



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:30 AM UTC

PDB ID : 7G3L / pdb_00007g3l

Title : Crystal Structure of rat Autotaxin in complex with 2-[(2-tert-butyl-5-chloro-4-cyanophenoxy)methyl]-N,3-dimethylimidazole-4-carboxamide, i.e. SMILES Clc1c(C#N)cc(C(C)(C)C)c(c1)OCC1=NC=C(C(=O)NC)N1C with IC50=0.0853541 microM

Authors : Stihle, M.; Benz, J.; Hunziker, D.; Green, L.; Rudolph, M.G.

Deposited on : 2023-06-05

Resolution : 1.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

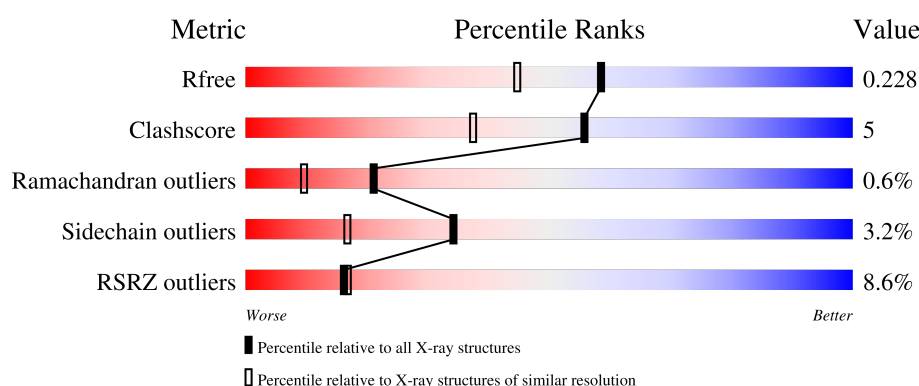
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	8% 79% 14% 5%
2	B	8	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	A	902	-	-	X	-

2 Entry composition [i](#)

There are 9 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.

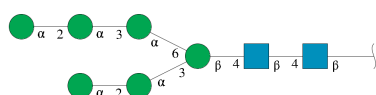
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	20	0
			6603	4191	1131	1228	53			

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

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

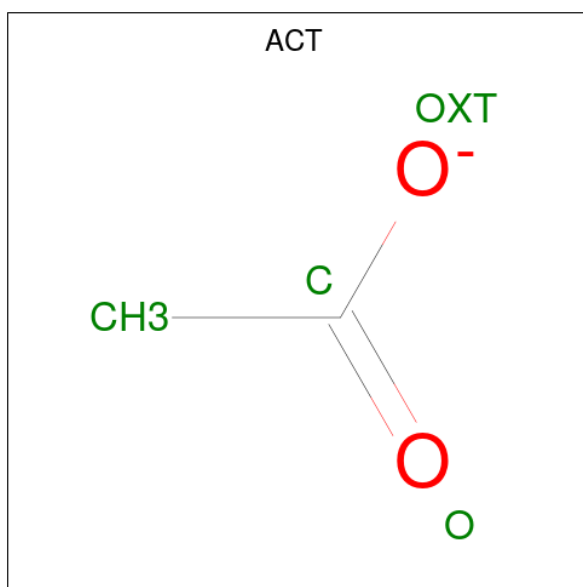
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

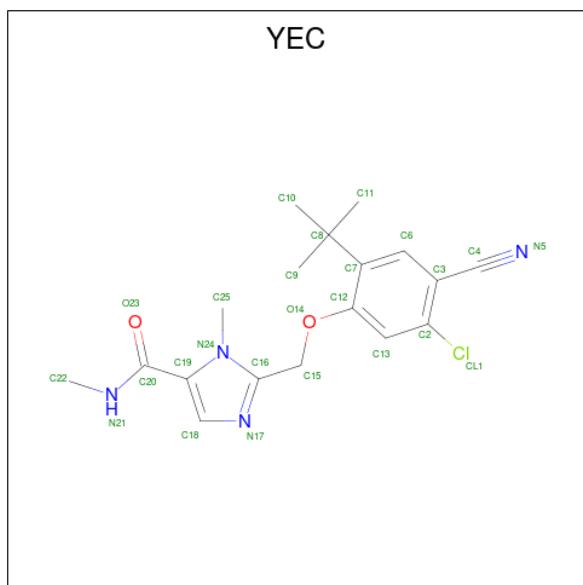
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 8 is 2-[(2-tert-butyl-5-chloro-4-cyanophenoxy)methyl]-N,1-dimethyl-1H-imidazole-5-carboxamide (CCD ID: YEC) (formula: $C_{18}H_{21}ClN_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Cl	N	O	0	0
			25	18	1	4	2		

