

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

#### Aug 20, 2023 – 02:20 PM EDT

PDB ID : 20PH

Title: Human dipeptidyl peptidase IV in complex with an alpha amino acid inhibitor

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Deposited on : 2007-01-29

Resolution : 2.40 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

buster-report : 1.1.7 (2018)

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

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

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

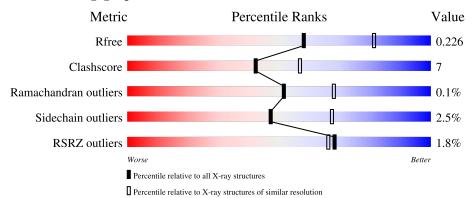
Validation Pipeline (wwPDB-VP) : 2.35

## 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 2.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	728	84%	15%	•						
1	В	728	85%	14%	•						
2	С	2	100%								
2	F	2	50% 50%								
3	D	2	100%								

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Mol	Chain		Quality of chain							
9	T.	0								
3	Е	2	100%							
3	G	2	100%							
	TT	0								
3	Н	2	50% 50%	_						
3	I	2	100%							
3	J	2	50% 50%							
	Т.7	0								
3	K	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:

Mol	Type	Chain	Res	Chirality	Geometry	Geometry   Clashes   Elec	
3	NAG	D	1	X	-	-	-
3	NAG	G	2	-	-	-	X
3	NAG	Н	2	-	-	-	X
4	NAG	A	1092	-	-	-	X
4	NAG	В	2092	-	-	-	X



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13182 atoms, of which 0 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.

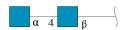
• Molecule 1 is a protein called Dipeptidyl peptidase 4 soluble form.

Mol	Chain	Residues		Atoms					AltConf	Trace
1	A	728	Total 5965	C 3828	N 982	O 1129	S 26	0	0	0
1	В	728	Total 5965	C 3828	N 982	O 1129	S 26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

	Chain	Residue   Modelled		Actual	Comment	Reference		
	A	39	39 THR		engineered mutation	UNP P27487		
Ī	В	39	THR	SER	engineered mutation	UNP P27487		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	С	2	Total 28				0	0	0
2	F	2	Total 28		N 2	O 10	0	0	0

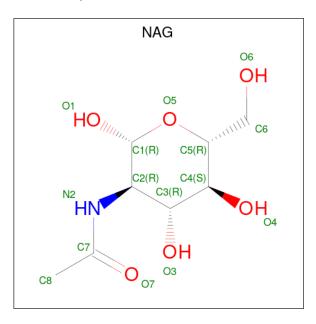
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0
3	E	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0
3	Н	2	Total C N O 28 16 2 10	0	0	0
3	I	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0
3	К	2	Total C N O 28 16 2 10	0	0	0

 $\bullet$  Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\rm C_8H_{15}NO_6).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	В	1	Total C N O 14 8 1 5	0	0

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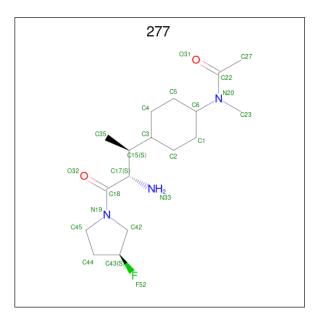
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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	В	1	Total 14				0	0
4	В	1	Total 14	C 8		O 5	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

• Molecule 6 is N-(TRANS-4- $\{(1S,2S)-2-AMINO-3-[(3S)-3-FLUOROPYRROLIDIN-1-YL]-1-METHYL-3-OXOPROPYL\}CYCLOHEXYL)-N-METHYLACETAMIDE (three-letter code: 277) (formula: <math>C_{17}H_{30}FN_3O_2$ ).



Mol	Chain	Residues	${f Atoms}$					ZeroOcc	AltConf	
6	Λ	1	Total	С	F	N	О	0	0	
U	0 A	1	23	17	1	3	2	0		
6	D	1	Total	С	F	N	О	0	0	
$\theta \mid B$	D	1	23	17	1	3	2	U		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	427	Total O 427 427	0	0

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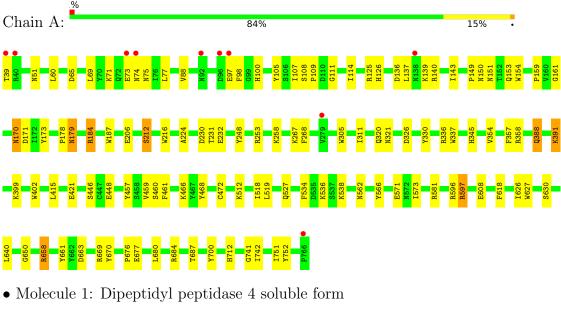
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	442	Total O 442 442	0	0

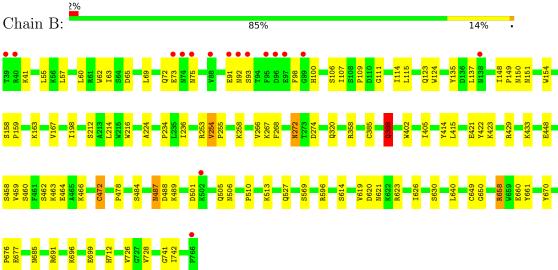


## 3 Residue-property plots (i)

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: Dipeptidyl peptidase 4 soluble form





