



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:21 PM BST

PDB ID : 6DD5  
Title : Crystal Structure of the Cas6 Domain of *Marinomonas mediterranea* MMB-1 Cas6-RT-Cas1 Fusion Protein  
Authors : Stamos, J.L.; Mohr, G.; Silas, S.; Makarova, K.S.; Markham, L.M.; Yao, J.; Lucas-Elio, P.; Sanchez-Amat, A.; Fire, A.Z.; Koonin, E.V.; Lambowitz, A.M.  
Deposited on : 2018-05-09  
Resolution : 2.85 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.

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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 : 2.13.1  
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) : 2.13.1

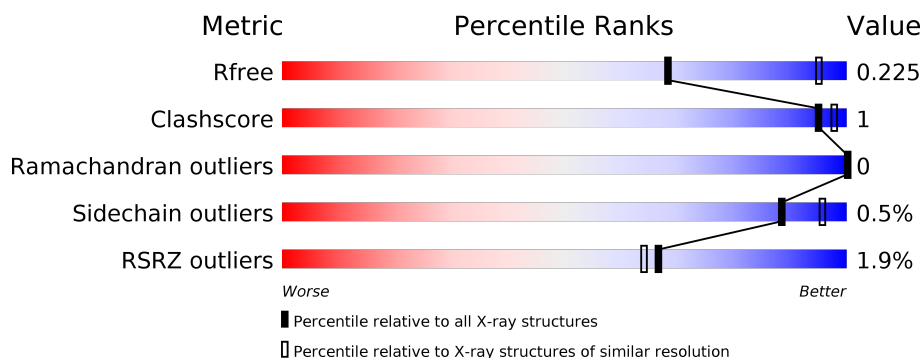
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	678	<div> <div style="width: 93%;"></div> <div>93%</div> </div>
1	B	678	<div> <div style="width: 91%;"></div> <div>91%</div> </div>
2	C	2	<div> <div style="width: 50%;"></div> <div>50%</div> </div>
2	D	2	<div> <div style="width: 50%;"></div> <div>50%</div> </div>

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
4	SO4	A	1411	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10268 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 MMB-1 Cas6 Fused to Maltose Binding Protein, CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	0	0
			5096	3264	858	961	13			
1	B	645	Total	C	N	O	S	0	0	0
			5029	3221	846	949	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEY0
A	360	ALA	-	linker	UNP P0AEY0
A	361	ALA	-	linker	UNP P0AEY0
A	362	LEU	-	linker	UNP P0AEY0
A	363	ALA	-	linker	UNP P0AEY0
A	364	ALA	-	linker	UNP P0AEY0
A	365	ALA	-	linker	UNP P0AEY0
A	366	GLN	-	linker	UNP P0AEY0
A	367	THR	-	linker	UNP P0AEY0
A	368	ALA	-	linker	UNP P0AEY0
A	369	ALA	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
A	371	ALA	-	linker	UNP P0AEY0
A	372	ALA	-	linker	UNP P0AEY0
A	1001	MET	-	linker	UNP P0AEY0
A	1002	VAL	-	linker	UNP P0AEY0
B	1	MET	-	initiating methionine	UNP P0AEY0
B	360	ALA	-	linker	UNP P0AEY0
B	361	ALA	-	linker	UNP P0AEY0
B	362	LEU	-	linker	UNP P0AEY0
B	363	ALA	-	linker	UNP P0AEY0
B	364	ALA	-	linker	UNP P0AEY0
B	365	ALA	-	linker	UNP P0AEY0
B	366	GLN	-	linker	UNP P0AEY0

