



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2026 – 01:26 pm BST

PDB ID : 9SCM / pdb_00009scm
Title : Crystal structure of Tc AChE with reactivator JDS364 Orthorhombic
Authors : de la Mora, E.; De Sousa, J.; Weik, M.; Nachon, F.; Baati, R.; Dias, J.
Deposited on : 2025-08-11
Resolution : 2.40 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 : 1.8.4, CSD as541be (2020)
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

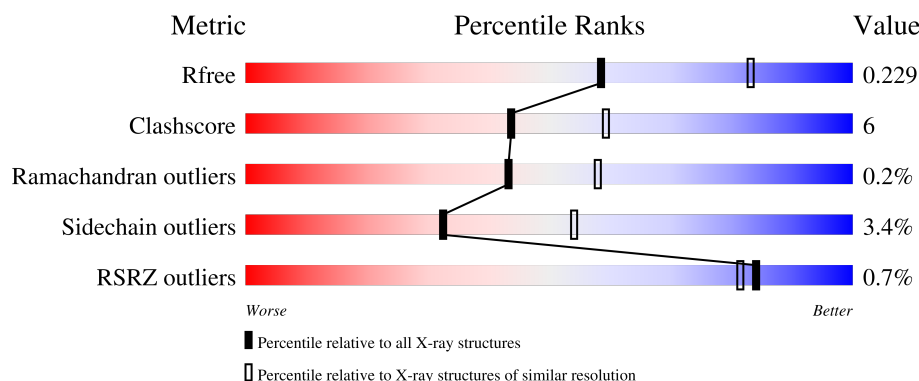
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	B	532	<div> <div></div> <div>88%</div> <div>12%</div> <div>.</div> </div>
1	D0Z0	532	<div> <div></div> <div>97%</div> <div>.</div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9277 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D0Z0	532	Total	C	N	O	S	0	21	0
			4403	2819	750	810	24			
1	B	532	Total	C	N	O	S	0	21	0
			4403	2819	750	810	24			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



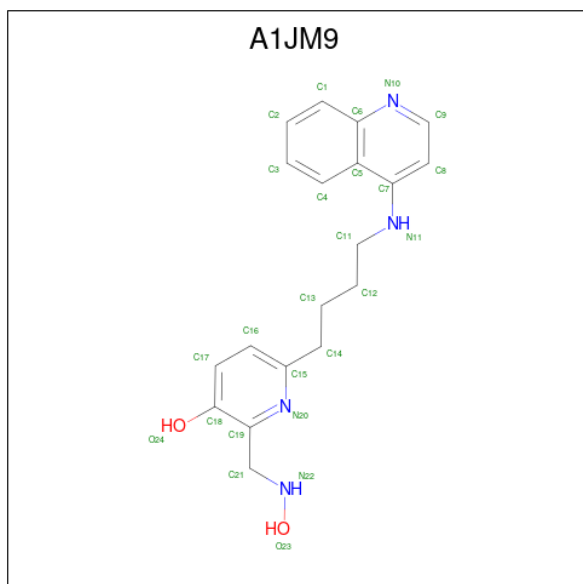
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D0Z0	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-[(oxidanylamino)methyl]-6-[4-(quinolin-4-ylamino)butyl]pyridin-3-ol (CCD ID: A1JM9) (formula: $C_{19}H_{22}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D0Z0	1	Total	C	N	O	11	0
			25	19	4	2		
4	B	1	Total	C	N	O	0	0
			25	19	4	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D0Z0	1	Total	C	O	0	0
			6	3	3		
5	D0Z0	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D0Z0	172	Total	O	0	0
			172	172		
6	B	189	Total	O	0	0
			189	189		

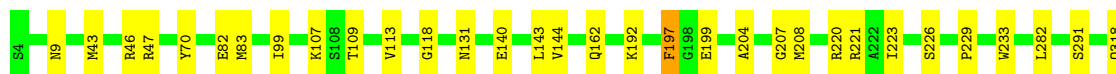
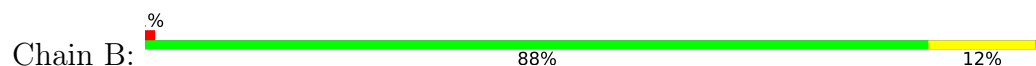
3 Residue-property plots [i](#)

