



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2025 – 04:30 pm BST

PDB ID : 9H1B / pdb\_00009h1b  
Title : Crystal structure of Angiotensin-1 converting enzyme N-domain in complex with dual ACE/NEP inhibitor AD015  
Authors : Cozier, G.E.; Acharya, K.R.  
Deposited on : 2024-10-09  
Resolution : 1.70 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](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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

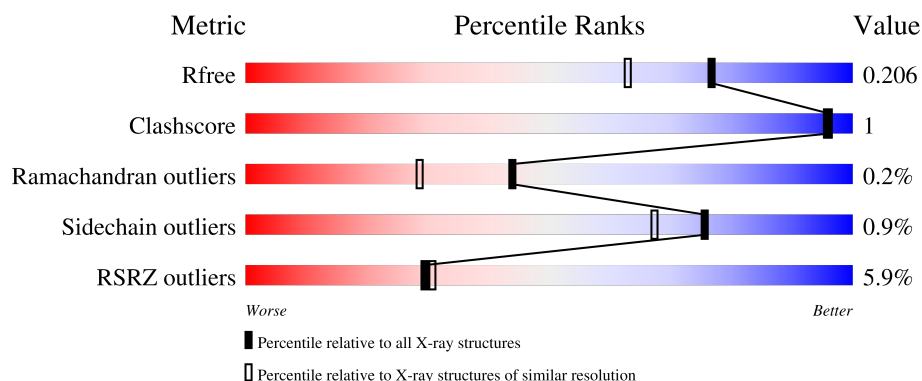
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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  $\geq 3$ , 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	628	
1	B	628	
2	C	4	
2	F	4	
3	D	2	

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Mol	Chain	Length	Quality of chain
3	G	2	 50%50%
4	E	2	 50%50%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 21119 atoms, of which 9918 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.

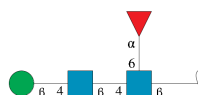
- Molecule 1 is a protein called Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	604	Total	C	H	N	O	S	0	9	0
			9789	3213	4774	869	914	19			
1	B	605	Total	C	H	N	O	S	0	6	0
			9749	3206	4753	858	913	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	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			
2	F	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.



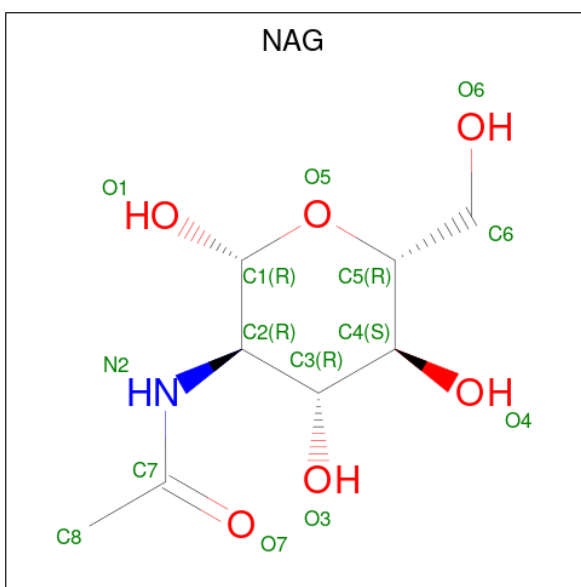
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
3	G	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

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



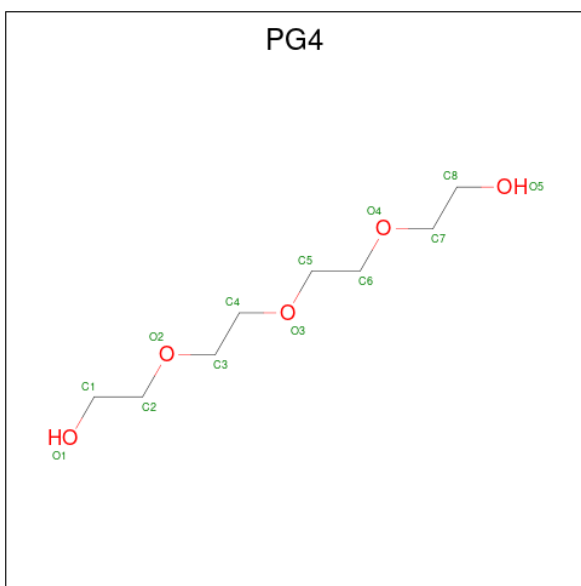
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



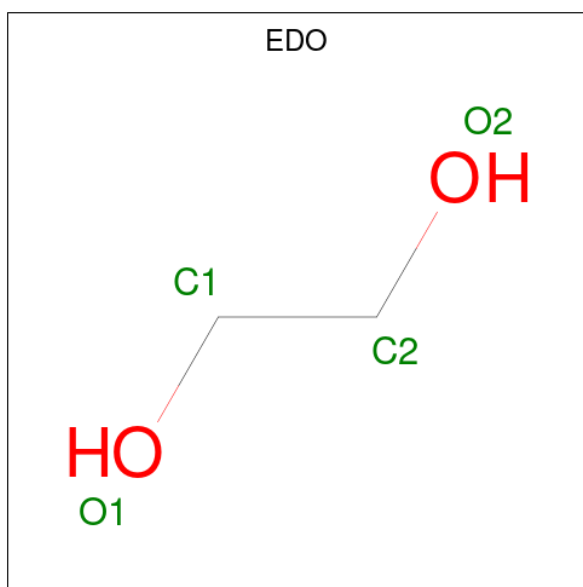
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	1
			31	8	18	5		

- Molecule 7 is ACETIC ACID (CCD ID: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



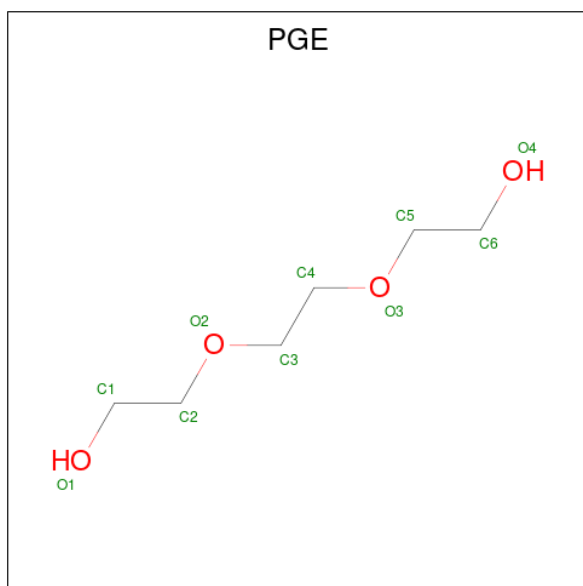
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		

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

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

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

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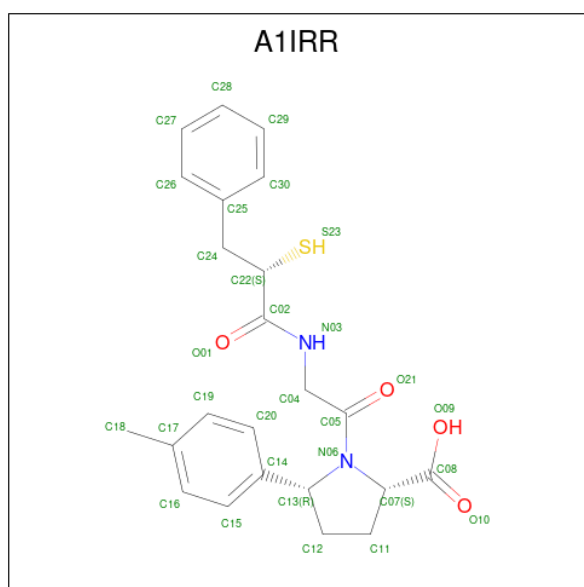
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Zn	0	0
			1	1		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 12 is (2 {S},5 {R})-5-(4-methylphenyl)-1-[2-[[[(2 {S})-3-phenyl-2-sulfanyl-propano yl]amino]ethanoyl]pyrrolidine-2-carboxylic acid (CCD ID: A1IRR) (formula: C<sub>23</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	A	1	Total	C	H	N	O	S	0	0
			55	23	25	2	4	1		
12	B	1	Total	C	H	N	O	S	0	0
			55	23	25	2	4	1		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

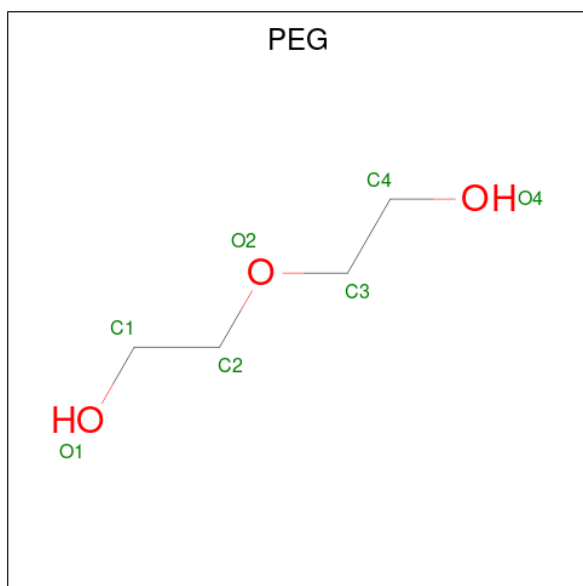
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Mg	0	0
			1	1		

