



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:18 PM BST

PDB ID : 6F5U  
Title : CRYSTAL STRUCTURE OF EBOLAVIRUS GLYCOPROTEIN IN COMPLEX WITH BEPRIDIL  
Authors : Ren, J.; Zhao, Y.; Fry, E.E.; Stuart, D.I.  
Deposited on : 2017-12-03  
Resolution : 2.07 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
buster-report	:	1.1.7 (2018)
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

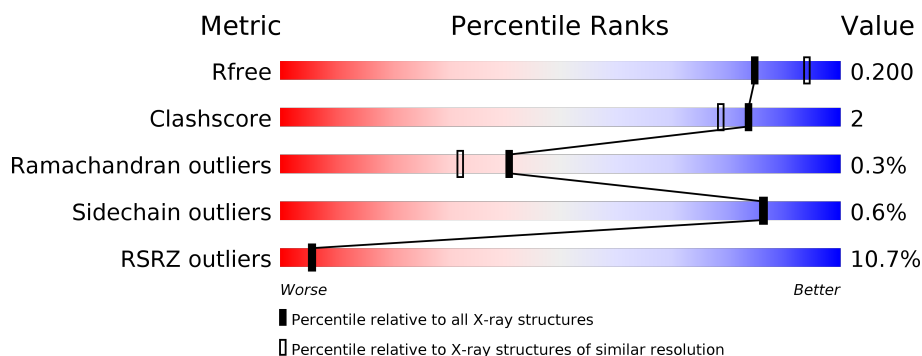
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	330	<div> <div>6%</div> <div>71%</div> <div>5%</div> <div>24%</div> </div>
2	B	168	<div> <div>13%</div> <div>73%</div> <div>5%</div> <div>22%</div> </div>
3	C	4	<div> <div>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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	C	4	-	-	-	X
4	NAG	A	603	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3297 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 Envelope glycoprotein,Envelope glycoprotein,GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1939	1240	327	367	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	-	expression tag	UNP Q05320
A	29	THR	-	expression tag	UNP Q05320
A	30	GLY	-	expression tag	UNP Q05320
A	31	ARG	-	expression tag	UNP Q05320
A	42	ALA	THR	engineered mutation	UNP Q05320

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1035	660	177	192	6			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	613	ALA	HIS	engineered mutation	UNP Q05320
B	633	GLY	-	expression tag	UNP Q05320
B	634	SER	-	expression tag	UNP Q05320
B	635	GLY	-	expression tag	UNP Q05320
B	636	TYR	-	expression tag	UNP Q05320
B	637	ILE	-	expression tag	UNP Q05320
B	638	PRO	-	expression tag	UNP Q05320
B	639	GLU	-	expression tag	UNP Q05320
B	640	ALA	-	expression tag	UNP Q05320
B	641	PRO	-	expression tag	UNP Q05320
B	642	ARG	-	expression tag	UNP Q05320

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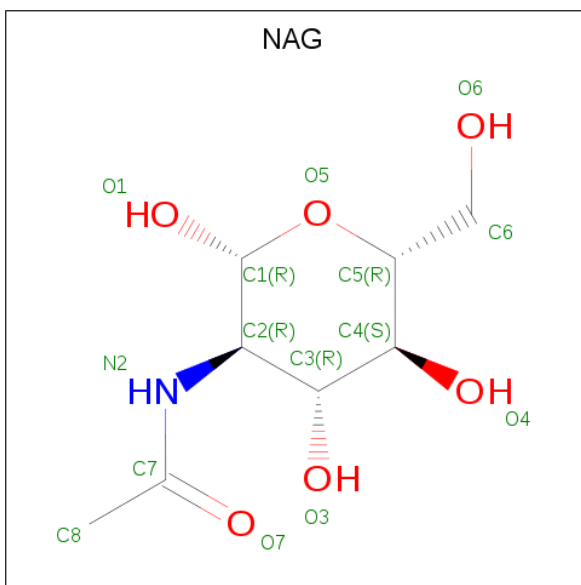
Chain	Residue	Modelled	Actual	Comment	Reference
B	643	ASP	-	expression tag	UNP Q05320
B	644	GLY	-	expression tag	UNP Q05320
B	645	GLN	-	expression tag	UNP Q05320
B	646	ALA	-	expression tag	UNP Q05320
B	647	TYR	-	expression tag	UNP Q05320
B	648	VAL	-	expression tag	UNP Q05320
B	649	ARG	-	expression tag	UNP Q05320
B	650	LYS	-	expression tag	UNP Q05320
B	651	ASP	-	expression tag	UNP Q05320
B	652	GLY	-	expression tag	UNP Q05320
B	653	GLU	-	expression tag	UNP Q05320
B	654	TRP	-	expression tag	UNP Q05320
B	655	VAL	-	expression tag	UNP Q05320
B	656	LEU	-	expression tag	UNP Q05320
B	657	LEU	-	expression tag	UNP Q05320
B	658	SER	-	expression tag	UNP Q05320
B	659	THR	-	expression tag	UNP Q05320
B	660	PHE	-	expression tag	UNP Q05320
B	661	LEU	-	expression tag	UNP Q05320
B	662	GLY	-	expression tag	UNP Q05320
B	663	THR	-	expression tag	UNP Q05320
B	664	HIS	-	expression tag	UNP Q05320
B	665	HIS	-	expression tag	UNP Q05320
B	666	HIS	-	expression tag	UNP Q05320
B	667	HIS	-	expression tag	UNP Q05320
B	668	HIS	-	expression tag	UNP Q05320
B	669	HIS	-	expression tag	UNP Q05320

