



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 09:16 pm GMT

PDB ID : 6I3J  
Title : Bilirubin oxidase from *Myrothecium verrucaria* in complex with ferricyanide  
Authors : Svecova, L.; Koval, T.; Skalova, T.; Kolenko, P.; Duskova, J.; Ostergaard, L.H.; Dohnalek, J.  
Deposited on : 2018-11-06  
Resolution : 2.59 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

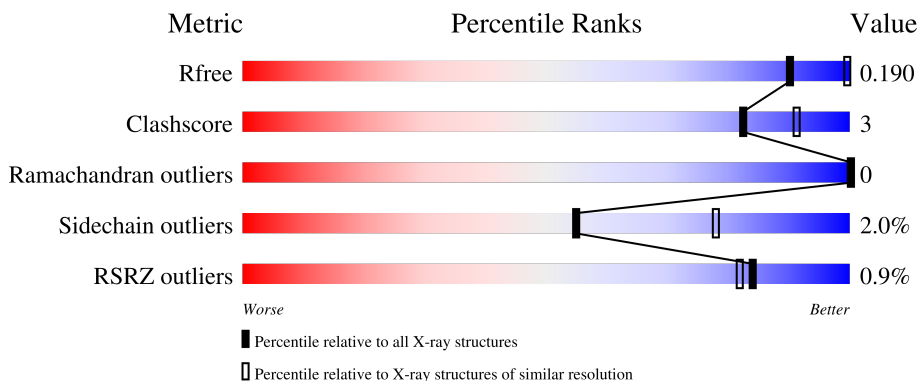
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\leq 5\%$ . 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	534	 90% 9% 2% 1%
1	B	534	 92% 8% 2% 1%
2	C	5	 100%
3	D	3	 33% 67%
4	E	4	 75% 25%

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Mol	Chain	Length	Quality of chain
5	F	2	 50% 50%

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
8	SIN	B	617	-	X	-	-

## 2 Entry composition [i](#)

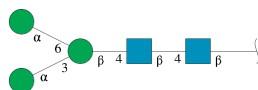
There are 12 unique types of molecules in this entry. The entry contains 9511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bilirubin oxidase.

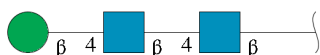
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	534	4327	2755	740	818	14	0	9	0
1	B	533	4280	2731	732	803	14	0	5	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



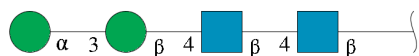
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	61	34	2	25	0	0	0

- Molecule 3 is an oligosaccharide called 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
			Total	C	N	O			
3	D	3	39	22	2	15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O			
4	E	4	50	28	2	20	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

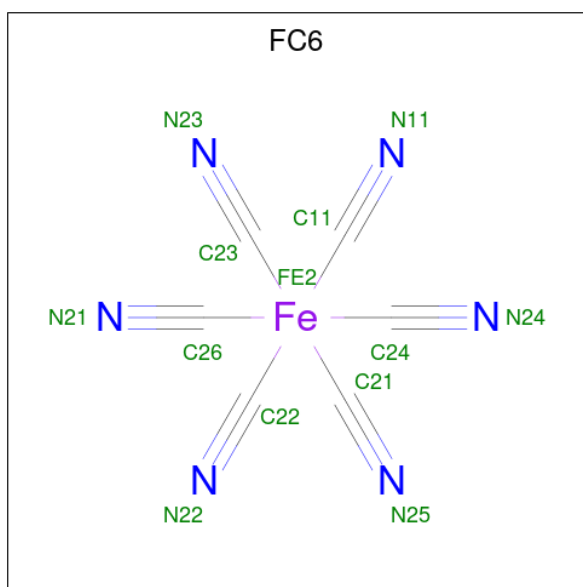


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	2	28	16	2	10	0	0	0

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

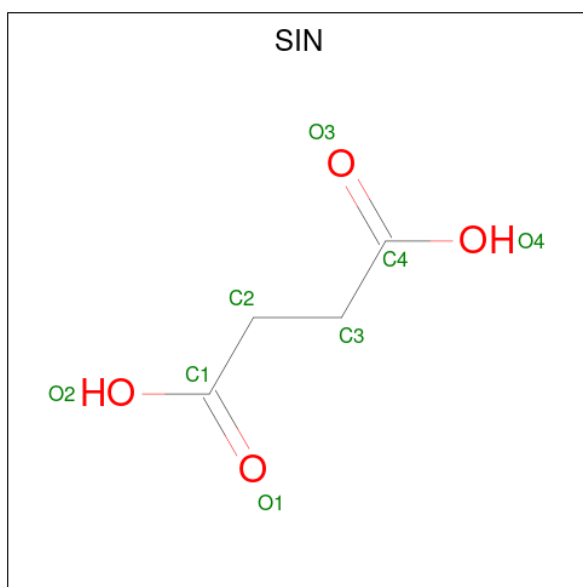
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Cu	0	0
			4	4		
6	B	4	Total	Cu	0	0
			4	4		

- Molecule 7 is HEXACYANOFERRATE(3-) (three-letter code: FC6) (formula: C<sub>6</sub>FeN<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Fe	N		
7	A	1	13	6	1	6	0	0
7	A	1	13	6	1	6	0	0
7	A	1	13	6	1	6	0	0
7	A	1	13	6	1	6	0	0
7	B	1	13	6	1	6	0	0
7	B	1	13	6	1	6	0	0
7	B	1	13	6	1	6	0	0
7	B	1	13	6	1	6	0	0
7	B	1	13	6	1	6	0	0

- Molecule 8 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 8 4 4	0	0
8	A	1	Total C O 8 4 4	0	0
8	A	1	Total C O 8 4 4	0	0
8	B	1	Total C O 8 4 4	0	0
8	B	1	Total C O 8 4 4	0	0

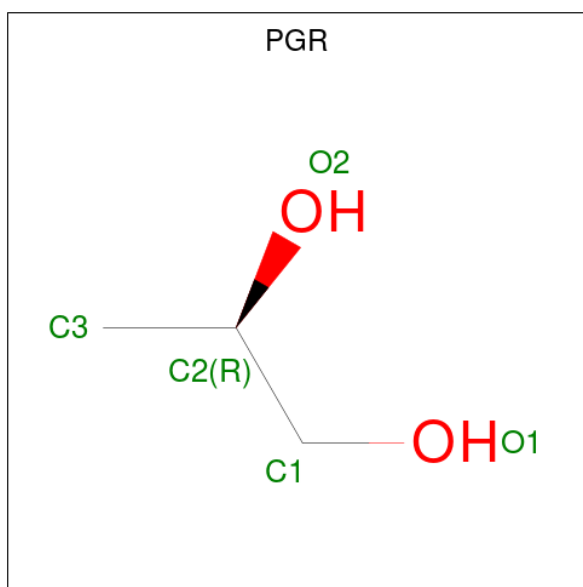
- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	5	Total Na 5 5	0	0
9	B	3	Total Na 3 3	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0

- Molecule 11 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 12 is water.

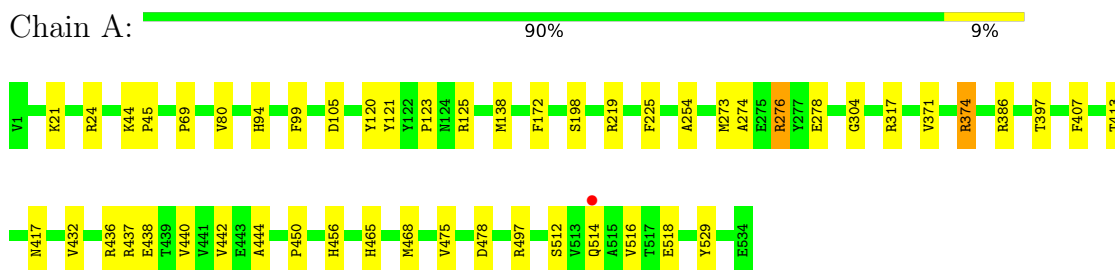
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	297	Total	O	0	0
			297	297		
12	B	250	Total	O	0	0
			250	250		



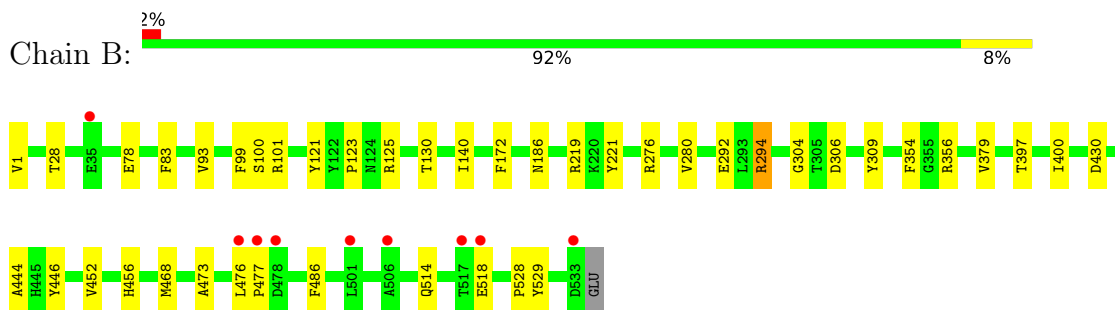
### 3 Residue-property plots [i](#)

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.

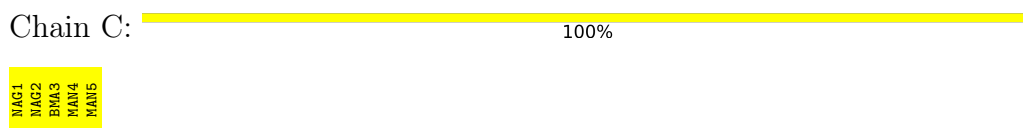
- Molecule 1: Bilirubin oxidase



- Molecule 1: Bilirubin oxidase



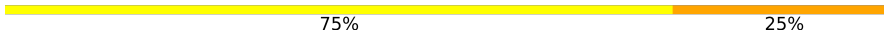
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain E:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.38Å 203.85Å 226.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.59 47.30 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.30-2.59) 99.9 (47.30-2.59)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.160 , 0.226 0.168 , 0.190	Depositor DCC
$R_{free}$ test set	2442 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtrriage
Anisotropy	0.375	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: CU, CL, BMA, PGR, FC6, NAG, MAN, SIN, NA

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	0.51	0/4460	0.71	0/6097
1	B	0.49	0/4417	0.70	0/6038
All	All	0.50	0/8877	0.70	0/12135

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	497	ARG	Sidechain
1	B	125[A]	ARG	Sidechain
1	B	294	ARG	Sidechain

## 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	4327	0	4084	23	0
1	B	4280	0	4068	21	0
2	C	61	0	52	0	0
3	D	39	0	33	0	0
4	E	50	0	43	1	0
5	F	28	0	24	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	52	0	0	1	0
7	B	65	0	0	1	0
8	A	24	0	12	0	0
8	B	16	0	8	1	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	A	1	0	0	0	0
11	B	5	0	8	0	0
12	A	297	0	0	3	0
12	B	250	0	0	1	0
All	All	9511	0	8332	44	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 3.

All (44) 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:465[B]:HIS:CD2	12:A:750:HOH:O	1.69	1.29
1:A:465[B]:HIS:HD2	12:A:750:HOH:O	1.12	1.02
1:B:276[B]:ARG:NH1	1:B:430:ASP:OD1	2.28	0.66
1:B:456:HIS:HB3	1:B:468:MET:HG3	1.77	0.66
1:A:456:HIS:HB3	1:A:468:MET:HG3	1.85	0.58
1:B:486:PHE:CZ	1:B:528:PRO:HB3	2.41	0.55
1:B:123:PRO:HB3	1:B:529:TYR:CG	2.41	0.55
1:A:432:VAL:HG21	1:A:440:VAL:HG11	1.88	0.54
1:A:437[A]:ARG:NH2	12:A:702:HOH:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ALA:HB3	1:A:278:GLU:HB2	1.90	0.52
1:B:172:PHE:CE1	1:B:219:ARG:HD3	2.46	0.51
1:B:354:PHE:CE2	1:B:400:ILE:HD12	2.46	0.50
1:A:21:LYS:HB2	1:A:69:PRO:HB2	1.95	0.49
1:B:379:VAL:O	1:B:473:ALA:HA	2.13	0.47
1:B:140:ILE:HA	12:B:828:HOH:O	2.14	0.47
1:A:172:PHE:CE1	1:A:219:ARG:HD3	2.50	0.47
1:A:407:PHE:HB3	1:A:444:ALA:HB2	1.98	0.46
1:B:130:THR:O	1:B:276[B]:ARG:HD2	2.15	0.46
1:A:304:GLY:O	1:A:436:ARG:HD2	2.16	0.46
1:A:123:PRO:HB3	1:A:529:TYR:CG	2.50	0.46
1:A:386:ARG:HH22	7:A:616:FC6:C21	2.27	0.46
1:B:476:LEU:HB3	1:B:477:PRO:HD2	1.98	0.46
1:B:78:GLU:OE2	8:B:616:SIN:O3	2.33	0.45
1:A:371:VAL:HA	1:A:374:ARG:HG2	1.98	0.45
1:B:444:ALA:HB3	1:B:446:TYR:CE1	2.51	0.45
1:B:292:GLU:HG2	1:B:294:ARG:HG3	1.98	0.45
1:A:450:PRO:HB3	1:A:475:VAL:HG13	1.98	0.44
1:B:130:THR:O	1:B:276[A]:ARG:NE	2.48	0.44
1:A:273:MET:O	1:A:274:ALA:HB3	2.18	0.44
1:B:304:GLY:HA2	1:B:397:THR:HG21	1.99	0.43
1:A:94:HIS:ND1	1:A:105:ASP:O	2.51	0.43
1:A:44:LYS:HB2	1:A:45:PRO:HD2	2.01	0.43
1:B:101:ARG:HG2	1:B:529:TYR:CE1	2.53	0.43
1:A:225:PHE:O	1:A:276:ARG:HA	2.18	0.43
1:A:304:GLY:HA2	1:A:397:THR:HG21	2.01	0.42
1:B:452:VAL:HG21	4:E:1:NAG:H82	2.01	0.42
1:A:386:ARG:HA	1:A:442:VAL:O	2.20	0.42
1:A:512:SER:O	1:A:516:VAL:HG23	2.19	0.42
1:B:186:ASN:HB2	7:B:612:FC6:N21	2.35	0.42
1:A:413:THR:O	1:A:438:GLU:HA	2.20	0.41
1:B:83:PHE:CG	1:B:93:VAL:HG21	2.56	0.41
1:A:80:VAL:HA	1:A:120:TYR:O	2.20	0.41
1:B:1:VAL:O	1:B:309:TYR:HA	2.21	0.41
1:B:221:TYR:O	1:B:280:VAL:HA	2.21	0.41