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: Acetylcholinesterase



- Molecule 1: Acetylcholinesterase



- Molecule 2: 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	92.06Å 107.01Å 151.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.48 – 2.40 39.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.48-2.40) 99.1 (39.48-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.229 0.192 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9277	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0950e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, NAG, A1JM9

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	B	0.36	0/4531	0.60	4/6150 (0.1%)
1	D0Z0	0.40	4/4531 (0.1%)	0.57	5/6150 (0.1%)
All	All	0.38	4/9062 (0.0%)	0.58	9/12300 (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	D0Z0	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D0Z0	329	SER	C-O	-6.05	1.17	1.24
1	D0Z0	331	PHE	C-O	-5.27	1.17	1.24
1	D0Z0	330[A]	PHE	CA-C	5.01	1.59	1.52
1	D0Z0	330[B]	PHE	CA-C	5.01	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330[A]	PHE	CA-C-O	10.31	135.26	120.51
1	B	330[B]	PHE	CA-C-O	10.31	135.26	120.51
1	D0Z0	329	SER	N-CA-C	8.66	121.50	111.11
1	B	330[A]	PHE	N-CA-C	7.41	126.59	110.80
1	B	330[B]	PHE	N-CA-C	7.41	126.59	110.80
1	D0Z0	330[A]	PHE	CA-C-O	7.38	128.42	119.49
1	D0Z0	330[B]	PHE	CA-C-O	7.38	128.42	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D0Z0	330[A]	PHE	N-CA-C	7.13	125.98	110.80
1	D0Z0	330[B]	PHE	N-CA-C	7.13	125.98	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D0Z0	330[A]	PHE	Mainchain

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	B	4403	0	4219	44	0
1	D0Z0	4403	0	0	0	0
2	C	28	0	25	3	0
3	D0Z0	14	0	0	0	0
4	B	25	0	0	1	0
4	D0Z0	25	0	0	0	0
5	B	6	0	8	3	0
5	D0Z0	12	0	0	0	0
6	B	189	0	0	15	0
6	D0Z0	172	0	0	0	0
All	All	9277	0	4252	48	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 (48) 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:B:118:GLY:HA2	5:B:601:GOL:H2	1.31	1.10
6:B:884:HOH:O	2:C:1:NAG:O6	1.84	0.95
1:B:514:GLN:O	6:B:701:HOH:O	1.85	0.94
1:B:483:ASN:OD1	6:B:702:HOH:O	1.86	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:O	6:B:703:HOH:O	1.89	0.91
1:B:499:GLU:OE1	6:B:704:HOH:O	1.91	0.89
1:B:374:GLN:OE1	6:B:705:HOH:O	1.96	0.84
1:B:321:LEU:HD11	1:B:408[A]:VAL:HG12	1.62	0.80
6:B:889:HOH:O	2:C:2:NAG:O4	2.00	0.78
1:B:199:GLU:OE2	6:B:706:HOH:O	2.04	0.75
1:B:355:GLY:HA3	1:B:391:LEU:HD11	1.72	0.70
1:B:482:PRO:O	6:B:710:HOH:O	2.13	0.66
1:B:427:ALA:HB3	1:B:430[B]:LEU:HD13	1.80	0.64
1:B:500:GLN:OE1	6:B:711:HOH:O	2.15	0.63
1:B:118:GLY:HA2	5:B:601:GOL:C2	2.19	0.59
1:B:118:GLY:CA	5:B:601:GOL:H2	2.20	0.56
1:B:226:SER:OG	6:B:709:HOH:O	2.12	0.55
4:B:602:A1JM9:C4	4:B:602:A1JM9:C11	2.85	0.54
1:B:430[A]:LEU:HD21	1:B:439:ILE:HD12	1.89	0.53
1:B:221[A]:ARG:NE	1:B:318:GLN:OE1	2.38	0.53
1:B:430[B]:LEU:HD12	6:B:784:HOH:O	2.09	0.53
1:B:220:ARG:HG3	1:B:221[A]:ARG:HG3	1.90	0.53
1:B:70:TYR:OH	6:B:708:HOH:O	2.11	0.52
1:B:47:ARG:NH1	1:B:162:GLN:OE1	2.35	0.52
1:B:197:PHE:HB3	1:B:223:ILE:HB	1.92	0.51
2:C:1:NAG:H3	2:C:1:NAG:H83	1.91	0.50
1:B:388:ARG:HD3	6:B:787:HOH:O	2.12	0.50
1:B:404:LEU:O	1:B:408[A]:VAL:HG13	2.11	0.50
1:B:405:MET:HA	1:B:408[B]:VAL:HG12	1.94	0.49
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.49	0.48
1:B:204:ALA:O	1:B:208:MET:HG3	2.15	0.47
1:B:223:ILE:HA	1:B:320:LEU:O	2.17	0.45
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.99	0.45
1:B:344[A]:GLU:OE1	1:B:346:LYS:HE3	2.17	0.45
1:B:43:MET:HG2	1:B:46[A]:ARG:HH21	1.82	0.44
1:B:344[A]:GLU:HG2	1:B:388:ARG:HH21	1.83	0.43
1:B:197:PHE:CB	1:B:223:ILE:HB	2.48	0.43
1:B:9[B]:ASN:N	1:B:9[B]:ASN:OD1	2.51	0.43
1:B:383:ASN:HB3	1:B:386:LYS:HB2	2.00	0.42
1:B:475:THR:HG22	1:B:481:ASN:O	2.19	0.42
1:B:43:MET:HA	1:B:46[A]:ARG:HG3	2.02	0.42
1:B:113:VAL:HG22	1:B:144:VAL:HB	2.01	0.42
1:B:233:TRP:CD1	1:B:233:TRP:H	2.37	0.42
1:B:43:MET:HE3	1:B:46[A]:ARG:CZ	2.51	0.41
1:B:362:HIS:CD2	1:B:362:HIS:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASN:HB2	6:B:794:HOH:O	2.20	0.41
1:B:43:MET:HE2	1:B:43:MET:HB3	1.91	0.40
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.97	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	B	551/532 (104%)	526 (96%)	24 (4%)	1 (0%)	43	58
1	D0Z0	551/532 (104%)	526 (96%)	24 (4%)	1 (0%)	43	58
All	All	1102/1064 (104%)	1052 (96%)	48 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	489	GLU
1	D0Z0	486	HIS

