



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:26 AM BST

PDB ID : 6QF7  
Title : Crystal structures of the recombinant beta-Factor XIIa protease with bound Thr-Arg and Pro-Arg substrate mimetics  
Authors : Pathak, M.; Mannal, R.; Li, C.; Bubacarr, G.K.; Badraddin, K.H.; Belviso, B.D.; Camila, R.B.; Dreveny, I.; Fischer, P.M.; Dekker, L.V.; Oliva, M.L.V.; Emsley, J.  
Deposited on : 2019-01-09  
Resolution : 4.00 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.

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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

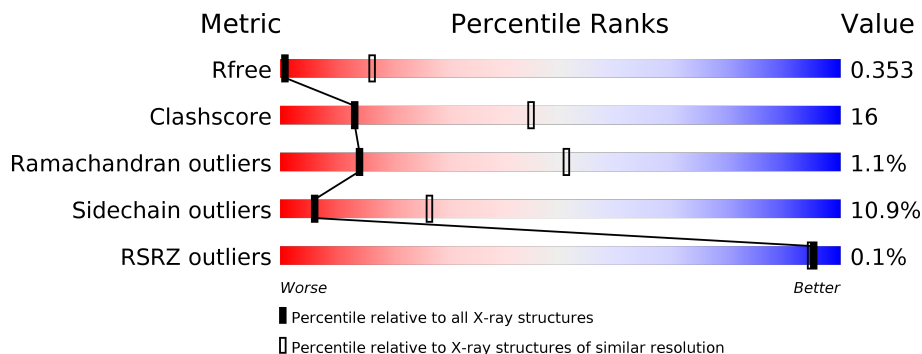
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.



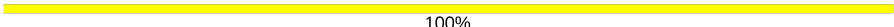
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	374	 90% 8% .
1	C	374	 91% 7% ..
2	B	254	 57% 28% 10% . .
2	D	254	 61% 24% 10% .
3	E	2	 100%
4	F	2	 100%

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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
3	NAG	E	2	X	-	-	-
4	GLC	F	2	-	-	X	-
5	NAG	B	701	X	-	-	X
6	0G6	D	703	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9512 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 Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	369	2839	1830	462	541	6	0	2	0
1	C	370	2845	1834	463	542	6	0	2	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP A0A376KDN7
A	0	SER	ALA	conflict	UNP A0A376KDN7
A	82	ALA	ASP	conflict	UNP A0A376KDN7
A	83	ALA	LYS	conflict	UNP A0A376KDN7
A	172	ALA	GLU	conflict	UNP A0A376KDN7
A	173	ALA	ASN	conflict	UNP A0A376KDN7
A	239	ALA	LYS	conflict	UNP A0A376KDN7
A	362	ALA	LYS	conflict	UNP A0A376KDN7
A	363	ALA	ASP	conflict	UNP A0A376KDN7
A	367	ASN	ARG	conflict	UNP A0A376KDN7
A	368	ALA	-	expression tag	UNP A0A376KDN7
A	369	ALA	-	expression tag	UNP A0A376KDN7
A	370	ALA	-	expression tag	UNP A0A376KDN7
A	371	ALA	-	expression tag	UNP A0A376KDN7
A	372	SER	-	expression tag	UNP A0A376KDN7
C	-1	ARG	-	expression tag	UNP A0A376KDN7
C	0	SER	ALA	conflict	UNP A0A376KDN7
C	82	ALA	ASP	conflict	UNP A0A376KDN7
C	83	ALA	LYS	conflict	UNP A0A376KDN7
C	172	ALA	GLU	conflict	UNP A0A376KDN7
C	173	ALA	ASN	conflict	UNP A0A376KDN7
C	239	ALA	LYS	conflict	UNP A0A376KDN7
C	362	ALA	LYS	conflict	UNP A0A376KDN7
C	363	ALA	ASP	conflict	UNP A0A376KDN7
C	367	ASN	ARG	conflict	UNP A0A376KDN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	368	ALA	-	expression tag	UNP A0A376KDN7
C	369	ALA	-	expression tag	UNP A0A376KDN7
C	370	ALA	-	expression tag	UNP A0A376KDN7
C	371	ALA	-	expression tag	UNP A0A376KDN7
C	372	SER	-	expression tag	UNP A0A376KDN7

- Molecule 2 is a protein called Coagulation factor XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1840	1153	325	347	15	3	0	0
2	D	244	Total	C	N	O	S			
			1840	1153	325	347	15	3	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	330	ALA	-	expression tag	UNP P00748
B	331	ALA	-	expression tag	UNP P00748
B	332	ALA	-	expression tag	UNP P00748
B	333	ALA	-	expression tag	UNP P00748
B	334	SER	THR	conflict	UNP P00748
B	335	GLU	ARG	conflict	UNP P00748
B	336	PHE	ASN	conflict	UNP P00748
B	?	-	LEU	deletion	UNP P00748
B	?	-	ARG	deletion	UNP P00748
B	?	-	LYS	deletion	UNP P00748
B	?	-	SER	deletion	UNP P00748
B	?	-	LEU	deletion	UNP P00748
B	?	-	SER	deletion	UNP P00748
B	?	-	SER	deletion	UNP P00748
B	?	-	MET	deletion	UNP P00748
B	?	-	THR	deletion	UNP P00748
B	?	-	ARG	deletion	UNP P00748
B	?	-	GLN	deletion	UNP P00748
B	?	-	ALA	deletion	UNP P00748
B	?	-	ALA	deletion	UNP P00748
B	?	-	GLU	deletion	UNP P00748
D	329	ALA	-	expression tag	UNP P00748
D	330	ALA	-	expression tag	UNP P00748
D	331	ALA	-	expression tag	UNP P00748
D	332	ALA	-	expression tag	UNP P00748

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Chain	Residue	Modelled	Actual	Comment	Reference
D	333	SER	THR	conflict	UNP P00748
D	334	GLU	ARG	conflict	UNP P00748
D	335	PHE	ASN	conflict	UNP P00748
D	?	-	LEU	deletion	UNP P00748
D	?	-	ARG	deletion	UNP P00748
D	?	-	LYS	deletion	UNP P00748
D	?	-	SER	deletion	UNP P00748
D	?	-	LEU	deletion	UNP P00748
D	?	-	SER	deletion	UNP P00748
D	?	-	SER	deletion	UNP P00748
D	?	-	MET	deletion	UNP P00748
D	?	-	THR	deletion	UNP P00748
D	?	-	ARG	deletion	UNP P00748
D	?	-	GLN	deletion	UNP P00748
D	?	-	ALA	deletion	UNP P00748
D	?	-	ALA	deletion	UNP P00748
D	?	-	GLU	deletion	UNP P00748