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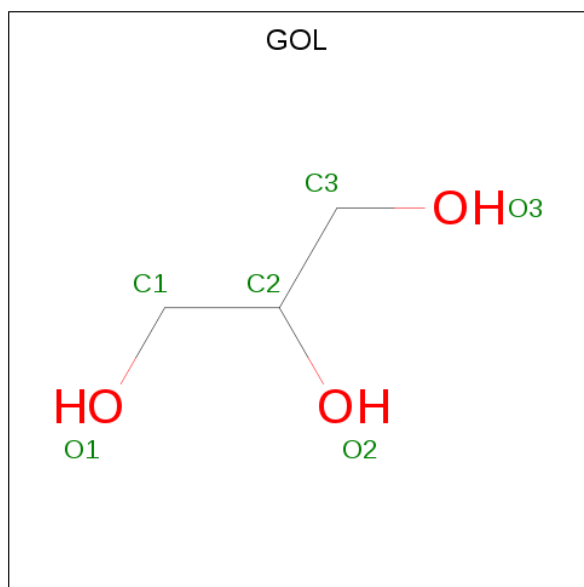
Chain	Residue	Modelled	Actual	Comment	Reference
B	367	THR	-	linker	UNP P0AEY0
B	368	ALA	-	linker	UNP P0AEY0
B	369	ALA	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
B	371	ALA	-	linker	UNP P0AEY0
B	372	ALA	-	linker	UNP P0AEY0
B	1001	MET	-	linker	UNP P0AEY0
B	1002	VAL	-	linker	UNP P0AEY0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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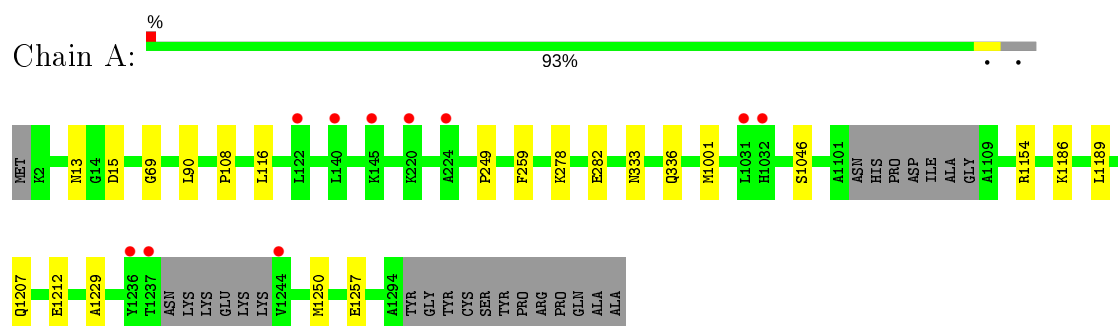
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

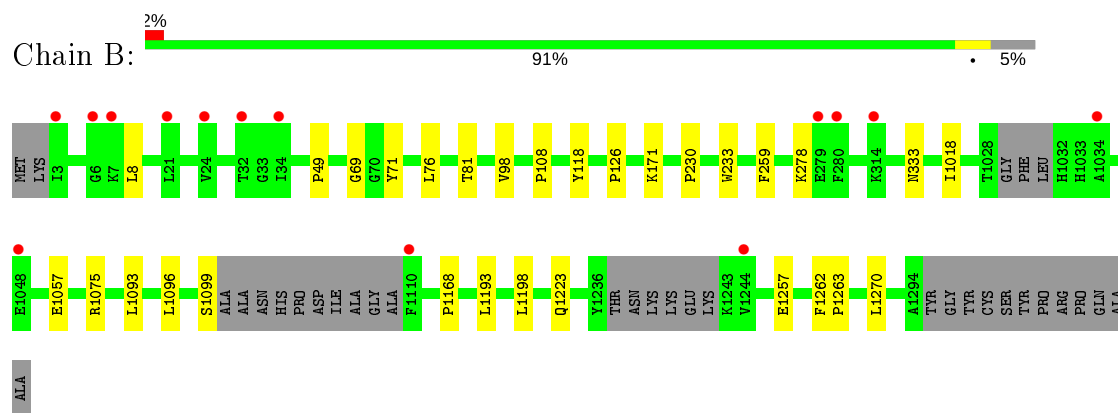
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: MMB-1 Cas6 Fused to Maltose Binding Protein,CRISPR-associated endonuclease Cas1



- Molecule 1: MMB-1 Cas6 Fused to Maltose Binding Protein,CRISPR-associated endonuclease Cas1



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.28Å 110.76Å 192.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.85 48.23 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.23-2.85) 100.0 (48.23-2.85)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.187 , 0.225 0.187 , 0.225	Depositor DCC
$R_{free}$ test set	2278 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GLC, SO4

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	0.33	0/5215	0.50	0/7081
1	B	0.33	0/5147	0.50	0/6994
All	All	0.33	0/10362	0.50	0/14075