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



Chain C:		100%	-
NDG2			
• Molecule 2: copyranose	2-acetamido-2-deoxy-alp	oha-D-glucopyranose-(1-4)-2-acetam	ido-2-deoxy-beta-D-glu
Chain F:	50%	50%	•
NDG2			
• Molecule 3: opyranose	2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamic	do-2-deoxy-beta-D-gluo
Chain D:		100%	•
NAG1 NAG2			
• Molecule 3: opyranose	2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamic	do-2-deoxy-beta-D-gluo
Chain E:		100%	•
NAG1 NAG2			
• Molecule 3: opyranose	2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamic	do-2-deoxy-beta-D-gluo
Chain G:		100%	•
NAG1 NAG2			
• Molecule 3: opyranose	2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamic	do-2-deoxy-beta-D-gluo
Chain H:	50%	50%	•
NAG1 NAG2			
• Molecule 3: opyranose	2-acetamido-2-deoxy-bet	ta-D-glucopyranose-(1-4)-2-acetamic	do-2-deoxy-beta-D-glud
Chain I:		100%	
NAG2			

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta	-D-gluc
opyranose	

Chain J: 50% 50%



 $\bullet$  Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	117.91Å 126.08Å 137.11Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.40	Depositor
Resolution (A)	46.40 - 2.36	EDS
% Data completeness	100.0 (30.00-2.40)	Depositor
(in resolution range)	98.3 (46.40-2.36)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.36 (at 2.37Å)	Xtriage
Refinement program	CNS, CNX	Depositor
D D.	0.188 , 0.238	Depositor
$R, R_{free}$	0.178 , 0.226	DCC
$R_{free}$ test set	4193 reflections $(5.05\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 39.3	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.70% 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: NDG, NAG, NA, 277

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		
MIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.49	0/6137	0.69	0/8346	
1	В	0.50	0/6137	0.68	1/8346 (0.0%)	
All	All	0.49	0/12274	0.68	1/16692 (0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	388	GLN	N-CA-C	-5.43	96.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	700	TYR	Sidechain

#### 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	5965	0	5677	75	0
1	В	5965	0	5679	90	0
2	С	28	0	24	0	0
2	F	28	0	24	2	0
3	D	28	0	25	2	0
3	Ε	28	0	25	0	0
3	G	28	0	25	0	0
3	Н	28	0	25	2	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
4	A	42	0	39	3	0
4	В	42	0	39	2	0
5	A	1	0	0	0	0
6	A	23	0	28	1	0
6	В	23	0	28	1	0
7	A	427	0	0	6	0
7	В	442	0	0	3	0
All	All	13182	0	11713	166	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 7.

The worst 5 of 166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} & ( ext{Å}) \end{aligned}$	Clash overlap (Å)	
1:A:149:PRO:HA	3:D:1:NAG:H82	1.48	0.96	
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.72	0.86	
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.71	0.86	
1:A:253:ARG:HH21	1:B:253:ARG:HH21	0.87	0.82	
1:B:75:ASN:HD21	4:B:2092:NAG:HN2	1.29	0.80	

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	726/728 (100%)	690 (95%)	35 (5%)	1 (0%)	51	68
1	В	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	51	68
All	All	1452/1456 (100%)	1386 (96%)	64 (4%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	320	GLN
1	A	320	GLN

#### 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	$653/653 \; (100\%)$	634 (97%)	19 (3%)	42 62		
1	В	$653/653 \; (100\%)$	640 (98%)	13 (2%)	55 74		
All	All	1306/1306 (100%)	1274 (98%)	32 (2%)	47 67		

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	506	ASN
1	В	621	ASN
1	A	472	CYS
1	A	448	GLU
1	В	658	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	345	HIS
1	В	572	ASN
1	В	712	HIS
1	В	533	HIS
1	В	74	ASN

#### 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)

18 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	Trino	Chain	Dag	Link	Во	ond leng	ths	В	ond ang	gles
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	С	1	2,1	14,14,15	0.79	0	17,19,21	1.23	2 (11%)
2	NDG	С	2	2	14,14,15	0.86	0	17,19,21	0.90	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.92	1 (7%)	17,19,21	0.71	0
3	NAG	D	2	3	14,14,15	0.88	1 (7%)	17,19,21	0.72	0
3	NAG	Е	1	3,1	14,14,15	0.58	0	17,19,21	0.66	1 (5%)
3	NAG	Е	2	3	14,14,15	0.80	0	17,19,21	0.87	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.83	0	17,19,21	0.90	0
2	NDG	F	2	2	14,14,15	0.80	1 (7%)	17,19,21	0.69	0
3	NAG	G	1	3,1	14,14,15	0.82	0	17,19,21	0.86	0
3	NAG	G	2	3	14,14,15	0.68	0	17,19,21	0.58	0
3	NAG	Н	1	3,1	14,14,15	0.72	0	17,19,21	0.62	0
3	NAG	Н	2	3	14,14,15	0.97	1 (7%)	17,19,21	0.76	0
3	NAG	I	1	3,1	14,14,15	0.49	0	17,19,21	0.71	0



