



# Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2024 – 06:14 PM JST

PDB ID : 8ZCK  
Title : Serial Femtosecond Crystallography Structure of Fc Fragment of Human IgG1 from Biosimilar VEGF-Trap  
Authors : Destan, E.; DeMirici, H.  
Deposited on : 2024-04-30  
Resolution : 2.00 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

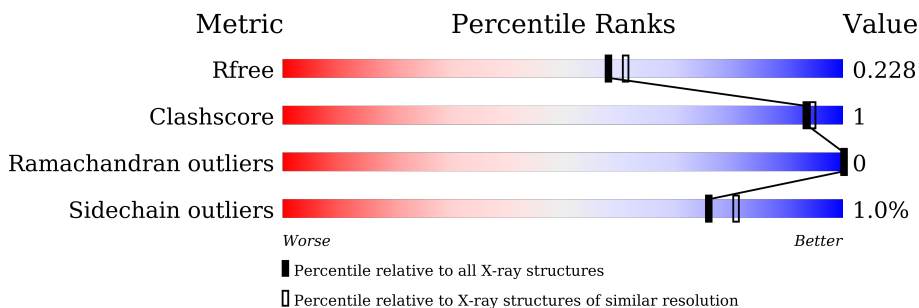
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	208	97%
1	B	208	97%
2	C	9	33%
3	D	7	71%

## 2 Entry composition i

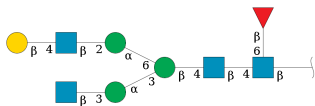
There are 4 unique types of molecules in this entry. The entry contains 3670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Immunoglobulin gamma-1 heavy chain.

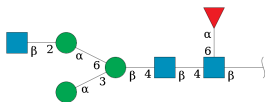
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total	C	N	O	S	0	2	0
			1666	1061	279	320	6			
1	B	208	Total	C	N	O	S	0	3	0
			1682	1072	284	320	6			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 4 is water.

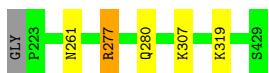
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	51	Total 51	O 51	0	0
4	B	76	Total 76	O 76	0	0

### 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.

- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain A:  97%

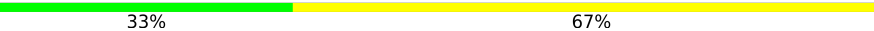


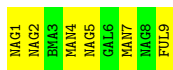
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain B:  97%



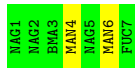
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  33% 67%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  71% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.47Å 79.99Å 143.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 2.00 29.20 – 1.30	Depositor EDS
% Data completeness (in resolution range)	88.6 (29.20-2.00) 57.7 (29.20-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.30Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.189 , 0.227 0.192 , 0.228	Depositor DCC
$R_{free}$ test set	2000 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtrriage
Anisotropy	0.119	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: GAL, FUC, FUL, BMA, NAG, MAN

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	0.28	0/1718	0.51	0/2340
1	B	0.28	0/1737	0.52	0/2366
All	All	0.28	0/3455	0.52	0/4706

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	1666	0	1636	5	0
1	B	1682	0	1660	3	0
2	C	110	0	93	3	0
3	D	85	0	73	0	0
4	A	51	0	0	0	0
4	B	76	0	0	1	0
All	All	3670	0	3462	10	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 (10) 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:261:ASN:HB2	1:A:307:LYS:HB3	1.82	0.61
2:C:1:NAG:H61	2:C:2:NAG:HN2	1.68	0.59
1:A:277:ARG:HH11	1:A:277:ARG:H	1.53	0.57
2:C:1:NAG:H61	2:C:2:NAG:N2	2.21	0.55
1:B:329:ARG:NH1	4:B:503:HOH:O	2.41	0.53
1:A:280:GLN:HG2	2:C:1:NAG:O6	2.12	0.49
1:A:277:ARG:H	1:A:277:ARG:HD2	1.78	0.47
1:B:244[B]:VAL:HG23	1:B:291:LEU:HB3	1.97	0.46
1:A:277:ARG:HH11	1:A:277:ARG:N	2.15	0.43
1:B:413:MET:HB3	1:B:413:MET:HE2	1.89	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	Allowed	Outliers	Percentiles	
1	A	207/208 (100%)	204 (99%)	3 (1%)	0	100	100
1	B	209/208 (100%)	208 (100%)	1 (0%)	0	100	100
All	All	416/416 (100%)	412 (99%)	4 (1%)	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	196/194 (101%)	194 (99%)	2 (1%)	76	81
1	B	197/194 (102%)	195 (99%)	2 (1%)	76	81
All	All	393/388 (101%)	389 (99%)	4 (1%)	76	81

