



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:01 PM BST

PDB ID : 6TT1  
Title : Crystal structure of 'Res\_S2 mutant human Angiotensin-1 converting enzyme N-domain in complex with 33RE.  
Authors : Cozier, G.E.; Acharya, K.R.  
Deposited on : 2019-12-23  
Resolution : 1.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

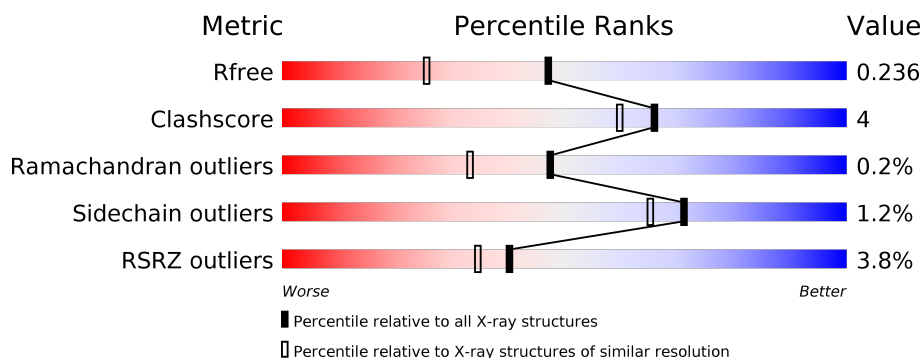
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	629	<div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	B	629	<div> <div>7%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
2	C	4	<div> <div>25%</div> <div>75%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	2	<div> <div>100%</div> </div>
4	F	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 20593 atoms, of which 9625 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
1	A	605	Total	C	H	N	O	S	0	8	0
			9719	3193	4750	850	907	19			
1	B	595	Total	C	H	N	O	S	0	8	0
			9514	3126	4647	833	889	19			

There are 34 discrepancies between the modelled and reference sequences:

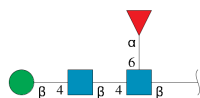
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	131	GLN	ASN	conflict	UNP P12821
A	260	THR	SER	conflict	UNP P12821
A	262	SER	GLU	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	354	GLU	ASP	conflict	UNP P12821
A	357	VAL	SER	conflict	UNP P12821
A	358	VAL	THR	conflict	UNP P12821
A	369	PHE	TYR	conflict	UNP P12821
A	381	GLU	ARG	conflict	UNP P12821
A	431	ASP	GLU	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	conflict	UNP P12821
B	25	GLN	ASN	conflict	UNP P12821
B	82	GLN	ASN	conflict	UNP P12821
B	117	GLN	ASN	conflict	UNP P12821
B	131	GLN	ASN	conflict	UNP P12821
B	260	THR	SER	conflict	UNP P12821
B	262	SER	GLU	conflict	UNP P12821
B	289	GLN	ASN	conflict	UNP P12821

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	354	GLU	ASP	conflict	UNP P12821
B	357	VAL	SER	conflict	UNP P12821
B	358	VAL	THR	conflict	UNP P12821
B	369	PHE	TYR	conflict	UNP P12821
B	381	GLU	ARG	conflict	UNP P12821
B	431	ASP	GLU	conflict	UNP P12821
B	545	ARG	GLN	conflict	UNP P12821
B	576	LEU	PRO	conflict	UNP P12821
B	629	LEU	-	expression tag	UNP P12821

- Molecule 2 is an oligosaccharide called 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
2	C	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
3	E	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

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



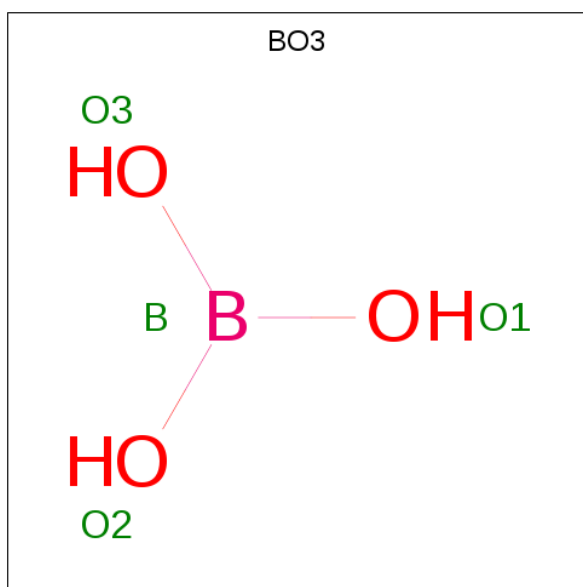
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 6 is BORIC ACID (three-letter code: BO3) (formula:  $BH_3O_3$ ).

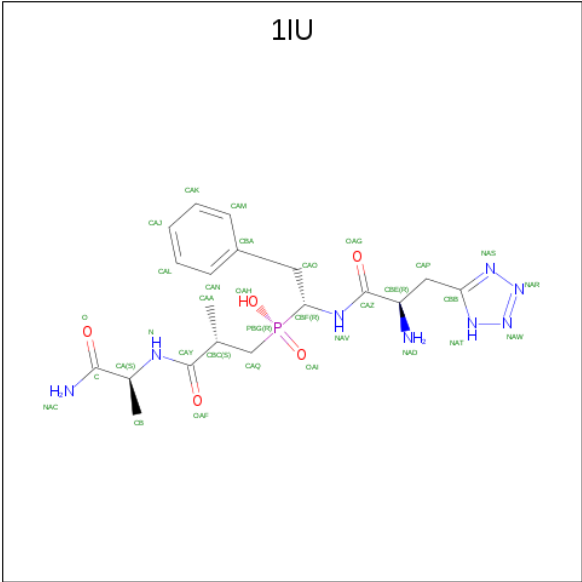


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	B	O	0	0
			4	1	3		
6	A	1	Total	B	O	0	0
			4	1	3		
6	B	1	Total	B	O	0	0
			4	1	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is [3-[(2S)-1-azanyl-1-oxidanylidene-propan-2-yl]amino]-2-methyl-3-oxidanylidene-propyl)-[(1R)-1-[(2R)-2-azanyl-3-(1H-1,2,3,4-tetrazol-5-yl)propanoyl]amino]-2-phenylethyl]phosphinic acid (three-letter code: IUU) (formula: C<sub>19</sub>H<sub>29</sub>N<sub>8</sub>O<sub>5</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			33	19	8	5	1		
8	B	1	Total	C	N	O	P	0	0
			33	19	8	5	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cl	0	0
			1	1		
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

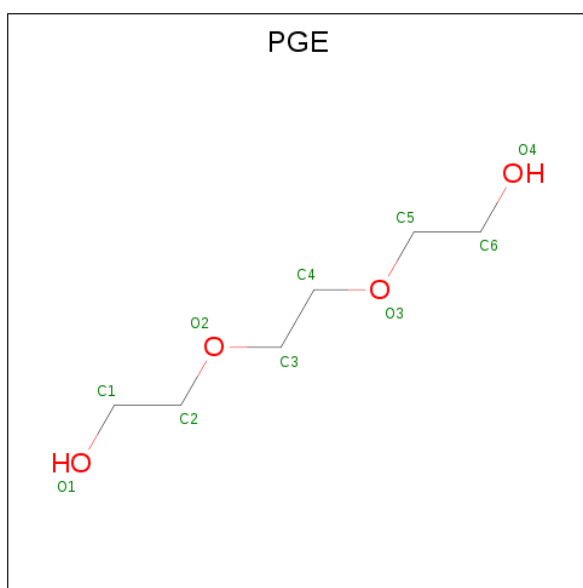
- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