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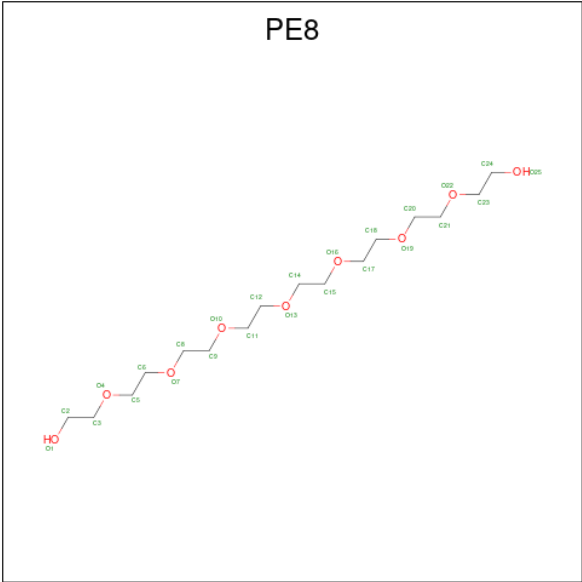
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	2	Total	Mg	0	0
			2	2		

- Molecule 14 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 15 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula:  $C_{16}H_{34}O_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	H	O	0	0
			59	16	34	9		

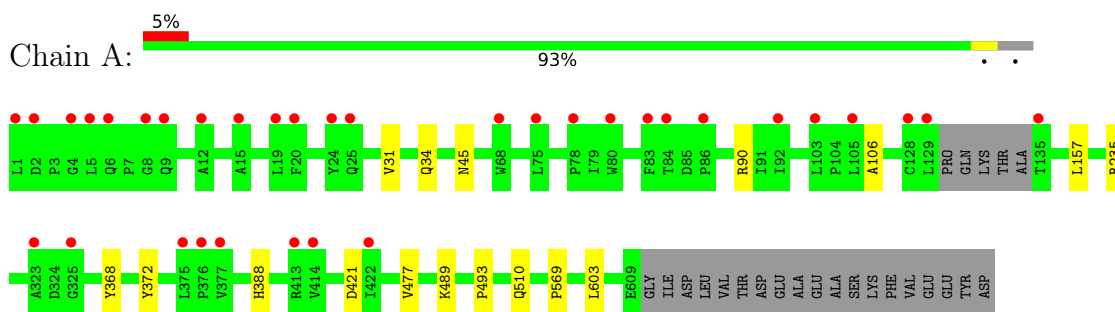
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	355	Total	O	0	2
			357	357		
16	B	451	Total	O	0	0
			451	451		

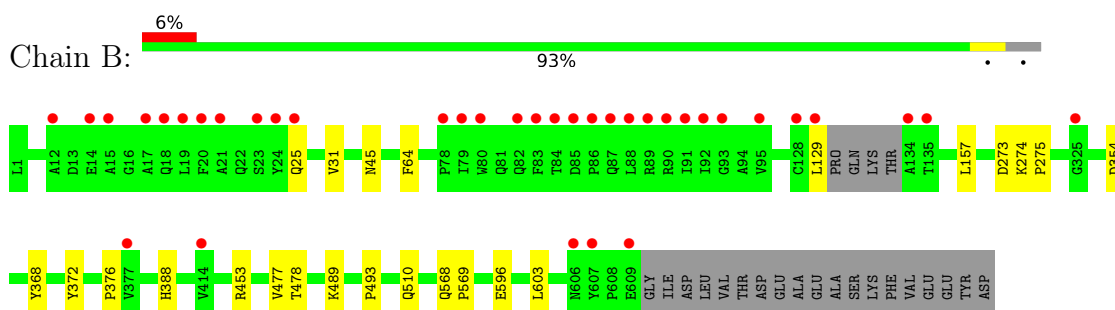
### 3 Residue-property plots

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, soluble form



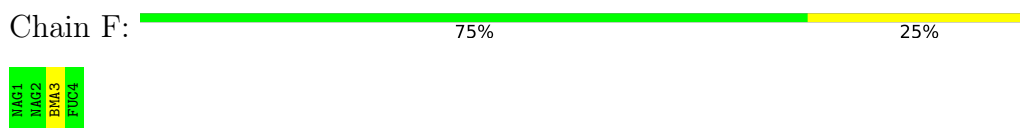
- Molecule 1: Angiotensin-converting enzyme, soluble form



- 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 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 G:  50% 50%

MAG1  
FUC2

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

Chain E:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.73Å 76.94Å 82.40Å 88.81° 64.37° 75.32°	Depositor
Resolution (Å)	56.13 – 1.70 56.13 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (56.13-1.70) 97.3 (56.13-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.180 , 0.209 0.178 , 0.206	Depositor DCC
$R_{free}$ test set	2024 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 45.5	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	0.97	EDS
Total number of atoms	21119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ACY, FUC, PGE, PG4, PE8, A1IRR, MG, ZN, CL, NAG, BMA, 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	0.47	0/5170	0.58	0/7037
1	B	0.53	0/5151	0.61	0/7015
All	All	0.50	0/10321	0.59	0/14052

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	5015	4774	4787	8	0
1	B	4996	4753	4764	12	0
2	C	49	43	43	0	0
2	F	49	43	43	0	0
3	D	24	22	22	1	0
3	G	24	22	22	1	0
4	E	28	25	25	0	0
5	A	14	13	13	0	0
6	A	13	18	13	0	0
7	A	4	3	3	0	0
7	B	8	6	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	16	24	24	0	0
8	B	16	24	24	0	0
9	A	10	14	14	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	30	25	0	0	0
12	B	30	25	0	1	0
13	A	1	0	0	0	0
13	B	2	0	0	0	0
14	B	35	50	44	0	0
15	B	25	34	34	0	0
16	A	357	0	0	3	0
16	B	451	0	0	2	0
All	All	11201	9918	9881	21	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASP:OD2	16:B:801:HOH:O	2.09	0.69
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.79	0.65
1:A:106:ALA:O	16:A:801:HOH:O	2.18	0.55
1:B:25:GLN:OE1	1:B:376:PRO:HB2	2.08	0.54
1:B:453:ARG:HD3	16:B:952:HOH:O	2.08	0.53
1:B:274:LYS:HB3	1:B:275:PRO:HD2	1.92	0.50
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.95	0.48
1:B:489:LYS:O	1:B:493:PRO:HD2	2.14	0.48
1:B:568:GLN:HB3	7:B:706:ACY:H2	1.95	0.47
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.96	0.47
1:A:31:VAL:O	1:A:34:GLN:HG3	2.14	0.47
1:B:31:VAL:HG21	1:B:64:PHE:CD1	2.51	0.46
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.97	0.46
1:A:489:LYS:O	1:A:493:PRO:HD2	2.17	0.45
12:B:715:A1IRR:O21	12:B:715:A1IRR:C08	2.65	0.44
1:B:596:GLU:OE2	3:D:1:NAG:O7	2.36	0.43
1:A:90:ARG:NH2	16:A:830:HOH:O	2.51	0.42
1:A:235:ARG:NH1	16:A:835:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLN:HG2	1:A:569:PRO:HG2	2.00	0.42
1:B:510:GLN:HG2	1:B:569:PRO:HG2	2.01	0.42
1:B:478:THR:HB	3:G:2:FUC:H2	2.02	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	609/628 (97%)	602 (99%)	6 (1%)	1 (0%)	44	29
1	B	607/628 (97%)	597 (98%)	9 (2%)	1 (0%)	44	29
All	All	1216/1256 (97%)	1199 (99%)	15 (1%)	2 (0%)	44	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	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	529/540 (98%)	525 (99%)	4 (1%)	79	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	526/540 (97%)	521 (99%)	5 (1%)	73	64
All	All	1055/1080 (98%)	1046 (99%)	9 (1%)	75	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	421	ASP
1	B	129	LEU
1	B	273	ASP
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS

Sometimes 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 [i](#)

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

## 5.5 Carbohydrates [i](#)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	2,1	14,14,15	0.84	1 (7%)	17,19,21	0.71	0
2	NAG	C	2	2	14,14,15	0.77	0	17,19,21	0.89	0
2	BMA	C	3	2	11,11,12	0.85	0	15,15,17	1.94	2 (13%)
2	FUC	C	4	2	10,10,11	0.80	0	14,14,16	0.99	0
3	NAG	D	1	1,3	14,14,15	0.57	0	17,19,21	1.03	1 (5%)
3	FUC	D	2	3	10,10,11	0.71	0	14,14,16	1.15	0
4	NAG	E	1	4,1	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
4	NAG	E	2	4	14,14,15	0.67	0	17,19,21	0.80	0
2	NAG	F	1	2,1	14,14,15	0.75	0	17,19,21	0.68	0
2	NAG	F	2	2	14,14,15	0.78	0	17,19,21	0.87	0
2	BMA	F	3	2	11,11,12	0.78	0	15,15,17	1.80	3 (20%)
2	FUC	F	4	2	10,10,11	0.73	0	14,14,16	0.75	0
3	NAG	G	1	1,3	14,14,15	0.63	0	17,19,21	1.01	1 (5%)
3	FUC	G	2	3	10,10,11	0.57	0	14,14,16	1.50	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	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	-	1/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	FUC	F	4	2	-	-	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-2.03	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	C1-O5-C5	5.56	119.73	112.19
2	F	3	BMA	C1-O5-C5	4.86	118.78	112.19
3	G	2	FUC	C1-O5-C5	3.17	119.95	112.78
4	E	1	NAG	C1-O5-C5	3.00	116.25	112.19
3	G	1	NAG	O5-C5-C6	2.86	111.69	107.20
2	F	3	BMA	O5-C5-C6	2.43	111.01	107.20
3	G	2	FUC	C1-C2-C3	2.34	112.55	109.67
3	D	1	NAG	C1-O5-C5	2.34	115.36	112.19
2	F	3	BMA	O4-C4-C3	-2.32	104.98	110.35
2	C	3	BMA	O4-C4-C3	-2.04	105.63	110.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

