



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:01 AM BST

PDB ID : 6F9T
Title : Crystal structure of human testis Angiotensin-1 converting enzyme in complex with Sampatrilat.
Authors : Cozier, G.E.; Acharya, K.R.
Deposited on : 2017-12-15
Resolution : 1.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

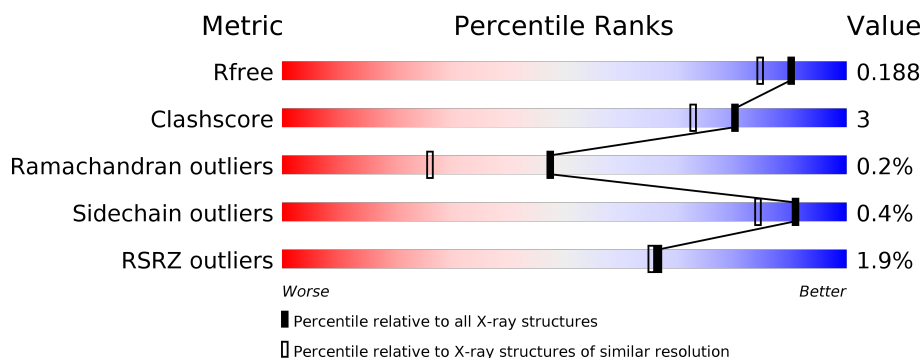
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	591	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	B	2	<div> <div></div> <div>100%</div> </div>
3	C	8	<div> <div>38%</div> <div>63%</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10715 atoms, of which 4921 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	586	9577	3117	4696	833	907	24	0	20	0

There are 5 discrepancies between the modelled and reference sequences:

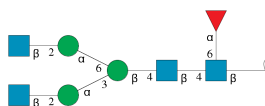
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLY	GLU	conflict	UNP P12821
A	90	GLN	ASN	conflict	UNP P12821
A	155	GLN	ASN	conflict	UNP P12821
A	337	GLN	ASN	conflict	UNP P12821
A	586	GLN	ASN	conflict	UNP P12821

- 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
			Total	C	H	N	O			
2	B	2	53	16	25	2	10	0	0	0

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

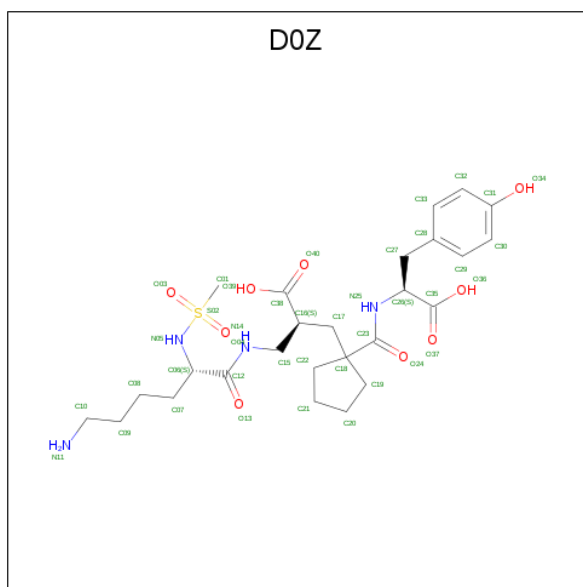


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	H	N	O	0	0	0
			186	56	87	4	39			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is Sampatrilat (three-letter code: D0Z) (formula: C₂₆H₄₀N₄O₉S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	0	0
			78	26	38	4	9	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

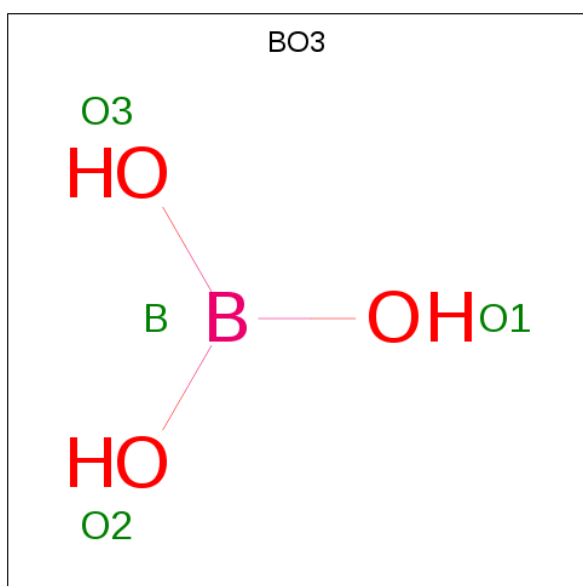
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cl	0	0
			2	2		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	N	0	0
			10	3	5	2		
7	A	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 8 is BORIC ACID (three-letter code: BO3) (formula: BH_3O_3).



