

# wwPDB X-ray Structure Validation Summary Report (i)

Feb 7, 2022 – 03:23 pm GMT

PDB ID : 7Q26

Title: Crystal structure of Angiotensin-1 converting enzyme N-domain in complex

with dual ACE/NEP inhibitor AD013

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Deposited on : 2021-10-23

Resolution : 1.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.26

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$ 

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

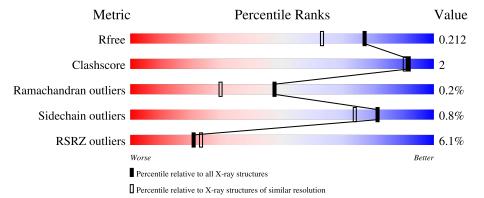
Validation Pipeline (wwPDB-VP) : 2.26

## 1 Overall quality at a glance (i)

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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 >=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 <=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	3%	93%		
1	В	629	8%	93%		
2	С	2	50	9%	50%	
3	D	4		75%		25%
3	F	4	25%	25%	50%	



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Mol	Chain	Length	Qual	ity of chain
4	Е	2	50%	50%
4	G	2		100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

$\mathbf{N}$	Iol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
	9	ACT	A	705	-	-	X	-
	9	ACT	В	709	_	-	X	-



# 2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 21101 atoms, of which 9951 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			Atom	S			ZeroOcc	AltConf	Trace
1	A	606	Total 9835	C 3223	H 4808	N 863	O 922	S 19	0	16	0
1	В	603	Total 9752	C 3201	H 4763	N 855	O 914	S 19	0	12	0

There are 18 discrepancies between the modelled and reference sequences:

Chain			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
A	629	LEU	-	expression tag	UNP P12821
В	9	GLN	ASN	engineered mutation	UNP P12821
В	25	GLN	ASN	engineered mutation	UNP P12821
В	82	GLN	ASN	engineered mutation	UNP P12821
В	117	GLN	ASN	engineered mutation	UNP P12821
В	131	GLN	ASN	engineered mutation	UNP P12821
В	289	GLN	ASN	engineered mutation	UNP P12821
В	545	ARG	GLN	engineered mutation	UNP P12821
В	576	LEU	PRO	engineered mutation	UNP P12821
В	629	629 LEU - expression tag		UNP P12821	

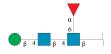
• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
9	С	9	Total	С	Н	N	О	0	0	0
			54	16	26	2	10	0	0	0

• Molecule 3 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		$\mathbf{At}$	$\overline{\mathrm{oms}}$			ZeroOcc	AltConf	Trace
2	D	4	Total	С	Н	N	О	0	0	0
3	ש	4	96	28	47	2	2 19			0
9	E	4	Total	С	Н	N	О	0	0	0
3	Г	F 4		28	45	2	19	U	0	U

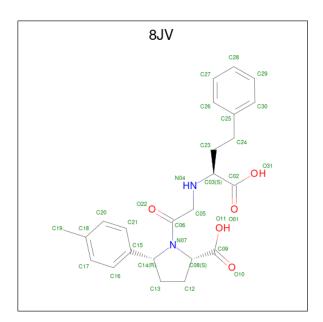
• Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
4	E	2	Total	С	Н	N	О	0	0	0
4	<u> 1</u> 2	2	47	14	23	1	9	U	0	U
1	С	2	Total	С	Н	N	О	0	0	0
4	G	2	47	14	23	1	9	U	U	U

• Molecule 5 is  $(2 \{S\}, 5 \{R\})$ -5-(4-methylphenyl)-1-[2- $[[(2 \{S\})$ -1-oxidanyl-1-oxidanylidene-4-phenyl-butan-2-yl]amino]ethanoyl]pyrrolidine-2-carboxylic acid (three-letter code: 8JV) (formula:  $C_{24}H_{28}N_2O_5$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
E	A	1	Total	С	Н	N	О	0	0	
5	A	1	57	24	26	2	5	U	U	
5	D	1	Total	С	Н	N	О	0	0	
5	Б	1	57	24	26	2	5	U	0	

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	В	1	Total Zn 1 1	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	В	1	Total Cl 1 1	0	0

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

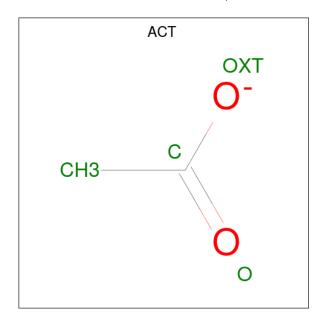
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total Mg 1 1	0	0

