



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 7G6M / pdb_00007g6m
Title : Crystal Structure of rat Autotaxin in complex with [(3aS,6aS)-5-[2-cyclopropyl-6-(oxan-4-ylmethoxy)pyridine-4-carbonyl]-1,3,3a,4,6,6a-hexahydropyrrolo[3,4-c]pyrrol-2-yl]-(1H-benzotriazol-5-yl)methanone, i.e. SMILES N1(C[C@@H]2[C@@H](C1)CN(C2)C(=O)c1cc(nc(c1)OCC1CCOCC1)C1CC1)C(=O)c1ccc2c(c1)N=NN2 with IC50=0.00159445 microM
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Mattei, P.; Rudolph, M.G.
Deposited on : 2023-06-05
Resolution : 2.13 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)

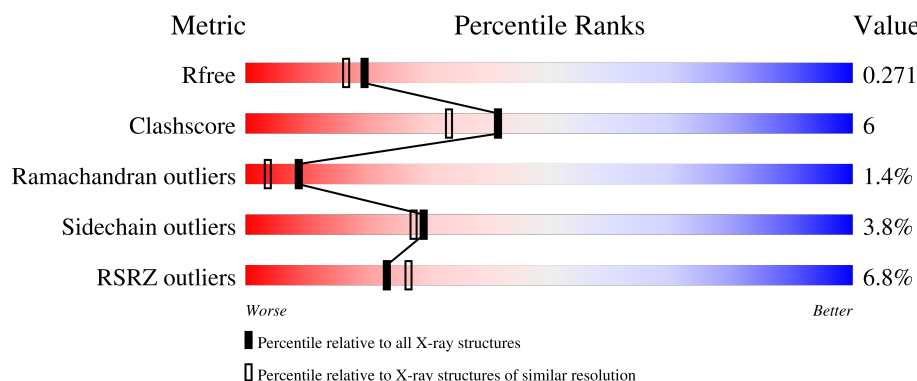
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

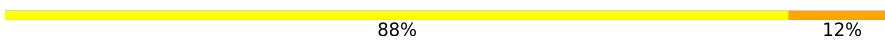
The reported resolution of this entry is 2.13 Å.

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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	

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

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6867 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.

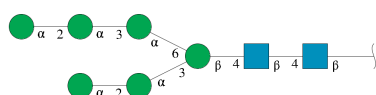
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	805	Total	C	N	O	S	0	0	0
			6500	4120	1121	1210	49			

There are 14 discrepancies between the modelled and reference sequences:

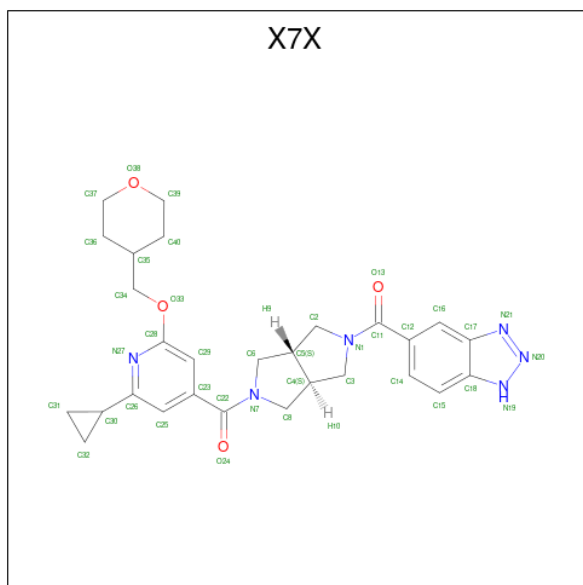
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
A	872	HIS	-	expression tag	UNP Q64610
A	873	HIS	-	expression tag	UNP Q64610

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



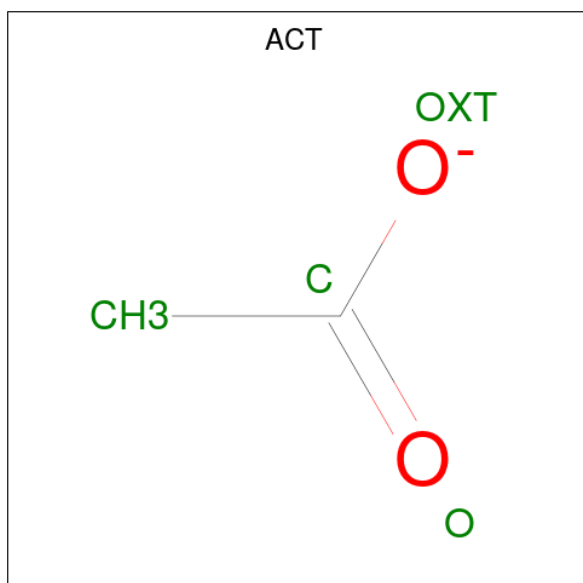
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 3 is [(3aR,6aS)-5-(1H-benzotriazole-5-carbonyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl]{2-cyclopropyl-6-[(oxan-4-yl)methoxy]pyridin-4-yl}methanone (CCD ID: X7X) (formula: C₂₈H₃₂N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			38	28	6	4		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