Mol	Type Chain Res Li		Link Bond lengths			Bond angles				
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	J	1	3,1	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
3	NAG	J	2	3	14,14,15	0.59	0	17,19,21	0.69	0
3	NAG	K	1	3,1	14,14,15	0.45	0	17,19,21	0.99	2 (11%)
3	NAG	K	2	3	14,14,15	0.77	0	17,19,21	0.88	1 (5%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NDG	С	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Е	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NDG	F	2	2	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Н	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Н	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\mathring{\mathbf{A}})$	$\operatorname{Ideal}(\text{\AA})$
3	D	1	NAG	C1-C2	2.62	1.56	1.52
3	Н	2	NAG	C1-C2	2.58	1.56	1.52
3	D	2	NAG	C1-C2	2.28	1.55	1.52
2	F	2	NDG	C1-C2	2.25	1.55	1.52

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



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	1	NAG	C4-C3-C2	-3.26	106.24	111.02
3	K	1	NAG	C4-C3-C2	-2.78	106.94	111.02
3	K	1	NAG	C2-N2-C7	-2.23	119.73	122.90
2	С	2	NDG	O5-C1-C2	-2.20	107.81	111.29
3	J	1	NAG	C2-N2-C7	-2.13	119.87	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	NAG	C1

5 of 19 torsion outliers are listed below:

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

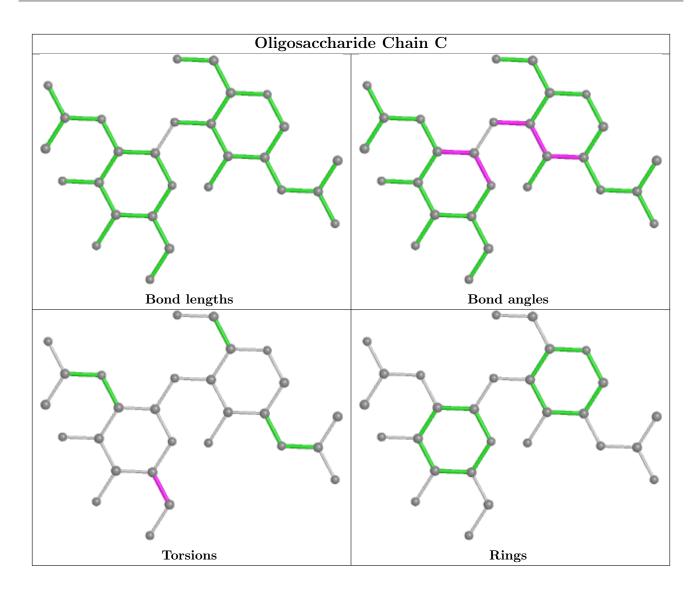
There are no ring outliers.

6 monomers are involved in 6 short contacts:

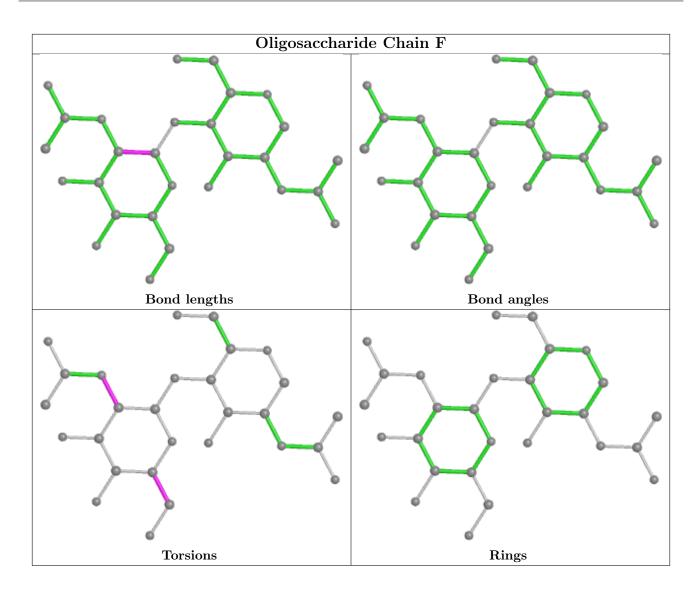
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	Н	1	NAG	2	0
2	F	1	NAG	1	0
2	F	2	NDG	2	0
3	Н	2	NAG	2	0
3	D	1	NAG	2	0

