



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 AM UTC

PDB ID : 9GH7 / pdb_00009gh7
Title : Complex of human TfR1 with a potent bicyclic peptide
Authors : Pellegrino, S.; Pernigo, S.; Swan, M.K.; Bezerra, G.A.; Chen, L.
Deposited on : 2024-08-15
Resolution : 2.08 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

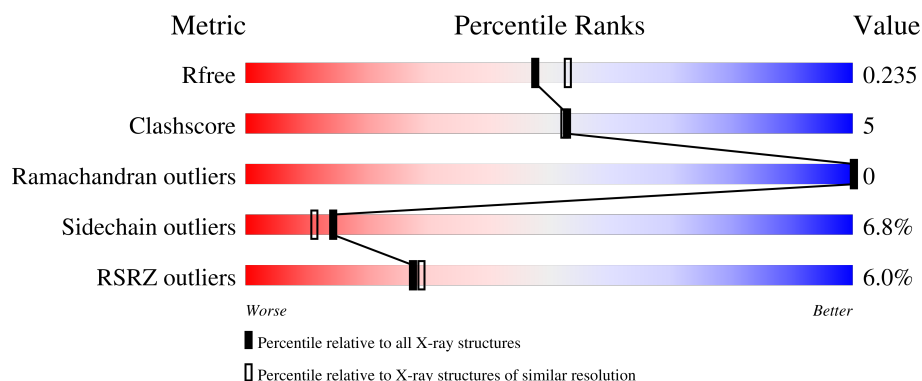
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	678	6% 78% 14% 6%
2	P	15	7% 93% 7%
3	B	2	100%
3	C	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5290 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			4998	3205	837	942	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	HIS	-	expression tag	UNP P02786
A	84	HIS	-	expression tag	UNP P02786
A	85	HIS	-	expression tag	UNP P02786
A	86	HIS	-	expression tag	UNP P02786
A	87	HIS	-	expression tag	UNP P02786
A	88	HIS	-	expression tag	UNP P02786

- Molecule 2 is a protein called Bicyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	S	0	0	0
			100	63	17	17	3			

- Molecule 3 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
3	B	2	Total	C	N	O		0	0	0
			28	16	2	10				
3	C	2	Total	C	N	O		0	0	0
			28	16	2	10				

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

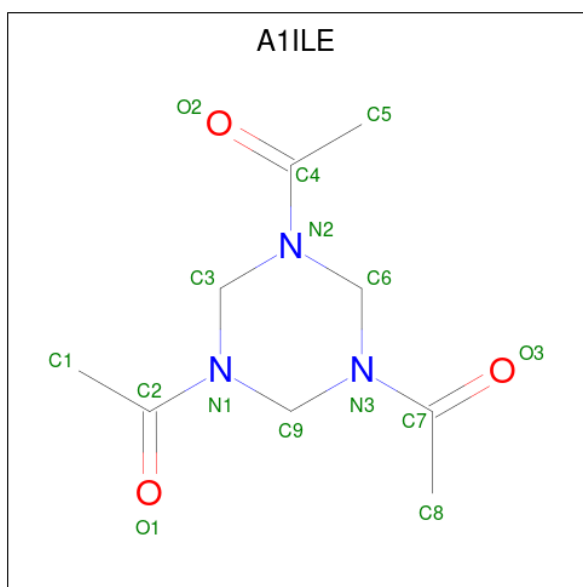
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 1-(3,5-diethanoyl-1,3,5-triazinan-1-yl)ethanone (CCD ID: A1ILE) (formula: C₉H₁₅N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	P	1	Total	C	N	O	0	0
			15	9	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	110	Total	O	0	0
			110	110		
7	P	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.95Å 94.95Å 226.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.54 – 2.08 87.54 – 2.08	Depositor EDS
% Data completeness (in resolution range)	76.4 (87.54-2.08) 76.5 (87.54-2.08)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.198 , 0.235 0.208 , 0.235	Depositor DCC
R_{free} test set	2438 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5290	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: GOL, A1ILE, CA, NAG

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	0.62	0/5118	1.16	18/6950 (0.3%)
2	P	0.65	0/104	0.97	0/143
All	All	0.62	0/5222	1.16	18/7093 (0.3%)