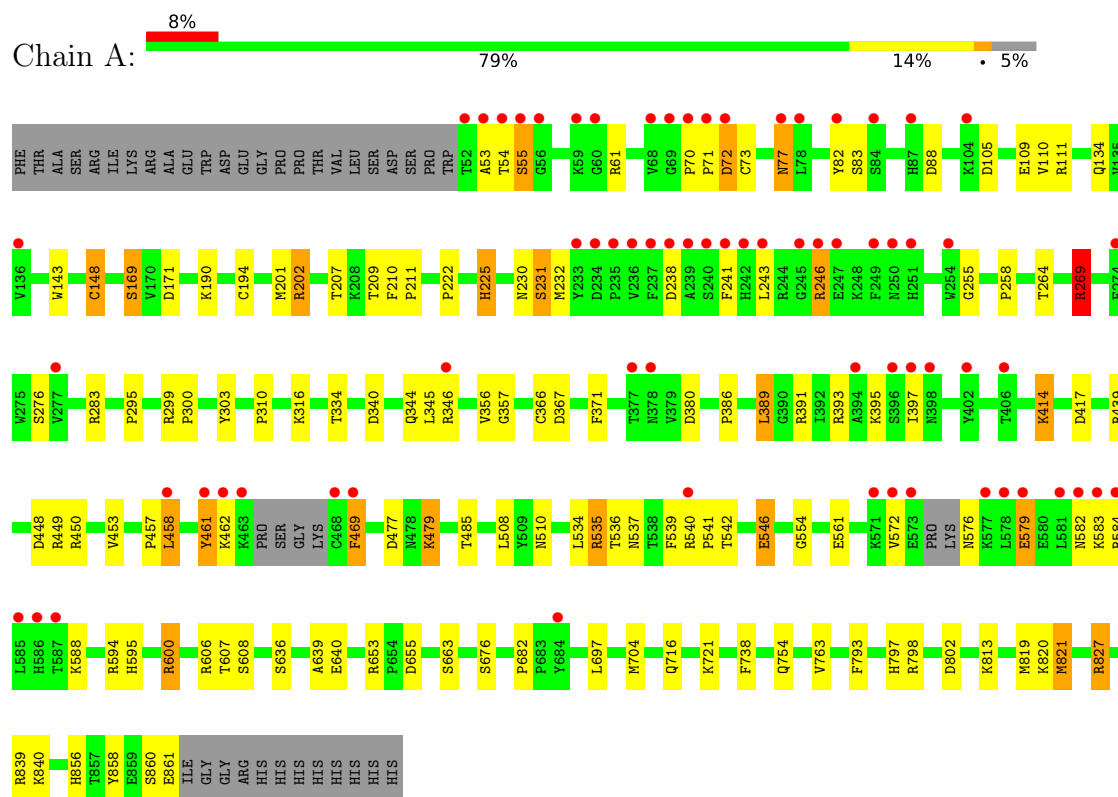
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	494	Total	O	0	0
			494	494		

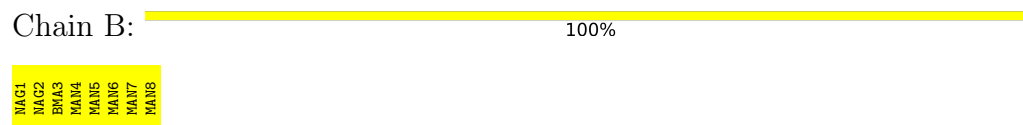
3 Residue-property plots [i](#)

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	84.11Å 91.82Å 120.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.03 – 1.84 73.03 – 1.84	Depositor EDS
% Data completeness (in resolution range)	79.2 (73.03-1.84) 79.6 (73.03-1.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.171 , 0.220 0.181 , 0.228	Depositor DCC
R_{free} test set	3373 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: ZN, NAG, CA, NA, BMA, K, MAN, ACT, YEC

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	1.20	32/6827 (0.5%)	1.19	13/9254 (0.1%)

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	14

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	ARG	C-O	-7.85	1.14	1.24
1	A	255	GLY	N-CA	6.49	1.51	1.45
1	A	207	THR	N-CA	-6.45	1.38	1.46
1	A	148[A]	CYS	C-O	-6.37	1.16	1.23
1	A	148[B]	CYS	C-O	-6.37	1.16	1.23
1	A	231	SER	N-CA	6.36	1.53	1.45
1	A	546	GLU	CD-OE1	6.18	1.37	1.25
1	A	655	ASP	C-O	-6.13	1.16	1.24
1	A	453	VAL	C-O	6.12	1.30	1.24
1	A	607	THR	C-O	-5.98	1.17	1.24
1	A	510	ASN	N-CA	5.83	1.53	1.46
1	A	366	CYS	C-O	-5.78	1.17	1.24
1	A	345	LEU	C-O	-5.73	1.16	1.24
1	A	169	SER	CA-CB	-5.66	1.44	1.53
1	A	561	GLU	C-O	-5.63	1.16	1.24
1	A	143	TRP	C-O	-5.53	1.17	1.24
1	A	697	LEU	N-CA	5.53	1.52	1.46
1	A	663	SER	C-O	-5.49	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	PRO	C-O	5.48	1.30	1.23
1	A	258	PRO	C-O	5.46	1.30	1.23
1	A	588	LYS	N-CA	5.44	1.53	1.46
1	A	461	TYR	N-CA	5.25	1.53	1.46
1	A	276	SER	N-CA	5.18	1.52	1.46
1	A	340	ASP	C-O	-5.17	1.18	1.24
1	A	676	SER	C-O	-5.16	1.17	1.24
1	A	608[A]	SER	C-O	-5.13	1.18	1.24
1	A	608[B]	SER	C-O	-5.13	1.18	1.24
1	A	88	ASP	N-CA	5.12	1.52	1.46
1	A	763	VAL	N-CA	-5.07	1.41	1.46
1	A	554	GLY	C-O	-5.03	1.19	1.23
1	A	448	ASP	N-CA	-5.03	1.39	1.46
1	A	738	PHE	N-CA	5.02	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	THR	CA-CB-OG1	-8.66	96.61	109.60
1	A	469	PHE	CA-CB-CG	7.93	121.73	113.80
1	A	225	HIS	CA-CB-CG	7.44	121.24	113.80
1	A	344	GLN	CB-CA-C	-7.42	98.47	110.79
1	A	813	LYS	CB-CA-C	-7.24	97.38	109.55
1	A	264	THR	CA-CB-OG1	-7.03	99.06	109.60
1	A	202	ARG	CA-C-O	6.25	123.95	119.32
1	A	827	ARG	CG-CD-NE	-5.58	99.72	112.00
1	A	367	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	595	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	840	LYS	CB-CA-C	-5.29	103.72	111.77
1	A	334	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	61	ARG	CB-CA-C	-5.17	102.65	111.02