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	F	2	23	12	11	0	0	0
4	G	2	23	12	11	0	0	0



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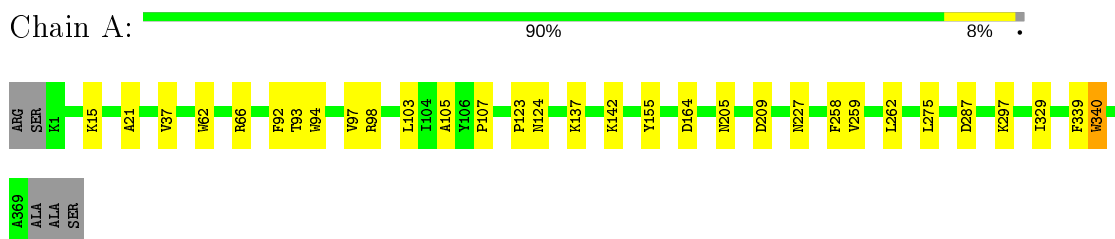
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	1	30	21	6	3	0	0



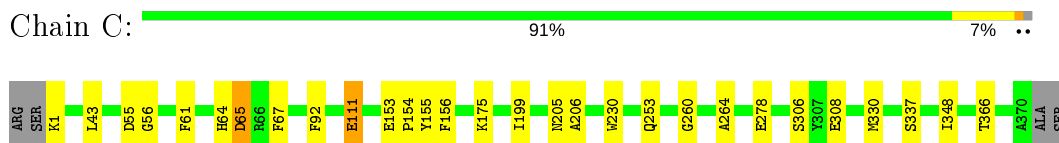
### 3 Residue-property plots [i](#)

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.

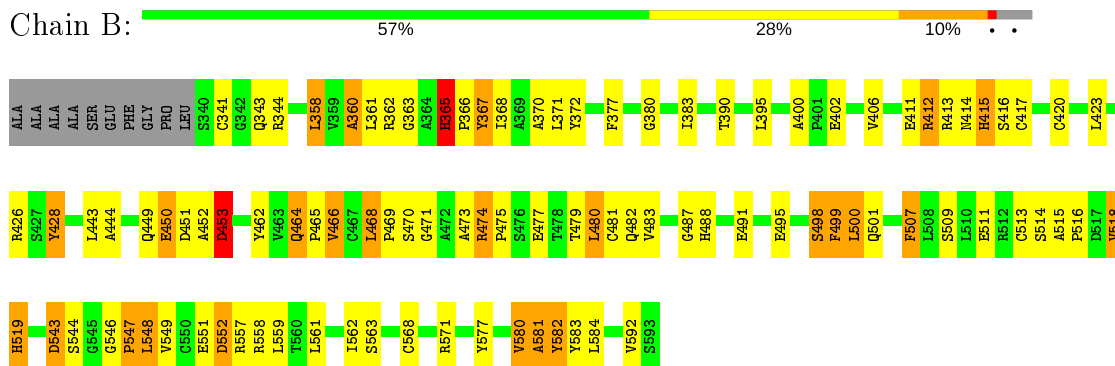
- Molecule 1: Maltodextrin-binding protein



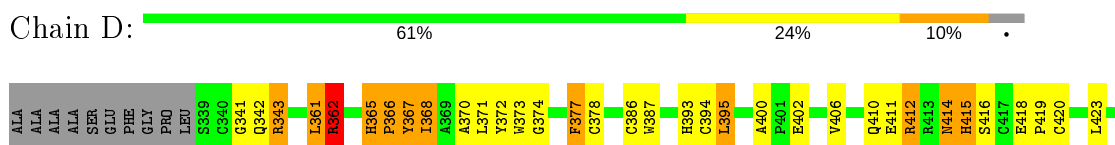
- Molecule 1: Maltodextrin-binding protein

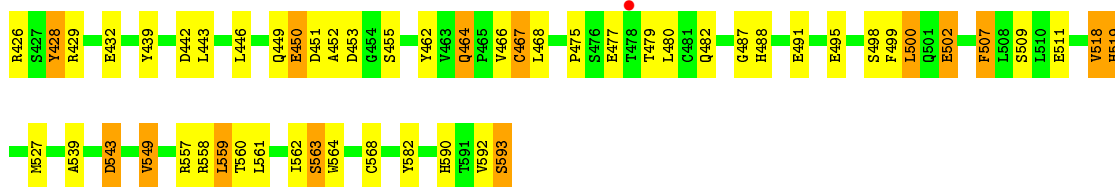


- Molecule 2: Coagulation factor XII



- Molecule 2: Coagulation factor XII






- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1  
MAG2

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

Chain F:  100%

GLC1  
GLC2

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

Chain G:  100%

GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.45Å 131.45Å 238.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.11 – 4.00 29.46 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (115.11-4.00) 93.4 (29.46-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.297 , 0.356 0.298 , 0.353	Depositor DCC
$R_{free}$ test set	1708 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , -2.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	9512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: 0G6, GLC, NAG

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	0.42	0/2914	0.57	0/3962
1	C	0.43	0/2920	0.56	0/3971
2	B	0.55	0/1886	0.82	2/2569 (0.1%)
2	D	0.58	0/1886	0.81	0/2569
All	All	0.49	0/9606	0.67	2/13071 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	499	PHE	CB-CA-C	7.09	124.59	110.40
2	B	360	ALA	N-CA-C	6.29	127.98	111.00

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	2839	0	2817	32	0
1	C	2845	0	2824	20	0
2	B	1840	0	1741	129	0
2	D	1840	0	1742	117	0
3	E	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	23	0	21	16	0
4	G	23	0	21	5	0
5	B	14	0	13	1	0
6	B	30	0	31	1	0
6	D	30	0	31	21	0
All	All	9512	0	9266	304	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 16.