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	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	VAL	N-CA-CB	10.21	121.34	110.62
1	A	658	THR	CA-CB-OG1	-7.04	99.04	109.60
1	A	504	THR	CA-CB-OG1	-6.87	99.30	109.60
1	A	753	VAL	CB-CA-C	-6.86	102.92	111.70
1	A	297	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	512	ASN	CB-CA-C	5.98	119.08	109.27
1	A	164	ASN	CB-CA-C	-5.79	101.18	110.79
1	A	495	LYS	CB-CA-C	5.74	119.87	109.37
1	A	531	LYS	CB-CA-C	-5.71	100.91	110.56
1	A	203	VAL	N-CA-CB	-5.67	102.39	111.58
1	A	251	ASN	CB-CA-C	5.63	116.72	109.80
1	A	362	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	729	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	697	PHE	N-CA-CB	-5.42	103.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	PHE	N-CA-CB	5.42	117.92	110.07
1	A	211	TYR	N-CA-CB	-5.34	101.46	110.49
1	A	536	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	531	LYS	N-CA-CB	5.03	117.91	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	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	4998	0	4888	51	0
2	P	100	0	89	0	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
6	P	15	0	0	1	0
7	A	110	0	0	2	0
7	P	4	0	0	0	0
All	All	5290	0	5035	51	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 (51) 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:249:PRO:HA	7:A:949:HOH:O	1.71	0.89
1:A:721:GLN:HE21	1:A:723:ASN:HB2	1.41	0.84
1:A:515:HIS:HD2	1:A:517:VAL:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:NH1	1:A:601:LEU:O	2.29	0.65
1:A:721:GLN:HG3	1:A:723:ASN:HD22	1.63	0.63
1:A:626:ASN:OD1	1:A:643:TYR:OH	2.13	0.62
1:A:561:THR:HG22	1:A:562:ASP:O	2.01	0.61
1:A:699:HIS:HD2	1:A:701:PHE:H	1.49	0.61
1:A:234:HIS:HD2	1:A:236:ASN:H	1.51	0.58
1:A:515:HIS:CD2	1:A:516:PRO:HD2	2.39	0.57
1:A:359:THR:HG22	1:A:360:ASP:H	1.71	0.55
1:A:397:VAL:HB	1:A:445:SER:HB3	1.90	0.54
1:A:514:LYS:HD2	1:A:519:GLY:O	2.09	0.53
1:A:588:ARG:HG3	1:A:588:ARG:HH11	1.74	0.53
1:A:428:LYS:HA	1:A:428:LYS:HE2	1.91	0.52
1:A:539:ASN:HD22	1:A:541:ALA:H	1.57	0.52
1:A:524:GLN:NE2	1:A:524:GLN:HA	2.26	0.50
1:A:201:ILE:HG22	1:A:212:LEU:HD12	1.92	0.50
1:A:446:ARG:NH2	1:A:604:ASP:O	2.45	0.50
1:A:623:ARG:HG2	1:A:623:ARG:HH21	1.78	0.49
