

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

### Apr 21, 2024 - 04:09 PM JST

PDB ID : 7F5P

Title : The crystal structure of VyPAL2-C214A, a dead mutant of VyPAL2 peptide

asparaginyl ligase in form I

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Deposited on : 2021-06-22

Resolution : 1.90 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
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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

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

Xtriage (Phenix) : 1.13 EDS : 2.36.2

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

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

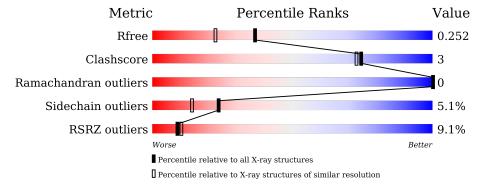
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 1.90 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
WIGHT	$(\# {\rm Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	289	9%	85%	12% ••			
2	В	3	33%	67%				
2	С	3	67%		33%			
2	Е	3		100%				
3	D	2		100%				
4	F	5		100%				



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2544 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 Peptide Asparaginyl Ligases.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	286	Total	С	N	О	S	0	1	0
1	A	200	2220	1410	361	438	11	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP A0A509GV09
A	172	HD0	HIS	conflict	UNP A0A509GV09
A	214	ALA	CYS	engineered mutation	UNP A0A509GV09

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	3	Total C N O 39 22 2 15	0	0	0
2	С	3	Total C N O 39 22 2 15	0	0	0
2	Е	3	Total C N O 39 22 2 15	0	0	0

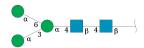
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total 28	C 16	N 2	O 10	0	0	0

 $\bullet \ \, \text{Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.}$ 



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
4	F	5	Total 61			O 25	0	0	0

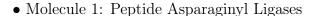
• Molecule 5 is water.

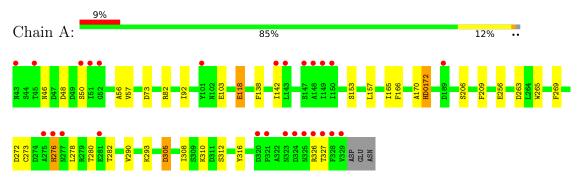
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	118	Total O 118 118	0	0



# 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 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose

Chain B: 33% 67%

NAG1 NAG2 MAN3

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

Chain C: 67% 33%

NAG1 NAG2 MAN3

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

Chain E: 100%

NAG1 NAG2 MAN3

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

Chain D: 100%





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

Chain F: 100%

NAG1 NAG2 MAN3 MAN4 MAN5



# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	95.00Å 81.15Å 47.65Å	Donogitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $113.62^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	40.91 - 1.90	Depositor	
resolution (A)	40.91 - 1.90	EDS	
% Data completeness	99.3 (40.91-1.90)	Depositor	
(in resolution range)	99.7 (40.91-1.90)	EDS	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.36 (at 1.89Å)	Xtriage	
Refinement program	BUSTER 2.10.3	Depositor	
P.P.	0.215 , $0.244$	Depositor	
$R, R_{free}$	0.217 , $0.252$	DCC	
$R_{free}$ test set	1304 reflections $(5.00\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage	
Anisotropy	0.455	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 62.0	EDS	
L-test for twinning <sup>2</sup>	$ < L > = 0.50, < L^2> = 0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.97	EDS	
Total number of atoms	2544	wwPDB-VP	
Average B, all atoms $(Å^2)$	72.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.74% 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: MAN, HD0, NAG

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).

Mal	Chain	Bond	lengths	Bond	angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.42	0/2260	0.59	0/3072

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	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ALA	Mainchain, Peptide
1	A	172	HD0	Mainchain, Peptide