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	B	478/465 (103%)	460 (96%)	18 (4%)	29	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D0Z0	478/465 (103%)	462 (97%)	16 (3%)	33	55
All	All	956/930 (103%)	922 (96%)	34 (4%)	32	52

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D0Z0	19[A]	ARG
1	D0Z0	19[B]	ARG
1	D0Z0	63	TYR
1	D0Z0	73	GLU
1	D0Z0	82	GLU
1	D0Z0	124	SER
1	D0Z0	133	LYS
1	D0Z0	197	PHE
1	D0Z0	253	ASN
1	D0Z0	288	PHE
1	D0Z0	344[A]	GLU
1	D0Z0	344[B]	GLU
1	D0Z0	350	GLU
1	D0Z0	357	LYS
1	D0Z0	473	TRP
1	D0Z0	494	LEU
1	B	82	GLU
1	B	83	MET
1	B	99	ILE
1	B	109	THR
1	B	140	GLU
1	B	143	LEU
1	B	192	LYS
1	B	197	PHE
1	B	291	SER
1	B	349	ARG
1	B	350	GLU
1	B	360	VAL
1	B	362	HIS
1	B	365	ASP
1	B	408[A]	VAL
1	B	408[B]	VAL
1	B	490	SER
1	B	535	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	181	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 ⓘ

2 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	C	1	2,1	14,14,15	0.74	0	17,19,21	2.01	4 (23%)
2	NAG	C	2	2	14,14,15	1.15	1 (7%)	17,19,21	2.62	9 (52%)

