



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:12 PM UTC

PDB ID : 6TT1 / pdb_00006tt1
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

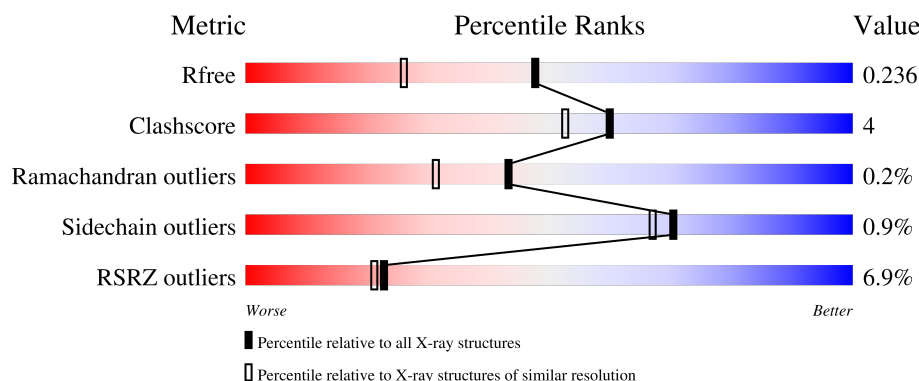
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	629	2% 89% 7% .
1	B	629	11% 83% 12% 5%
2	C	4	25% 75%
3	D	2	50% 50%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
4	F	2	

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:

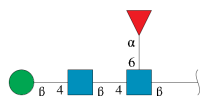
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	131	GLN	ASN	conflict	UNP P12821
A	260	THR	SER	conflict	UNP P12821
A	262	SER	GLU	conflict	UNP P12821
A	289	GLN	ASN	conflict	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

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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.



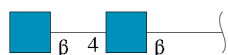
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

- 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.



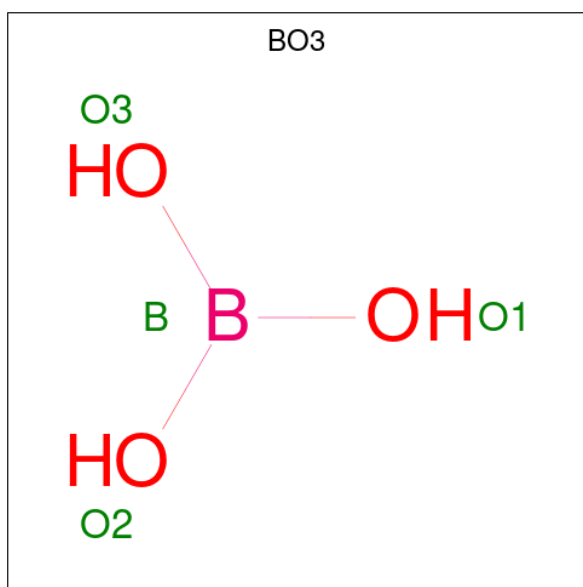
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	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-phenyl-ethyl]phosphinic acid (CCD ID: 1IU) (formula: C₁₉H₂₉N₈O₅P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



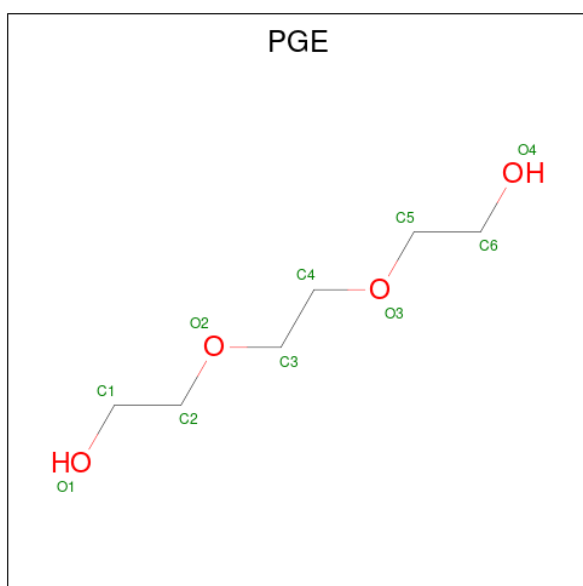
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



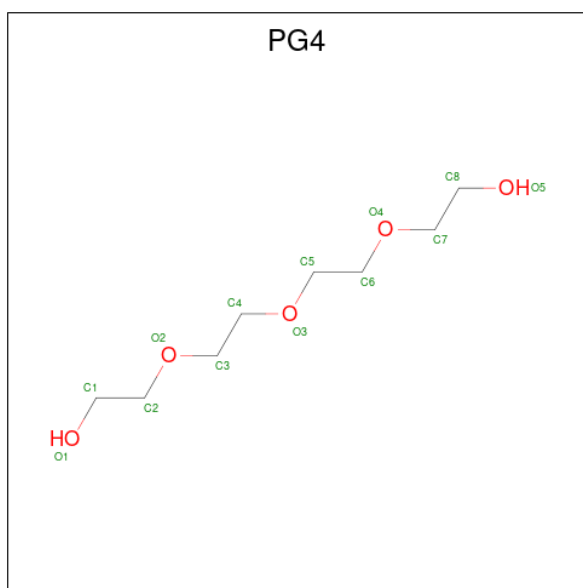
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		
11	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

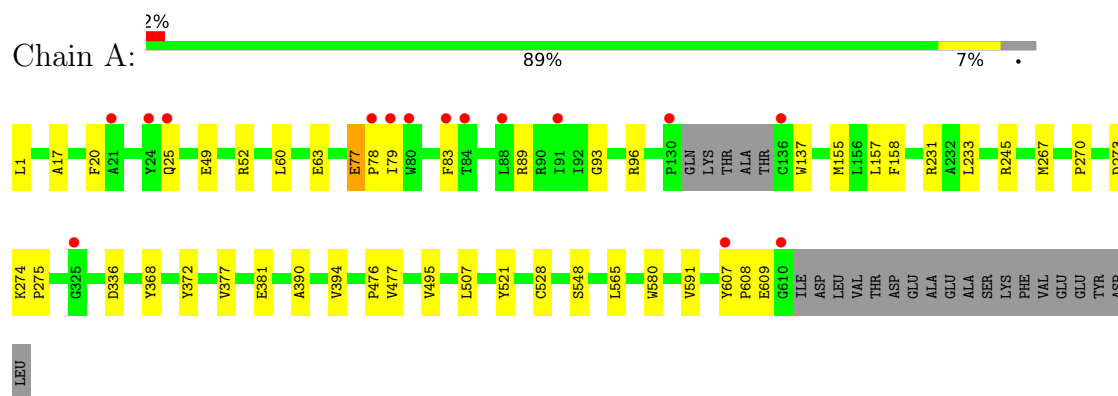
- Molecule 14 is water.