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



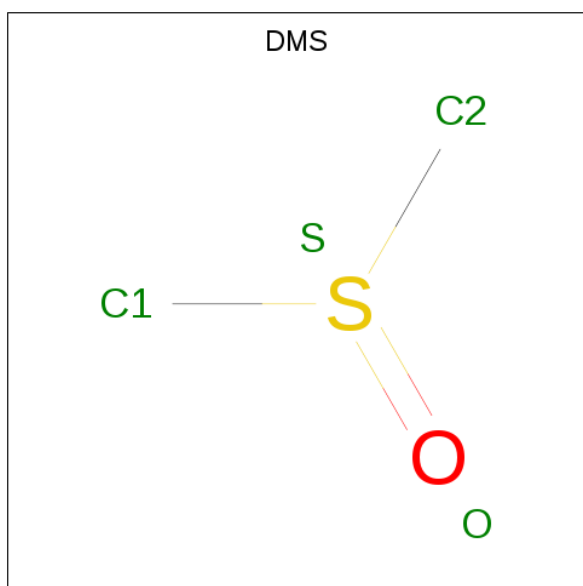
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



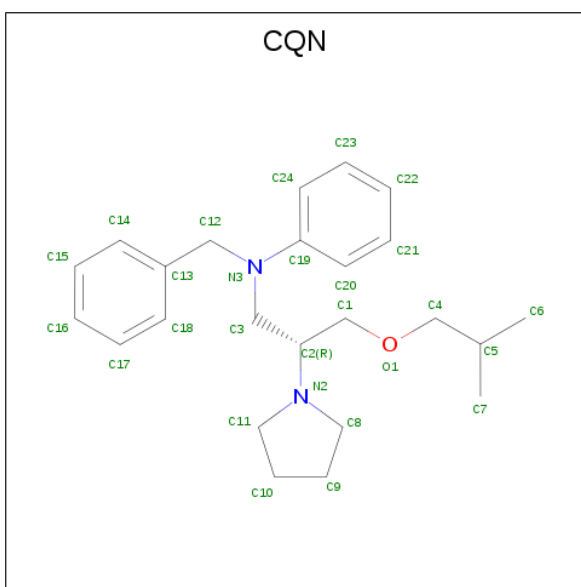
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 7 is Bepridil (three-letter code: CQN) (formula:  $C_{24}H_{34}N_2O$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			27	24	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	84	Total O 84 84	0	0
8	B	64	Total O 64 64	0	0



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.

- [illegible]

- Chain B:
- 
- | Position | Most Conserved Residue | Information Content (bits) |
|----------|------------------------|----------------------------|
| 1        | GLY                    | 0.25                       |
| 2        | GLY                    | 0.20                       |
| 3        | GLY                    | 0.20                       |
| 4        | THR                    | 0.15                       |
| 5        | THR                    | 0.15                       |
| 6        | THR                    | 0.15                       |
| 7        | THR                    | 0.15                       |
| 8        | THR                    | 0.15                       |
| 9        | THR                    | 0.15                       |
| 10       | THR                    | 0.15                       |
| 11       | THR                    | 0.15                       |
| 12       | THR                    | 0.15                       |
| 13       | GLY                    | 0.05                       |
| 14       | GLY                    | 0.05                       |
| 15       | GLY                    | 0.05                       |
| 16       | GLY                    | 0.05                       |
| 17       | GLY                    | 0.05                       |
| 18       | GLY                    | 0.05                       |
| 19       | GLY                    | 0.05                       |
| 20       | GLY                    | 0.05                       |
| 21       | GLY                    | 0.05                       |
| 22       | GLY                    | 0.05                       |
| 23       | GLY                    | 0.05                       |
| 24       | GLY                    | 0.05                       |
| 25       | GLY                    | 0.05                       |
| 26       | GLY                    | 0.05                       |
| 27       | GLY                    | 0.05                       |
| 28       | GLY                    | 0.05                       |
| 29       | GLY                    | 0.05                       |
| 30       | GLY                    | 0.05                       |
| 31       | GLY                    | 0.05                       |
| 32       | GLY                    | 0.05                       |

