



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 9, 2025 – 08:12 PM EDT

PDB ID : 6E0W / pdb\_00006e0w  
Title : Crystal structure of the colanidase tailspike protein gp150 of Phage Phi92 complexed with one repeating unit of colanic acid  
Authors : Plattner, M.; Browning, C.; Gerardy-Schahn, R.; Shneider, M.M.; Leiman, P.G.; Schwarzer, D.  
Deposited on : 2018-07-07  
Resolution : 1.80 Å(reported)

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	<b>FAILED</b>
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

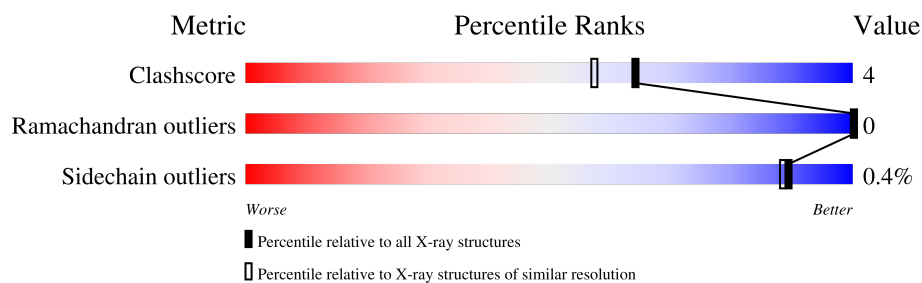
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)

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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	626	
1	B	626	
2	C	6	
2	D	6	

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	Clashes	Electron density
3	SO4	B	906	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10586 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.

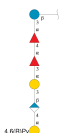
- Molecule 1 is a protein called Bacteriophage Phi92 gp150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	4	0
			4590	2878	779	907	26			
1	B	602	Total	C	N	O	S	0	6	0
			4605	2886	781	912	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP I7I026
B	179	SER	-	expression tag	UNP I7I026

- Molecule 2 is an oligosaccharide called 4,6-O-[(1R)-1-carboxyethylidene]-D-galactopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-alpha-D-galactopyranose-(1-3)-alpha-L-fucopyranose-(1-4)-alpha-L-fucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	6	Total	C	O	0	0	0
			71	39	32			
2	D	6	Total	C	O	0	0	0
			71	39	32			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

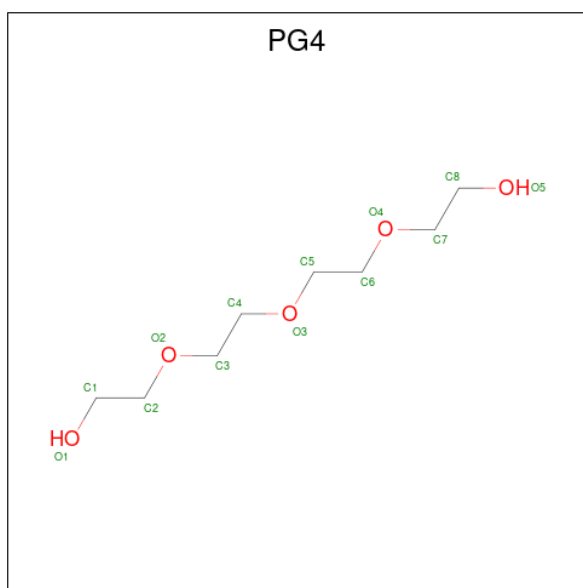
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	604	Total 604	O 604	0	0
7	B	575	Total 575	O 575	0	0

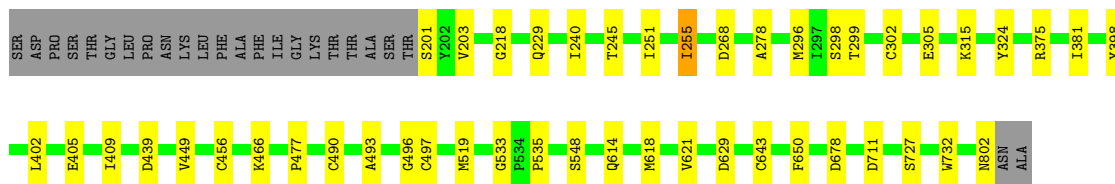
### 3 Residue-property plots

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. 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. 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.