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

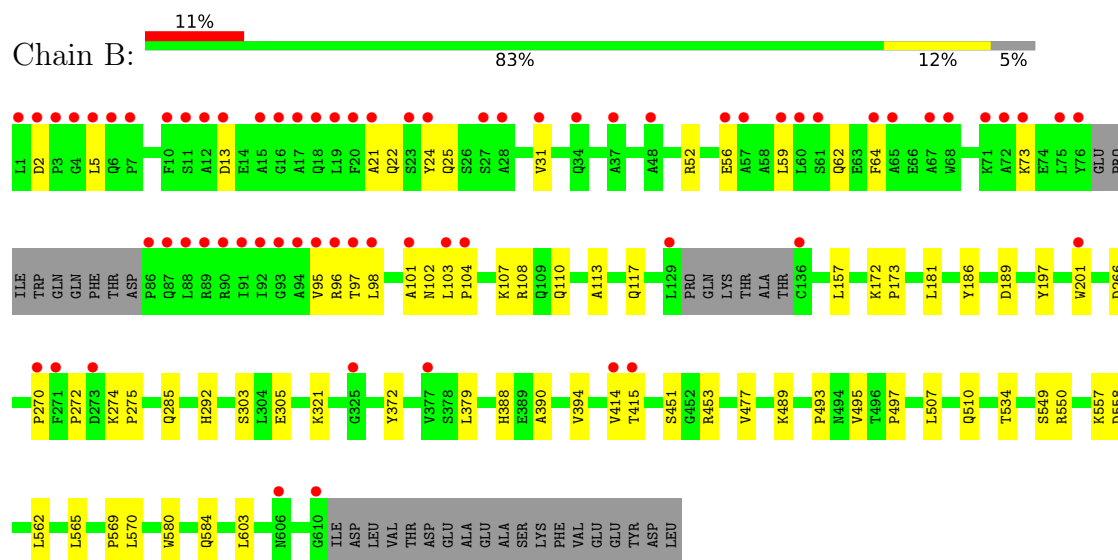
3 Residue-property plots [i](#)

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: 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

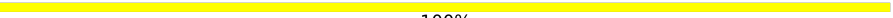


- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

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, α , β , γ	73.17Å 77.13Å 82.87Å 88.93° 64.53° 75.15°	Depositor
Resolution (Å)	44.59 – 1.80 44.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.59-1.80) 97.4 (44.59-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.200 , 0.237 0.200 , 0.236	Depositor DCC
R_{free} test set	2111 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.3	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	20593	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, EDO, BO3, BMA, 1IU, PEG, CL, FUC, PG4

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	0.46	0/5167	0.60	0/7038
1	B	0.40	0/5051	0.58	1/6879 (0.0%)
All	All	0.43	0/10218	0.59	1/13917 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	PRO	N-CA-C	5.29	120.48	113.86

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	4969	4750	4715	27	0
1	B	4867	4647	4615	45	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	6	0	0
6	B	4	0	3	0	0
7	A	1	0	0	0	0
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	6	2
All	All	10968	9625	9679	85	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 85 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%)	36	25
1	B	597/629 (95%)	573 (96%)	24 (4%)	0	100	100
All	All	1206/1258 (96%)	1170 (97%)	34 (3%)	2 (0%)	43	31

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%)	523 (99%)	5 (1%)	70	67
1	B	515/541 (95%)	511 (99%)	4 (1%)	73	70
All	All	1043/1082 (96%)	1034 (99%)	9 (1%)	70	67

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	372	TYR
1	B	388	HIS
1	A	372	TYR
1	A	609	GLU

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Mol	Chain	Res	Type
1	B	285	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	371	GLN
1	B	527	GLN
1	B	606	ASN
1	A	371	GLN
1	A	70	GLN

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	0.57	0	17,19,21	0.65	0
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
2	BMA	C	3	2	11,11,12	1.29	2 (18%)	15,15,17	0.97	0
2	FUC	C	4	2	10,10,11	0.96	1 (10%)	14,14,16	0.88	0
3	NAG	D	1	1,3	14,14,15	0.41	0	17,19,21	0.64	0
3	FUC	D	2	3	10,10,11	1.17	1 (10%)	14,14,16	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.97	1 (7%)	17,19,21	0.68	0
3	FUC	E	2	3	10,10,11	0.88	0	14,14,16	1.31	2 (14%)
4	NAG	F	1	1,4	14,14,15	0.60	0	17,19,21	0.55	0
4	NAG	F	2	4	14,14,15	0.68	1 (7%)	17,19,21	0.58	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	-3.31	1.38	1.43
3	E	1	NAG	C1-C2	3.00	1.56	1.52
2	C	3	BMA	C1-C2	2.37	1.57	1.52
4	F	2	NAG	C1-C2	2.25	1.55	1.52
2	C	3	BMA	C4-C5	2.09	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	FUC	C1-C2-C3	3.21	114.32	109.64
3	E	2	FUC	O5-C1-C2	2.72	117.27	110.79
2	C	2	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

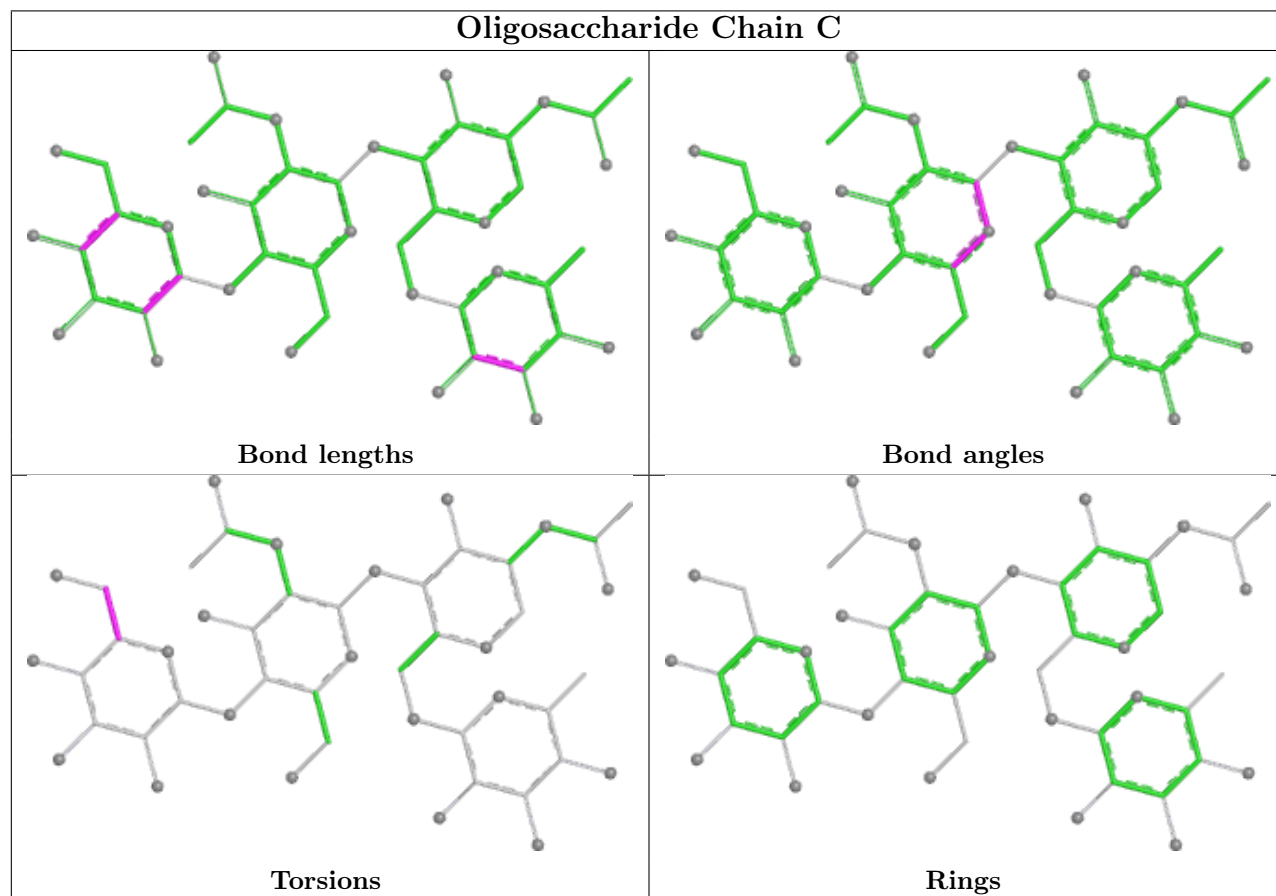
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6