The worst 5 of 304 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:D:377:PHE:HD1	2:D:378:CYS:N	1.32	1.25
2:B:362:ARG:HG3	2:B:363:GLY:N	1.37	1.23
2:B:360:ALA:HB2	2:B:500:LEU:O	1.42	1.17
2:B:367:TYR:HD2	2:B:466:VAL:CG1	1.58	1.15
2:B:367:TYR:CD2	2:B:466:VAL:HG11	1.82	1.14

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	369/374 (99%)	337 (91%)	31 (8%)	1 (0%)	41	75
1	C	370/374 (99%)	344 (93%)	25 (7%)	1 (0%)	41	75
2	B	238/254 (94%)	199 (84%)	32 (13%)	7 (3%)	4	32
2	D	238/254 (94%)	206 (87%)	28 (12%)	4 (2%)	9	43
All	All	1215/1256 (97%)	1086 (89%)	116 (10%)	13 (1%)	14	51

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	466	VAL
2	B	453	ASP
2	B	465	PRO
2	B	581	ALA
1	C	67	PHE

### 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	288/289 (100%)	276 (96%)	12 (4%)	30	56
1	C	288/289 (100%)	275 (96%)	13 (4%)	27	55
2	B	194/199 (98%)	154 (79%)	40 (21%)	1	7
2	D	194/199 (98%)	154 (79%)	40 (21%)	1	7
All	All	964/976 (99%)	859 (89%)	105 (11%)	6	26

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	558	ARG
1	C	205	ASN
2	D	549	VAL
2	B	563	SER
1	C	43	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	342	GLN
2	D	415	HIS
2	D	482	GLN
1	C	253	GLN
2	D	449	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 [i](#)

6 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	E	1	3	14,14,15	0.95	0	17,19,21	1.37	3 (17%)
3	NAG	E	2	3	14,14,15	1.01	1 (7%)	17,19,21	1.33	4 (23%)
4	GLC	F	1	4	12,12,12	0.44	0	17,17,17	0.53	0
4	GLC	F	2	4	11,11,12	0.22	0	15,15,17	0.62	0
4	GLC	G	1	4	12,12,12	0.44	0	17,17,17	0.56	0
4	GLC	G	2	4	11,11,12	0.27	0	15,15,17	0.64	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	NAG	E	1	3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	1/1/5/7	2/6/23/26	0/1/1/1
4	GLC	F	1	4	-	0/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1
4	GLC	G	1	4	-	0/2/22/22	0/1/1/1
4	GLC	G	2	4	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	3.00	1.56	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O4-C4-C3	-2.89	103.66	110.35
3	E	1	NAG	C3-C4-C5	-2.82	105.21	110.24
3	E	2	NAG	C4-C3-C2	2.72	115.00	111.02
3	E	2	NAG	O5-C5-C6	2.64	111.34	107.20
3	E	1	NAG	C2-N2-C7	-2.18	119.80	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	NAG	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

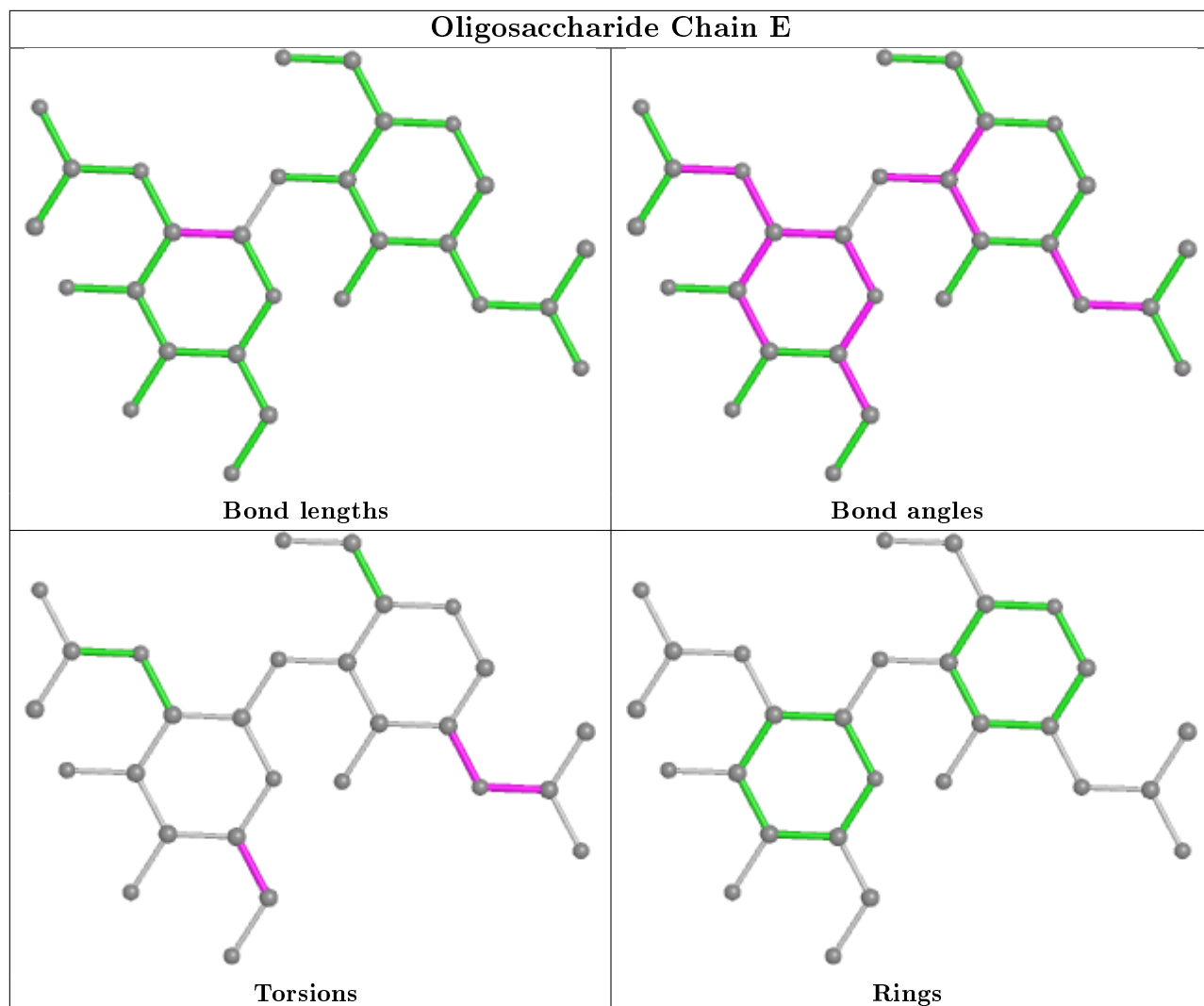
There are no ring outliers.