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

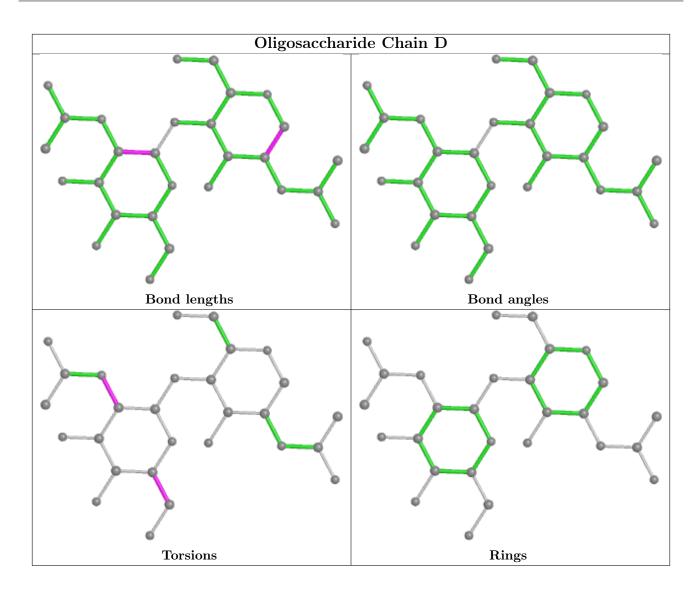




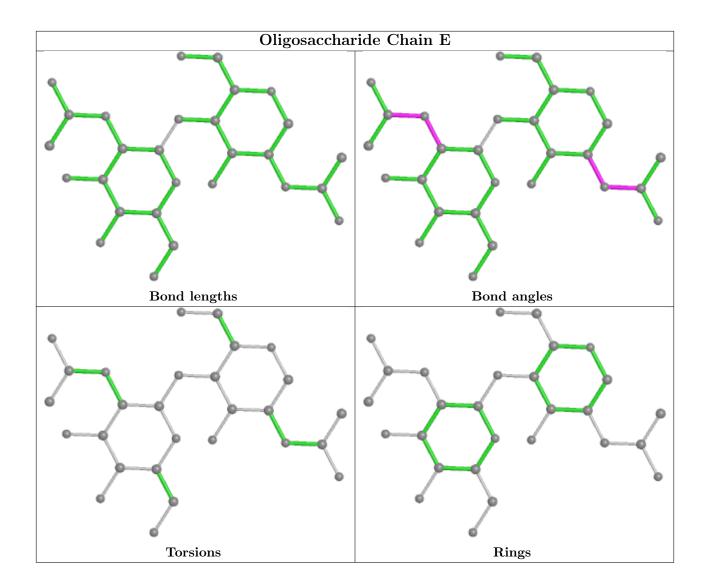




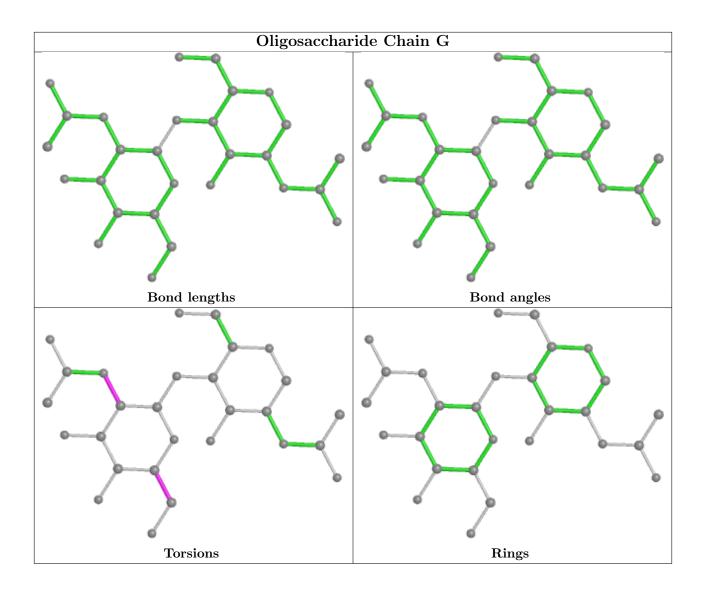




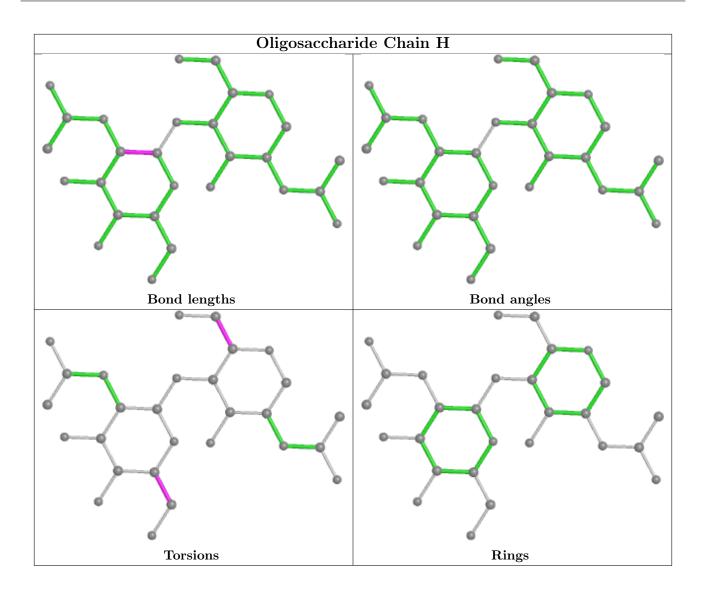




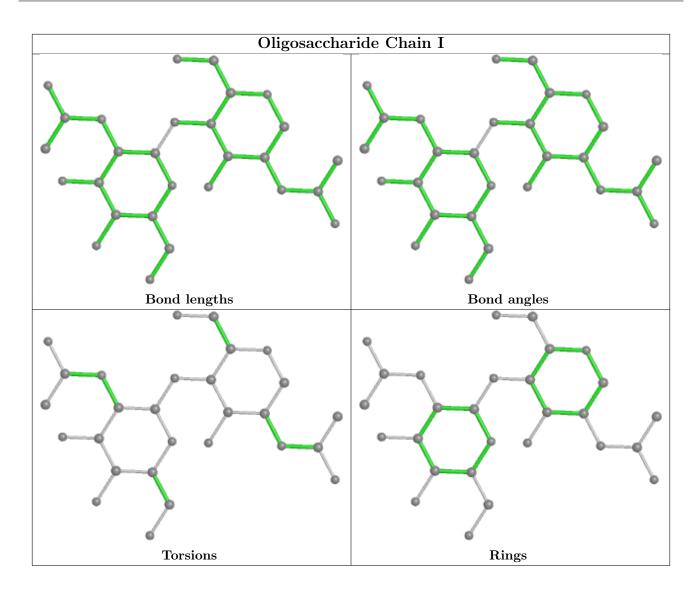




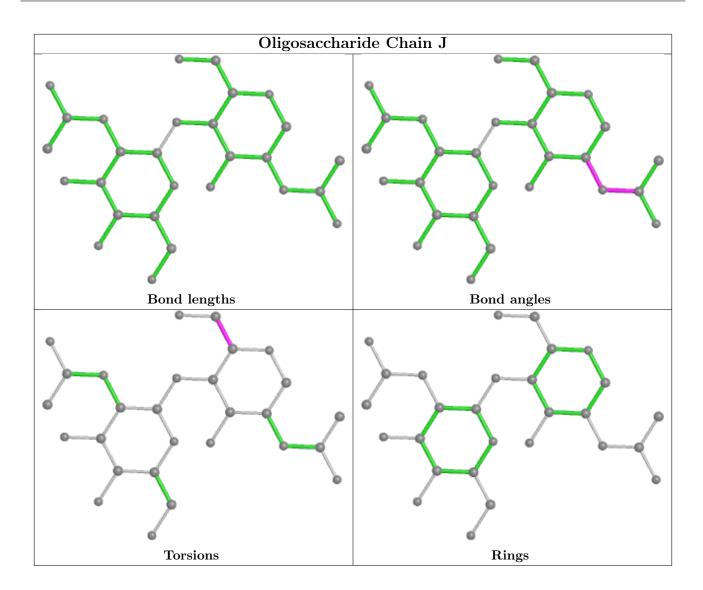




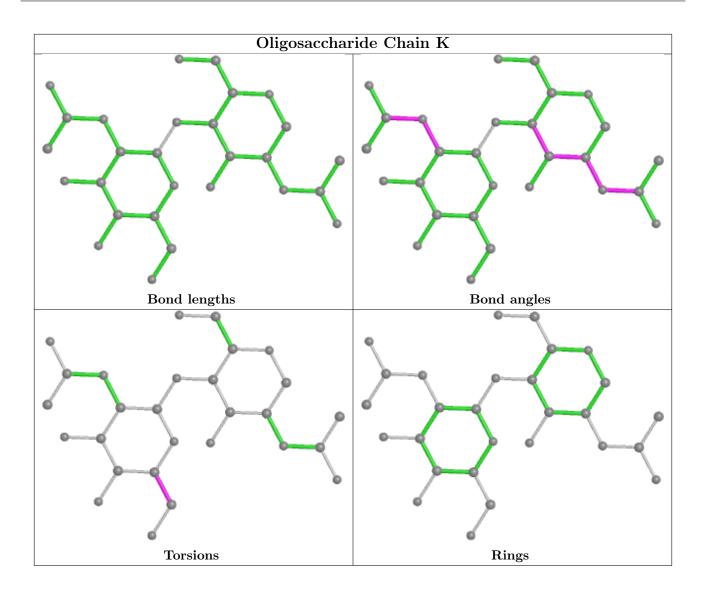












#### 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	Tuno	Chain	Res	Link	Bond lengths				Bond angles		
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
6	277	A	1001	-	23,24,24	2.81	4 (17%)	30,34,34	1.08	3 (10%)	
4	NAG	A	1092	1	14,14,15	0.92	1 (7%)	17,19,21	0.61	0	
4	NAG	A	1281	1	14,14,15	0.82	0	17,19,21	1.06	1 (5%)	



Mol	Tuno	Chain	Res	Link	Вс	ond leng	ths	Bond angles		
MIOI	Type			Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	В	2150	1	14,14,15	0.91	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	В	2321	1	14,14,15	0.65	0	17,19,21	1.01	1 (5%)
4	NAG	A	1520	1	14,14,15	0.88	1 (7%)	17,19,21	0.90	0
4	NAG	В	2092	1	14,14,15	0.84	0	17,19,21	0.78	0