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	541/534 (101%)	513 (95%)	28 (5%)	0	100	100
1	B	536/534 (100%)	504 (94%)	32 (6%)	0	100	100
All	All	1077/1068 (101%)	1017 (94%)	60 (6%)	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	462/453 (102%)	451 (98%)	11 (2%)	49	74
1	B	457/453 (101%)	447 (98%)	10 (2%)	52	76
All	All	919/906 (101%)	898 (98%)	21 (2%)	55	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	PHE
1	A	121	TYR
1	A	138	MET
1	A	198	SER
1	A	276	ARG
1	A	374	ARG
1	A	417	ASN
1	A	478[A]	ASP

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Mol	Chain	Res	Type
1	A	478[B]	ASP
1	A	514	GLN
1	A	518	GLU
1	B	28	THR
1	B	99	PHE
1	B	100	SER
1	B	121	TYR
1	B	306	ASP
1	B	356[A]	ARG
1	B	356[B]	ARG
1	B	514	GLN
1	B	518[A]	GLU
1	B	518[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	72	GLN
1	B	510	GLN
1	B	514	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](#)

14 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	0.61	0	17,19,21	1.42	3 (17%)
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	1.15	1 (5%)
2	BMA	C	3	2	11,11,12	1.15	1 (9%)	15,15,17	1.93	4 (26%)
2	MAN	C	4	2	11,11,12	1.05	0	15,15,17	1.76	1 (6%)
2	MAN	C	5	2	11,11,12	0.69	0	15,15,17	1.11	1 (6%)
3	NAG	D	1	1,9,3	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	0.77	0
3	BMA	D	3	3	11,11,12	0.49	0	15,15,17	1.18	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	1.45	4 (23%)
4	BMA	E	3	4	11,11,12	0.95	0	15,15,17	2.17	6 (40%)
4	MAN	E	4	4	11,11,12	0.78	0	15,15,17	1.27	2 (13%)
5	NAG	F	1	1,9,5	14,14,15	0.69	0	17,19,21	0.93	0
5	NAG	F	2	5	14,14,15	0.68	0	17,19,21	1.35	1 (5%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,9,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	1,9,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	BMA	C2-C3	2.21	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	6.31	120.74	112.19
2	C	3	BMA	C3-C4-C5	4.20	117.73	110.24
2	C	2	NAG	C1-O5-C5	4.15	117.81	112.19
5	F	2	NAG	C1-O5-C5	4.04	117.66	112.19
4	E	1	NAG	C1-C2-N2	-3.96	103.73	110.49
2	C	3	BMA	O5-C1-C2	-3.85	104.83	110.77
4	E	3	BMA	O2-C2-C3	3.79	117.72	110.14
4	E	3	BMA	O5-C5-C6	3.57	112.80	107.20
4	E	3	BMA	C3-C4-C5	3.47	116.42	110.24
4	E	4	MAN	C1-C2-C3	3.07	113.44	109.67
4	E	3	BMA	O3-C3-C2	3.06	115.86	109.99
2	C	3	BMA	O2-C2-C3	3.03	116.21	110.14
4	E	3	BMA	C1-C2-C3	-3.01	105.96	109.67
3	D	1	NAG	O5-C5-C6	2.93	111.80	107.20
4	E	2	NAG	C4-C3-C2	-2.90	106.77	111.02
2	C	1	NAG	O5-C1-C2	-2.89	106.72	111.29
4	E	2	NAG	O4-C4-C5	2.85	116.37	109.30
3	D	3	BMA	C1-C2-C3	-2.54	106.54	109.67
2	C	1	NAG	O4-C4-C3	-2.37	104.88	110.35
2	C	1	NAG	C1-C2-N2	-2.36	106.47	110.49
4	E	1	NAG	O4-C4-C3	-2.35	104.91	110.35
4	E	2	NAG	C3-C4-C5	-2.29	106.15	110.24
2	C	5	MAN	C1-C2-C3	2.29	112.48	109.67
4	E	4	MAN	O5-C5-C6	2.28	110.78	107.20
2	C	3	BMA	C2-C3-C4	2.18	114.67	110.89
3	D	3	BMA	C3-C4-C5	2.18	114.13	110.24
4	E	3	BMA	C1-O5-C5	-2.17	109.25	112.19
3	D	1	NAG	O5-C1-C2	-2.15	107.89	111.29
4	E	2	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	BMA	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6

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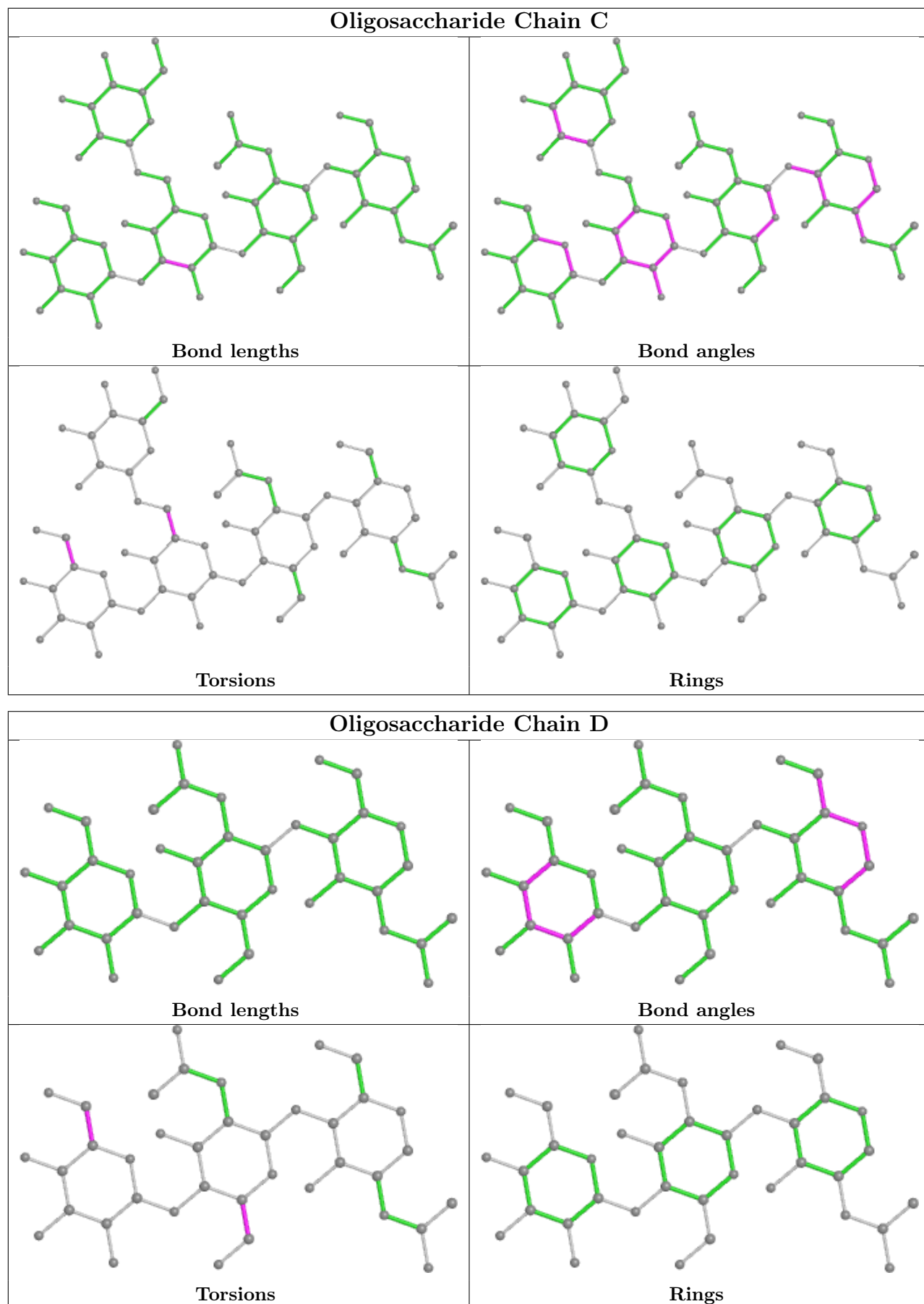
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6

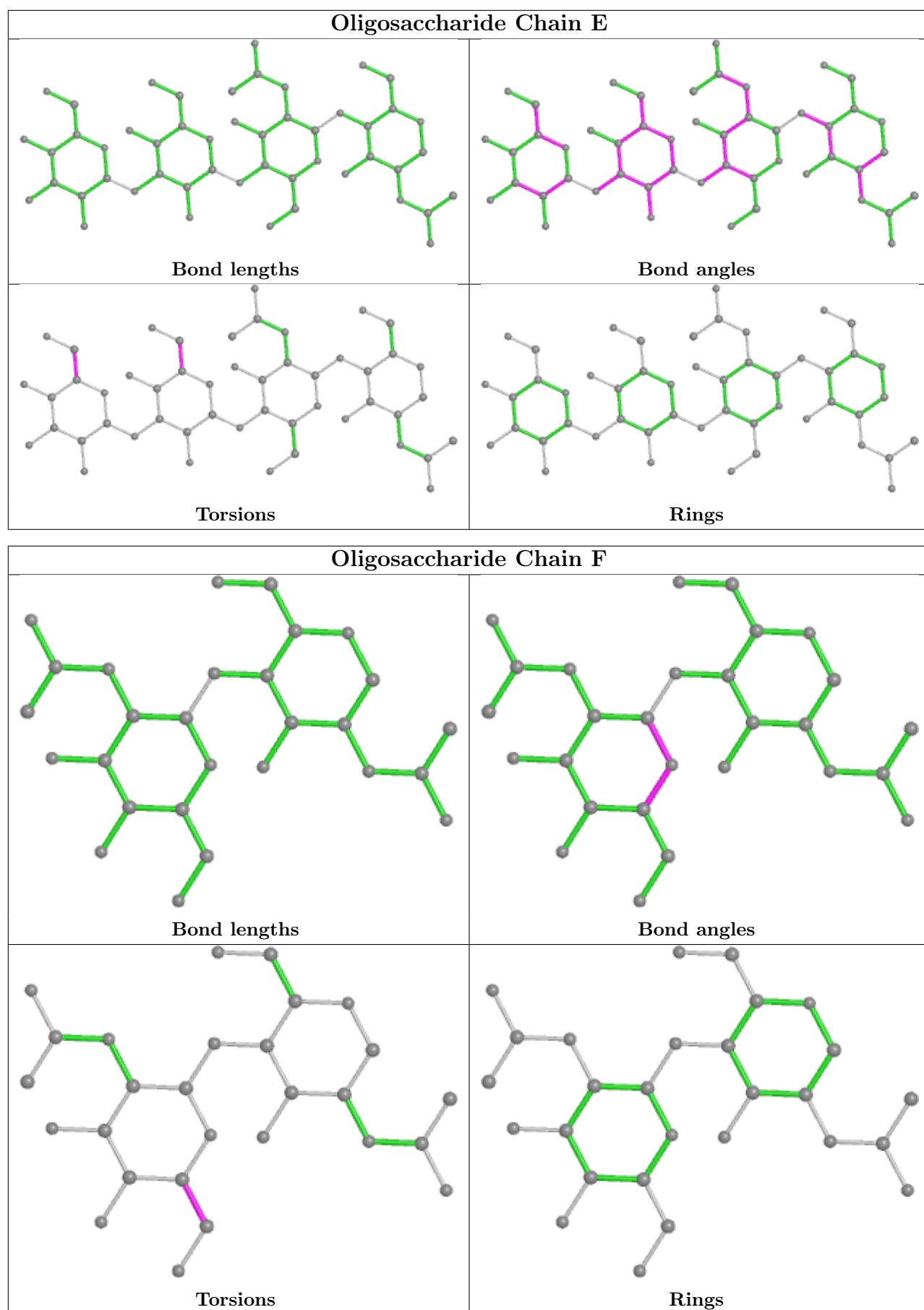
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	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 oligosaccharide.