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	C	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	3.86	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-C2-N2	5.16	119.30	110.49
2	C	1	NAG	C2-N2-C7	5.14	130.23	122.90
2	C	2	NAG	C4-C3-C2	-4.49	104.44	111.02
2	C	2	NAG	C1-O5-C5	4.26	117.96	112.19
2	C	2	NAG	O5-C5-C6	-3.81	101.24	107.20
2	C	1	NAG	C1-C2-N2	3.64	116.70	110.49
2	C	1	NAG	C3-C4-C5	3.27	116.07	110.24
2	C	2	NAG	O3-C3-C4	3.21	117.77	110.35
2	C	2	NAG	O3-C3-C2	2.76	115.18	109.47
2	C	2	NAG	O6-C6-C5	-2.54	102.59	111.29
2	C	2	NAG	C2-N2-C7	2.26	126.12	122.90
2	C	1	NAG	C1-O5-C5	2.11	115.05	112.19
2	C	2	NAG	O5-C5-C4	2.09	115.92	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

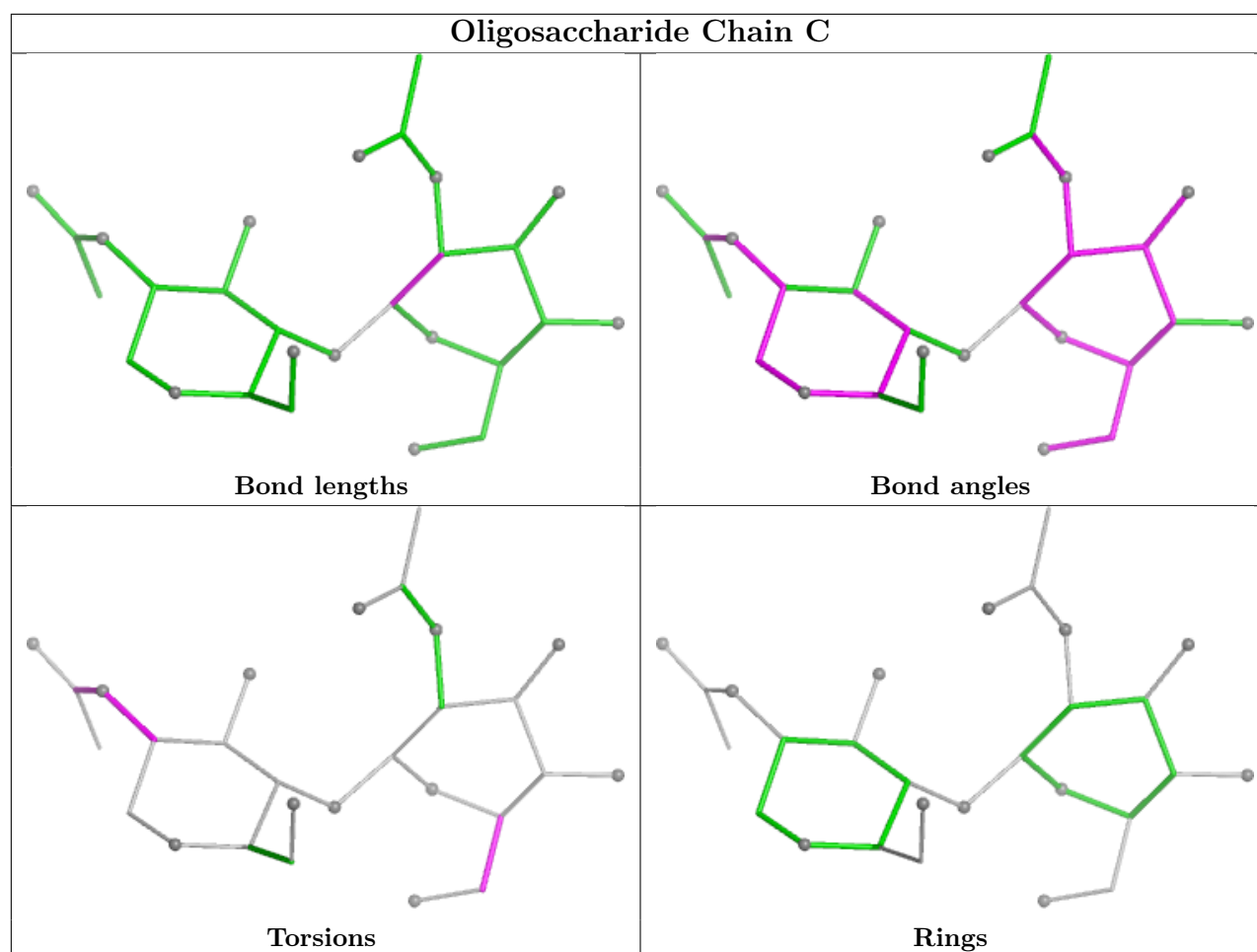
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	C	2	NAG	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](#)