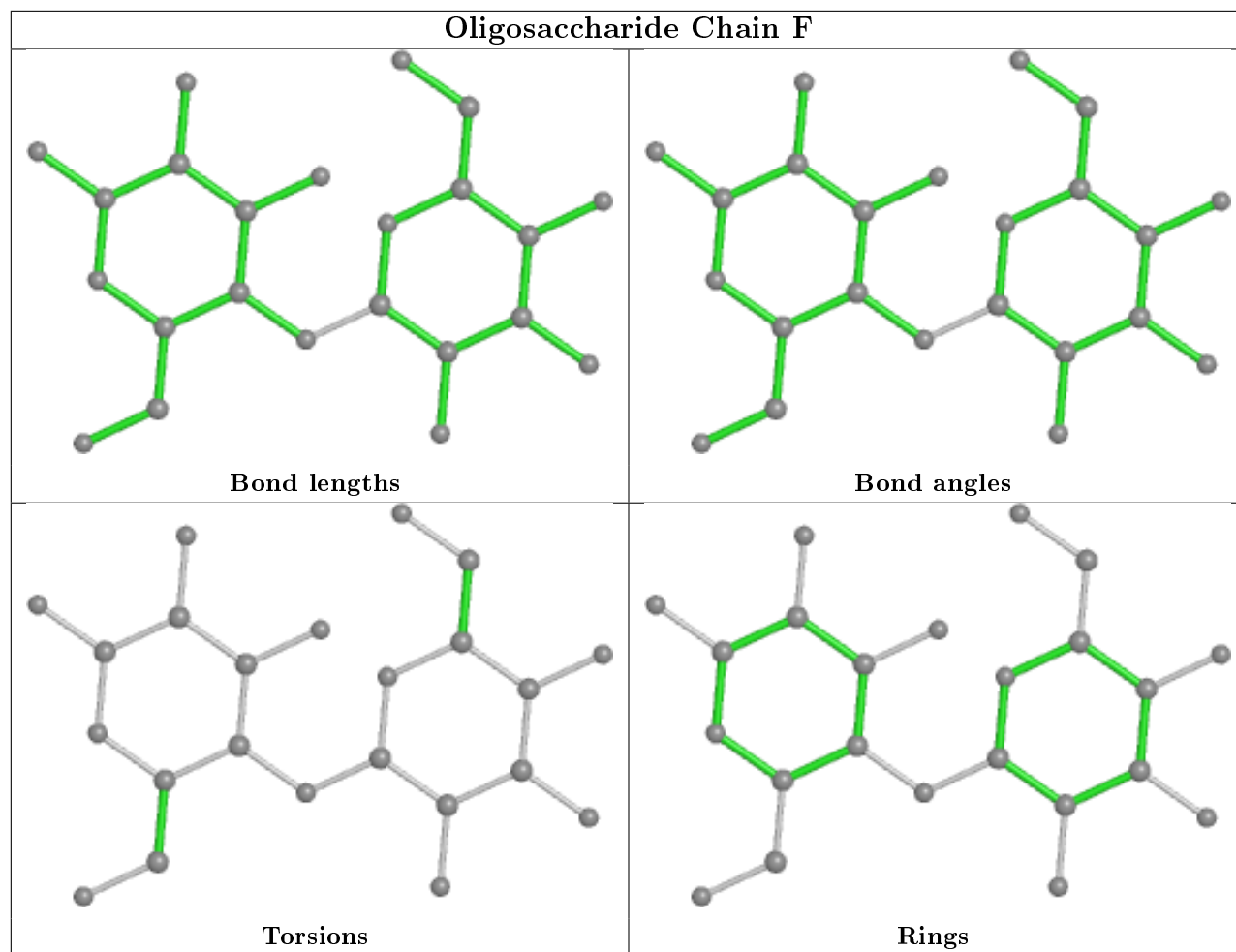
6 monomers are involved in 23 short contacts:

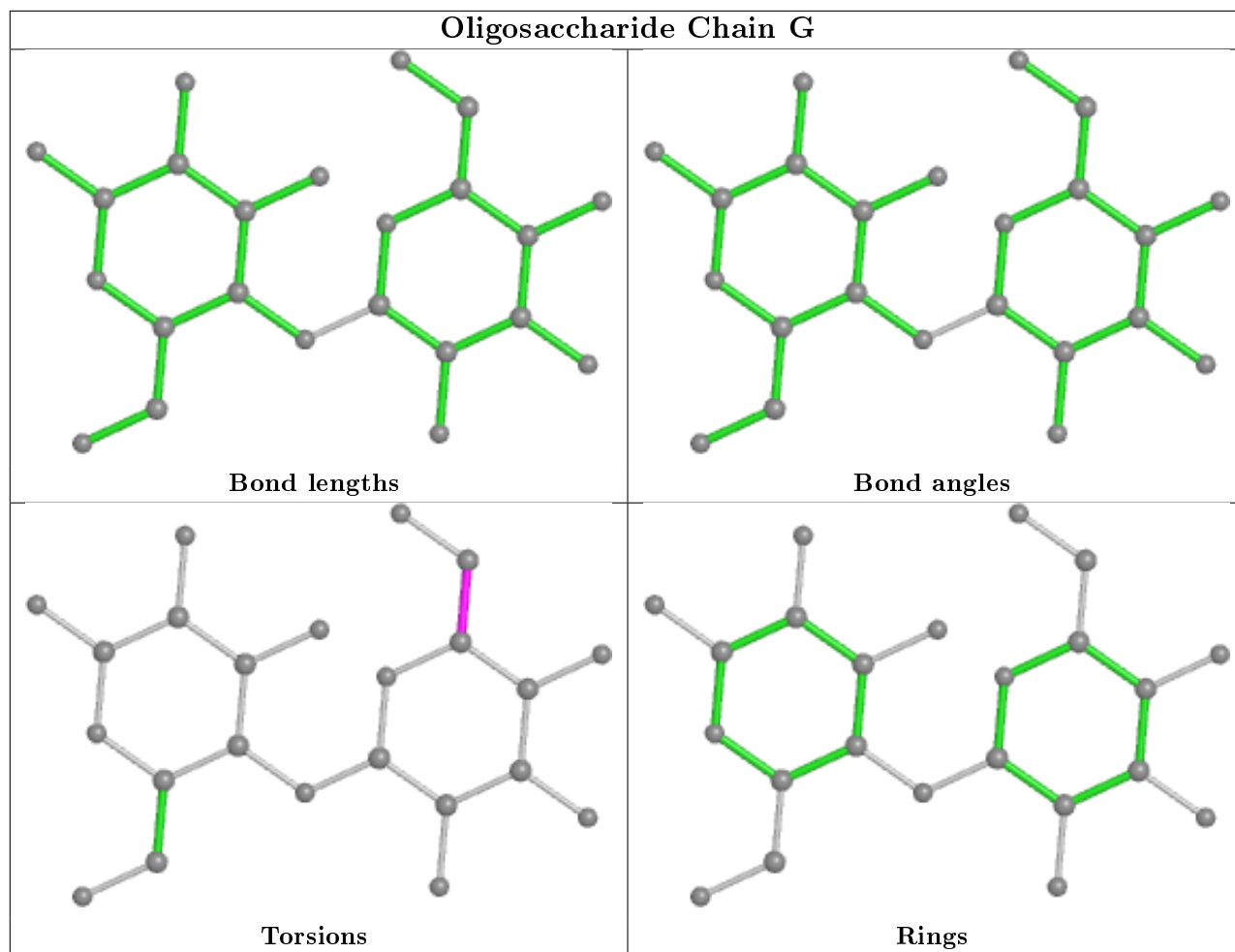
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	4	0
3	E	2	NAG	1	0
4	G	2	GLC	1	0
4	F	2	GLC	16	0
4	F	1	GLC	1	0
3	E	1	NAG	2	0

