



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 04:09 PM JST

PDB ID : 7F5J  
Title : The crystal structure of VyPAL2-I244V, a more efficient mutant of VyPAL2 peptide asparaginyl ligase in its active enzyme form  
Authors : Hu, S.; Sahili, A.; Lescar, J.  
Deposited on : 2021-06-22  
Resolution : 1.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

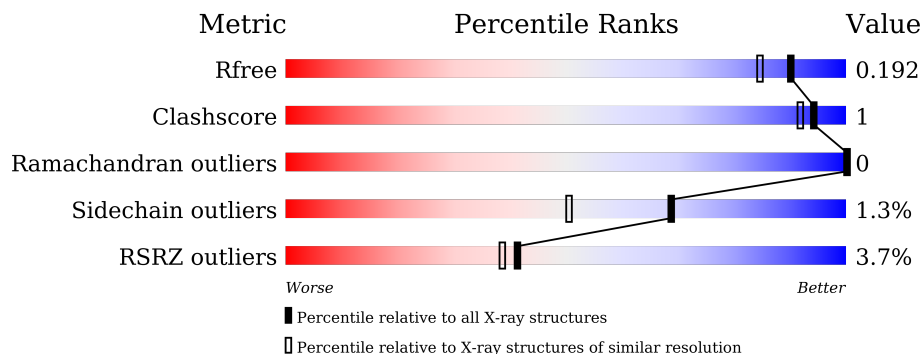
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

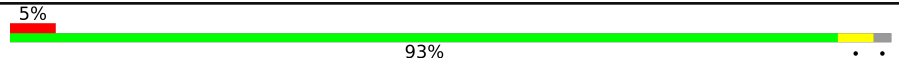
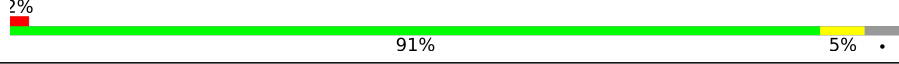
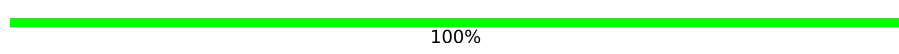

The reported resolution of this entry is 1.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	 5% 93% 2% 2%
1	B	282	 2% 91% 5% 2%
2	C	2	 100%
3	D	2	 50% 50%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	409	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 4919 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
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	3	0
			2145	1368	349	416	12			
1	B	271	Total	C	N	O	S	0	4	0
			2118	1353	341	412	12			

There are 6 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	244	VAL	ILE	engineered mutation	UNP A0A509GV09
B	?	-	ASP	deletion	UNP A0A509GV09
B	172	HD0	HIS	conflict	UNP A0A509GV09
B	244	VAL	ILE	engineered mutation	UNP A0A509GV09

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



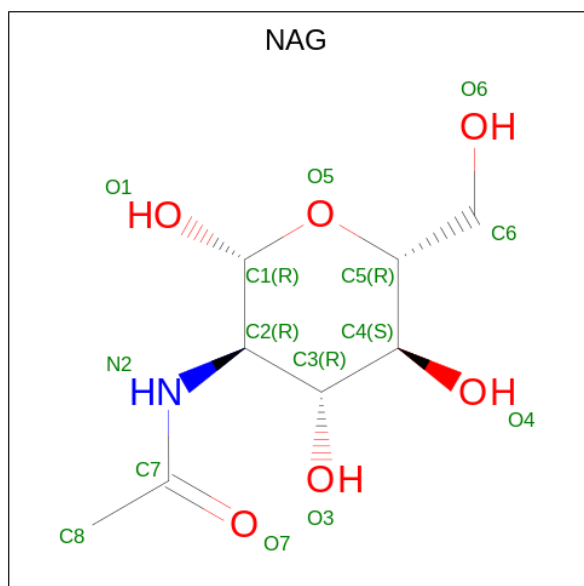
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