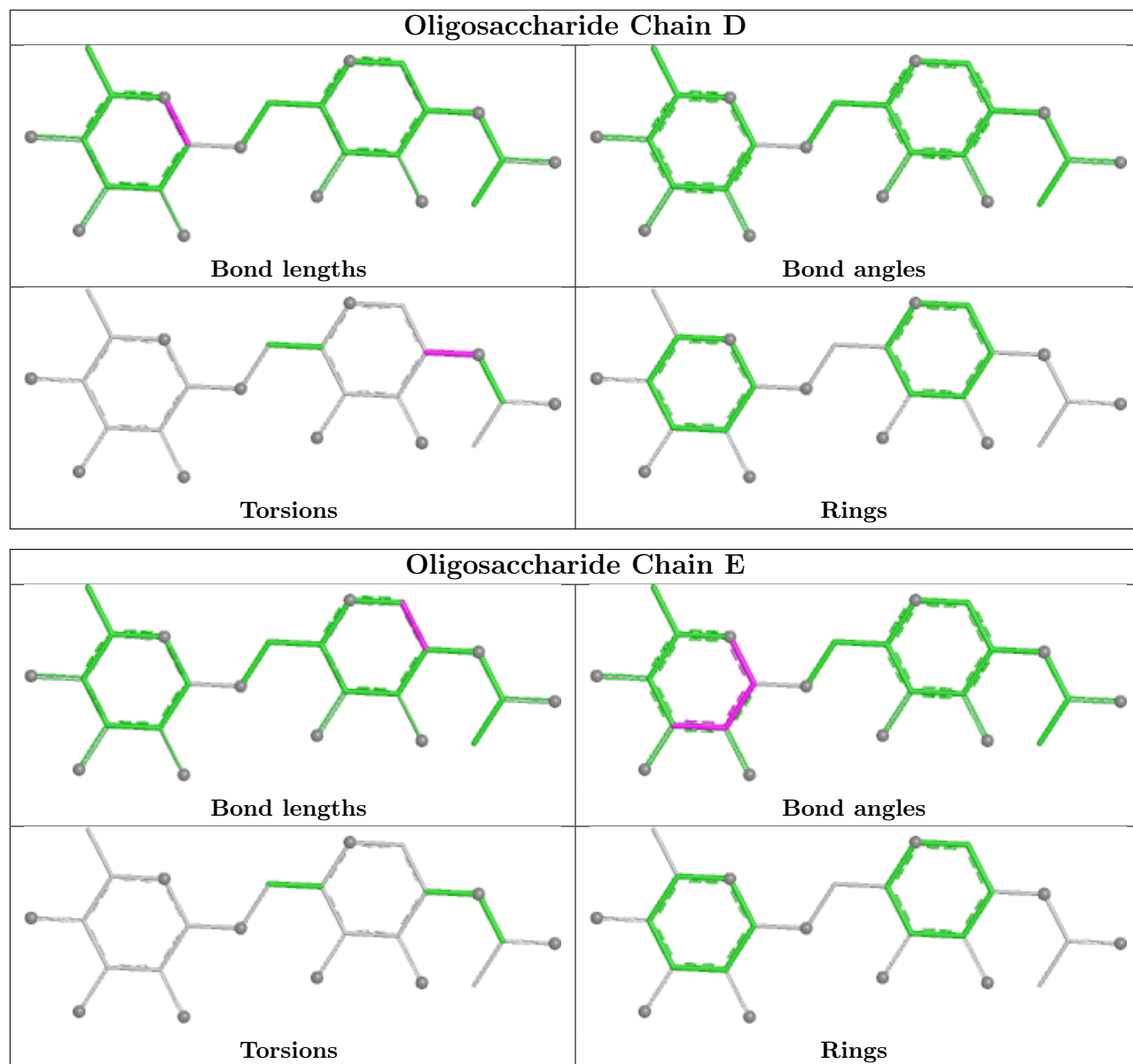
There are no ring outliers.