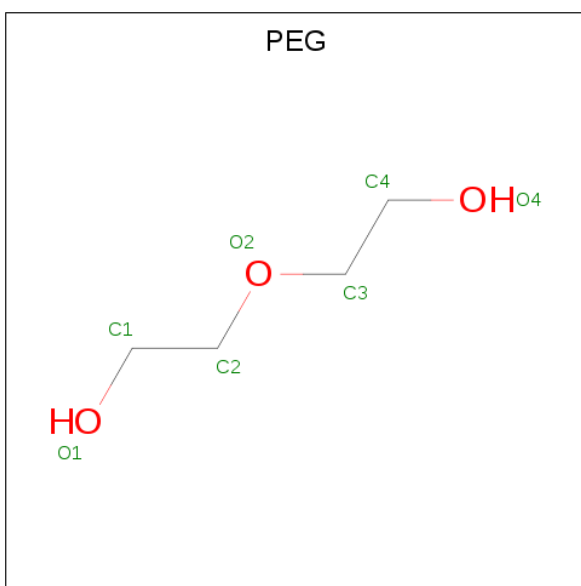
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	B	H	O	0	0
			7	1	3	3		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



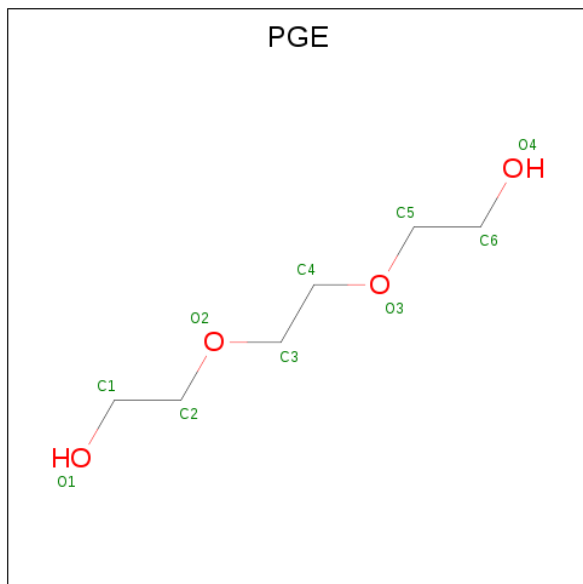
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			17	4	10	3		
10	A	1	Total	C	H	O	0	0
			17	4	10	3		
10	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

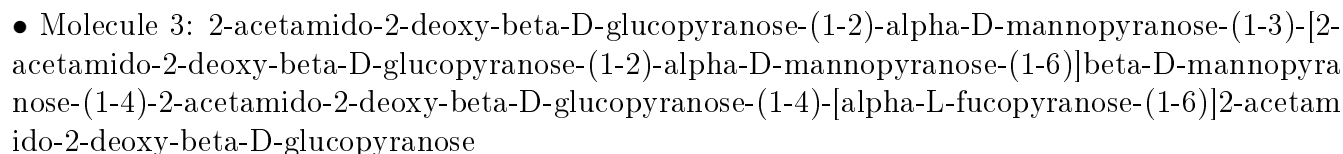
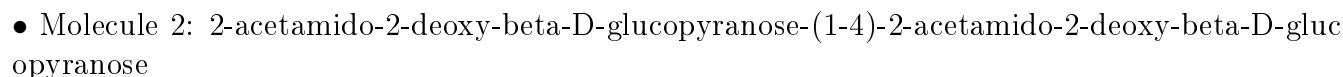


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	678	Total	O	0	9
			686	686		

- Molecule 1: Angiotensin-converting enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.10Å 84.76Å 133.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.63 – 1.60 71.63 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (71.63-1.60) 98.8 (71.63-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.165 , 0.187 0.165 , 0.188	Depositor DCC
R_{free} test set	2215 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10715	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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, PGE, NAG, CL, BO3, D0Z, EDO, BMA, FUC, IMD, CSO, PEG, MAN

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	0.47	0/5080	0.62	0/6905

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4881	4696	4619	22	0
2	B	28	25	25	0	0
3	C	99	87	85	0	0
4	A	1	0	0	0	0
5	A	40	38	0	2	0
6	A	2	0	0	0	0
7	A	10	10	10	1	0
8	A	4	3	3	0	0
9	A	12	18	18	0	0
10	A	21	30	30	5	0
11	A	10	14	14	0	0
12	A	686	0	0	11	1
All	All	5794	4921	4804	27	1

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 3.

All (27) 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:624:ASN:ND2	12:A:802:HOH:O	2.22	0.70
1:A:239:GLU:OE2	12:A:801:HOH:O	2.10	0.69
5:A:712:D0Z:N11	12:A:805:HOH:O	2.29	0.64
1:A:617:PRO:HD2	12:A:997:HOH:O	2.03	0.58
1:A:496:CSO:OD	1:A:623:PRO:HD3	2.07	0.55
10:A:721:PEG:H32	12:A:1198:HOH:O	2.10	0.51
1:A:496:CSO:OD	1:A:623:PRO:CD	2.59	0.50
1:A:282[B]:THR:HG23	12:A:1152:HOH:O	2.12	0.50
1:A:593:LEU:HD22	12:A:1422:HOH:O	2.13	0.49
1:A:179:LEU:HD11	1:A:499:VAL:HG23	1.94	0.49
5:A:712:D0Z:C22	5:A:712:D0Z:C38	2.93	0.46
1:A:618:GLN:HG3	1:A:621:TRP:HB2	1.97	0.46
1:A:86:MET:O	1:A:90:GLN:HG3	2.16	0.45
1:A:511:LYS:O	1:A:515:PRO:HD2	2.17	0.45
1:A:313:ARG:HG3	12:A:1249:HOH:O	2.17	0.45
1:A:353:HIS:CG	10:A:722:PEG:H22	2.52	0.44
1:A:85:ASN:O	1:A:88:ILE:HG22	2.17	0.44
1:A:546:PRO:HG2	10:A:723:PEG:H42	2.01	0.43
1:A:411:GLU:HB2	1:A:526:SER:HB2	2.02	0.42
10:A:722:PEG:C4	12:A:836:HOH:O	2.68	0.42
1:A:462:TYR:O	1:A:466:GLN:HG2	2.21	0.41
1:A:507:ASP:N	1:A:508:PRO:CD	2.83	0.41
1:A:485:TRP:CD2	1:A:508:PRO:HG3	2.55	0.41
1:A:372:THR:HG23	12:A:974:HOH:O	2.20	0.41
1:A:443:ASP:OD2	10:A:723:PEG:H41	2.22	0.40
7:A:716:IMD:H2	12:A:989:HOH:O	2.22	0.40
1:A:104:VAL:HG13	1:A:113:LYS:CG	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1051:HOH:O	12:A:1062:HOH:O[1_655]	2.15	0.05