6	277	В	1002	-	23,24,24	2.79	3 (13%)	30,34,34	1.02	3 (10%)

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
6	277	A	1001	-	-	0/24/43/43	0/2/2/2
4	NAG	A	1092	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1281	1	-	2/6/23/26	0/1/1/1
4	NAG	В	2150	1	-	0/6/23/26	0/1/1/1
4	NAG	В	2321	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1520	1	-	2/6/23/26	0/1/1/1
4	NAG	В	2092	1	-	4/6/23/26	0/1/1/1
6	277	В	1002	-	-	0/24/43/43	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\mathring{\mathrm{A}})$	Ideal(A)
6	A	1001	277	C17-N33	-11.96	1.12	1.47
6	В	1002	277	C17-N33	-11.44	1.13	1.47
6	В	1002	277	C17-C18	4.11	1.57	1.53
6	A	1001	277	C17-C18	3.43	1.57	1.53
6	В	1002	277	C15-C17	2.76	1.58	1.54

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathbf{Ideal}(^o)$
6	В	1002	277	C6-N20-C22	3.01	126.52	119.59
6	A	1001	277	C6-N20-C22	2.96	126.41	119.59
4	В	2321	NAG	C2-N2-C7	-2.75	118.98	122.90
4	A	1281	NAG	C2-N2-C7	-2.47	119.38	122.90
6	A	1001	277	C23-N20-C22	-2.46	114.03	120.04

There are no chirality outliers.