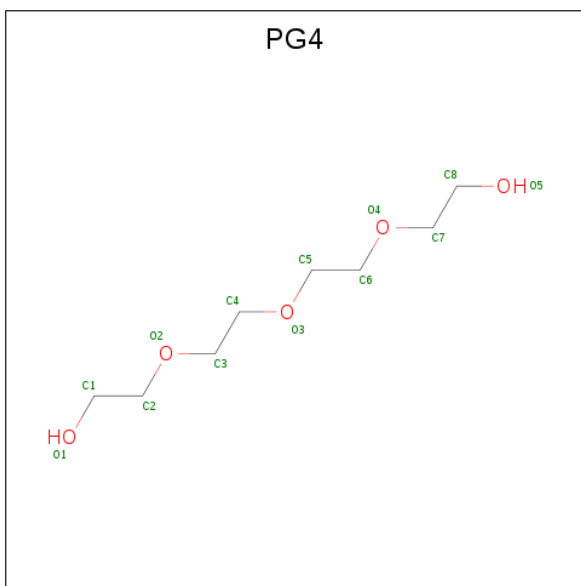
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		
11	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	1
			48	12	28	8		
12	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 13 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	1
			26	16	10		

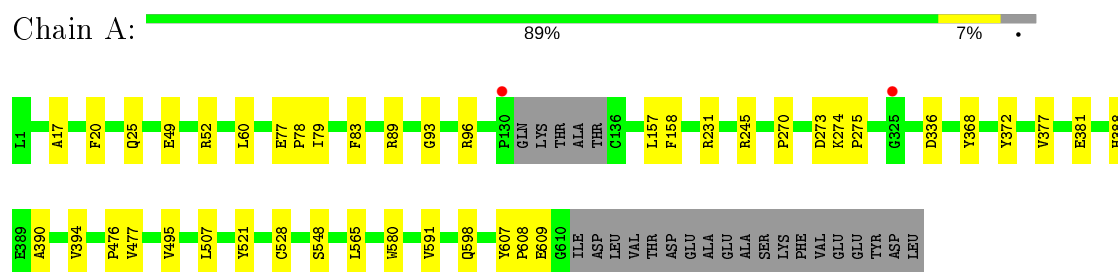
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	489	Total	O	0	7
			496	496		
14	B	295	Total	O	0	4
			299	299		

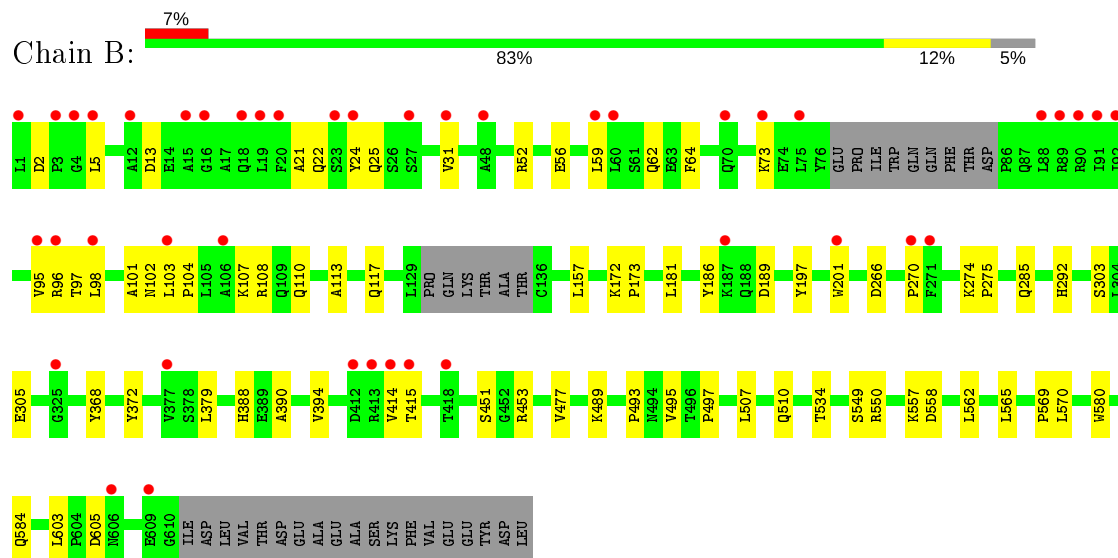
### 3 Residue-property plots

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: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- Molecule 2: 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



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

MAG1  
FUC2

- Molecule 3:  $\alpha$ -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1  
FUC2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.17Å 77.13Å 82.87Å 88.93° 64.53° 75.15°	Depositor
Resolution (Å)	44.59 – 1.80 74.14 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.59-1.80) 97.4 (74.14-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.200 , 0.237 0.199 , 0.236	Depositor DCC
$R_{free}$ test set	2111 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, BO3, EDO, PG4, PGE, FUC, 1IU, PEG

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	0.52	0/5167	0.64	0/7038
1	B	0.47	0/5051	0.61	0/6879
All	All	0.50	0/10218	0.62	0/13917

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

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	4969	4750	4715	23	0
1	B	4867	4647	4615	44	0
2	C	49	43	43	0	0
3	D	24	22	22	1	0
3	E	24	22	22	0	0
4	F	28	25	25	0	0
5	A	14	13	13	0	0
5	B	14	13	13	0	0
6	A	8	0	6	0	0
6	B	4	0	3	0	0
7	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	33	0	28	2	0
8	B	33	0	28	4	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	16	24	24	3	0
10	B	16	24	24	4	0
11	A	7	0	10	0	0
11	B	7	0	10	2	0
12	A	20	28	28	3	0
12	B	10	14	14	0	0
13	B	26	0	36	4	0
14	A	496	0	0	4	2
14	B	299	0	0	5	2
All	All	10968	9625	9679	80	2

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.