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

Mol	Chain	Res	Type
1	A	277	ARG
1	A	319	LYS
1	B	343	LEU
1	B	398	ASP

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](#)

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

## 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).

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	0.23	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.38	0	17,19,21	0.43	0
2	BMA	C	3	2	11,11,12	0.59	0	15,15,17	0.96	0
2	MAN	C	4	2	11,11,12	0.96	1 (9%)	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	5	2	14,14,15	1.12	1 (7%)	17,19,21	1.72	1 (5%)
2	GAL	C	6	2	11,11,12	0.80	0	15,15,17	0.91	0
2	MAN	C	7	2	11,11,12	0.86	1 (9%)	15,15,17	1.46	2 (13%)
2	NAG	C	8	2	14,14,15	0.40	0	17,19,21	0.34	0
2	FUL	C	9	2	10,10,11	1.55	2 (20%)	14,14,16	2.04	4 (28%)
3	NAG	D	1	1,3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	D	2	3	14,14,15	0.29	0	17,19,21	0.52	0
3	BMA	D	3	3	11,11,12	0.84	0	15,15,17	1.03	0
3	MAN	D	4	3	11,11,12	0.74	0	15,15,17	1.26	2 (13%)
3	NAG	D	5	3	14,14,15	0.25	0	17,19,21	0.42	0
3	MAN	D	6	3	11,11,12	0.88	1 (9%)	15,15,17	0.83	1 (6%)
3	FUC	D	7	3	10,10,11	0.79	0	14,14,16	0.83	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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	0/6/23/26	0/1/1/1
2	GAL	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	1/1/1/1
2	NAG	C	8	2	-	2/6/23/26	0/1/1/1
2	FUL	C	9	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	FUC	D	7	3	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	NAG	O5-C1	4.05	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9	FUL	O5-C1	3.78	1.49	1.43
2	C	4	MAN	C1-C2	2.56	1.58	1.52
3	D	6	MAN	O5-C1	-2.24	1.40	1.43
2	C	9	FUL	C2-C3	-2.09	1.49	1.52
2	C	7	MAN	C1-C2	2.06	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	NAG	C1-O5-C5	6.59	121.13	112.19
2	C	9	FUL	C3-C4-C5	4.29	116.46	109.77
2	C	7	MAN	C1-O5-C5	4.05	117.68	112.19
2	C	9	FUL	C2-C3-C4	3.71	117.32	110.89
3	D	4	MAN	O2-C2-C3	-3.27	103.58	110.14
2	C	9	FUL	C1-C2-C3	3.20	113.61	109.67
3	D	4	MAN	C1-O5-C5	2.80	115.98	112.19
2	C	7	MAN	O2-C2-C3	-2.67	104.80	110.14
2	C	4	MAN	C1-O5-C5	2.62	115.74	112.19
2	C	4	MAN	O2-C2-C3	-2.03	106.07	110.14
2	C	9	FUL	C6-C5-C4	-2.02	109.34	113.07
3	D	6	MAN	O2-C2-C3	-2.01	106.11	110.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	8	NAG	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
2	C	7	MAN	O5-C5-C6-O6
2	C	8	NAG	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	C	3	BMA	O5-C5-C6-O6

