



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 04:22 AM UTC

PDB ID : 7G3R / pdb_00007g3r
Title : Crystal Structure of rat Autotaxin in complex with 5-tert-butyl-2-methyl-4-[(6-oxo-4,5-dihydro-1H-pyridazin-3-yl)methoxy]benzonitrile, i.e. SMILES O=C1NN=C(CC1)COc1cc(C)c(C#N)cc1C(C)(C)C with IC50=0.0299365 microM
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Ratni, H.; Rudolph, M.G.
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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

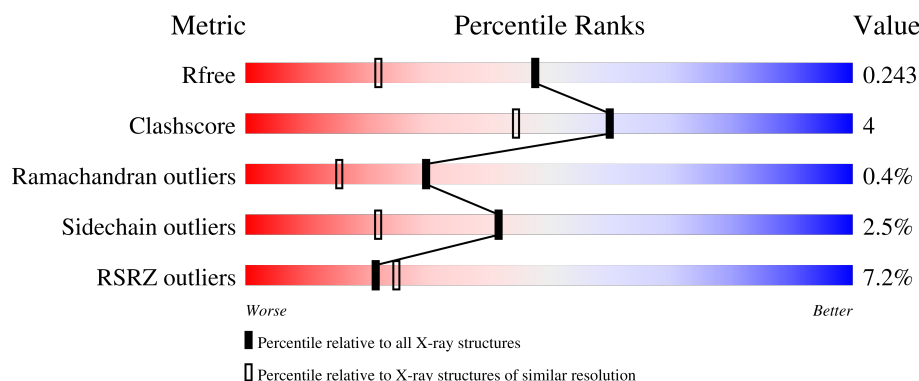
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	
2	B	8	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7273 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	805	6603	4193	1135	1223	52	0	17	0

There are 14 discrepancies between the modelled and reference sequences:

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

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

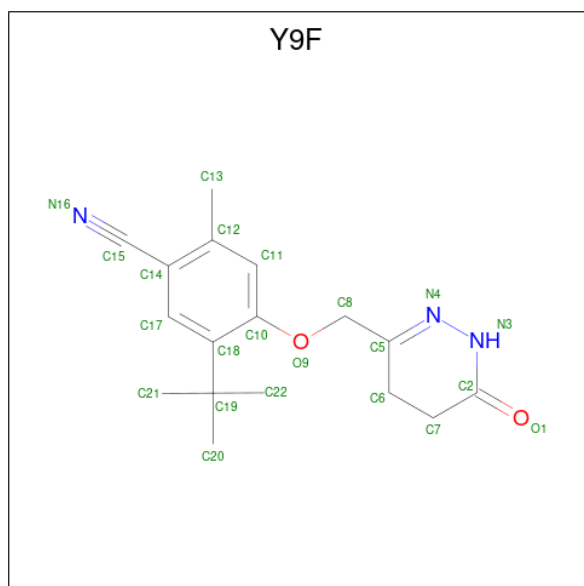


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is 5-tert-butyl-2-methyl-4-[(6-oxo-1,4,5,6-tetrahydropyridazin-3-yl)methoxy]benzonitrile (CCD ID: Y9F) (formula: C₁₇H₂₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			44	34	6	4		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

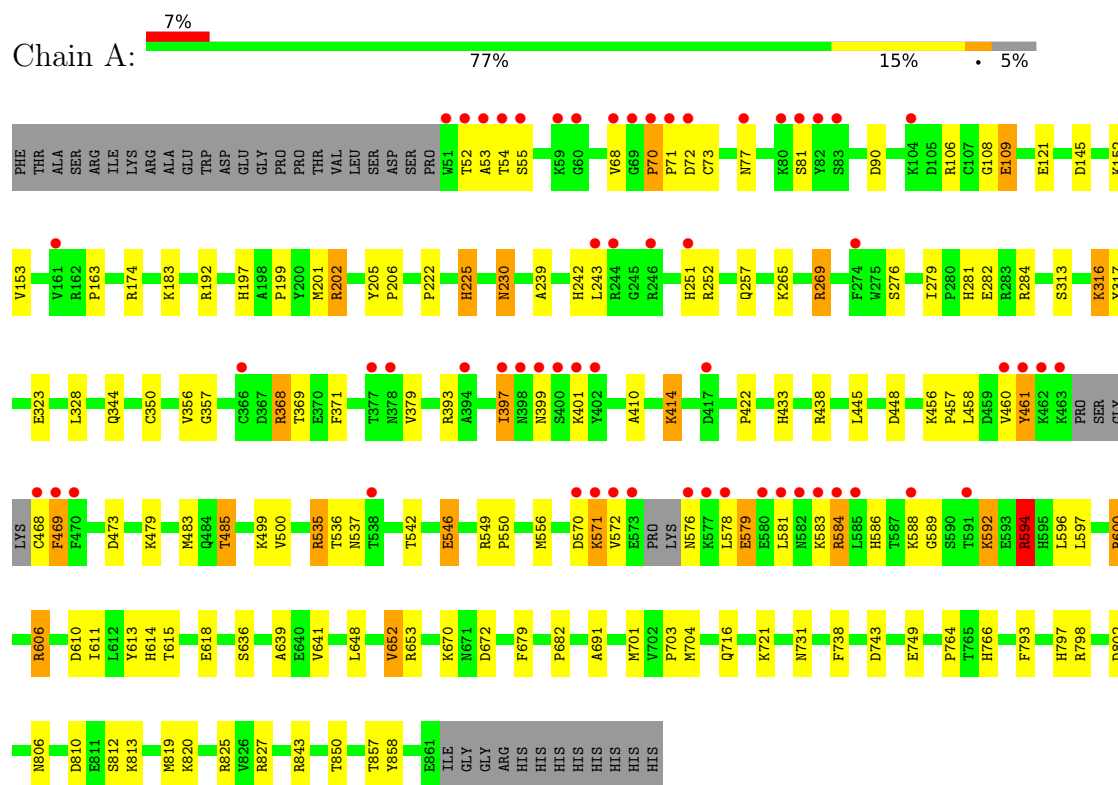
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	519	Total	O	0	0
			519	519		