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

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



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

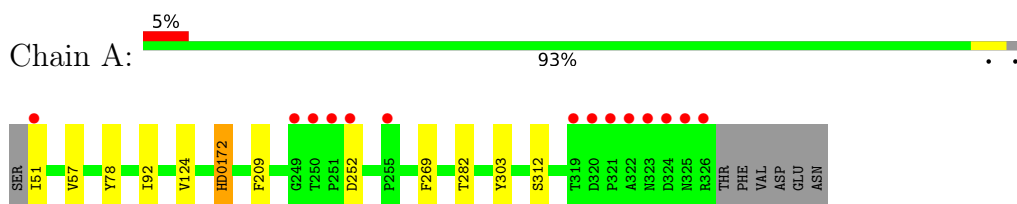
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	251	Total O 251 251	0	0
7	B	249	Total O 249 249	0	0

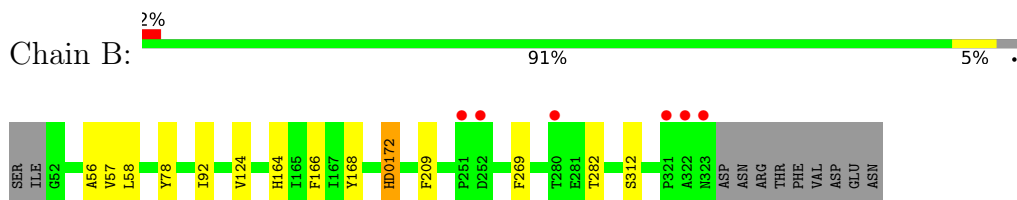
### 3 Residue-property plots [i](#)

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.

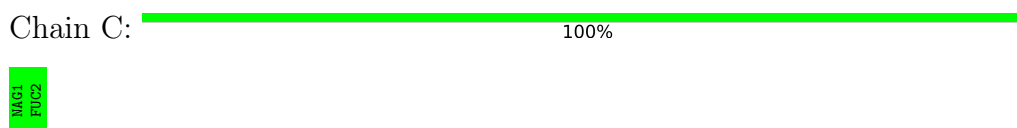
- Molecule 1: Peptide Asparaginyl Ligases



- Molecule 1: Peptide Asparaginyl Ligases



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.27Å 78.98Å 92.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.06 – 1.59 47.14 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.06-1.59) 99.3 (47.14-1.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 1.59Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.163 , 0.193 0.164 , 0.192	Depositor DCC
$R_{free}$ test set	3721 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, EDO, GOL, FUC, HD0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/2190	0.58	0/2975
1	B	0.41	0/2166	0.57	0/2943
All	All	0.41	0/4356	0.57	0/5918

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	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	172	HD0	Peptide,Mainchain
1	B	172	HD0	Peptide,Mainchain

### 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	2145	0	2055	4	0
1	B	2118	0	2026	7	0
2	C	24	0	22	0	0
3	D	28	0	25	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	16	0	24	0	0
5	B	8	0	12	0	0
6	A	18	0	24	1	0
6	B	6	0	8	0	0
7	A	251	0	0	0	0
7	B	249	0	0	3	0
All	All	4919	0	4248	11	0

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

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:HA	1:A:312:SER:HA	1.95	0.48
1:A:78:TYR:CD2	1:A:124:VAL:HG22	2.51	0.45
1:B:282:THR:HA	1:B:312:SER:HA	1.98	0.45
1:B:56:ALA:HA	1:B:166:PHE:O	2.18	0.44
1:B:57:VAL:HG22	1:B:92:ILE:HD12	2.00	0.43
1:A:57:VAL:HG22	1:A:92:ILE:HD12	2.02	0.42
1:A:303:TYR:HD2	6:A:406:GOL:H2	1.84	0.42
1:B:168:TYR:HD2	7:B:673:HOH:O	2.03	0.41
1:B:164:HIS:HD2	7:B:683:HOH:O	2.03	0.41
1:B:58:LEU:HB3	7:B:673:HOH:O	2.20	0.41
1:B:78:TYR:CD2	1:B:124:VAL:HG22	2.55	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/282 (98%)	270 (98%)	5 (2%)	0	100	100
1	B	272/282 (96%)	268 (98%)	4 (2%)	0	100	100
All	All	547/564 (97%)	538 (98%)	9 (2%)	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	230/234 (98%)	226 (98%)	4 (2%)	60	38
1	B	227/234 (97%)	225 (99%)	2 (1%)	78	65
All	All	457/468 (98%)	451 (99%)	6 (1%)	69	50