## 5.6 Ligand geometry

Of 32 ligands modelled in this entry, 17 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	FC6	A	616	-	12,12,12	0.57	0	-		
8	SIN	B	616	-	7,7,7	1.15	0	8,8,8	1.10	0
7	FC6	B	612	-	12,12,12	0.61	0	-		
8	SIN	A	617	-	7,7,7	0.85	0	8,8,8	1.54	3 (37%)
8	SIN	A	619	-	7,7,7	1.05	0	8,8,8	1.09	0
7	FC6	A	614	-	12,12,12	0.42	0	-		
7	FC6	B	611	-	12,12,12	0.47	0	-		
7	FC6	A	613	-	12,12,12	0.35	0	-		
8	SIN	B	617	-	7,7,7	1.38	1 (14%)	8,8,8	2.01	3 (37%)
7	FC6	B	614	-	12,12,12	0.47	0	-		
11	PGR	B	621	-	3,4,4	0.86	0	1,4,4	0.34	0
7	FC6	B	613	-	12,12,12	0.67	0	-		
7	FC6	A	615	-	12,12,12	0.45	0	-		
8	SIN	A	618	-	7,7,7	1.64	2 (28%)	8,8,8	1.09	1 (12%)
7	FC6	B	615	-	12,12,12	0.33	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
8	SIN	B	616	-	-	1/5/5/5	-
8	SIN	A	617	-	-	0/5/5/5	-
8	SIN	A	619	-	-	3/5/5/5	-
8	SIN	B	617	-	-	5/5/5/5	-
11	PGR	B	621	-	-	0/2/2/2	-
8	SIN	A	618	-	-	0/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	618	SIN	C3-C4	2.39	1.56	1.50
8	B	617	SIN	C2-C1	2.20	1.55	1.50
8	A	618	SIN	O3-C4	2.06	1.29	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	617	SIN	O2-C1-C2	3.31	124.67	114.03
8	B	617	SIN	O4-C4-C3	2.52	122.14	114.03
8	A	618	SIN	C2-C3-C4	2.47	118.92	113.60
8	A	617	SIN	O4-C4-C3	2.21	121.14	114.03
8	B	617	SIN	O1-C1-C2	-2.20	116.01	123.08
8	A	617	SIN	O3-C4-C3	-2.18	116.07	123.08
8	A	617	SIN	O1-C1-C2	-2.15	116.16	123.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	616	SIN	C1-C2-C3-C4
8	A	619	SIN	C1-C2-C3-C4
8	B	617	SIN	C1-C2-C3-C4
8	A	619	SIN	O1-C1-C2-C3
8	B	617	SIN	C2-C3-C4-O3
8	A	619	SIN	O2-C1-C2-C3
8	B	617	SIN	C2-C3-C4-O4
8	B	617	SIN	O2-C1-C2-C3
8	B	617	SIN	O1-C1-C2-C3

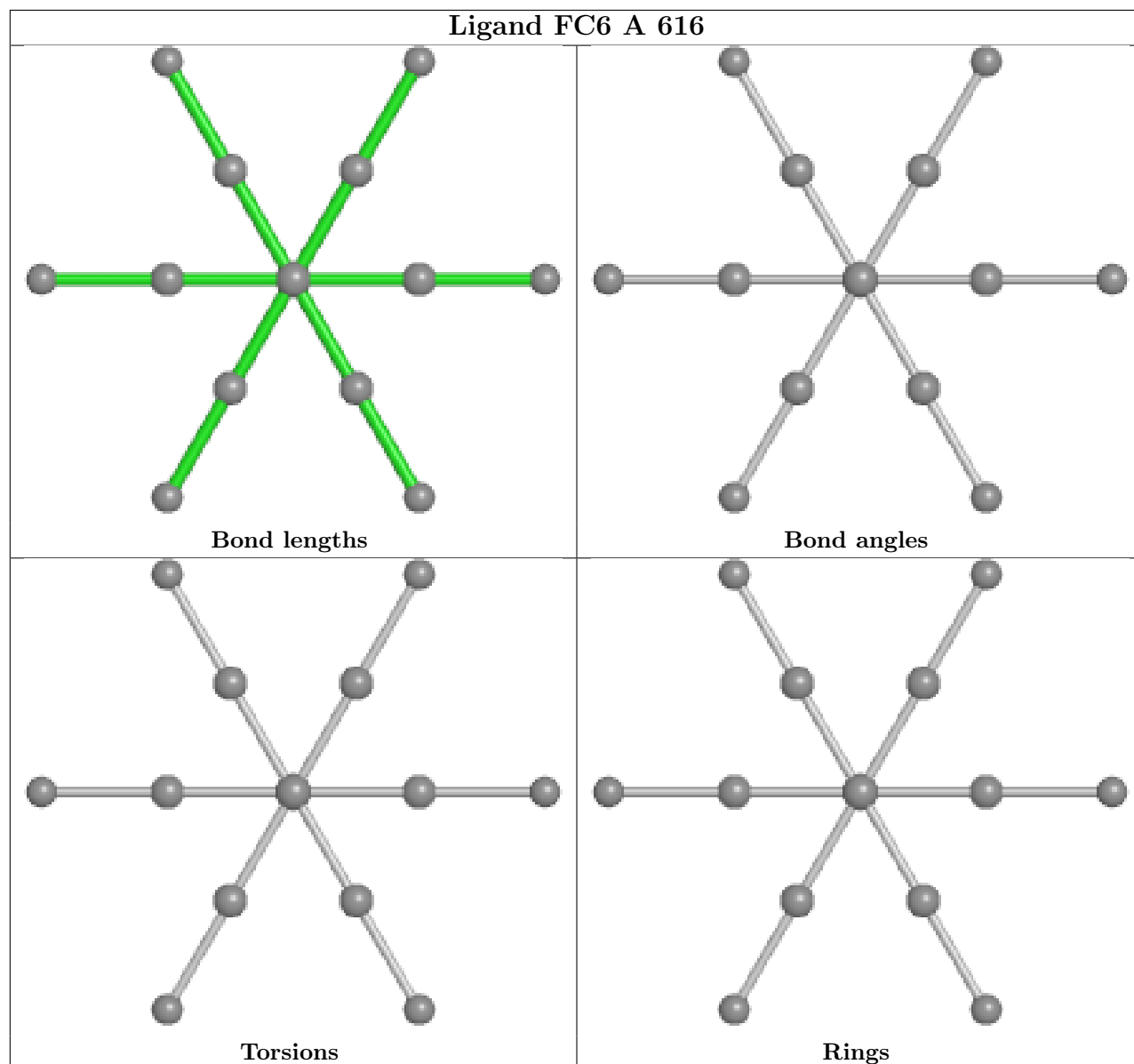
There are no ring outliers.

3 monomers are involved in 3 short contacts:

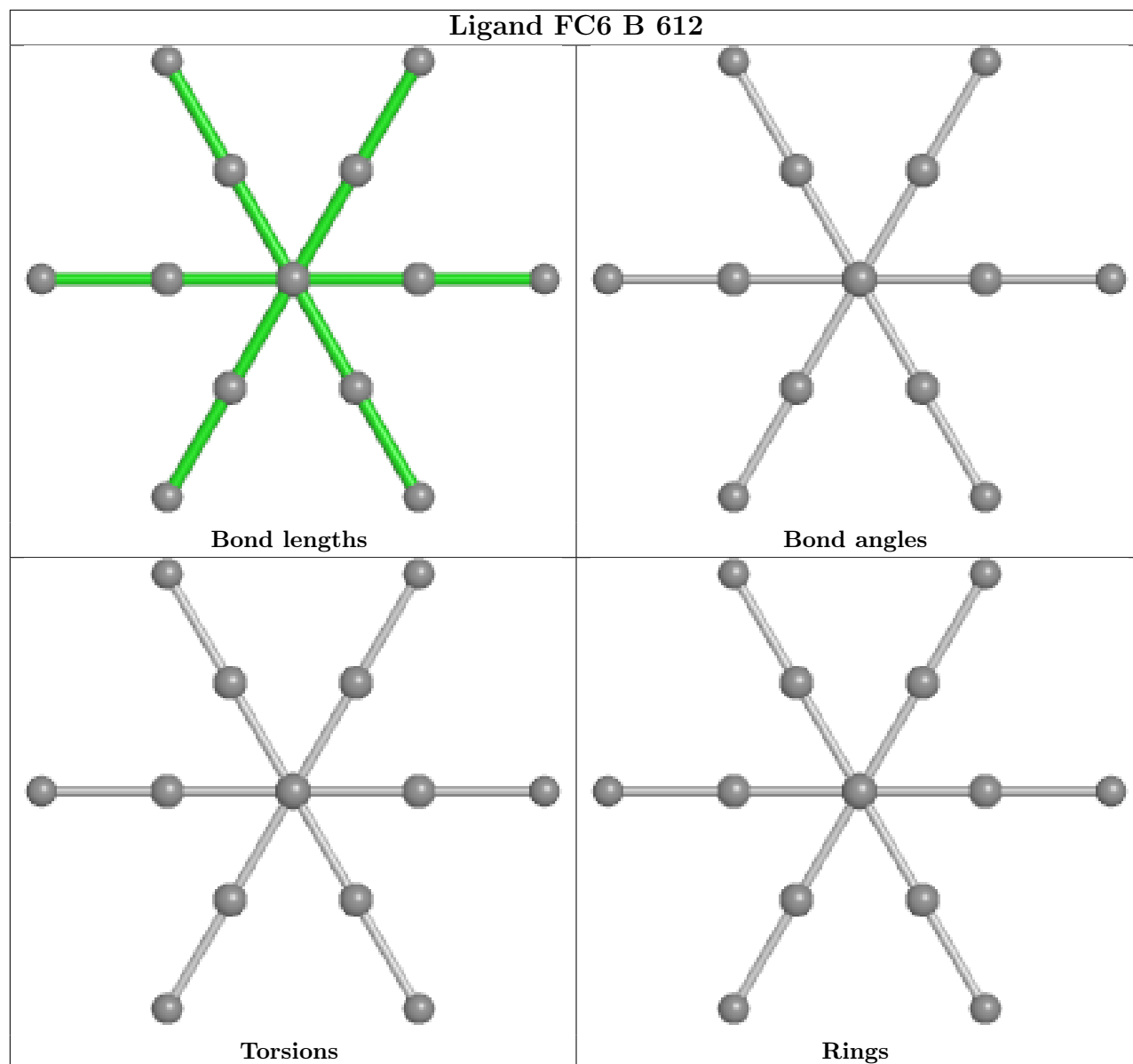
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	616	FC6	1	0
8	B	616	SIN	1	0
7	B	612	FC6	1	0

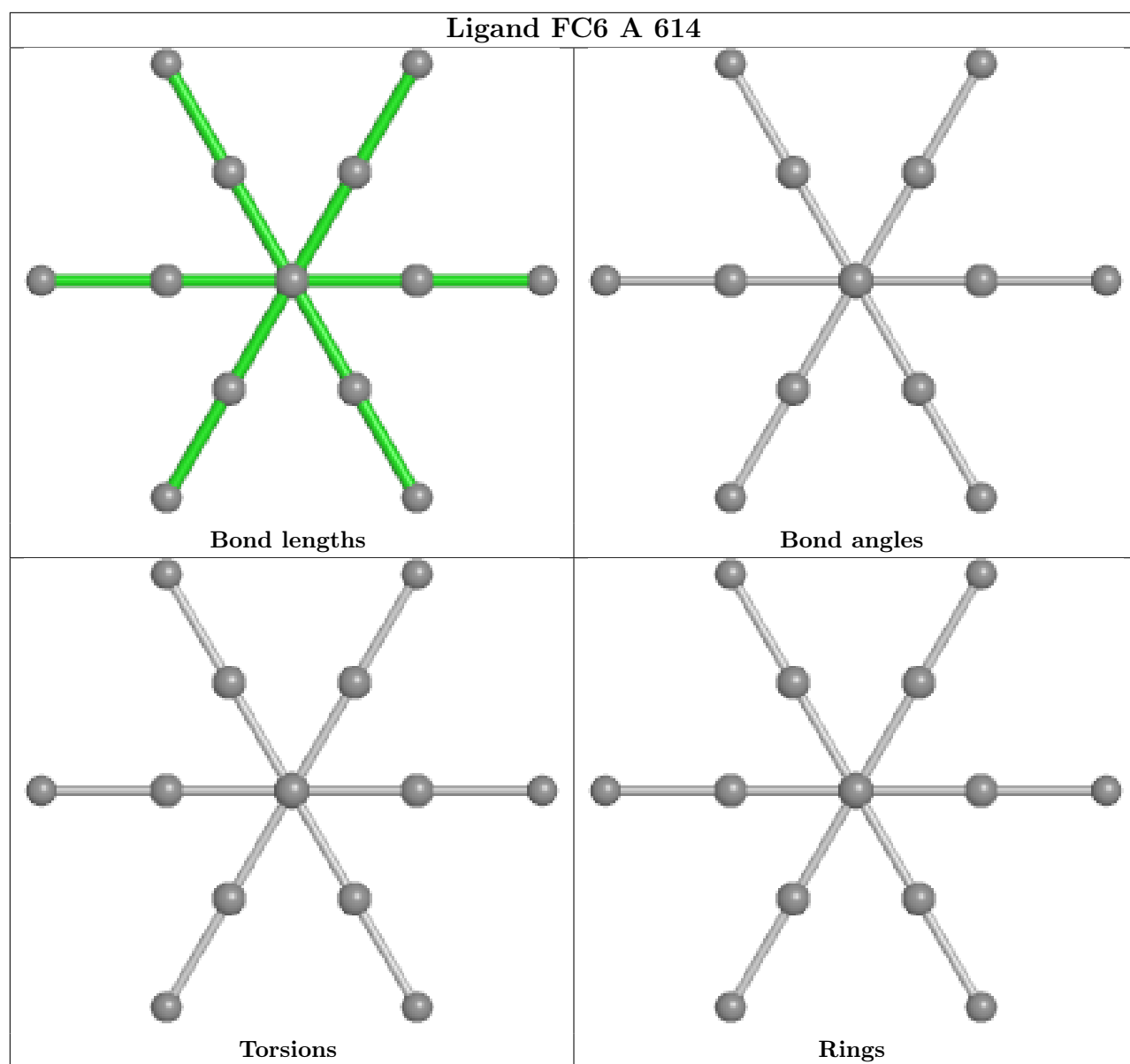
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