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	ARG	Sidechain
1	A	246	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	346	ARG	Sidechain
1	A	391	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	393	ARG	Sidechain
1	A	439	ARG	Sidechain
1	A	584	ARG	Sidechain
1	A	600	ARG	Sidechain
1	A	653	ARG	Sidechain
1	A	798	ARG	Sidechain
1	A	827	ARG	Sidechain
1	A	839	ARG	Sidechain

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	6603	0	6384	62	0
2	B	94	0	79	0	0
3	A	1	0	0	0	0
4	A	2	0	0	2	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	12	0	9	0	0
8	A	25	0	0	0	0
9	A	494	0	0	10	0
All	All	7233	0	6472	62	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 5.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539[A]:PHE:O	1:A:541:PRO:HD3	1.73	0.88
1:A:230:ASN:ND2	9:A:1002:HOH:O	1.97	0.79
1:A:134:GLN:NE2	9:A:1004:HOH:O	2.06	0.78
1:A:77:ASN:O	1:A:77:ASN:ND2	2.14	0.78
1:A:639:ALA:HB2	9:A:1131:HOH:O	1.84	0.76
1:A:821:MET:HA	1:A:821:MET:HE2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLN:HG3	9:A:1336:HOH:O	1.85	0.74
1:A:754:GLN:CG	9:A:1336:HOH:O	2.37	0.70
1:A:754:GLN:CD	9:A:1336:HOH:O	2.41	0.64
1:A:534:LEU:HD12	1:A:537[B]:ASN:ND2	2.16	0.60
1:A:209:THR:OG1	4:A:902:CA:CA	1.78	0.60
1:A:594:ARG:HH22	1:A:636:SER:HB3	1.67	0.59
1:A:458:LEU:HD13	1:A:462:LYS:HD3	1.84	0.58
1:A:576:ASN:HD21	1:A:579:GLU:CD	2.11	0.58
1:A:190:LYS:O	1:A:194[B]:CYS:HB2	2.03	0.58
1:A:539[A]:PHE:O	1:A:541:PRO:CD	2.50	0.57
1:A:82:TYR:HA	1:A:246:ARG:HH22	1.70	0.57
1:A:171:ASP:O	1:A:310:PRO:HD2	2.06	0.56
1:A:77:ASN:ND2	1:A:77:ASN:C	2.66	0.54
1:A:209:THR:HG1	4:A:902:CA:CA	1.48	0.53
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.44	0.53
1:A:449:ARG:O	1:A:450[A]:ARG:HB2	2.08	0.51
1:A:793:PHE:CE2	1:A:819:MET:HE3	2.45	0.51
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.94	0.49
1:A:269:ARG:HB3	1:A:300:PRO:HA	1.95	0.49
1:A:110:VAL:O	1:A:111:ARG:C	2.54	0.49
1:A:201:MET:HE1	1:A:356:VAL:CG2	2.42	0.49
1:A:458:LEU:C	1:A:458:LEU:HD12	2.38	0.49
1:A:210:PHE:N	1:A:211:PRO:CD	2.76	0.48
1:A:540:ARG:NH1	9:A:1025:HOH:O	2.46	0.48
1:A:546:GLU:CD	1:A:600:ARG:HH22	2.21	0.48
1:A:389:LEU:HD23	1:A:389:LEU:N	2.28	0.48
1:A:579:GLU:HA	1:A:582:ASN:CB	2.44	0.47
1:A:54:THR:HA	1:A:73:CYS:HB3	1.96	0.47
1:A:579:GLU:HA	1:A:582:ASN:HB2	1.95	0.47
1:A:721:LYS:HD2	9:A:1399:HOH:O	2.14	0.46
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.51	0.45
1:A:535:ARG:HG2	1:A:536[A]:THR:HG23	1.96	0.45
1:A:380:ASP:O	1:A:395:LYS:HD3	2.16	0.45
1:A:856:HIS:CD2	1:A:858[A]:TYR:CE1	3.04	0.45
1:A:449:ARG:O	1:A:450[B]:ARG:HB2	2.16	0.45
1:A:414:LYS:HD3	1:A:414:LYS:HA	1.72	0.45
1:A:232:MET:HE3	1:A:241:PHE:CG	2.52	0.44
1:A:821:MET:HA	1:A:821:MET:CE	2.42	0.44
1:A:269:ARG:NH2	1:A:299:ARG:O	2.50	0.44
1:A:536[A]:THR:O	1:A:537[A]:ASN:HB2	2.17	0.44
1:A:820:LYS:HG2	1:A:858[B]:TYR:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:C	1:A:55:SER:H	2.26	0.44
1:A:704:MET:HA	1:A:797:HIS:NE2	2.33	0.44
1:A:105:ASP:OD1	1:A:105:ASP:N	2.43	0.43
1:A:210:PHE:HE2	1:A:243:LEU:HD23	1.82	0.43
1:A:458:LEU:HA	1:A:461:TYR:CE2	2.53	0.43
1:A:479:LYS:HE2	1:A:821:MET:HE1	2.01	0.43
1:A:357:GLY:HA3	1:A:485:THR:OG1	2.18	0.43
1:A:479:LYS:HE2	1:A:821:MET:CE	2.49	0.42
1:A:72:ASP:OD1	1:A:72:ASP:N	2.53	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.90	0.41
1:A:606:ARG:HD2	9:A:1144:HOH:O	2.21	0.41
1:A:802:ASP:HA	9:A:1111:HOH:O	2.20	0.41
1:A:540:ARG:HD3	1:A:540:ARG:HA	1.59	0.41
1:A:300:PRO:HD2	1:A:303:TYR:OH	2.22	0.40
1:A:169:SER:HA	1:A:356:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	818/846 (97%)	786 (96%)	27 (3%)	5 (1%)	21 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	70	PRO
1	A	238	ASP
1	A	477	ASP
1	A	572	VAL