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

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	5096	0	5020	10	0
1	B	5029	0	4918	14	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	45	0	0	0	0
4	B	40	0	0	0	0
All	All	10268	0	9996	24	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 (24) 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:13:ASN:ND2	1:A:15:ASP:OD1	2.35	0.58
1:B:81:THR:O	1:B:278:LYS:NZ	2.37	0.57
1:A:1189:LEU:HD21	1:A:1250:MET:HE1	1.88	0.53
1:B:1223:GLN:HB2	1:B:1257:GLU:HB2	1.90	0.52
1:A:90:LEU:HD23	1:A:108:PRO:HG2	1.93	0.50
1:B:98:VAL:HG21	1:B:108:PRO:HD3	1.94	0.50
1:B:49:PRO:HG3	1:B:71:TYR:CE1	2.48	0.48
1:A:1154:ARG:HG2	1:A:1257:GLU:HG2	1.97	0.47
1:A:336:GLN:OE1	1:A:1001:MET:HG2	2.16	0.45
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.52	0.45
1:B:69:GLY:HA3	1:B:333:ASN:O	2.16	0.45
1:B:1168:PRO:HD3	1:B:1193:LEU:HD13	1.99	0.44
1:A:69:GLY:HA3	1:A:333:ASN:O	2.18	0.43
1:A:278:LYS:HE3	1:A:282:GLU:OE2	2.19	0.43
1:B:118:TYR:CE1	1:B:126:PRO:HD3	2.55	0.42
1:A:116:LEU:HD22	1:A:249:PRO:HD3	2.02	0.41
1:B:1057:GLU:OE1	1:B:1075:ARG:NH2	2.44	0.41
1:B:1096:LEU:HD23	1:B:1099:SER:HB2	2.01	0.41
1:B:1018:ILE:HD13	1:B:1093:LEU:HD11	2.01	0.41
1:A:1186:LYS:HG3	1:A:1229:ALA:HB3	2.03	0.41
1:B:1198:LEU:HD21	1:B:1270:LEU:HA	2.04	0.40
1:B:171:LYS:HD2	1:B:171:LYS:HA	1.89	0.40
1:B:1262:PHE:HA	1:B:1263:PRO:HD3	1.96	0.40
1:A:1207:GLN:HA	1:A:1212:GLU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	646/678 (95%)	632 (98%)	14 (2%)	0	100	100
1	B	637/678 (94%)	625 (98%)	12 (2%)	0	100	100
All	All	1283/1356 (95%)	1257 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	530/553 (96%)	528 (100%)	2 (0%)	91	96
1	B	521/553 (94%)	518 (99%)	3 (1%)	86	95
All	All	1051/1106 (95%)	1046 (100%)	5 (0%)	88	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	PHE
1	A	1046	SER
1	B	8	LEU
1	B	76	LEU
1	B	259	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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	GLC	C	1	2	12,12,12	0.55	0	17,17,17	0.76	0
2	GLC	C	2	2	11,11,12	0.67	0	15,15,17	1.06	1 (6%)
2	GLC	D	1	2	12,12,12	0.63	0	17,17,17	0.90	0
2	GLC	D	2	2	11,11,12	0.65	0	15,15,17	1.13	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	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C1-O5-C5	2.47	115.54	112.19
2	D	2	GLC	O5-C5-C6	2.34	110.87	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6