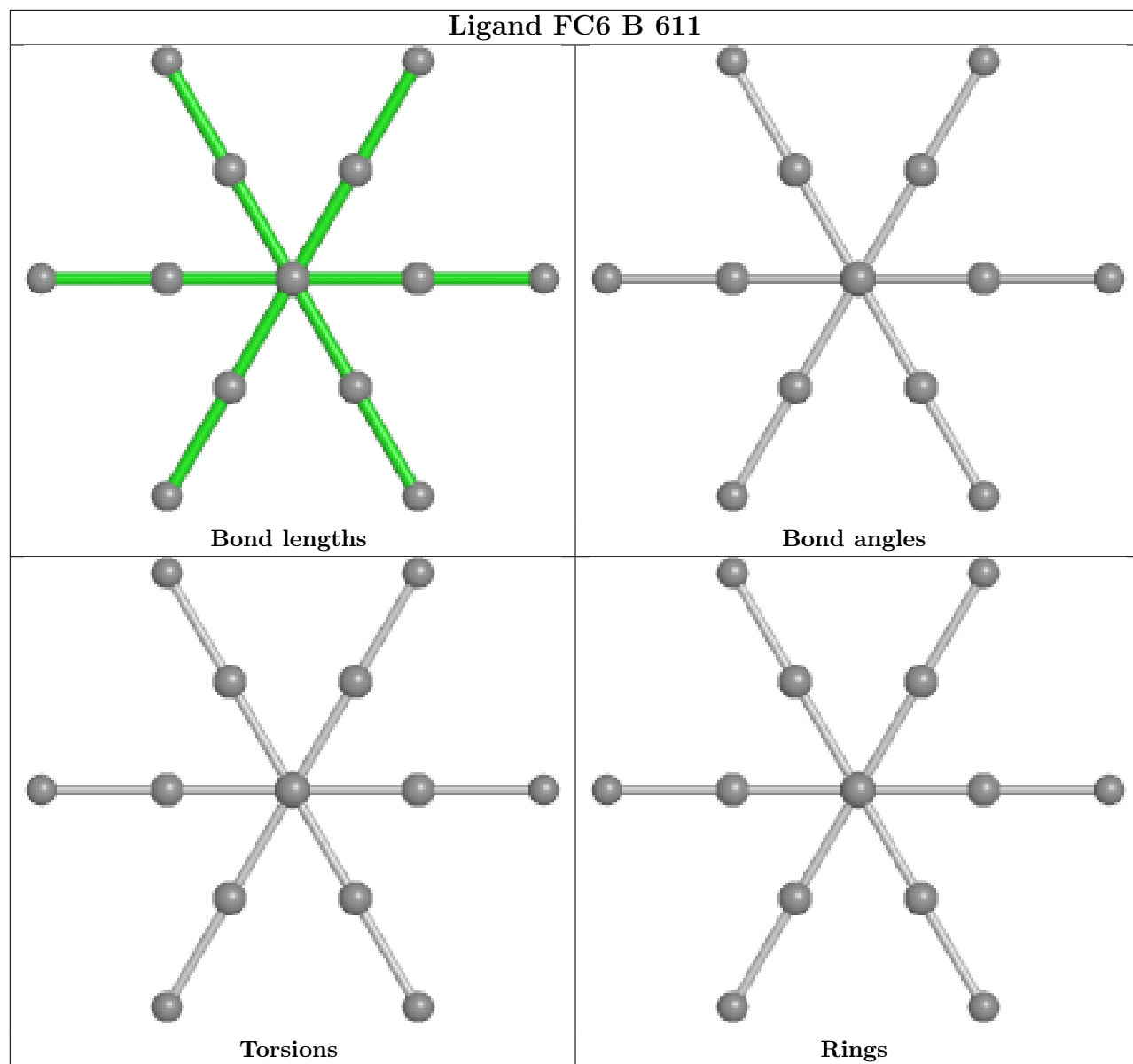
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