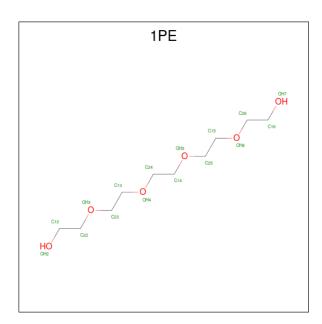
 $\bullet$  Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 



Mol	Chain	Residues	$\mathbf{A}$	Atoms			ZeroOcc	AltConf
9	A	1	Total 7				0	0
9	A	1	Total 7				0	0
9	В	1	Total 7		Н 3	O 2	0	0

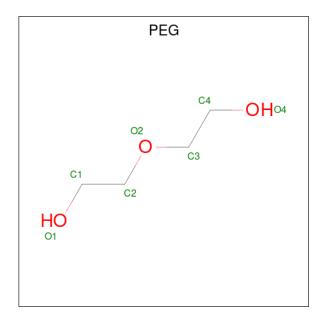
 $\bullet$  Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $\mathrm{C_{10}H_{22}O_6}).$ 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	0 A	A 1	Total	С	Н	О	0	0
10			38	10	22	6		
10	D	1	Total	С	Н	О	0	0
10	D	В 1	38	10	22	6		U

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



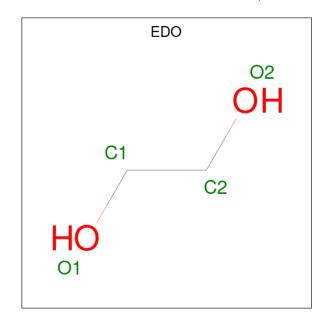
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total 17	C 4	H 10	O 3	0	0



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$\mathbf{M}$	ol	Chain	Residues	A	ltor	ns		ZeroOcc	AltConf
1	1	В	1	Total	C 4	H 10	O 3	0	0

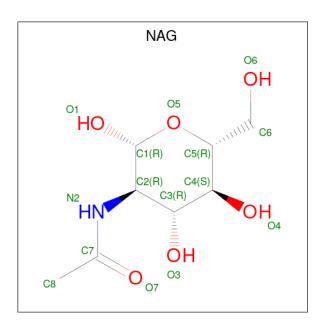
• Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf
12	A	1	Total 10			0	0
12	A	1	Total 10			0	0

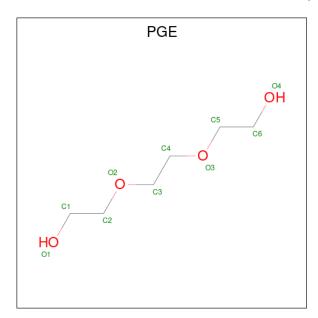
 $\bullet$  Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6).$ 





$\overline{\text{Mol}}$	Chain	Residues		At	oms			ZeroOcc	AltConf
19	D	1	Total	С	Н	N	О	0	0
19	D	1	27	8	13	1	5	U	U

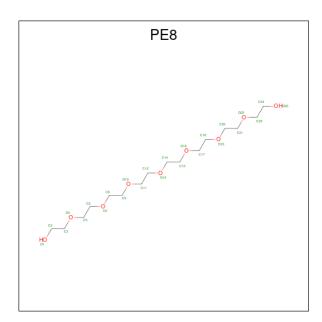
 $\bullet$  Molecule 14 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $\mathrm{C_6H_{14}O_4}).$ 



Me	l Cha	ain	Residues	Atoms				ZeroOcc	AltConf
14	Е	3	1	Total 24	C 6	H 14	O 4	0	0

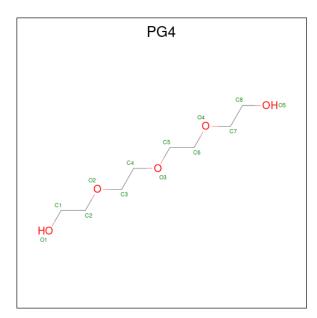
• Molecule 15 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula:  $C_{16}H_{34}O_9$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	D	1	Total	С	Н	О	0	0
15	Ъ	1	59	16	34	9	0	0

 $\bullet$  Molecule 16 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $\mathrm{C_8H_{18}O_5}).$ 



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	С	Н	О	0	0
10	Б	1	31	8	18	5	U	0

• Molecule 17 is water.