## 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	2220	0	2103	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	39	0	34	0	0
2	С	39	0	34	0	0
2	Ε	39	0	34	0	0
3	D	28	0	25	0	0
4	F	61	0	52	0	0
5	A	118	0	0	0	0
All	All	2544	0	2282	15	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 3.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:A:282:THR:HA	1:A:312:SER:HA	1.82	0.62
1:A:157:LEU:HD13	1:A:165:ILE:HD13	1.84	0.59
1:A:48:ASP:OD2	1:A:50:SER:HB3	2.04	0.58
1:A:272:ASP:OD1	1:A:276:HIS:NE2	2.33	0.56
1:A:305:ASP:HB3	1:A:308:ILE:HG12	1.91	0.51
1:A:73:ASP:OD2	1:A:263:ASP:OD1	2.29	0.51
1:A:57:VAL:HG22	1:A:92:ILE:HD12	1.95	0.49
1:A:280:THR:HG21	1:A:327:THR:HG22	1.94	0.48
1:A:138:PHE:CZ	1:A:142:ILE:HD11	2.49	0.48
1:A:273:CYS:HA	1:A:278:LEU:HD21	1.96	0.46
1:A:206:SER:OG	1:A:316:TYR:OH	2.29	0.46
1:A:265:TRP:CD1	1:A:290:VAL:HG11	2.55	0.42
1:A:103:GLU:CD	1:A:103:GLU:H	2.24	0.41
1:A:118:GLU:H	1:A:118:GLU:HG2	1.76	0.41
1:A:56:ALA:HA	1:A:166:PHE:O	2.21	0.40

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	Favoured Allowed		Percentiles	
1	A	284/289 (98%)	274 (96%)	10 (4%)	0	100 100	

There are no Ramachandran outliers to report.

#### 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	238/240 (99%)	225 (94%)	13 (6%)	21 12		

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	82	ARG
1	A	118	GLU
1	A	153[A]	SER
1	A	153[B]	SER
1	A	209	PHE
1	A	256	GLU
1	A	269	PHE
1	A	276	HIS
1	A	293	LYS
1	A	305	ASP
1	A	310	LYS
1	A	326	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	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)

1 non-standard protein/DNA/RNA residue is 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).

1	Mol Type	Chain	Dog	Tiple	Bond lengths			Bond angles			
10.		туре	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
	1	HD0	A	172	1	11,18,19	3.11	3 (27%)	14,25,27	4.37	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HD0	A	172	1	-	0/9/26/28	0/2/2/2

#### All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	A	172	HD0	CAW-CAX	8.11	1.62	1.50
1	A	172	HD0	CAU-NAS	5.34	1.49	1.39
1	A	172	HD0	CAX-NAS	2.21	1.42	1.39

#### All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	172	HD0	CB-C1-NAS	14.16	130.25	112.32
1	A	172	HD0	CAW-CAX-NAS	-6.70	102.35	107.53
1	A	172	HD0	OAY-CAX-CAW	2.97	131.57	127.24

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

16 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	Trino	Chain	Res	T inle	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	В	1	2,1	14,14,15	0.34	0	17,19,21	0.75	0
2	NAG	В	2	2	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
2	MAN	В	3	2	11,11,12	0.54	0	15,15,17	1.19	2 (13%)
2	NAG	С	1	2,1	14,14,15	0.27	0	17,19,21	0.42	0
2	NAG	С	2	2	14,14,15	0.22	0	17,19,21	0.95	1 (5%)
2	MAN	С	3	2	11,11,12	0.28	0	15,15,17	0.74	0
3	NAG	D	1	3,1	14,14,15	0.29	0	17,19,21	1.87	3 (17%)
3	NAG	D	2	3	14,14,15	0.28	0	17,19,21	1.17	1 (5%)
2	NAG	Е	1	2,1	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
2	NAG	Е	2	2	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
2	MAN	Е	3	2	11,11,12	0.65	0	15,15,17	1.87	3 (20%)
4	NAG	F	1	4,1	14,14,15	0.25	0	17,19,21	0.70	1 (5%)
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	1.13	1 (5%)
4	MAN	F	3	4	11,11,12	0.60	0	15,15,17	1.49	2 (13%)
4	MAN	F	4	4	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
4	MAN	F	5	4	11,11,12	0.27	0	15,15,17	0.79	1 (6%)