Note EDS failed to run properly.

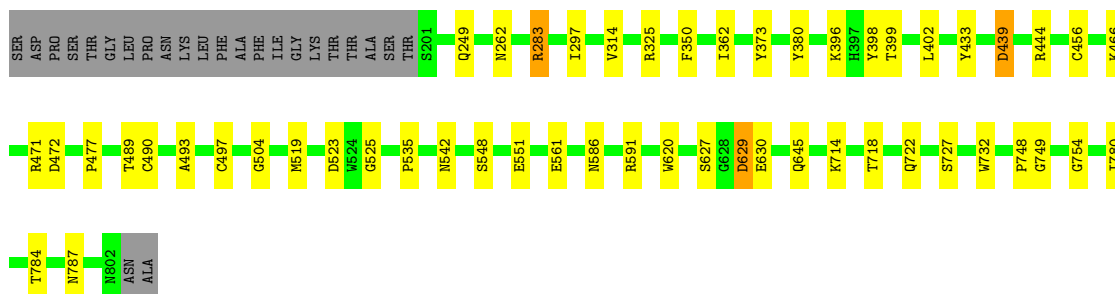
- Molecule 1: Bacteriophage Phi92 gp150

Chain A: 




- Molecule 1: Bacteriophage Phi92 gp150

Chain B: 



- Molecule 2: 4,6-O-[(1R)-1-carboxyethylidene]-D-galactopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-alpha-D-galactopyranose-(1-3)-alpha-L-fucopyranose-(1-4)-alpha-L-fucopyranose-(1-3)-beta-D-glucopyranose

Chain C: 



- Molecule 2: 4,6-O-[(1R)-1-carboxyethylidene]-D-galactopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-alpha-D-galactopyranose-(1-3)-alpha-L-fucopyranose-(1-4)-alpha-L-fucopyranose-(1-3)-beta-D-glucopyranose

Chain D: 



BGC1  
FUC2  
FUC3  
GLA4  
BDF5  
HLA6

## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.62Å 117.62Å 308.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.46 – 1.80	Depositor
% Data completeness (in resolution range)	95.6 (61.46-1.80)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.81Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, $R_{free}$	0.153 , 0.176	Depositor
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.557	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.068 for -h-k,k,-l	Xtriage
Total number of atoms	10586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: GLA, EDO, MG, SO4, PG4, BGC, HLA, BDP, FUC

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	0.68	2/4688 (0.0%)	0.70	0/6376
1	B	0.74	2/4703 (0.0%)	0.72	3/6397 (0.0%)
All	All	0.71	4/9391 (0.0%)	0.71	3/12773 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	TYR	CD1-CE1	6.97	1.49	1.39
1	B	380	TYR	CD1-CE1	6.24	1.48	1.39
1	A	650	PHE	CE2-CZ	5.46	1.47	1.37
1	A	621	VAL	CB-CG1	5.01	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	B	523	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	325	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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	4590	0	4396	31	0
1	B	4605	0	4405	35	0
2	C	71	0	44	2	0
2	D	71	0	44	0	0
3	A	20	0	0	0	0
3	B	30	0	0	0	7
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	B	4	0	6	1	0
6	B	13	0	18	1	0
7	A	604	0	0	13	6
7	B	575	0	0	15	1
All	All	10586	0	8913	69	13

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 4.