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	604/591 (102%)	595 (98%)	8 (1%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	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	530/514 (103%)	528 (100%)	2 (0%)	91 84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	TYR
1	A	394	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSO	A	496	1	3,6,7	0.71	0	0,6,8	0.00	-

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
1	CSO	A	496	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	496	CSO	2	0

5.5 Carbohydrates ⓘ

10 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	1,2	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
2	NAG	B	2	2	14,14,15	0.31	0	17,19,21	0.82	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	C	2	3	14,14,15	0.75	1 (7%)	17,19,21	0.44	0
3	BMA	C	3	3	11,11,12	0.92	0	15,15,17	1.00	0
3	MAN	C	4	3	11,11,12	0.87	1 (9%)	15,15,17	1.88	2 (13%)
3	NAG	C	5	3	14,14,15	0.17	0	17,19,21	0.74	1 (5%)
3	MAN	C	6	3	11,11,12	1.07	0	15,15,17	1.08	1 (6%)
3	NAG	C	7	3	14,14,15	0.29	0	17,19,21	0.40	0
3	FUC	C	8	3	10,10,11	0.77	1 (10%)	14,14,16	0.65	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	4/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	NAG	C	7	3	-	0/6/23/26	0/1/1/1
3	FUC	C	8	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	-2.75	1.39	1.43
3	C	4	MAN	C1-C2	2.17	1.57	1.52
3	C	8	FUC	O5-C1	-2.07	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	5.14	119.15	112.19
3	C	4	MAN	O2-C2-C3	-4.54	101.05	110.14
2	B	1	NAG	C1-O5-C5	2.67	115.80	112.19
3	C	6	MAN	O2-C2-C3	-2.48	105.18	110.14
3	C	5	NAG	C1-O5-C5	2.27	115.27	112.19
2	B	2	NAG	C1-O5-C5	2.27	115.27	112.19

There are no chirality outliers.

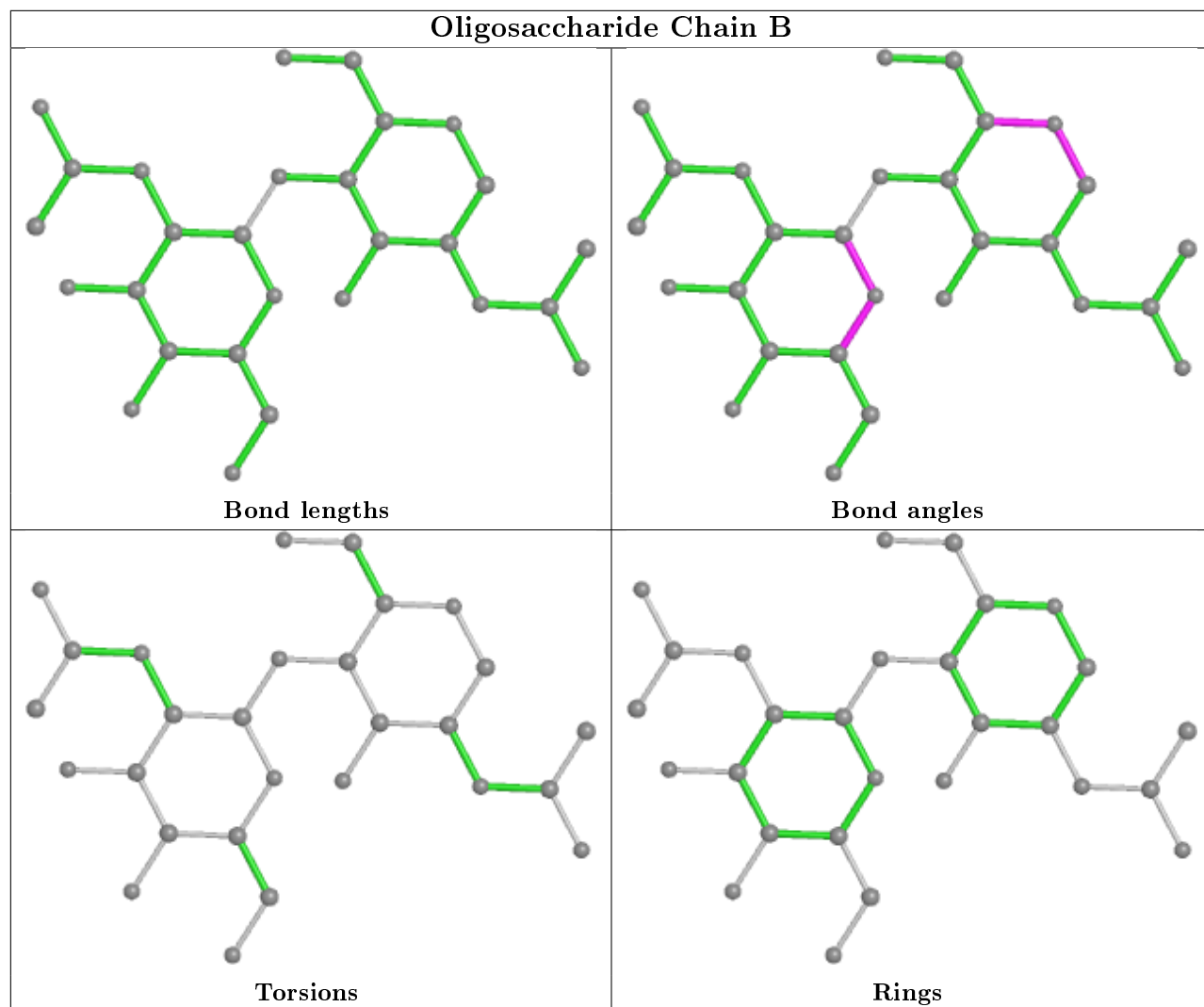
All (6) torsion outliers are listed below:

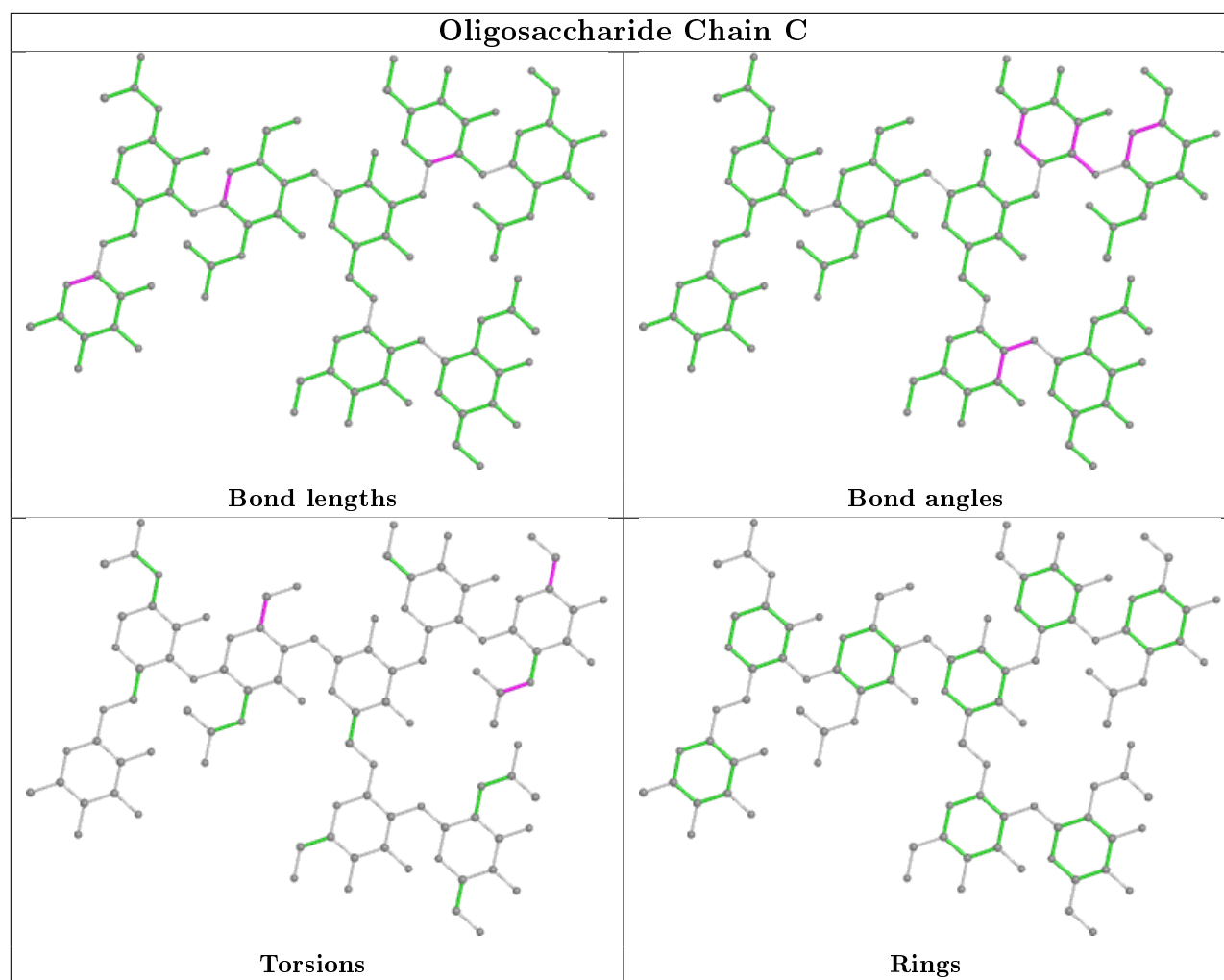
Mol	Chain	Res	Type	Atoms
3	C	5	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	5	NAG	C8-C7-N2-C2
3	C	5	NAG	O7-C7-N2-C2
3	C	5	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