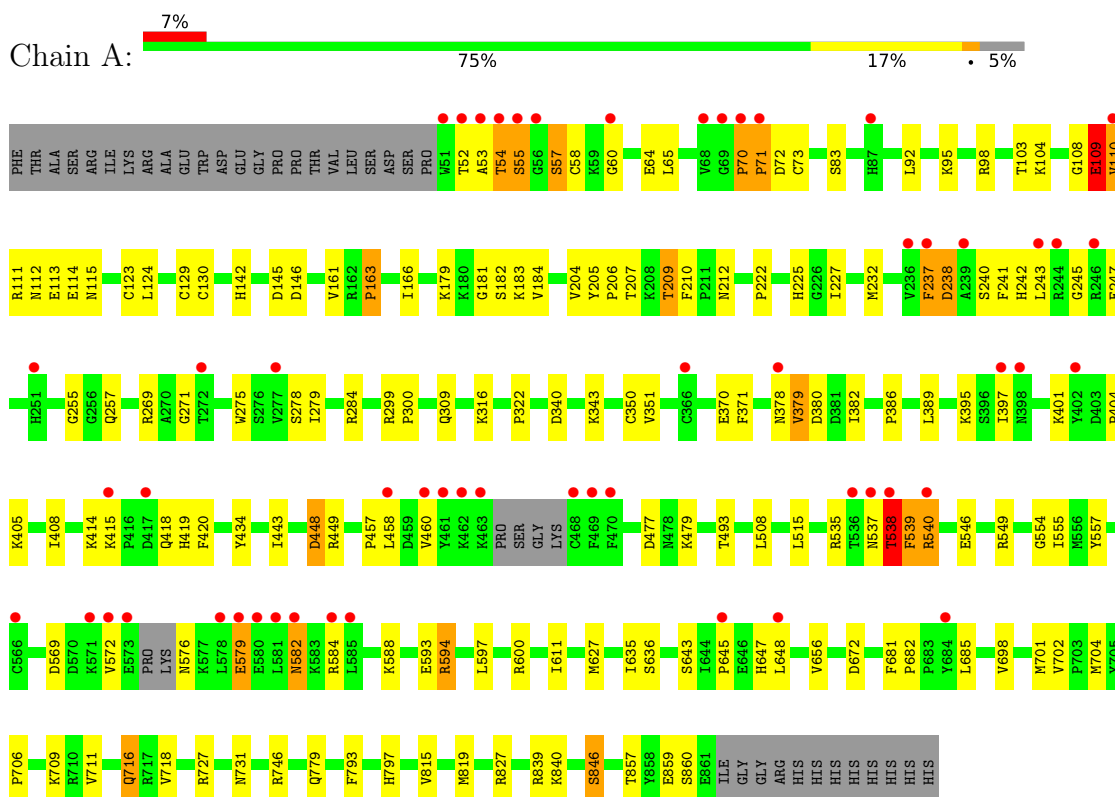
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	226	Total O 226 226	0	0

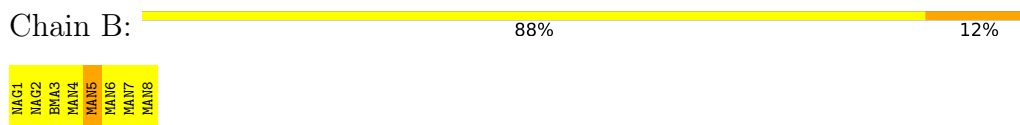
3 Residue-property plots [i](#)

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	84.69Å 92.56Å 120.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.28 – 2.13 46.28 – 2.13	Depositor EDS
% Data completeness (in resolution range)	93.0 (46.28-2.13) 93.0 (46.28-2.13)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.214 , 0.271 0.214 , 0.271	Depositor DCC
R_{free} test set	2641 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: X7X, CL, CA, NAG, MAN, NA, ACT, BMA, 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	1.19	8/6682 (0.1%)	1.28	40/9062 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	PRO	CA-C	6.53	1.58	1.52
1	A	163	PRO	CA-C	6.07	1.57	1.52
1	A	535	ARG	C-O	-5.98	1.17	1.24
1	A	207	THR	N-CA	-5.95	1.39	1.46
1	A	181	GLY	C-O	-5.72	1.20	1.24
1	A	397	ILE	N-CA	5.26	1.53	1.46
1	A	672	ASP	C-O	5.11	1.30	1.23
1	A	257	GLN	N-CA	-5.02	1.41	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	MET	CA-C-N	-11.00	108.48	120.14
1	A	627	MET	C-N-CA	-11.00	108.48	120.14
1	A	540	ARG	CA-C-N	-8.95	111.53	120.31
1	A	540	ARG	C-N-CA	-8.95	111.53	120.31
1	A	539	PHE	N-CA-C	-8.73	95.16	109.40
1	A	279	ILE	CA-C-N	-8.28	112.33	120.52
1	A	279	ILE	C-N-CA	-8.28	112.33	120.52
1	A	681	PHE	N-CA-C	-7.46	100.39	109.72
1	A	299	ARG	CA-C-N	-7.44	112.67	120.03
1	A	299	ARG	C-N-CA	-7.44	112.67	120.03
1	A	702	VAL	N-CA-C	7.34	115.21	109.19
1	A	237	PHE	N-CA-C	-7.23	104.26	113.23
1	A	130	CYS	N-CA-C	-6.95	100.19	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ASN	N-CA-C	6.64	118.60	111.36
1	A	389	LEU	CA-C-N	-6.60	117.51	122.33
1	A	389	LEU	C-N-CA	-6.60	117.51	122.33
1	A	779	GLN	CA-C-N	-6.39	113.71	120.03
1	A	779	GLN	C-N-CA	-6.39	113.71	120.03
1	A	702	VAL	CA-C-N	-6.28	113.21	119.99
1	A	702	VAL	C-N-CA	-6.28	113.21	119.99
1	A	611	ILE	CB-CA-C	-6.05	103.29	111.15
1	A	271	GLY	N-CA-C	-5.85	105.20	111.93
1	A	540	ARG	CB-CA-C	5.75	115.61	110.44
1	A	857	THR	CB-CA-C	-5.66	99.79	109.65
1	A	434	TYR	N-CA-C	5.55	116.37	108.54
1	A	245	GLY	N-CA-C	5.55	117.68	112.08
1	A	716	GLN	N-CA-C	5.50	117.35	111.36
1	A	204	VAL	CB-CA-C	-5.47	103.55	112.03
1	A	538	THR	N-CA-C	-5.38	103.39	110.33
1	A	109	GLU	N-CA-C	5.37	122.23	110.80
1	A	508	LEU	N-CA-C	5.34	117.18	111.36
1	A	582	ASN	N-CA-C	5.27	116.71	110.97
1	A	182	SER	N-CA-C	5.22	117.64	111.33
1	A	340	ASP	N-CA-C	-5.13	105.86	111.82
1	A	448	ASP	N-CA-C	5.09	117.42	110.24
1	A	554	GLY	N-CA-C	-5.09	105.59	112.57
1	A	209	THR	N-CA-C	5.08	116.51	110.97
1	A	718	VAL	N-CA-C	5.01	116.43	111.67
1	A	827	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	A	55	SER	N-CA-C	5.01	119.54	113.38