The worst 5 of 69 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:678:ASP:OD2	7:A:1001:HOH:O	1.98	0.81
1:A:203:VAL:O	7:A:1002:HOH:O	2.00	0.80
1:B:561:GLU:OE1	7:B:1001:HOH:O	2.03	0.75
1:A:439:ASP:HB3	7:A:1018:HOH:O	1.88	0.73
1:B:262:ASN:OD1	7:B:1002:HOH:O	2.08	0.72

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:906:SO4:O2	3:B:906:SO4:O4[3_455]	0.02	2.18
3:B:906:SO4:O2	3:B:906:SO4:O3[2_565]	0.03	2.17
3:B:906:SO4:O3	3:B:906:SO4:O4[2_565]	0.04	2.16
3:B:906:SO4:S	3:B:906:SO4:O1[2_565]	1.46	0.74
3:B:906:SO4:S	3:B:906:SO4:O4[2_565]	1.46	0.74

## 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	604/626 (96%)	580 (96%)	24 (4%)	0	100	100
1	B	606/626 (97%)	582 (96%)	24 (4%)	0	100	100
All	All	1210/1252 (97%)	1162 (96%)	48 (4%)	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	494/509 (97%)	493 (100%)	1 (0%)	92	91
1	B	496/509 (97%)	493 (99%)	3 (1%)	84	82
All	All	990/1018 (97%)	986 (100%)	4 (0%)	89	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ILE
1	B	439	ASP
1	B	629	ASP
1	B	722	GLN

Sometimes 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 ⓘ

12 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	BGC	C	1	2	12,12,12	1.11	1 (8%)	17,17,17	0.93	1 (5%)
2	FUC	C	2	2	10,10,11	1.34	1 (10%)	14,14,16	0.97	1 (7%)
2	FUC	C	3	2	10,10,11	0.97	0	14,14,16	0.88	1 (7%)
2	GLA	C	4	2	11,11,12	1.76	3 (27%)	15,15,17	1.23	1 (6%)
2	BDP	C	5	2	12,12,13	1.82	3 (25%)	14,17,19	1.21	1 (7%)
2	HLA	C	6	2	16,17,18	2.10	2 (12%)	19,26,28	1.56	2 (10%)
2	BGC	D	1	2	12,12,12	1.24	1 (8%)	17,17,17	0.93	0
2	FUC	D	2	2	10,10,11	1.46	1 (10%)	14,14,16	0.74	0
2	FUC	D	3	2	10,10,11	0.70	0	14,14,16	1.11	1 (7%)
2	GLA	D	4	2	11,11,12	1.57	3 (27%)	15,15,17	1.55	2 (13%)
2	BDP	D	5	2	12,12,13	1.59	2 (16%)	14,17,19	1.39	1 (7%)
2	HLA	D	6	2	16,17,18	2.30	2 (12%)	19,26,28	1.85	4 (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
2	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	GLA	C	4	2	-	1/2/19/22	0/1/1/1
2	BDP	C	5	2	-	0/4/21/24	0/1/1/1
2	HLA	C	6	2	-	0/6/34/37	0/2/2/2
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1
2	BDP	D	5	2	-	1/4/21/24	0/1/1/1
2	HLA	D	6	2	-	0/6/34/37	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	HLA	O6-CAM	7.87	1.48	1.41
2	C	6	HLA	O6-CAM	6.80	1.47	1.41
2	C	4	GLA	O5-C1	4.58	1.51	1.43
2	C	5	BDP	O5-C1	4.48	1.51	1.43
2	D	6	HLA	O4-CAM	3.64	1.47	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	HLA	O6-CAM-CAN	5.04	110.21	106.89
2	C	6	HLA	O4-C4-C3	4.43	113.86	109.28
2	D	4	GLA	C1-O5-C5	-4.14	106.63	112.19
2	D	5	BDP	C1-C2-C3	3.84	115.24	109.64
2	D	4	GLA	C3-C4-C5	3.44	116.48	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