6 ligands 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	$\# Z > 2$
4	A1JM9	B	602	-	26,27,27	1.81	7 (26%)	28,35,35	1.86	7 (25%)
5	GOL	D0Z0	604	4	5,5,5	0.19	0	5,5,5	0.54	0
4	A1JM9	D0Z0	602	5	26,27,27	1.74	4 (15%)	28,35,35	1.84	7 (25%)
5	GOL	B	601	-	5,5,5	0.35	0	5,5,5	0.72	0
3	NAG	D0Z0	601	1	14,14,15	1.51	1 (7%)	17,19,21	1.05	1 (5%)
5	GOL	D0Z0	603	-	5,5,5	0.26	0	5,5,5	0.61	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	A1JM9	B	602	-	-	8/10/11/11	0/3/3/3
5	GOL	D0Z0	604	4	-	4/4/4/4	-
4	A1JM9	D0Z0	602	5	-	3/10/11/11	0/3/3/3
5	GOL	B	601	-	-	4/4/4/4	-
3	NAG	D0Z0	601	1	-	2/6/23/26	0/1/1/1
5	GOL	D0Z0	603	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	A1JM9	C5-C6	-5.63	1.33	1.42
3	D0Z0	601	NAG	O5-C1	5.53	1.52	1.43
4	D0Z0	602	A1JM9	C5-C6	-5.05	1.34	1.42
4	D0Z0	602	A1JM9	C7-N11	4.09	1.46	1.36
4	D0Z0	602	A1JM9	C21-C19	3.75	1.58	1.51
4	B	602	A1JM9	C7-N11	3.69	1.45	1.36
4	D0Z0	602	A1JM9	O24-C18	3.02	1.42	1.36
4	B	602	A1JM9	O24-C18	2.57	1.41	1.36
4	B	602	A1JM9	C21-C19	2.39	1.55	1.51
4	B	602	A1JM9	C19-N20	-2.18	1.30	1.34
4	B	602	A1JM9	C15-N20	-2.07	1.31	1.34
4	B	602	A1JM9	C14-C15	2.06	1.55	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	A1JM9	C5-C7-N11	5.03	125.54	119.66
4	B	602	A1JM9	C7-C5-C6	4.56	120.95	118.06
4	D0Z0	602	A1JM9	C7-C5-C6	4.11	120.66	118.06
4	D0Z0	602	A1JM9	C15-N20-C19	3.80	122.78	118.16
4	D0Z0	602	A1JM9	C5-C7-N11	3.34	123.56	119.66
4	D0Z0	602	A1JM9	C14-C15-N20	3.29	120.84	115.95
3	D0Z0	601	NAG	C1-O5-C5	3.07	116.36	112.19
4	B	602	A1JM9	C15-N20-C19	2.77	121.53	118.16
4	B	602	A1JM9	C16-C17-C18	-2.55	117.88	120.50
4	B	602	A1JM9	C8-C7-N11	-2.53	119.44	122.30
4	D0Z0	602	A1JM9	C11-N11-C7	2.41	127.27	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	A1JM9	C8-C7-C5	-2.39	115.01	119.68
4	B	602	A1JM9	C4-C5-C7	-2.21	119.48	123.00
4	D0Z0	602	A1JM9	C8-C7-N11	-2.06	119.98	122.30
4	D0Z0	602	A1JM9	C14-C15-C16	-2.02	117.61	121.58

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D0Z0	602	A1JM9	C12-C13-C14-C15
4	B	602	A1JM9	C5-C7-N11-C11
4	B	602	A1JM9	C8-C7-N11-C11
5	D0Z0	604	GOL	O1-C1-C2-C3
5	D0Z0	604	GOL	C1-C2-C3-O3
5	B	601	GOL	O1-C1-C2-C3
5	B	601	GOL	C1-C2-C3-O3
3	D0Z0	601	NAG	O5-C5-C6-O6
3	D0Z0	601	NAG	C4-C5-C6-O6
5	B	601	GOL	O2-C2-C3-O3
5	D0Z0	604	GOL	O1-C1-C2-O2
5	D0Z0	604	GOL	O2-C2-C3-O3
5	B	601	GOL	O1-C1-C2-O2
4	B	602	A1JM9	C12-C13-C14-C15
4	B	602	A1JM9	C11-C12-C13-C14
4	B	602	A1JM9	C13-C14-C15-N20
4	B	602	A1JM9	C18-C19-C21-N22
4	B	602	A1JM9	C13-C14-C15-C16
4	B	602	A1JM9	N11-C11-C12-C13
4	D0Z0	602	A1JM9	N11-C11-C12-C13
4	D0Z0	602	A1JM9	N20-C19-C21-N22