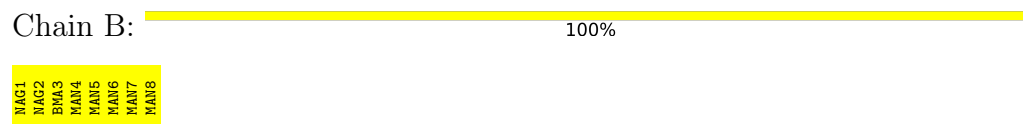
3 Residue-property plots [i](#)

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	84.06Å 92.12Å 120.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.20 – 1.76 73.20 – 1.76	Depositor EDS
% Data completeness (in resolution range)	71.3 (73.20-1.76) 71.4 (73.20-1.76)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.180 , 0.239 0.189 , 0.243	Depositor DCC
R_{free} test set	3470 reflections (3.71%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.2	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	0.95	EDS
Total number of atoms	7273	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MAN, NA, BMA, CA, NAG, ACT, Y9F

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	1.25	42/6831 (0.6%)	1.24	18/9256 (0.2%)

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	16

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	THR	C-O	-9.14	1.14	1.24
1	A	670	LYS	C-O	-7.51	1.15	1.24
1	A	473	ASP	C-O	-7.49	1.15	1.23
1	A	257	GLN	N-CA	-7.00	1.39	1.46
1	A	500	VAL	N-CA	-6.95	1.40	1.46
1	A	121	GLU	C-O	-6.89	1.15	1.24
1	A	197	HIS	CE1-NE2	6.81	1.39	1.32
1	A	672	ASP	C-O	6.80	1.32	1.24
1	A	546	GLU	CD-OE1	6.62	1.38	1.25
1	A	153	VAL	N-CA	-6.46	1.39	1.46
1	A	328	LEU	C-O	6.25	1.31	1.24
1	A	461	TYR	N-CA	6.24	1.54	1.46
1	A	738	PHE	N-CA	6.23	1.53	1.46
1	A	313	SER	N-CA	-6.22	1.38	1.46
1	A	766	HIS	CE1-NE2	6.22	1.38	1.32
1	A	535	ARG	C-O	-6.21	1.16	1.24
1	A	281	HIS	C-O	-6.09	1.17	1.24
1	A	397	ILE	N-CA	6.07	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	586	HIS	CE1-NE2	5.99	1.38	1.32
1	A	174	ARG	C-O	-5.93	1.16	1.23
1	A	652	VAL	C-O	-5.88	1.18	1.24
1	A	145	ASP	C-O	-5.86	1.16	1.24
1	A	433	HIS	C-O	5.79	1.31	1.23
1	A	239	ALA	C-O	5.56	1.30	1.23
1	A	265	LYS	C-O	-5.54	1.17	1.24
1	A	571	LYS	N-CA	5.54	1.52	1.46
1	A	152	LYS	C-O	-5.50	1.17	1.24
1	A	445	LEU	N-CA	-5.49	1.39	1.46
1	A	225	HIS	CE1-NE2	5.42	1.38	1.32
1	A	610	ASP	C-O	-5.37	1.17	1.24
1	A	850	THR	N-CA	-5.33	1.40	1.46
1	A	284	ARG	C-O	-5.32	1.18	1.24
1	A	691	ALA	N-CA	5.30	1.53	1.46
1	A	679	PHE	N-CA	-5.29	1.39	1.45
1	A	230	ASN	N-CA	5.21	1.52	1.46
1	A	282	GLU	C-O	-5.16	1.18	1.24
1	A	369	THR	N-CA	-5.16	1.39	1.46
1	A	448	ASP	N-CA	-5.09	1.39	1.46
1	A	316	LYS	C-O	-5.09	1.17	1.24
1	A	648	LEU	N-CA	5.02	1.52	1.46
1	A	731	ASN	N-CA	-5.01	1.39	1.46
1	A	556	MET	C-O	-5.00	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	HIS	CA-CB-CG	7.89	121.69	113.80
1	A	202	ARG	CA-C-O	7.78	125.08	119.32
1	A	70	PRO	C-N-CD	-7.30	104.54	120.60
1	A	806	ASN	CB-CA-C	-7.00	98.71	110.81
1	A	827	ARG	CG-CD-NE	-6.22	98.31	112.00
1	A	537	ASN	CA-CB-CG	-5.98	106.62	112.60
1	A	813	LYS	CB-CA-C	-5.89	99.66	109.55
1	A	743	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	583	LYS	CA-C-N	5.46	127.60	120.28
1	A	583	LYS	C-N-CA	5.46	127.60	120.28
1	A	344	GLN	CB-CA-C	-5.42	101.80	110.79
1	A	546	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	90	ASP	CB-CA-C	-5.33	102.51	110.88
1	A	581	LEU	CA-C-N	5.28	127.36	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	LEU	C-N-CA	5.28	127.36	120.28
1	A	422	PRO	CB-CA-C	-5.26	103.10	110.63
1	A	368	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	542	THR	CA-CB-OG1	-5.04	102.05	109.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	192	ARG	Sidechain
1	A	202	ARG	Sidechain
1	A	252	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	438	ARG	Sidechain
1	A	549	ARG	Sidechain
1	A	594	ARG	Sidechain
1	A	600	ARG	Sidechain
1	A	606[A]	ARG	Sidechain
1	A	606[B]	ARG	Sidechain
1	A	653	ARG	Sidechain
1	A	798	ARG	Sidechain
1	A	825	ARG	Sidechain
1	A	843	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	6603	0	6396	57	0
2	B	94	0	79	0	0
3	A	2	0	0	0	0
4	A	44	0	0	0	0
5	A	8	0	6	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	519	0	0	8	0
All	All	7273	0	6481	57	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 4.