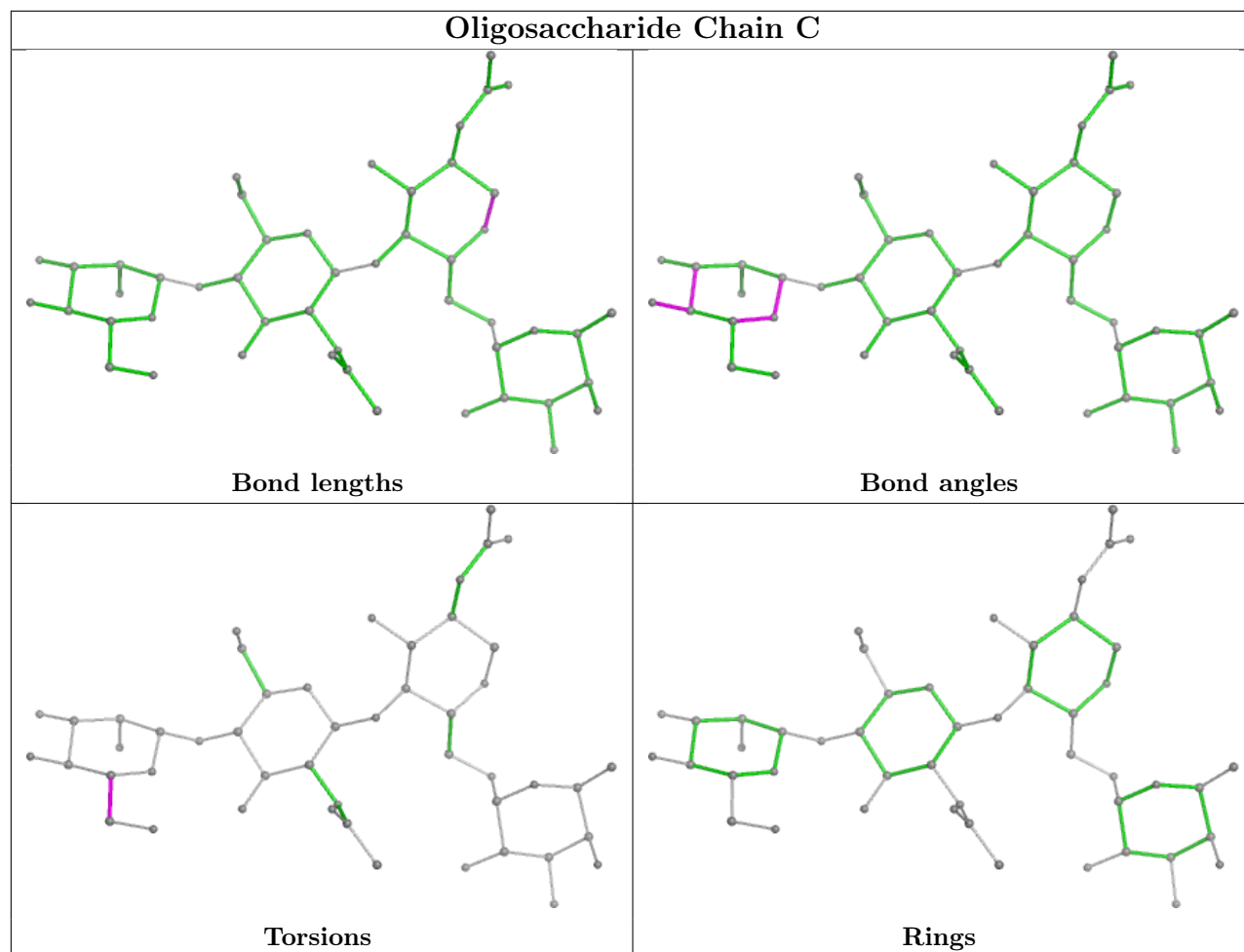
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

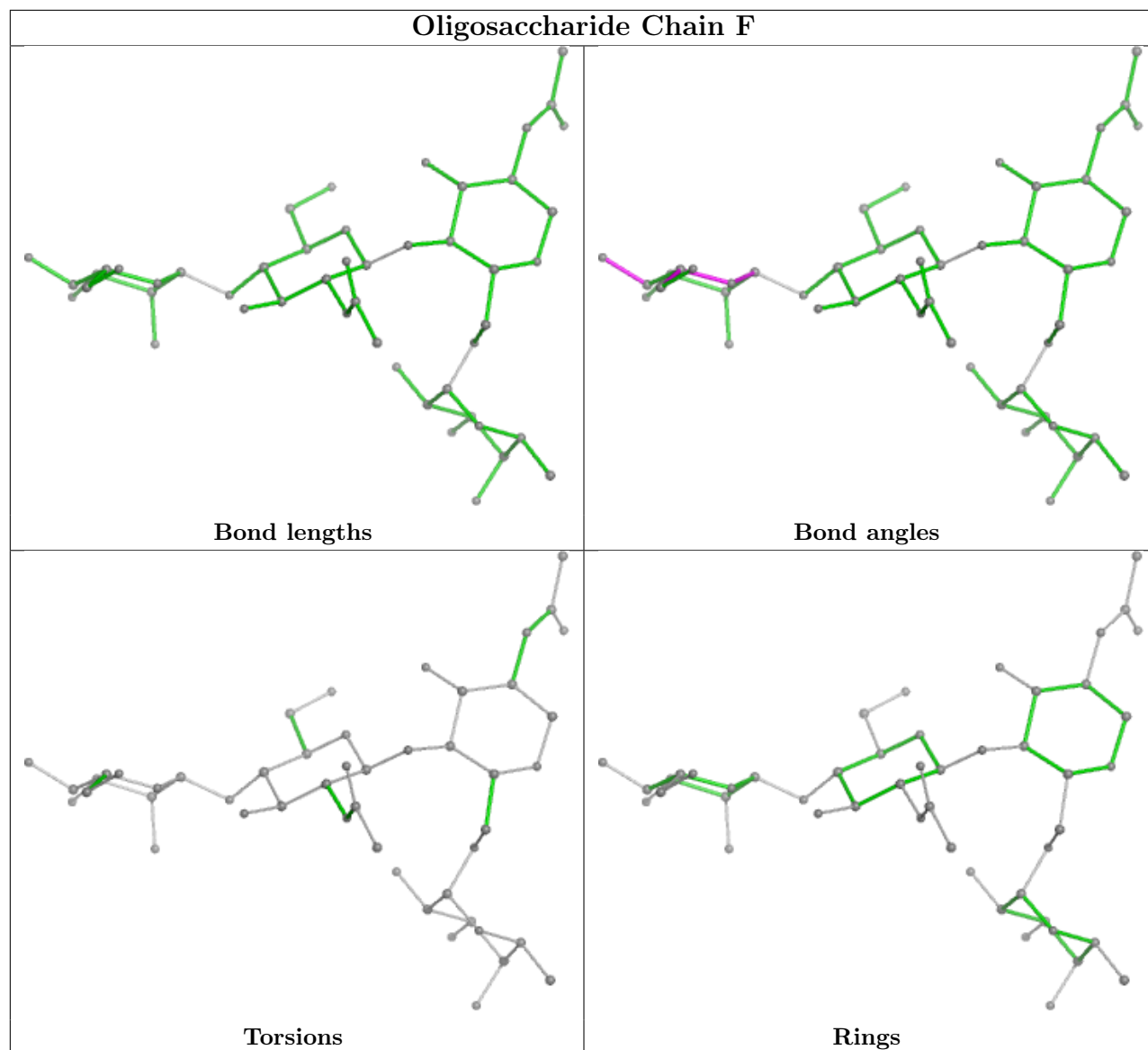
There are no ring outliers.

2 monomers are involved in 2 short contacts:

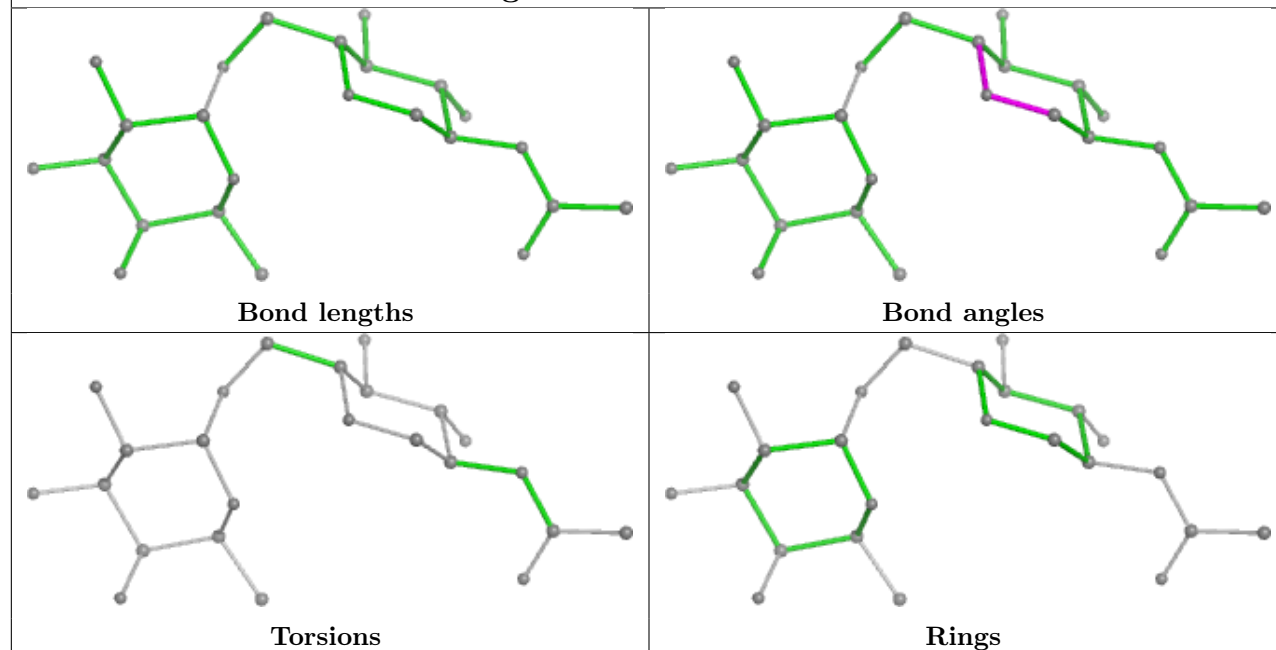
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	G	2	FUC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