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 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\# Z > 2$
5	D0Z	A	712	4	33,41,41	2.40	9 (27%)	40,57,57	1.56	8 (20%)
7	IMD	A	716	-	3,5,5	0.36	0	4,5,5	0.54	0
10	PEG	A	721	-	6,6,6	0.55	0	5,5,5	0.33	0
7	IMD	A	715	-	3,5,5	0.48	0	4,5,5	0.70	0
9	EDO	A	719	-	3,3,3	0.46	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PEG	A	723	-	6,6,6	0.50	0	5,5,5	0.21	0
10	PEG	A	722	-	6,6,6	0.49	0	5,5,5	0.42	0
8	BO3	A	717	-	3,3,3	0.22	0	3,3,3	0.09	0
11	PGE	A	724	-	9,9,9	0.36	0	8,8,8	0.48	0
9	EDO	A	718	-	3,3,3	0.44	0	2,2,2	0.33	0
9	EDO	A	720	-	3,3,3	0.50	0	2,2,2	0.25	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
5	D0Z	A	712	4	-	6/38/55/55	0/2/2/2
7	IMD	A	716	-	-	-	0/1/1/1
10	PEG	A	721	-	-	1/4/4/4	-
7	IMD	A	715	-	-	-	0/1/1/1
9	EDO	A	719	-	-	1/1/1/1	-
10	PEG	A	723	-	-	3/4/4/4	-
10	PEG	A	722	-	-	3/4/4/4	-
11	PGE	A	724	-	-	1/7/7/7	-
9	EDO	A	718	-	-	1/1/1/1	-
9	EDO	A	720	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	712	D0Z	C19-C18	6.33	1.68	1.54
5	A	712	D0Z	C22-C18	-6.23	1.41	1.54
5	A	712	D0Z	C12-N14	5.36	1.45	1.33
5	A	712	D0Z	C23-N25	5.09	1.44	1.34
5	A	712	D0Z	C19-C20	-3.56	1.40	1.52
5	A	712	D0Z	S02-N05	3.13	1.68	1.62
5	A	712	D0Z	O13-C12	-2.75	1.17	1.23
5	A	712	D0Z	C22-C21	2.51	1.60	1.52
5	A	712	D0Z	C01-S02	2.35	1.81	1.75

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	712	D0Z	O04-S02-O03	-5.13	111.47	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	712	D0Z	O03-S02-C01	3.54	113.96	108.28
5	A	712	D0Z	C16-C15-N14	-2.89	108.69	112.55
5	A	712	D0Z	C22-C18-C19	2.61	105.60	102.35
5	A	712	D0Z	C21-C22-C18	2.48	107.98	105.00
5	A	712	D0Z	C22-C21-C20	-2.48	99.13	105.79
5	A	712	D0Z	C07-C06-C12	-2.35	104.70	110.20
5	A	712	D0Z	C33-C28-C29	2.11	121.48	118.17

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	712	D0Z	C19-C18-C23-O24
5	A	712	D0Z	C22-C18-C23-O24
10	A	722	PEG	C4-C3-O2-C2
11	A	724	PGE	C3-C4-O3-C5
10	A	723	PEG	O2-C3-C4-O4
10	A	723	PEG	O1-C1-C2-O2
9	A	718	EDO	O1-C1-C2-O2
9	A	720	EDO	O1-C1-C2-O2
10	A	722	PEG	O1-C1-C2-O2
9	A	719	EDO	O1-C1-C2-O2
5	A	712	D0Z	C19-C18-C23-N25
5	A	712	D0Z	C22-C18-C23-N25
10	A	721	PEG	O2-C3-C4-O4
5	A	712	D0Z	N25-C26-C27-C28
10	A	722	PEG	O2-C3-C4-O4
5	A	712	D0Z	C17-C18-C23-O24
10	A	723	PEG	C4-C3-O2-C2