All (57) 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:479[A]:LYS:NZ	8:A:1001:HOH:O	1.98	0.96
1:A:468:CYS:SG	1:A:469:PHE:N	2.56	0.75
1:A:576:ASN:HB3	1:A:579:GLU:HG3	1.74	0.70
1:A:652:VAL:HG21	1:A:701[B]:MET:HE1	1.75	0.69
1:A:251:HIS:HB3	8:A:1440:HOH:O	1.93	0.67
1:A:77:ASN:O	1:A:276:SER:OG	2.17	0.63
1:A:243:LEU:HD21	8:A:1466:HOH:O	2.01	0.60
1:A:578:LEU:H	1:A:578:LEU:HD23	1.66	0.60
1:A:410:ALA:O	1:A:414:LYS:HG3	2.02	0.60
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.84	0.59
1:A:458:LEU:HA	1:A:461:TYR:CE2	2.38	0.59
1:A:230:ASN:ND2	8:A:1003:HOH:O	2.20	0.58
1:A:576:ASN:ND2	1:A:578:LEU:HD21	2.19	0.57
1:A:606[B]:ARG:HG2	1:A:606[B]:ARG:NH1	2.19	0.57
1:A:316:LYS:HD2	8:A:1025:HOH:O	2.04	0.57
1:A:201:MET:HE1	1:A:356:VAL:CG2	2.35	0.57
1:A:639:ALA:HB2	8:A:1099:HOH:O	2.04	0.55
1:A:458:LEU:HA	1:A:461:TYR:CZ	2.43	0.54
1:A:810:ASP:OD2	1:A:812:SER:OG	2.21	0.53
1:A:546:GLU:CD	1:A:600:ARG:HH22	2.17	0.53
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.45	0.52
1:A:594:ARG:HH12	1:A:636:SER:HB3	1.74	0.51
1:A:108:GLY:O	1:A:109:GLU:C	2.53	0.51
1:A:108:GLY:O	1:A:109:GLU:O	2.28	0.51
1:A:54:THR:HA	1:A:73:CYS:HB3	1.95	0.49
1:A:317:TYR:CD2	1:A:323:GLU:HB2	2.47	0.49
1:A:550:PRO:HB2	1:A:611:ILE:HG12	1.96	0.48
1:A:596:LEU:HD22	1:A:618[A]:GLU:OE1	2.14	0.48
1:A:199:PRO:HG3	1:A:499[B]:LYS:HE3	1.95	0.47
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.49	0.47
1:A:703:PRO:HG2	1:A:764:PRO:HD3	1.97	0.47
1:A:570:ASP:C	1:A:571:LYS:HG2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ASP:HA	8:A:1242:HOH:O	2.16	0.46
1:A:793:PHE:CE2	1:A:819:MET:HE3	2.52	0.45
1:A:584:ARG:NH1	8:A:1038:HOH:O	2.50	0.45
1:A:483:MET:HA	1:A:483:MET:HE2	1.99	0.44
1:A:163:PRO:HB3	1:A:350:CYS:O	2.18	0.44
1:A:596:LEU:HD22	1:A:618[A]:GLU:CD	2.43	0.44
1:A:276:SER:HB2	1:A:279:ILE:HD12	2.00	0.43
1:A:53:ALA:C	1:A:55:SER:H	2.26	0.43
1:A:70:PRO:HA	1:A:71:PRO:HA	1.80	0.43
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.54	0.42
1:A:357:GLY:HA3	1:A:485:THR:OG1	2.19	0.42
1:A:479[B]:LYS:HB2	1:A:857[B]:THR:HG21	2.02	0.42
1:A:614:HIS:O	1:A:615:THR:C	2.62	0.42
1:A:704:MET:HA	1:A:797:HIS:NE2	2.35	0.42
1:A:613:TYR:HA	1:A:618[B]:GLU:OE1	2.20	0.41
1:A:820:LYS:HG2	1:A:858[B]:TYR:CZ	2.56	0.41
1:A:535:ARG:HG2	1:A:536:THR:HG23	2.02	0.41
1:A:456[A]:LYS:HE3	1:A:458:LEU:CD2	2.51	0.41
1:A:641:VAL:HG23	1:A:721[B]:LYS:HD3	2.01	0.41
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.88	0.41
1:A:589:GLY:O	1:A:592:LYS:HB3	2.21	0.41
1:A:550:PRO:CB	1:A:611:ILE:HG12	2.51	0.41
1:A:52:THR:HB	1:A:54:THR:HG23	2.03	0.40
1:A:199:PRO:HG3	1:A:499[B]:LYS:CE	2.50	0.40
1:A:368:ARG:HH11	1:A:368:ARG:HD3	1.70	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	817/846 (97%)	782 (96%)	32 (4%)	3 (0%)	30 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	572	VAL
1	A	399	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	746/765 (98%)	728 (98%)	18 (2%)	43	23