- Chain C: 
- | Category | Percentage |
|----------|------------|
| NAG1     | 10%        |
| NAG2     | 10%        |
| BMA3     | 10%        |
| MAN4     | 10%        |

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.05Å 114.05Å 307.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.17 – 2.07 83.08 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.17-2.07) 99.9 (83.08-2.07)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.07Å)	Xtriage
Refinement program	PHENIX (dev_2940: ???)	Depositor
R, $R_{free}$	0.187 , 0.200 0.186 , 0.200	Depositor DCC
$R_{free}$ test set	2350 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.5	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	0.97	EDS
Total number of atoms	3297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, BMA, NAG, DMS, MAN, CQN

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	0.26	0/1950	0.46	0/2650
2	B	0.25	0/1060	0.42	0/1445
All	All	0.26	0/3010	0.45	0/4095

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	1939	0	1850	9	0
2	B	1035	0	1001	5	0
3	C	50	0	43	0	0
4	A	56	0	52	3	0
5	A	24	0	32	0	0
5	B	6	0	8	0	0
6	A	4	0	6	0	0
6	B	8	0	12	0	0
7	A	27	0	0	1	0
8	A	84	0	0	0	0
8	B	64	0	0	0	0
All	All	3297	0	3004	15	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 2.

All (15) 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:264:GLY:O	4:A:603:NAG:O3	1.98	0.80
1:A:45:VAL:HG23	2:B:504:ILE:HD11	1.68	0.75
1:A:106:GLU:HG3	1:A:290:PHE:CD1	2.36	0.60
1:A:248:PHE:HA	1:A:283:THR:HG21	1.85	0.57
2:B:508:GLN:HE21	2:B:560:GLN:HE22	1.52	0.56
1:A:71:GLU:OE2	1:A:107:ASN:N	2.41	0.54
1:A:277:VAL:HG13	1:A:281:ILE:HD12	1.93	0.51
4:A:603:NAG:H83	4:A:603:NAG:O3	2.10	0.51
1:A:228:ASN:OD1	1:A:229:GLU:N	2.47	0.47
7:A:610:CQN:C21	2:B:558:LEU:HD21	2.47	0.44
1:A:114:LYS:O	1:A:144:THR:HA	2.18	0.44
2:B:612:PRO:O	2:B:616:THR:HG23	2.19	0.43
2:B:508:GLN:HE21	2:B:560:GLN:NE2	2.16	0.41
4:A:603:NAG:C8	4:A:603:NAG:C3	2.98	0.41
1:A:142:SER:O	1:A:221:GLN:HA	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	235/330 (71%)	230 (98%)	5 (2%)	0	100	100
2	B	129/168 (77%)	123 (95%)	5 (4%)	1 (1%)	19	9
All	All	364/498 (73%)	353 (97%)	10 (3%)	1 (0%)	41	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	525	ALA

### 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	205/245 (84%)	204 (100%)	1 (0%)	88	89
2	B	109/139 (78%)	108 (99%)	1 (1%)	78	78
All	All	314/384 (82%)	312 (99%)	2 (1%)	86	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
2	B	522	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	139	HIS
1	A	221	GLN
2	B	514	ASN
2	B	560	GLN

### 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 ⓘ

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
3	NAG	C	1	3,2	14,14,15	0.22	0	17,19,21	0.58	0
3	NAG	C	2	3	14,14,15	0.26	0	17,19,21	0.59	0
3	BMA	C	3	3	11,11,12	0.53	0	15,15,17	0.87	1 (6%)
3	MAN	C	4	3	11,11,12	1.61	2 (18%)	15,15,17	2.22	4 (26%)

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	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	MAN	C1-C2	4.15	1.61	1.52
3	C	4	MAN	O5-C1	3.01	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	6.52	121.03	112.19
3	C	4	MAN	C1-C2-C3	3.85	114.39	109.67
3	C	4	MAN	O5-C1-C2	2.76	115.03	110.77
3	C	4	MAN	O2-C2-C3	-2.42	105.29	110.14
3	C	3	BMA	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