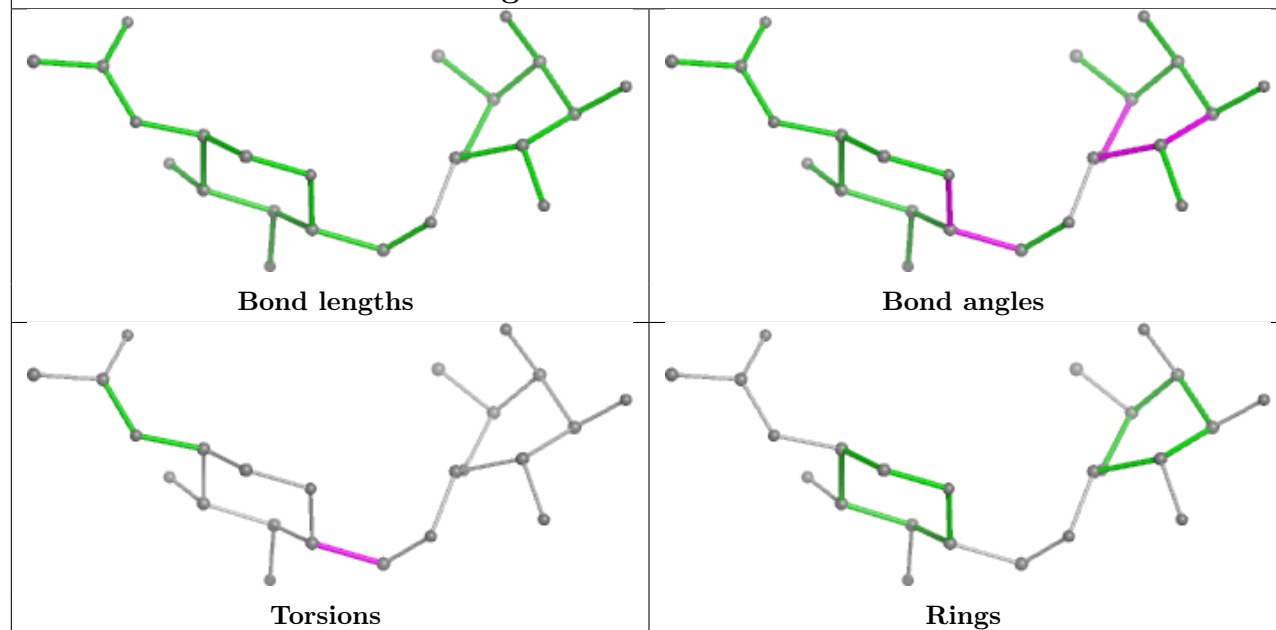


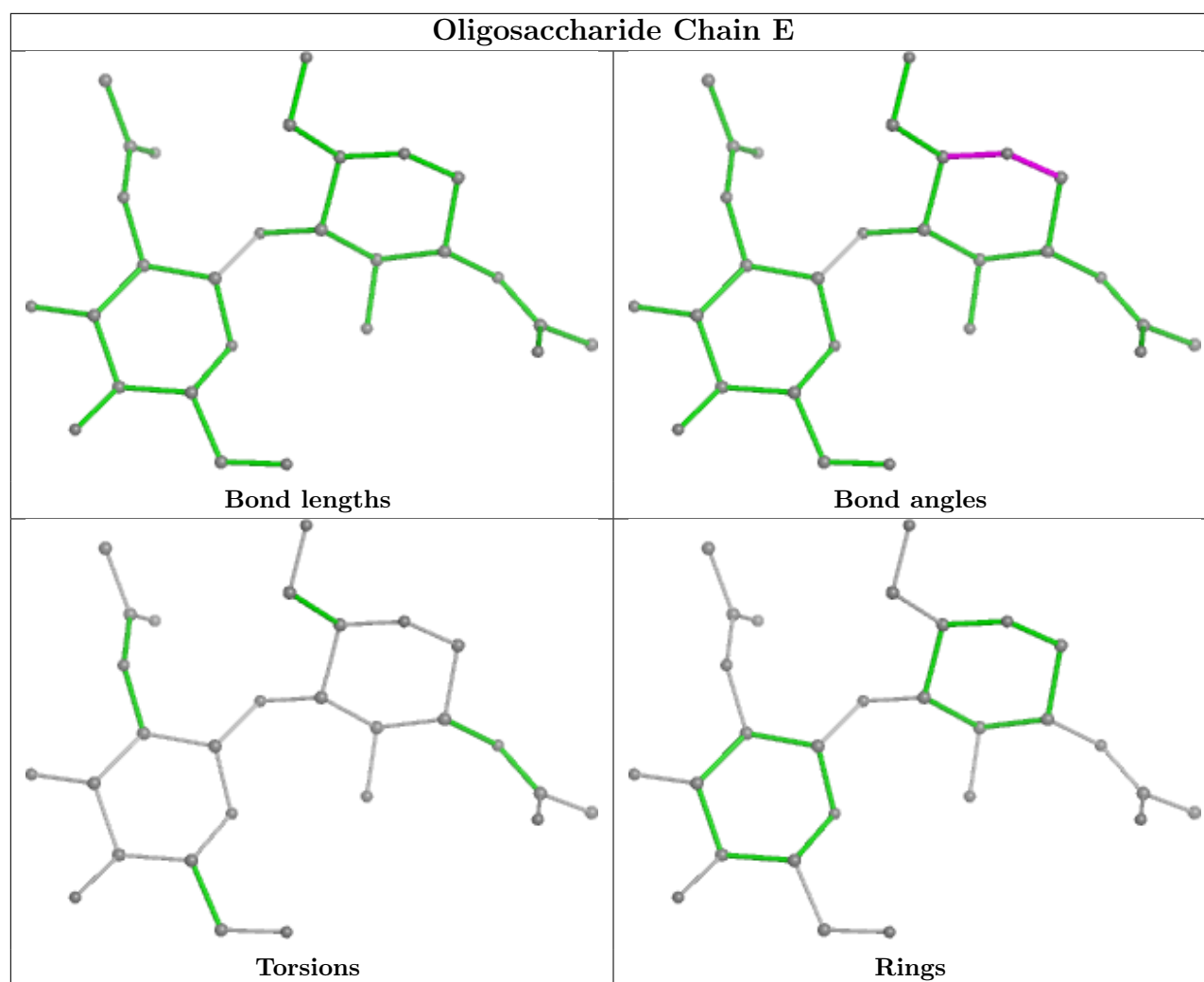


## Oligosaccharide Chain D



## Oligosaccharide Chain G





## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 7 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
12	A1IRR	A	711	10	31,32,32	2.77	6 (19%)	38,44,44	1.66	10 (26%)
14	PEG	B	705	-	6,6,6	0.22	0	5,5,5	0.30	0
8	EDO	A	708	-	3,3,3	0.27	0	2,2,2	0.34	0
12	A1IRR	B	715	10	31,32,32	2.86	7 (22%)	38,44,44	1.85	12 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ACY	A	703	-	3,3,3	1.30	0	3,3,3	1.21	0
8	EDO	B	709	-	3,3,3	0.31	0	2,2,2	0.16	0
14	PEG	B	704	-	6,6,6	0.26	0	5,5,5	0.27	0
8	EDO	B	707	-	3,3,3	0.21	0	2,2,2	0.14	0
14	PEG	B	701	-	6,6,6	0.27	0	5,5,5	0.49	0
7	ACY	B	711	-	3,3,3	1.24	0	3,3,3	1.08	0
8	EDO	A	707	-	3,3,3	0.29	0	2,2,2	0.11	0
14	PEG	B	712[B]	-	6,6,6	0.25	0	5,5,5	0.36	0
7	ACY	B	706	-	3,3,3	1.24	0	3,3,3	1.01	0
8	EDO	A	704	-	3,3,3	0.28	0	2,2,2	0.02	0
6	PG4	A	702[A]	-	12,12,12	0.33	0	11,11,11	0.27	0
9	PGE	A	705	-	9,9,9	0.24	0	8,8,8	0.52	0
8	EDO	B	708	-	3,3,3	0.28	0	2,2,2	0.29	0
8	EDO	B	710	-	3,3,3	0.27	0	2,2,2	0.26	0
8	EDO	A	706	-	3,3,3	0.28	0	2,2,2	0.20	0
15	PE8	B	702	-	24,24,24	0.28	0	23,23,23	0.23	0
5	NAG	A	701	1	14,14,15	0.53	0	17,19,21	0.97	1 (5%)
14	PEG	B	703	-	6,6,6	0.24	0	5,5,5	0.40	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
12	A1IRR	A	711	10	-	1/23/38/38	0/3/3/3
14	PEG	B	705	-	-	2/4/4/4	-
8	EDO	A	708	-	-	0/1/1/1	-
12	A1IRR	B	715	10	-	1/23/38/38	0/3/3/3
8	EDO	B	709	-	-	0/1/1/1	-
14	PEG	B	704	-	-	1/4/4/4	-
8	EDO	B	707	-	-	0/1/1/1	-
14	PEG	B	701	-	-	0/4/4/4	-
8	EDO	A	707	-	-	0/1/1/1	-
14	PEG	B	712[B]	-	-	1/4/4/4	-
8	EDO	A	704	-	-	0/1/1/1	-
6	PG4	A	702[A]	-	-	4/10/10/10	-
9	PGE	A	705	-	-	1/7/7/7	-
8	EDO	B	708	-	-	0/1/1/1	-
8	EDO	B	710	-	-	1/1/1/1	-
8	EDO	A	706	-	-	0/1/1/1	-
15	PE8	B	702	-	-	9/22/22/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	701	1	-	1/6/23/26	0/1/1/1
14	PEG	B	703	-	-	1/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	715	A1IRR	C07-N06	-9.24	1.34	1.46
12	A	711	A1IRR	C07-N06	-8.81	1.34	1.46
12	A	711	A1IRR	C05-N06	8.13	1.46	1.36
12	B	715	A1IRR	C05-N06	7.76	1.46	1.36
12	B	715	A1IRR	C12-C13	-5.61	1.39	1.54
12	B	715	A1IRR	C13-N06	5.20	1.60	1.47
12	A	711	A1IRR	C12-C13	-5.05	1.41	1.54
12	A	711	A1IRR	C02-N03	4.71	1.43	1.33
12	A	711	A1IRR	C13-N06	4.70	1.59	1.47
12	B	715	A1IRR	C02-N03	4.60	1.43	1.33
12	A	711	A1IRR	C24-C25	2.45	1.57	1.51
12	B	715	A1IRR	C20-C19	2.08	1.42	1.38
12	B	715	A1IRR	O10-C08	2.01	1.28	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	715	A1IRR	O21-C05-N06	-4.61	117.43	122.29
12	B	715	A1IRR	C12-C13-N06	3.98	104.62	101.97
12	A	711	A1IRR	C12-C13-N06	3.79	104.49	101.97
12	A	711	A1IRR	C12-C13-C14	-3.55	106.73	113.61
12	B	715	A1IRR	C12-C13-C14	-3.36	107.10	113.61
12	A	711	A1IRR	C04-N03-C02	-3.15	113.58	121.37
12	B	715	A1IRR	C04-N03-C02	-3.02	113.89	121.37
12	B	715	A1IRR	C08-C07-N06	-2.86	107.47	113.01
12	B	715	A1IRR	C19-C20-C14	-2.80	118.38	121.20
5	A	701	NAG	C1-O5-C5	2.59	115.70	112.19
12	B	715	A1IRR	C15-C14-C13	-2.51	116.00	120.76
12	B	715	A1IRR	C20-C14-C15	2.41	121.30	118.29
12	B	715	A1IRR	C24-C22-C02	-2.39	106.71	112.10
12	A	711	A1IRR	C19-C20-C14	-2.39	118.79	121.20
12	A	711	A1IRR	O21-C05-N06	-2.38	119.78	122.29
12	A	711	A1IRR	C24-C22-C02	-2.38	106.74	112.10
12	A	711	A1IRR	C14-C13-N06	2.33	118.42	113.98
12	A	711	A1IRR	C15-C14-C13	-2.28	116.44	120.76
12	B	715	A1IRR	C12-C11-C07	-2.26	100.74	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	711	A1IRR	C20-C14-C15	2.24	121.09	118.29
12	B	715	A1IRR	C14-C13-N06	2.21	118.20	113.98
12	A	711	A1IRR	O09-C08-O10	-2.16	119.17	124.09
12	B	715	A1IRR	C11-C07-N06	2.11	105.12	103.09