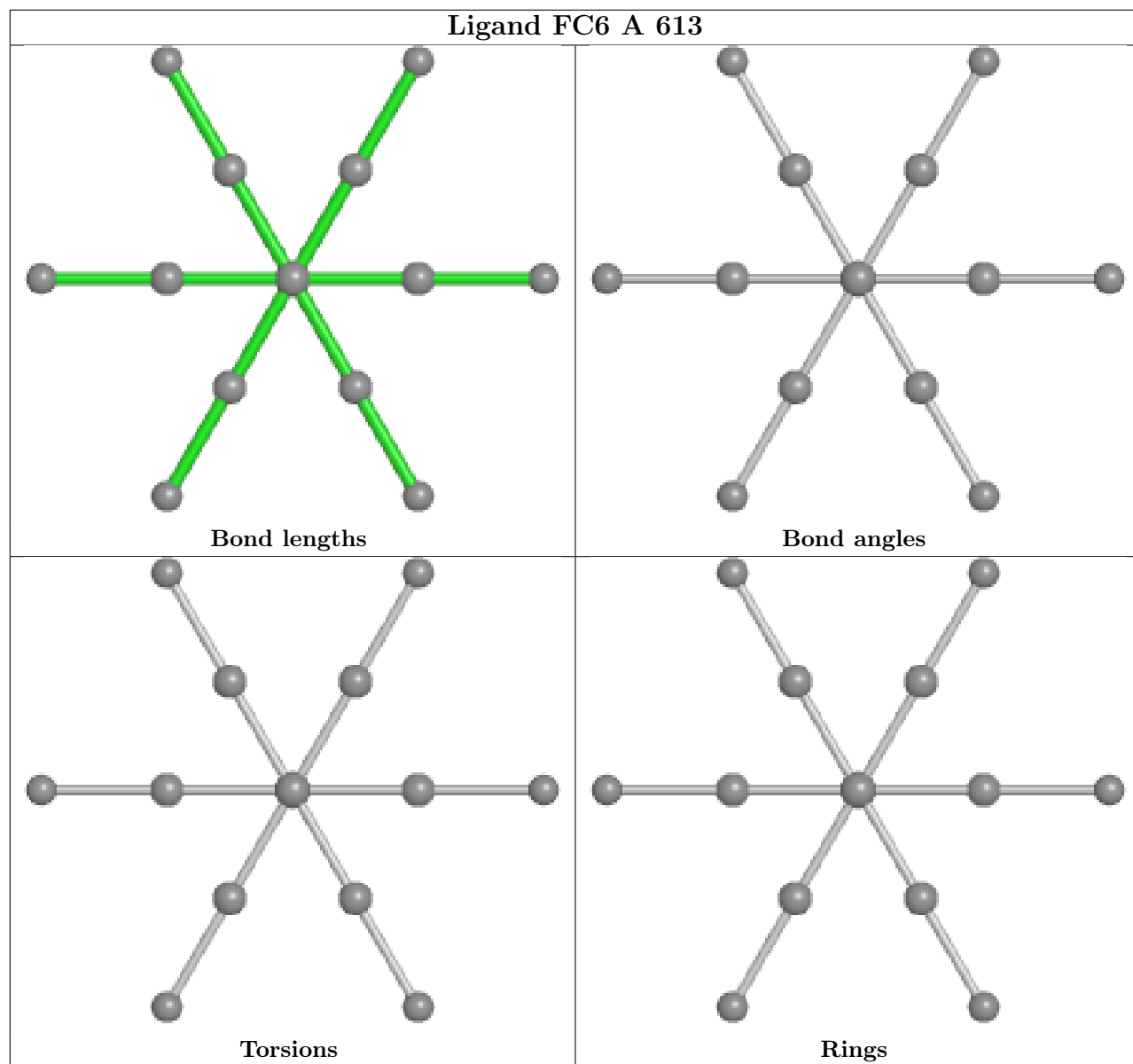


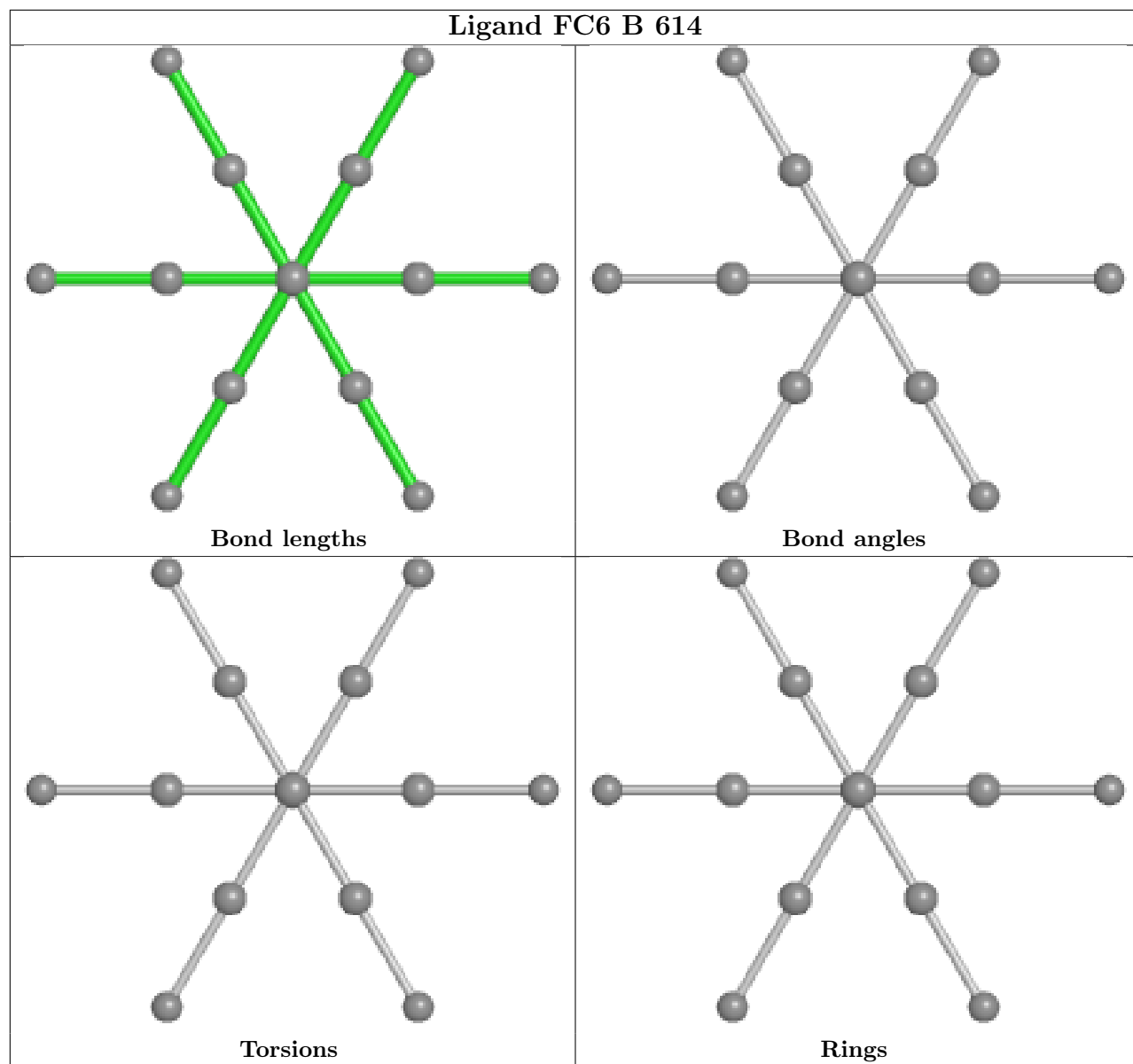


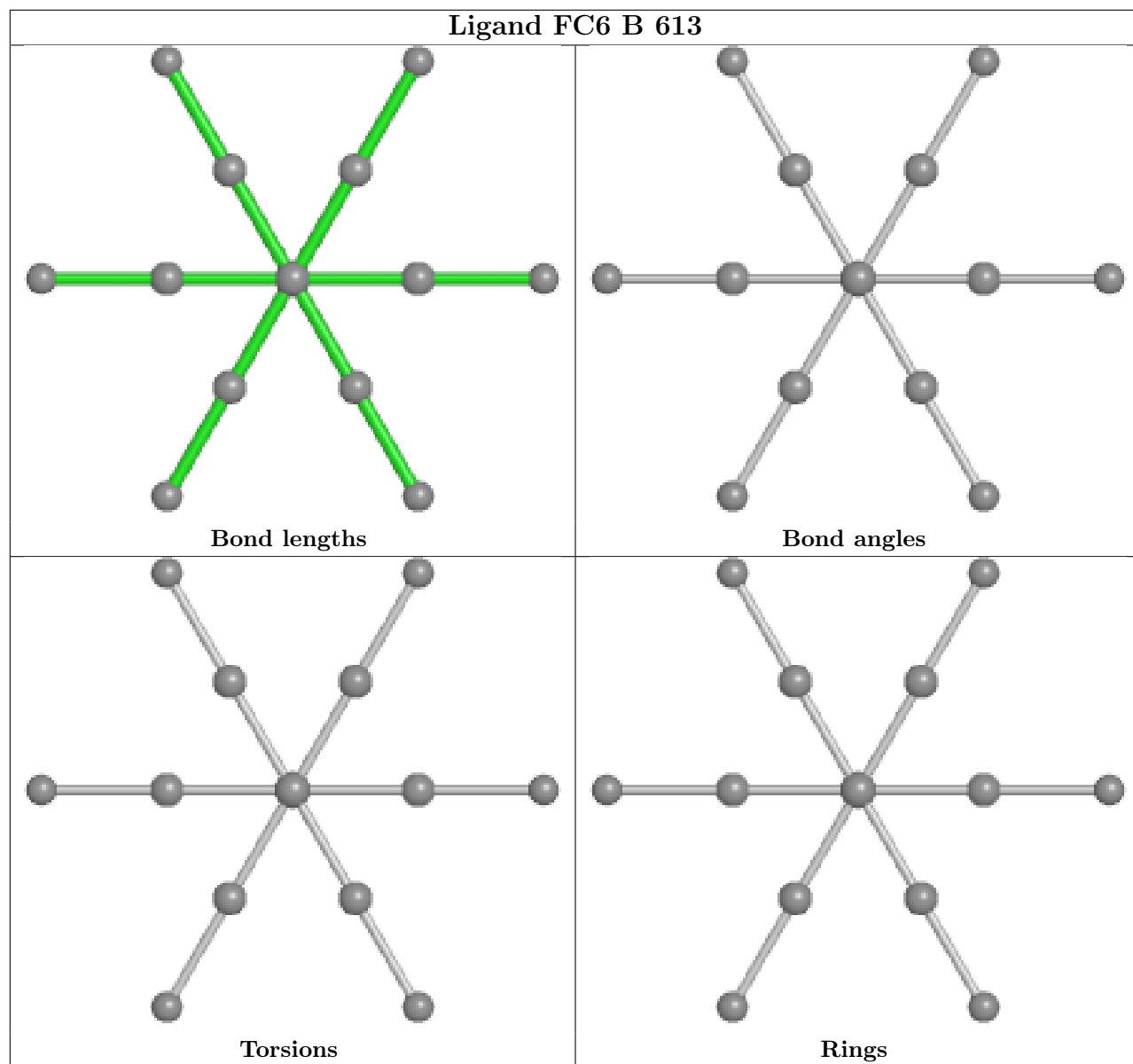


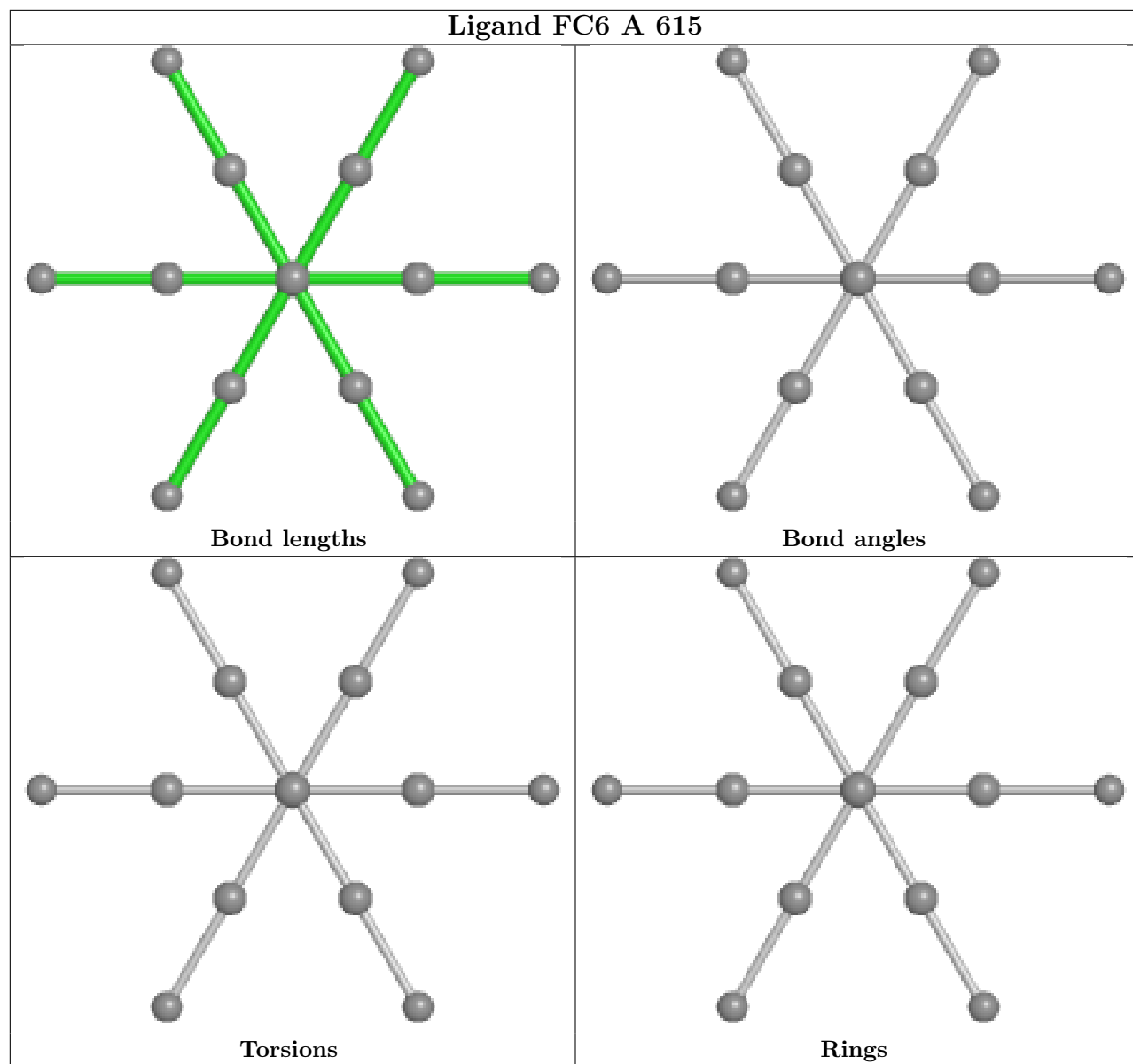


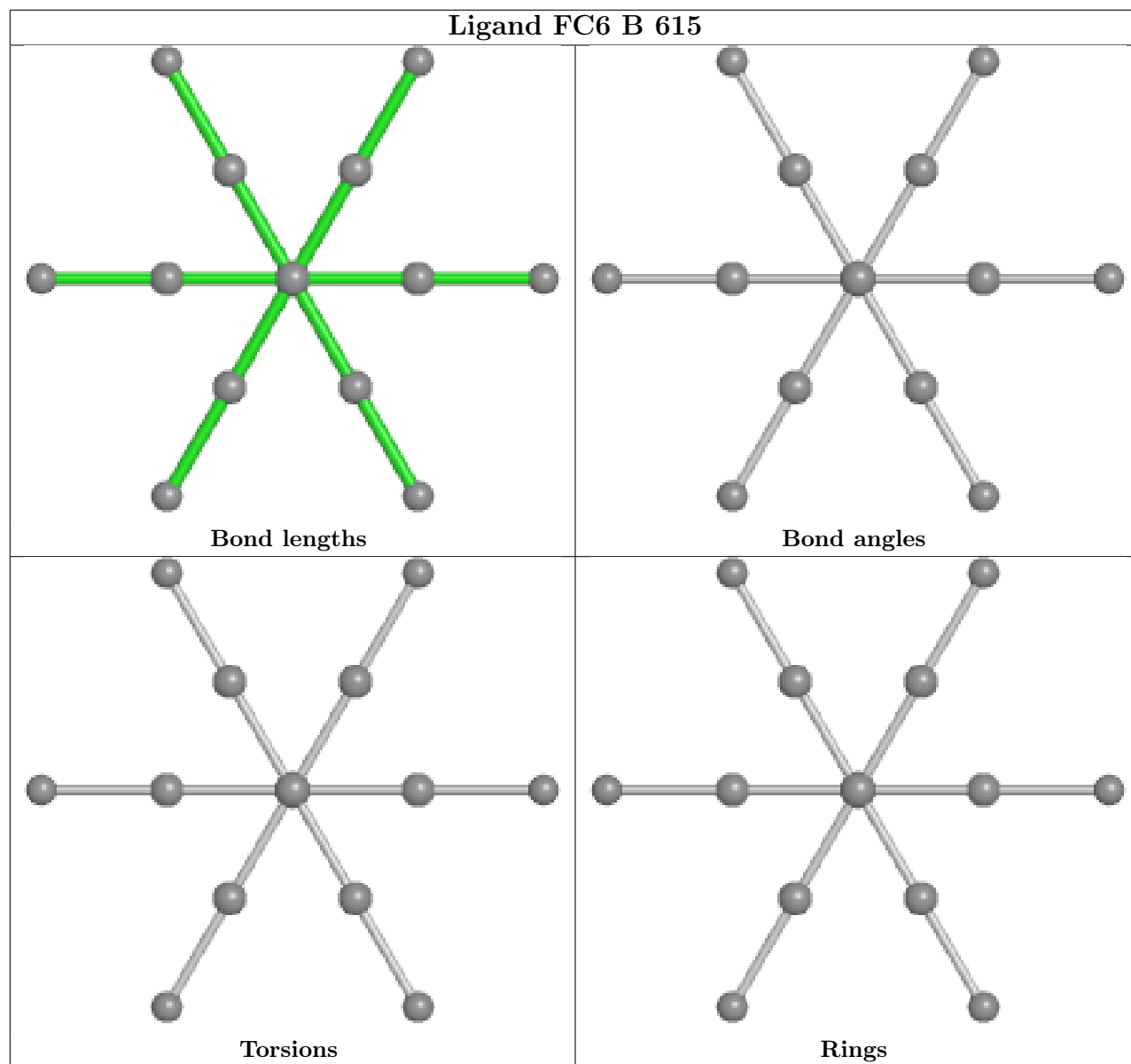












## 5.7 Other polymers [i](#)

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 [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	534/534 (100%)	-0.48	1 (0%) 95 95	18, 30, 48, 71	0
1	B	533/534 (99%)	-0.30	9 (1%) 70 66	24, 38, 65, 114	2 (0%)
All	All	1067/1068 (99%)	-0.39	10 (0%) 84 82	18, 34, 60, 114	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	LEU	4.1
1	A	514	GLN	3.2
1	B	478	ASP	3.2
1	B	35	GLU	2.9
1	B	518[A]	GLU	2.6
1	B	533	ASP	2.5
1	B	506	ALA	2.3
1	B	501	LEU	2.3
1	B	477	PRO	2.2
1	B	517	THR	2.1