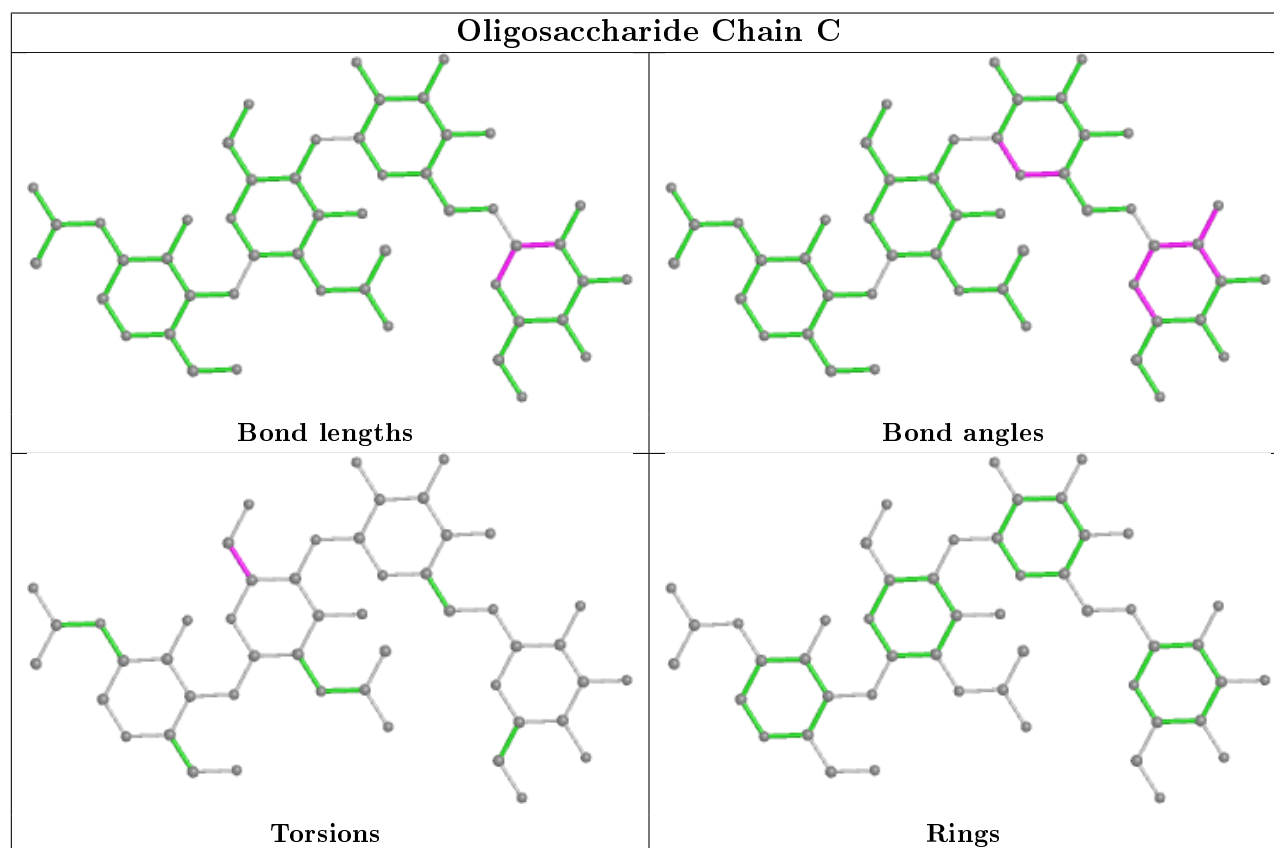
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-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](#)

13 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	A	603	1	14,14,15	0.63	0	17,19,21	2.65	3 (17%)
5	GOL	A	608	-	5,5,5	0.83	0	5,5,5	1.02	0
4	NAG	A	602	1	14,14,15	0.30	0	17,19,21	0.32	0
6	DMS	B	706	-	3,3,3	0.64	0	3,3,3	0.49	0
5	GOL	A	607	-	5,5,5	0.89	0	5,5,5	0.94	0
4	NAG	A	604	1	14,14,15	0.26	0	17,19,21	0.41	0
6	DMS	A	609	-	3,3,3	0.65	0	3,3,3	0.51	0
5	GOL	A	605	-	5,5,5	0.84	0	5,5,5	1.01	0
6	DMS	B	707	-	3,3,3	0.64	0	3,3,3	0.56	0
5	GOL	A	606	-	5,5,5	0.85	0	5,5,5	0.95	0
5	GOL	B	705	-	5,5,5	0.83	0	5,5,5	1.02	0
4	NAG	A	601	1	14,14,15	0.21	0	17,19,21	0.53	0
7	CQN	A	610	-	29,29,29	3.95	19 (65%)	35,37,37	1.95	5 (14%)