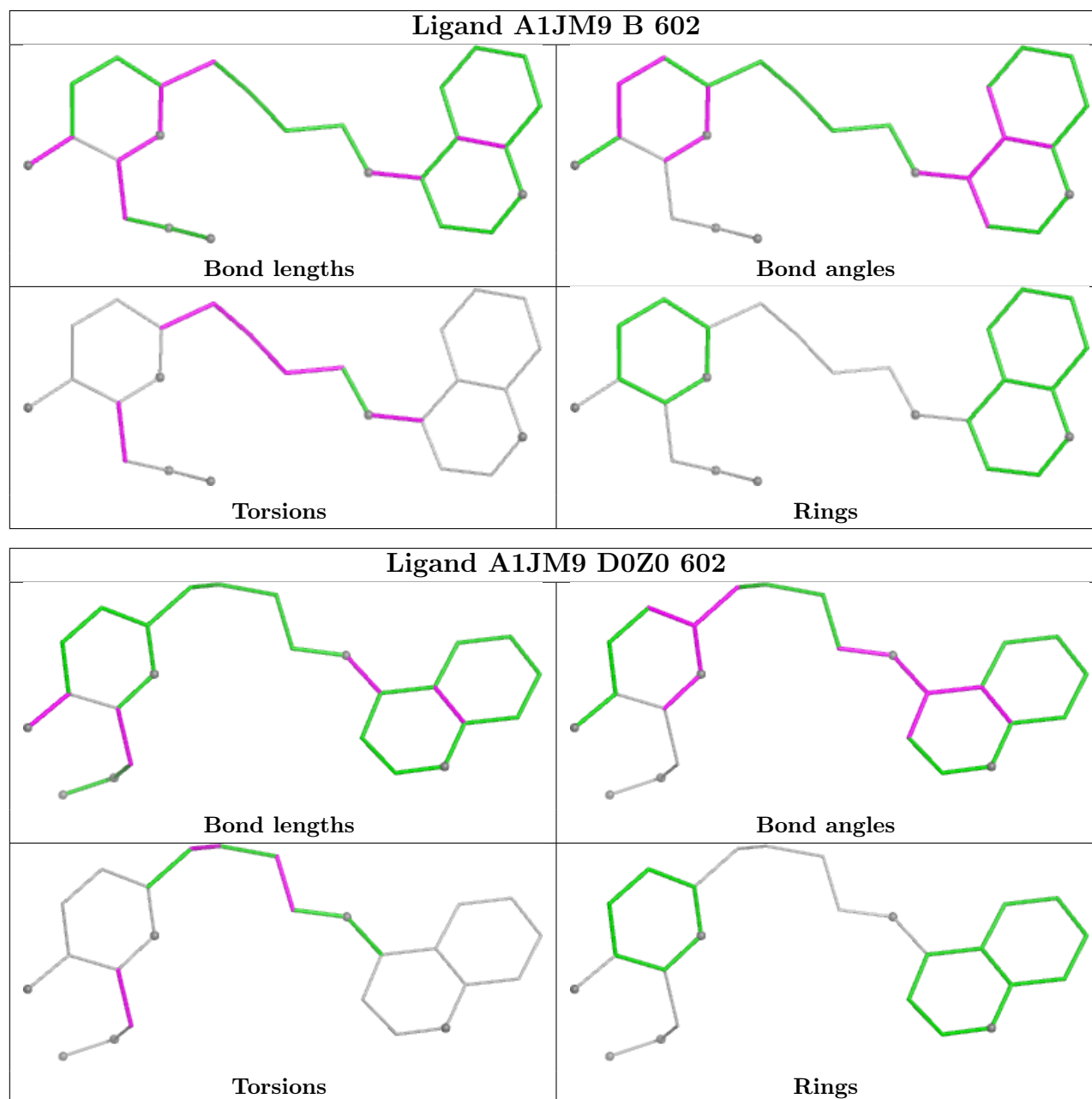
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	A1JM9	1	0
5	B	601	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	532/532 (100%)	-0.42	4 (0%) 82 80	11, 29, 46, 89	21 (3%)
1	D0Z0	532/532 (100%)	-0.43	3 (0%) 85 83	10, 29, 48, 118	21 (3%)
All	All	1064/1064 (100%)	-0.43	7 (0%) 84 81	10, 29, 47, 118	42 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D0Z0	486	HIS	3.9
1	B	486	HIS	3.0
1	D0Z0	485	PRO	2.8
1	B	362	HIS	2.8
1	D0Z0	487	SER	2.7
1	B	535	THR	2.7
1	B	485	PRO	2.5