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	209	PHE
1	A	252	ASP
1	A	269	PHE
1	B	209	PHE
1	B	269	PHE

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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HD0	A	172	1	11,18,19	3.16	4 (36%)	14,25,27	2.12	3 (21%)
1	HD0	B	172	1	11,18,19	3.28	4 (36%)	14,25,27	2.05	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	-	1/9/26/28	0/2/2/2
1	HD0	B	172	1	-	0/9/26/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	HD0	CAW-CAX	8.28	1.63	1.50
1	A	172	HD0	CAW-CAX	8.19	1.63	1.50
1	B	172	HD0	CAU-NAS	5.00	1.48	1.39
1	A	172	HD0	CAU-NAS	4.55	1.47	1.39
1	B	172	HD0	OAV-CAU	-3.50	1.16	1.22
1	A	172	HD0	CAX-NAS	2.62	1.43	1.39
1	B	172	HD0	CAX-NAS	2.47	1.43	1.39
1	A	172	HD0	OAV-CAU	-2.42	1.18	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	HD0	CAW-CAX-NAS	-5.26	103.46	107.53
1	B	172	HD0	CAW-CAX-NAS	-5.25	103.47	107.53
1	A	172	HD0	CB-C1-NAS	3.93	117.29	112.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	HD0	C1-NAS-CAU	-3.23	116.90	123.23
1	B	172	HD0	OAY-CAX-CAW	2.84	131.38	127.24
1	A	172	HD0	C1-NAS-CAU	-2.29	118.73	123.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	HD0	CB-C1-NAS-CAX

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	2,1	14,14,15	0.30	0	17,19,21	0.40	0
2	FUC	C	2	2	10,10,11	0.32	0	14,14,16	0.81	0
3	NAG	D	1	3,1	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
3	NAG	D	2	3	14,14,15	0.29	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	O5-C1-C2	-2.70	107.02	111.29

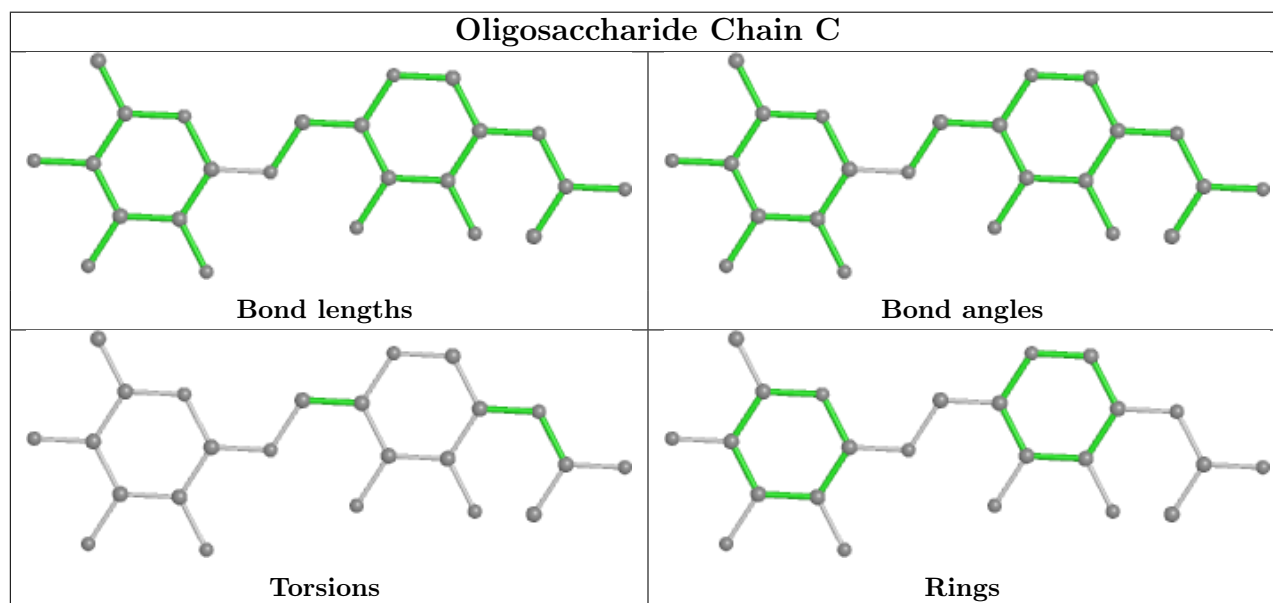
There are no chirality outliers.