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	6500	0	6244	83	0
2	B	94	0	79	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	38	0	0	0	0
4	A	4	0	3	0	0
5	A	1	0	0	0	0
6	A	2	0	0	1	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	226	0	0	7	0
All	All	6867	0	6326	83	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 6.

All (83) 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:569:ASP:OD2	1:A:647:HIS:HB2	1.67	0.93
1:A:52:THR:HB	1:A:54:THR:HG22	1.53	0.91
1:A:52:THR:HA	1:A:71:PRO:HB3	1.58	0.85
1:A:539:PHE:HA	9:A:1007:HOH:O	1.77	0.82
1:A:209:THR:OG1	6:A:904:CA:CA	1.66	0.71
1:A:576:ASN:ND2	1:A:579:GLU:HB2	2.08	0.69
1:A:110:VAL:O	1:A:111:ARG:C	2.41	0.64
1:A:269:ARG:HB3	1:A:300:PRO:HA	1.80	0.64
1:A:370:GLU:OE2	1:A:419:HIS:HD2	1.85	0.60
1:A:540:ARG:NH1	9:A:1006:HOH:O	2.35	0.59
1:A:647:HIS:CD2	1:A:648:LEU:HG	2.39	0.57
1:A:635:ILE:HD12	1:A:685:LEU:HD13	1.89	0.55
1:A:163:PRO:HB3	1:A:350:CYS:O	2.07	0.55
1:A:746:ARG:NH2	9:A:1001:HOH:O	2.10	0.55
1:A:232:MET:HE3	1:A:241:PHE:CG	2.43	0.54
1:A:322:PRO:O	9:A:1002:HOH:O	2.18	0.54
1:A:382:ILE:O	1:A:382:ILE:HG13	2.07	0.54
1:A:404:PRO:HB3	1:A:443:ILE:HD11	1.89	0.53
1:A:142:HIS:HB2	1:A:145:ASP:OD2	2.09	0.53
1:A:584:ARG:O	1:A:588:LYS:HG2	2.09	0.52
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.90	0.52
1:A:52:THR:HB	1:A:54:THR:CG2	2.34	0.52
1:A:698:VAL:HG23	1:A:701:MET:HE2	1.91	0.52
1:A:161:VAL:HG22	1:A:161:VAL:O	2.09	0.51
1:A:54:THR:HA	1:A:73:CYS:HB3	1.93	0.51
1:A:255:GLY:HA3	2:B:5:MAN:O3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:SER:O	1:A:645:PRO:HD3	2.10	0.51
1:A:537:ASN:O	1:A:538:THR:O	2.30	0.50
1:A:839:ARG:O	1:A:840:LYS:HD3	2.11	0.50
1:A:537:ASN:O	1:A:538:THR:C	2.54	0.50
1:A:846:SER:HB3	9:A:1221:HOH:O	2.11	0.50
1:A:555:ILE:HG23	1:A:656:VAL:HG23	1.94	0.49
1:A:576:ASN:HD21	1:A:579:GLU:HB2	1.76	0.49
1:A:53:ALA:H	1:A:71:PRO:HB2	1.78	0.49
1:A:92:LEU:O	1:A:95:LYS:HE3	2.13	0.49
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.60	0.48
1:A:237:PHE:O	1:A:238:ASP:C	2.53	0.48
1:A:98:ARG:HG3	1:A:115:ASN:OD1	2.13	0.48
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.48	0.48
1:A:546:GLU:CD	1:A:600:ARG:HH22	2.22	0.48
1:A:378:ASN:O	1:A:380:ASP:N	2.47	0.48
1:A:112:ASN:OD1	1:A:114:GLU:HB2	2.13	0.47
1:A:711:VAL:HG13	1:A:815:VAL:HG13	1.95	0.47
1:A:275:TRP:CD2	1:A:284:ARG:HG2	2.50	0.47
1:A:53:ALA:C	1:A:55:SER:H	2.23	0.46
1:A:537:ASN:C	1:A:538:THR:O	2.56	0.46
1:A:635:ILE:CD1	1:A:685:LEU:HD13	2.45	0.46
1:A:793:PHE:CE2	1:A:819:MET:HE3	2.50	0.46
1:A:408:ILE:HD11	1:A:443:ILE:HG12	1.98	0.46
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.98	0.46
1:A:210:PHE:HE1	1:A:243:LEU:HD23	1.82	0.45
1:A:161:VAL:O	1:A:161:VAL:CG2	2.63	0.45
1:A:555:ILE:HG23	1:A:656:VAL:CG2	2.47	0.45
1:A:540:ARG:HD3	1:A:540:ARG:HA	1.66	0.45
1:A:70:PRO:HA	1:A:71:PRO:HA	1.69	0.44
1:A:448:ASP:O	1:A:449:ARG:C	2.60	0.44
1:A:309:GLN:HA	1:A:309:GLN:OE1	2.18	0.44
1:A:123:CYS:O	1:A:124:LEU:C	2.59	0.43
1:A:370:GLU:OE2	1:A:419:HIS:CD2	2.68	0.43
1:A:704:MET:HA	1:A:797:HIS:NE2	2.33	0.43
1:A:275:TRP:CE3	1:A:284:ARG:HG2	2.54	0.43
1:A:240:SER:O	1:A:247:GLU:HG2	2.18	0.43
1:A:594:ARG:NH1	1:A:636:SER:HB3	2.34	0.43
1:A:108:GLY:O	1:A:109:GLU:O	2.36	0.42
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.54	0.42
1:A:124:LEU:N	1:A:129:CYS:SG	2.92	0.42
1:A:225:HIS:CE1	1:A:227:ILE:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:TYR:O	1:A:656:VAL:HB	2.19	0.42
1:A:597:LEU:HD12	1:A:731:ASN:HB2	2.01	0.42
1:A:237:PHE:O	1:A:238:ASP:O	2.38	0.42
1:A:709:LYS:HB3	1:A:709:LYS:HE2	1.85	0.41
1:A:57:SER:OG	1:A:58:CYS:N	2.53	0.41
1:A:493:THR:HG21	1:A:515:LEU:HD23	2.02	0.41
1:A:594:ARG:HH12	1:A:636:SER:HB3	1.84	0.41
1:A:698:VAL:HG22	1:A:698:VAL:O	2.20	0.41
1:A:146:ASP:OD2	1:A:343:LYS:NZ	2.45	0.41
1:A:479:LYS:O	1:A:859:GLU:HG3	2.21	0.41
1:A:414:LYS:HD3	1:A:414:LYS:HA	1.51	0.41
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.56	0.40
1:A:420:PHE:CD1	1:A:420:PHE:C	3.00	0.40
1:A:112:ASN:C	1:A:114:GLU:H	2.28	0.40
1:A:706:PRO:HD2	9:A:1069:HOH:O	2.22	0.40
1:A:727:ARG:NH2	9:A:1005:HOH:O	2.33	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	799/846 (94%)	739 (92%)	49 (6%)	11 (1%)	9 4

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	379	VAL
1	A	64	GLU
1	A	418	GLN
1	A	579	GLU

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Mol	Chain	Res	Type
1	A	113	GLU
1	A	238	ASP
1	A	477	ASP
1	A	60	GLY
1	A	386	PRO
1	A	71	PRO

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	728/765 (95%)	700 (96%)	28 (4%)	29	28

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	57	SER
1	A	72	ASP
1	A	83	SER
1	A	103	THR
1	A	104	LYS
1	A	110	VAL
1	A	179	LYS
1	A	183	LYS
1	A	184	VAL
1	A	242	HIS
1	A	278	SER
1	A	316	LYS
1	A	379	VAL
1	A	395	LYS
1	A	401	LYS
1	A	405	LYS
1	A	415	LYS
1	A	458	LEU
1	A	460	VAL