5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1281	NAG	C4-C5-C6-O6
4	В	2092	NAG	C1-C2-N2-C7
4	A	1281	NAG	O5-C5-C6-O6
4	В	2092	NAG	C4-C5-C6-O6
4	В	2092	NAG	C3-C2-N2-C7

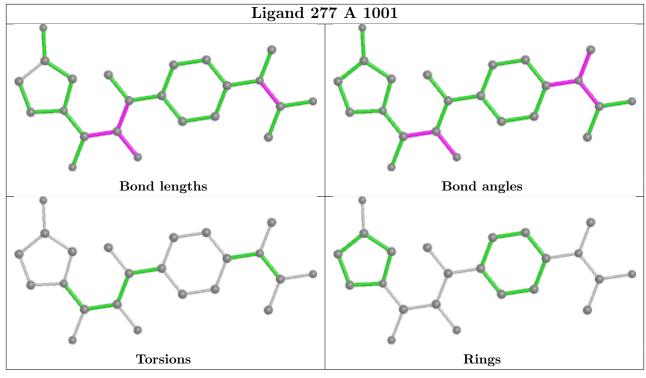
There are no ring outliers.

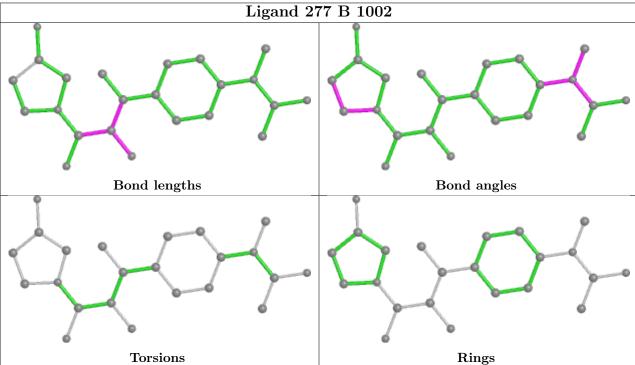
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	277	1	0
4	A	1092	NAG	1	0
4	A	1520	NAG	2	0
4	В	2092	NAG	2	0
6	В	1002	277	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	<RSRZ $>$	$ ightarrow \# \mathrm{RSRZ} {>} 2$		$OWAB(A^2)$	Q < 0.9
1	A	728/728 (100%)	-0.40	10 (1%) 75	73	12, 23, 44, 59	0
1	В	728/728 (100%)	-0.36	16 (2%) 62	60	12, 24, 43, 60	0
All	All	1456/1456 (100%)	-0.38	26 (1%) 68	66	12, 24, 44, 60	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	39	THR	7.3
1	В	39	THR	4.2
1	В	74	ASN	3.6
1	В	91	GLU	3.3
1	A	97	GLU	3.3

#### 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	$\operatorname{Res}$	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	NAG	Н	2	14/15	0.49	0.49	60,63,67,67	0
3	NAG	D	2	14/15	0.54	0.32	55,60,64,64	0
2	NDG	С	2	14/15	0.56	0.31	55,58,60,60	0
3	NAG	G	2	14/15	0.58	0.43	58,60,63,64	0
3	NAG	D	1	14/15	0.67	0.35	54,57,59,59	0

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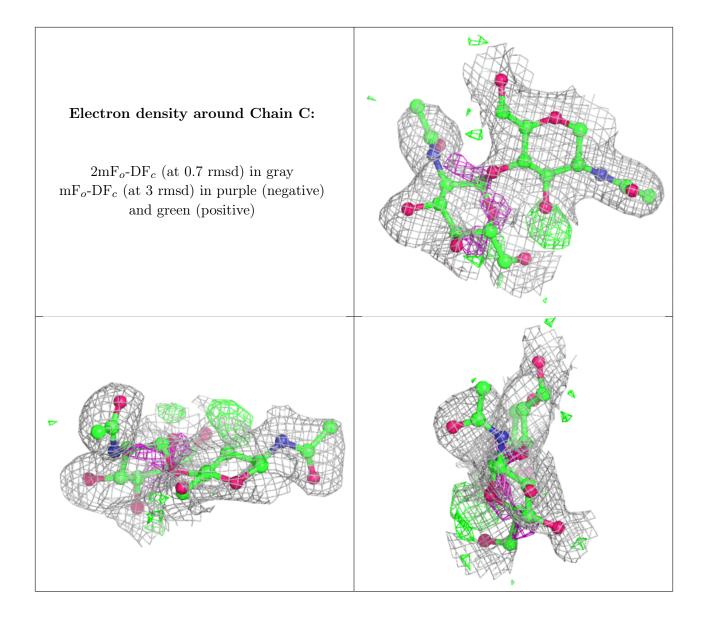