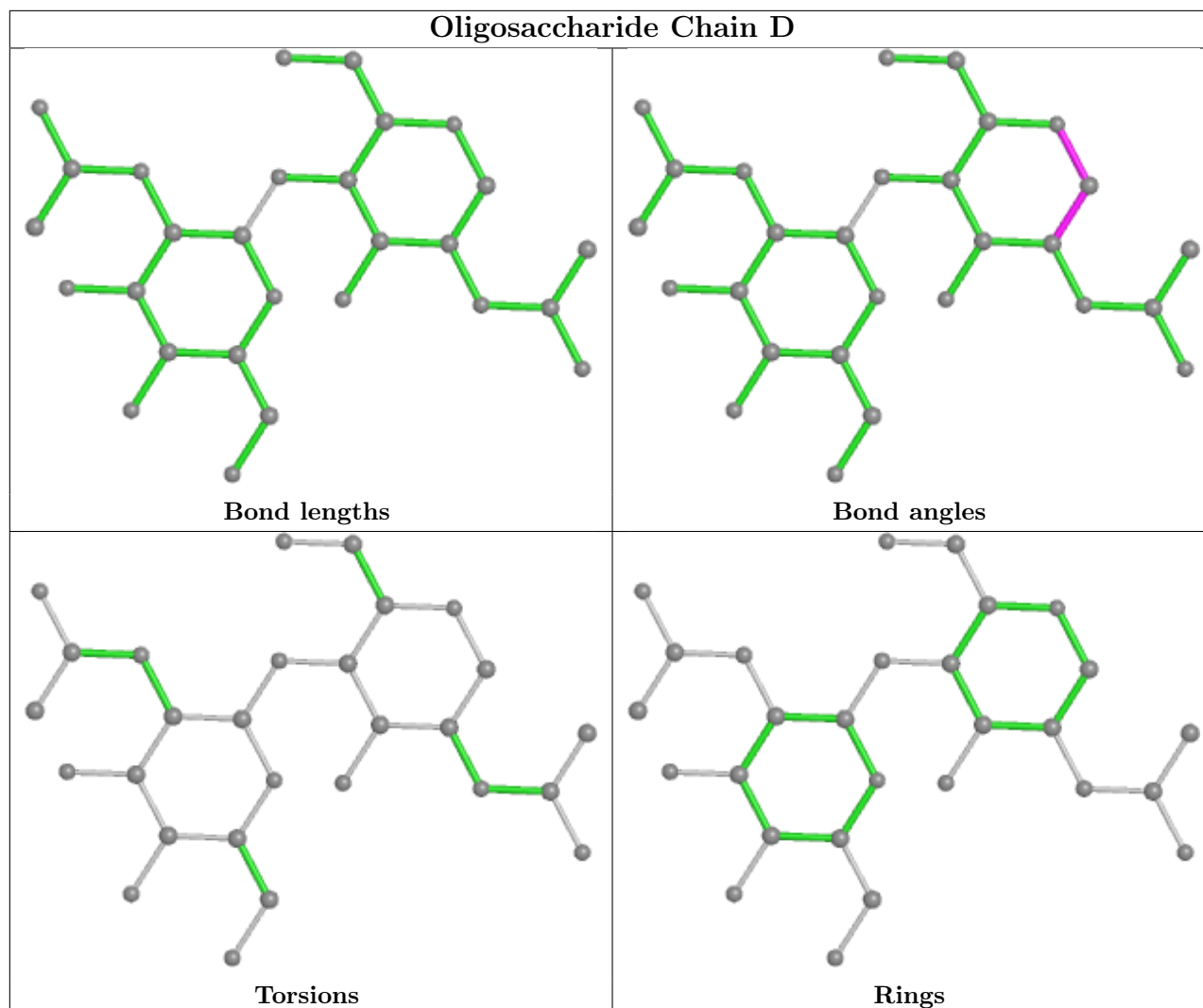
There are no torsion outliers.