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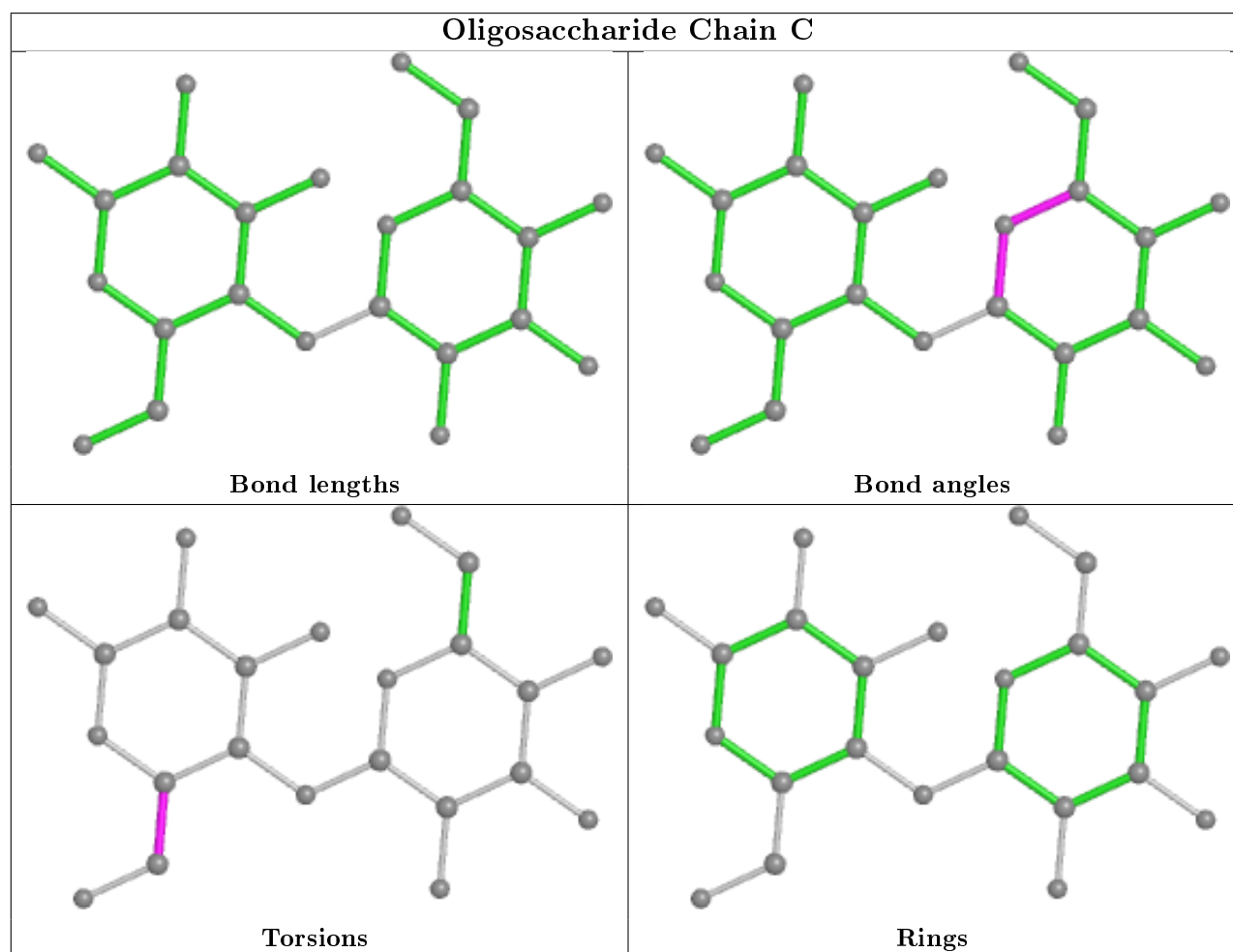
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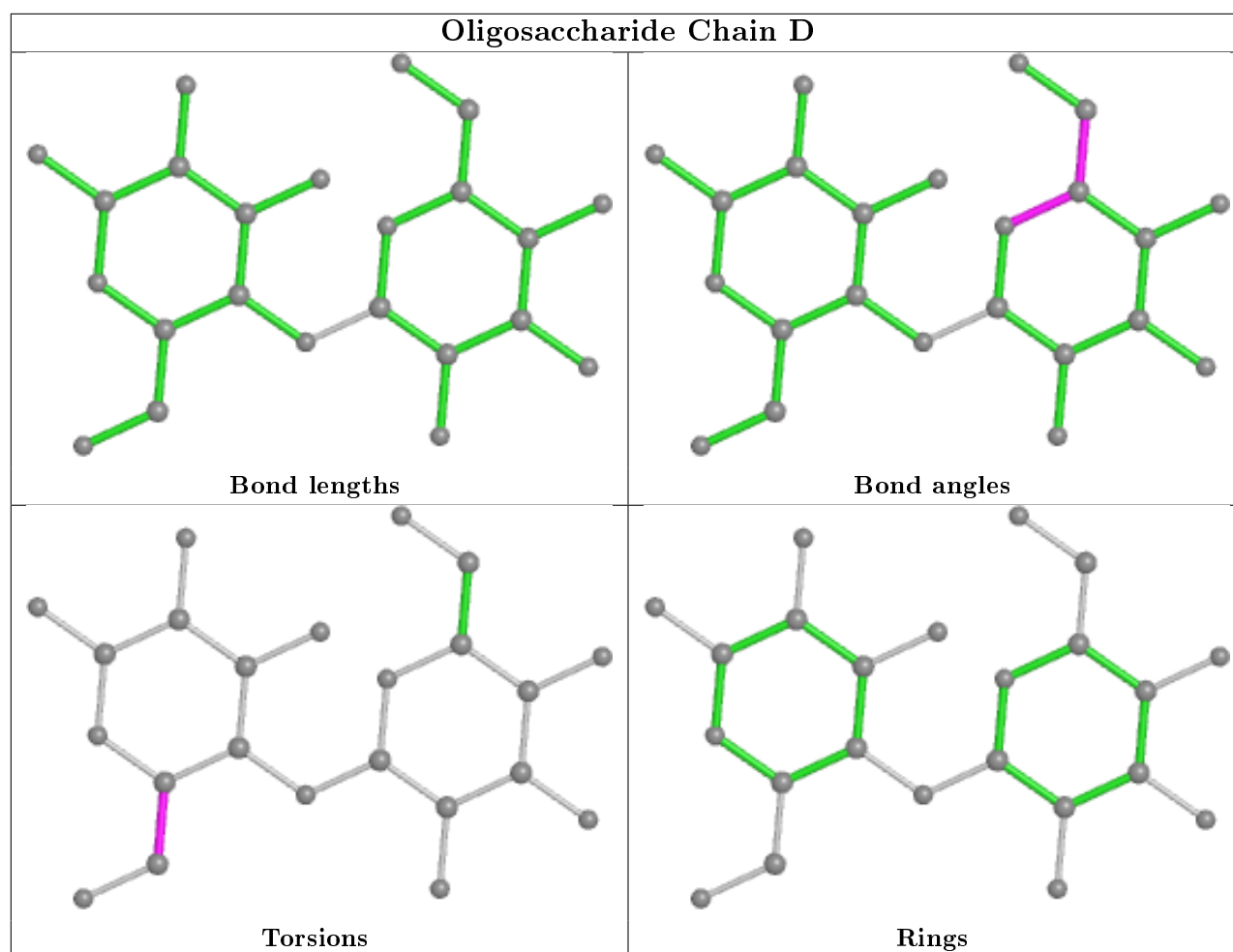
Mol	Chain	Res	Type	Atoms
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