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	72	ASP
1	A	81	SER
1	A	183	LYS
1	A	242	HIS
1	A	269	ARG
1	A	379	VAL
1	A	397	ILE
1	A	401	LYS
1	A	414	LYS
1	A	460	VAL
1	A	469	PHE
1	A	579	GLU
1	A	584	ARG
1	A	588	LYS
1	A	592	LYS
1	A	594	ARG
1	A	749	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	398	ASN
1	A	436	ASN
1	A	471	GLN
1	A	576	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 ⓘ

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	1.19	1 (7%)	17,19,21	2.19	6 (35%)
2	NAG	B	2	2	14,14,15	0.98	0	17,19,21	1.44	3 (17%)
2	BMA	B	3	2	11,11,12	1.46	2 (18%)	15,15,17	1.76	4 (26%)
2	MAN	B	4	2	11,11,12	1.83	3 (27%)	15,15,17	3.13	10 (66%)
2	MAN	B	5	2	11,11,12	1.46	2 (18%)	15,15,17	2.15	7 (46%)
2	MAN	B	6	2	11,11,12	1.30	1 (9%)	15,15,17	1.20	1 (6%)
2	MAN	B	7	2	11,11,12	1.51	1 (9%)	15,15,17	2.48	4 (26%)
2	MAN	B	8	2	11,11,12	1.56	2 (18%)	15,15,17	2.38	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	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	1/1/1/1
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	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	MAN	C1-C2	3.65	1.60	1.52
2	B	8	MAN	C2-C3	3.63	1.58	1.52
2	B	3	BMA	C2-C3	3.44	1.57	1.52
2	B	4	MAN	O5-C5	3.01	1.49	1.43
2	B	4	MAN	O5-C1	2.69	1.48	1.43
2	B	4	MAN	C6-C5	2.65	1.60	1.51
2	B	5	MAN	C4-C5	2.54	1.58	1.53
2	B	6	MAN	O5-C5	2.43	1.48	1.43
2	B	3	BMA	O3-C3	2.18	1.48	1.43
2	B	5	MAN	C1-C2	2.17	1.57	1.52
2	B	1	NAG	O5-C5	-2.16	1.39	1.43
2	B	8	MAN	O3-C3	2.03	1.48	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	C1-O5-C5	6.68	121.13	112.19
2	B	7	MAN	C1-C2-C3	5.61	117.82	109.64
2	B	8	MAN	O3-C3-C2	5.56	121.40	110.05
2	B	1	NAG	O4-C4-C5	-4.89	97.28	109.32
2	B	7	MAN	O2-C2-C3	-4.80	100.20	110.15
2	B	4	MAN	O6-C6-C5	4.18	125.58	111.33
2	B	4	MAN	O5-C5-C6	4.11	115.67	107.66
2	B	5	MAN	C1-O5-C5	4.09	117.67	112.19
2	B	3	BMA	C1-C2-C3	3.96	115.41	109.64
2	B	8	MAN	O2-C2-C3	3.90	118.22	110.15
2	B	4	MAN	O4-C4-C3	-3.72	101.61	110.38
2	B	4	MAN	O4-C4-C5	3.63	118.25	109.32
2	B	4	MAN	O3-C3-C2	3.57	117.34	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	MAN	O2-C2-C3	-3.47	102.97	110.15
2	B	8	MAN	O5-C5-C6	3.29	114.06	107.66
2	B	1	NAG	O3-C3-C4	-3.17	102.91	110.38
2	B	8	MAN	O5-C5-C4	-3.15	103.15	110.83
2	B	5	MAN	C3-C4-C5	3.15	115.94	110.23
2	B	7	MAN	O2-C2-C1	3.13	116.40	109.22
2	B	7	MAN	O3-C3-C4	-3.12	103.01	110.38
2	B	1	NAG	O5-C1-C2	-2.99	106.67	111.29
2	B	1	NAG	O7-C7-C8	2.92	127.25	122.05
2	B	4	MAN	C6-C5-C4	2.87	120.06	113.02
2	B	5	MAN	O2-C2-C1	2.69	115.38	109.22
2	B	1	NAG	C2-N2-C7	2.69	126.50	122.90
2	B	2	NAG	C4-C3-C2	-2.61	107.19	111.02
2	B	2	NAG	O5-C1-C2	-2.60	107.27	111.29
2	B	8	MAN	C2-C3-C4	-2.59	106.30	110.86
2	B	3	BMA	C1-O5-C5	2.50	115.54	112.19
2	B	3	BMA	O2-C2-C1	-2.42	103.67	109.22
2	B	3	BMA	C3-C4-C5	2.29	114.38	110.23
2	B	1	NAG	C1-O5-C5	2.28	115.25	112.19
2	B	6	MAN	O5-C5-C6	2.24	112.01	107.66
2	B	5	MAN	O4-C4-C5	2.21	114.78	109.32
2	B	5	MAN	O4-C4-C3	-2.11	105.39	110.38
2	B	2	NAG	O7-C7-C8	-2.08	118.35	122.05
2	B	4	MAN	O2-C2-C1	2.07	113.97	109.22
2	B	4	MAN	O5-C5-C4	-2.00	105.95	110.83
2	B	4	MAN	C3-C4-C5	2.00	113.86	110.23
2	B	5	MAN	O5-C5-C6	-2.00	103.77	107.66