1:A:682:GLU:OE2	1:A:699:HIS:HE1	1.95	0.49
1:A:623:ARG:NH2	1:A:624:ASP:OD1	2.42	0.48
1:A:250:VAL:O	1:A:251:ASN:C	2.57	0.48
1:A:515:HIS:HB3	1:A:518:THR:HG23	1.95	0.48
1:A:667:ASP:CG	1:A:670:VAL:HG13	2.39	0.47
1:A:313:PHE:HB2	1:A:314:PRO:HD2	1.95	0.47
1:A:440:ASP:N	1:A:440:ASP:OD1	2.45	0.47
1:A:293:ALA:HB2	1:A:339:ARG:NH2	2.29	0.47
1:A:134:LYS:NZ	1:A:440:ASP:OD2	2.49	0.46
1:A:249:PRO:CA	7:A:949:HOH:O	2.45	0.46
1:A:721:GLN:NE2	1:A:723:ASN:HB2	2.19	0.46
1:A:699:HIS:CD2	1:A:701:PHE:H	2.32	0.45
1:A:147:LEU:CD2	1:A:165:LEU:HD11	2.47	0.44
1:A:607:LEU:O	1:A:608:ASN:HB2	2.19	0.43
1:A:563:TYR:HD1	1:A:566:LEU:HD13	1.83	0.43
1:A:214:GLU:OE2	1:A:338:SER:OG	2.33	0.42
1:A:210:VAL:O	1:A:211:TYR:HB2	2.20	0.42
1:A:550:ILE:O	1:A:551:PRO:C	2.62	0.42
1:A:413:GLY:HA2	6:P:101:A1ILE:O1	2.20	0.42
1:A:525:ASP:OD1	1:A:525:ASP:C	2.62	0.42
1:A:133:GLU:O	1:A:134:LYS:C	2.63	0.42
1:A:491:THR:O	1:A:515:HIS:CE1	2.73	0.42
1:A:353:CYS:O	1:A:354:PRO:C	2.63	0.41
1:A:314:PRO:HA	1:A:465:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD22	1:A:165:LEU:HD11	2.02	0.41
1:A:232:LEU:HB3	1:A:367:THR:HG23	2.03	0.41
1:A:211:TYR:OH	1:A:344:LYS:HG2	2.20	0.41
1:A:234:HIS:HE1	1:A:282:TYR:OH	2.04	0.41
1:A:582:GLU:O	1:A:583:LEU:C	2.62	0.41
1:A:234:HIS:CD2	1:A:236:ASN:H	2.33	0.41
1:A:402:TYR:HB3	1:A:447:SER:HB2	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	634/678 (94%)	609 (96%)	25 (4%)	0	100	100
2	P	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
All	All	646/693 (93%)	620 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	537/580 (93%)	500 (93%)	37 (7%)	14	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	11/11 (100%)	11 (100%)	0	100	100
All	All	548/591 (93%)	511 (93%)	37 (7%)	14	11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LYS
1	A	132	SER
1	A	148	ASN
1	A	177	LYS
1	A	200	VAL
1	A	203	VAL
1	A	248	THR
1	A	274	LEU
1	A	331	ASN
1	A	359	THR
1	A	360	ASP
1	A	367	THR
1	A	373	VAL
1	A	377	VAL
1	A	426	LEU
1	A	429	LEU
1	A	438	LEU
1	A	440	ASP
1	A	445	SER
1	A	489	LEU
1	A	495	LYS
1	A	518	THR
1	A	526	SER
1	A	539	ASN
1	A	566	LEU
1	A	585	LYS
1	A	588	ARG
1	A	618	LEU
1	A	633	LYS
1	A	670	VAL
1	A	677	ARG
1	A	695	SER
1	A	709	LEU
1	A	714	GLU
1	A	719	ARG
1	A	721	GLN