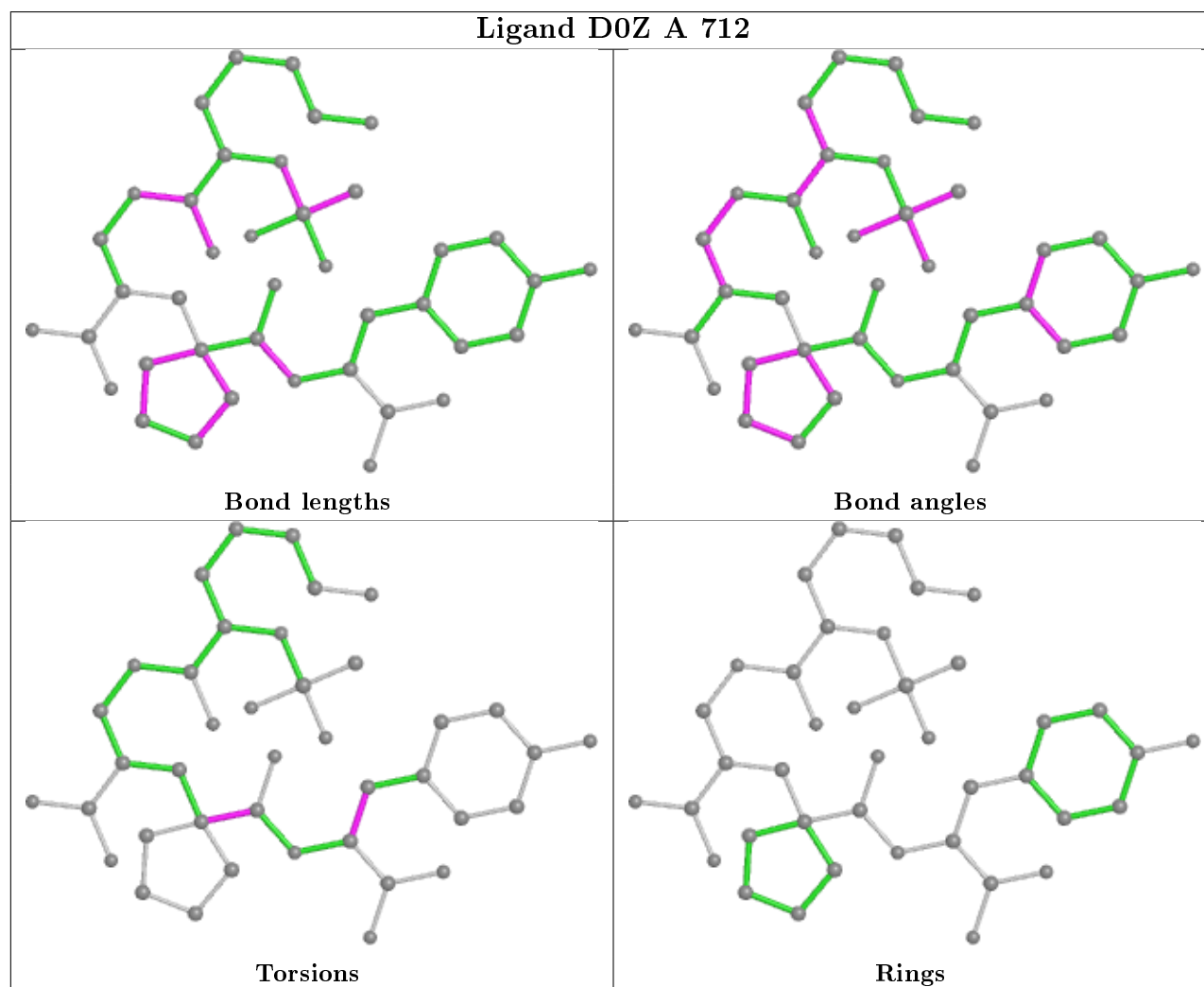
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	712	D0Z	2	0
7	A	716	IMD	1	0
10	A	721	PEG	1	0
10	A	723	PEG	2	0
10	A	722	PEG	2	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 [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	A	585/591 (98%)	-0.30	11 (1%) 66 65	9, 18, 40, 67	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	TRP	4.5
1	A	619	TYR	4.0
1	A	623	PRO	3.6
1	A	437	GLY	3.2
1	A	625	SER	3.2
1	A	622	THR	3.1
1	A	155	GLN	2.9
1	A	624	ASN	2.8
1	A	438	GLY	2.7
1	A	617	PRO	2.6
1	A	618	GLN	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	496	7/8	0.99	0.07	9,13,17,19	0

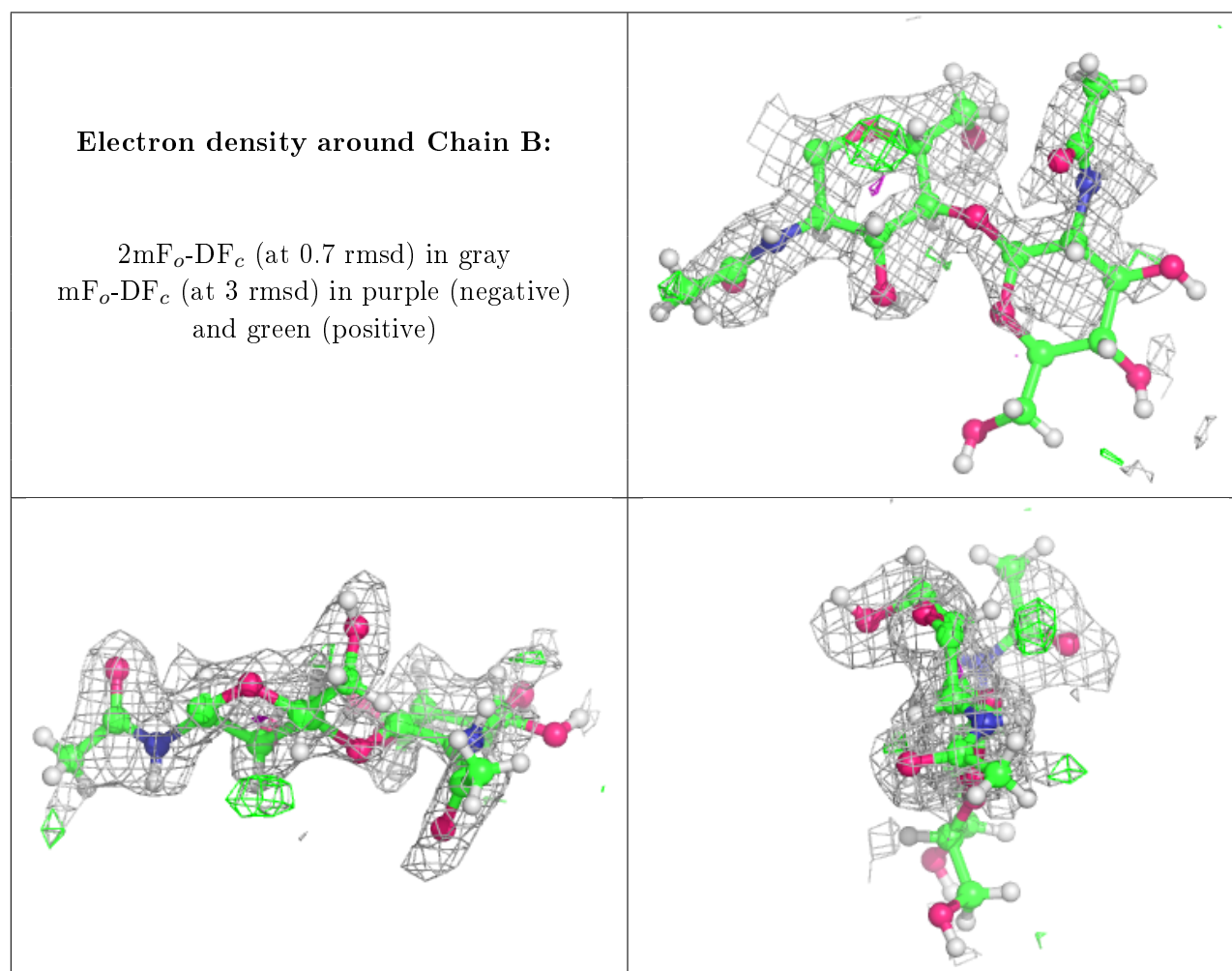
6.3 Carbohydrates [i](#)