There are no chirality outliers.

All (7) torsion outliers are listed below:

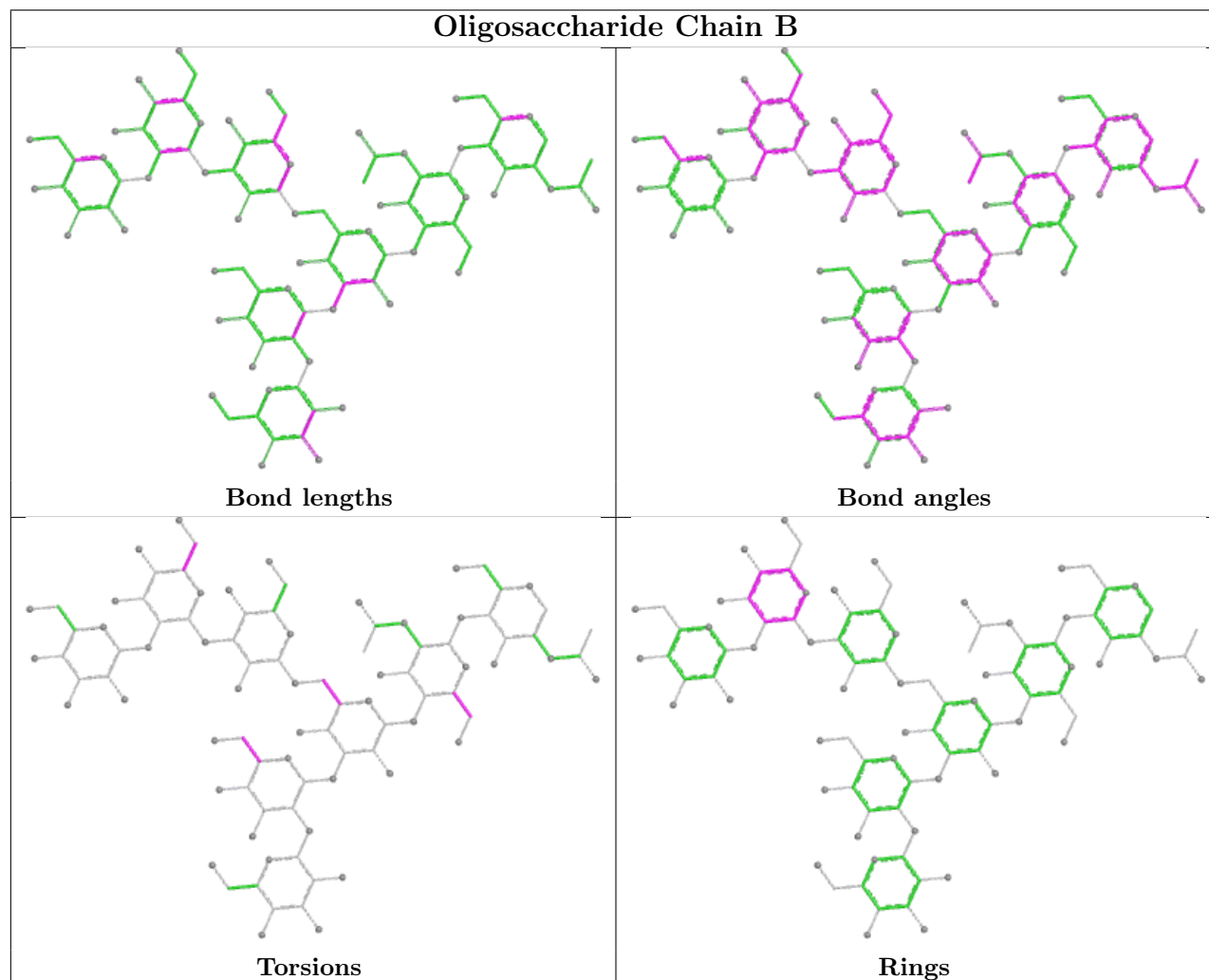
Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	C1-C2-C3-C4-C5-O5