There are no ring outliers.

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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	403	1	14,14,15	0.26	0	17,19,21	0.61	0
5	EDO	A	405	-	3,3,3	0.63	0	2,2,2	0.21	0
5	EDO	A	407	-	3,3,3	0.61	0	2,2,2	0.33	0
4	NAG	B	401	1	14,14,15	0.32	0	17,19,21	0.50	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	403	-	3,3,3	0.58	0	2,2,2	0.29	0
6	GOL	A	408	-	5,5,5	0.10	0	5,5,5	0.46	0
5	EDO	B	404	-	3,3,3	0.60	0	2,2,2	0.30	0
5	EDO	B	405	-	3,3,3	0.68	0	2,2,2	0.28	0
6	GOL	A	406	-	5,5,5	0.10	0	5,5,5	0.47	0
6	GOL	A	409	-	5,5,5	0.03	0	5,5,5	0.12	0
4	NAG	A	404	1	14,14,15	0.27	0	17,19,21	0.44	0
6	GOL	B	402	-	5,5,5	0.05	0	5,5,5	0.18	0
4	NAG	A	401	1	14,14,15	0.25	0	17,19,21	0.77	1 (5%)
5	EDO	A	402	-	3,3,3	0.51	0	2,2,2	0.52	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
4	NAG	B	403	1	-	0/6/23/26	0/1/1/1
5	EDO	A	405	-	-	0/1/1/1	-
5	EDO	A	407	-	-	0/1/1/1	-
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
5	EDO	A	403	-	-	0/1/1/1	-
6	GOL	A	408	-	-	0/4/4/4	-
5	EDO	B	404	-	-	0/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
6	GOL	A	406	-	-	4/4/4/4	-
6	GOL	A	409	-	-	0/4/4/4	-
4	NAG	A	404	1	-	0/6/23/26	0/1/1/1
6	GOL	B	402	-	-	0/4/4/4	-
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	EDO	A	402	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	NAG	C1-C2-N2	-2.20	106.73	110.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	406	GOL	O1-C1-C2-C3
6	A	406	GOL	O2-C2-C3-O3
6	A	406	GOL	O1-C1-C2-O2
6	A	406	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	406	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	274/282 (97%)	-0.21	14 (5%) 28 26	23, 33, 52, 84	0
1	B	270/282 (95%)	-0.32	6 (2%) 62 60	25, 34, 49, 67	0
All	All	544/564 (96%)	-0.27	20 (3%) 41 39	23, 34, 50, 84	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	PRO	6.5
1	A	249	GLY	6.2
1	A	321	PRO	5.9
1	B	251	PRO	5.2
1	A	322	ALA	5.0
1	A	325	ASN	4.9
1	B	322	ALA	4.1
1	A	324	ASP	4.0
1	A	320	ASP	3.9
1	A	252	ASP	3.5
1	A	255	PRO	3.5
1	A	250	THR	3.4
1	A	326	ARG	3.4
1	A	51	ILE	3.3
1	A	323	ASN	3.3
1	A	319	THR	3.1
1	B	252	ASP	3.1
1	B	321	PRO	2.9
1	B	323	ASN	2.3
1	B	280	THR	2.3