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Mol	Chain	Res	Type
1	A	538	THR
1	A	549	ARG
1	A	572	VAL
1	A	582	ASN
1	A	593	GLU
1	A	594	ARG
1	A	846	SER
1	A	860	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	378	ASN
1	A	398	ASN
1	A	419	HIS
1	A	436	ASN
1	A	471	GLN
1	A	537	ASN
1	A	576	ASN
1	A	638	GLN
1	A	647	HIS
1	A	731	ASN
1	A	806	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	2,1	14,14,15	0.92	0	17,19,21	2.11	3 (17%)
2	NAG	B	2	2	14,14,15	0.74	0	17,19,21	1.97	3 (17%)
2	BMA	B	3	2	11,11,12	0.98	1 (9%)	15,15,17	1.96	3 (20%)
2	MAN	B	4	2	11,11,12	1.22	1 (9%)	15,15,17	1.98	6 (40%)
2	MAN	B	5	2	11,11,12	0.79	0	15,15,17	2.05	4 (26%)
2	MAN	B	6	2	11,11,12	0.94	0	15,15,17	2.12	3 (20%)
2	MAN	B	7	2	11,11,12	1.66	2 (18%)	15,15,17	1.99	4 (26%)
2	MAN	B	8	2	11,11,12	0.97	0	15,15,17	1.11	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	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	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	-	1/2/19/22	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	MAN	C2-C3	3.70	1.58	1.52
2	B	4	MAN	C2-C3	2.96	1.57	1.52
2	B	7	MAN	C1-C2	2.62	1.58	1.52
2	B	3	BMA	C2-C3	2.61	1.56	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	6.60	121.04	112.19
2	B	6	MAN	C1-O5-C5	6.41	120.78	112.19
2	B	1	NAG	O5-C1-C2	-6.24	101.64	111.29