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	747/765 (98%)	723 (97%)	24 (3%)	34 17

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	71	PRO
1	A	72	ASP
1	A	77	ASN
1	A	83	SER
1	A	148[A]	CYS
1	A	148[B]	CYS
1	A	231	SER
1	A	269	ARG
1	A	316	LYS
1	A	386	PRO
1	A	389	LEU
1	A	397	ILE
1	A	414	LYS
1	A	417	ASP
1	A	458	LEU
1	A	469	PHE
1	A	479	LYS
1	A	579	GLU
1	A	583	LYS
1	A	640	GLU
1	A	821	MET
1	A	860	SER
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	436	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	471	GLN
1	A	484	GLN
1	A	576	ASN
1	A	647	HIS
1	A	856	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 ⓘ

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	1.14	1 (7%)	17,19,21	1.43	2 (11%)
2	NAG	B	2	2	14,14,15	1.19	2 (14%)	17,19,21	2.22	3 (17%)
2	BMA	B	3	2	11,11,12	1.41	1 (9%)	15,15,17	3.32	11 (73%)
2	MAN	B	4	2	11,11,12	1.60	2 (18%)	15,15,17	2.68	8 (53%)
2	MAN	B	5	2	11,11,12	1.20	1 (9%)	15,15,17	2.22	8 (53%)
2	MAN	B	6	2	11,11,12	0.99	0	15,15,17	1.96	4 (26%)
2	MAN	B	7	2	11,11,12	1.42	1 (9%)	15,15,17	2.90	5 (33%)
2	MAN	B	8	2	11,11,12	1.22	1 (9%)	15,15,17	2.31	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	1/2/19/22	0/1/1/1
2	MAN	B	8	2	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	MAN	C2-C3	3.30	1.57	1.52
2	B	4	MAN	C2-C3	2.82	1.56	1.52
2	B	7	MAN	C1-C2	2.65	1.58	1.52
2	B	1	NAG	C1-C2	-2.56	1.48	1.52
2	B	3	BMA	C2-C3	2.55	1.56	1.52
2	B	2	NAG	C8-C7	2.41	1.55	1.50
2	B	4	MAN	C6-C5	2.33	1.59	1.51
2	B	2	NAG	C6-C5	2.30	1.59	1.51
2	B	5	MAN	C2-C3	2.27	1.56	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	9.02	124.28	112.19
2	B	2	NAG	C1-O5-C5	7.28	121.94	112.19
2	B	7	MAN	C1-C2-C3	7.25	120.20	109.64
2	B	4	MAN	C1-O5-C5	7.06	121.65	112.19
2	B	8	MAN	O3-C3-C2	5.84	121.97	110.05
2	B	7	MAN	O2-C2-C3	-5.20	99.37	110.15
2	B	6	MAN	C1-O5-C5	5.05	118.95	112.19
2	B	5	MAN	C1-C2-C3	4.47	116.15	109.64
2	B	8	MAN	O2-C2-C3	4.13	118.71	110.15
2	B	3	BMA	C1-C2-C3	4.06	115.55	109.64
2	B	3	BMA	O2-C2-C1	-3.44	101.35	109.22
2	B	1	NAG	O5-C1-C2	-3.38	106.06	111.29
2	B	3	BMA	O6-C6-C5	-3.37	99.86	111.33
2	B	5	MAN	O5-C5-C4	3.35	118.97	110.83
2	B	4	MAN	O3-C3-C2	3.33	116.85	110.05
2	B	3	BMA	O4-C4-C5	-3.29	101.23	109.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	O5-C5-C4	3.17	118.53	110.83
2	B	5	MAN	O6-C6-C5	-3.16	100.56	111.33
2	B	4	MAN	O6-C6-C5	3.02	121.63	111.33
2	B	2	NAG	C3-C4-C5	2.94	115.56	110.23
2	B	3	BMA	C2-C3-C4	-2.85	105.86	110.86
2	B	6	MAN	O3-C3-C2	-2.81	104.31	110.05
2	B	7	MAN	C3-C4-C5	2.79	115.29	110.23
2	B	7	MAN	C2-C3-C4	2.78	115.75	110.86
2	B	8	MAN	C1-C2-C3	-2.51	106.00	109.64
2	B	5	MAN	O5-C5-C6	-2.46	102.87	107.66
2	B	5	MAN	C3-C4-C5	2.43	114.63	110.23
2	B	2	NAG	O3-C3-C2	-2.41	104.39	109.40
2	B	5	MAN	C1-O5-C5	2.33	115.31	112.19
2	B	8	MAN	O4-C4-C5	2.31	115.02	109.32
2	B	5	MAN	O2-C2-C3	-2.25	105.49	110.15
2	B	4	MAN	O4-C4-C5	2.21	114.78	109.32
2	B	3	BMA	O5-C1-C2	2.21	116.07	110.79
2	B	6	MAN	O2-C2-C3	-2.20	105.60	110.15
2	B	4	MAN	O4-C4-C3	-2.19	105.22	110.38
2	B	3	BMA	O2-C2-C3	2.18	114.67	110.15
2	B	4	MAN	C1-C2-C3	2.13	112.74	109.64
2	B	3	BMA	C3-C4-C5	2.10	114.04	110.23
2	B	4	MAN	C3-C4-C5	2.08	114.00	110.23
2	B	1	NAG	O4-C4-C5	-2.07	104.22	109.32
2	B	5	MAN	O5-C1-C2	-2.07	105.85	110.79
2	B	8	MAN	O5-C5-C4	-2.07	105.79	110.83
2	B	3	BMA	O5-C5-C4	2.06	115.84	110.83
2	B	4	MAN	C6-C5-C4	2.04	118.04	113.02
2	B	3	BMA	O3-C3-C2	2.01	114.17	110.05
2	B	6	MAN	O5-C1-C2	2.01	115.59	110.79