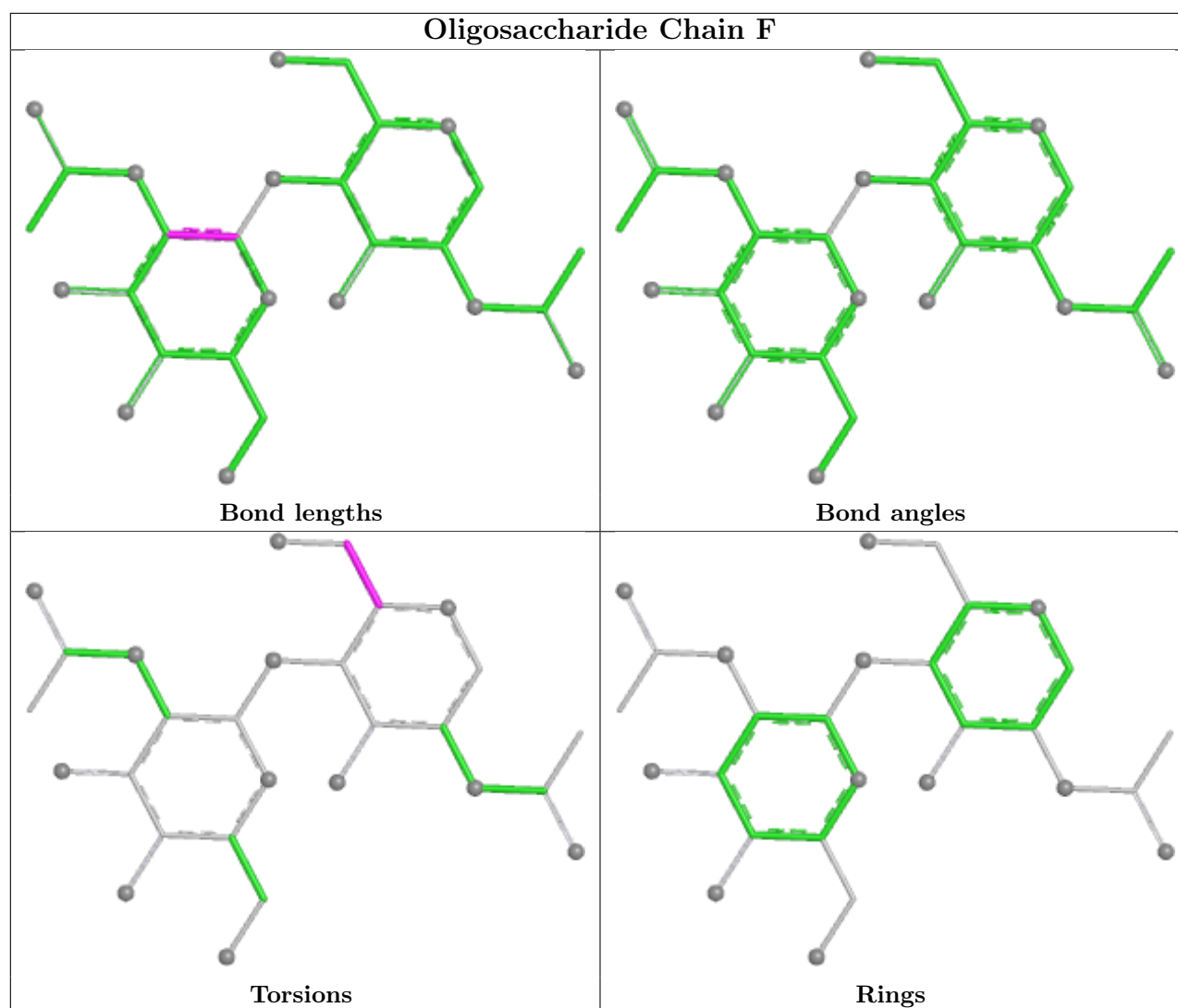
1 monomer is involved in 1 short contact:

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 [i](#)

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	$\# Z > 2$
13	PG4	B	710[A]	-	12,12,12	0.54	0	11,11,11	0.30	0
5	NAG	B	703	1	14,14,15	0.58	0	17,19,21	0.64	0
13	PG4	B	710[B]	-	12,12,12	0.53	0	11,11,11	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	A	713	-	3,3,3	0.36	0	2,2,2	0.55	0
10	EDO	A	716	-	3,3,3	0.47	0	2,2,2	0.43	0
11	PEG	A	717	-	6,6,6	0.50	0	5,5,5	0.30	0
8	1IU	A	711	7	31,34,34	2.13	6 (19%)	38,47,47	1.66	5 (13%)
6	BO3	A	708	-	3,3,3	0.30	0	3,3,3	0.43	0
5	NAG	A	701	1	14,14,15	0.49	0	17,19,21	0.80	1 (5%)
10	EDO	A	714	-	3,3,3	0.58	0	2,2,2	0.37	0
6	BO3	A	709	-	3,3,3	0.29	0	3,3,3	0.27	0
10	EDO	B	712	-	3,3,3	0.42	0	2,2,2	0.53	0
10	EDO	B	711	-	3,3,3	0.53	0	2,2,2	0.19	0
10	EDO	B	714	-	3,3,3	0.47	0	2,2,2	0.48	0
11	PEG	B	715	-	6,6,6	0.48	0	5,5,5	0.34	0
6	BO3	B	706	-	3,3,3	0.30	0	3,3,3	0.29	0
10	EDO	A	715	-	3,3,3	0.56	0	2,2,2	0.21	0
12	PGE	A	718[A]	-	9,9,9	0.41	0	8,8,8	0.69	0
10	EDO	B	713	-	3,3,3	0.49	0	2,2,2	0.34	0
12	PGE	A	718[B]	-	9,9,9	0.36	0	8,8,8	0.61	0
12	PGE	B	716	-	9,9,9	0.40	0	8,8,8	0.47	0
8	1IU	B	708	7	31,34,34	2.06	6 (19%)	38,47,47	1.68	8 (21%)

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
13	PG4	B	710[A]	-	-	4/10/10/10	-
5	NAG	B	703	1	-	2/6/23/26	0/1/1/1
13	PG4	B	710[B]	-	-	3/10/10/10	-
10	EDO	A	713	-	-	0/1/1/1	-
10	EDO	A	716	-	-	0/1/1/1	-
11	PEG	A	717	-	-	1/4/4/4	-
8	1IU	A	711	7	-	9/34/39/39	0/2/2/2
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
10	EDO	A	714	-	-	1/1/1/1	-
10	EDO	B	712	-	-	1/1/1/1	-
10	EDO	B	711	-	-	1/1/1/1	-
10	EDO	B	714	-	-	1/1/1/1	-
11	PEG	B	715	-	-	1/4/4/4	-
10	EDO	A	715	-	-	0/1/1/1	-
12	PGE	A	718[A]	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	B	713	-	-	0/1/1/1	-
12	PGE	A	718[B]	-	-	3/7/7/7	-
12	PGE	B	716	-	-	3/7/7/7	-
8	1IU	B	708	7	-	6/34/39/39	0/2/2/2

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	5.74	1.46	1.34
8	A	711	1IU	CAZ-NAV	5.64	1.46	1.34
8	A	711	1IU	CAY-N	5.59	1.46	1.34
8	B	708	1IU	C-NAC	4.93	1.44	1.32
8	A	711	1IU	PBG-CAQ	4.86	1.84	1.79

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	711	1IU	CBE-CAZ-NAV	5.78	124.03	116.21
8	B	708	1IU	CBE-CAZ-NAV	5.43	123.56	116.21
8	A	711	1IU	CBA-CAO-CBF	-4.55	103.44	113.34
8	B	708	1IU	CBA-CAO-CBF	-3.76	105.16	113.34
8	A	711	1IU	NAS-NAR-NAW	-2.86	107.09	110.50

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	711	1IU	CBE-CAP-CBB-NAT
8	A	711	1IU	OAG-CAZ-CBE-CAP
8	A	711	1IU	NAV-CAZ-CBE-CAP
8	B	708	1IU	CBE-CAP-CBB-NAT
8	B	708	1IU	OAG-CAZ-CBE-CAP

There are no ring outliers.