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	711	A1IRR	S23-C22-C24-C25
9	A	705	PGE	O2-C3-C4-O3
6	A	702[A]	PG4	O4-C7-C8-O5
15	B	702	PE8	O19-C20-C21-O22
15	B	702	PE8	O4-C5-C6-O7
14	B	705	PEG	O2-C3-C4-O4
6	A	702[A]	PG4	O3-C5-C6-O4
14	B	712[B]	PEG	O2-C3-C4-O4
15	B	702	PE8	O10-C11-C12-O13
14	B	703	PEG	C4-C3-O2-C2
15	B	702	PE8	C12-C11-O10-C9
15	B	702	PE8	C20-C21-O22-C23
6	A	702[A]	PG4	C8-C7-O4-C6
14	B	705	PEG	O1-C1-C2-O2
15	B	702	PE8	O16-C17-C18-O19
15	B	702	PE8	O7-C8-C9-O10
15	B	702	PE8	C5-C6-O7-C8
15	B	702	PE8	C11-C12-O13-C14
8	B	710	EDO	O1-C1-C2-O2
6	A	702[A]	PG4	O2-C3-C4-O3
12	B	715	A1IRR	S23-C22-C24-C25
14	B	704	PEG	C1-C2-O2-C3
5	A	701	NAG	C4-C5-C6-O6

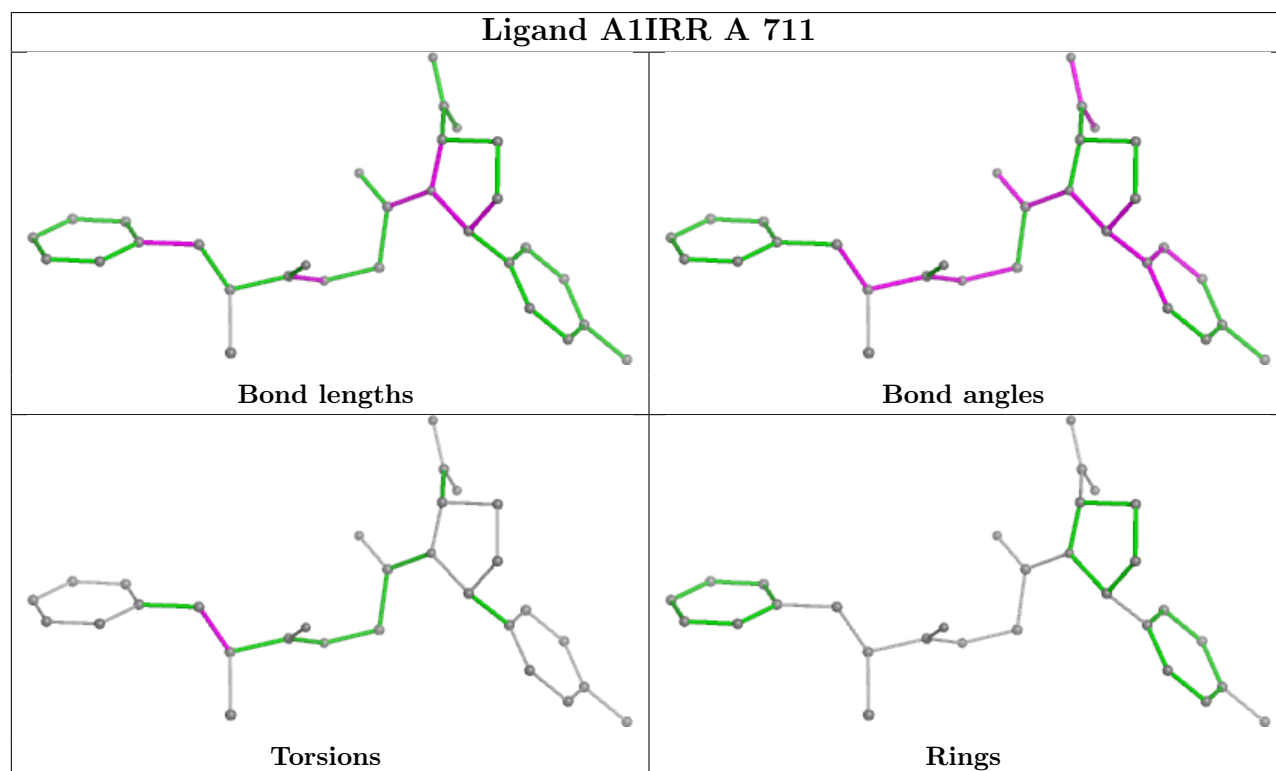
There are no ring outliers.

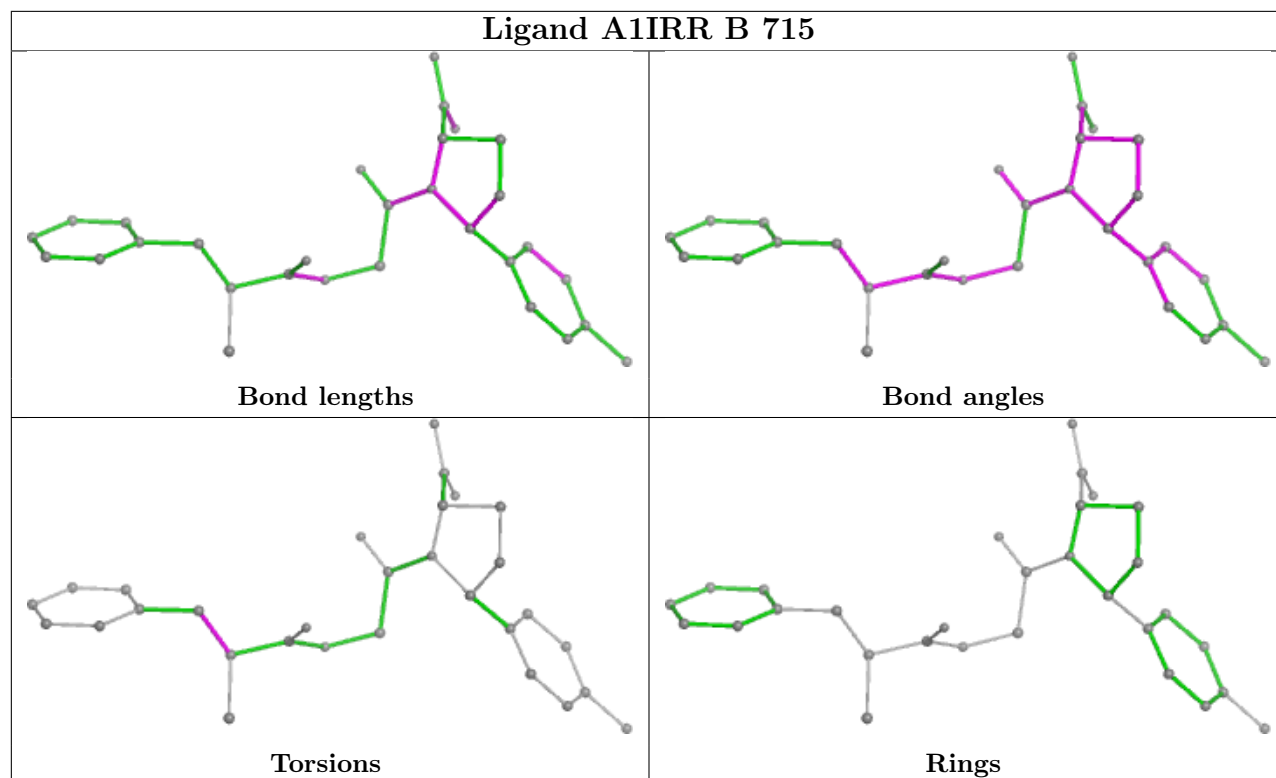
2 monomers are involved in 2 short contacts:

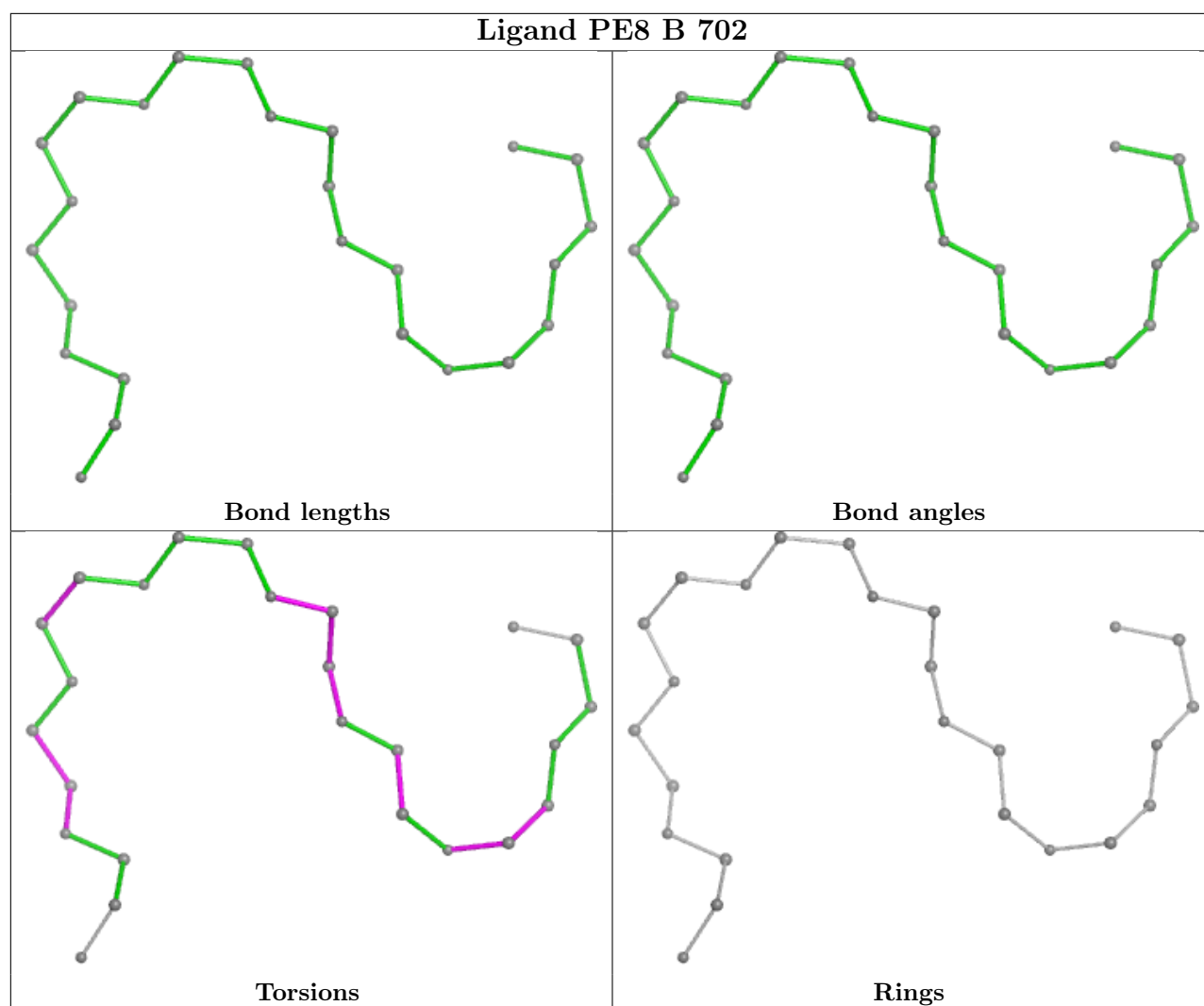
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	715	A1IRR	1	0
7	B	706	ACY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	604/628 (96%)	0.14	34 (5%) 31 33	13, 44, 76, 105	9 (1%)
1	B	605/628 (96%)	-0.16	37 (6%) 28 29	12, 36, 69, 102	6 (0%)
All	All	1209/1256 (96%)	-0.01	71 (5%) 29 31	12, 40, 74, 105	15 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	5.2
1	B	129	LEU	5.0
1	B	607	TYR	4.8
1	B	86	PRO	4.6
1	B	83	PHE	3.8
1	B	91	ILE	3.8
1	A	1	LEU	3.8
1	B	85	ASP	3.7
1	A	105	LEU	3.6
1	B	17	ALA	3.6
1	A	414	VAL	3.5
1	B	88	LEU	3.5
1	B	24	TYR	3.5
1	B	84	THR	3.4
1	A	135	THR	3.3
1	A	4	GLY	3.3
1	A	25	GLN	3.3
1	B	92	ILE	3.2
1	B	19	LEU	3.2
1	B	134	ALA	3.2
1	B	414	VAL	3.2
1	B	25	GLN	3.1
1	B	606	ASN	3.1
1	B	325	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	2.9
1	B	12	ALA	2.9
1	A	6	GLN	2.9
1	B	21	ALA	2.8
1	B	80	TRP	2.7
1	B	18	GLN	2.7
1	B	20	PHE	2.7
1	B	78	PRO	2.7
1	B	87	GLN	2.7
1	A	19	LEU	2.7
1	A	9	GLN	2.6
1	B	15	ALA	2.6
1	A	377	VAL	2.6
1	A	24	TYR	2.6
1	A	325	GLY	2.5
1	A	376	PRO	2.5
1	A	78	PRO	2.5
1	B	90	ARG	2.5
1	A	103	LEU	2.4
1	B	93	GLY	2.4
1	B	14	GLU	2.4
1	B	79	ILE	2.3
1	A	80	TRP	2.3
1	A	84	THR	2.3
1	A	75	LEU	2.3
1	A	128	CYS	2.2
1	A	92	ILE	2.2
1	A	83	PHE	2.2
1	A	422	ILE	2.2
1	A	12	ALA	2.2
1	B	23	SER	2.2
1	A	413	ARG	2.2
1	A	15	ALA	2.2
1	B	135	THR	2.2
1	B	377	VAL	2.2
1	A	68	TRP	2.1
1	B	128	CYS	2.1
1	B	89	ARG	2.1
1	B	609	GLU	2.1
1	A	375	LEU	2.1
1	B	82	GLN	2.1
1	A	2	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	323	ALA	2.1
1	A	8	GLY	2.1
1	A	20	PHE	2.0
1	B	95	VAL	2.0
1	A	86	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

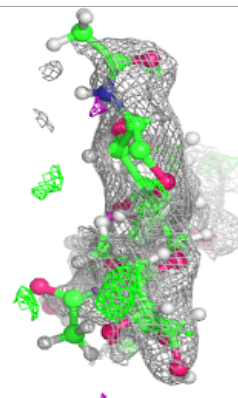
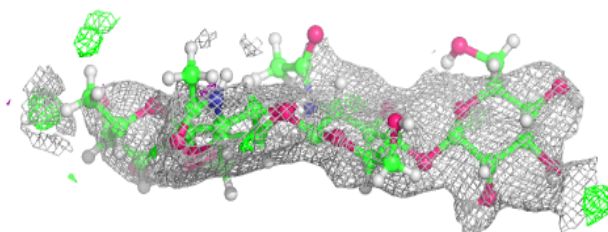
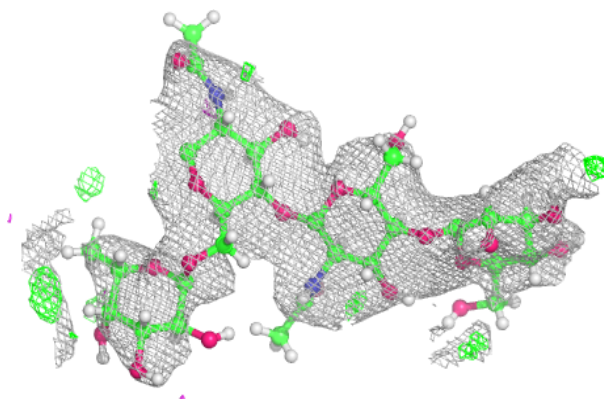
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	FUC	G	2	10/11	0.58	0.19	63,80,94,94	0
2	FUC	C	4	10/11	0.65	0.17	74,90,112,112	0
2	BMA	C	3	11/12	0.65	0.14	92,98,118,122	0
3	FUC	D	2	10/11	0.68	0.17	58,80,95,98	0
4	NAG	E	2	14/15	0.70	0.14	60,87,115,120	0
2	BMA	F	3	11/12	0.80	0.12	62,74,89,92	0
2	NAG	C	1	14/15	0.80	0.12	72,84,103,104	0
3	NAG	D	1	14/15	0.83	0.12	44,62,76,86	0
4	NAG	E	1	14/15	0.85	0.12	43,67,81,83	0
2	NAG	C	2	14/15	0.85	0.12	78,88,106,106	0
3	NAG	G	1	14/15	0.86	0.14	39,59,71,76	0
2	FUC	F	4	10/11	0.87	0.11	46,63,75,83	0
2	NAG	F	2	14/15	0.89	0.10	41,64,72,77	0
2	NAG	F	1	14/15	0.94	0.07	38,48,62,62	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.