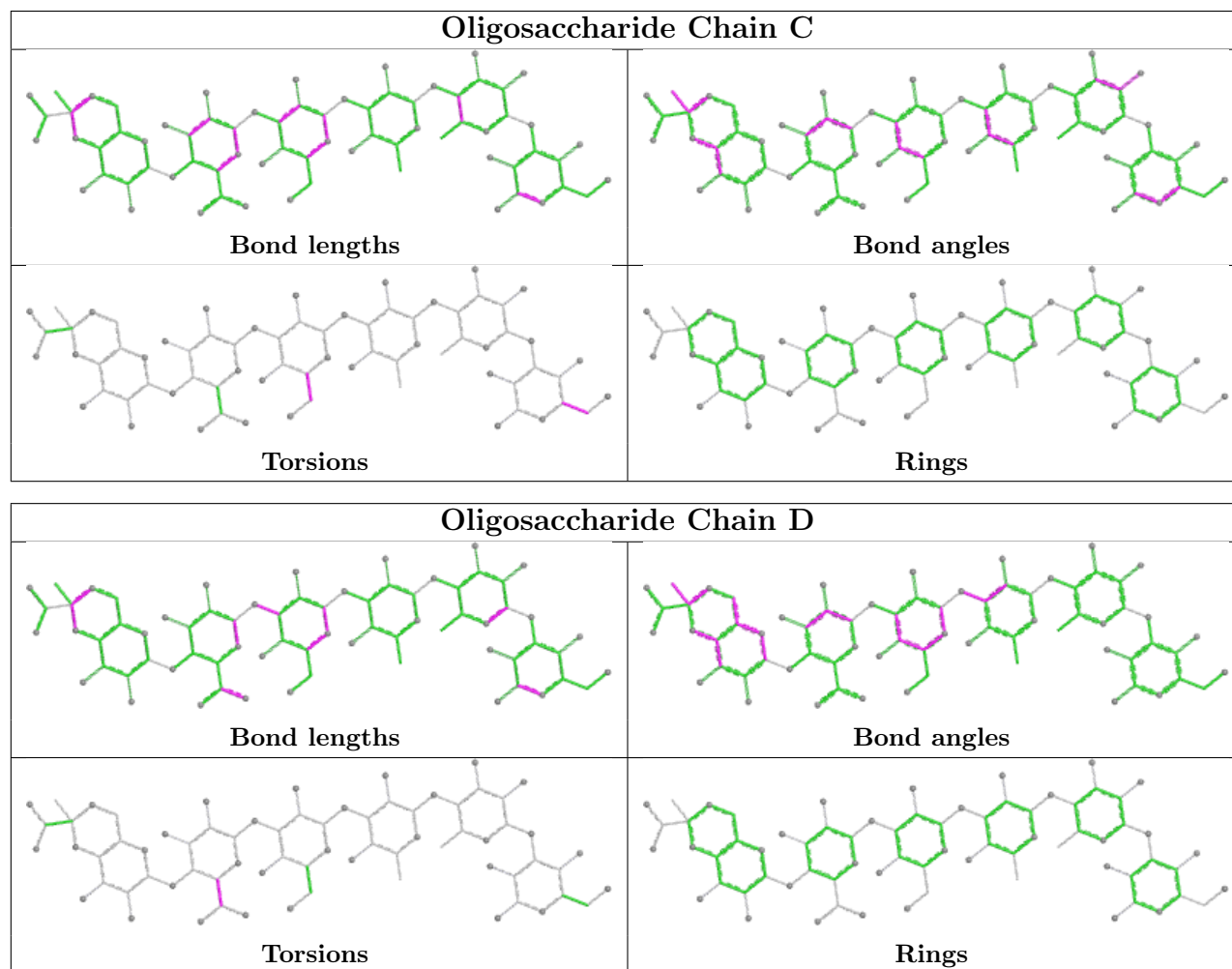
Mol	Chain	Res	Type	Atoms
2	C	1	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	C	4	GLA	C4-C5-C6-O6
2	D	5	BDP	O5-C5-C6-O6A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	GLA	1	0
2	C	6	HLA	1	0