The worst 5 of 80 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:93:GLY:O	14:A:802:HOH:O	2.04	0.75
8:B:708:1IU:HAD1	10:B:712:EDO:H11	1.55	0.71
8:A:711:1IU:HAD1	10:A:713:EDO:H22	1.61	0.65
8:B:708:1IU:HAD1	10:B:712:EDO:C1	2.13	0.62
1:A:231:ARG:NH2	14:A:803:HOH:O	2.32	0.60

All (2) 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)
14:A:1112:HOH:O	14:B:801:HOH:O[1_654]	2.12	0.08
14:A:1000:HOH:O	14:B:1044:HOH:O[1_554]	2.19	0.01

## 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	609/629 (97%)	597 (98%)	10 (2%)	2 (0%)	41	27
1	B	597/629 (95%)	573 (96%)	24 (4%)	0	100	100
All	All	1206/1258 (96%)	1170 (97%)	34 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	78	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	528/541 (98%)	522 (99%)	6 (1%)	73	68
1	B	515/541 (95%)	509 (99%)	6 (1%)	71	65
All	All	1043/1082 (96%)	1031 (99%)	12 (1%)	71	65

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	609	GLU
1	B	285	GLN
1	B	372	TYR
1	A	598	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	368	TYR

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

### 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 ⓘ

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	C	1	1,2	14,14,15	0.58	0	17,19,21	0.63	0
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
2	BMA	C	3	2	11,11,12	1.32	2 (18%)	15,15,17	1.01	0
2	FUC	C	4	2	10,10,11	0.99	1 (10%)	14,14,16	0.93	0
3	NAG	D	1	1,3	14,14,15	0.40	0	17,19,21	0.62	0
3	FUC	D	2	3	10,10,11	1.22	1 (10%)	14,14,16	1.00	1 (7%)
3	NAG	E	1	1,3	14,14,15	0.92	1 (7%)	17,19,21	0.67	0
3	FUC	E	2	3	10,10,11	0.90	0	14,14,16	1.66	2 (14%)
4	NAG	F	1	1,4	14,14,15	0.59	0	17,19,21	0.53	0
4	NAG	F	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.56	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	FUC	O5-C1	-3.50	1.38	1.43
3	E	1	NAG	C1-C2	2.74	1.56	1.52
2	C	3	BMA	C1-C2	2.48	1.57	1.52
2	C	3	BMA	C4-C5	2.11	1.57	1.53
2	C	4	FUC	C2-C3	2.09	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	FUC	O5-C1-C2	4.21	117.27	110.77
3	E	2	FUC	C1-C2-C3	3.79	114.32	109.67
3	D	2	FUC	C1-C2-C3	2.18	112.35	109.67
2	C	2	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

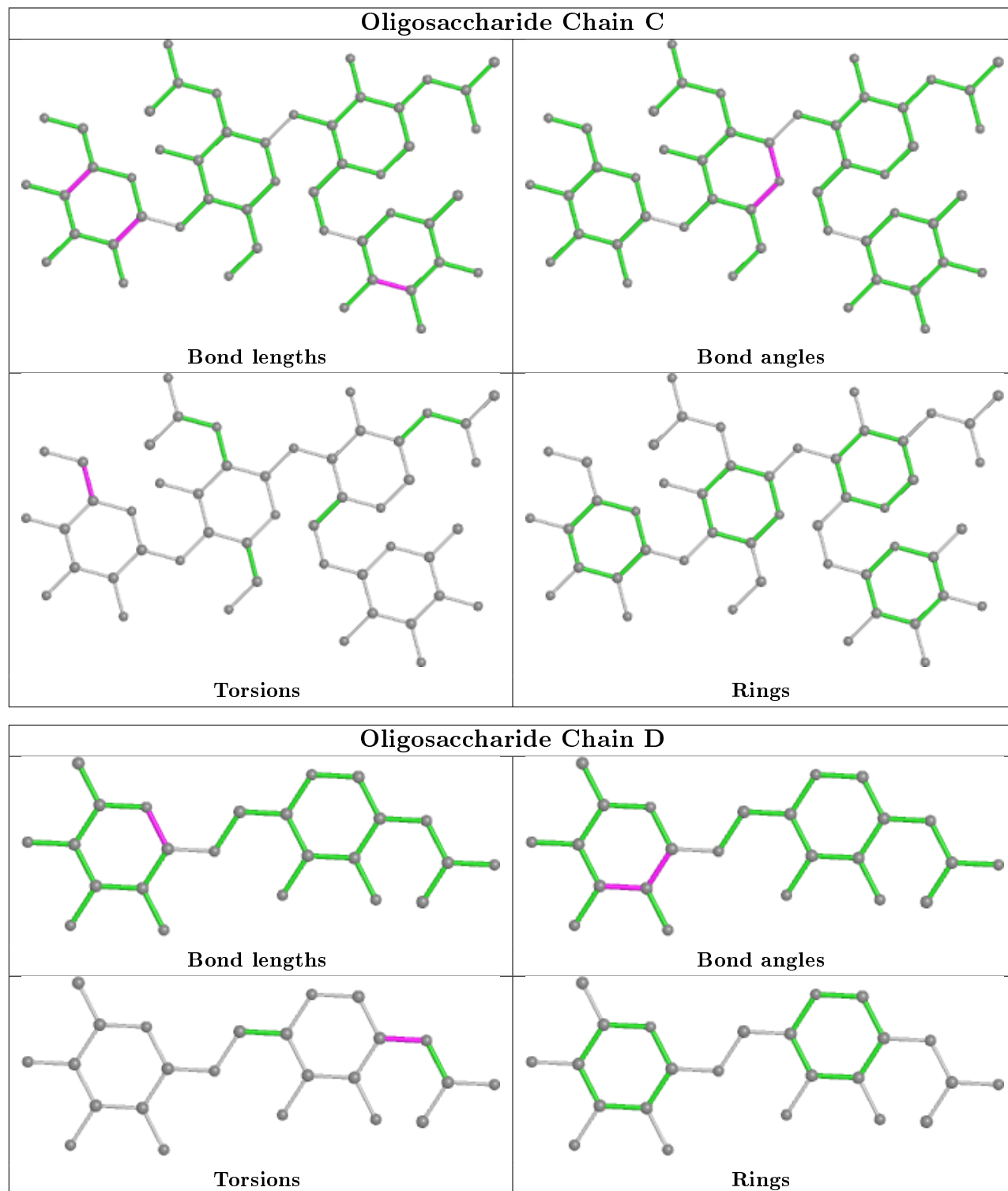
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7
3	D	1	NAG	C1-C2-N2-C7