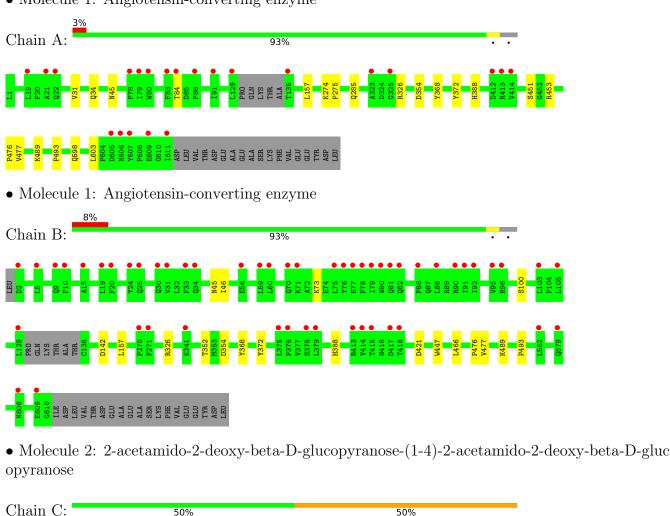
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	440	Total O 445 445	0	6
17	В	317	Total O 319 319	0	2



#### 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



Chain C: 50%

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)|2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 75% 25%





 $\bullet \ \, Molecule \ 3: \ beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose$ 

Chain F: 25% 25% 50%



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	72.89Å 77.10Å 82.62Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$88.63^{\circ}$ $64.18^{\circ}$ $74.79^{\circ}$	Depositor
Resolution (Å)	55.27 - 1.70	Depositor
Resolution (A)	73.97 - 1.70	EDS
% Data completeness	97.0 (55.27-1.70)	Depositor
(in resolution range)	97.0 (73.97-1.70)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.84 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
D D.	0.195 , 0.215	Depositor
$R, R_{free}$	0.193 , $0.212$	DCC
$R_{free}$ test set	1949 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.51, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21101	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 5.79% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: 8JV, ZN, PGE, BMA, ACT, PEG, NAG, 1PE, PE8, MG, EDO, 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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.26	0/5230	0.50	0/7122	
1	В	0.26	0/5170	0.49	0/7041	
All	All	0.26	0/10400	0.50	0/14163	

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	5027	4808	4759	13	0
1	В	4989	4763	4732	11	0
2	С	28	26	25	1	0
3	D	49	47	43	0	0
3	F	49	45	43	4	0
4	Ε	24	23	22	0	0
4	G	24	23	22	0	0
5	A	31	26	0	0	0
5	В	31	26	0	0	0
6	A	1	0	0	0	0
6	В	1	0	0	0	0



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Mol	Chain		H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	В	1	0	0	0	0
8	A	1	0	0	0	0
8	В	1	0	0	0	0
9	A	8	6	6	2	0
9	В	4	3	3	3	0
10	A	16	22	22	0	0
10	В	16	22	22	1	0
11	A	7	10	10	0	0
11	В	7	10	10	0	0
12	A	8	12	12	0	0
13	В	14	13	13	1	0
14	В	10	14	14	0	0
15	В	25	34	34	0	0
16	В	13	18	18	0	0
17	A	445	0	0	7	1
17	В	319	0	0	6	0
All	All	11150	9951	9810	33	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	$\begin{array}{c cccc} & & & & & & & Interaton \\ \hline & & & & & distance \end{array}$		$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:84:THR:OG1	17:A:801[A]:HOH:O	2.07	0.72
1:B:46:ILE:O	17:B:801:HOH:O	2.10	0.69
9:A:705:ACT:H3	17:A:978:HOH:O	1.95	0.65
1:B:100:SER:O	17:B:802:HOH:O	2.15	0.65
1:A:354:ASP:OD1	17:A:802:HOH:O	2.16	0.62

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

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
17:A:1212:HOH:O	17:A:1214:HOH:O[1_655]	2.05	0.15



## 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	Percentile	es
1	A	618/629 (98%)	608 (98%)	9 (2%)	1 (0%)	47 30	
1	В	$611/629 \ (97\%)$	600 (98%)	10 (2%)	1 (0%)	47 30	
All	All	1229/1258 (98%)	1208 (98%)	19 (2%)	2 (0%)	47 30	

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	45	ASN
1	A	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	Rotameric Outliers		Percentiles		
1	A	536/541 (99%)	532 (99%)	4 (1%)	84	77		
1	В	529/541 (98%)	525 (99%)	4 (1%)	81	74		
All	All	1065/1082 (98%)	1057 (99%)	8 (1%)	81	74		

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	421	ASP
1	В	388	HIS
1	В	368	TYR
1	A	598	GLN



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Mol	Chain	Res	Type
1	В	372	TYR

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).