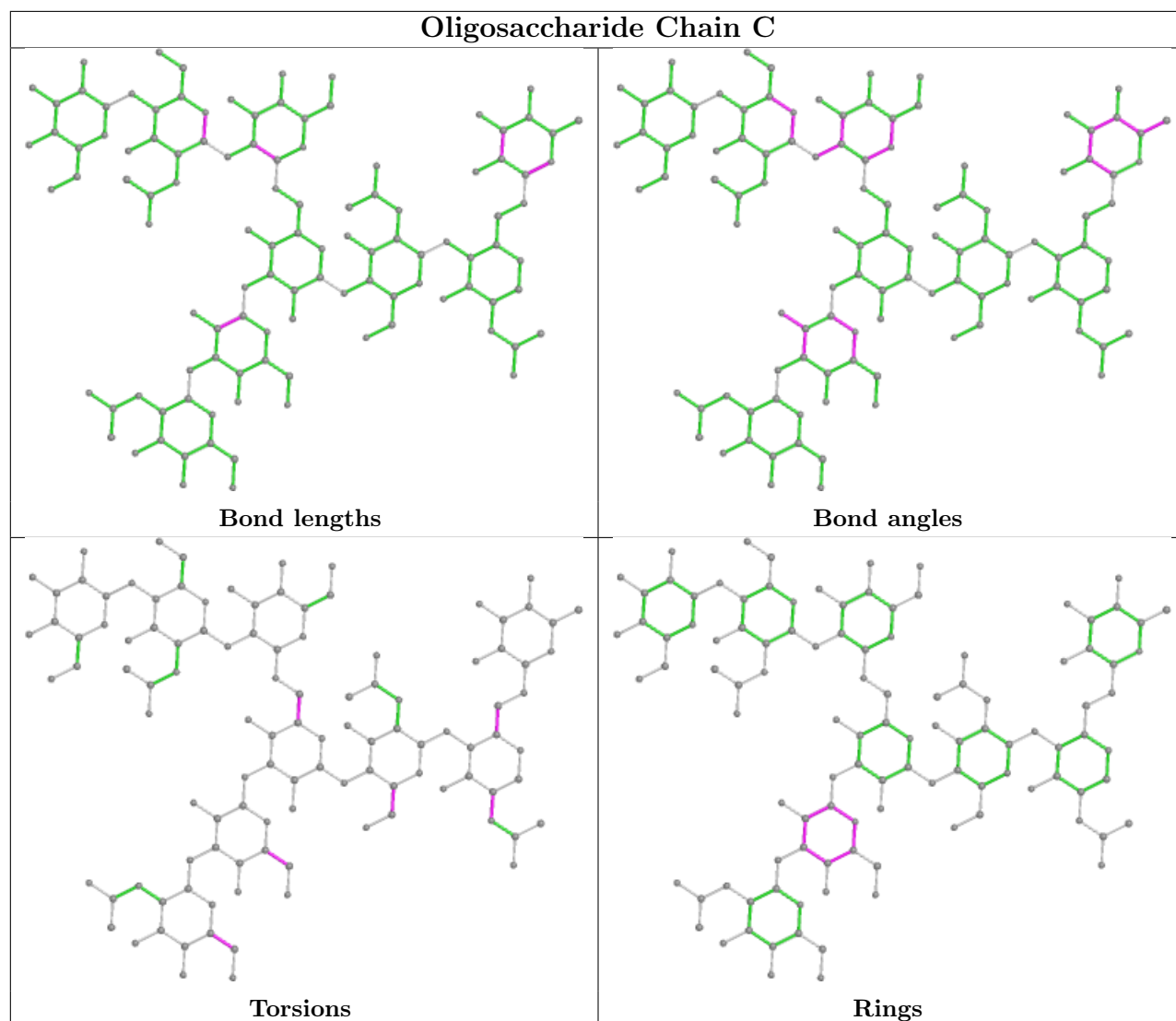
All (1) ring outliers are listed below:

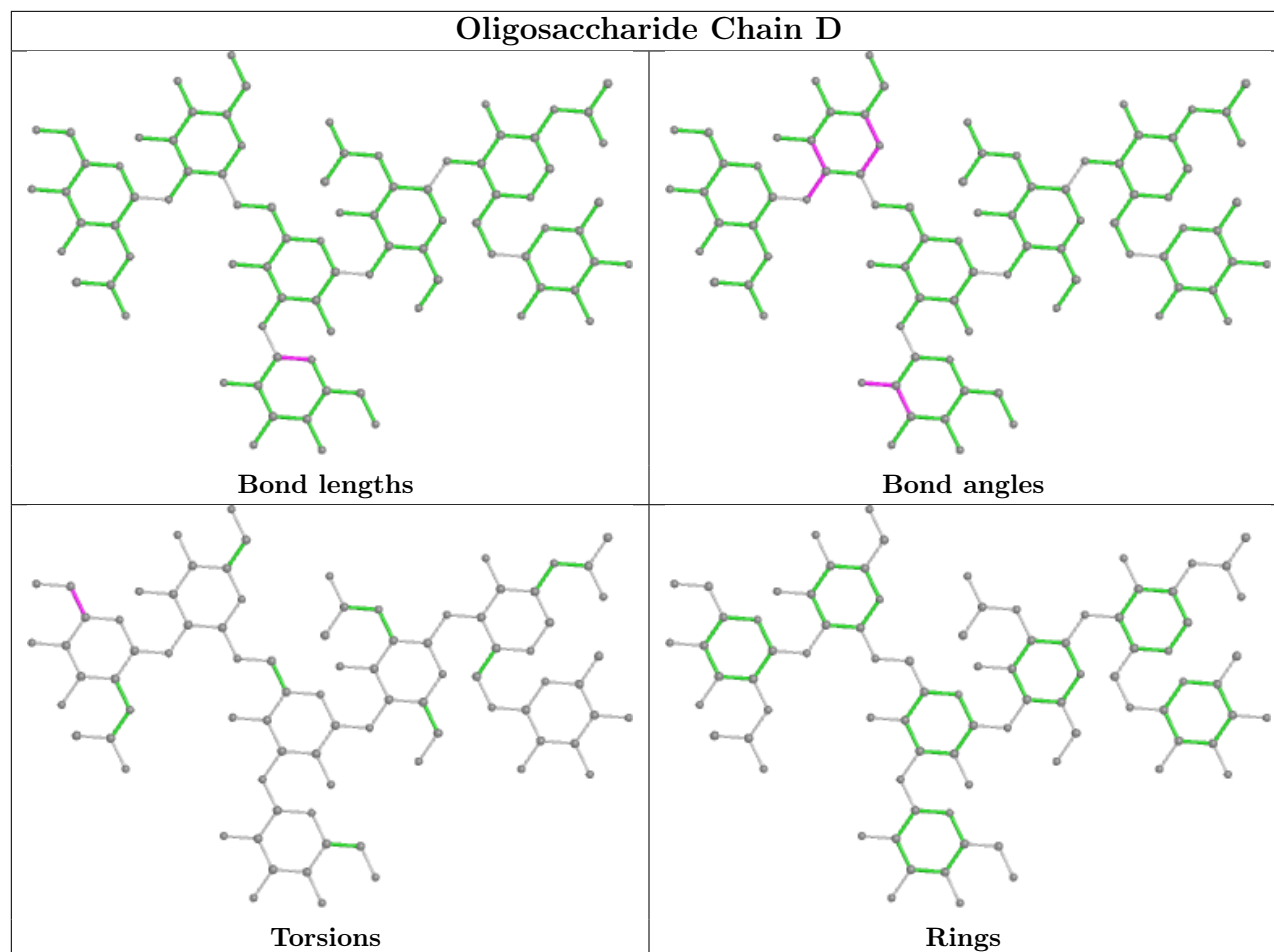
Mol	Chain	Res	Type	Atoms
2	C	7	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	C	1	NAG	3	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](#)