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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	NAG	В	1	2,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1
2	MAN	В	3	2	-	1/2/19/22	0/1/1/1
2	NAG	С	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1
2	MAN	С	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
2	NAG	Е	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	0/6/23/26	0/1/1/1
2	MAN	Е	3	2	-	0/2/19/22	1/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	MAN	F	3	4	-	0/2/19/22	1/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	Е	3	MAN	C1-O5-C5	6.20	120.60	112.19
3	D	1	NAG	C1-O5-C5	5.57	119.74	112.19
4	F	3	MAN	C1-O5-C5	4.29	118.00	112.19
3	D	2	NAG	O5-C1-C2	-4.18	104.68	111.29
4	F	2	NAG	O5-C1-C2	-3.93	105.08	111.29
3	D	1	NAG	C3-C4-C5	3.86	117.12	110.24
2	Е	2	NAG	O5-C1-C2	-3.75	105.36	111.29
4	F	3	MAN	C1-C2-C3	3.37	113.81	109.67
2	В	3	MAN	C1-C2-C3	3.31	113.73	109.67
4	F	4	MAN	C1-O5-C5	2.51	115.59	112.19
2	Е	3	MAN	C1-C2-C3	2.47	112.70	109.67
2	В	2	NAG	O5-C1-C2	-2.44	107.44	111.29
4	F	5	MAN	C1-O5-C5	2.42	115.47	112.19
2	В	3	MAN	C1-O5-C5	2.29	115.30	112.19
3	D	1	NAG	O5-C1-C2	-2.27	107.70	111.29
2	С	2	NAG	C1-O5-C5	2.25	115.24	112.19
4	F	1	NAG	C1-O5-C5	2.24	115.23	112.19
2	Е	3	MAN	C2-C3-C4	2.17	114.65	110.89
2	Е	1	NAG	O5-C1-C2	-2.03	108.09	111.29

There are no chirality outliers.



All (4) torsion outliers are listed below:

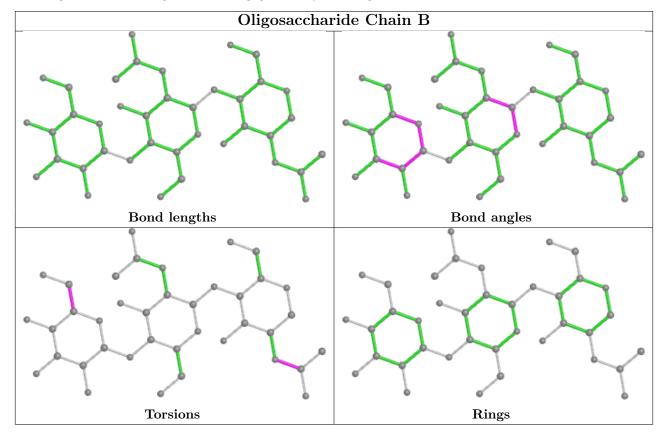
Mol	Chain	Res	Type	Atoms
2	В	3	MAN	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	В	1	NAG	C8-C7-N2-C2
2	С	1	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

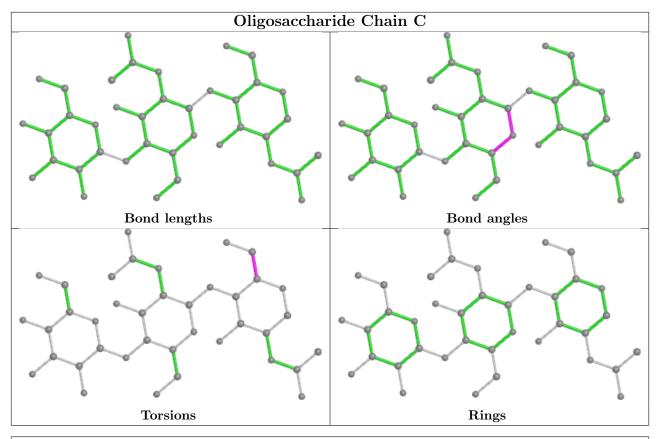
Mol	Chain	Res	Type	Atoms
2	Е	3	MAN	C1-C2-C3-C4-C5-O5
4	F	3	MAN	C1-C2-C3-C4-C5-O5

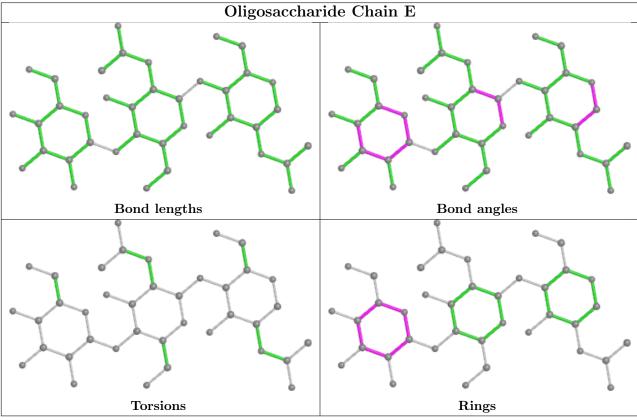
No monomer is involved in short contacts.

