



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:46 PM BST

PDB ID : 2WNU  
Title : Complex between c1q globular heads and heparan sulfate  
Authors : Garlatti, V.; Chouquet, A.; Lunardi, T.; Thielens, N.M.; Arlaud, G.J.; Gaboriaud, C.  
Deposited on : 2009-07-20  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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

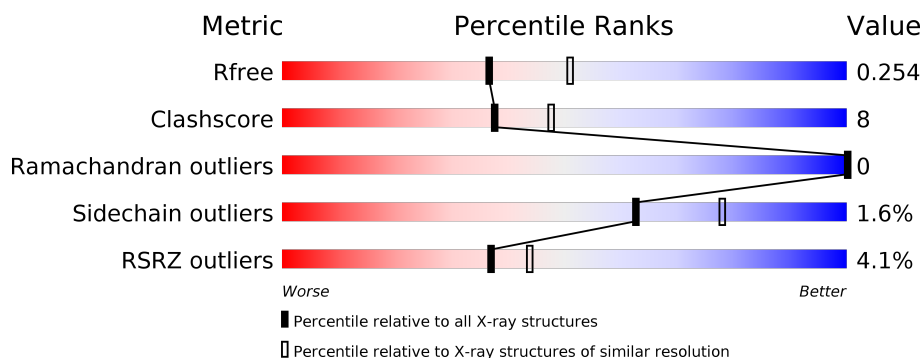
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



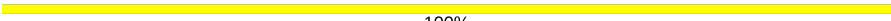
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	134	<div> <div>3%</div> <div>83%</div> <div>16%</div> <div>..</div> </div>
1	D	134	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	136	<div> <div>9%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
2	E	136	<div> <div>9%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
3	C	131	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
3	F	131	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	G	2	 100%

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
4	IDU	G	2	X	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6514 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 COMPLEMENT C1Q SUBCOMPONENT SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	3	0
			1056	676	181	194	5			
1	D	133	Total	C	N	O	S	0	3	0
			1056	676	181	194	5			

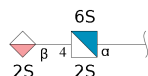
- Molecule 2 is a protein called COMPLEMENT C1Q SUBCOMPONENT SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	2	1
			1062	670	189	196	7			
2	E	133	Total	C	N	O	S	3	2	1
			1060	669	187	197	7			

- Molecule 3 is a protein called COMPLEMENT C1Q SUBCOMPONENT SUBUNIT C.

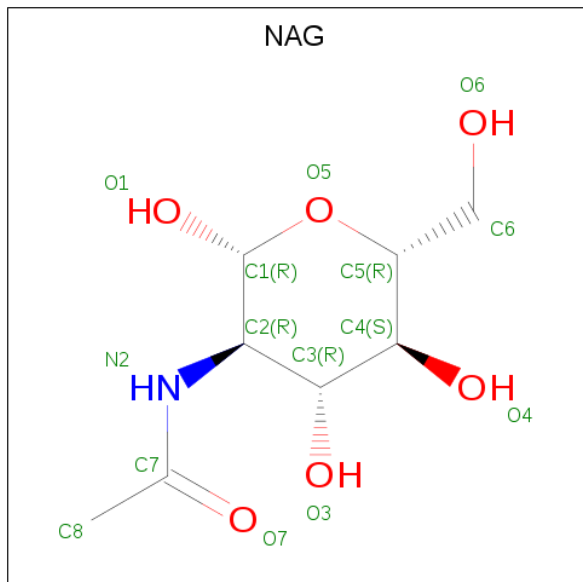
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	5	0
			1027	659	173	191	4			
3	F	129	Total	C	N	O	S	0	5	0
			1027	659	173	191	4			

- Molecule 4 is an oligosaccharide called 2-O-sulfo-beta-L-altropyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	S	0	0	0
			35	12	1	19	3			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	1	6		


- Molecule 6 is water.