2	B	5	MAN	C1-O5-C5	5.94	120.15	112.19
2	B	3	BMA	C1-O5-C5	4.66	118.44	112.19
2	B	7	MAN	C1-C2-C3	4.58	116.32	109.64
2	B	4	MAN	O3-C3-C2	3.96	118.13	110.05
2	B	7	MAN	C2-C3-C4	3.27	116.61	110.86
2	B	2	NAG	O7-C7-C8	-3.19	116.37	122.05
2	B	1	NAG	C2-N2-C7	-3.17	118.65	122.90
2	B	3	BMA	O2-C2-C3	3.07	116.50	110.15
2	B	4	MAN	C1-C2-C3	2.87	113.82	109.64
2	B	3	BMA	O4-C4-C3	2.82	117.02	110.38
2	B	4	MAN	C6-C5-C4	2.70	119.64	113.02
2	B	7	MAN	C3-C4-C5	2.65	115.03	110.23
2	B	4	MAN	O4-C4-C3	-2.59	104.27	110.38
2	B	8	MAN	C1-O5-C5	2.59	115.66	112.19
2	B	6	MAN	C2-C3-C4	2.55	115.35	110.86
2	B	6	MAN	O5-C1-C2	2.50	116.75	110.79
2	B	5	MAN	O4-C4-C5	2.33	115.06	109.32
2	B	4	MAN	C1-O5-C5	2.32	115.29	112.19
2	B	4	MAN	O6-C6-C5	2.31	119.19	111.33
2	B	5	MAN	C6-C5-C4	-2.30	107.38	113.02
2	B	1	NAG	O5-C5-C4	-2.29	105.25	110.83
2	B	7	MAN	O5-C5-C6	2.19	111.93	107.66
2	B	8	MAN	O3-C3-C2	2.11	114.37	110.05
2	B	5	MAN	O5-C5-C4	2.05	115.82	110.83
2	B	2	NAG	C8-C7-N2	2.00	119.44	116.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

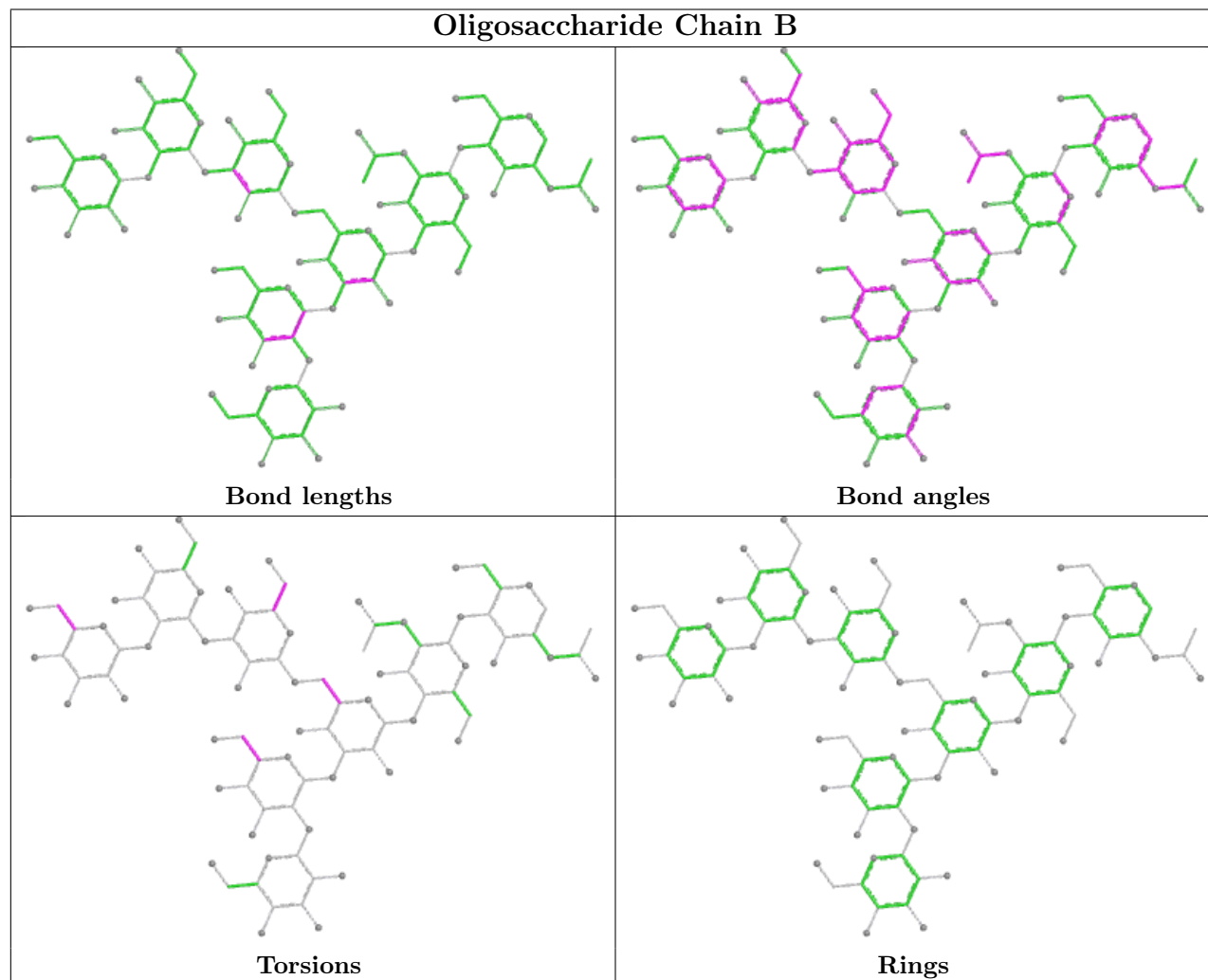
Mol	Chain	Res	Type	Atoms
2	B	7	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	MAN	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	ACT	A	902	-	3,3,3	1.11	0	3,3,3	1.32	0
3	X7X	A	901	7	44,44,44	1.76	10 (22%)	60,64,64	1.80	18 (30%)