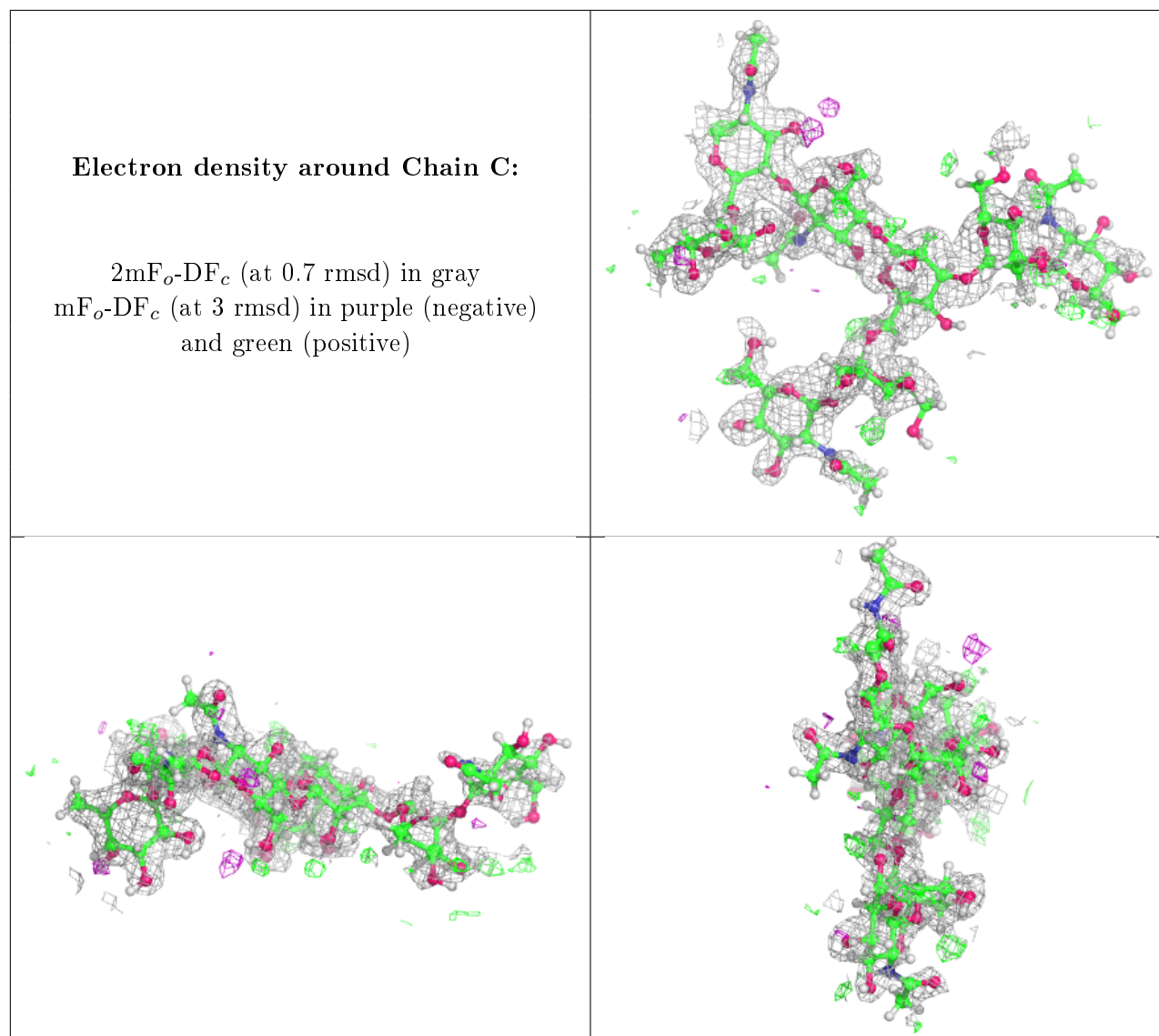
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	B	2	14/15	0.62	0.28	59,80,107,120	0
3	MAN	C	6	11/12	0.71	0.18	42,61,77,81	0
3	BMA	C	3	11/12	0.76	0.15	48,59,75,90	0
2	NAG	B	1	14/15	0.76	0.14	45,59,73,76	0
3	NAG	C	5	14/15	0.76	0.27	74,89,99,101	0
3	NAG	C	7	14/15	0.79	0.17	27,46,54,60	28
3	MAN	C	4	11/12	0.80	0.21	58,83,104,104	0
3	FUC	C	8	10/11	0.89	0.12	28,41,50,52	0
3	NAG	C	2	14/15	0.90	0.12	29,41,61,70	0
3	NAG	C	1	14/15	0.92	0.08	25,36,49,49	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.