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



## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	909	-	3,3,3	0.43	0	2,2,2	0.47	0
3	SO4	A	902	-	4,4,4	0.21	0	6,6,6	0.25	0
3	SO4	B	903	-	4,4,4	0.48	0	6,6,6	0.34	0
3	SO4	A	904	-	4,4,4	0.61	0	6,6,6	0.56	0
3	SO4	B	905	-	4,4,4	0.23	0	6,6,6	0.29	0
6	PG4	B	910	-	12,12,12	0.54	0	11,11,11	0.64	0
3	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.42	0
3	SO4	B	901	-	4,4,4	0.24	0	6,6,6	0.50	0
3	SO4	B	904	-	4,4,4	0.39	0	6,6,6	0.85	0
3	SO4	B	902	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	B	906	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	A	903	-	4,4,4	0.58	0	6,6,6	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
5	EDO	B	909	-	-	1/1/1/1	-
6	PG4	B	910	-	-	2/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	910	PG4	O4-C7-C8-O5
6	B	910	PG4	O3-C5-C6-O4
5	B	909	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	909	EDO	1	0
6	B	910	PG4	1	0
3	B	906	SO4	0	7

## 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](#)

EDS failed to run properly - this section is therefore empty.

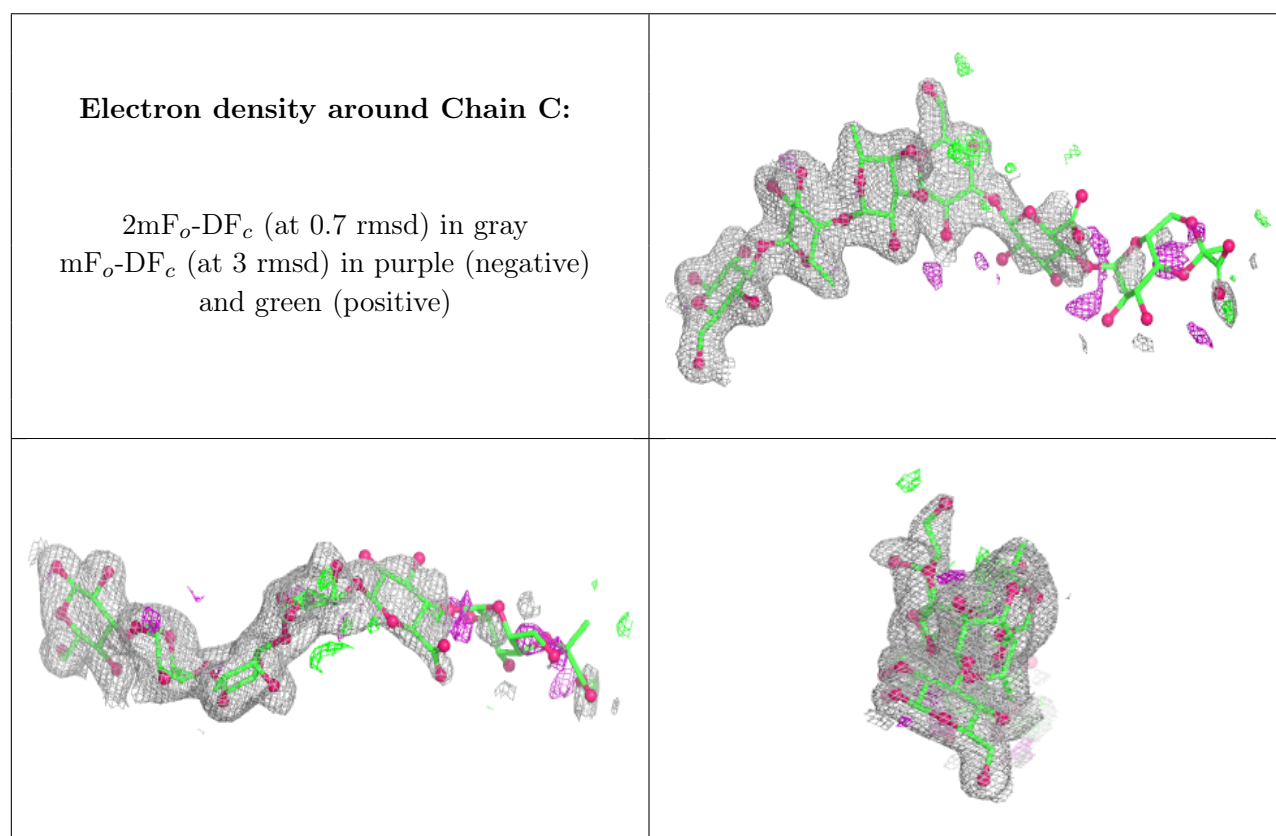
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