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](#)

19 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	SO4	A	1403	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	A	1408	-	4,4,4	0.17	0	6,6,6	0.10	0
4	SO4	A	1410	-	4,4,4	0.15	0	6,6,6	0.26	0
4	SO4	A	1407	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	A	1406	-	4,4,4	0.19	0	6,6,6	0.24	0
4	SO4	B	1406	-	4,4,4	0.17	0	6,6,6	0.13	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	1404	-	4,4,4	0.13	0	6,6,6	0.15	0
4	SO4	B	1408	-	4,4,4	0.15	0	6,6,6	0.50	0
4	SO4	B	1403	-	4,4,4	0.11	0	6,6,6	0.45	0
4	SO4	A	1405	-	4,4,4	0.16	0	6,6,6	0.29	0
4	SO4	A	1411	-	4,4,4	0.13	0	6,6,6	0.38	0
4	SO4	B	1407	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	A	1409	-	4,4,4	0.13	0	6,6,6	0.20	0
4	SO4	B	1409	-	4,4,4	0.14	0	6,6,6	0.77	0
3	GOL	B	1402	-	5,5,5	0.90	0	5,5,5	0.91	0
4	SO4	B	1405	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SO4	B	1404	-	4,4,4	0.12	0	6,6,6	0.22	0
4	SO4	B	1410	-	4,4,4	0.13	0	6,6,6	0.19	0
3	GOL	A	1402	-	5,5,5	0.79	0	5,5,5	1.04	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
3	GOL	B	1402	-	-	1/4/4/4	-
3	GOL	A	1402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1402	GOL	O1-C1-C2-O2
3	A	1402	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	652/678 (96%)	0.06	10 (1%) 73 72	23, 45, 91, 143	0
1	B	645/678 (95%)	0.10	14 (2%) 62 59	27, 52, 99, 143	0
All	All	1297/1356 (95%)	0.08	24 (1%) 66 64	23, 49, 97, 143	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1244	VAL	4.2
1	A	1236	TYR	3.7
1	B	24	VAL	3.5
1	A	145	LYS	3.4
1	B	34	ILE	3.4
1	B	280	PHE	3.3
1	A	1237	THR	3.2
1	B	21	LEU	3.1
1	B	6	GLY	2.9
1	A	1032	HIS	2.9
1	B	1244	VAL	2.8
1	A	122	LEU	2.7
1	A	140	LEU	2.6
1	B	279	GLU	2.6
1	B	3	ILE	2.5
1	B	1048	GLU	2.5
1	B	32	THR	2.4
1	A	1031	LEU	2.4
1	A	220	LYS	2.4
1	B	1110	PHE	2.3
1	A	224	ALA	2.1
1	B	314	LYS	2.1
1	B	7	LYS	2.0
1	B	1034	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