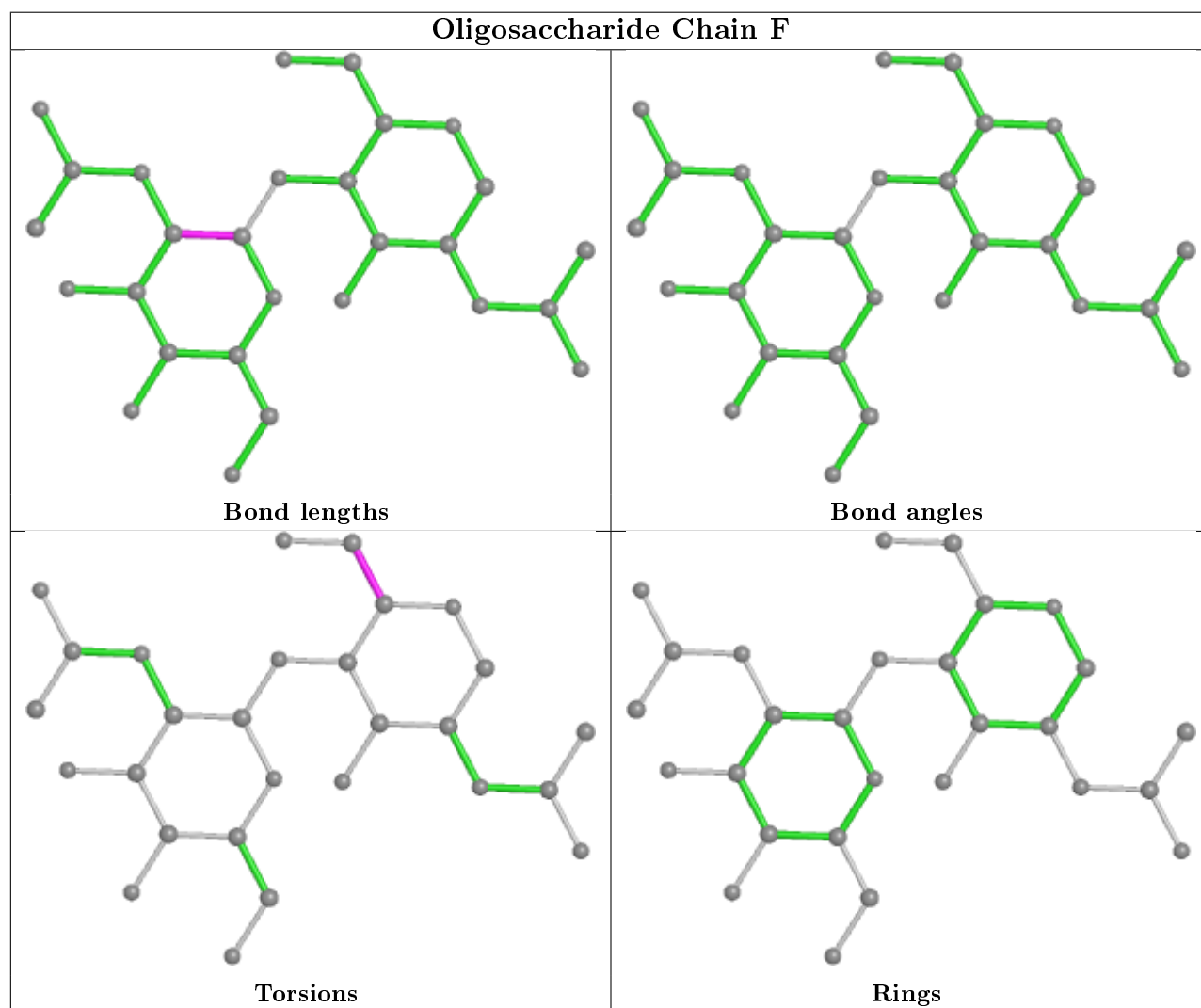
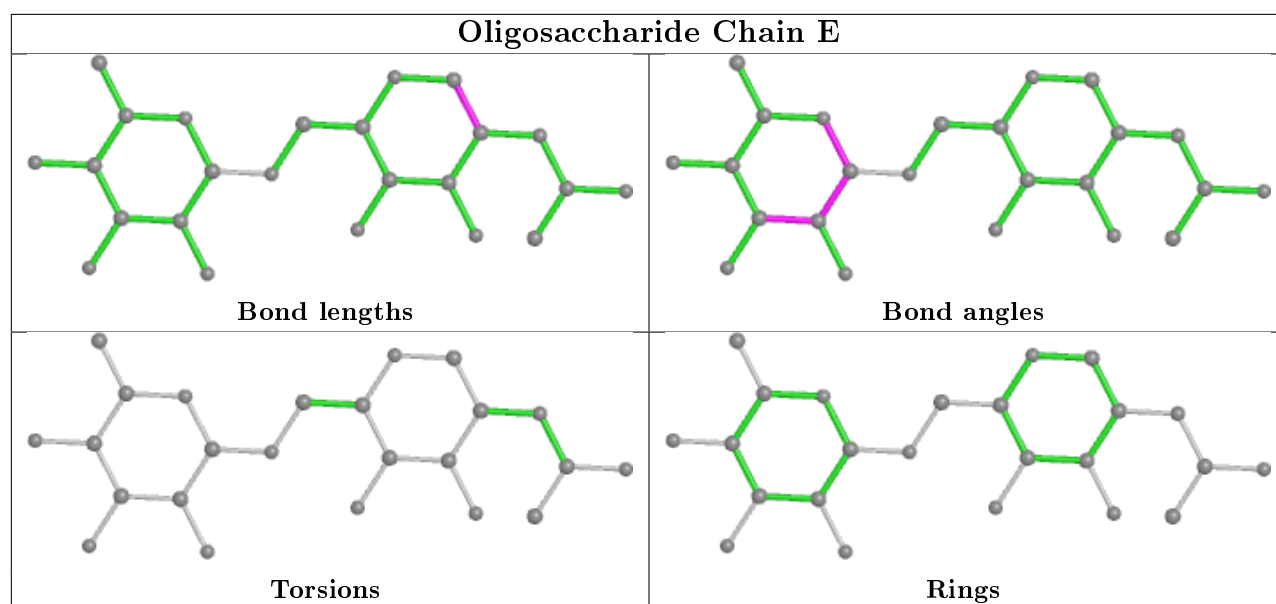
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	FUC	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

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	BO3	B	706	-	3,3,3	0.26	0	3,3,3	0.28	0
13	PG4	B	710[B]	-	12,12,12	0.51	0	11,11,11	0.39	0
10	EDO	B	712	-	3,3,3	0.44	0	2,2,2	0.49	0
11	PEG	A	717	-	6,6,6	0.49	0	5,5,5	0.30	0
10	EDO	A	713	-	3,3,3	0.39	0	2,2,2	0.51	0
10	EDO	B	711	-	3,3,3	0.56	0	2,2,2	0.14	0
10	EDO	B	714	-	3,3,3	0.49	0	2,2,2	0.45	0
10	EDO	A	715	-	3,3,3	0.59	0	2,2,2	0.16	0
12	PGE	A	718[A]	-	9,9,9	0.41	0	8,8,8	0.69	0
12	PGE	B	716	-	9,9,9	0.39	0	8,8,8	0.47	0
12	PGE	A	718[B]	-	9,9,9	0.36	0	8,8,8	0.61	0
5	NAG	A	701	1	14,14,15	0.46	0	17,19,21	0.78	1 (5%)
5	NAG	B	703	1	14,14,15	0.56	0	17,19,21	0.63	0
10	EDO	B	713	-	3,3,3	0.53	0	2,2,2	0.29	0
8	1IU	B	708	7	30,34,34	2.00	6 (20%)	34,47,47	1.98	11 (32%)
10	EDO	A	716	-	3,3,3	0.51	0	2,2,2	0.39	0
8	1IU	A	711	7	30,34,34	2.07	6 (20%)	34,47,47	2.04	8 (23%)
11	PEG	B	715	-	6,6,6	0.47	0	5,5,5	0.34	0
6	BO3	A	709	-	3,3,3	0.24	0	3,3,3	0.26	0
6	BO3	A	708	-	3,3,3	0.25	0	3,3,3	0.41	0
10	EDO	A	714	-	3,3,3	0.61	0	2,2,2	0.33	0
13	PG4	B	710[A]	-	12,12,12	0.53	0	11,11,11	0.30	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
10	EDO	A	713	-	-	0/1/1/1	-
12	PGE	B	716	-	-	3/7/7/7	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	B	711	-	-	1/1/1/1	-
8	1IU	B	708	7	-	6/32/39/39	0/2/2/2
10	EDO	B	712	-	-	1/1/1/1	-
13	PG4	B	710[B]	-	-	3/10/10/10	-
8	1IU	A	711	7	-	6/32/39/39	0/2/2/2
10	EDO	B	714	-	-	1/1/1/1	-
10	EDO	A	714	-	-	1/1/1/1	-
10	EDO	A	715	-	-	0/1/1/1	-
10	EDO	A	716	-	-	0/1/1/1	-
5	NAG	B	703	1	-	2/6/23/26	0/1/1/1
11	PEG	B	715	-	-	1/4/4/4	-
12	PGE	A	718[B]	-	-	3/7/7/7	-
11	PEG	A	717	-	-	1/4/4/4	-
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
13	PG4	B	710[A]	-	-	4/10/10/10	-
12	PGE	A	718[A]	-	-	5/7/7/7	-
10	EDO	B	713	-	-	0/1/1/1	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	708	1IU	CAZ-NAV	5.59	1.46	1.34
8	A	711	1IU	CAZ-NAV	5.49	1.46	1.34
8	A	711	1IU	CAY-N	5.44	1.46	1.34
8	A	711	1IU	PBG-CAQ	4.86	1.84	1.79
8	B	708	1IU	PBG-CAQ	4.72	1.84	1.79