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](#)

3 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	$\# Z  > 2$
6	0G6	B	702	2	30,31,32	0.40	0	37,41,42	0.78	1 (2%)
6	0G6	D	703	2	30,31,32	0.39	0	37,41,42	0.78	1 (2%)
5	NAG	B	701	2	14,14,15	0.30	0	17,19,21	0.64	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
6	0G6	B	702	2	-	20/31/41/43	0/2/2/2
6	0G6	D	703	2	-	20/31/41/43	0/2/2/2
5	NAG	B	701	2	1/1/5/7	4/6/23/26	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(°)
6	B	702	0G6	CG-CB-CA	-2.26	109.42	114.13
6	D	703	0G6	CG-CB-CA	-2.25	109.45	114.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	701	NAG	C1

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	702	0G6	N1-C-CA-N
6	B	702	0G6	N-CA-CB-CG
6	B	702	0G6	CA-C-N1-CA1
6	B	702	0G6	CA-C-N1-CD
6	B	702	0G6	O-C-N1-CA1

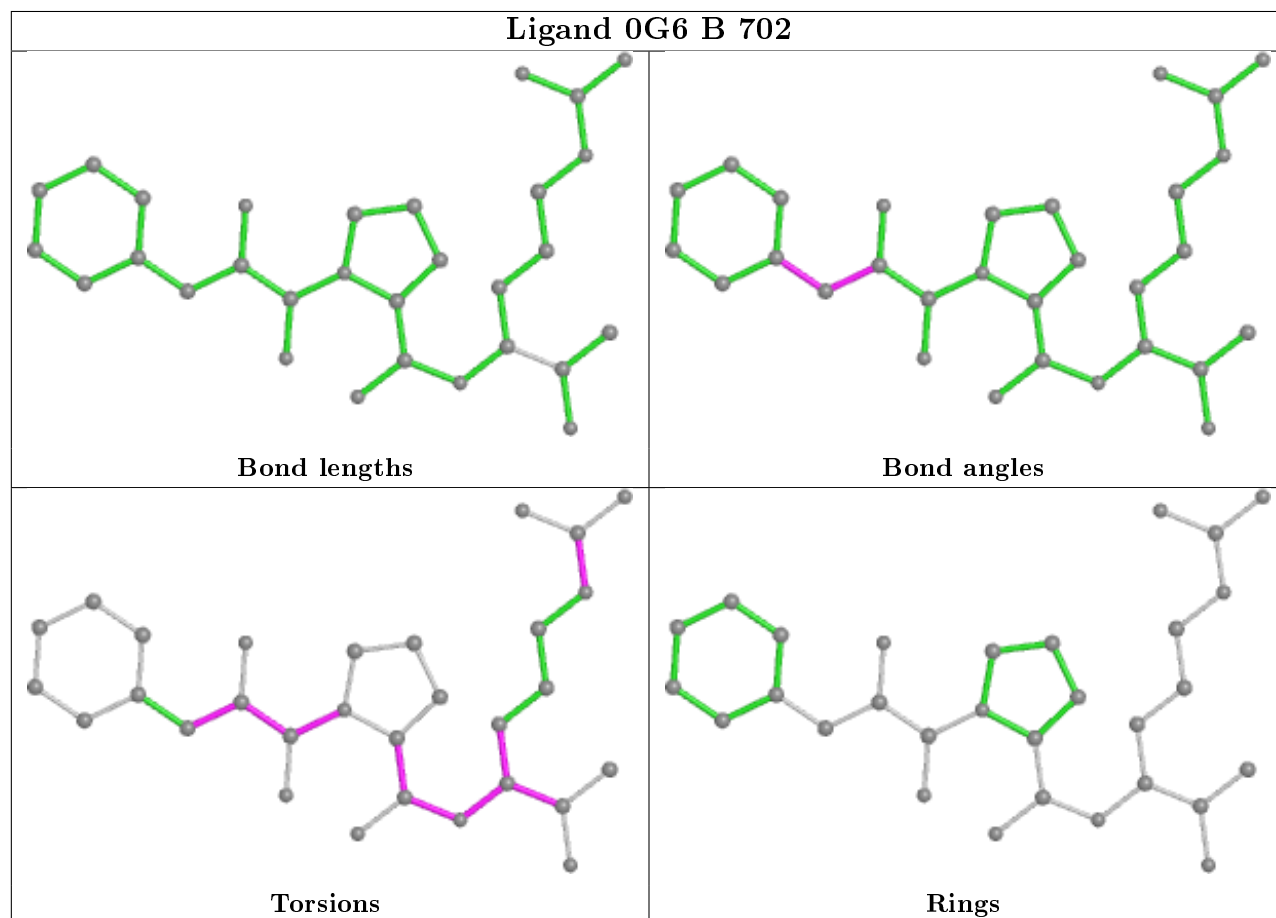
There are no ring outliers.