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	A	603	1	-	5/6/23/26	0/1/1/1
5	GOL	A	608	-	-	4/4/4/4	-
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
5	GOL	A	607	-	-	2/4/4/4	-
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
5	GOL	A	605	-	-	2/4/4/4	-
5	GOL	A	606	-	-	0/4/4/4	-
5	GOL	B	705	-	-	2/4/4/4	-
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	CQN	A	610	-	-	8/22/29/29	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	610	CQN	C24-C19	7.46	1.54	1.39
7	A	610	CQN	C18-C13	7.09	1.54	1.38
7	A	610	CQN	C15-C14	7.07	1.53	1.38
7	A	610	CQN	C21-C20	6.93	1.53	1.38
7	A	610	CQN	C2-N2	-6.41	1.31	1.48
7	A	610	CQN	C23-C22	5.76	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	610	CQN	C17-C16	5.54	1.52	1.38
7	A	610	CQN	C8-N2	-4.62	1.35	1.47
7	A	610	CQN	C11-N2	-4.13	1.37	1.47
7	A	610	CQN	C3-N3	4.01	1.50	1.46
7	A	610	CQN	C20-C19	-3.47	1.32	1.39
7	A	610	CQN	C1-C2	3.39	1.60	1.52
7	A	610	CQN	C14-C13	-3.33	1.31	1.38
7	A	610	CQN	C23-C24	-3.24	1.32	1.38
7	A	610	CQN	C17-C18	-3.16	1.32	1.38
7	A	610	CQN	C19-N3	2.90	1.46	1.38
7	A	610	CQN	C3-C2	2.77	1.61	1.53
7	A	610	CQN	C22-C21	-2.06	1.32	1.38
7	A	610	CQN	C12-C13	2.03	1.55	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	C2-N2-C7	9.82	136.89	122.90
7	A	610	CQN	C1-C2-N2	-6.55	104.16	115.07
7	A	610	CQN	C8-N2-C2	-5.40	108.89	114.12
7	A	610	CQN	C13-C12-N3	-4.66	106.69	114.18
7	A	610	CQN	C12-N3-C19	-3.68	114.46	120.78
7	A	610	CQN	C24-C19-N3	-3.02	117.22	121.38
4	A	603	NAG	C1-O5-C5	2.85	116.05	112.19
4	A	603	NAG	C8-C7-N2	2.06	119.58	116.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	NAG	C3-C2-N2-C7
5	A	608	GOL	C1-C2-C3-O3
5	A	607	GOL	O2-C2-C3-O3
5	A	605	GOL	O1-C1-C2-C3
5	B	705	GOL	O1-C1-C2-C3
7	A	610	CQN	O1-C1-C2-C3
7	A	610	CQN	O1-C1-C2-N2
7	A	610	CQN	O1-C4-C5-C7
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6