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

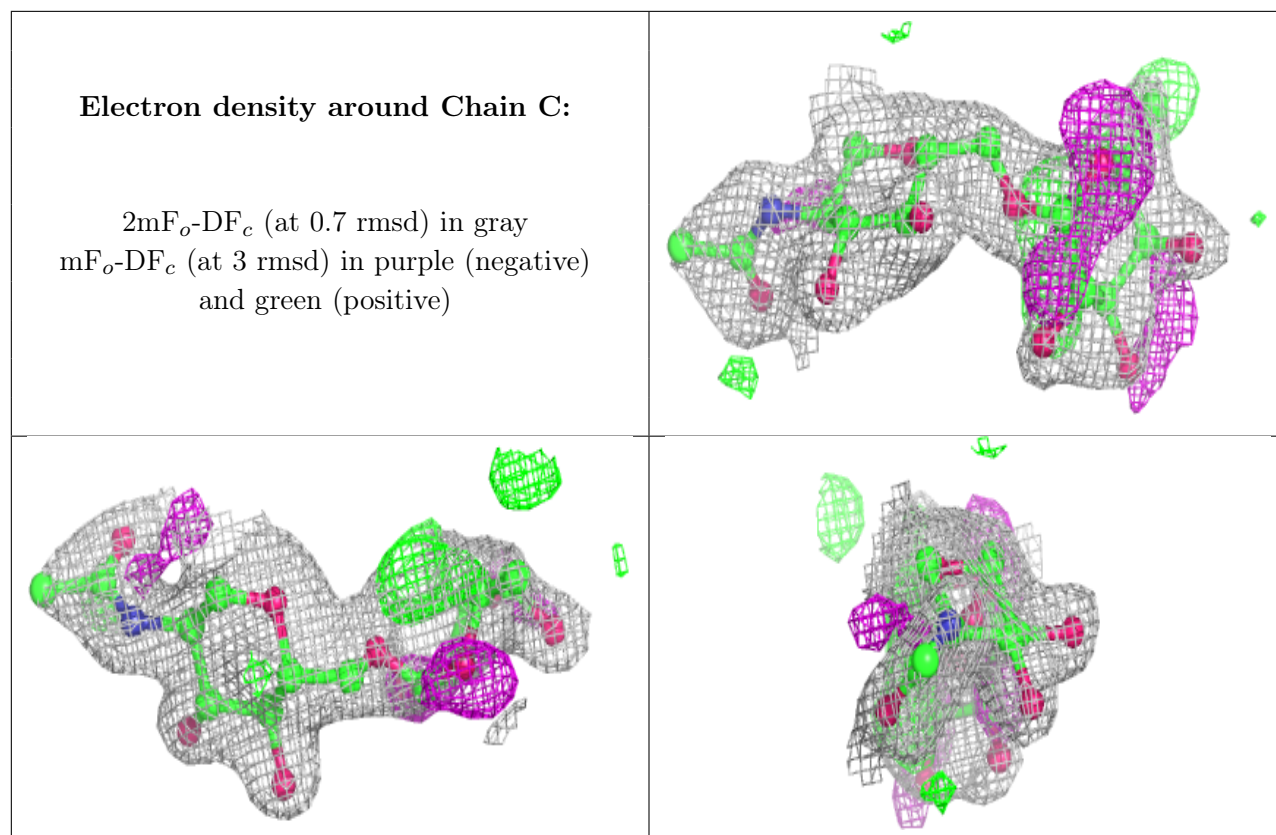
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	HD0	B	172	17/18	0.95	0.10	26,31,39,40	5
1	HD0	A	172	17/18	0.96	0.07	23,28,38,38	5