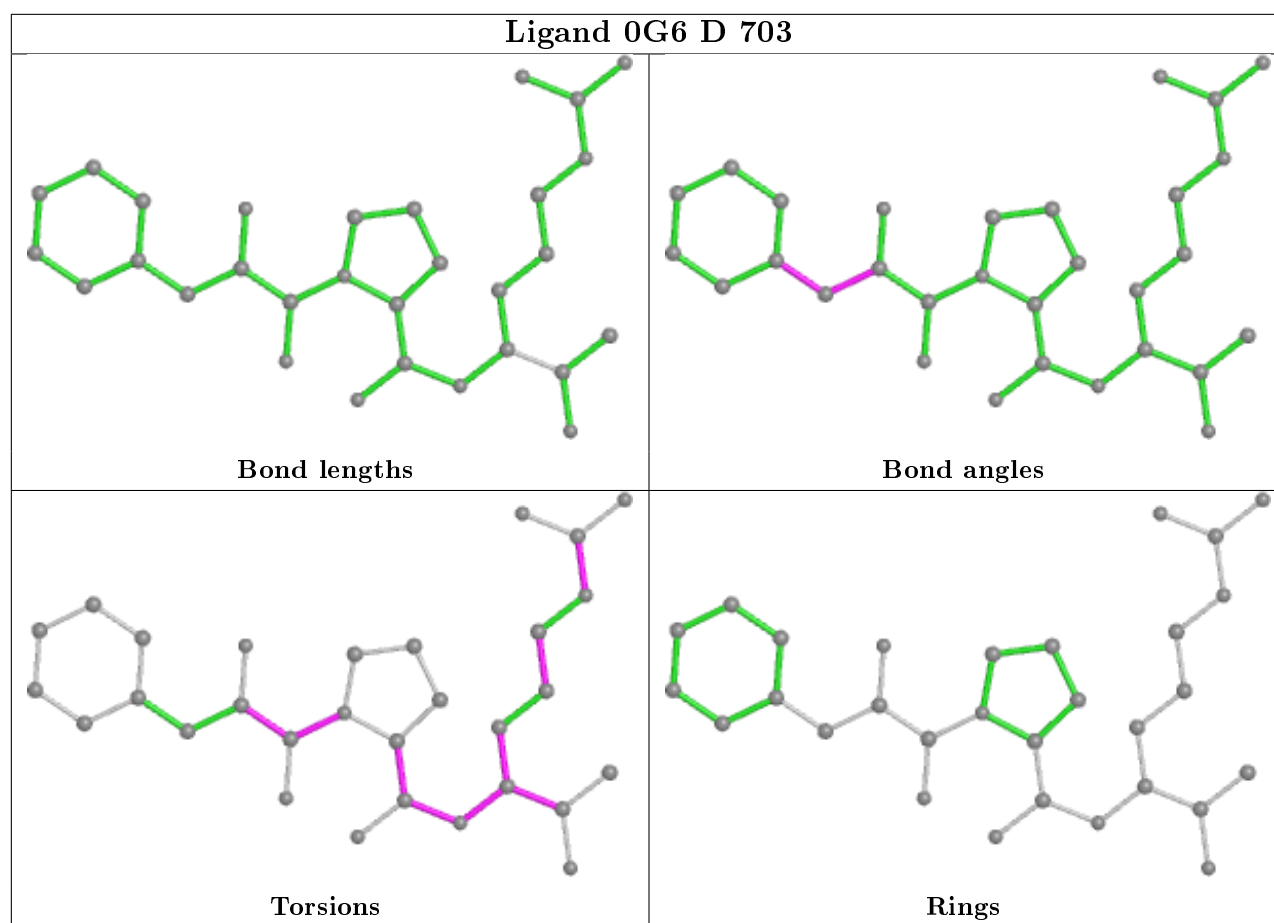
3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	702	0G6	1	0
6	D	703	0G6	21	0
5	B	701	NAG	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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	344:ARG	C	354:VAL	N	22.66
1	D	343:ARG	C	354:VAL	N	22.36
1	D	552:ASP	C	557:ARG	N	6.48
1	B	552:ASP	C	557:ARG	N	5.00

## 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	369/374 (98%)	-0.53	0 <a href="#">100</a> <a href="#">100</a>	19, 35, 68, 94	0
1	C	370/374 (98%)	-0.45	0 <a href="#">100</a> <a href="#">100</a>	19, 40, 61, 75	0
2	B	244/254 (96%)	-0.47	0 <a href="#">100</a> <a href="#">100</a>	20, 38, 75, 94	1 (0%)
2	D	244/254 (96%)	-0.46	1 (0%) <a href="#">92</a> <a href="#">87</a>	18, 29, 74, 107	1 (0%)
All	All	1227/1256 (97%)	-0.48	1 (0%) <a href="#">95</a> <a href="#">94</a>	18, 36, 67, 107	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	478	THR	3.6

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

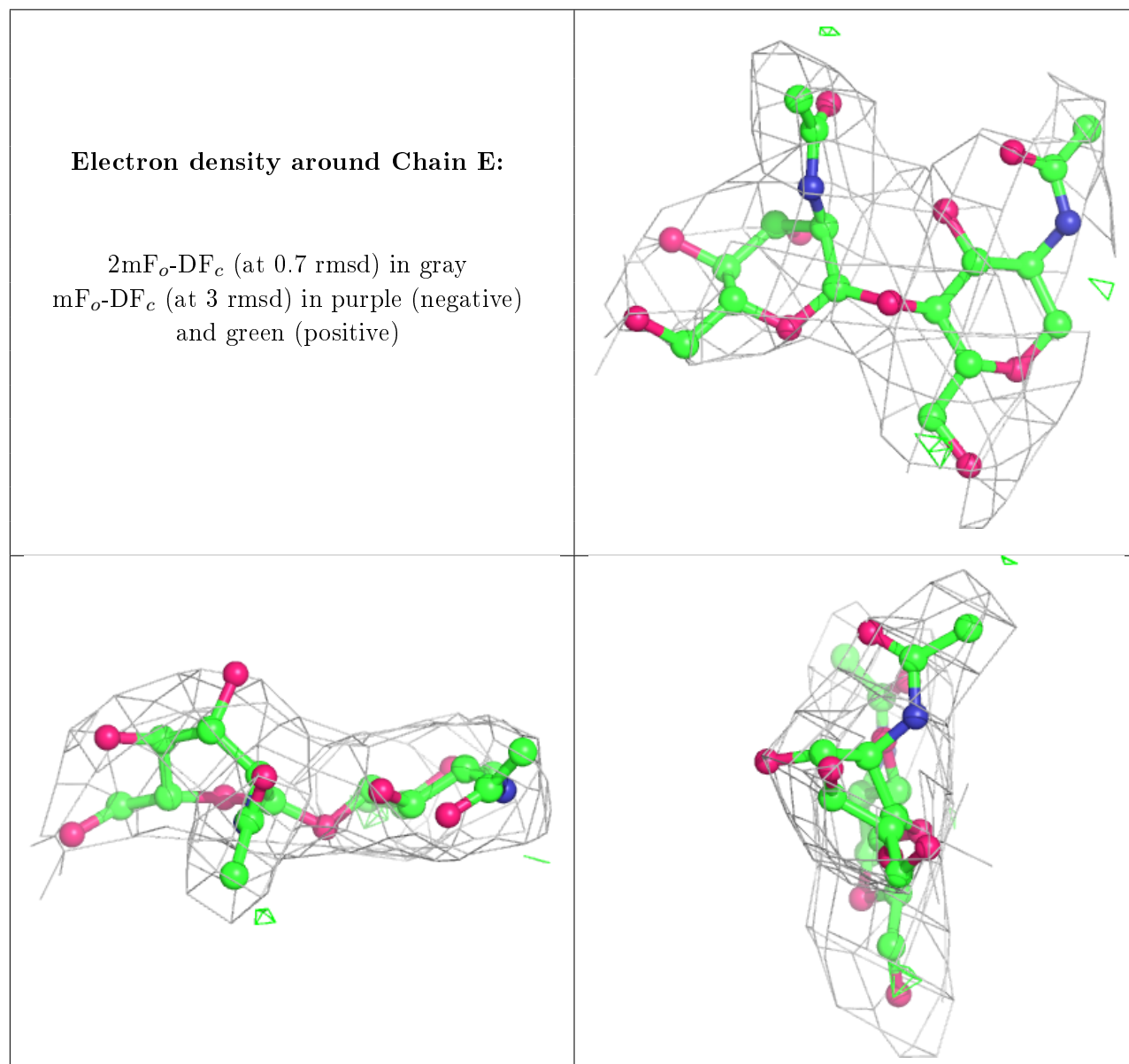
There are no non-standard protein/DNA/RNA residues in this entry.