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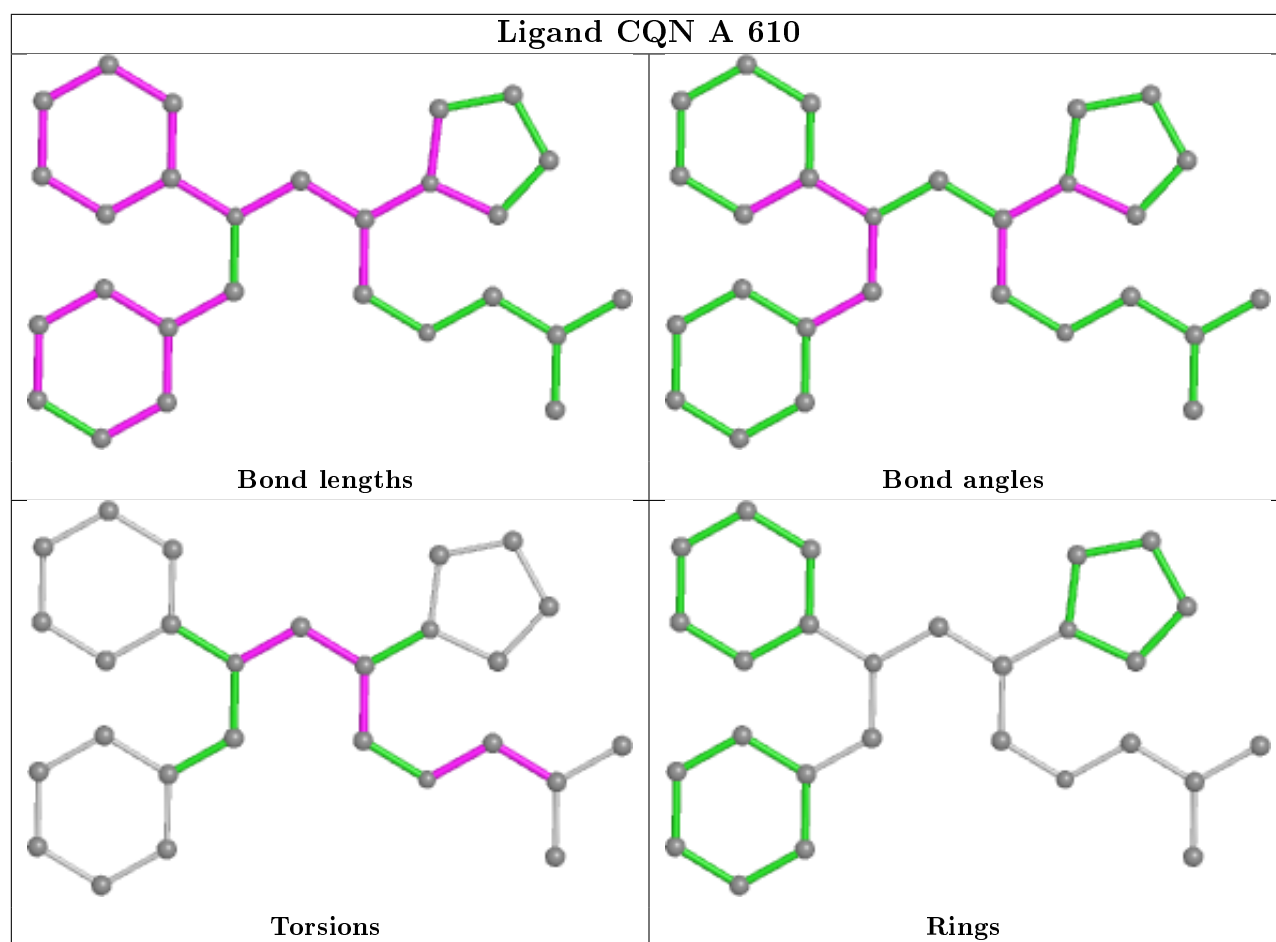
Mol	Chain	Res	Type	Atoms
5	A	608	GOL	O1-C1-C2-C3
5	A	607	GOL	C1-C2-C3-O3
5	A	605	GOL	O1-C1-C2-O2
5	B	705	GOL	O1-C1-C2-O2
7	A	610	CQN	O1-C4-C5-C6
5	A	608	GOL	O2-C2-C3-O3
7	A	610	CQN	C5-C4-O1-C1
7	A	610	CQN	N2-C2-C3-N3
5	A	608	GOL	O1-C1-C2-O2
7	A	610	CQN	C2-C3-N3-C19
7	A	610	CQN	C1-C2-C3-N3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	NAG	3	0
7	A	610	CQN	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	243/330 (73%)	0.79	19 (7%) 13 13	41, 61, 133, 169	0
2	B	131/168 (77%)	1.32	21 (16%) 1 1	41, 59, 182, 191	0
All	All	374/498 (75%)	0.98	40 (10%) 6 5	41, 60, 151, 191	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	626	ILE	10.5
2	B	620	THR	10.0
2	B	627	ILE	9.8
2	B	630	PHE	9.4
2	B	619	ILE	9.2
2	B	631	VAL	8.6
2	B	632	ASP	8.0
1	A	310	VAL	7.5
2	B	623	ILE	7.4
1	A	308	PHE	7.4
2	B	629	ASP	7.2
2	B	615	TRP	7.1
2	B	628	HIS	6.3
1	A	309	THR	6.0
1	A	281	ILE	5.9
2	B	616	THR	5.8
1	A	311	VAL	5.8
1	A	284	THR	5.6
2	B	625	GLN	5.5
1	A	211	SER	5.0
2	B	617	LYS	4.9
2	B	624	ASP	4.6
2	B	621	ASP	4.6
2	B	522	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	280	GLU	3.9
1	A	278	ASN	3.9
1	A	283	THR	3.7
1	A	307	SER	3.6
1	A	282	ASP	3.2
1	A	306	LEU	3.2
2	B	622	LYS	2.9
2	B	618	ASN	2.6
1	A	271	GLY	2.6
2	B	613	ALA	2.5
1	A	214	TYR	2.5
1	A	262	THR	2.4
1	A	288	TRP	2.4
1	A	275	TRP	2.1
1	A	270	THR	2.1
2	B	523	GLU	2.1