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
4	Y9F	A	902[A]	-	21,23,23	0.44	0	29,33,33	0.62	0
5	ACT	A	903	-	3,3,3	1.10	0	3,3,3	1.06	0
5	ACT	A	904	-	3,3,3	1.05	0	3,3,3	1.70	1 (33%)
4	Y9F	A	902[B]	-	21,23,23	0.41	0	29,33,33	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y9F	A	902[A]	-	-	0/12/23/23	0/2/2/2
4	Y9F	A	902[B]	-	-	0/12/23/23	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	ACT	OXT-C-O	-2.26	113.65	122.03

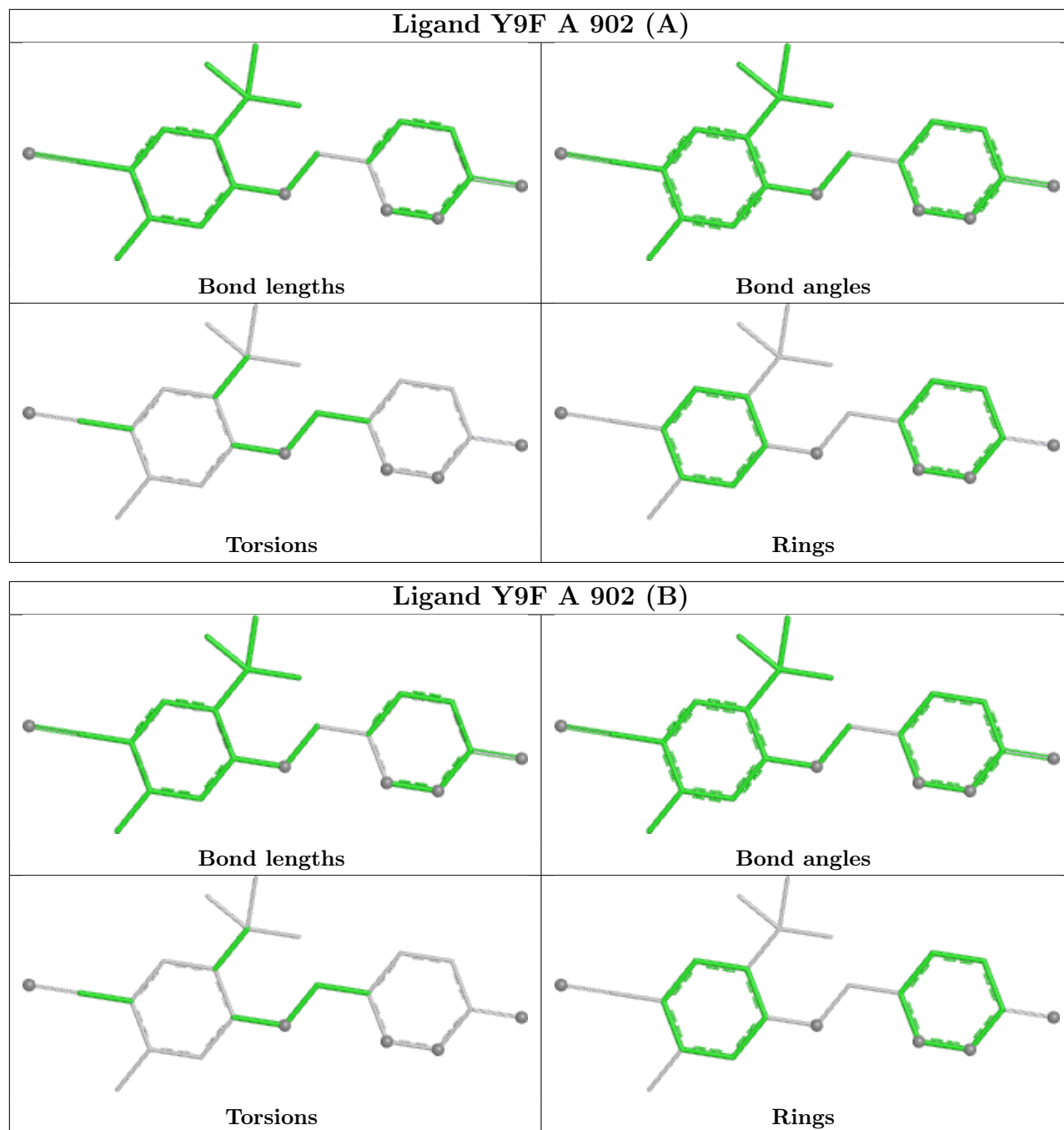
There are no chirality outliers.

There are no torsion outliers.