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

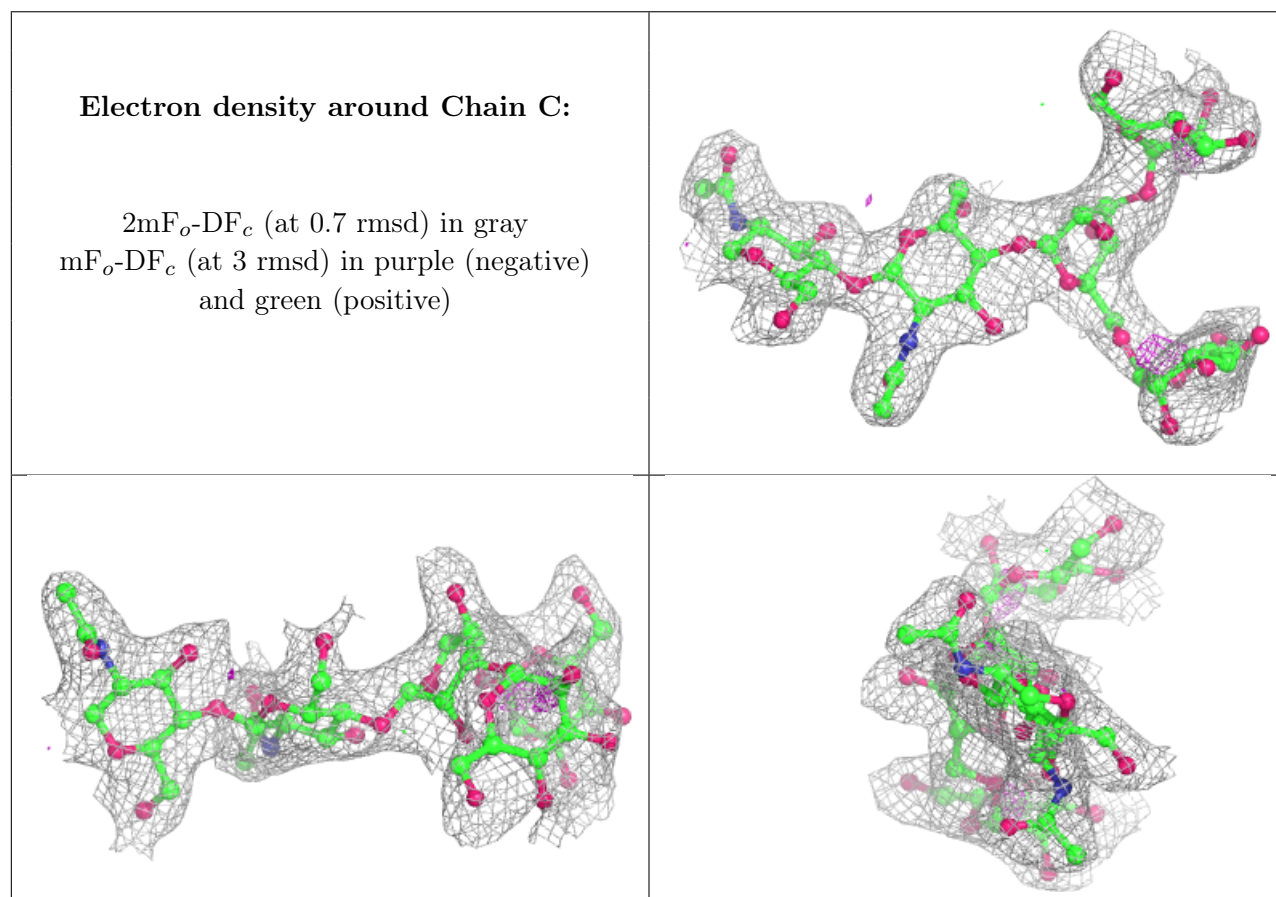
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

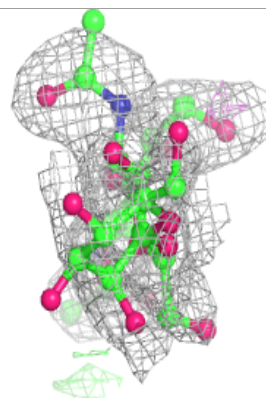
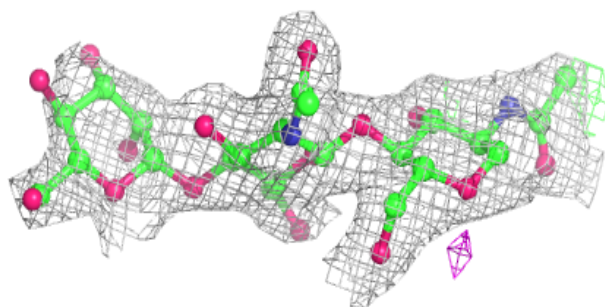
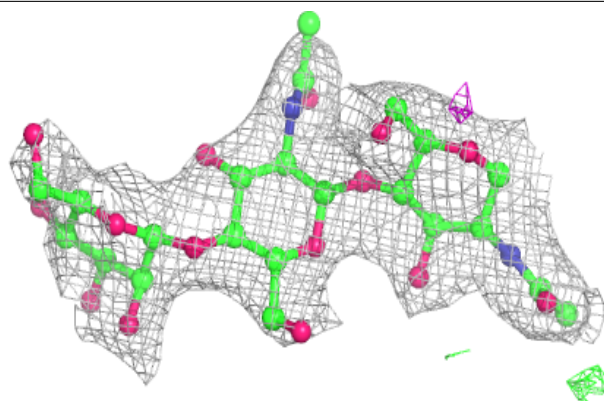
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	C	5	11/12	0.67	0.36	79,96,102,104	0
4	MAN	E	4	11/12	0.72	0.28	88,110,114,115	0
4	BMA	E	3	11/12	0.82	0.25	99,109,116,118	0
2	MAN	C	4	11/12	0.82	0.32	72,82,89,89	0
2	BMA	C	3	11/12	0.83	0.25	75,80,92,106	0
3	BMA	D	3	11/12	0.84	0.36	87,103,111,121	0
5	NAG	F	2	14/15	0.91	0.26	61,78,84,88	0
5	NAG	F	1	14/15	0.93	0.21	59,62,66,71	0
4	NAG	E	2	14/15	0.93	0.19	69,82,102,112	0
2	NAG	C	2	14/15	0.94	0.19	45,63,73,73	0
3	NAG	D	2	14/15	0.96	0.28	46,61,74,86	0
4	NAG	E	1	14/15	0.97	0.09	43,49,56,63	0
2	NAG	C	1	14/15	0.97	0.12	38,41,45,54	0
3	NAG	D	1	14/15	0.97	0.15	37,39,43,46	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.

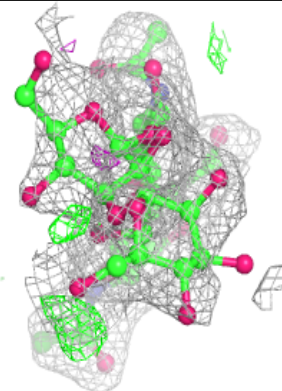
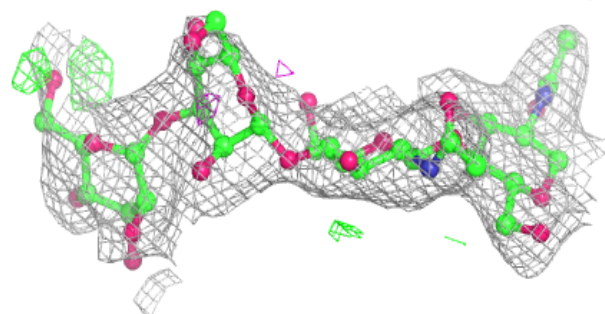
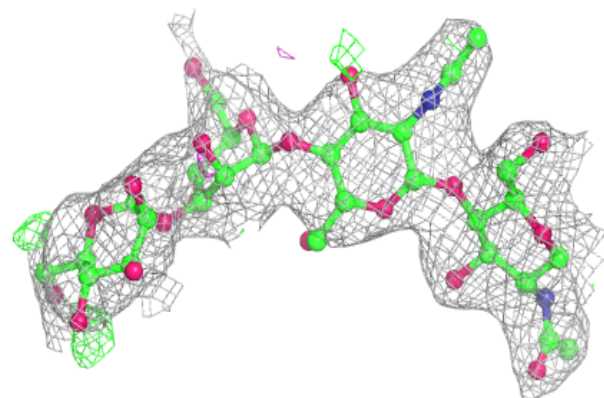


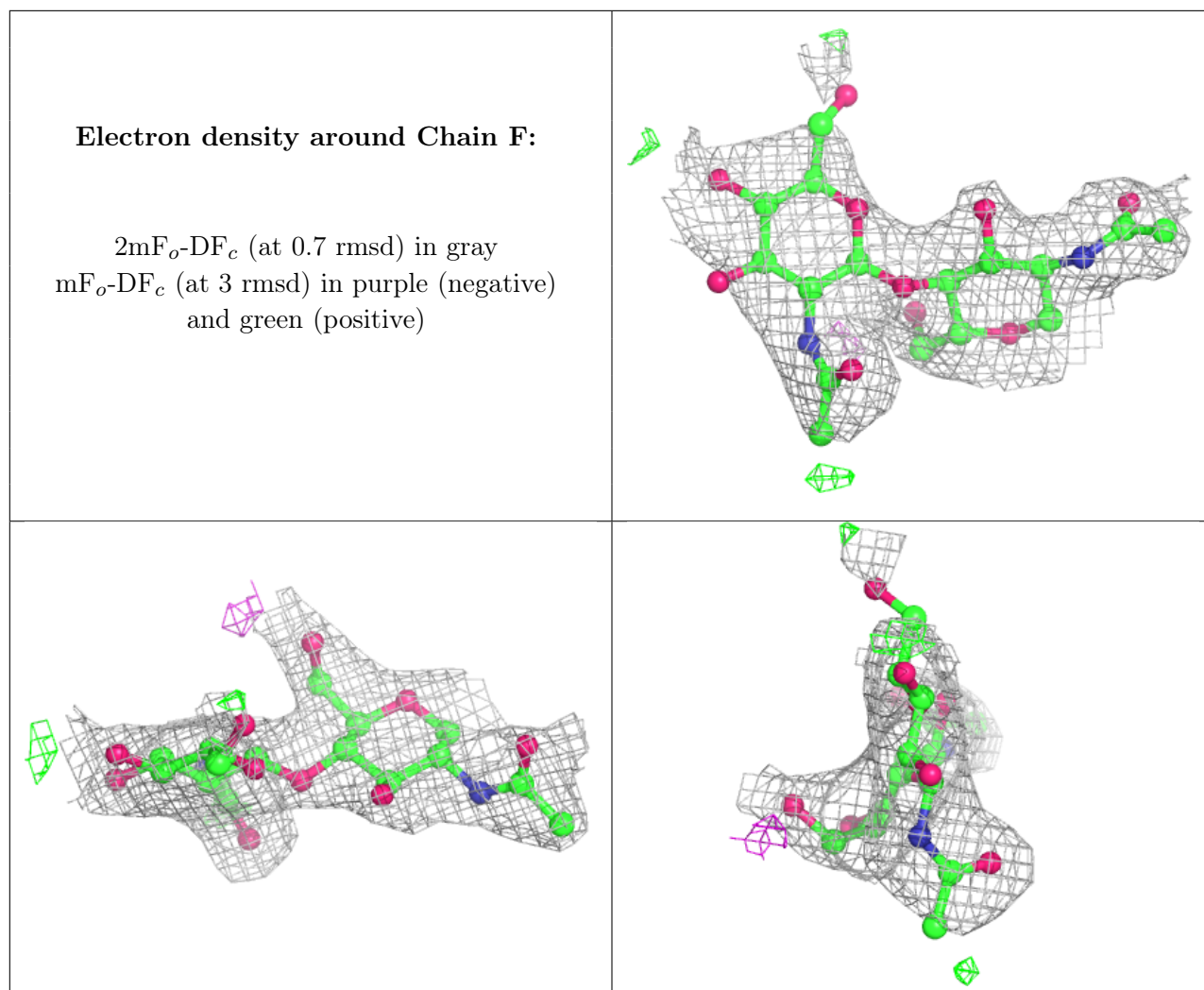
**Electron density around Chain D:**

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

**Electron density around Chain E:**

$2mF_o-DF_c$  (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
8	SIN	A	619	8/8	0.81	0.24	65,76,85,92	0
7	FC6	B	612	13/13	0.87	0.38	75,96,106,113	0
7	FC6	B	613	13/13	0.90	0.28	68,86,91,98	0
10	CL	A	625	1/1	0.90	0.17	63,63,63,63	0
11	PGR	B	621	5/5	0.90	0.20	45,46,53,54	0
8	SIN	B	617	8/8	0.91	0.19	46,54,56,56	0
7	FC6	A	614	13/13	0.93	0.31	48,59,65,66	13
7	FC6	B	611	13/13	0.93	0.24	60,69,81,81	13
7	FC6	B	615	13/13	0.94	0.28	73,87,95,96	0