There are no chirality outliers.

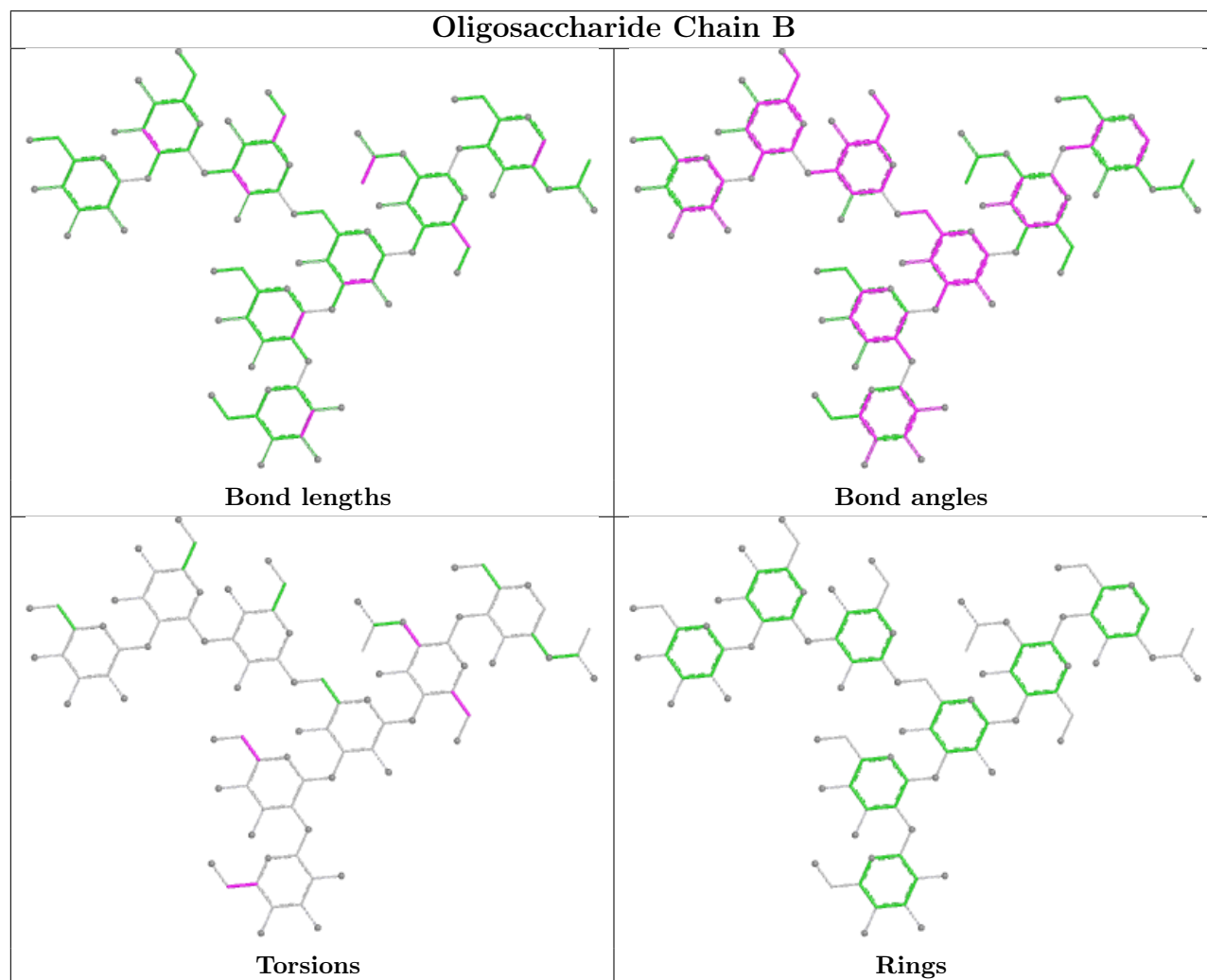
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	8	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6
2	B	7	MAN	O5-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, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ACT	A	906	-	3,3,3	1.17	0	3,3,3	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	A	907	4,3	3,3,3	1.01	0	3,3,3	3.14	2 (66%)
7	ACT	A	908	6	3,3,3	1.16	0	3,3,3	1.94	1 (33%)
8	YEC	A	909	-	26,26,26	2.80	12 (46%)	34,38,38	2.42	11 (32%)