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%)	0.26	58 (7%)	21 25	11, 25, 66, 143	17 (2%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	8.0
1	A	578	LEU	7.9
1	A	397	ILE	7.7
1	A	469	PHE	7.4
1	A	572	VAL	6.3
1	A	581	LEU	6.0
1	A	463	LYS	4.7
1	A	468	CYS	4.7
1	A	53	ALA	4.4
1	A	71	PRO	4.1
1	A	244	ARG	3.9
1	A	573	GLU	3.7
1	A	378	ASN	3.7
1	A	585	LEU	3.7
1	A	52	THR	3.6
1	A	54	THR	3.5
1	A	577	LYS	3.5
1	A	68	VAL	3.5
1	A	398	ASN	3.4
1	A	243	LEU	3.4
1	A	461	TYR	3.2
1	A	401	LYS	3.1
1	A	576	ASN	3.1
1	A	70	PRO	3.0
1	A	402	TYR	2.9
1	A	470	PHE	2.9
1	A	588	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	377	THR	2.8
1	A	580	GLU	2.8
1	A	584	ARG	2.8
1	A	400	SER	2.8
1	A	571	LYS	2.7
1	A	82	TYR	2.6
1	A	161	VAL	2.6
1	A	570	ASP	2.5
1	A	394	ALA	2.5
1	A	591	THR	2.5
1	A	104	LYS	2.4
1	A	55	SER	2.4
1	A	582	ASN	2.4
1	A	417	ASP	2.4
1	A	538	THR	2.4
1	A	80	LYS	2.4
1	A	399	ASN	2.3
1	A	462	LYS	2.3
1	A	77	ASN	2.3
1	A	366	CYS	2.3
1	A	274	PHE	2.3
1	A	59	LYS	2.3
1	A	60	GLY	2.3
1	A	460	VAL	2.2
1	A	246	ARG	2.2
1	A	583	LYS	2.2
1	A	72	ASP	2.1
1	A	69	GLY	2.1
1	A	83	SER	2.1
1	A	251	HIS	2.0
1	A	81	SER	2.0

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

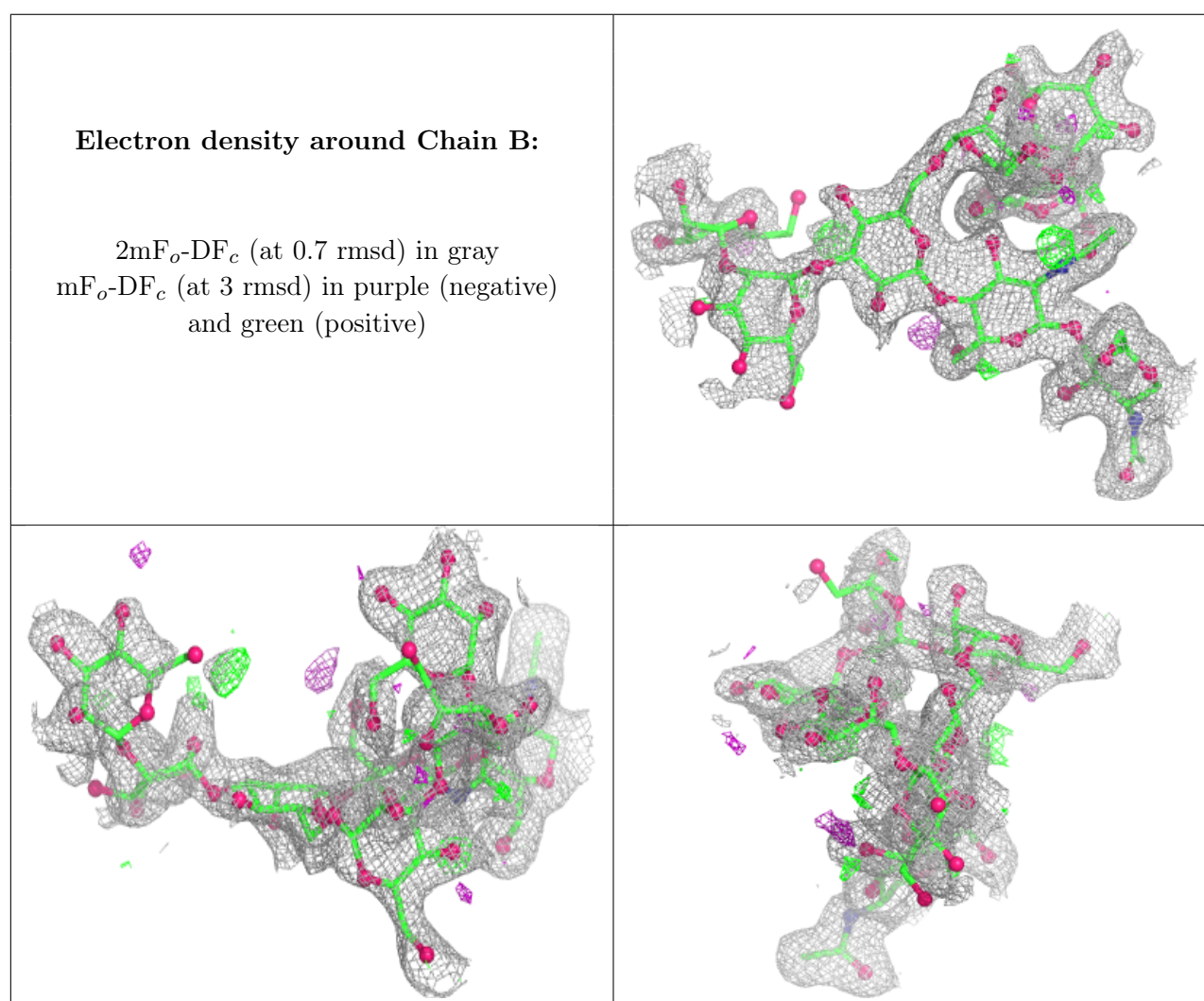
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.46	0.18	82,90,95,100	0
2	MAN	B	8	11/12	0.62	0.18	45,83,98,111	0
2	MAN	B	5	11/12	0.76	0.15	43,64,73,75	0
2	MAN	B	4	11/12	0.78	0.13	50,62,65,65	0
2	BMA	B	3	11/12	0.79	0.12	54,60,69,76	0
2	MAN	B	6	11/12	0.86	0.14	41,47,55,56	0
2	NAG	B	2	14/15	0.92	0.08	27,33,46,56	0
2	NAG	B	1	14/15	0.96	0.06	15,17,19,19	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,