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

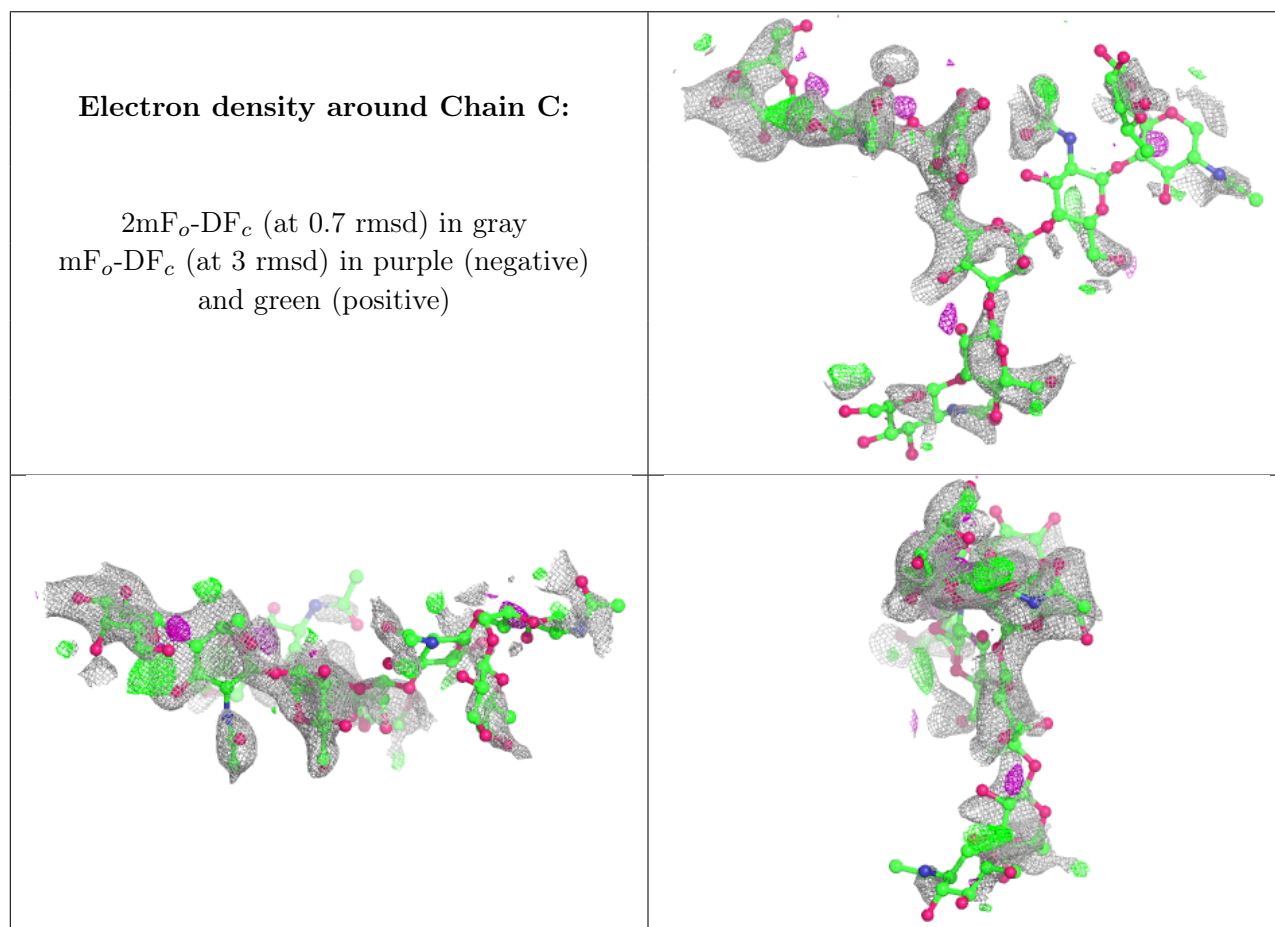
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