Mal	Т	Classia.	Dag	T : 1-	Во	ond leng	ths	В	ond ang	eles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	С	1	1,2	14,14,15	0.22	0	17,19,21	0.96	1 (5%)
2	NAG	С	2	2	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	D	1	1,3	14,14,15	0.44	0	17,19,21	0.50	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.49	0
3	BMA	D	3	3	11,11,12	0.54	0	15,15,17	0.91	1 (6%)
3	FUC	D	4	3	10,10,11	0.65	0	14,14,16	0.66	0
4	NAG	Е	1	1,4	14,14,15	0.43	0	17,19,21	0.89	0
4	FUC	Е	2	4	10,10,11	0.80	1 (10%)	14,14,16	1.84	4 (28%)
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.85	1 (5%)
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.75	1 (5%)
3	BMA	F	3	3	11,11,12	0.60	0	15,15,17	0.73	0
3	FUC	F	4	3	10,10,11	1.83	2 (20%)	14,14,16	1.33	1 (7%)
4	NAG	G	1	1,4	14,14,15	0.21	0	17,19,21	0.72	0
4	FUC	G	2	4	10,10,11	0.97	0	14,14,16	0.85	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	С	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	NAG	Е	1	1,4	-	3/6/23/26	0/1/1/1
4	FUC	Е	2	4	-	-	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	F	4	FUC	C1-C2	4.71	1.62	1.52
3	F	4	FUC	O5-C5	2.13	1.48	1.43
4	Е	2	FUC	C1-C2	2.09	1.57	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
4	Е	2	FUC	C1-O5-C5	3.71	121.18	112.78
4	Е	2	FUC	O5-C1-C2	3.71	116.49	110.77
3	F	4	FUC	O2-C2-C1	3.35	116.02	109.15
2	С	1	NAG	C1-O5-C5	3.34	116.71	112.19
4	Е	2	FUC	C1-C2-C3	3.32	113.75	109.67

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6



Continued from previous page...

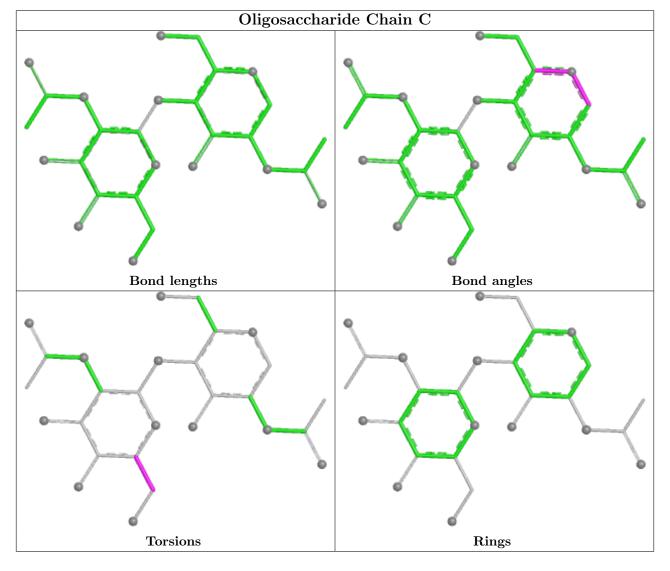
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6

There are no ring outliers.

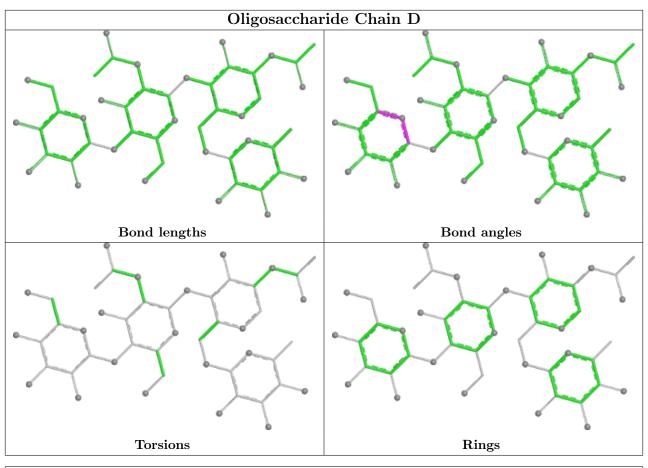
3 monomers are involved in 5 short contacts:

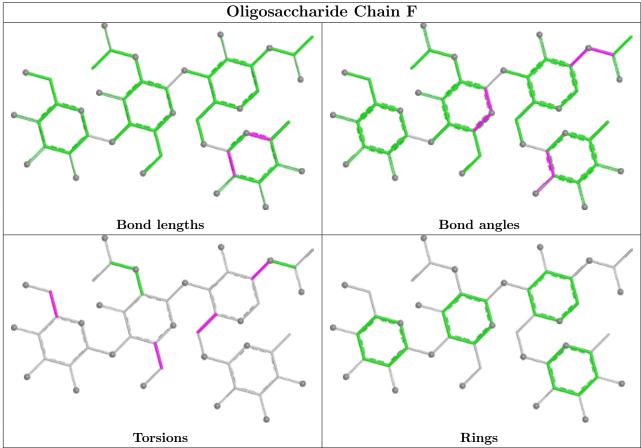
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	FUC	2	0
3	F	1	NAG	4	0
2	С	1	NAG	1	0

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

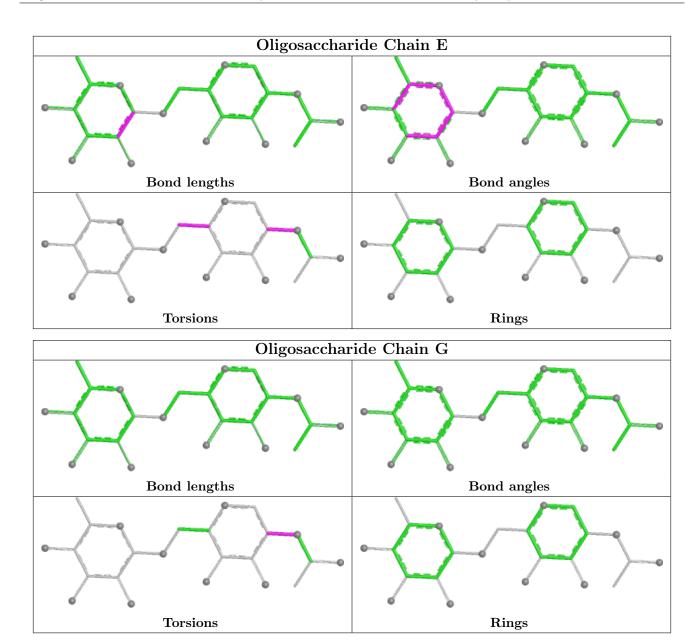












## 5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	В	ond leng	$\operatorname{gths}$	В	ond ang	gles	
MIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
	1	1	1								
Mol	Type	Chain	Res	Res	Link	$ \mathbf{B} $	ond leng	${ m gths}$	B	ond ang	
IVIOI	Турс	Chain	ICS	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
15	PE8	В	704	_	24,24,24	0.54	0	23,23,23	0.23	0	
16	PG4	В	708	_	12,12,12	0.51	0	11,11,11	0.48	0	
12	EDO	A	709	_	3,3,3	0.46	0	2,2,2	0.28	0	
12	EDO	A	710	-	3,3,3	0.47	0	2,2,2	0.20	0	
14	PGE	В	703	-	9,9,9	0.30	0	8,8,8	0.36	0	
11	PEG	A	708	_	6,6,6	0.48	0	5,5,5	0.35	0	
5	8JV	A	701	6	27,33,33	2.89	6 (22%)	32,45,45	1.92	5 (15%)	
10	1PE	В	710	-	15,15,15	0.52	0	14,14,14	0.34	0	
9	ACT	A	705	-	1,3,3	5.51	1 (100%)	0,3,3	_	-	
9	ACT	A	706	-	1,3,3	6.02	1 (100%)	0,3,3	_	-	
5	8JV	В	701	6	27,33,33	2.91	7 (25%)	32,45,45	1.76	4 (12%)	
9	ACT	В	709	-	1,3,3	6.18	1 (100%)	0,3,3	-	-	
11	PEG	В	711	-	6,6,6	0.49	0	5,5,5	0.28	0	
13	NAG	В	702	1	14,14,15	0.45	0	17,19,21	0.73	1 (5%)	
10	1PE	A	707	-	15,15,15	0.52	0	14,14,14	0.26	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
15	PE8	В	704	-	-	8/22/22/22	-
16	PG4	В	708	-	-	5/10/10/10	-
12	EDO	A	709	-	-	1/1/1/1	-
12	EDO	A	710	-	-	1/1/1/1	-
14	PGE	В	703	-	-	0/7/7/7	-
11	PEG	A	708	-	1	1/4/4/4	-
5	8JV	A	701	6	-	2/18/39/39	0/3/3/3
10	1PE	В	710	-	-	6/13/13/13	-
5	8JV	В	701	6	-	2/18/39/39	0/3/3/3
11	PEG	В	711	-	-	1/4/4/4	-
13	NAG	В	702	1	-	0/6/23/26	0/1/1/1
10	1PE	A	707	-	-	2/13/13/13	-