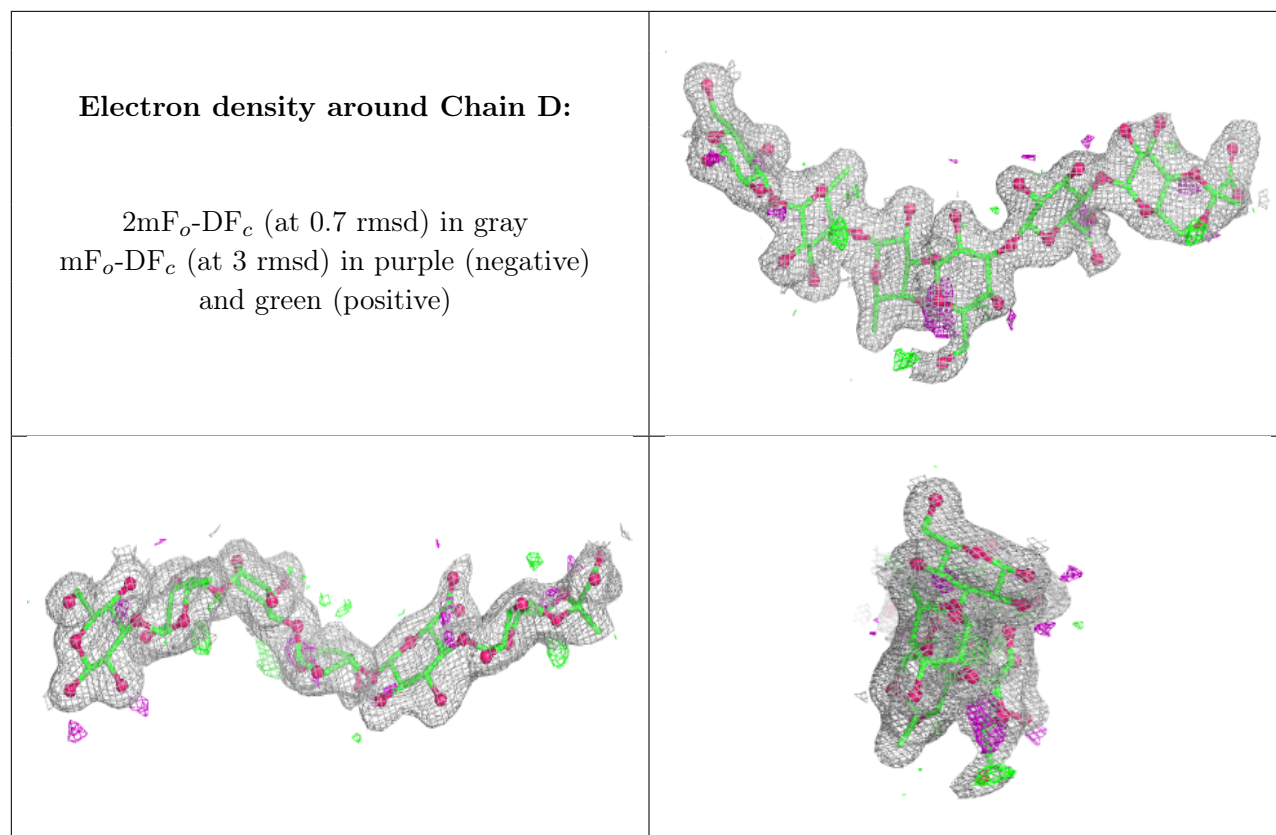
EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

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](#)

EDS failed to run properly - this section is therefore empty.

## 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.