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

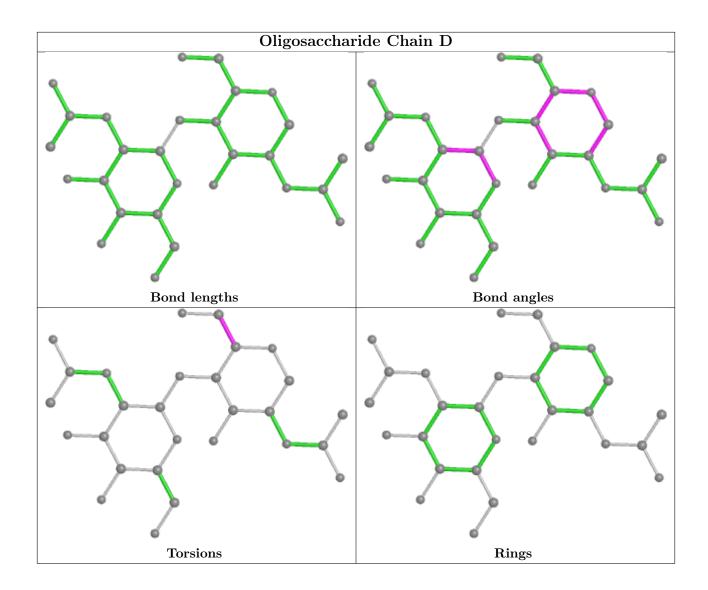




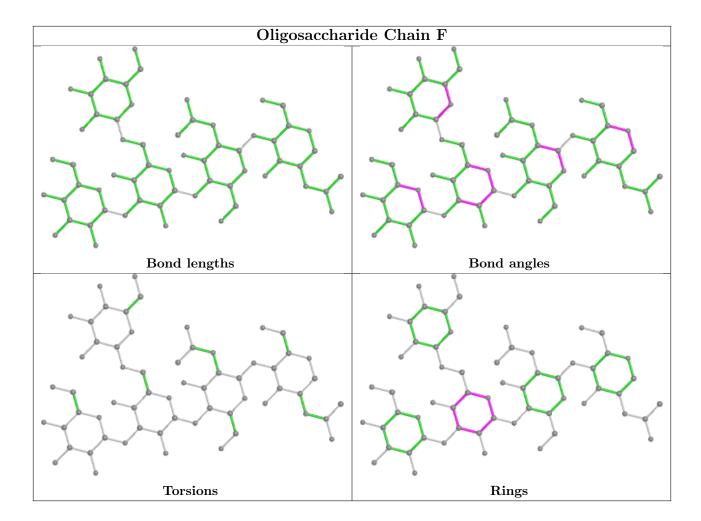












## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 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></rsrz>	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	285/289 (98%)	0.72	26 (9%) 9 10	43, 66, 92, 148	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	ILE	7.4
1	A	148	ALA	6.1
1	A	329	VAL	5.0
1	A	328	PHE	4.7
1	A	43	ASN	4.5
1	A	325	ASN	4.3
1	A	327	THR	4.1
1	A	326	ARG	3.6
1	A	275	ALA	3.6
1	A	149	ILE	3.3
1	A	277	ASN	3.2
1	A	52	GLY	3.1
1	A	320	ASP	2.7
1	A	143	LEU	2.7
1	A	324	ASP	2.7
1	A	51	ILE	2.6
1	A	276	HIS	2.5
1	A	189	ASP	2.5
1	A	147	SER	2.5
1	A	281	GLU	2.5
1	A	321	PRO	2.4
1	A	142	ILE	2.3
1	A	50	SER	2.3
1	A	45	THR	2.1
1	A	101	TYR	2.1
1	A	323	ASN	2.1



## 6.2 Non-standard residues in protein, DNA, RNA chains (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
1	HD0	A	172	17/18	0.96	0.14	43,48,57,57	0

