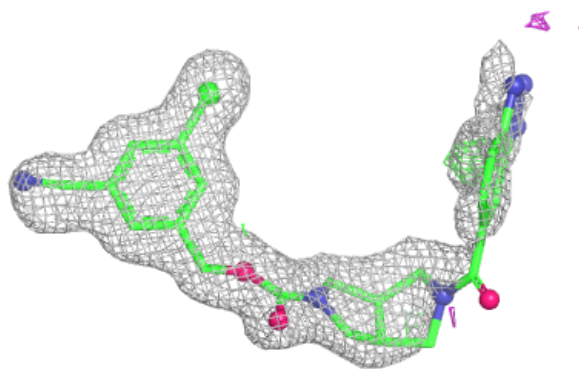
Electron density around XU6 A 902 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XU6 A 902 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.