The worst 5 of 16 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
5	В	701	8JV	C06-N07	9.01	1.48	1.36
5	A	701	8JV	C06-N07	8.57	1.47	1.36
5	A	701	8JV	C13-C12	-6.95	1.34	1.54
5	В	701	8JV	C13-C12	-6.82	1.35	1.54
9	В	709	ACT	СН3-С	6.18	1.56	1.48

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	701	8JV	C12-C08-N07	7.25	106.79	101.97
5	В	701	8JV	C12-C08-N07	6.82	106.51	101.97
5	A	701	8JV	C13-C14-C15	-4.27	105.34	113.61
5	В	701	8JV	C13-C14-C15	-3.87	106.12	113.61
5	A	701	8JV	O22-C06-N07	-3.41	118.70	122.29

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	В	708	PG4	C3-C4-O3-C5
10	В	710	1PE	OH5-C14-C24-OH4
15	В	704	PE8	O4-C5-C6-O7
10	В	710	1PE	OH6-C15-C25-OH5
16	В	708	PG4	O1-C1-C2-O2

There are no ring outliers.

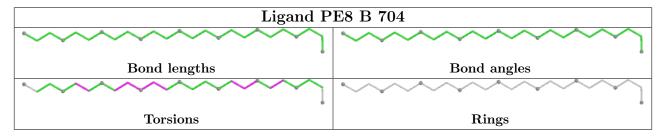
4 monomers are involved in 7 short contacts:

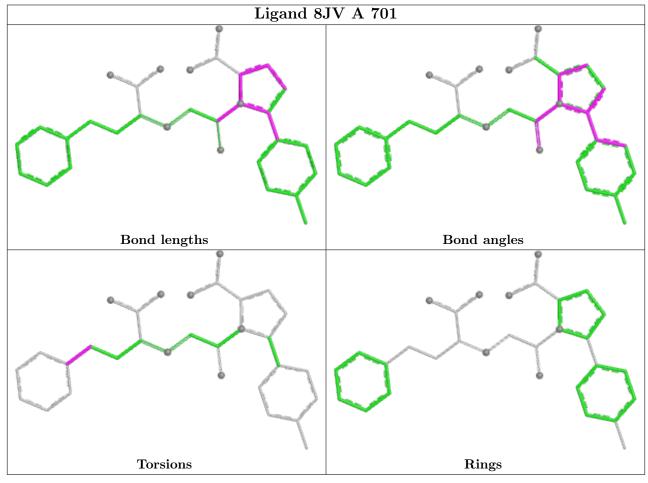
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	В	710	1PE	1	0
9	A	705	ACT	2	0
9	В	709	ACT	3	0
13	В	702	NAG	1	0

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 then 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

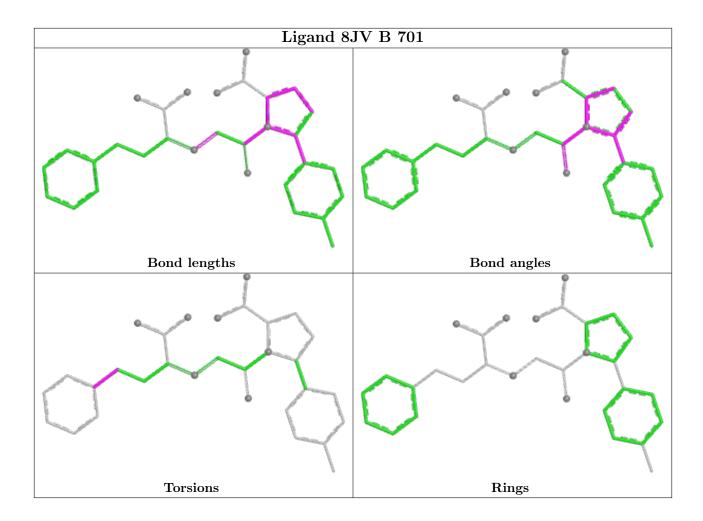


any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	606/629 (96%)	0.38	22 (3%) 42 47	17, 31, 56, 89	0
1	В	603/629 (95%)	0.60	52 (8%) 10 12	19, 41, 74, 105	0
All	All	1209/1258 (96%)	0.49	74 (6%) 21 23	17, 35, 69, 105	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	611	ILE	6.9
1	A	325	GLY	6.3
1	A	414	VAL	5.1
1	В	129	LEU	4.9
1	В	105	LEU	4.9

## 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,  $95^{th}$  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.