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Mol	Chain	Res	Type
1	A	753	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS
1	A	215	ASN
1	A	234	HIS
1	A	285	GLN
1	A	443	GLN
1	A	483	ASN
1	A	515	HIS
1	A	524	GLN
1	A	539	ASN
1	A	603	HIS
1	A	627	GLN
1	A	699	HIS
1	A	721	GLN
1	A	722	ASN
1	A	723	ASN

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 ⓘ

4 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
3	NAG	B	1	3,1	14,14,15	0.32	0	17,19,21	1.13	1 (5%)
3	NAG	B	2	3	14,14,15	0.47	0	17,19,21	2.06	2 (11%)
3	NAG	C	1	3,1	14,14,15	0.43	0	17,19,21	0.81	0
3	NAG	C	2	3	14,14,15	0.51	0	17,19,21	0.92	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C2-N2-C7	6.80	132.02	122.90
3	B	2	NAG	C1-C2-N2	-3.88	104.32	110.43
3	B	1	NAG	C2-N2-C7	3.31	127.33	122.90
3	C	2	NAG	C1-C2-N2	2.15	113.82	110.43

There are no chirality outliers.

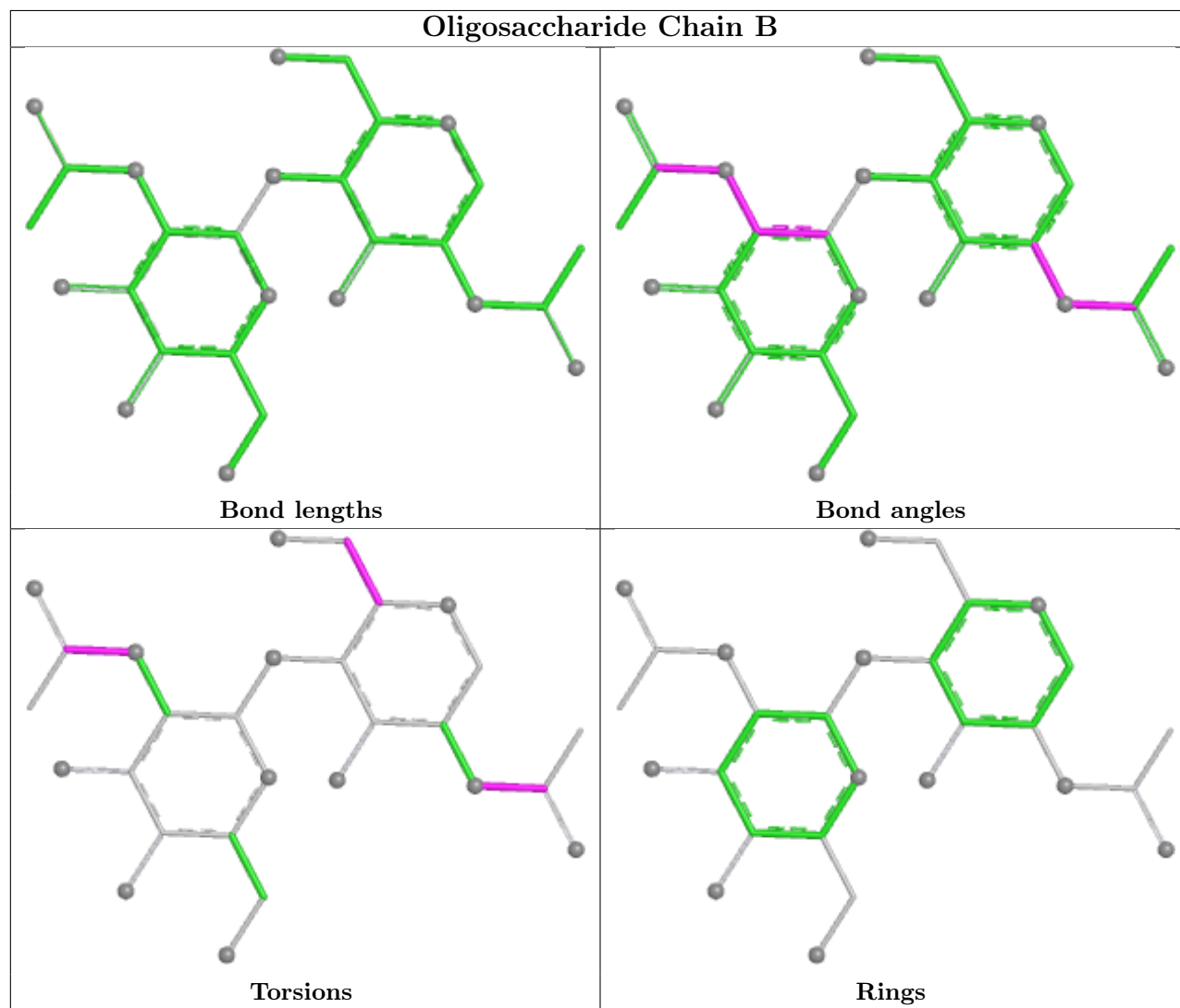
All (10) torsion outliers are listed below:

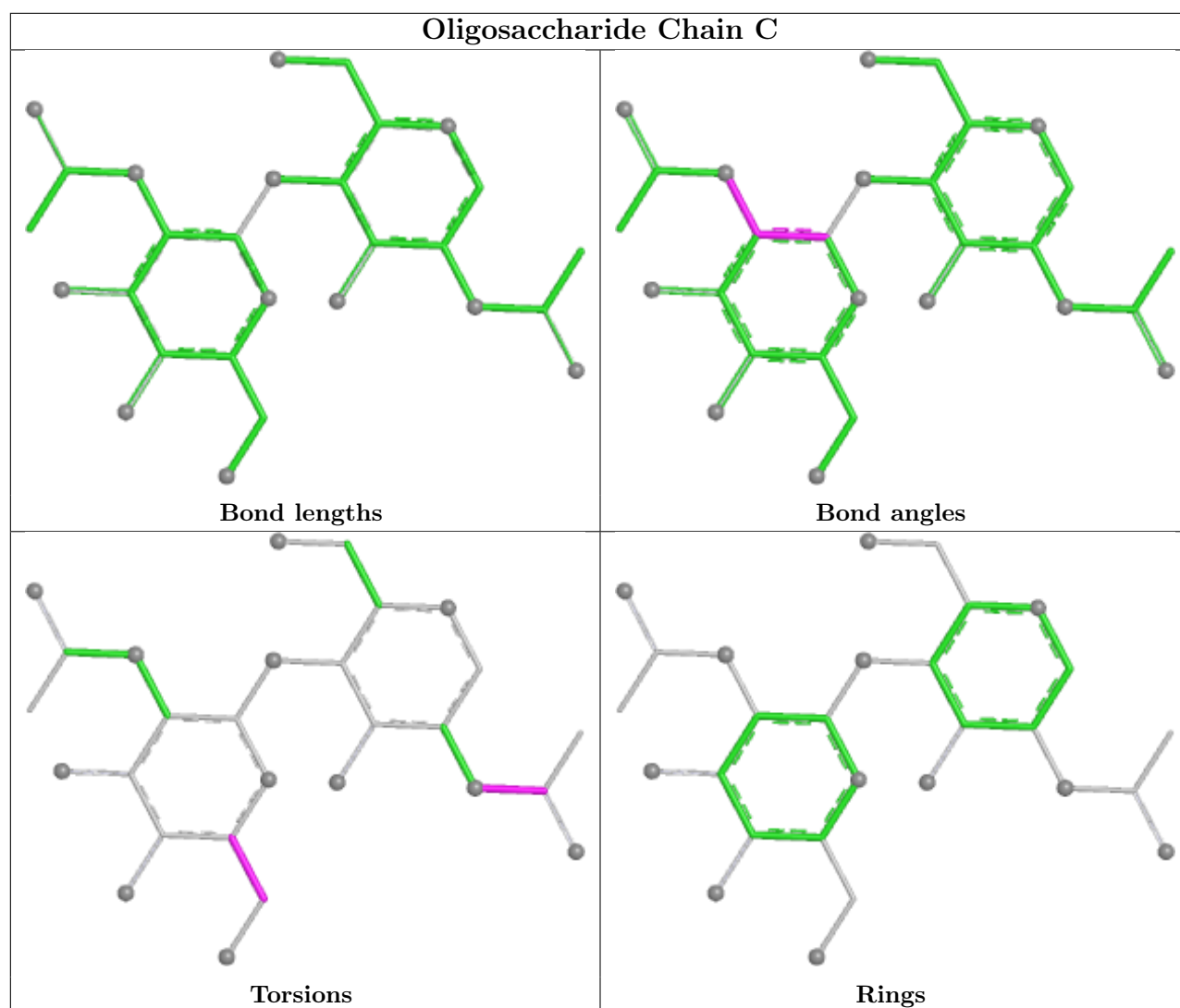
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	A1ILE	P	101	2	15,15,15	0.49	0	21,21,21	0.77	0
5	GOL	A	802	-	5,5,5	0.17	0	5,5,5	0.51	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
6	A1ILE	P	101	2	-	0/12/24/24	0/0/1/1
5	GOL	A	802	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