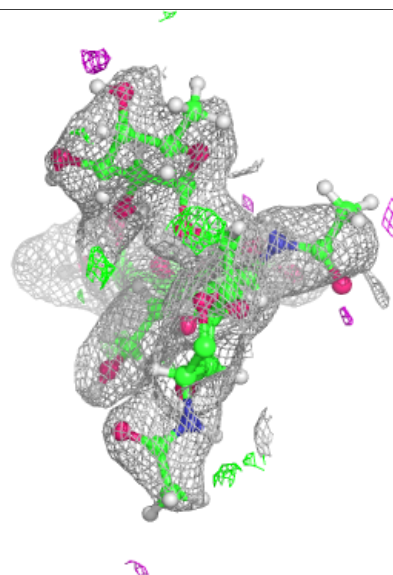
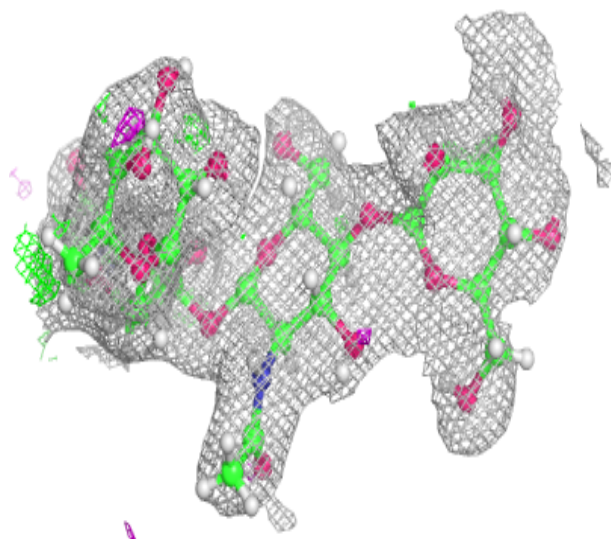
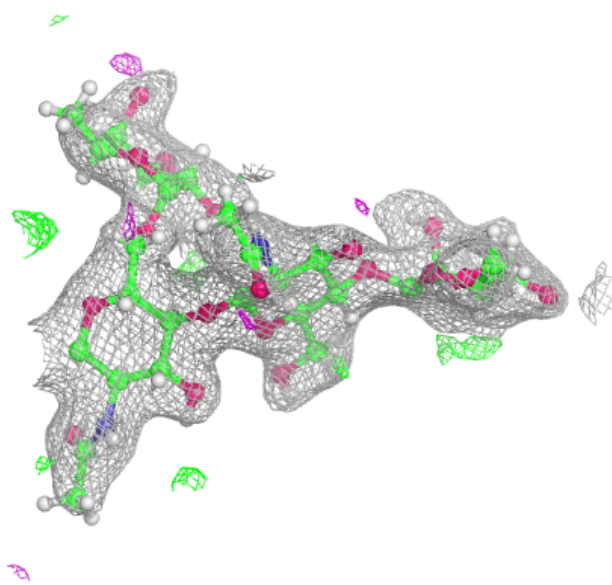
**Electron density around Chain C:**

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



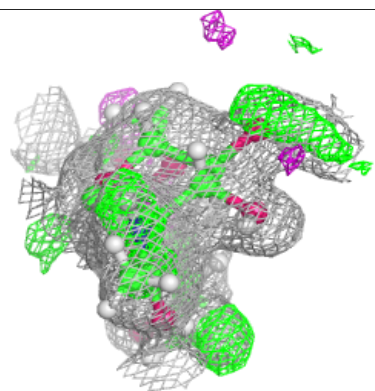
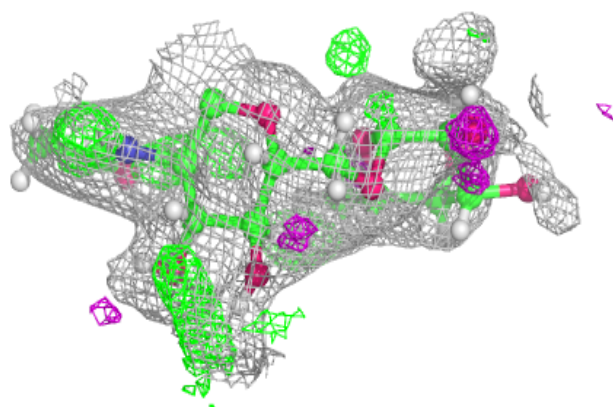
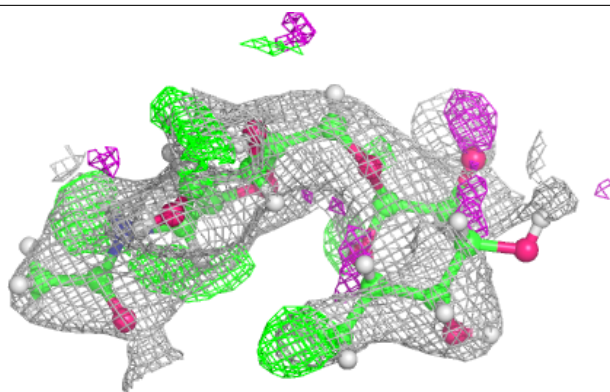
**Electron density around Chain F:**

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

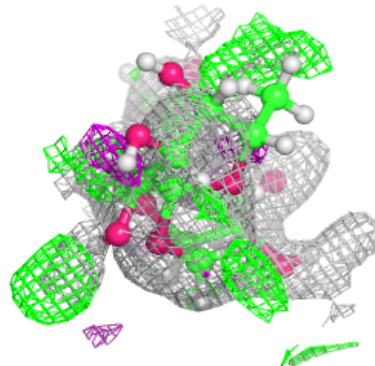
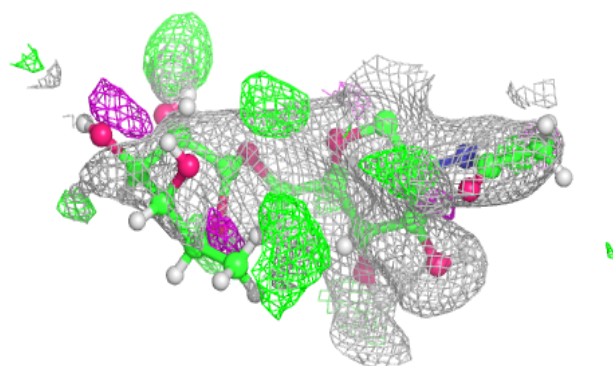
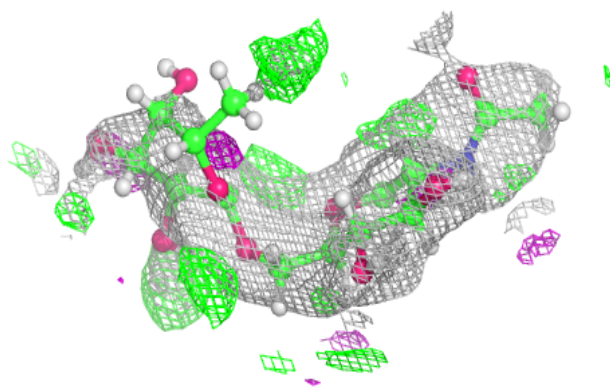