### 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(Å <sup>2</sup> )	Q<0.9
3	NAG	E	2	14/15	0.84	0.43	30,30,31,31	0
3	NAG	E	1	14/15	0.88	0.28	27,28,29,29	0
4	GLC	G	2	11/12	0.90	0.23	19,19,19,20	0
4	GLC	G	1	12/12	0.93	0.20	19,19,19,19	3
4	GLC	F	2	11/12	0.94	0.19	19,19,19,20	2
4	GLC	F	1	12/12	0.95	0.16	19,19,19,20	0

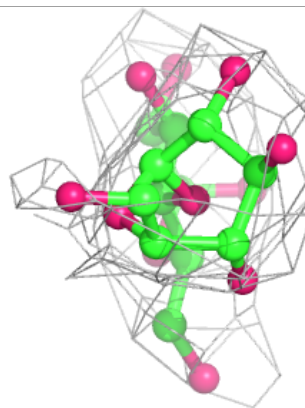
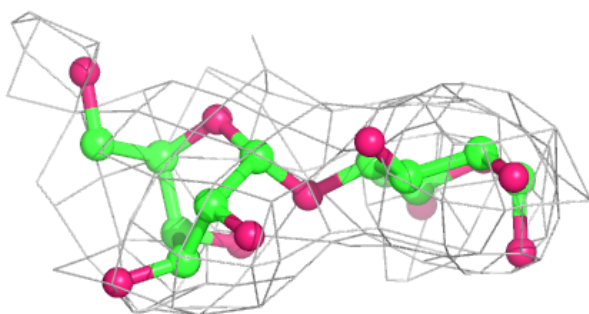
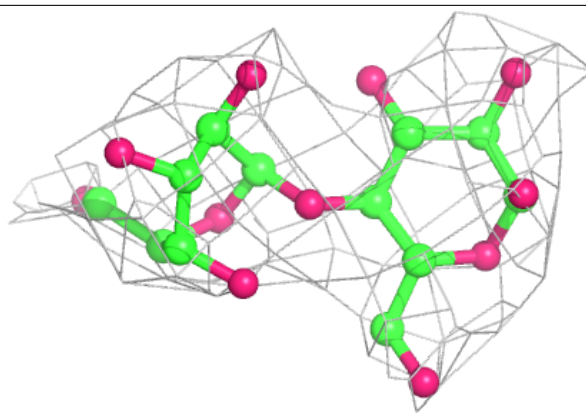
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