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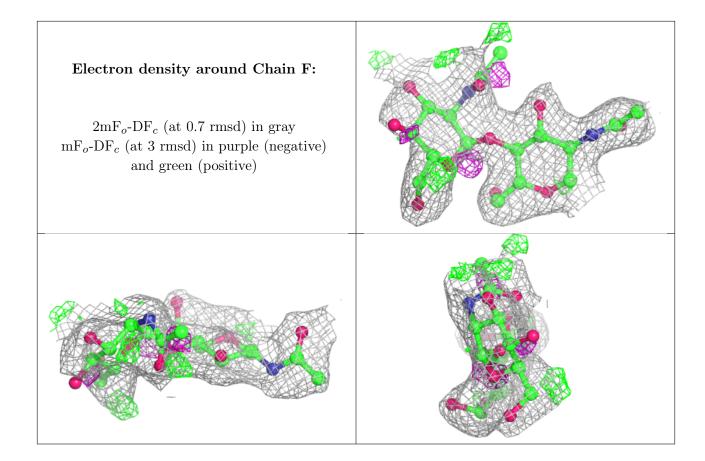
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
3	NAG	K	2	14/15	0.69	0.21	44,47,48,49	0
2	NDG	F	2	14/15	0.74	0.30	51,54,58,58	0
3	NAG	Е	2	14/15	0.80	0.26	46,50,54,54	0
3	NAG	G	1	14/15	0.82	0.27	45,48,50,55	0
3	NAG	Н	1	14/15	0.83	0.20	45,49,55,56	0
2	NAG	С	1	14/15	0.84	0.17	42,44,48,53	0
3	NAG	J	2	14/15	0.86	0.23	41,45,48,49	0
2	NAG	F	1	14/15	0.88	0.17	34,37,40,45	0
3	NAG	Е	1	14/15	0.90	0.18	38,43,46,47	0
3	NAG	K	1	14/15	0.91	0.14	28,32,41,42	0
3	NAG	I	2	14/15	0.91	0.19	41,44,46,47	0
3	NAG	J	1	14/15	0.95	0.13	30,33,38,40	0
3	NAG	I	1	14/15	0.95	0.14	33,39,43,44	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.