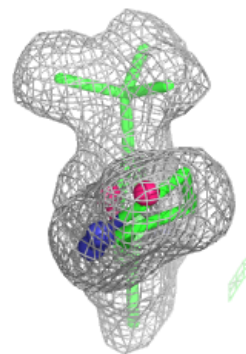
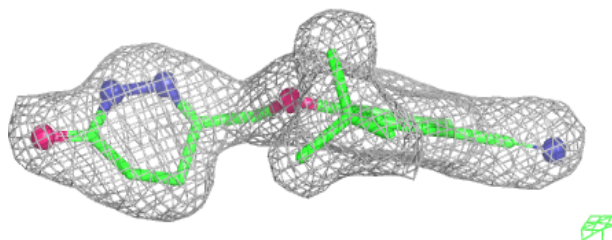
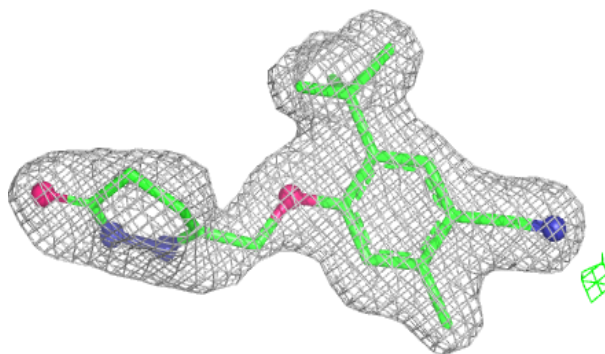
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	903	4/4	0.83	0.17	37,39,43,45	0
4	Y9F	A	902[B]	22/22	0.90	0.10	26,28,40,42	22
4	Y9F	A	902[A]	22/22	0.90	0.10	25,27,40,42	22
5	ACT	A	904	4/4	0.93	0.12	31,31,33,35	0
7	NA	A	906	1/1	0.97	0.04	32,32,32,32	0
7	NA	A	908	1/1	0.98	0.04	16,16,16,16	0
3	CA	A	901	1/1	0.99	0.07	39,39,39,39	0
3	CA	A	907	1/1	0.99	0.03	18,18,18,18	0
6	ZN	A	905	1/1	1.00	0.01	21,21,21,21	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.

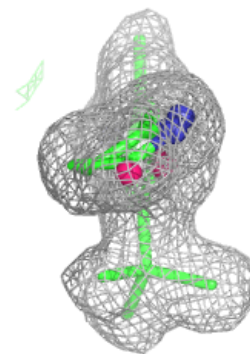
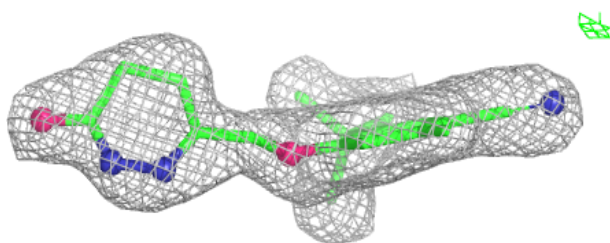
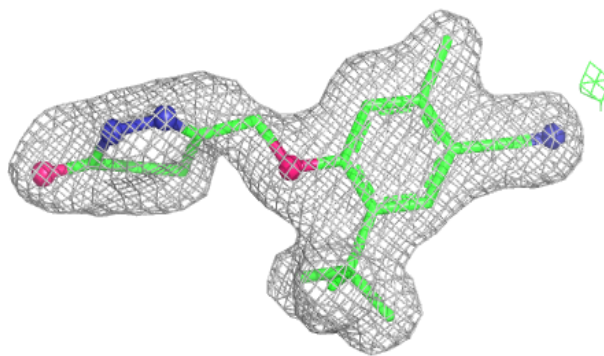
Electron density around Y9F A 902 (B):

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



Electron density around Y9F 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.