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

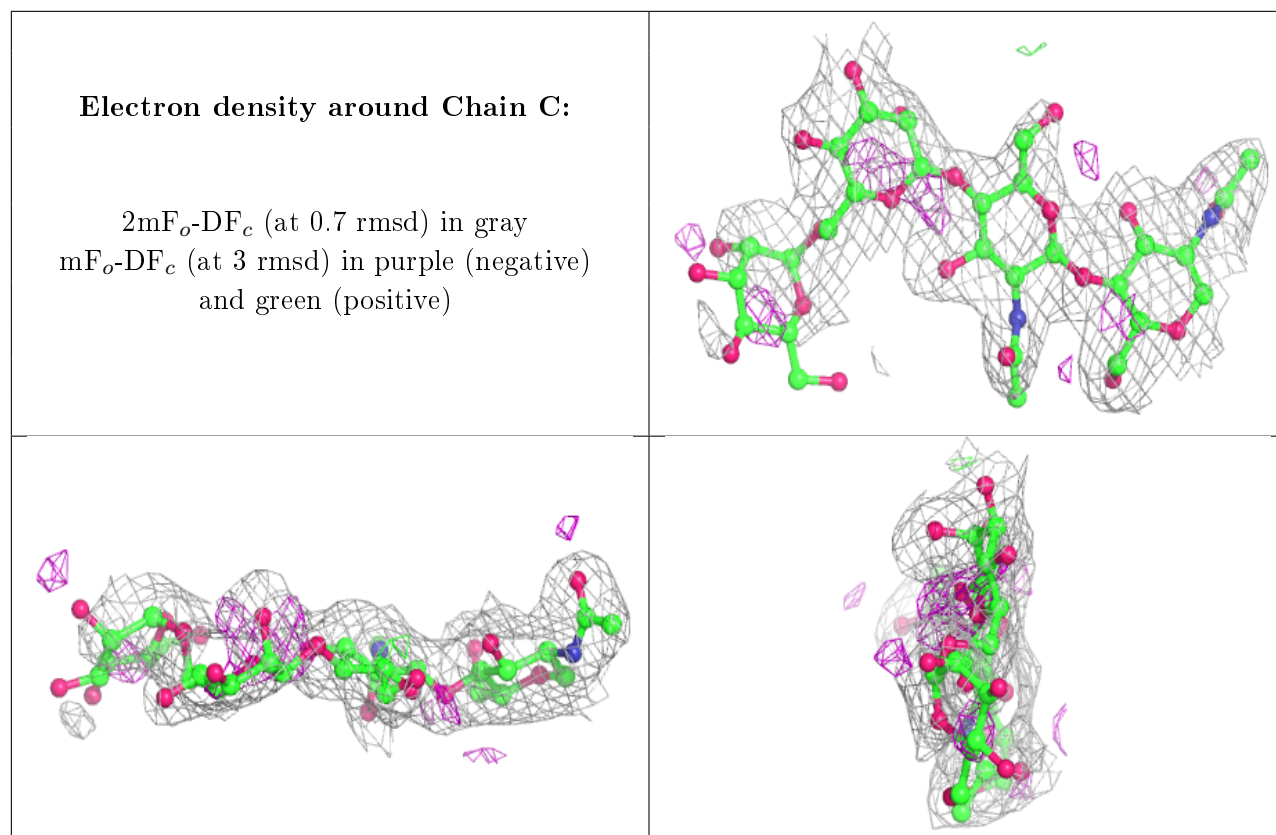
There are no non-standard protein/DNA/RNA residues in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
3	MAN	C	4	11/12	0.50	0.47	146,151,157,157	0
3	BMA	C	3	11/12	0.53	0.25	111,120,129,136	0
3	NAG	C	2	14/15	0.87	0.21	89,104,111,121	0
3	NAG	C	1	14/15	0.95	0.11	48,56,62,73	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.