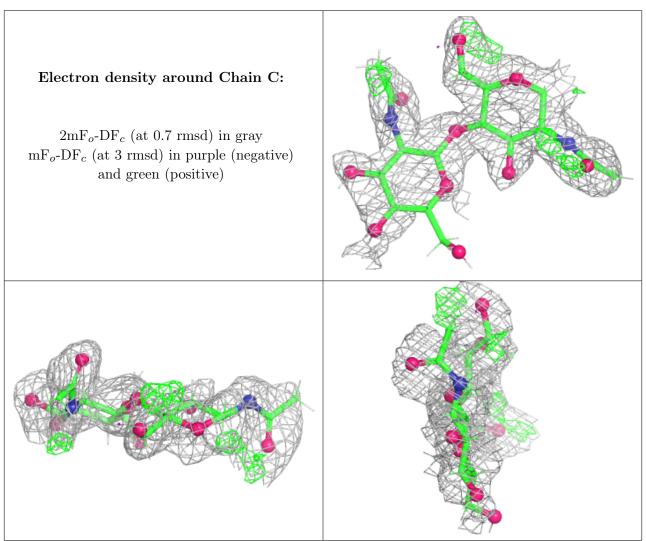
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	BMA	F	3	11/12	0.51	0.34	88,104,122,126	0
2	NAG	С	2	14/15	0.66	0.27	73,91,117,119	0
2	NAG	С	1	14/15	0.67	0.18	53,71,85,91	0
3	BMA	D	3	11/12	0.68	0.17	68,74,88,89	0
3	FUC	F	4	10/11	0.76	0.31	77,86,102,103	0



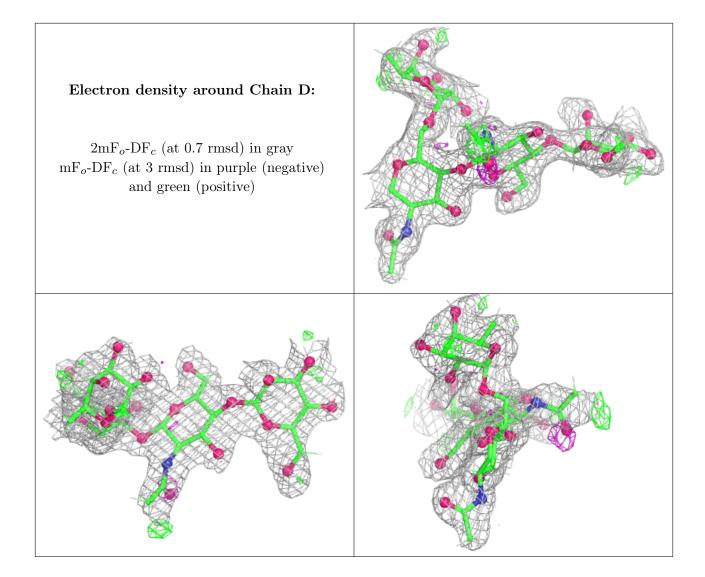
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	FUC	D	4	10/11	0.77	0.17	57,63,72,76	0
3	NAG	F	1	14/15	0.79	0.22	70,82,91,99	0
4	FUC	G	2	10/11	0.81	0.20	58,72,86,86	0
3	NAG	F	2	14/15	0.82	0.22	75,83,98,100	0
4	NAG	G	1	14/15	0.84	0.12	42,53,66,72	0
4	FUC	E	2	10/11	0.84	0.27	57,79,100,100	0
3	NAG	D	2	14/15	0.85	0.15	50,60,72,72	0
4	NAG	E	1	14/15	0.86	0.13	40,50,60,63	0
3	NAG	D	1	14/15	0.91	0.12	44,51,58,62	0

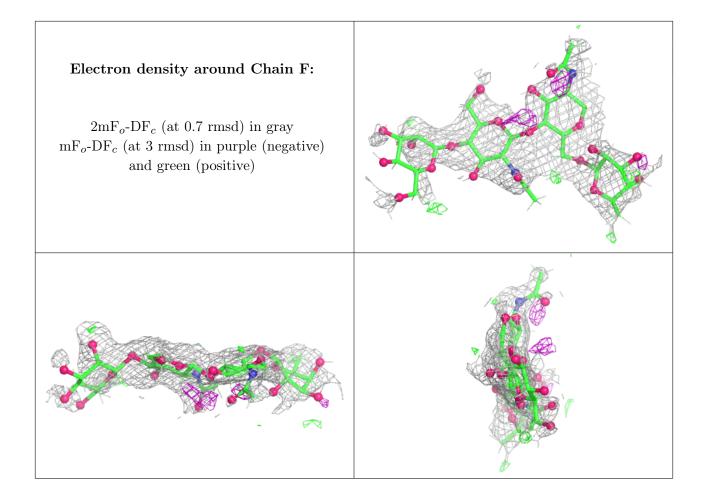
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.