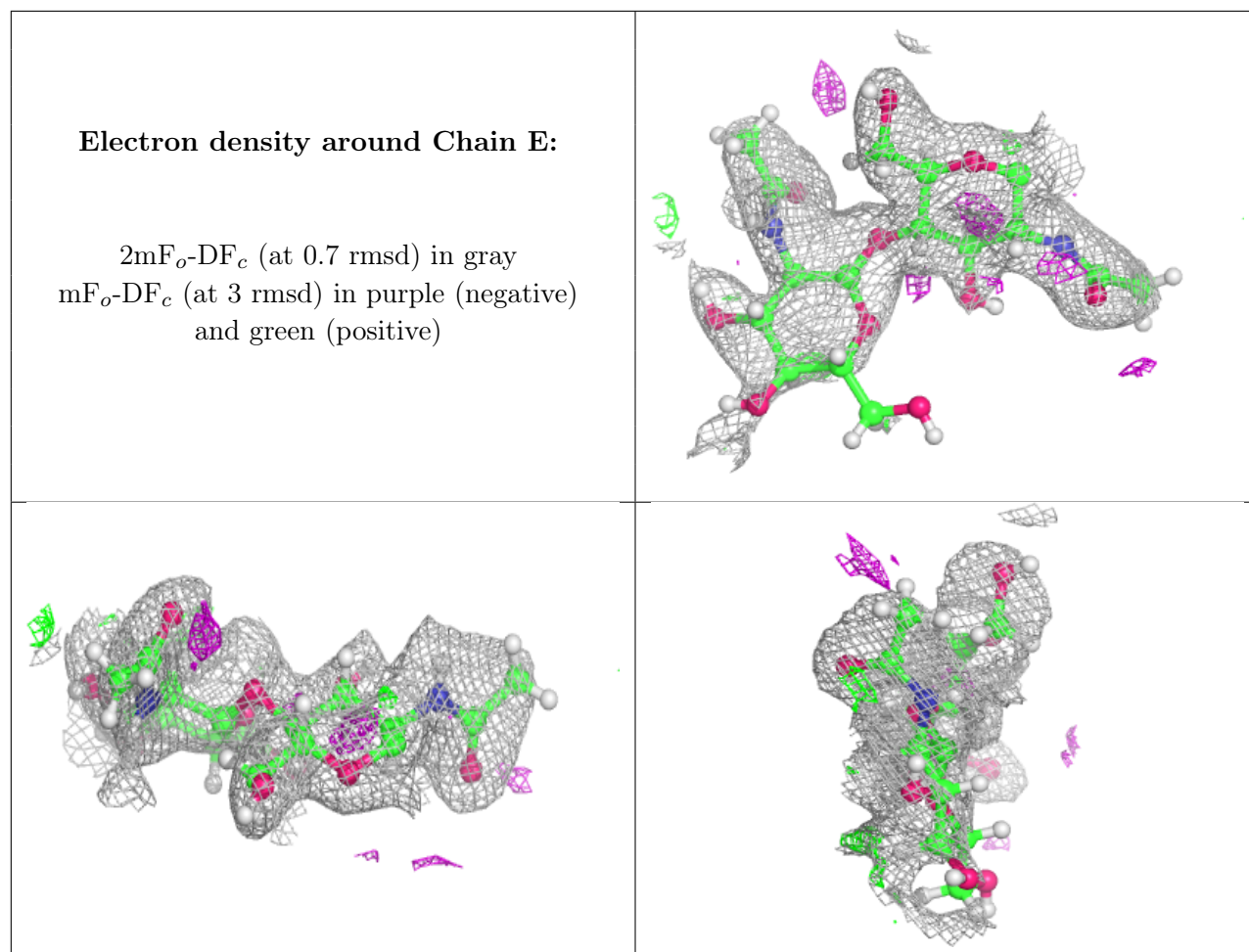
**Electron density around Chain D:**

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

**Electron density around Chain G:**

$2mF_o-DF_c$  (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, 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( $\text{\AA}^2$ )	Q<0.9
13	MG	B	717	1/1	0.68	0.34	67,67,67,67	0
8	EDO	A	707	4/4	0.81	0.13	57,69,79,84	0
5	NAG	A	701	14/15	0.82	0.13	51,66,79,81	0
8	EDO	B	708	4/4	0.83	0.11	53,64,74,75	0
6	PG4	A	702[A]	13/13	0.83	0.16	33,45,53,60	31
9	PGE	A	705	10/10	0.85	0.13	55,73,87,87	0
15	PE8	B	702	25/25	0.85	0.14	45,60,71,83	0
8	EDO	B	710	4/4	0.87	0.12	50,60,71,78	0
8	EDO	A	704	4/4	0.87	0.12	51,62,67,73	0
8	EDO	A	706	4/4	0.87	0.12	55,66,74,75	0
14	PEG	B	703	7/7	0.87	0.12	41,56,69,69	0

*Continued on next page...*



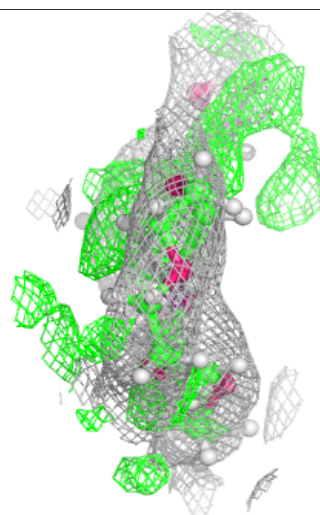
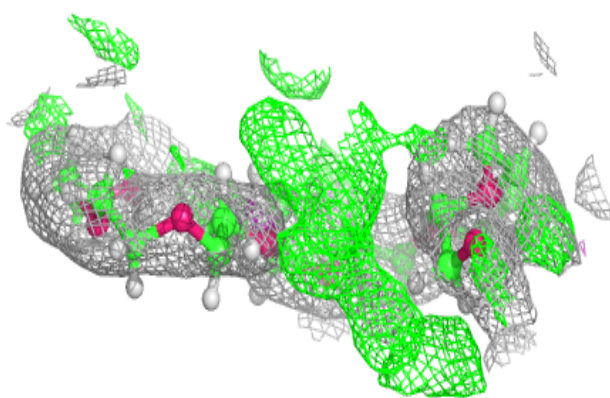
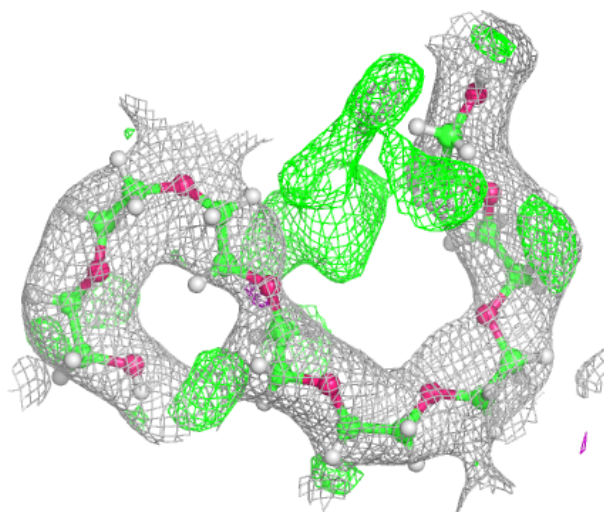
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	PEG	B	705	7/7	0.87	0.14	48,58,67,70	0
14	PEG	B	712[B]	7/7	0.87	0.16	39,47,51,52	17
8	EDO	B	709	4/4	0.87	0.13	56,68,72,80	0
8	EDO	A	708	4/4	0.88	0.18	46,67,73,82	0
14	PEG	B	701	7/7	0.88	0.14	43,61,70,77	0
14	PEG	B	704	7/7	0.89	0.11	49,59,72,79	0
13	MG	A	712	1/1	0.89	0.12	50,50,50,50	0
7	ACY	A	703	4/4	0.90	0.17	35,43,53,55	0
7	ACY	B	711	4/4	0.91	0.18	29,35,49,54	0
8	EDO	B	707	4/4	0.91	0.21	46,56,59,65	0
7	ACY	B	706	4/4	0.93	0.15	49,53,59,59	0
12	A1IRR	B	715	30/30	0.95	0.08	22,38,53,64	0
13	MG	B	716	1/1	0.96	0.07	46,46,46,46	0
12	A1IRR	A	711	30/30	0.96	0.08	26,38,52,63	0
11	CL	A	710	1/1	0.98	0.04	28,28,28,28	0
10	ZN	B	713	1/1	0.99	0.02	26,26,26,26	0
11	CL	B	714	1/1	1.00	0.02	23,23,23,23	0
10	ZN	A	709	1/1	1.00	0.02	26,26,26,26	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.

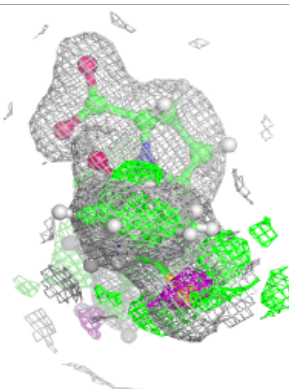
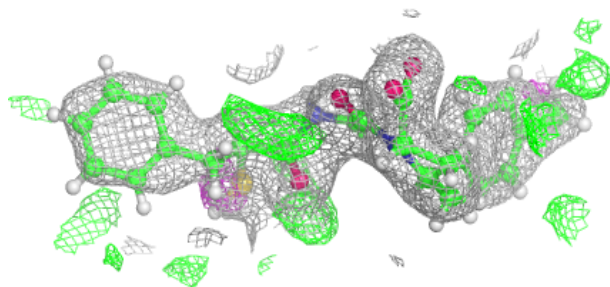
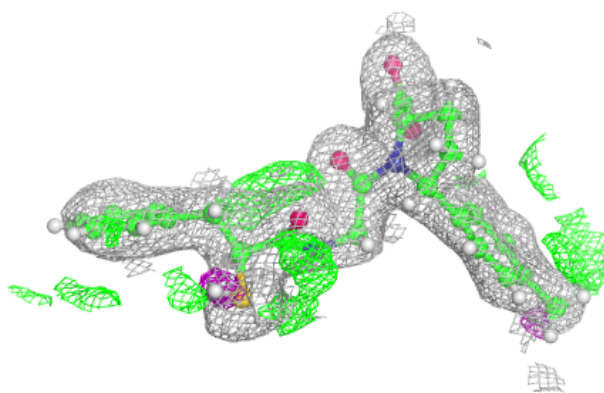
**Electron density around PE8 B 702:**

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

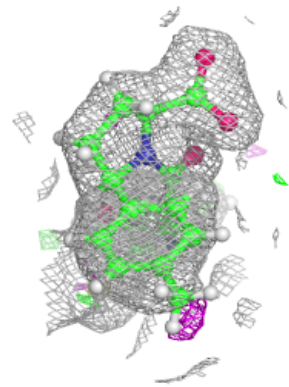
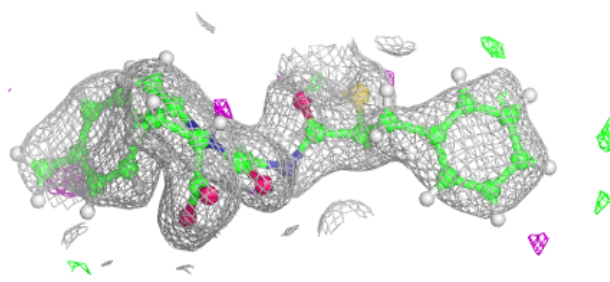
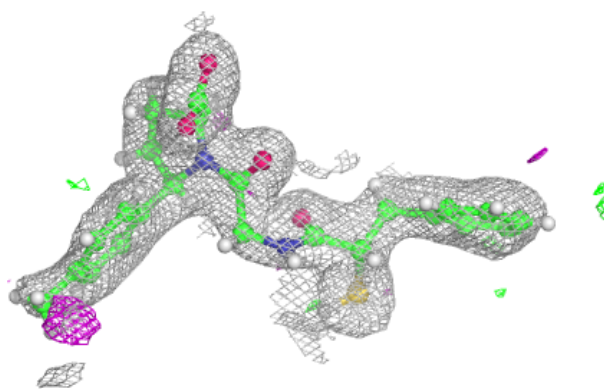


**Electron density around A1IRR B 715:**

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

**Electron density around A1IRR 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.