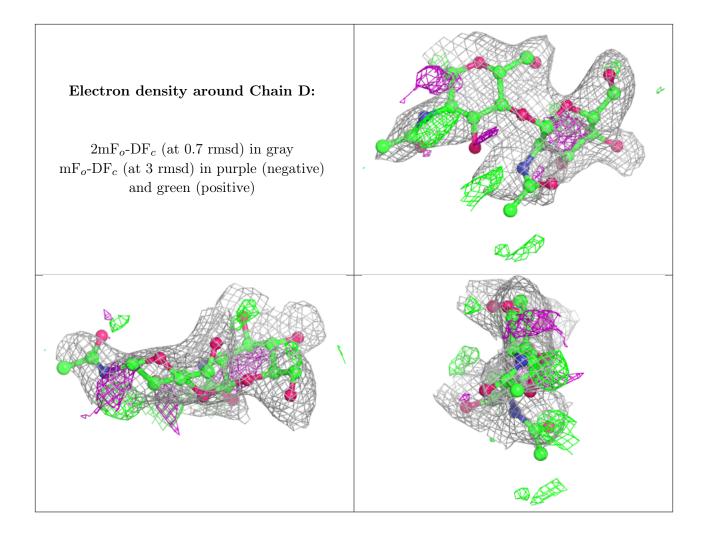








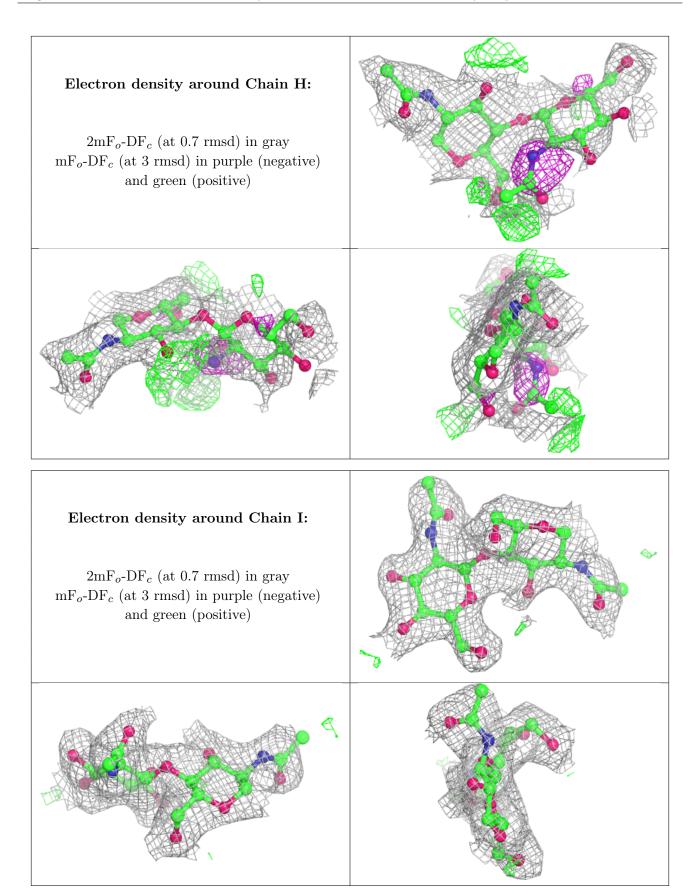




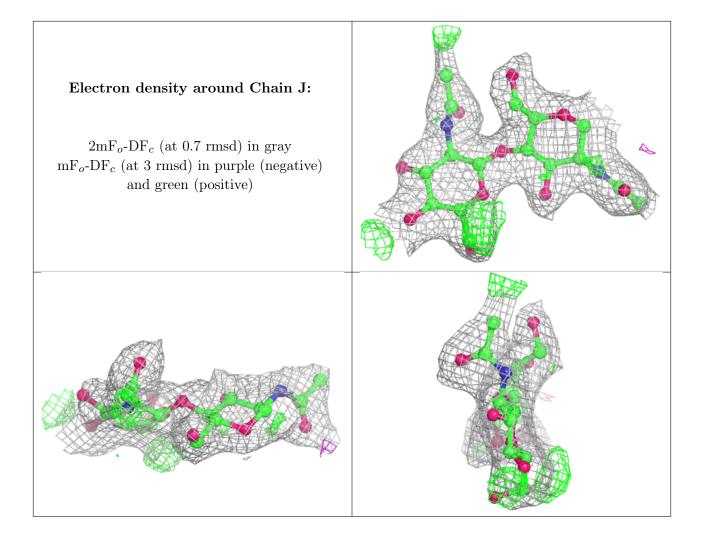


# Electron density around Chain E: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around Chain G: $2mF_o$ -DF<sub>c</sub> (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

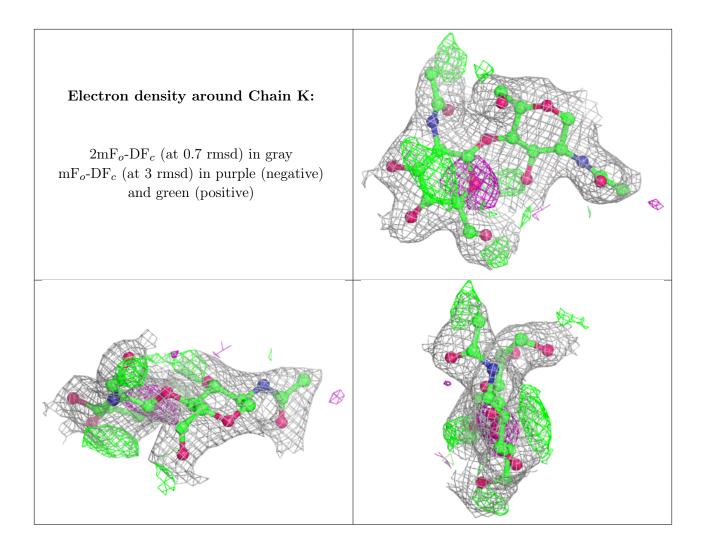












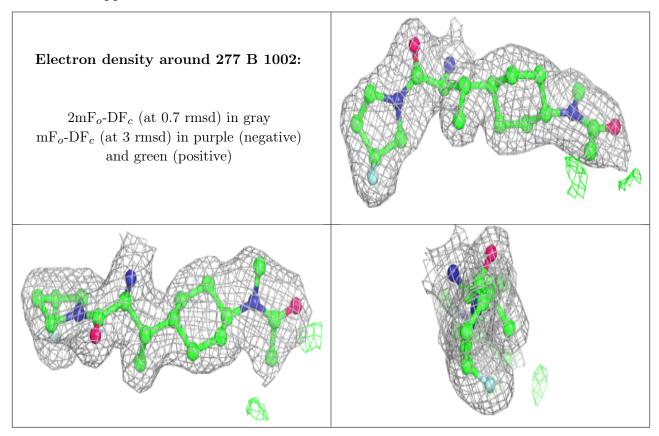
### 6.4 Ligands (i)

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.

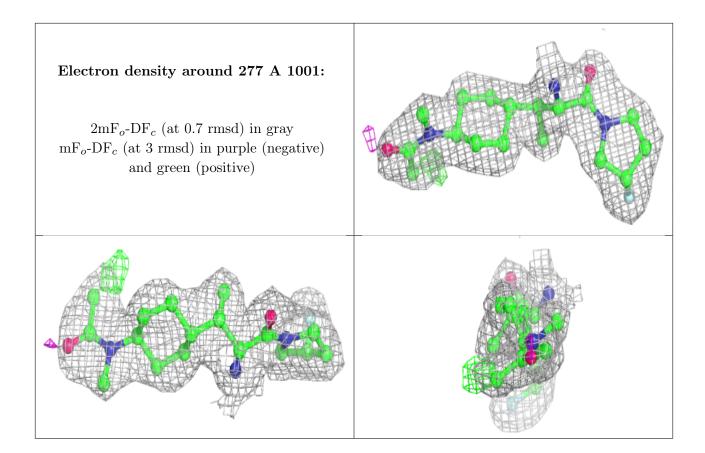
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NAG	A	1520	14/15	0.61	0.33	55,59,62,62	0
4	NAG	A	1092	14/15	0.66	0.47	62,63,64,64	0
4	NAG	В	2092	14/15	0.71	0.42	56,58,59,59	0
4	NAG	В	2150	14/15	0.76	0.35	47,51,53,55	0
4	NAG	В	2321	14/15	0.81	0.25	42,44,46,46	0
4	NAG	A	1281	14/15	0.84	0.18	41,45,46,47	0
5	NA	A	901	1/1	0.90	0.10	29,29,29,29	0
6	277	В	1002	23/23	0.95	0.20	14,17,27,31	0
6	277	A	1001	23/23	0.96	0.20	16,20,25,30	0



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







## 6.5 Other polymers (i)

There are no such residues in this entry.