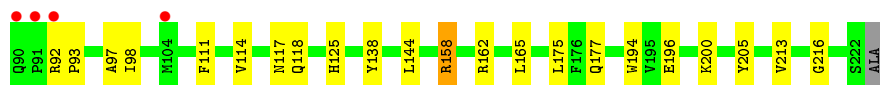
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	19	Total	O	0	0
			19	19		
6	C	39	Total	O	0	0
			39	39		
6	D	33	Total	O	0	0
			33	33		
6	E	19	Total	O	0	0
			19	19		
6	F	35	Total	O	0	0
			35	35		

### 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.

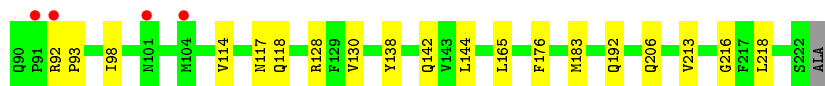
- Molecule 1: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT A

Chain A: 



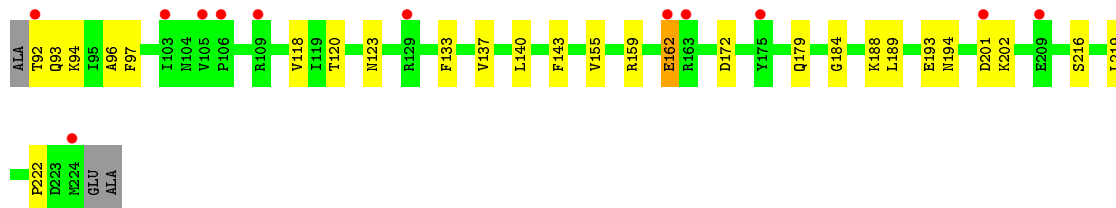
- Molecule 1: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT A

Chain D: 




- Molecule 2: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT B

Chain B: 




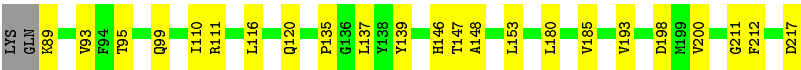
- Molecule 2: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT B

Chain E: 

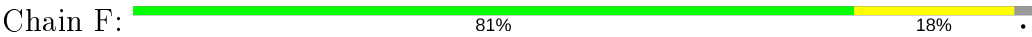


- Molecule 3: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT C

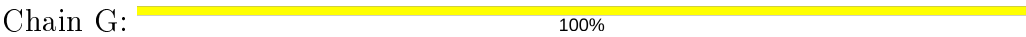
Chain C: 



● Molecule 3: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT C



● Molecule 4: 2-O-sulfo-beta-L-altropyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.09 Å 48.16 Å 87.73 Å 92.86° 92.20° 113.64°	Depositor
Resolution (Å)	19.65 – 2.30 19.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.65-2.30) 91.1 (19.65-2.30)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.30 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.198 , 0.256 0.198 , 0.254	Depositor DCC
$R_{free}$ test set	1451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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: IDU, NAG, SGN

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	0.49	0/1102	0.59	0/1494
1	D	0.46	0/1102	0.60	0/1494
2	B	0.49	0/1087	0.59	0/1468
2	E	0.92	3/1085 (0.3%)	0.69	1/1466 (0.1%)
3	C	0.50	0/1074	0.60	0/1462
3	F	0.50	0/1074	0.61	0/1462
All	All	0.58	3/6524 (0.0%)	0.61	1/8846 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	92	THR	CB-OG1	17.59	1.78	1.43
2	E	149	SER	CB-OG	-14.71	1.23	1.42
2	E	92	THR	CB-CG2	11.01	1.88	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	92	THR	OG1-CB-CG2	-12.17	82.01	110.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1056	0	1020	19	0
1	D	1056	0	1020	17	0
2	B	1062	0	1037	19	0
2	E	1060	0	1032	11	0
3	C	1027	0	1003	23	0
3	F	1027	0	1003	25	0
4	G	35	0	13	0	0
5	A	15	0	15	0	0
6	A	31	0	0	6	0
6	B	19	0	0	4	0
6	C	39	0	0	1	0
6	D	33	0	0	4	0
6	E	19	0	0	3	0
6	F	35	0	0	8	0
All	All	6514	0	6143	97	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 8.