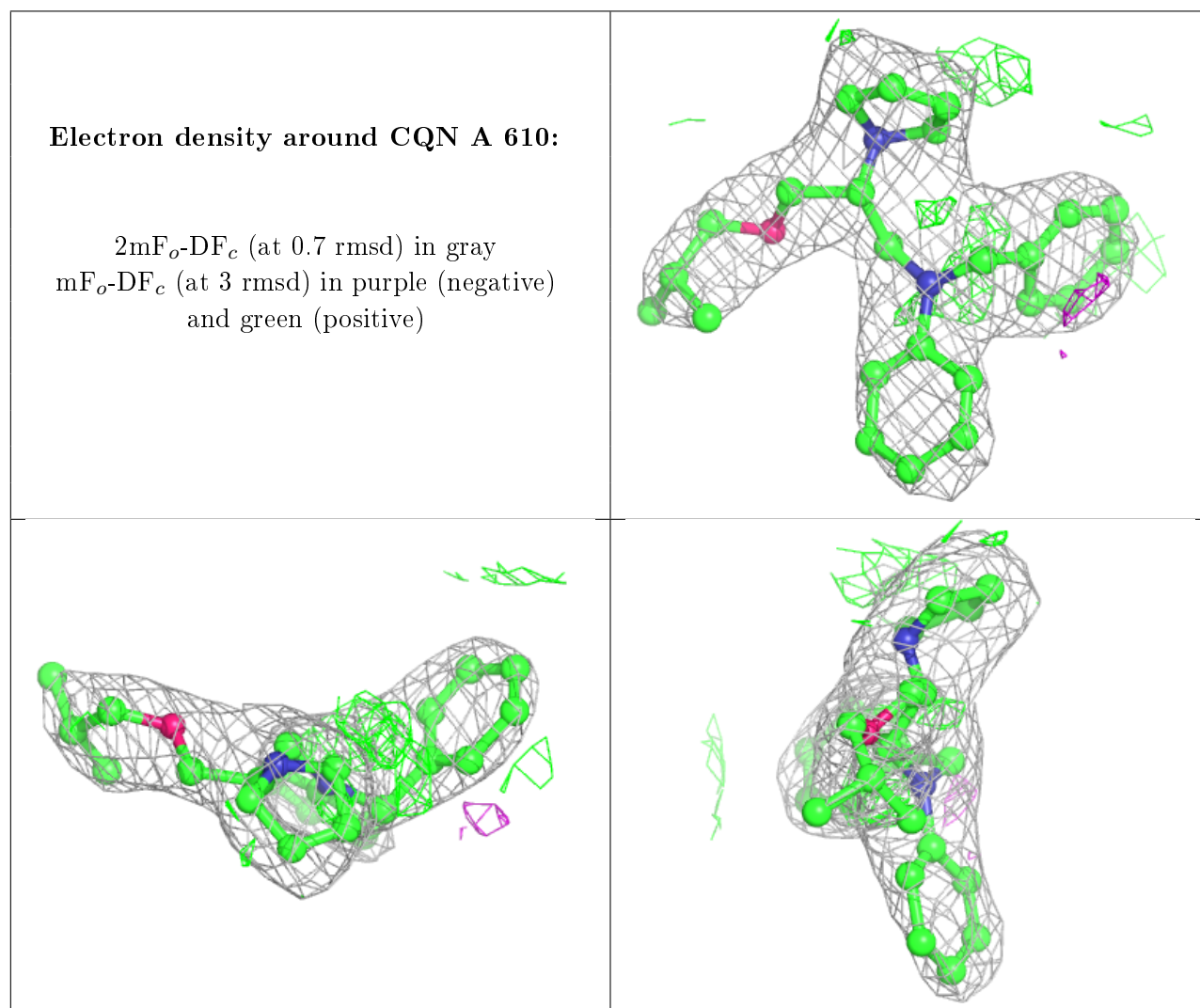


## 6.4 Ligands ⓘ

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	A	603	14/15	0.68	0.46	112,126,131,136	0
5	GOL	A	608	6/6	0.71	0.16	102,109,117,122	0
6	DMS	B	706	4/4	0.71	0.19	123,126,130,131	0
5	GOL	A	607	6/6	0.73	0.25	85,105,108,109	0
5	GOL	A	606	6/6	0.73	0.26	81,89,92,95	0
4	NAG	A	604	14/15	0.81	0.32	140,149,154,156	0
6	DMS	B	707	4/4	0.83	0.22	139,149,164,175	0
4	NAG	A	602	14/15	0.87	0.20	103,122,127,128	0
6	DMS	A	609	4/4	0.88	0.15	115,118,122,123	0
5	GOL	A	605	6/6	0.89	0.20	69,91,94,99	0
7	CQN	A	610	27/27	0.93	0.23	65,78,97,99	0
4	NAG	A	601	14/15	0.94	0.16	63,76,81,86	0
5	GOL	B	705	6/6	0.94	0.25	59,76,86,87	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.