## 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.

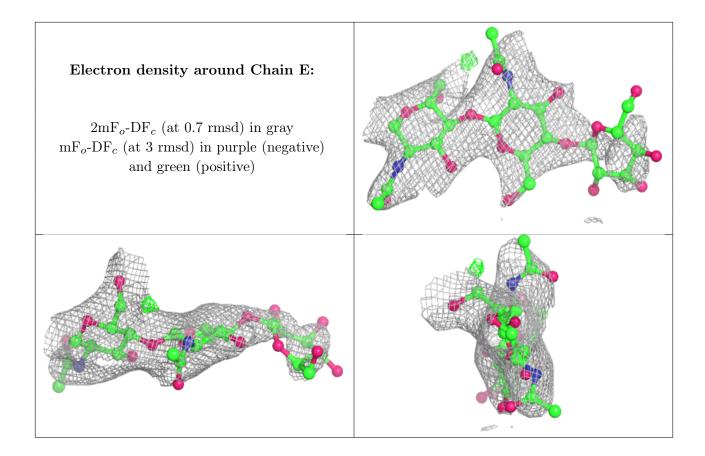
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q<0.9
3	NAG	D	1	14/15	0.44	0.39	155,157,158,158	0
2	MAN	С	3	11/12	0.54	0.31	112,115,115,115	0
4	MAN	F	3	11/12	0.59	0.22	160,161,161,162	0
3	NAG	D	2	14/15	0.66	0.38	156,156,156,156	0
4	NAG	F	1	14/15	0.73	0.40	165,166,167,167	0
2	MAN	В	3	11/12	0.79	0.23	98,100,101,101	0
2	MAN	Е	3	11/12	0.82	0.60	117,118,118,119	0
4	NAG	F	2	14/15	0.85	0.18	162,163,166,167	0
2	NAG	Е	2	14/15	0.86	0.38	111,113,114,115	0
2	NAG	В	2	14/15	0.87	0.12	85,88,92,95	0
4	MAN	F	5	11/12	0.88	0.27	159,160,160,160	0
2	NAG	С	2	14/15	0.89	0.16	101,104,106,109	0
4	MAN	F	4	11/12	0.90	0.20	162,163,163,163	0
2	NAG	С	1	14/15	0.91	0.11	88,90,93,97	0
2	NAG	Е	1	14/15	0.92	0.30	103,104,107,109	0
2	NAG	В	1	14/15	0.93	0.13	72,74,77,81	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.

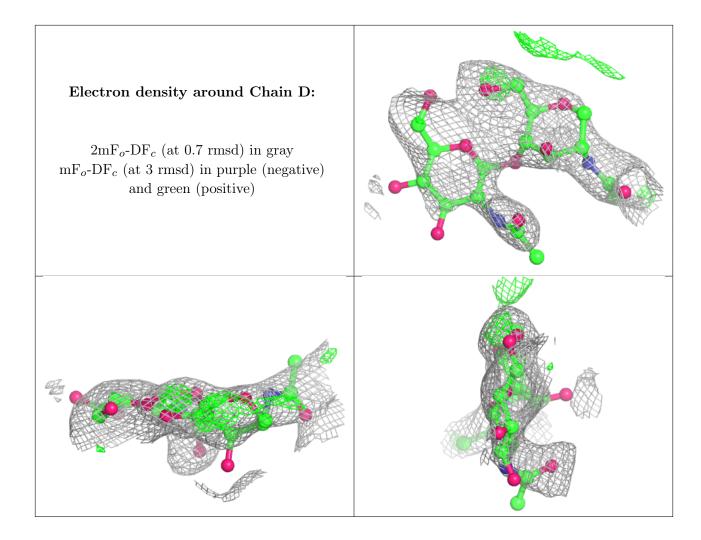


# Electron density around Chain B: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around Chain C: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $mF_o$ -DF<sub>c</sub> (at 3 rmsd)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

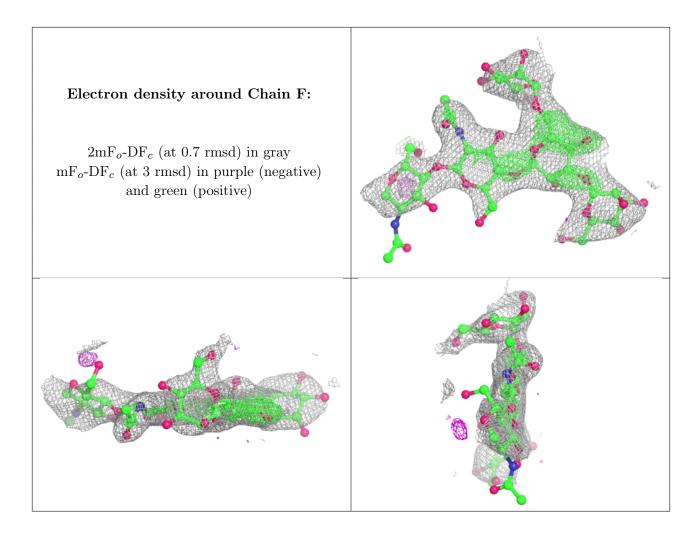












# 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