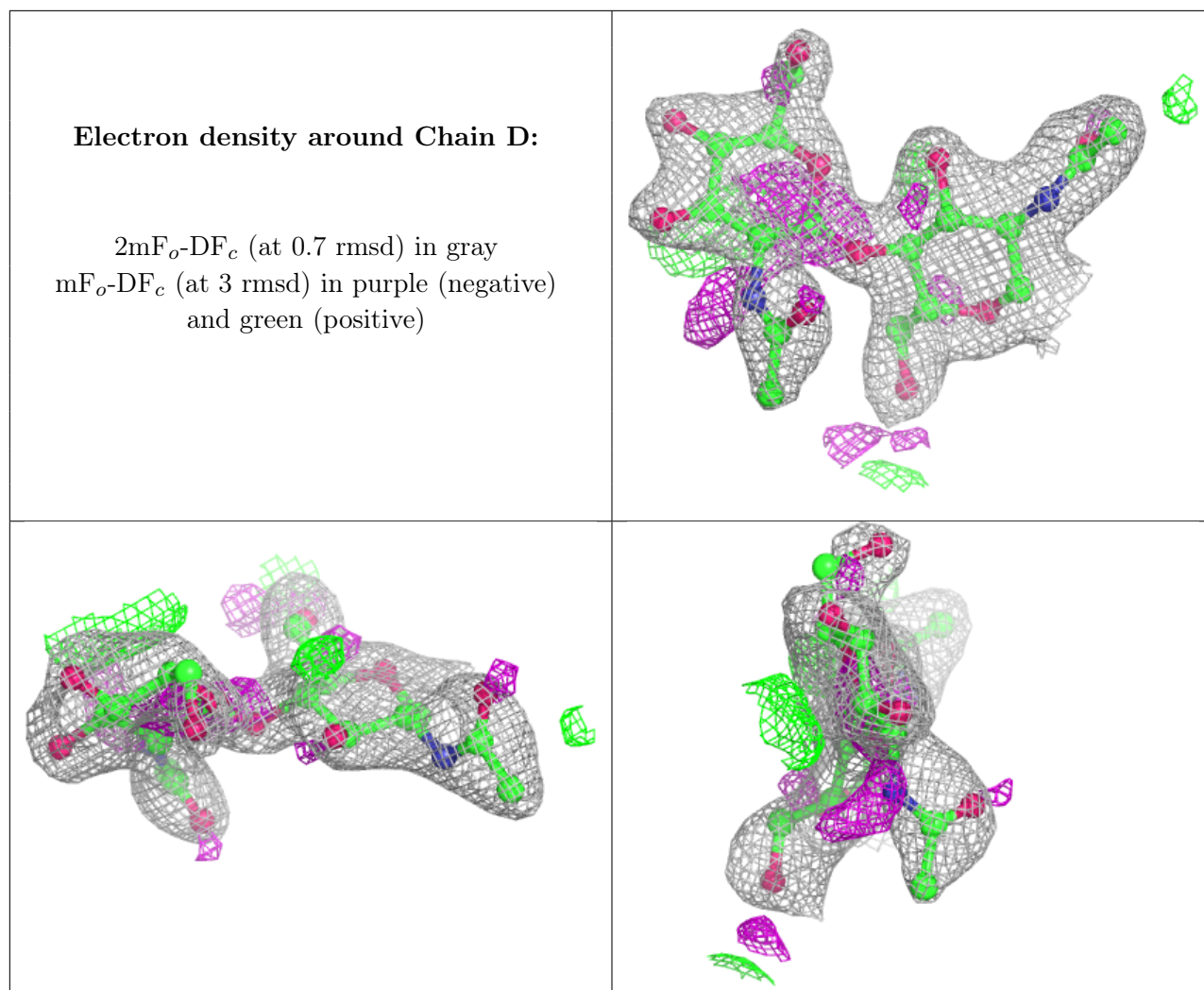
## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	C	2	10/11	0.61	0.25	57,58,59,59	0
3	NAG	D	2	14/15	0.77	0.24	55,56,59,59	0
2	NAG	C	1	14/15	0.85	0.12	48,51,53,55	0
3	NAG	D	1	14/15	0.87	0.13	45,47,49,52	0

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	403	14/15	0.56	0.38	67,69,70,70	0
6	GOL	A	409	6/6	0.60	0.47	114,114,114,114	0
6	GOL	A	406	6/6	0.67	0.19	54,57,58,59	0
5	EDO	A	407	4/4	0.68	0.20	43,45,46,47	0
5	EDO	B	405	4/4	0.68	0.16	52,54,55,55	0
5	EDO	A	405	4/4	0.72	0.13	62,62,62,62	0
5	EDO	B	404	4/4	0.79	0.11	45,47,48,49	0
4	NAG	A	404	14/15	0.81	0.22	57,59,60,60	0
5	EDO	A	403	4/4	0.84	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	408	6/6	0.86	0.13	53,53,54,54	0
6	GOL	B	402	6/6	0.86	0.11	68,68,68,68	0
4	NAG	B	401	14/15	0.87	0.17	51,54,55,55	0
4	NAG	A	401	14/15	0.88	0.14	46,49,50,51	0
5	EDO	A	402	4/4	0.89	0.10	39,41,42,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.