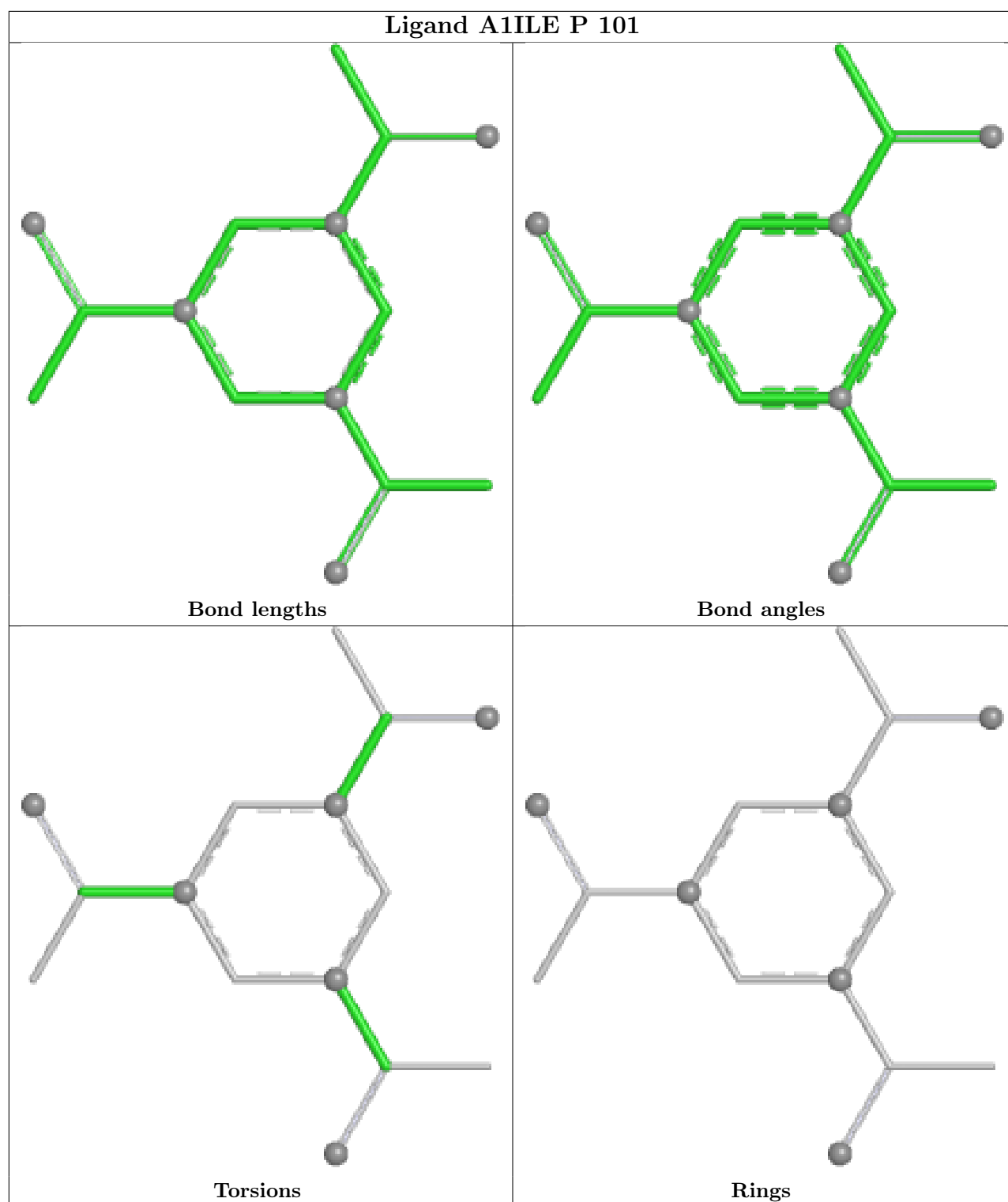
Mol	Chain	Res	Type	Atoms
5	A	802	GOL	O1-C1-C2-O2
5	A	802	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	101	A1ILE	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 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 ⓘ

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	636/678 (93%)	0.52	38 (5%) 27 29	33, 51, 81, 118	0
2	P	14/15 (93%)	0.80	1 (7%) 22 23	45, 52, 72, 84	0
All	All	650/693 (93%)	0.52	39 (6%) 27 29	33, 51, 81, 118	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	TYR	5.2
1	A	669	PHE	5.0
1	A	211	TYR	4.1
1	A	359	THR	3.9
1	A	197	GLN	3.6
1	A	210	VAL	3.5
1	A	248	THR	3.0
1	A	291	VAL	3.0
1	A	721	GLN	3.0
2	P	0	ALA	2.9
1	A	208	ARG	2.8
1	A	725	ALA	2.8
1	A	286	THR	2.7
1	A	643	TYR	2.5
1	A	603	HIS	2.5
1	A	344	LYS	2.5
1	A	526	SER	2.5
1	A	439	LYS	2.5
1	A	495	LYS	2.5
1	A	351	GLY	2.5
1	A	724	GLY	2.5
1	A	201	ILE	2.5
1	A	370	SER	2.4
1	A	438	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	129	ARG	2.4
1	A	130	LYS	2.3
1	A	561	THR	2.3
1	A	577	ILE	2.2
1	A	148	ASN	2.2
1	A	253	SER	2.2
1	A	209	LEU	2.2
1	A	378	SER	2.2
1	A	368	SER	2.1
1	A	205	LYS	2.1
1	A	714	GLU	2.1
1	A	207	GLY	2.1
1	A	213	VAL	2.1
1	A	327	SER	2.1
1	A	668	ARG	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](#)