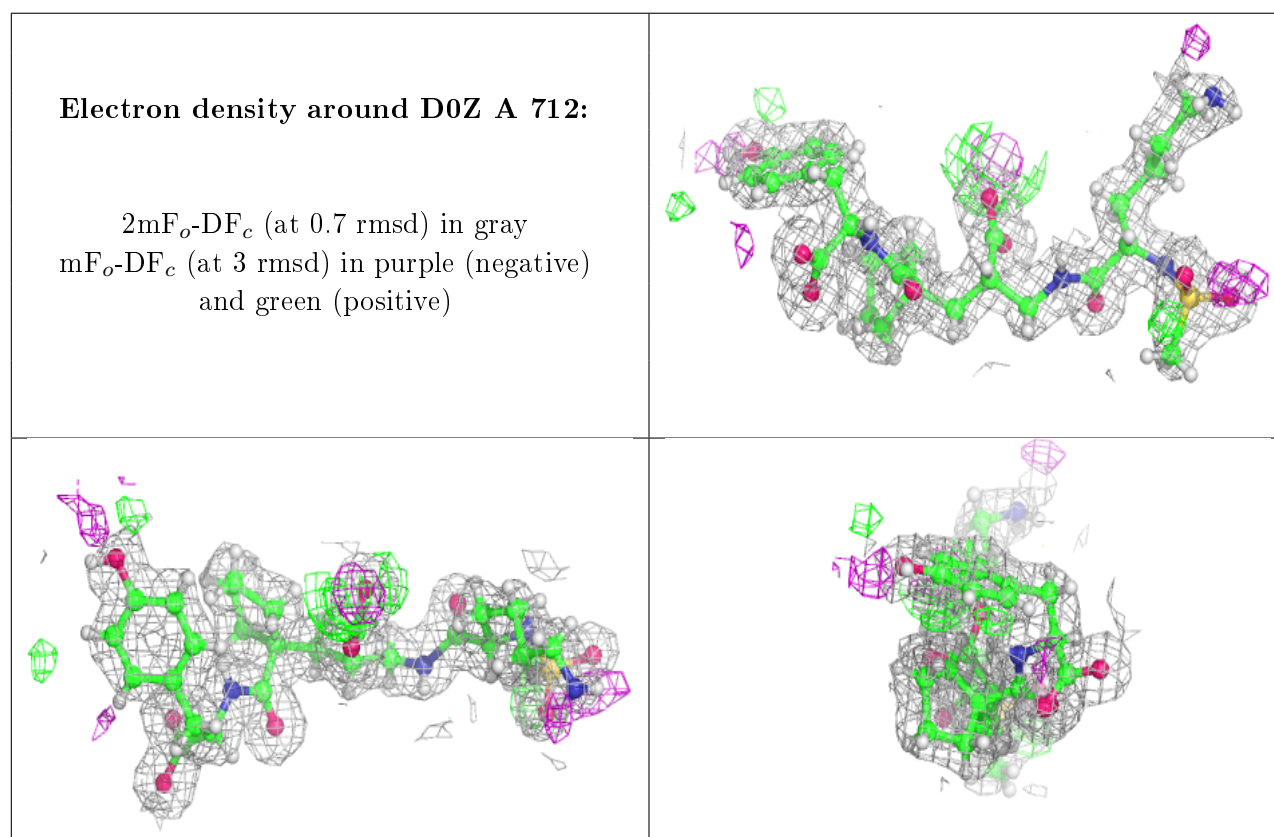
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PEG	A	721	7/7	0.69	0.31	37,50,61,63	0
9	EDO	A	720	4/4	0.73	0.24	45,54,63,76	0
9	EDO	A	719	4/4	0.76	0.31	38,48,58,62	0
10	PEG	A	723	7/7	0.76	0.26	41,50,58,65	0
7	IMD	A	716	5/5	0.79	0.26	39,48,60,61	0
9	EDO	A	718	4/4	0.82	0.13	37,45,52,58	0
10	PEG	A	722	7/7	0.86	0.21	34,43,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	BO3	A	717	4/4	0.89	0.10	28,32,38,41	0
11	PGE	A	724	10/10	0.90	0.21	29,47,59,64	0
7	IMD	A	715	5/5	0.95	0.10	17,21,26,27	0
5	D0Z	A	712	40/40	0.97	0.09	10,16,38,39	0
6	CL	A	713	1/1	1.00	0.12	14,14,14,14	0
6	CL	A	714	1/1	1.00	0.04	12,12,12,12	0
4	ZN	A	711	1/1	1.00	0.01	6,6,6,6	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 ⓘ

There are no such residues in this entry.