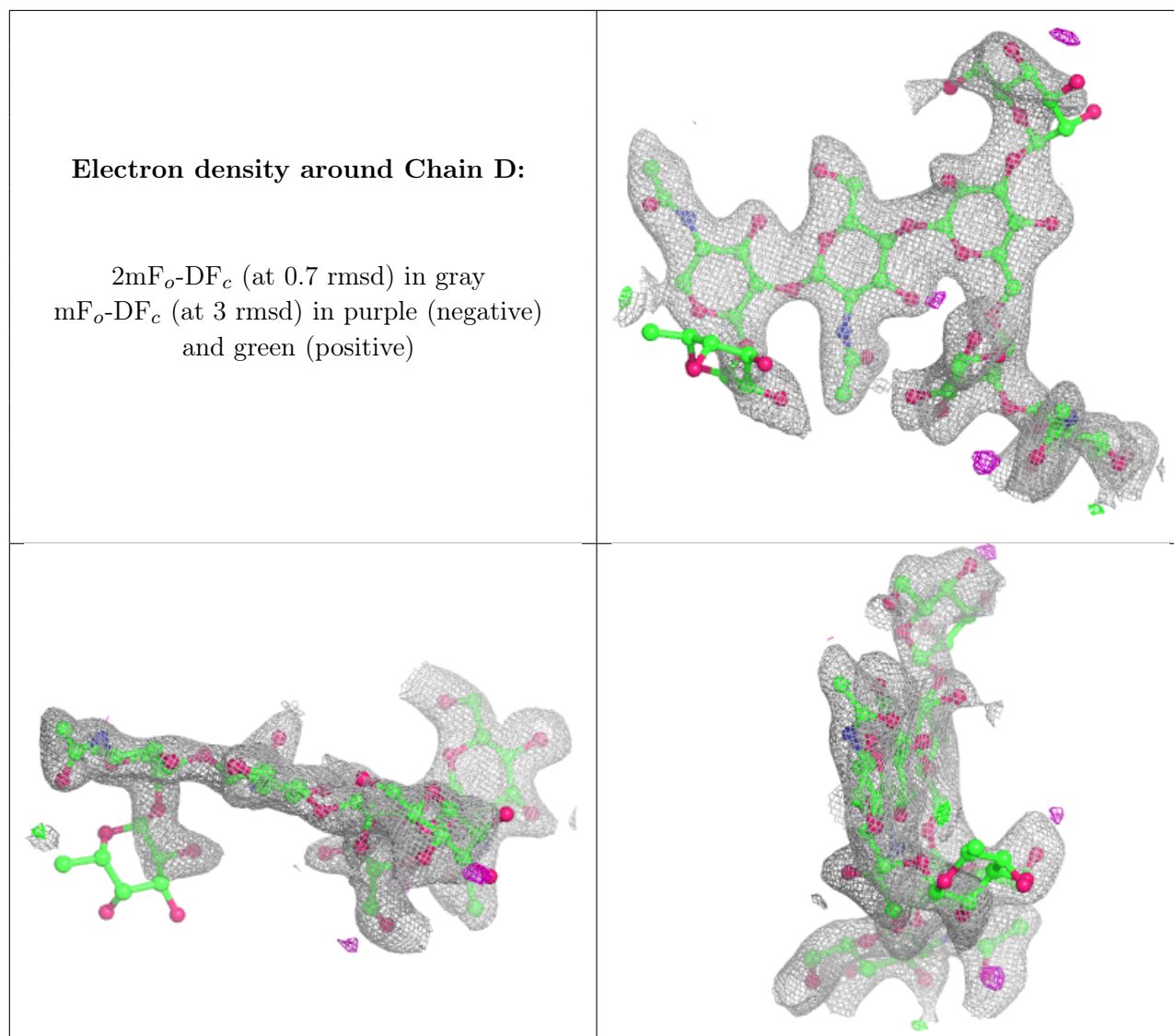
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - 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](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.