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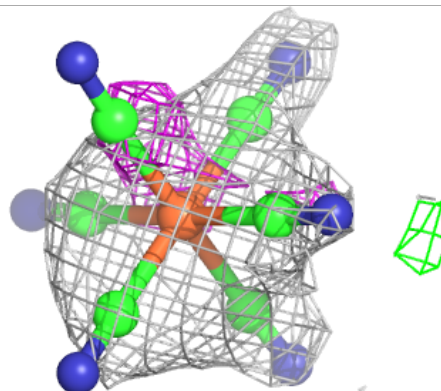
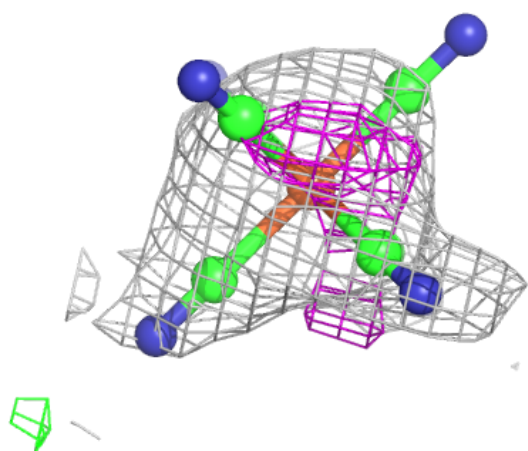
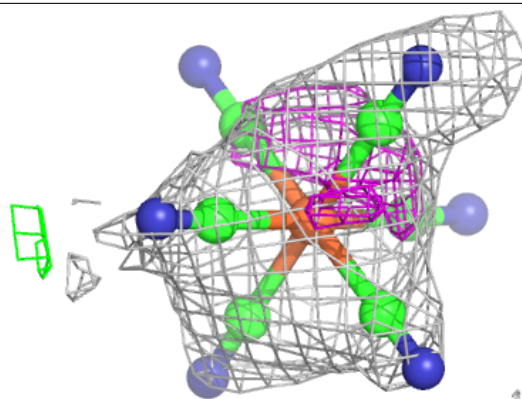
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NA	A	620	1/1	0.94	0.34	54,54,54,54	0
9	NA	A	623	1/1	0.94	0.13	41,41,41,41	0
9	NA	B	618	1/1	0.94	0.57	53,53,53,53	0
9	NA	B	619	1/1	0.94	0.14	43,43,43,43	0
7	FC6	A	616	13/13	0.94	0.22	58,75,86,88	0
8	SIN	B	616	8/8	0.94	0.17	53,64,70,80	0
8	SIN	A	618	8/8	0.95	0.12	32,37,40,41	0
7	FC6	A	615	13/13	0.95	0.19	43,52,55,62	13
9	NA	A	621	1/1	0.95	0.12	36,36,36,36	0
7	FC6	A	613	13/13	0.95	0.18	54,70,80,80	13
9	NA	A	622	1/1	0.96	0.07	40,40,40,40	0
9	NA	B	620	1/1	0.96	0.10	45,45,45,45	0
7	FC6	B	614	13/13	0.97	0.24	47,58,69,74	0
9	NA	A	624	1/1	0.99	0.06	32,32,32,32	0
6	CU	A	601	1/1	0.99	0.06	35,35,35,35	0
8	SIN	A	617	8/8	0.99	0.11	31,32,36,36	0
6	CU	B	601	1/1	1.00	0.05	38,38,38,38	0
6	CU	B	602	1/1	1.00	0.09	35,35,35,35	0
6	CU	B	603	1/1	1.00	0.11	40,40,40,40	0
6	CU	B	604	1/1	1.00	0.09	73,73,73,73	0
6	CU	A	602	1/1	1.00	0.11	30,30,30,30	0
6	CU	A	603	1/1	1.00	0.12	34,34,34,34	0
6	CU	A	604	1/1	1.00	0.07	57,57,57,57	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.

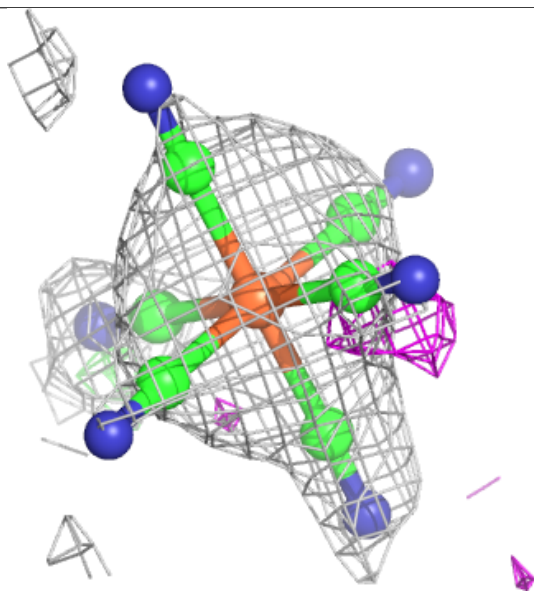
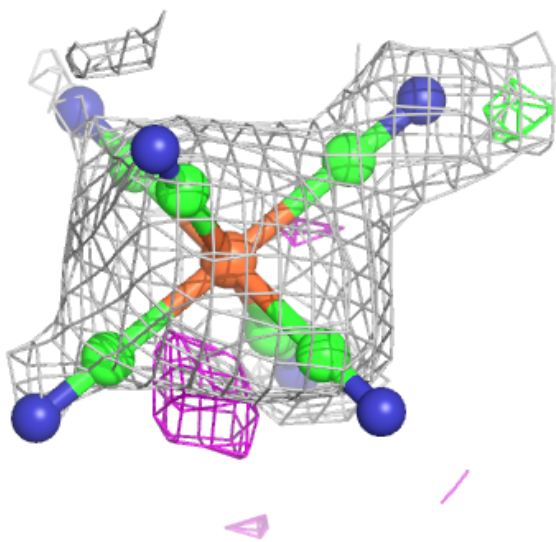
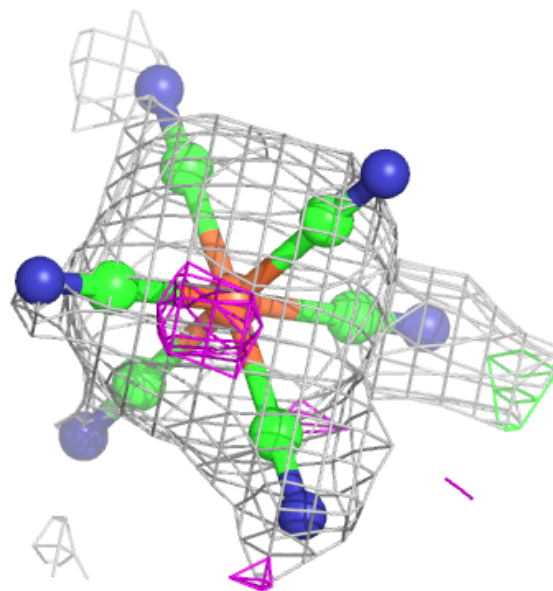
**Electron density around FC6 B 612:**

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



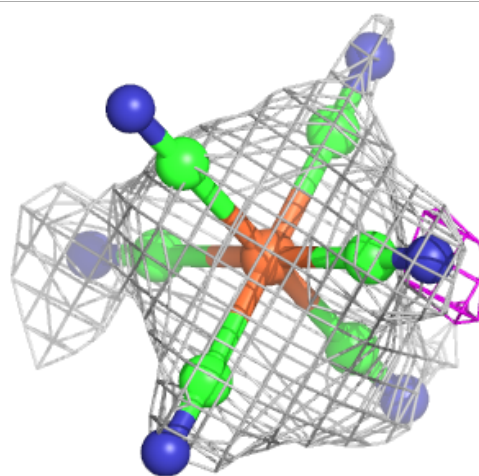
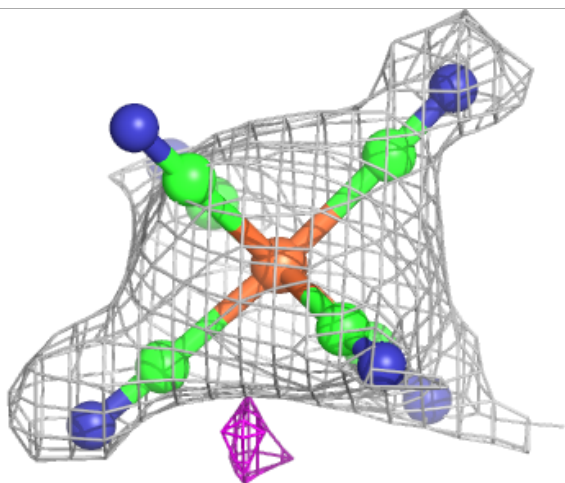
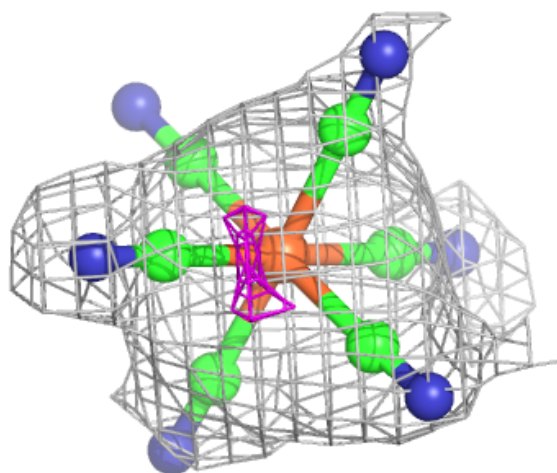
**Electron density around FC6 B 613:**

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



**Electron density around FC6 A 614:**

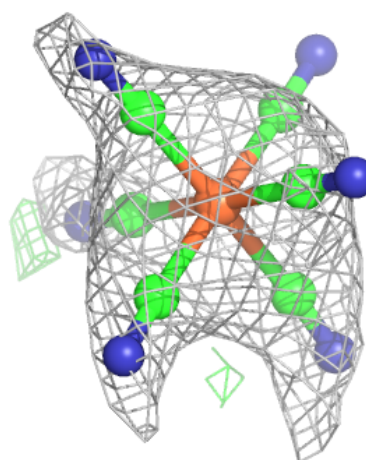
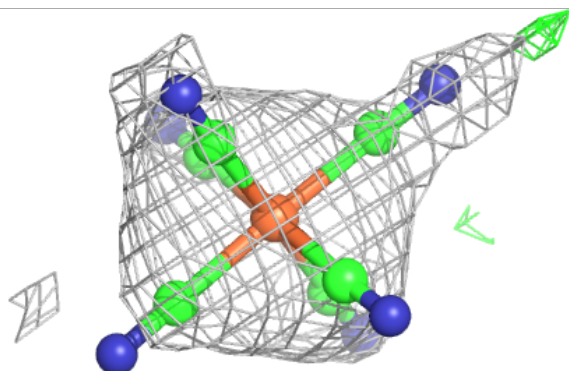
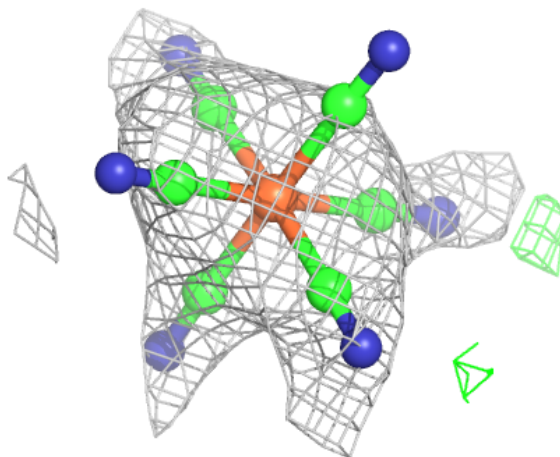
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





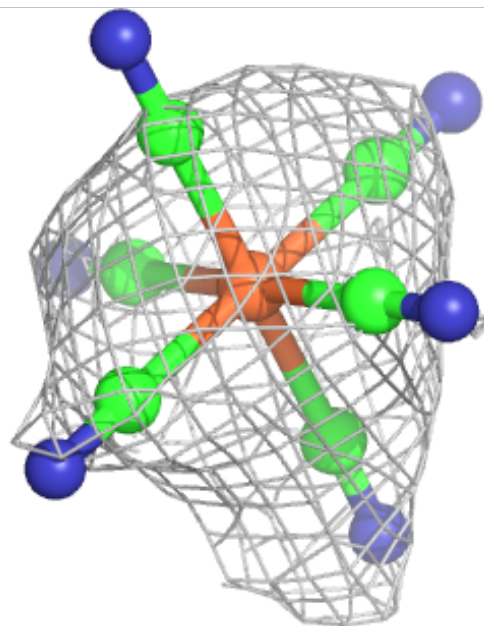
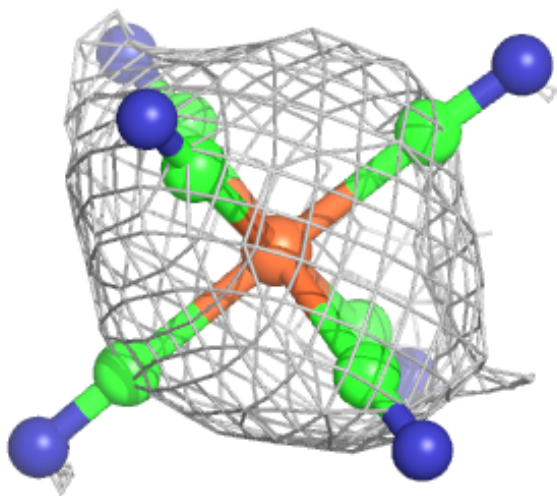
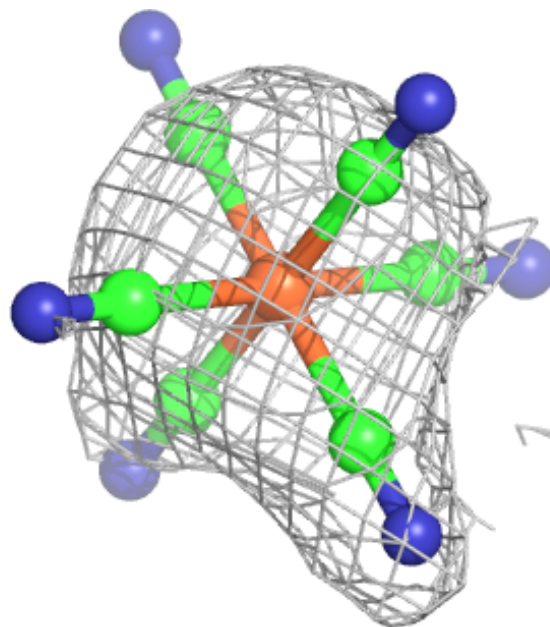
**Electron density around FC6 B 611:**