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
8	YEC	A	909	-	-	1/19/19/19	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	909	YEC	C6-C3	-6.04	1.30	1.39
8	A	909	YEC	C16-N17	5.91	1.39	1.32
8	A	909	YEC	C8-C7	-4.90	1.46	1.54
8	A	909	YEC	C2-CL1	-3.99	1.64	1.73
8	A	909	YEC	C18-C19	3.53	1.41	1.37
8	A	909	YEC	O14-C12	-3.34	1.31	1.37
8	A	909	YEC	C13-C12	-3.22	1.33	1.38
8	A	909	YEC	C3-C2	-2.89	1.37	1.40
8	A	909	YEC	C10-C8	2.86	1.62	1.53
8	A	909	YEC	C13-C2	-2.70	1.34	1.38
8	A	909	YEC	C4-N5	2.30	1.19	1.14
8	A	909	YEC	C20-N21	-2.10	1.30	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	909	YEC	C3-C2-CL1	7.16	125.54	119.45
8	A	909	YEC	O23-C20-N21	-5.79	113.05	122.84
8	A	909	YEC	C13-C2-CL1	-5.41	109.60	118.45
7	A	907	ACT	OXT-C-CH3	4.24	132.82	115.05
8	A	909	YEC	C2-C3-C4	3.29	124.59	121.18
8	A	909	YEC	O14-C12-C7	3.27	120.47	116.78
7	A	907	ACT	O-C-CH3	-3.21	109.36	122.53
8	A	909	YEC	C6-C3-C2	-3.04	115.23	118.29
8	A	909	YEC	C10-C8-C7	-2.86	105.42	110.87
8	A	909	YEC	O23-C20-C19	2.84	126.55	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	908	ACT	OXT-C-CH3	2.67	126.25	115.05
8	A	909	YEC	C19-C20-N21	2.64	120.39	116.21
8	A	909	YEC	C13-C12-C7	-2.49	119.55	122.11
8	A	909	YEC	C25-N24-C16	-2.25	124.41	126.96

There are no chirality outliers.

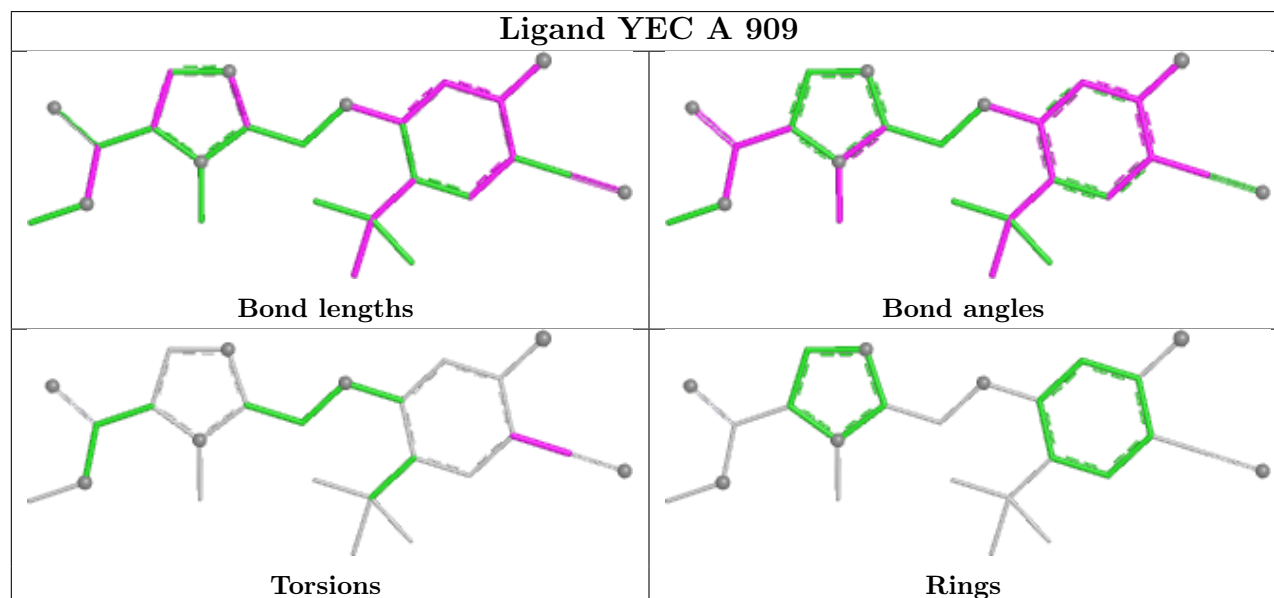
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	909	YEC	C2-C3-C4-N5