11 monomers are involved in 15 short contacts:

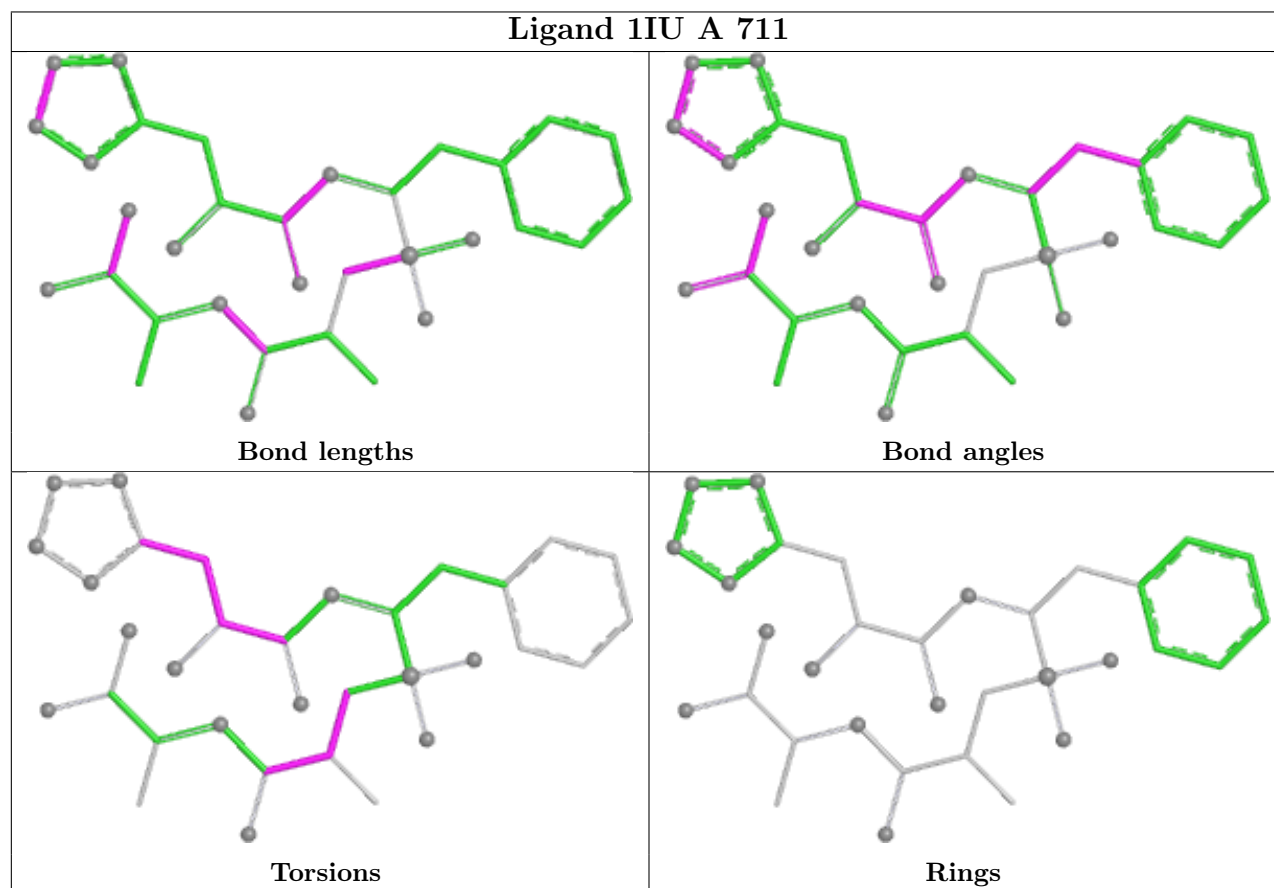
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	710[A]	PG4	3	0
13	B	710[B]	PG4	1	0
10	A	713	EDO	2	0

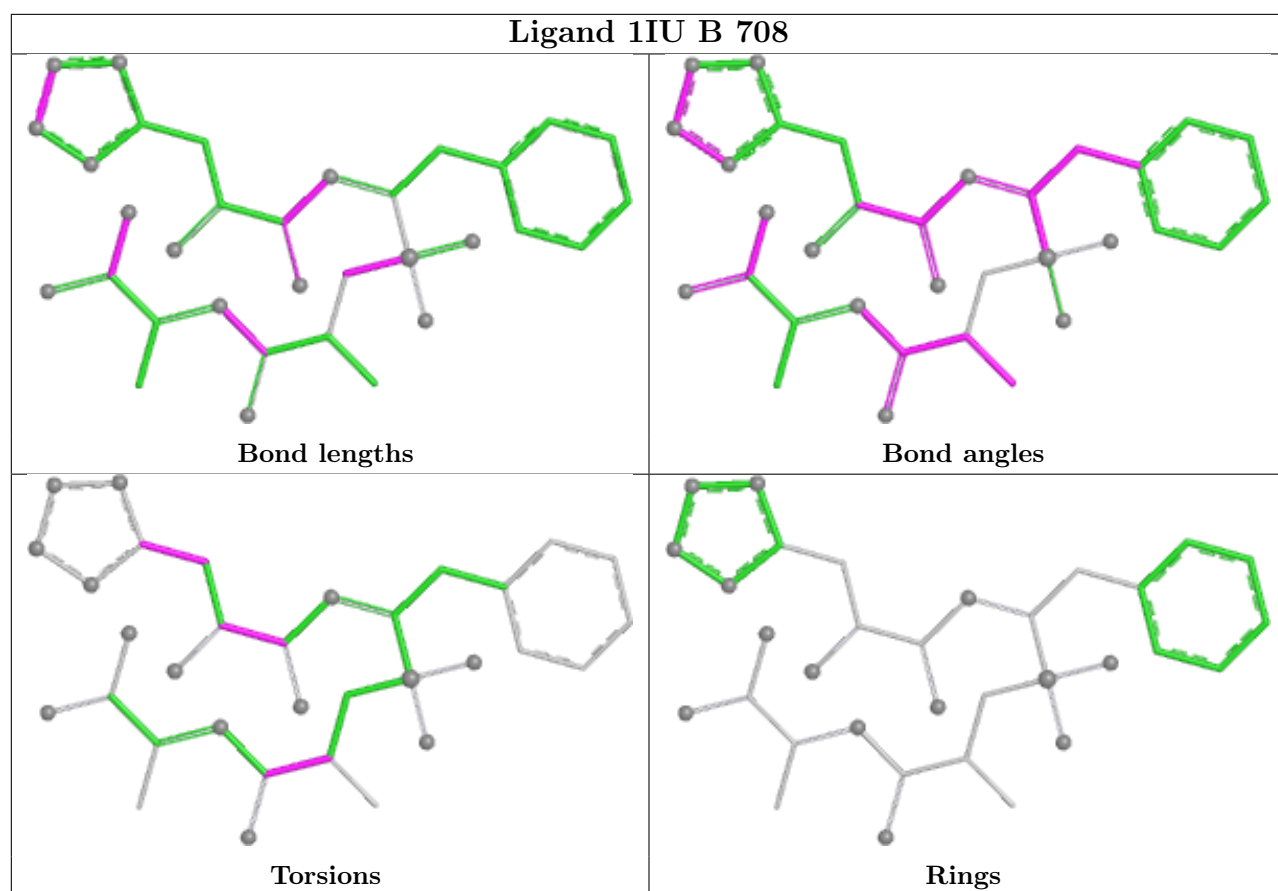
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	711	1IU	2	0
10	A	714	EDO	1	0
10	B	712	EDO	2	0
10	B	714	EDO	2	0
11	B	715	PEG	2	0
12	A	718[A]	PGE	2	0
12	A	718[B]	PGE	1	0
8	B	708	1IU	4	0