# Electron density around Chain E: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around Chain G: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (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,  $95^{th}$  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.

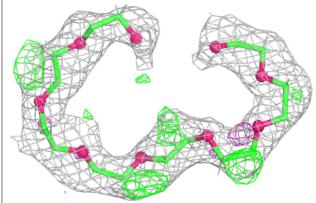
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
13	NAG	В	702	14/15	0.66	0.23	61,78,93,95	0
9	ACT	В	709	4/4	0.75	0.20	33,40,43,44	0
15	PE8	В	704	25/25	0.79	0.17	41,63,81,85	0
12	EDO	A	709	4/4	0.81	0.24	46,55,65,65	0
12	EDO	A	710	4/4	0.83	0.34	37,47,52,63	0
10	1PE	В	710	16/16	0.85	0.22	34,45,59,62	0
14	PGE	В	703	10/10	0.86	0.15	39,57,80,88	0
9	ACT	A	705	4/4	0.88	0.15	26,31,33,35	0
11	PEG	В	711	7/7	0.89	0.10	56,69,78,86	0
11	PEG	A	708	7/7	0.91	0.11	39,53,64,71	0
5	8JV	A	701	31/31	0.93	0.12	22,30,40,43	0
16	PG4	В	708	13/13	0.93	0.12	31,40,53,62	0
5	8JV	В	701	31/31	0.94	0.11	22,29,39,42	0
10	1PE	A	707	16/16	0.95	0.11	29,38,60,65	0
9	ACT	A	706	4/4	0.95	0.13	39,42,54,54	0
8	MG	В	707	1/1	0.97	0.10	40,40,40,40	0
8	MG	A	704	1/1	0.97	0.07	35,35,35,35	0
6	ZN	A	702	1/1	0.99	0.12	21,21,21,21	0
7	CL	A	703	1/1	0.99	0.14	19,19,19,19	0
7	CL	В	706	1/1	0.99	0.14	25,25,25,25	0
6	ZN	В	705	1/1	1.00	0.10	20,20,20,20	0

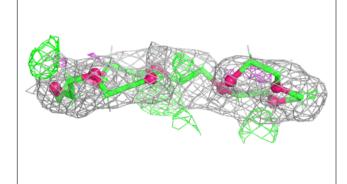
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

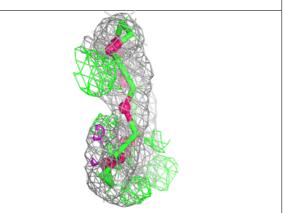


# Electron density around PE8 B 704:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

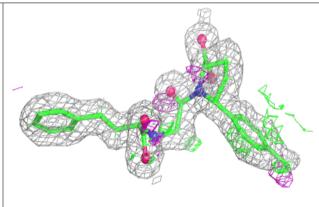


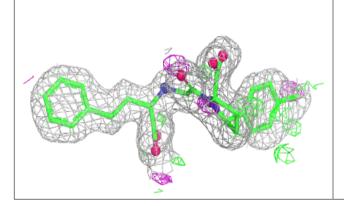


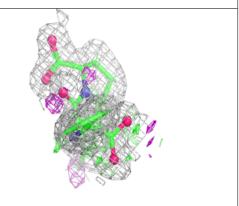


#### Electron density around 8JV A 701:

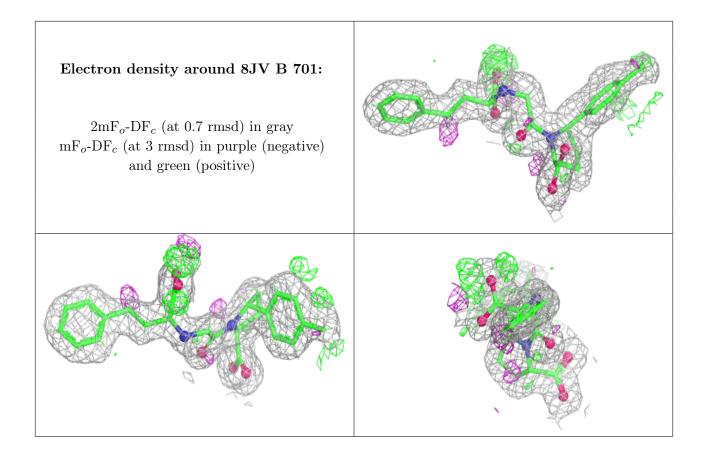
 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)











## 6.5 Other polymers (i)

There are no such residues in this entry.