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	X7X	A	901	7	-	2/25/55/55	0/7/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	X7X	C18-C17	4.53	1.46	1.40
3	A	901	X7X	C16-C17	3.32	1.45	1.40
3	A	901	X7X	C26-N27	3.32	1.38	1.34
3	A	901	X7X	O33-C28	3.00	1.42	1.36
3	A	901	X7X	C2-N1	2.81	1.52	1.46
3	A	901	X7X	C28-N27	2.72	1.37	1.33
3	A	901	X7X	C8-N7	2.63	1.51	1.46
3	A	901	X7X	C18-N19	2.59	1.41	1.36
3	A	901	X7X	C25-C23	2.25	1.42	1.39
3	A	901	X7X	C3-N1	2.18	1.50	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	X7X	C31-C30-C26	-4.68	114.95	120.30
3	A	901	X7X	C2-C5-C4	-4.53	97.09	103.56
3	A	901	X7X	C4-C3-N1	-4.29	96.54	103.02
3	A	901	X7X	C14-C12-C16	3.92	123.78	119.25
3	A	901	X7X	C23-C25-C26	-3.09	116.30	119.77
3	A	901	X7X	C5-C2-N1	-3.02	98.46	103.02
3	A	901	X7X	C12-C16-C17	-2.98	114.53	118.61
3	A	901	X7X	C36-C35-C34	-2.57	104.58	111.42
3	A	901	X7X	C14-C12-C11	-2.44	114.03	120.28
3	A	901	X7X	C29-C23-C25	2.40	122.47	119.65
3	A	901	X7X	C25-C23-C22	-2.39	114.82	120.13
3	A	901	X7X	O13-C11-N1	-2.37	118.62	122.35
3	A	901	X7X	C8-C4-C5	-2.22	100.39	103.56
3	A	901	X7X	C34-O33-C28	-2.20	114.81	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	X7X	C37-C36-C35	-2.19	105.93	112.03
3	A	901	X7X	O38-C37-C36	-2.13	108.06	111.74
3	A	901	X7X	C39-O38-C37	2.02	116.40	109.88
3	A	901	X7X	C15-C18-C17	-2.02	119.89	122.10

There are no chirality outliers.