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



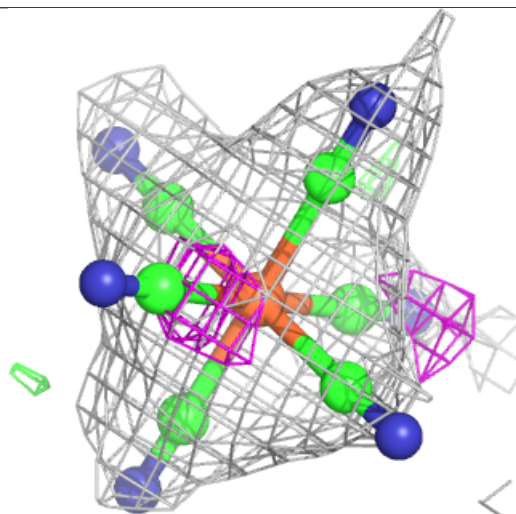
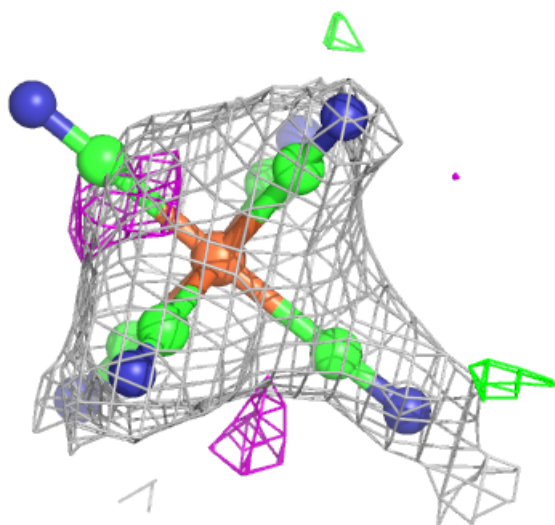
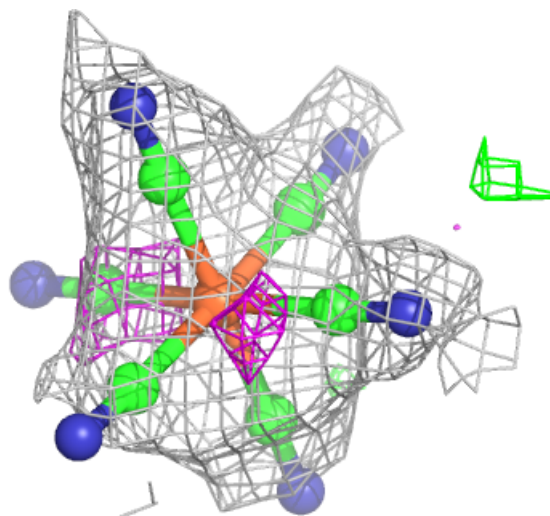
**Electron density around FC6 B 615:**

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



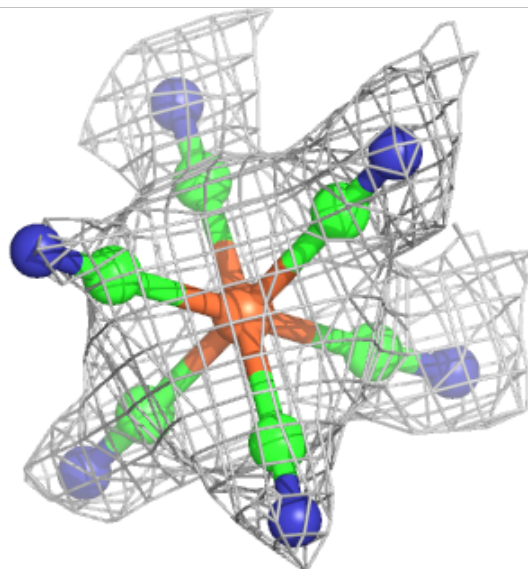
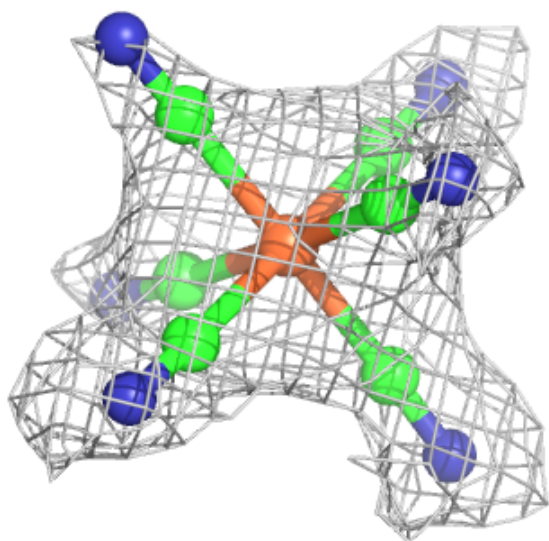
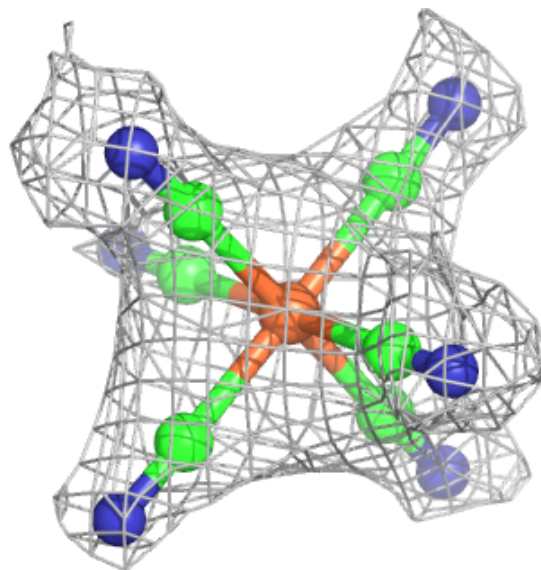
**Electron density around FC6 A 616:**

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



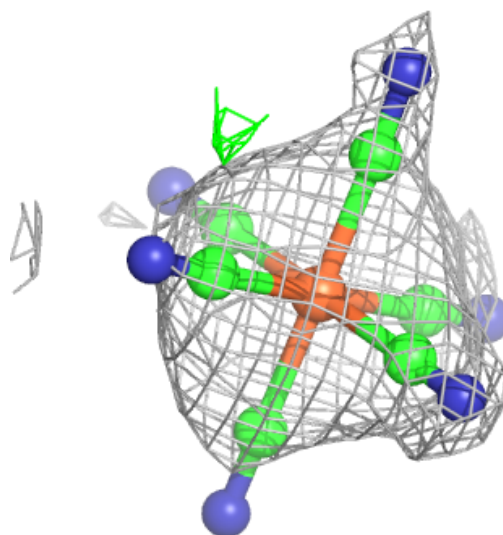
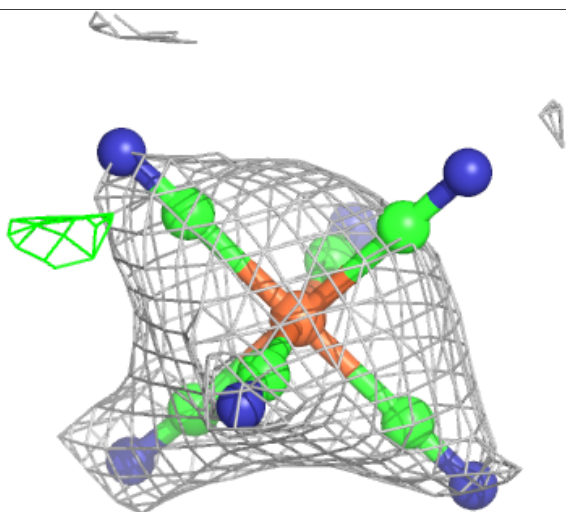
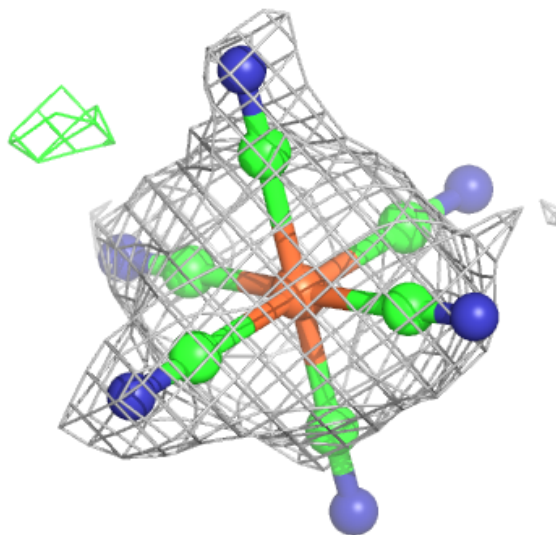
**Electron density around FC6 A 615:**

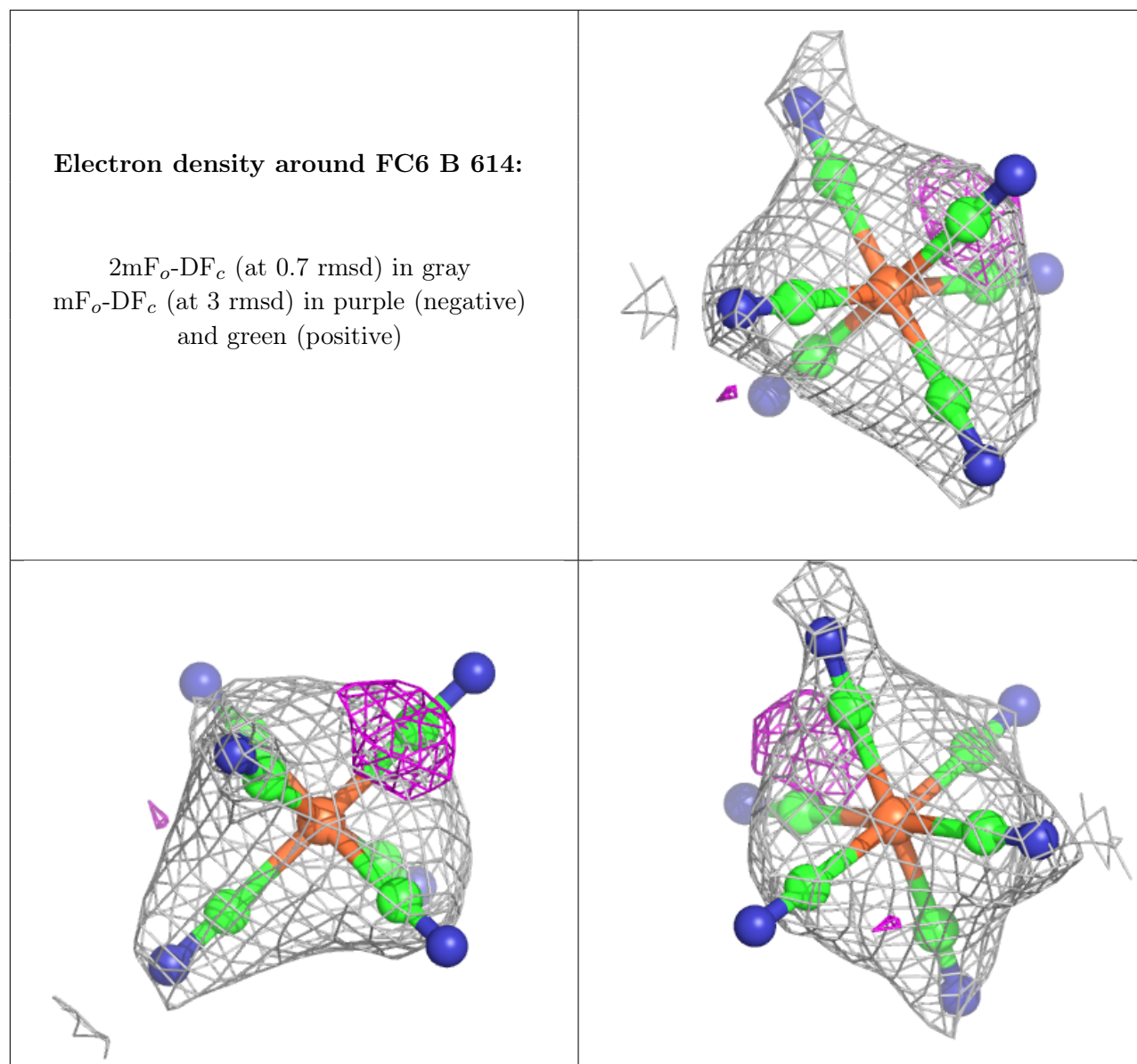
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FC6 A 613:**

$2mF_o-DF_c$  (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.