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	711	1IU	CBE-CAZ-NAV	5.68	124.03	116.15
8	B	708	1IU	CBE-CAZ-NAV	5.34	123.56	116.15
8	A	711	1IU	CBA-CAO-CBF	-4.51	103.44	113.38
8	B	708	1IU	NAT-NAW-NAR	-3.99	106.93	109.53
8	A	711	1IU	NAS-NAR-NAW	-3.74	107.09	109.53

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	708	1IU	OAG-CAZ-CBE-CAP
8	B	708	1IU	NAV-CAZ-CBE-CAP
8	A	711	1IU	OAG-CAZ-CBE-CAP
8	A	711	1IU	NAV-CAZ-CBE-CAP
12	A	718[A]	PGE	O3-C5-C6-O4

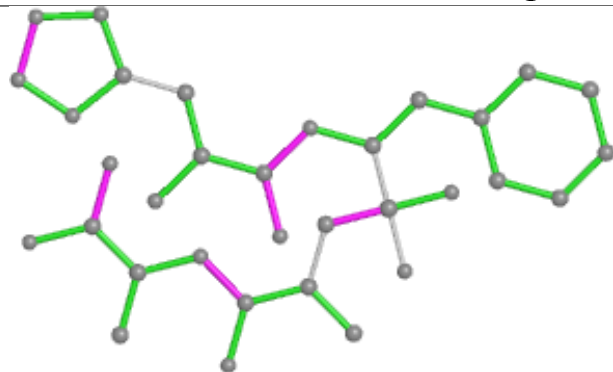
There are no ring outliers.

11 monomers are involved in 15 short contacts:

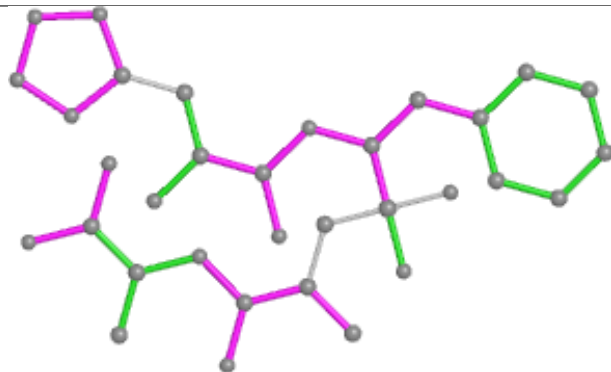
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	710[B]	PG4	1	0
10	B	712	EDO	2	0
10	A	713	EDO	2	0
10	B	714	EDO	2	0
12	A	718[A]	PGE	2	0
12	A	718[B]	PGE	1	0
8	B	708	1IU	4	0
8	A	711	1IU	2	0
11	B	715	PEG	2	0
10	A	714	EDO	1	0
13	B	710[A]	PG4	3	0

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.