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	A	605/629 (96%)	-0.17	15 (2%) 58 58	12, 35, 57, 85	4 (0%)
1	B	595/629 (94%)	0.55	68 (11%) 10 8	15, 44, 85, 103	4 (0%)
All	All	1200/1258 (95%)	0.18	83 (6%) 23 21	12, 39, 75, 103	8 (0%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	ILE	6.6
1	B	5	LEU	5.3
1	B	88	LEU	5.2
1	B	24	TYR	5.1
1	B	20	PHE	5.1

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.

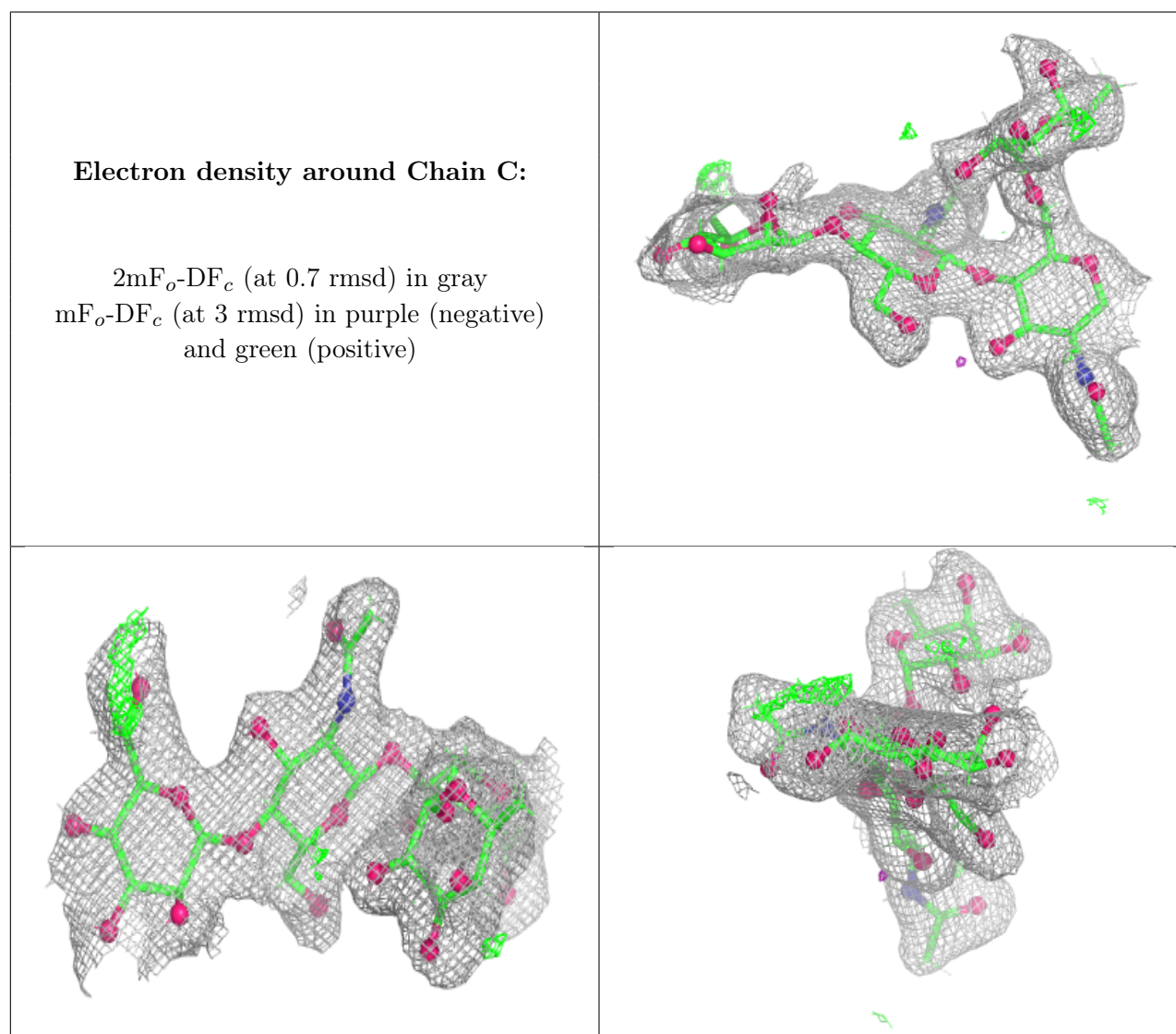
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.75	0.12	59,70,83,86	0
4	NAG	F	1	14/15	0.80	0.10	61,71,81,86	0
3	FUC	E	2	10/11	0.81	0.14	51,61,72,73	20
4	NAG	F	2	14/15	0.82	0.11	67,78,92,95	0
3	NAG	E	1	14/15	0.85	0.11	44,54,65,76	0

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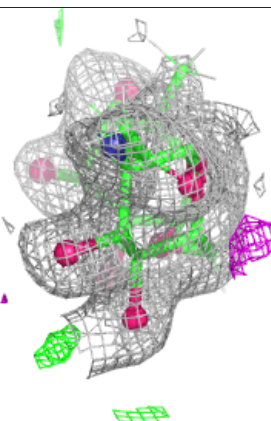
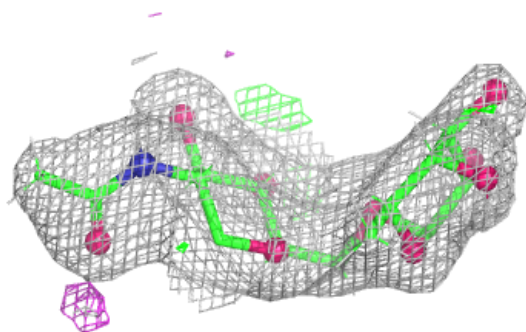
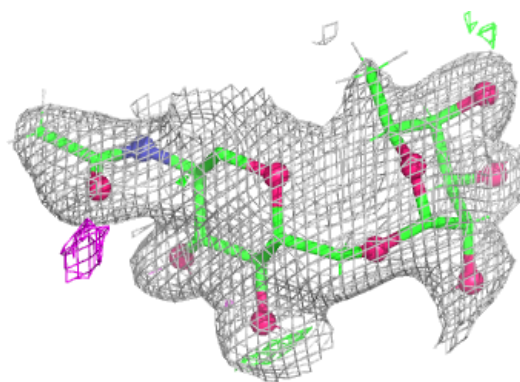
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	C	4	10/11	0.88	0.10	44,50,60,60	20
3	FUC	D	2	10/11	0.88	0.11	43,51,61,62	20
2	NAG	C	2	14/15	0.89	0.09	42,56,64,65	0
3	NAG	D	1	14/15	0.93	0.09	41,53,63,64	0
2	NAG	C	1	14/15	0.93	0.07	37,42,51,52	0

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.