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

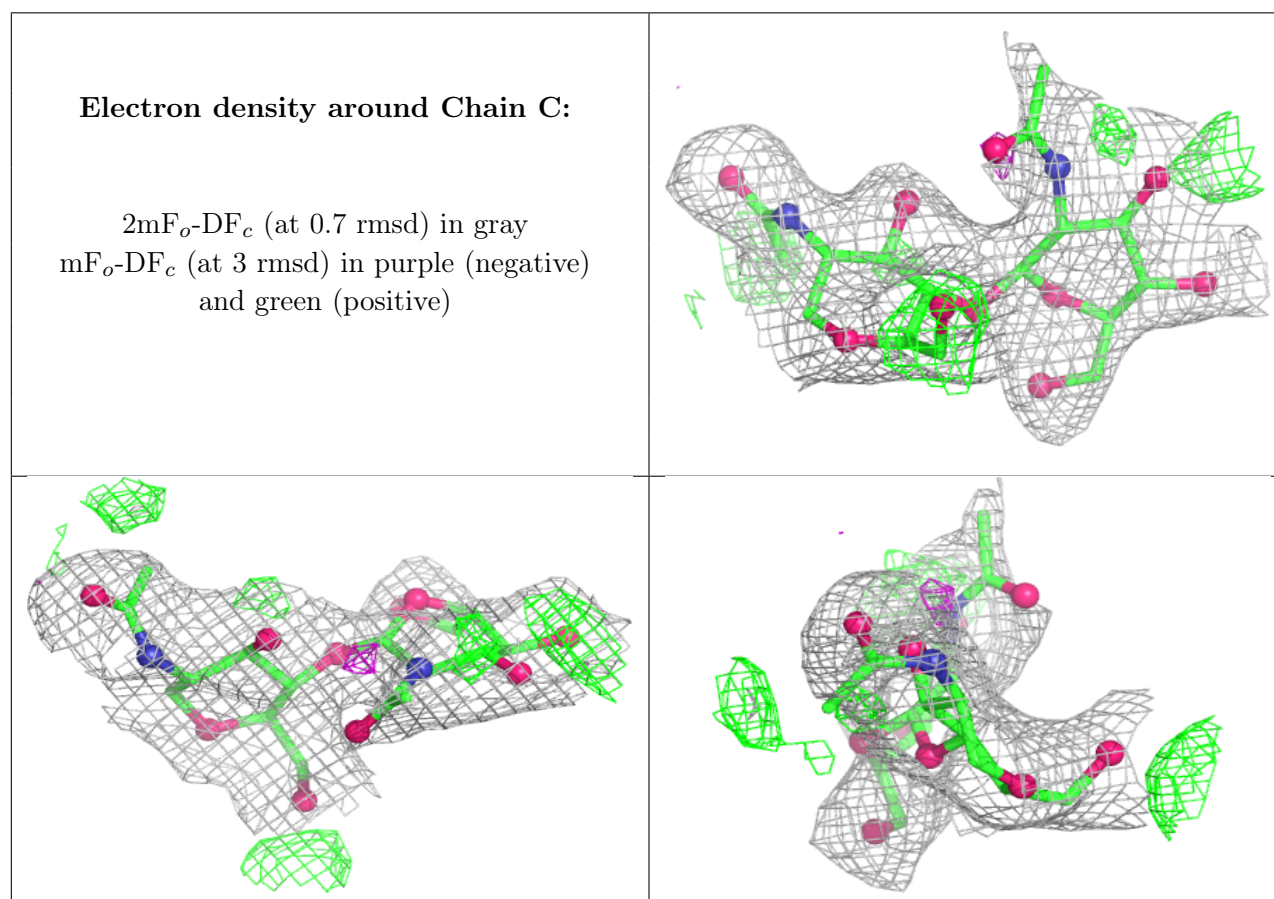
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.72	0.18	53,78,95,97	0
2	NAG	C	1	14/15	0.81	0.13	39,59,72,78	0