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	804/846 (95%)	0.19	69 (8%) 16 17	12, 29, 85, 144	20 (2%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PHE	7.9
1	A	236	VAL	6.3
1	A	469	PHE	6.0
1	A	578	LEU	5.1
1	A	243	LEU	4.9
1	A	68	VAL	4.6
1	A	572	VAL	4.4
1	A	397	ILE	4.3
1	A	581	LEU	4.2
1	A	71	PRO	4.1
1	A	239	ALA	3.8
1	A	468	CYS	3.8
1	A	70	PRO	3.7
1	A	54	THR	3.6
1	A	242	HIS	3.6
1	A	249	PHE	3.6
1	A	233	TYR	3.6
1	A	585	LEU	3.5
1	A	378	ASN	3.4
1	A	52	THR	3.2
1	A	55	SER	3.1
1	A	235	PRO	3.1
1	A	463	LYS	3.0
1	A	77	ASN	3.0
1	A	587	THR	2.9
1	A	240	SER	2.8
1	A	247	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	2.7
1	A	59	LYS	2.7
1	A	573	GLU	2.7
1	A	274	PHE	2.6
1	A	246	ARG	2.6
1	A	82	TYR	2.6
1	A	104	LYS	2.6
1	A	69	GLY	2.6
1	A	584	ARG	2.5
1	A	56	GLY	2.5
1	A	398	ASN	2.5
1	A	60	GLY	2.5
1	A	402	TYR	2.4
1	A	251	HIS	2.4
1	A	586	HIS	2.4
1	A	245	GLY	2.4
1	A	377	THR	2.3
1	A	582	ASN	2.3
1	A	571	LYS	2.3
1	A	577	LYS	2.3
1	A	579	GLU	2.3
1	A	254	TRP	2.3
1	A	241	PHE	2.3
1	A	583	LYS	2.3
1	A	234	ASP	2.3
1	A	78	LEU	2.3
1	A	136	VAL	2.2
1	A	461	TYR	2.2
1	A	462	LYS	2.2
1	A	84	SER	2.1
1	A	458	LEU	2.1
1	A	250	ASN	2.1
1	A	238	ASP	2.1
1	A	277	VAL	2.1
1	A	346	ARG	2.1
1	A	396	SER	2.0
1	A	87	HIS	2.0
1	A	394	ALA	2.0
1	A	72	ASP	2.0
1	A	406	THR	2.0
1	A	684	TYR	2.0
1	A	540	ARG	2.0

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

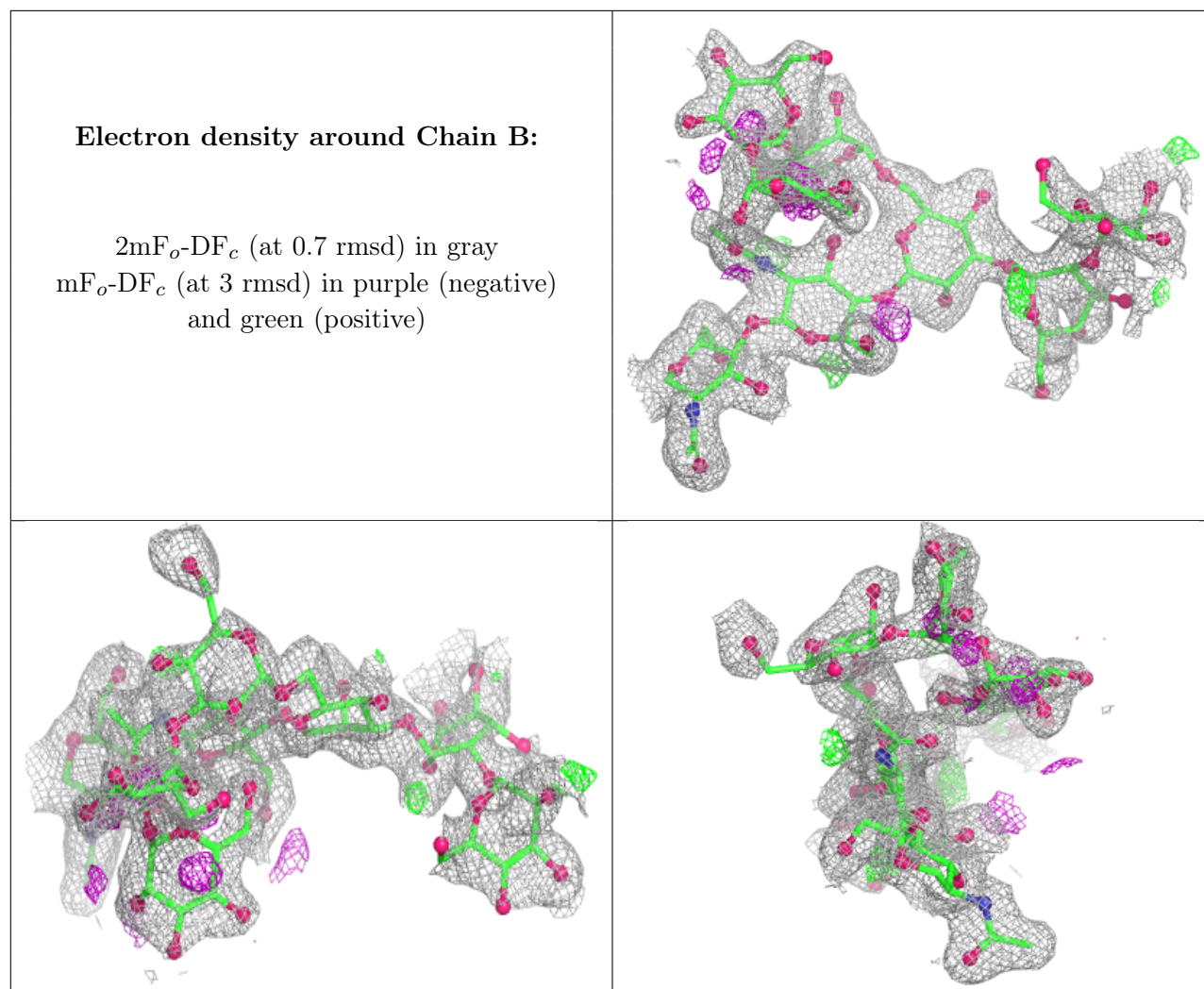
There are no non-standard protein/DNA/RNA residues in this entry.