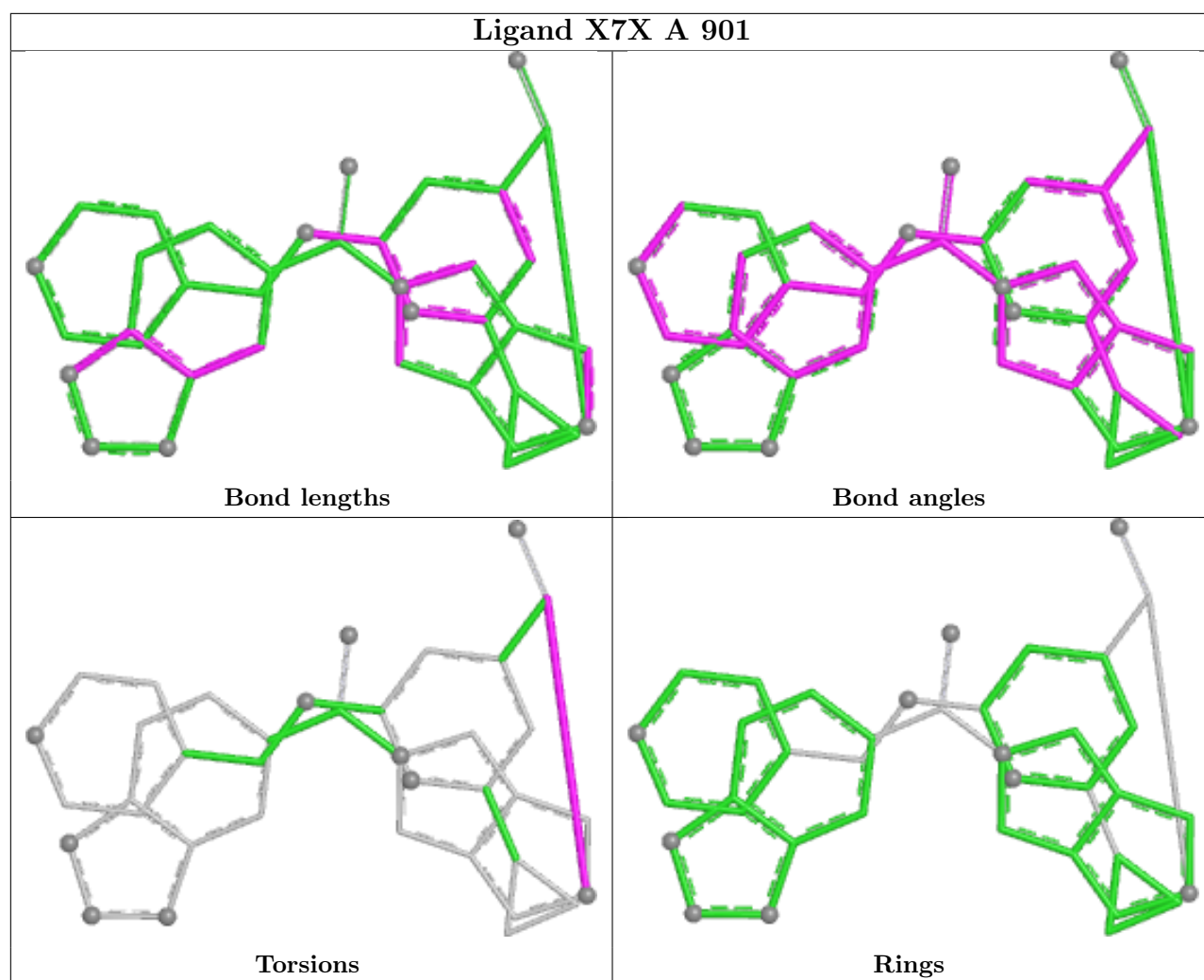
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	X7X	O24-C22-N7-C8
3	A	901	X7X	C23-C22-N7-C8

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.



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	805/846 (95%)	0.28	55 (6%)	23 27	23, 42, 79, 80	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	6.2
1	A	572	VAL	5.6
1	A	578	LEU	5.3
1	A	70	PRO	4.9
1	A	469	PHE	4.3
1	A	54	THR	4.2
1	A	581	LEU	4.0
1	A	69	GLY	4.0
1	A	461	TYR	3.9
1	A	68	VAL	3.9
1	A	468	CYS	3.9
1	A	71	PRO	3.8
1	A	52	THR	3.8
1	A	397	ILE	3.7
1	A	585	LEU	3.7
1	A	243	LEU	3.2
1	A	237	PHE	3.0
1	A	536	THR	3.0
1	A	53	ALA	2.9
1	A	246	ARG	2.8
1	A	463	LYS	2.7
1	A	684	TYR	2.7
1	A	87	HIS	2.6
1	A	378	ASN	2.5
1	A	579	GLU	2.5
1	A	584	ARG	2.5
1	A	398	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLY	2.5
1	A	60	GLY	2.4
1	A	648	LEU	2.3
1	A	580	GLU	2.3
1	A	239	ALA	2.3
1	A	236	VAL	2.3
1	A	251	HIS	2.2
1	A	110	VAL	2.2
1	A	366	CYS	2.2
1	A	573	GLU	2.2
1	A	458	LEU	2.2
1	A	402	TYR	2.2
1	A	571	LYS	2.2
1	A	417	ASP	2.2
1	A	538	THR	2.2
1	A	470	PHE	2.1
1	A	244	ARG	2.1
1	A	277	VAL	2.1
1	A	55	SER	2.1
1	A	645	PRO	2.1
1	A	460	VAL	2.1
1	A	415	LYS	2.1
1	A	582	ASN	2.1
1	A	272	THR	2.1
1	A	540	ARG	2.1
1	A	462	LYS	2.1
1	A	537	ASN	2.0
1	A	566	CYS	2.0