The worst 5 of 97 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)
2:E:180:VAL:HG11	6:F:2028:HOH:O	1.61	1.00
2:B:159[B]:ARG:NH2	2:B:188:LYS:O	2.12	0.83
1:A:111:PHE:CD2	6:A:2001:HOH:O	2.37	0.77
2:B:179:GLN:OE1	6:B:2014:HOH:O	2.04	0.73
3:F:175:ASN:OD1	6:F:2028:HOH:O	2.05	0.73

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	134/134 (100%)	127 (95%)	7 (5%)	0	100	100
1	D	134/134 (100%)	126 (94%)	8 (6%)	0	100	100
2	B	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
2	E	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
3	C	132/131 (101%)	127 (96%)	5 (4%)	0	100	100
3	F	132/131 (101%)	127 (96%)	5 (4%)	0	100	100
All	All	798/802 (100%)	755 (95%)	43 (5%)	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	120/117 (103%)	119 (99%)	1 (1%)	81	91
1	D	120/117 (103%)	120 (100%)	0	100	100
2	B	116/117 (99%)	111 (96%)	5 (4%)	29	40
2	E	116/117 (99%)	111 (96%)	5 (4%)	29	40
3	C	118/115 (103%)	118 (100%)	0	100	100
3	F	118/115 (103%)	118 (100%)	0	100	100
All	All	708/698 (101%)	697 (98%)	11 (2%)	62	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	162	GLU
2	B	189	LEU
2	E	149	SER
2	B	123	ASN
2	E	123	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	146	HIS
1	D	172	ASN
3	F	101	HIS
3	C	102	GLN
1	D	189	GLN

### 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 ⓘ

2 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	$\# Z  > 2$
4	SGN	G	1	4	19,20,20	1.41	2 (10%)	24,31,31	1.21	2 (8%)
4	IDU	G	2	4	12,15,17	1.23	2 (16%)	12,22,26	1.62	3 (25%)

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	SGN	G	1	4	-	3/11/31/31	0/1/1/1
4	IDU	G	2	4	1/1/5/7	3/5/22/29	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	SGN	O2S-S1	4.04	1.46	1.42
4	G	1	SGN	O1S-S1	3.84	1.46	1.42
4	G	2	IDU	O2-C2	-2.79	1.43	1.47
4	G	2	IDU	O2-S	2.27	1.64	1.57

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	IDU	C1-C2-C3	3.68	115.14	109.94
4	G	1	SGN	O2S-S1-O1S	-3.42	112.07	120.16
4	G	2	IDU	C4-C3-C2	2.51	114.02	110.77
4	G	2	IDU	O5-C1-C2	2.32	114.10	109.41
4	G	1	SGN	C4-C3-C2	2.21	113.58	110.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	2	IDU	C1