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	7	11/12	0.40	0.19	86,97,104,107	0
2	MAN	B	8	11/12	0.72	0.16	44,94,103,113	0
2	MAN	B	4	11/12	0.74	0.14	64,74,83,86	0
2	MAN	B	5	11/12	0.76	0.15	65,79,89,90	0
2	BMA	B	3	11/12	0.77	0.12	54,66,71,75	0
2	MAN	B	6	11/12	0.87	0.17	40,60,70,73	0
2	NAG	B	2	14/15	0.91	0.08	29,35,43,56	0
2	NAG	B	1	14/15	0.97	0.05	18,21,25,25	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.

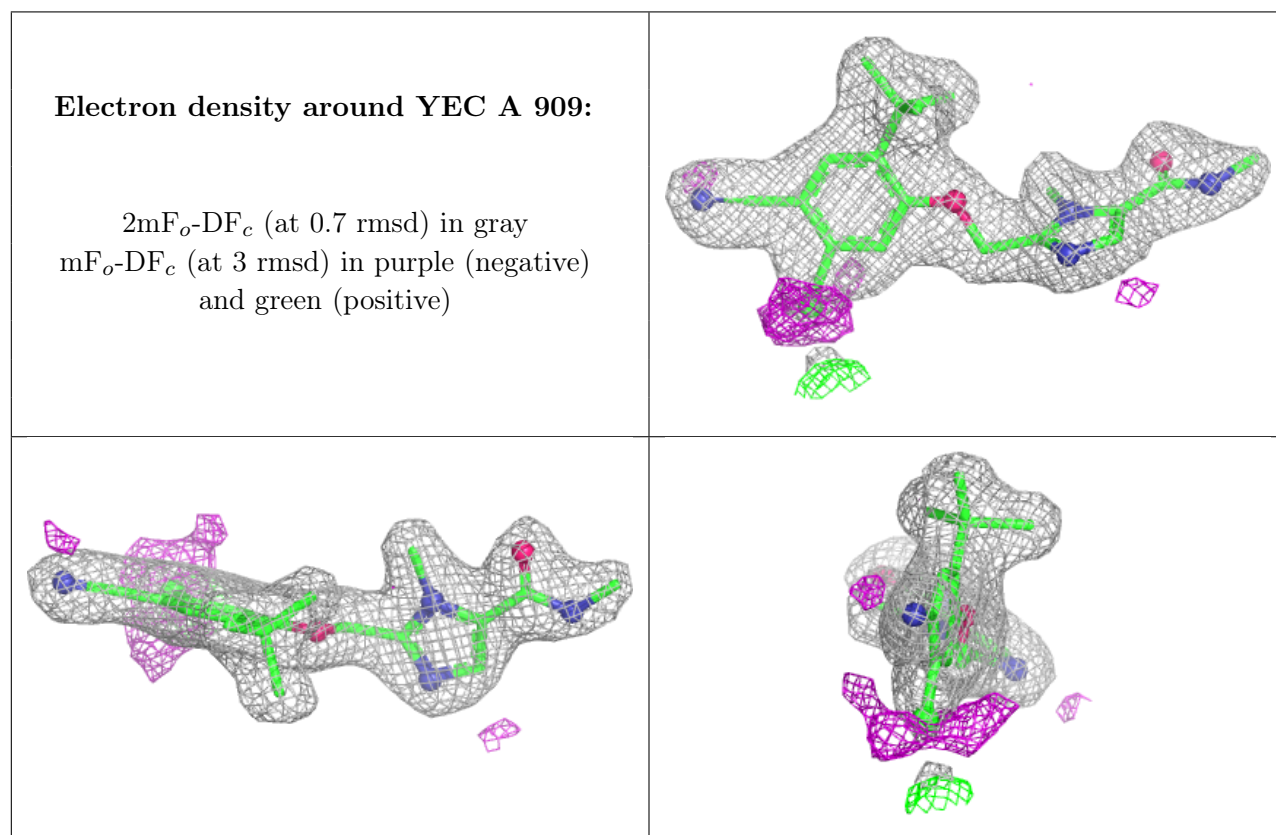


6.4 Ligands ⓘ

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
7	ACT	A	906	4/4	0.87	0.14	36,39,40,46	0
7	ACT	A	908	4/4	0.88	0.15	39,42,44,49	0
7	ACT	A	907	4/4	0.91	0.14	38,38,48,50	0
8	YEC	A	909	25/25	0.91	0.09	26,31,44,73	0
5	NA	A	903	1/1	0.96	0.06	38,38,38,38	0
6	K	A	905	1/1	0.98	0.04	33,33,33,33	0
4	CA	A	904	1/1	0.99	0.03	21,21,21,21	0
4	CA	A	902	1/1	1.00	0.02	24,24,24,24	0
3	ZN	A	901	1/1	1.00	0.01	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.