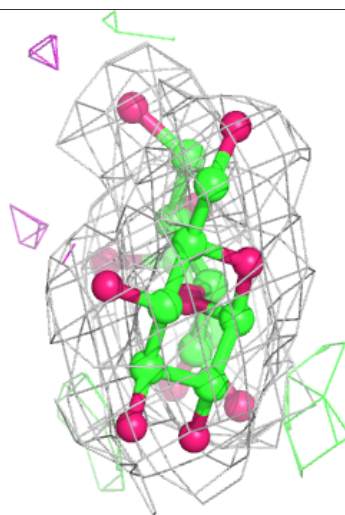
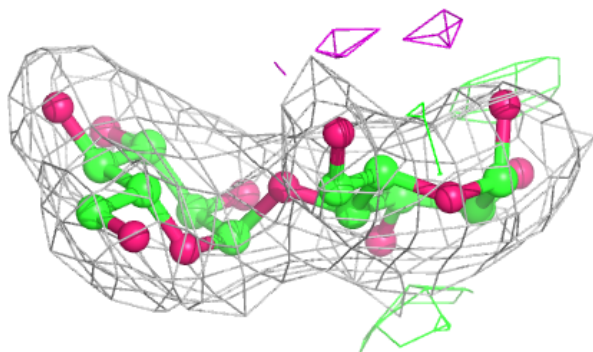
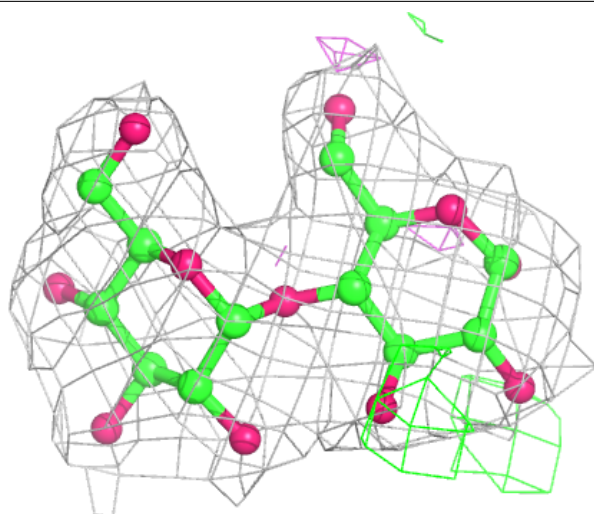
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