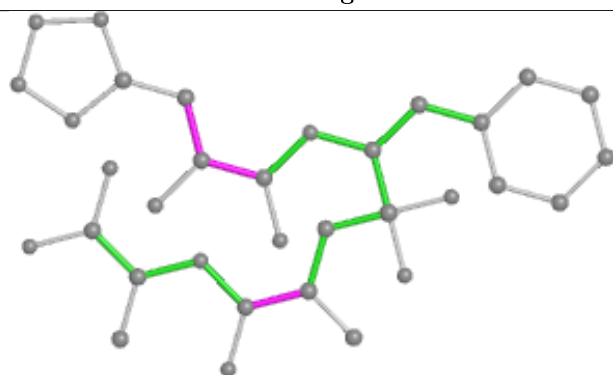
## Ligand 1IU B 708



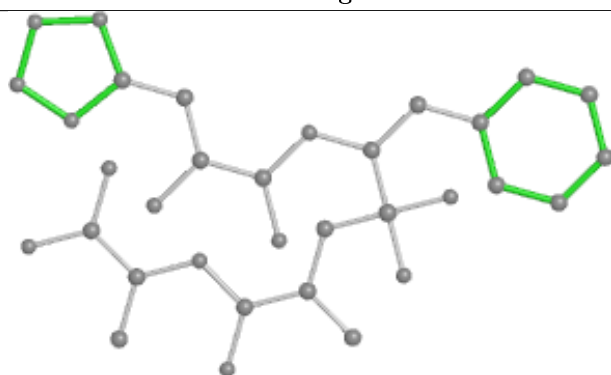
Bond lengths



Bond angles

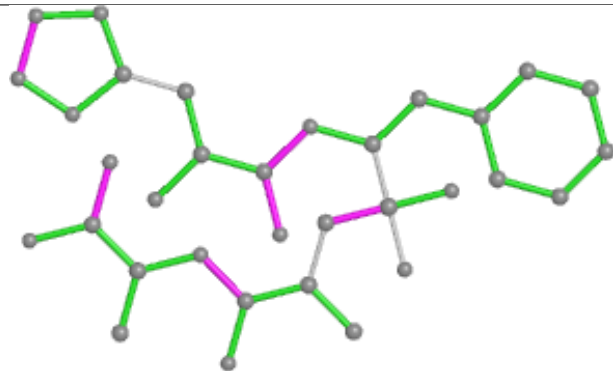


Torsions

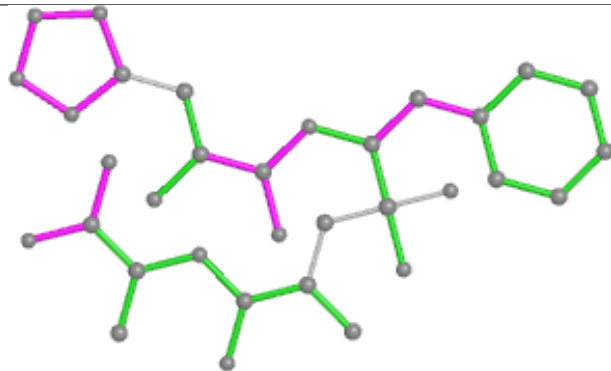


Rings

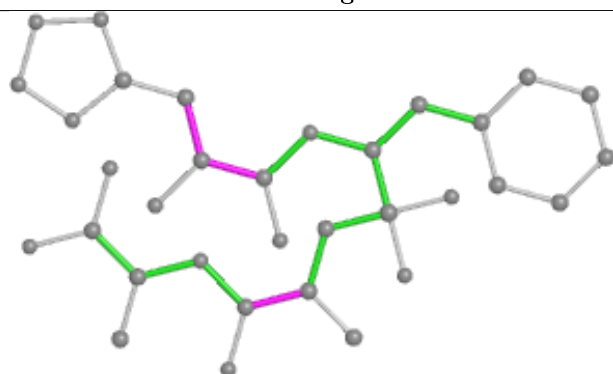
## Ligand 1IU A 711



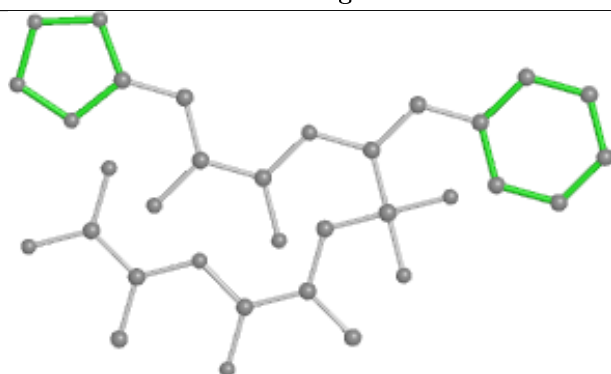
Bond lengths



Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	605/629 (96%)	-0.02	2 (0%) 94 92	19, 31, 52, 78	0
1	B	595/629 (94%)	0.33	43 (7%) 15 12	21, 41, 77, 93	0
All	All	1200/1258 (95%)	0.15	45 (3%) 40 35	19, 35, 69, 93	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	ILE	6.7
1	B	414	VAL	6.4
1	B	1	LEU	5.3
1	B	12	ALA	5.2
1	B	15	ALA	5.2

### 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, 95<sup>th</sup> 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.

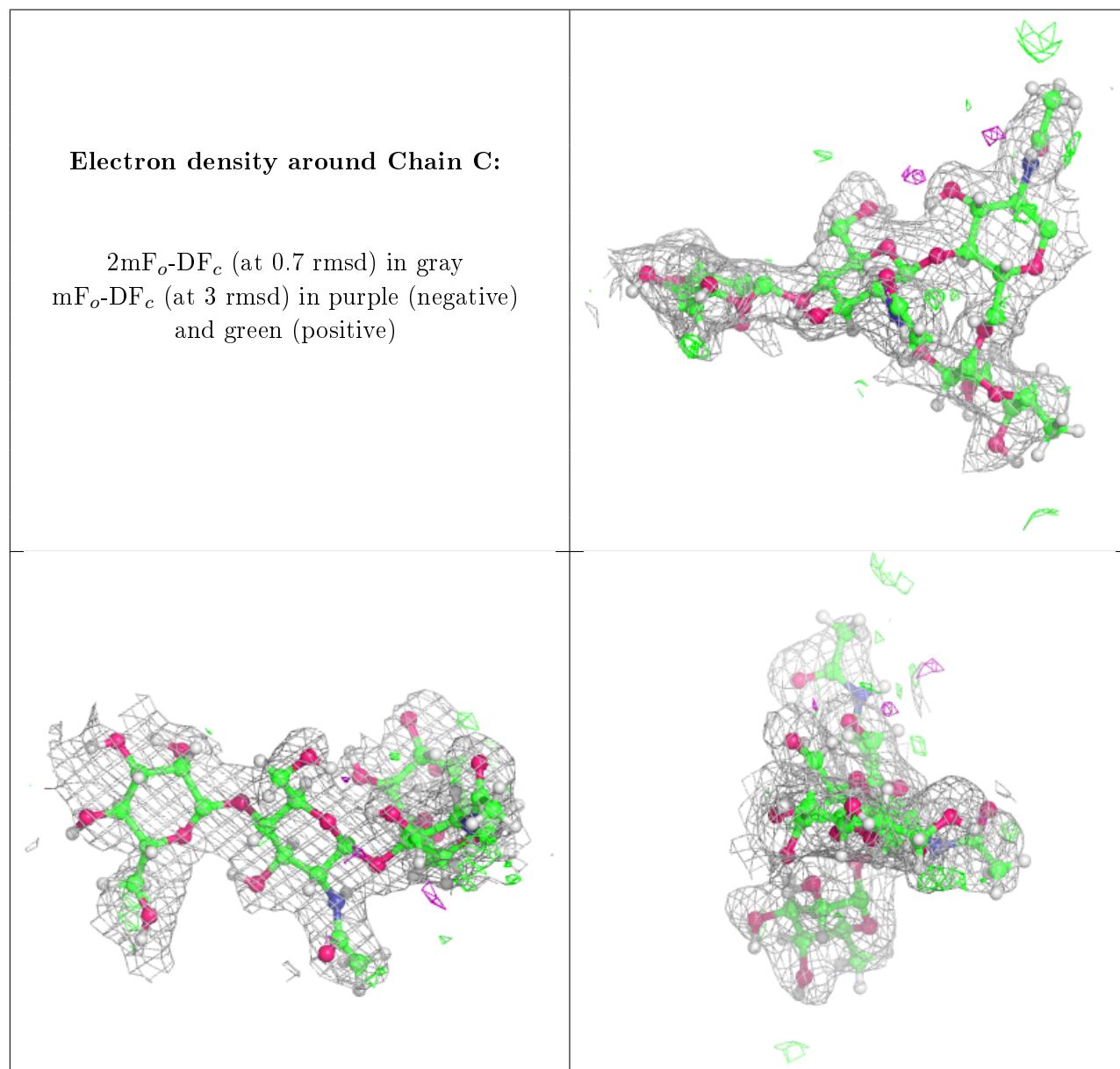
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	C	3	11/12	0.65	0.13	59,70,83,86	0
4	NAG	F	1	14/15	0.82	0.15	61,71,81,86	0
3	FUC	E	2	10/11	0.82	0.18	51,61,72,73	20
4	NAG	F	2	14/15	0.83	0.24	67,78,92,95	0
3	NAG	E	1	14/15	0.88	0.11	44,54,65,76	0