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



6.4 Ligands [i](#)

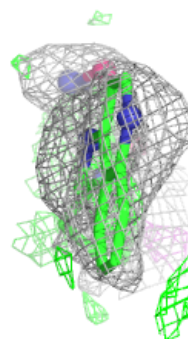
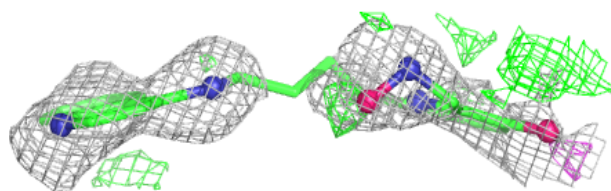
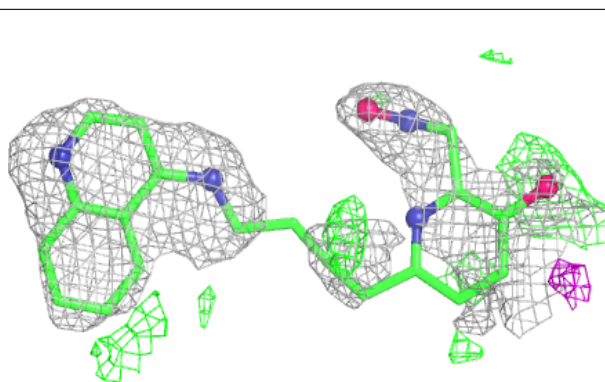
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	601	6/6	0.65	0.25	32,36,41,41	6
3	NAG	D0Z0	601	14/15	0.76	0.12	48,65,73,76	0
5	GOL	D0Z0	603	6/6	0.79	0.17	43,50,56,59	0
4	A1JM9	B	602	25/25	0.80	0.23	27,35,56,63	13
5	GOL	D0Z0	604	6/6	0.83	0.20	29,34,37,40	6
4	A1JM9	D0Z0	602	25/25	0.89	0.13	27,34,41,42	25

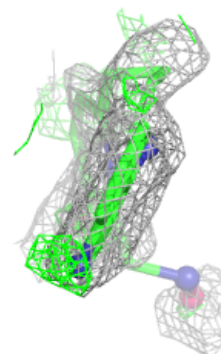
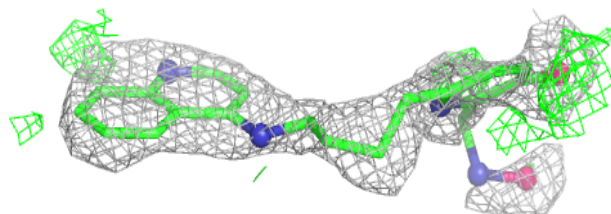
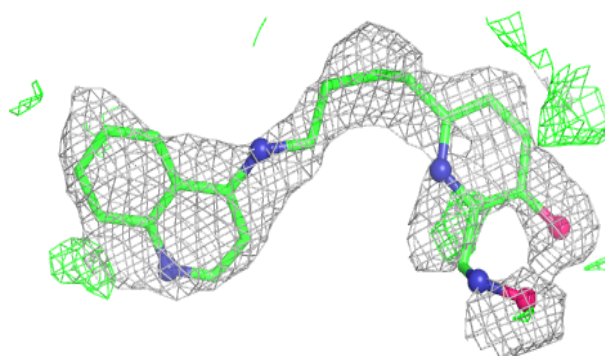
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1JM9 B 602:

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

**Electron density around A1JM9 D0Z0 602:**

$2mF_o-DF_c$ (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.