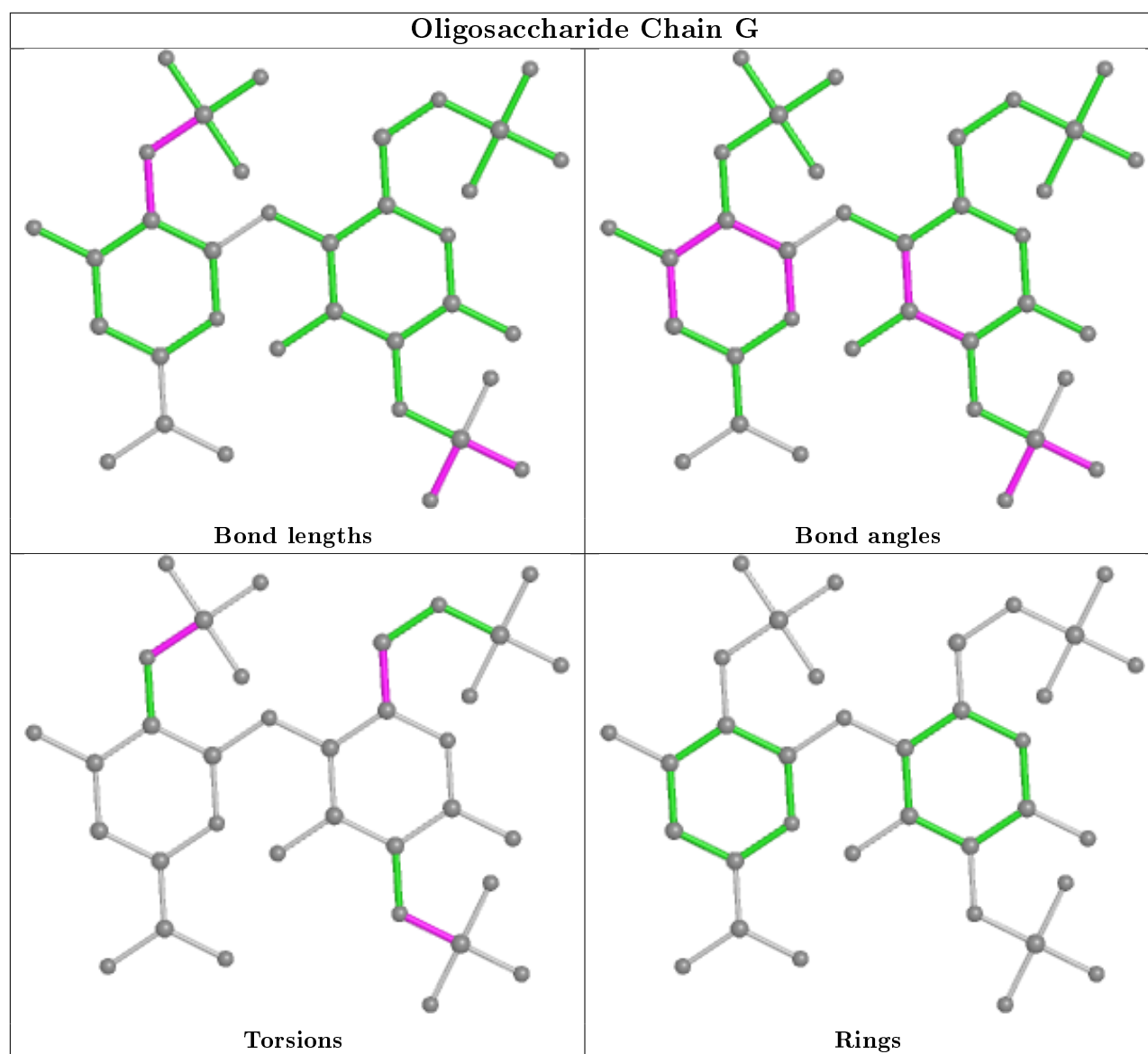
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	SGN	O5-C5-C6-O6
4	G	2	IDU	C2-O2-S-O3S
4	G	2	IDU	C2-O2-S-O1S
4	G	1	SGN	C4-C5-C6-O6
4	G	1	SGN	C2-N2-S1-O2S

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](#)

1 ligand 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	1223	-	15,15,15	0.42	0	21,21,21	0.63	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	NAG	A	1223	-	-	2/6/26/26	0/1/1/1

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
5	A	1223	NAG	C8-C7-N2-C2
5	A	1223	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	133/134 (99%)	0.01	4 (3%)	50 57	4, 12, 26, 34	0
1	D	133/134 (99%)	-0.06	4 (3%)	50 57	5, 13, 27, 32	0
2	B	133/136 (97%)	0.30	12 (9%)	9 12	8, 18, 32, 35	0
2	E	133/136 (97%)	0.32	12 (9%)	9 12	8, 18, 32, 35	2 (1%)
3	C	129/131 (98%)	-0.29	0	100 100	3, 9, 18, 25	0
3	F	129/131 (98%)	-0.36	0	100 100	3, 8, 17, 25	0
All	All	790/802 (98%)	-0.01	32 (4%)	37 44	3, 13, 28, 35	2 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	201	ASP	4.3
2	E	224	MET	4.3
2	B	92	THR	3.7
1	D	104	MET	3.7
1	A	90	GLN	3.5