*Continued on next page...*

*Continued from previous page...*

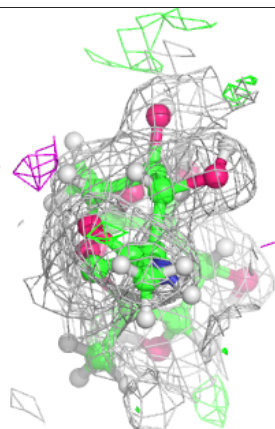
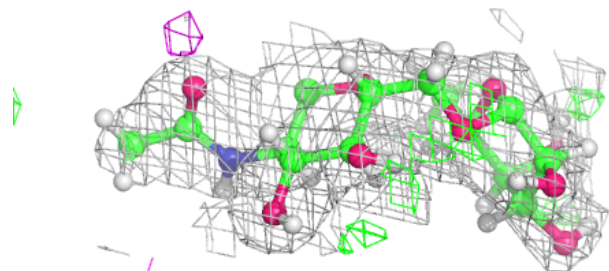
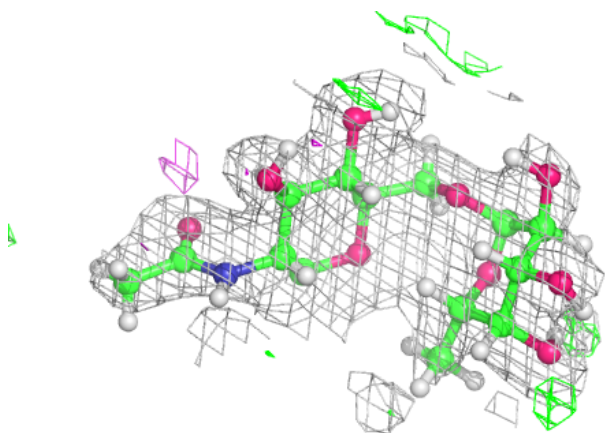
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	1	14/15	0.89	0.10	41,53,63,64	0
2	FUC	C	4	10/11	0.90	0.11	44,50,60,60	20
2	NAG	C	2	14/15	0.92	0.10	42,56,64,65	0
3	FUC	D	2	10/11	0.92	0.12	43,51,61,62	20
2	NAG	C	1	14/15	0.94	0.09	37,42,51,52	0

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.

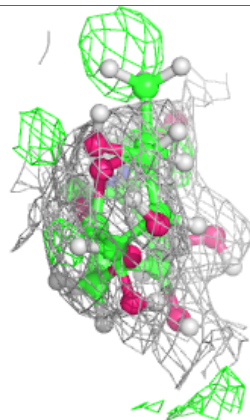
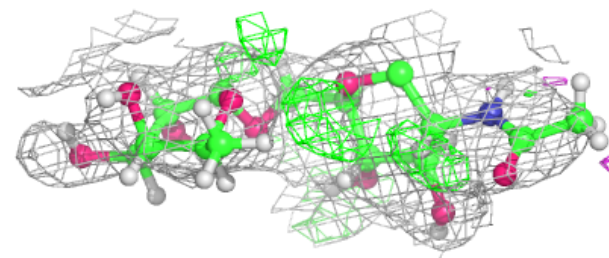
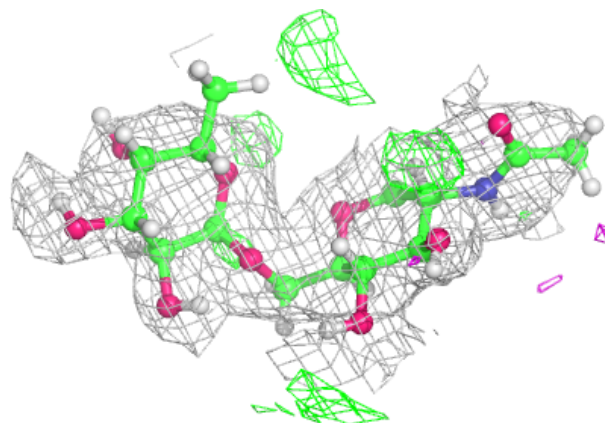


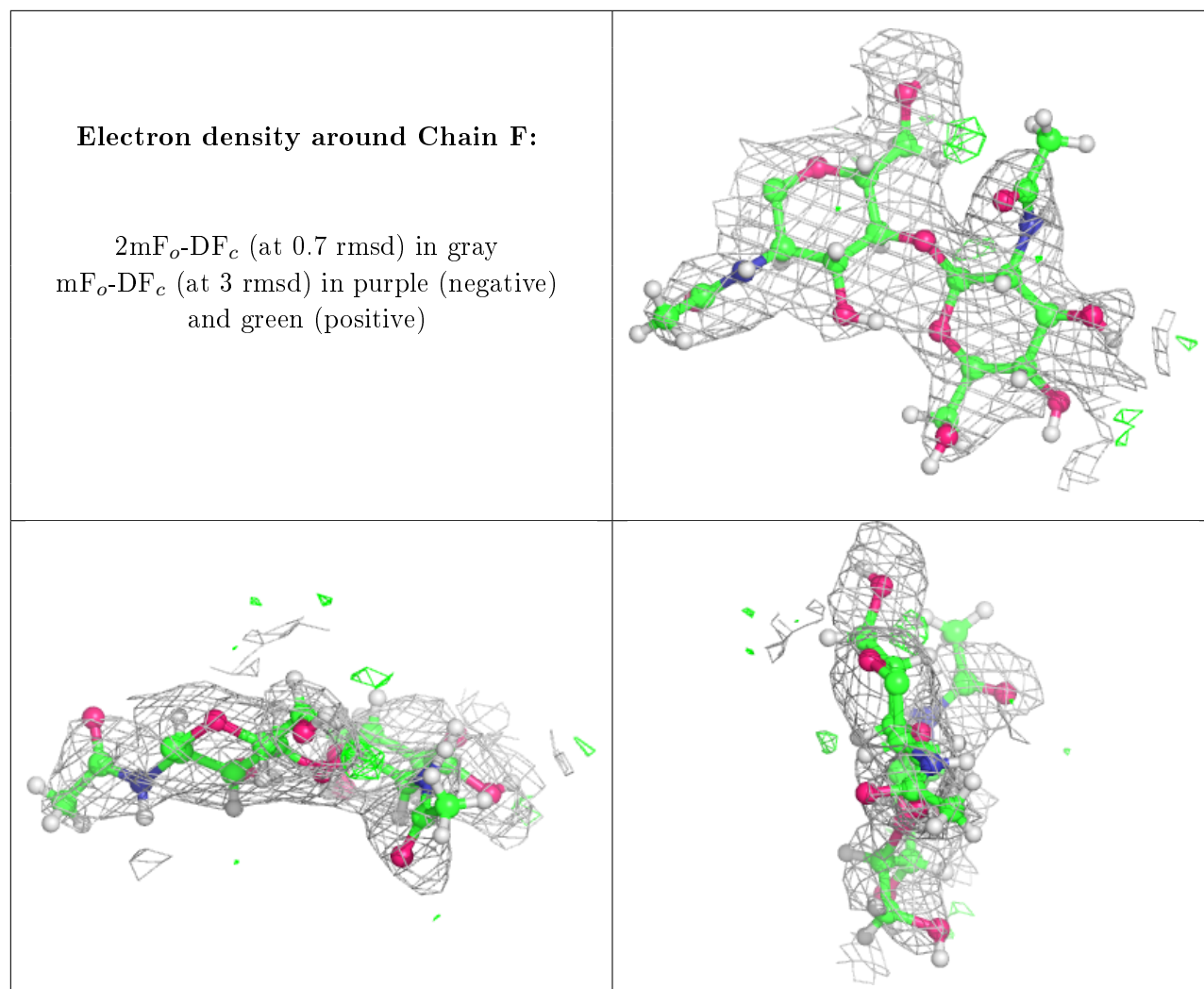
**Electron density around Chain D:**

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

**Electron density around Chain E:**

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





## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	B	703	14/15	0.64	0.21	61,78,94,98	0
10	EDO	A	716	4/4	0.73	0.15	52,62,65,65	0
5	NAG	A	701	14/15	0.74	0.20	49,63,76,77	0
13	PG4	B	710[B]	13/13	0.77	0.14	40,45,48,50	13
13	PG4	B	710[A]	13/13	0.77	0.14	38,45,49,50	13
10	EDO	A	714	4/4	0.80	0.15	34,41,43,47	10
6	BO3	B	706	4/4	0.82	0.17	38,44,45,48	0
10	EDO	B	711	4/4	0.83	0.13	50,60,67,70	0
12	PGE	A	718[B]	10/10	0.84	0.16	27,35,41,42	24