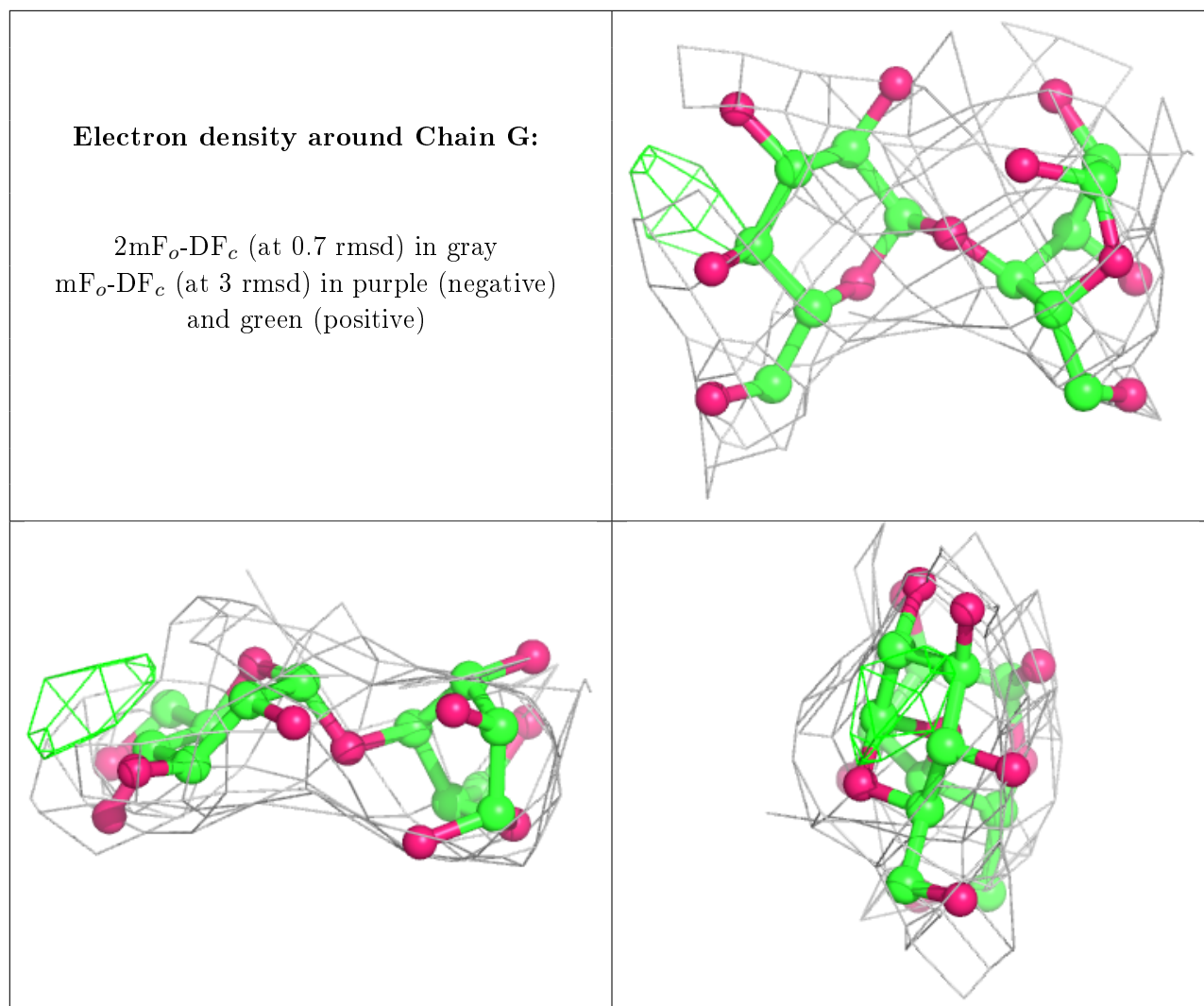




**Electron density around Chain F:**

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





## 6.4 Ligands [\(i\)](#)

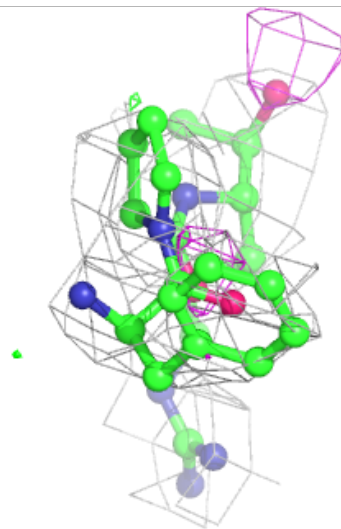
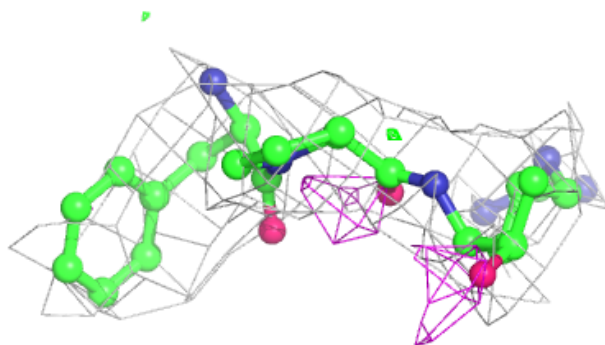
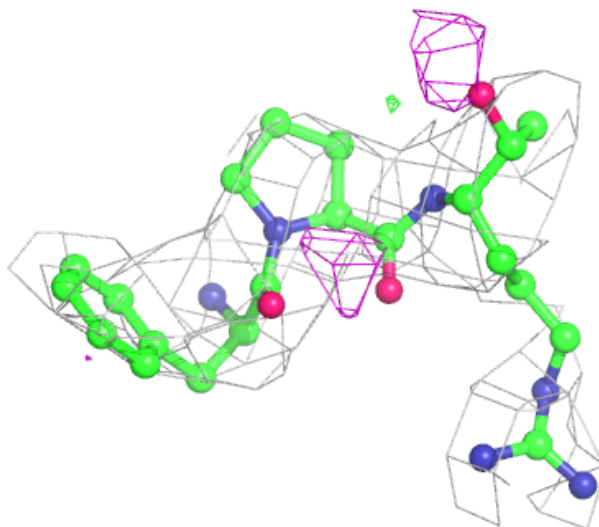
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

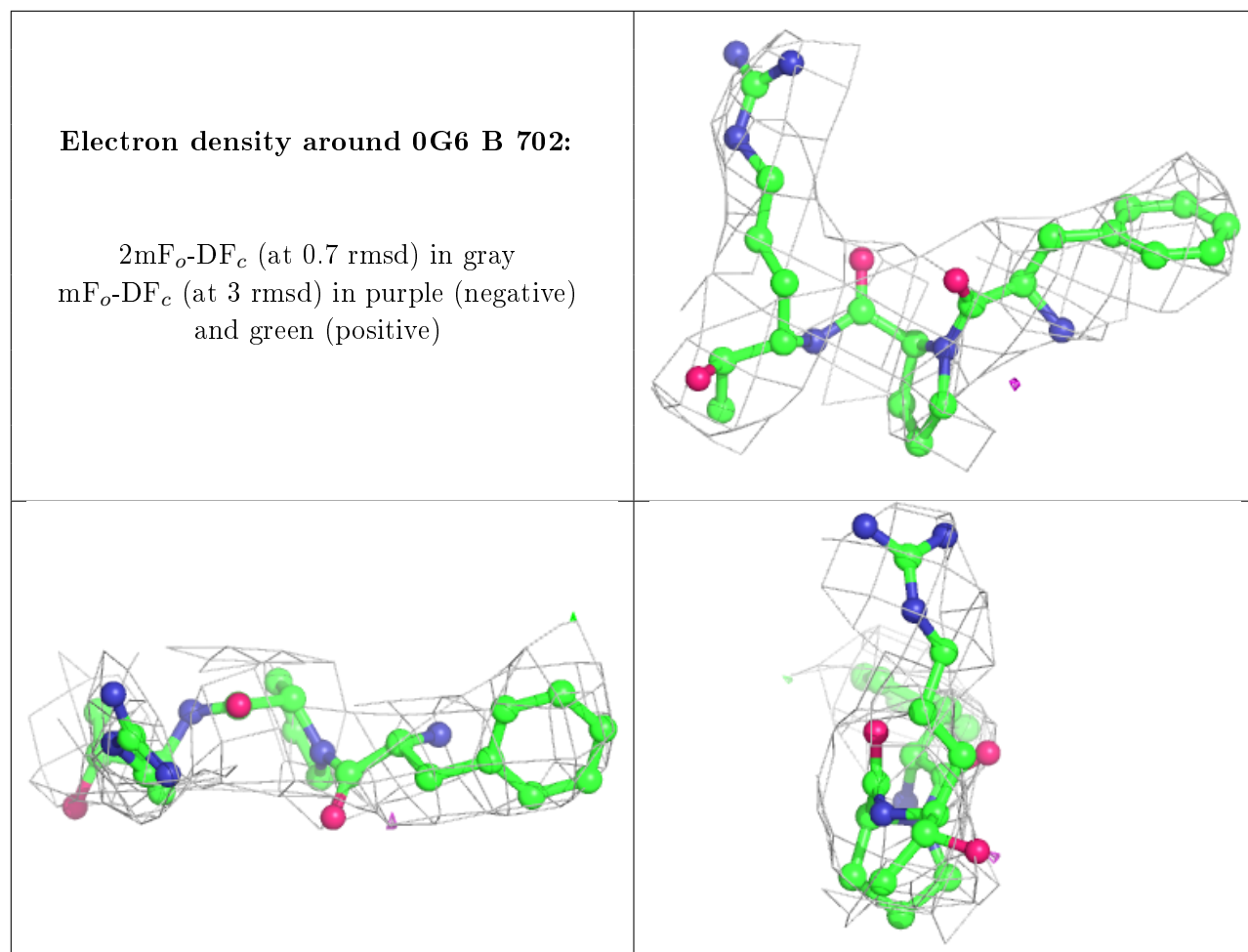
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	701	14/15	0.57	0.49	40,42,42,42	6
6	0G6	D	703	30/31	0.90	0.22	14,18,19,19	3
6	0G6	B	702	30/31	0.92	0.21	27,28,29,29	0

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.

**Electron density around 0G6 D 703:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.