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

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

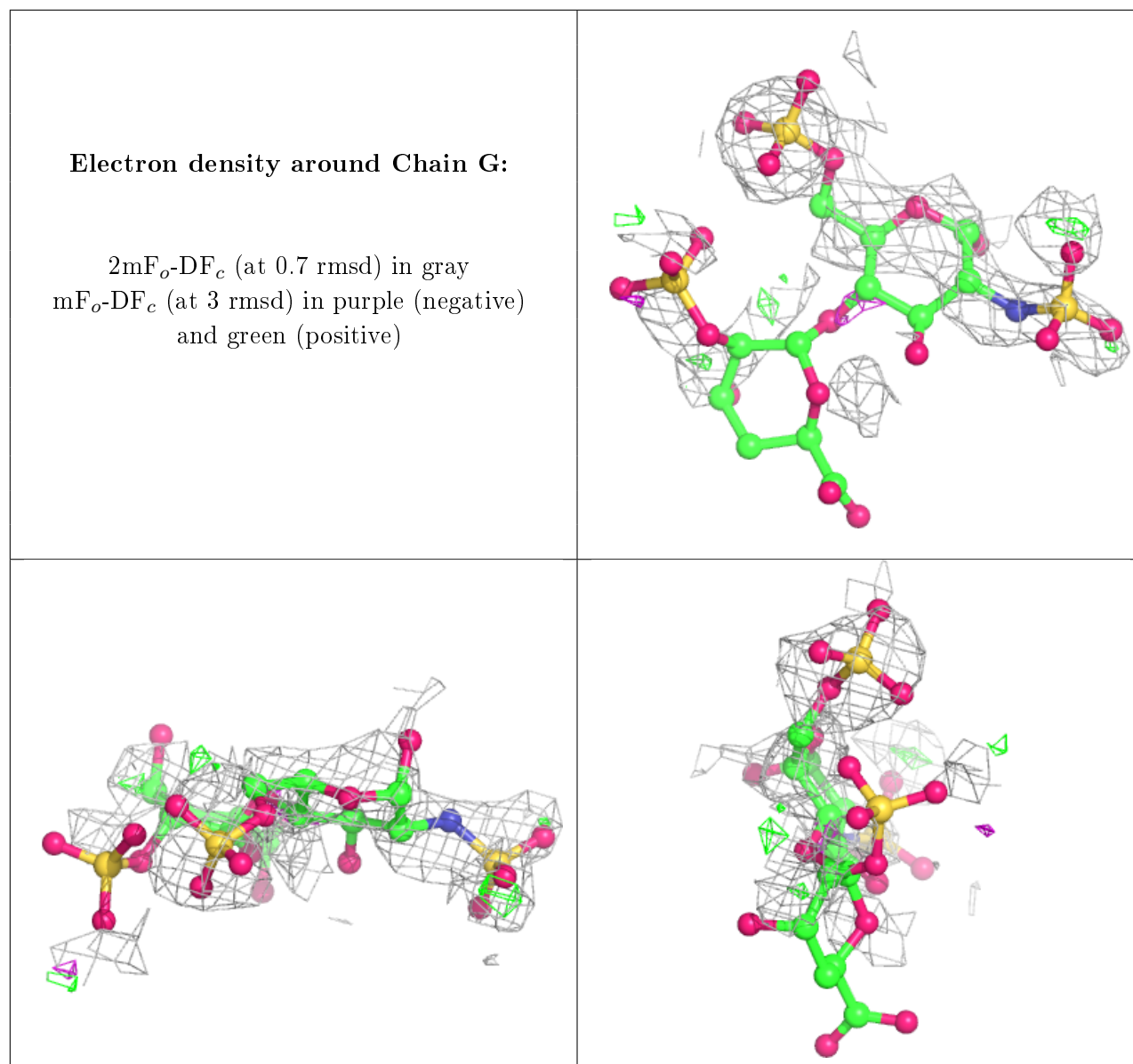
### 6.3 Carbohydrates [i](#)

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( $\text{\AA}^2$ )	Q<0.9
4	IDU	G	2	15/17	0.21	0.79	80,81,81,81	15
4	SGN	G	1	20/20	0.70	0.40	80,81,81,81	6

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 ⓘ

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
5	NAG	A	1223	15/15	0.67	0.29	62,63,64,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.