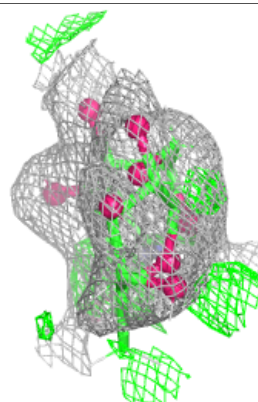
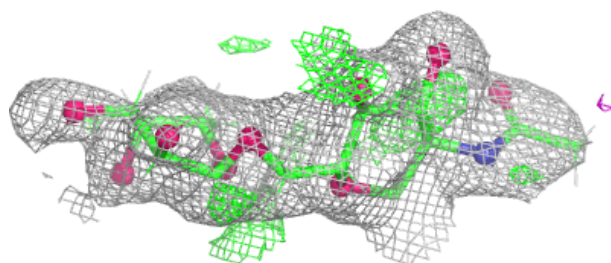
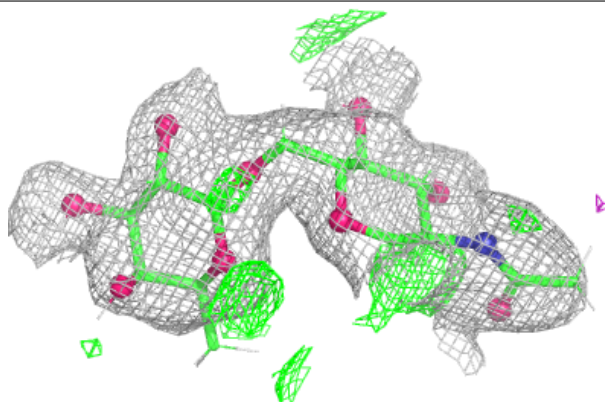


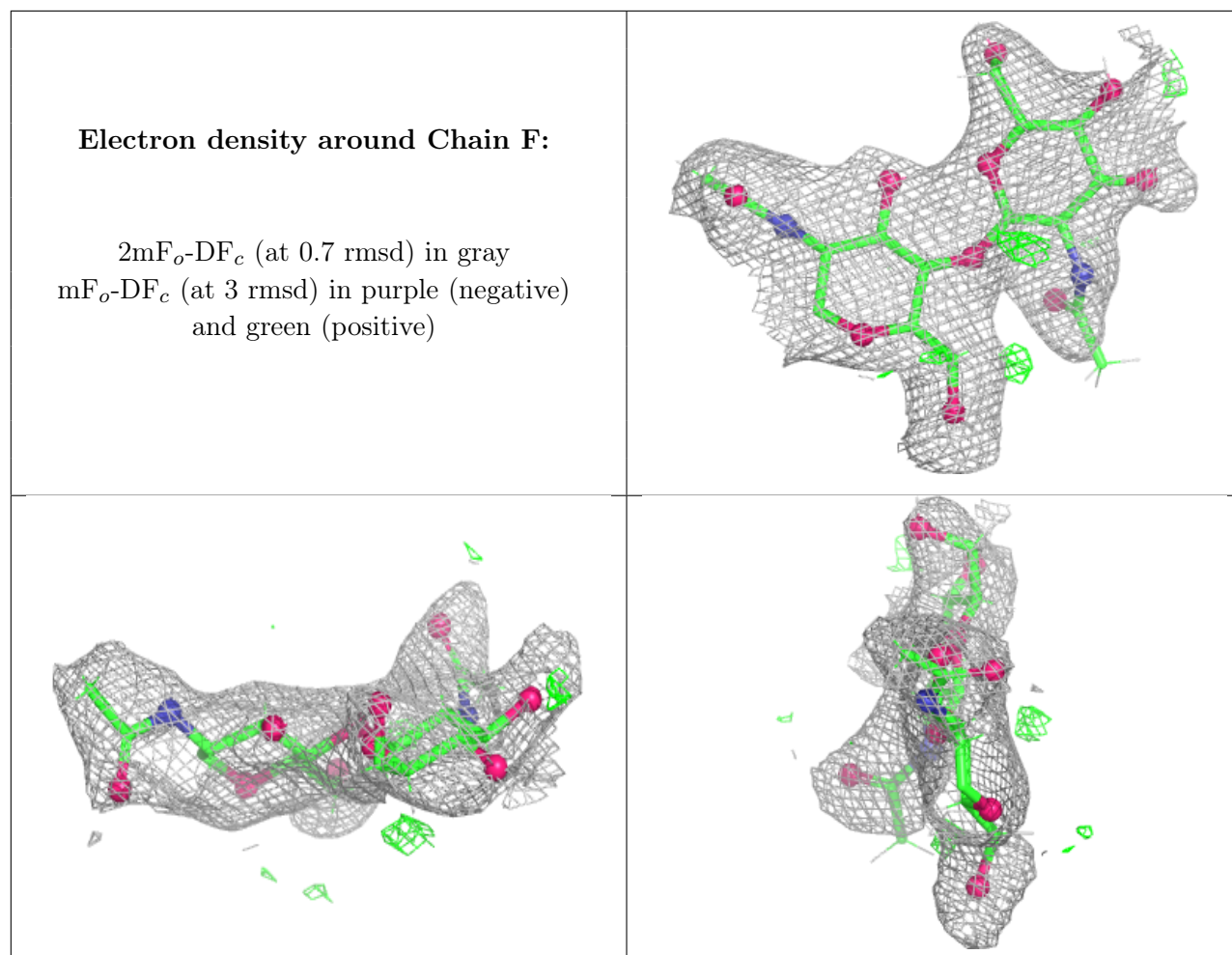
Electron density around Chain D:

$2mF_o-DF_c$ (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 [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	NAG	B	703	14/15	0.74	0.14	61,78,94,98	0
13	PG4	B	710[A]	13/13	0.75	0.18	38,45,49,50	13
13	PG4	B	710[B]	13/13	0.75	0.18	40,45,48,50	13
10	EDO	A	716	4/4	0.77	0.14	52,62,65,65	0
10	EDO	A	714	4/4	0.82	0.14	34,41,43,47	10
12	PGE	A	718[A]	10/10	0.84	0.13	30,37,44,44	24
12	PGE	A	718[B]	10/10	0.84	0.13	27,35,41,42	24
5	NAG	A	701	14/15	0.85	0.12	49,63,76,77	0
11	PEG	A	717	7/7	0.89	0.12	46,48,55,58	0
10	EDO	A	715	4/4	0.89	0.11	36,43,50,54	0