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

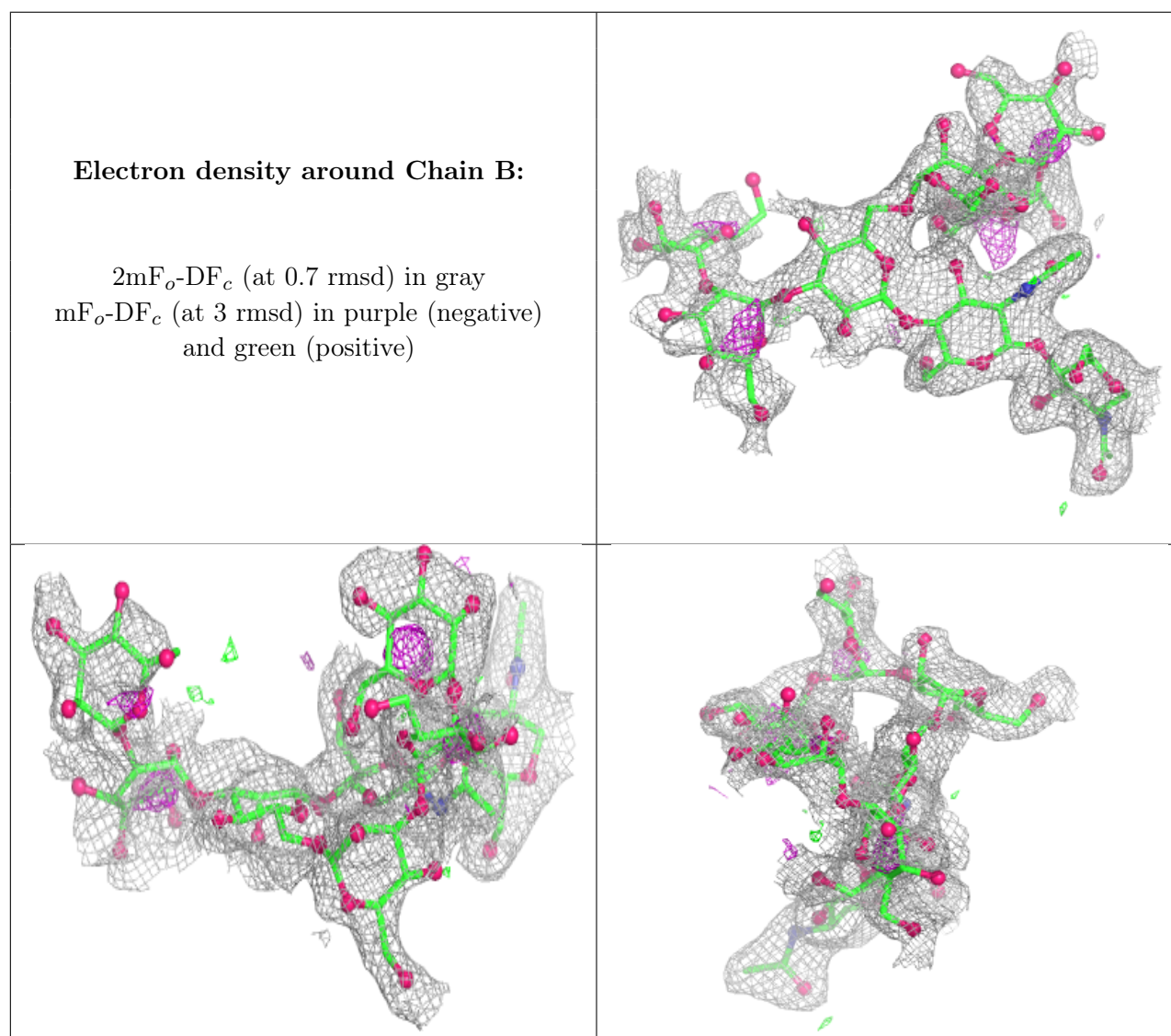
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	B	7	11/12	0.45	0.16	80,80,80,80	0
2	BMA	B	3	11/12	0.62	0.14	78,80,80,80	0
2	MAN	B	8	11/12	0.63	0.14	64,80,80,80	0
2	MAN	B	4	11/12	0.74	0.12	65,78,80,80	0
2	MAN	B	5	11/12	0.75	0.17	80,80,80,80	0
2	MAN	B	6	11/12	0.81	0.16	63,76,80,80	0
2	NAG	B	2	14/15	0.91	0.09	37,49,55,64	0
2	NAG	B	1	14/15	0.95	0.07	28,31,33,36	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

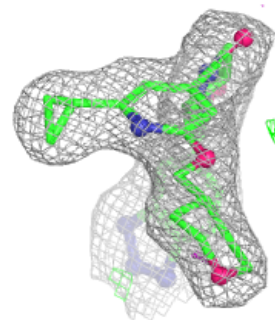
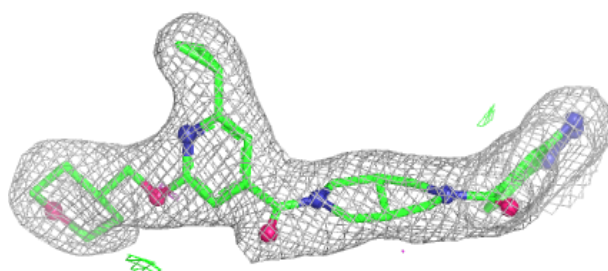
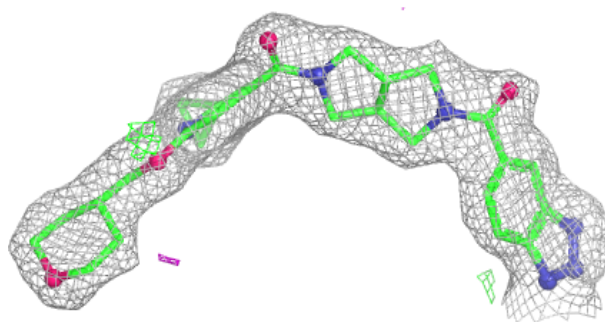
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	ACT	A	902	4/4	0.78	0.18	43,48,51,52	0
3	X7X	A	901	38/38	0.95	0.07	30,41,54,60	0
5	CL	A	903	1/1	0.96	0.07	50,50,50,50	0
6	CA	A	904	1/1	0.99	0.04	49,49,49,49	0
6	CA	A	906	1/1	0.99	0.02	34,34,34,34	0
8	NA	A	907	1/1	0.99	0.04	38,38,38,38	0
7	ZN	A	905	1/1	1.00	0.02	35,35,35,35	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 X7X A 901:

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.