*Continued on next page...*

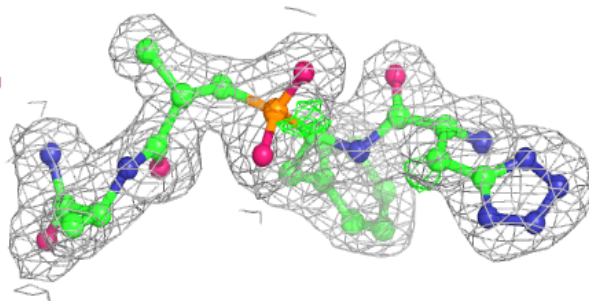
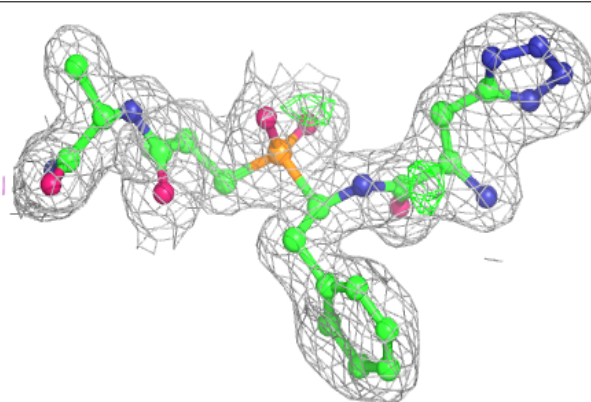
*Continued from previous page...*

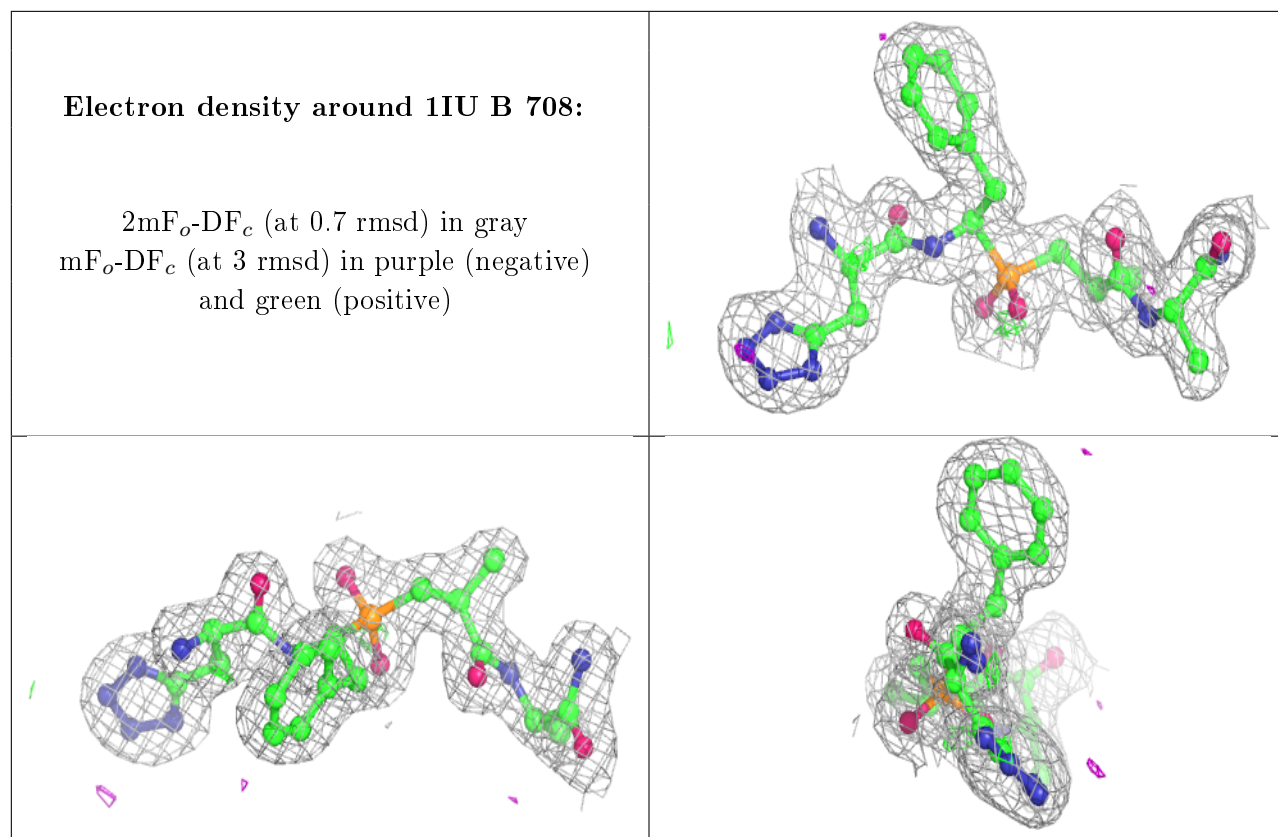
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	PGE	A	718[A]	10/10	0.84	0.16	30,37,44,44	24
10	EDO	B	712	4/4	0.89	0.16	40,48,53,53	0
10	EDO	B	714	4/4	0.89	0.16	40,48,52,56	0
10	EDO	A	713	4/4	0.89	0.10	37,44,45,48	10
11	PEG	A	717	7/7	0.90	0.10	46,48,55,58	0
10	EDO	A	715	4/4	0.90	0.09	36,43,50,54	0
10	EDO	B	713	4/4	0.90	0.17	52,62,64,67	0
12	PGE	B	716	10/10	0.92	0.08	34,46,57,57	0
6	BO3	A	709	4/4	0.92	0.08	45,46,48,55	0
6	BO3	A	708	4/4	0.93	0.17	36,39,40,40	0
11	PEG	B	715	7/7	0.94	0.07	38,42,47,48	0
8	1IU	A	711	33/33	0.97	0.11	19,24,32,33	0
8	1IU	B	708	33/33	0.98	0.10	19,26,38,40	0
9	CL	A	712	1/1	0.99	0.11	22,22,22,22	0
9	CL	B	709	1/1	0.99	0.11	30,30,30,30	0
7	ZN	A	710	1/1	1.00	0.13	25,25,25,25	0
7	ZN	B	707	1/1	1.00	0.12	25,25,25,25	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 1IU A 711:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.