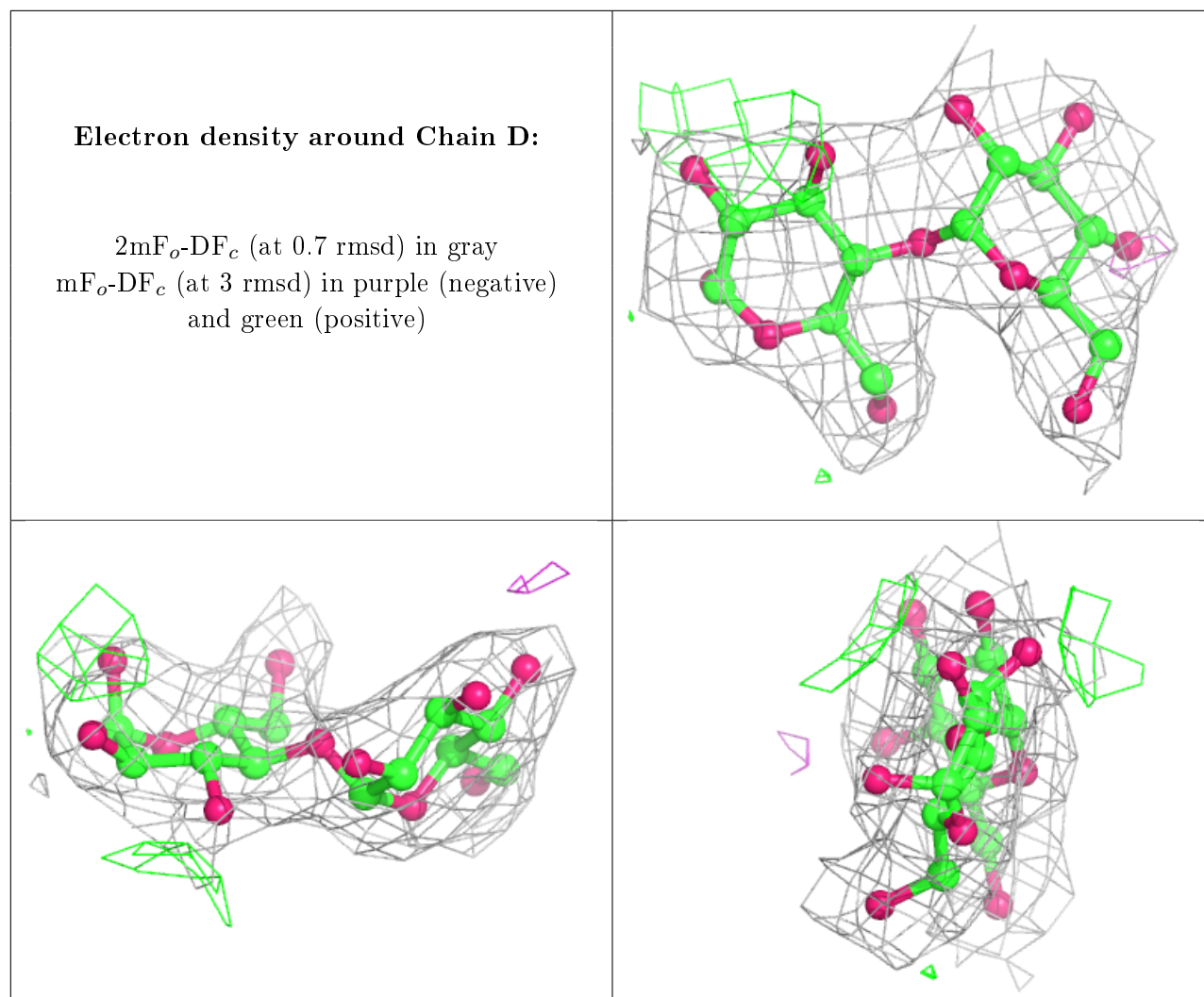
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	D	1	12/12	0.95	0.12	34,45,50,51	0
2	GLC	C	1	12/12	0.97	0.15	22,26,35,36	0
2	GLC	D	2	11/12	0.99	0.14	33,35,40,40	0
2	GLC	C	2	11/12	0.99	0.18	22,24,26,27	0

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

**Electron density around Chain C:**

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





## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	1411	5/5	0.77	0.41	119,122,124,134	0
4	SO4	A	1409	5/5	0.77	0.33	136,136,138,139	0
4	SO4	B	1408	5/5	0.79	0.32	134,134,136,136	0
3	GOL	B	1402	6/6	0.85	0.17	72,72,76,79	0
4	SO4	B	1410	5/5	0.88	0.41	124,125,128,129	0
4	SO4	A	1406	5/5	0.90	0.19	89,94,95,97	0
4	SO4	A	1407	5/5	0.91	0.19	110,111,112,114	0
4	SO4	A	1410	5/5	0.92	0.19	126,127,128,129	0
3	GOL	A	1402	6/6	0.92	0.15	65,69,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	1407	5/5	0.93	0.15	94,95,96,101	0
4	SO4	B	1409	5/5	0.93	0.38	145,146,147,147	0
4	SO4	B	1405	5/5	0.94	0.17	72,79,85,85	0
4	SO4	B	1406	5/5	0.94	0.17	97,100,101,102	0
4	SO4	B	1404	5/5	0.95	0.20	100,101,104,104	0
4	SO4	A	1408	5/5	0.95	0.15	100,101,102,102	0
4	SO4	A	1404	5/5	0.96	0.11	89,90,92,94	0
4	SO4	A	1405	5/5	0.96	0.21	79,84,88,89	0
4	SO4	A	1403	5/5	0.98	0.15	43,45,48,56	0
4	SO4	B	1403	5/5	0.98	0.14	48,51,53,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.