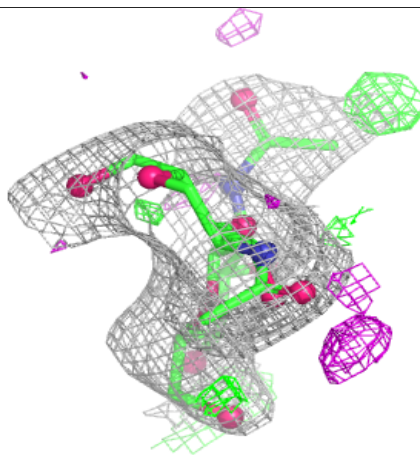
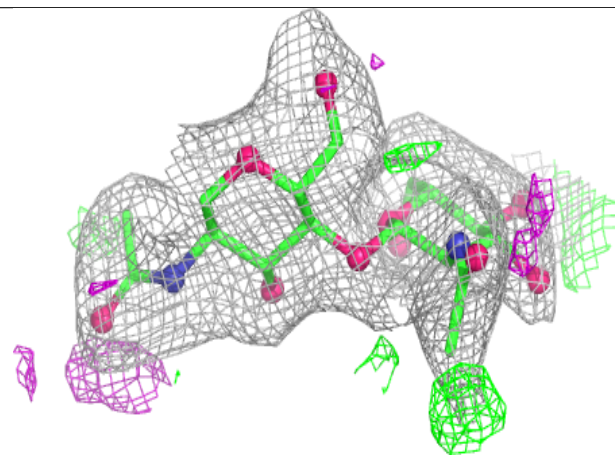
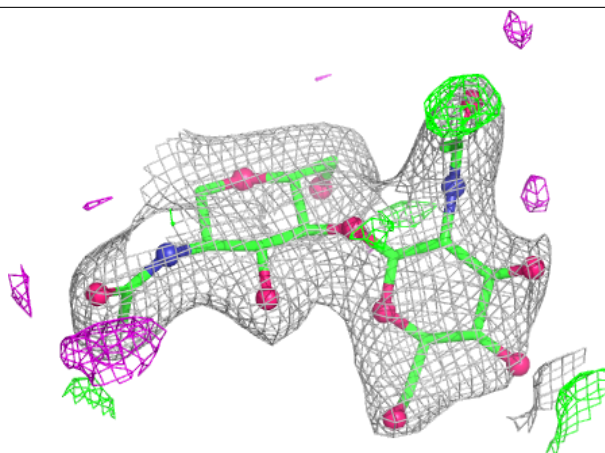
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

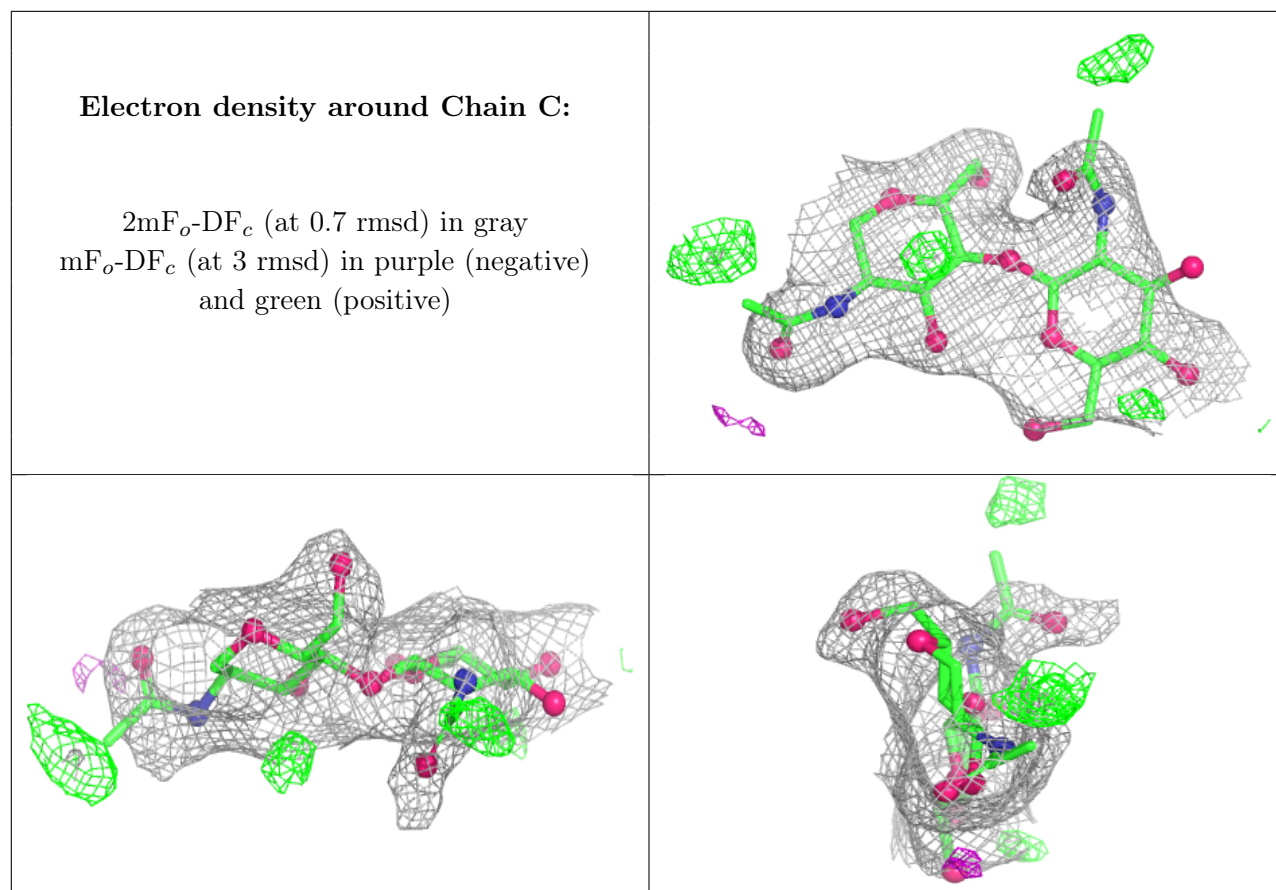
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	47,56,62,69	0
3	NAG	B	2	14/15	-	-	58,77,91,104	0
3	NAG	C	2	14/15	0.75	0.16	79,97,102,104	0
3	NAG	C	1	14/15	0.87	0.12	60,69,84,84	0