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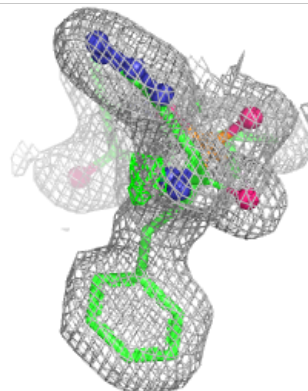
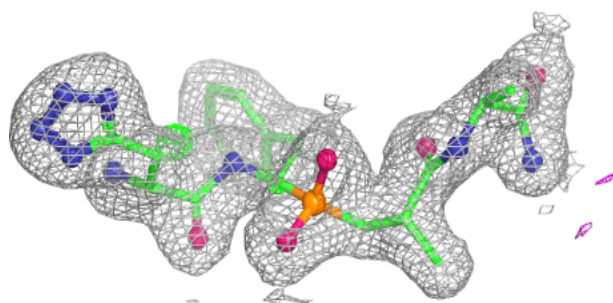
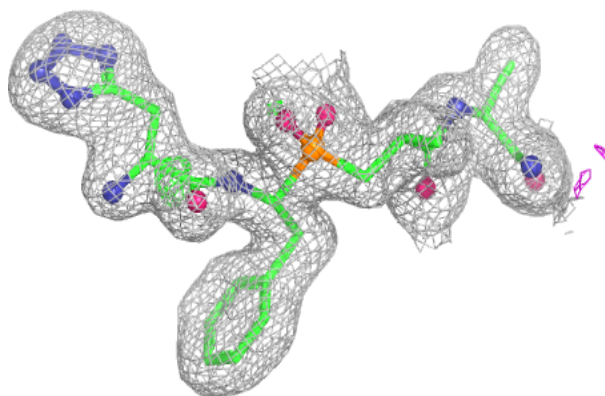
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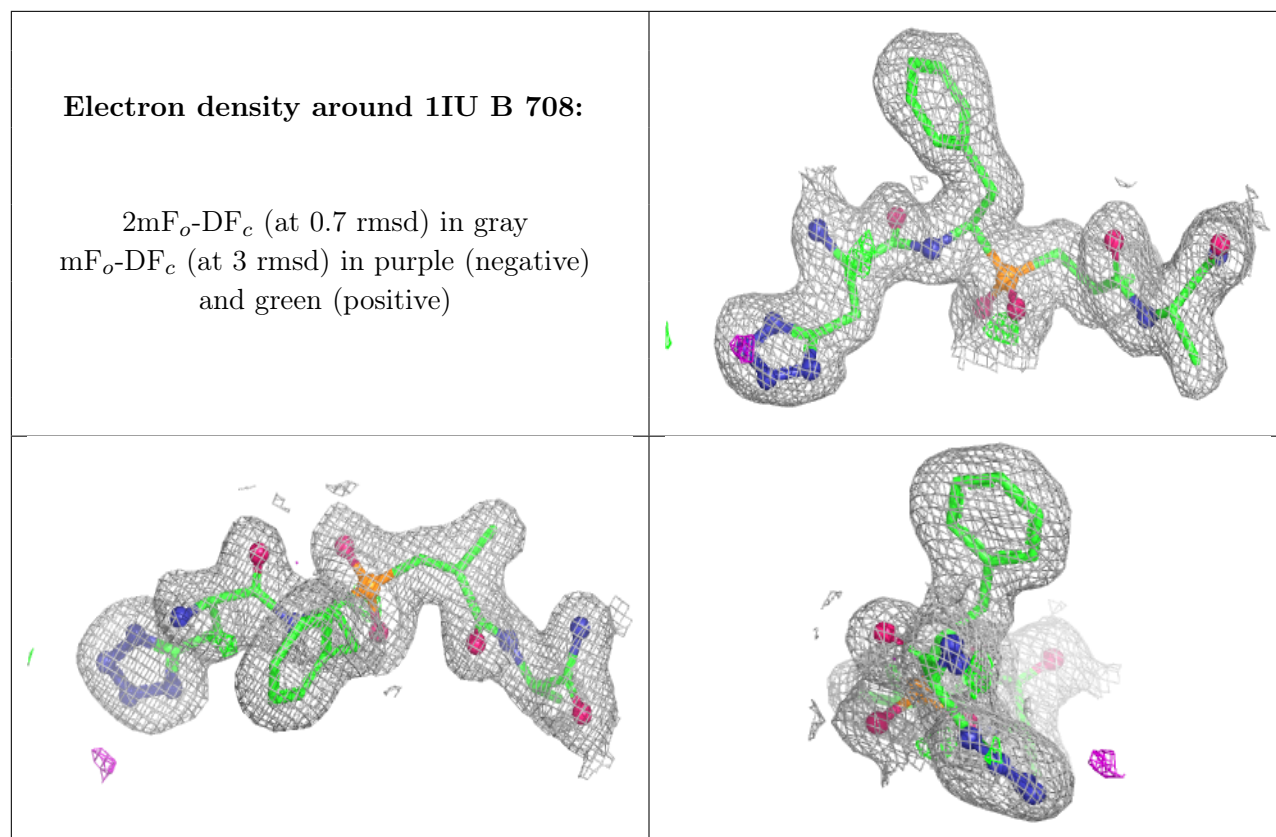
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	EDO	B	711	4/4	0.89	0.11	50,60,67,70	0
10	EDO	B	713	4/4	0.89	0.11	52,62,64,67	0
10	EDO	B	714	4/4	0.89	0.14	40,48,52,56	0
10	EDO	A	713	4/4	0.90	0.10	37,44,45,48	10
6	BO3	B	706	4/4	0.90	0.13	38,44,45,48	0
10	EDO	B	712	4/4	0.92	0.10	40,48,53,53	0
12	PGE	B	716	10/10	0.92	0.09	34,46,57,57	0
11	PEG	B	715	7/7	0.93	0.09	38,42,47,48	0
6	BO3	A	708	4/4	0.93	0.15	36,39,40,40	0
6	BO3	A	709	4/4	0.96	0.08	45,46,48,55	0
8	1IU	A	711	33/33	0.97	0.06	19,24,32,33	0
8	1IU	B	708	33/33	0.97	0.07	19,26,38,40	0
9	CL	B	709	1/1	0.97	0.05	30,30,30,30	0
9	CL	A	712	1/1	0.99	0.05	22,22,22,22	0
7	ZN	B	707	1/1	1.00	0.01	25,25,25,25	0
7	ZN	A	710	1/1	1.00	0.01	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_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.