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.

Electron density around Chain B:

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





6.4 Ligands [i](#)

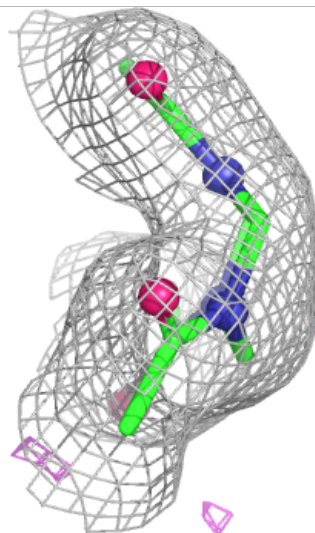
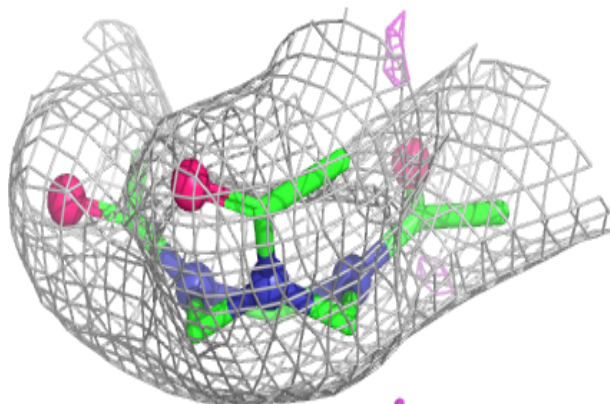
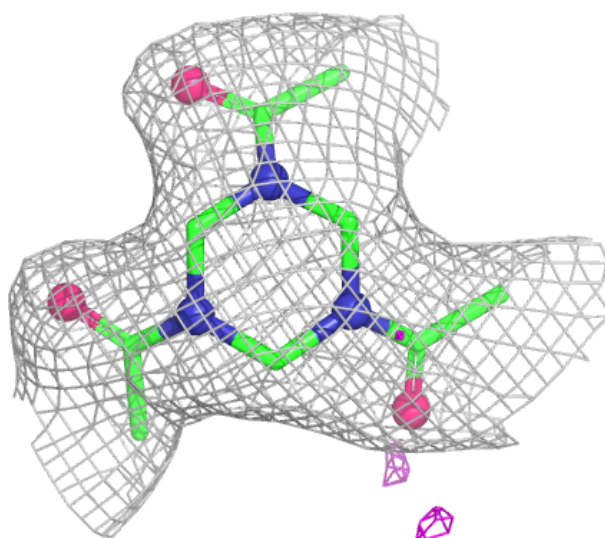
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	802	6/6	0.92	0.12	59,75,78,79	0
6	A1ILE	P	101	15/15	0.95	0.08	43,52,64,68	0
4	CA	A	801	1/1	1.00	0.02	37,37,37,37	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 A1ILE P 101:

$2mF_o-DF_c$ (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.