



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:12 PM UTC

PDB ID : 7W1E / pdb_00007w1e
Title : Crystal structure of Klebsiella pneumoniae K1 capsule-specific polysaccharide lyase in complex with products
Authors : Tu, I.F.; Huang, K.F.; Wu, S.H.
Deposited on : 2021-11-19
Resolution : 1.46 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

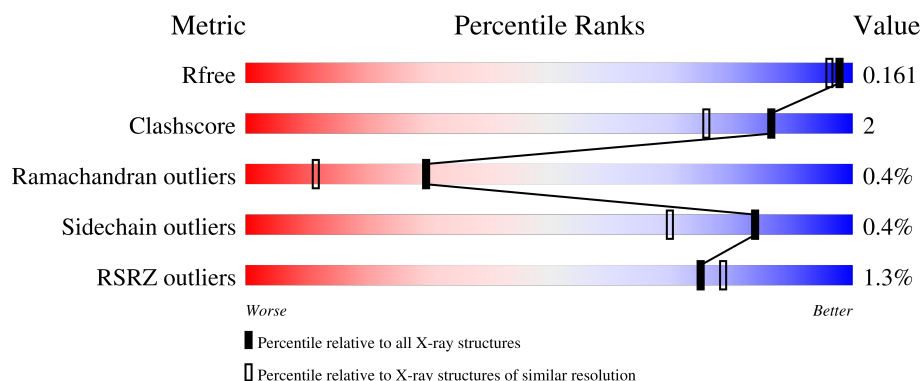
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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.



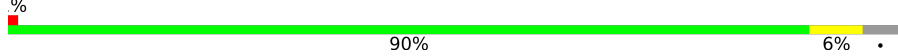
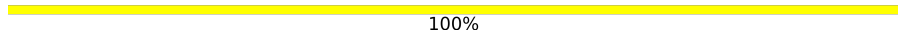
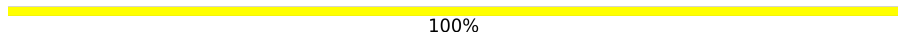
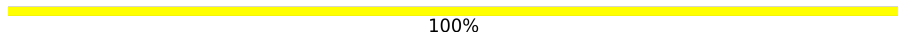
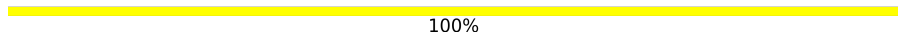
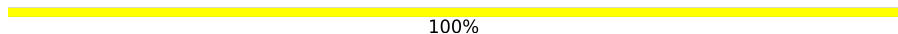
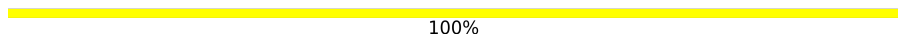
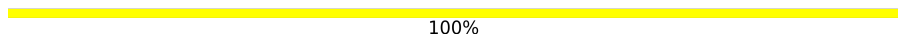
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 ≥ 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	671	91% 5% .
1	B	671	2% 89% 6% 6%
1	C	671	2% 91% . .
1	D	671	% 87% 6% 7%
1	E	671	% 91% 5% .

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Mol	Chain	Length	Quality of chain
1	F	671	
2	G	2	
2	H	2	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	702	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34447 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 K1 LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	4	0
			4880	3070	842	949	19			
1	B	634	Total	C	N	O	S	0	3	0
			4814	3025	832	938	19			
1	C	642	Total	C	N	O	S	0	1	0
			4863	3060	840	944	19			
1	D	622	Total	C	N	O	S	0	2	0
			4704	2957	815	914	18			
1	E	644	Total	C	N	O	S	0	4	0
			4895	3080	845	951	19			
1	F	642	Total	C	N	O	S	0	2	0
			4870	3062	841	948	19			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
A	-18	GLY	-	expression tag	UNP A0A068Q5Q5
A	-17	SER	-	expression tag	UNP A0A068Q5Q5
A	-16	SER	-	expression tag	UNP A0A068Q5Q5
A	-15	HIS	-	expression tag	UNP A0A068Q5Q5
A	-14	HIS	-	expression tag	UNP A0A068Q5Q5
A	-13	HIS	-	expression tag	UNP A0A068Q5Q5
A	-12	HIS	-	expression tag	UNP A0A068Q5Q5
A	-11	HIS	-	expression tag	UNP A0A068Q5Q5
A	-10	HIS	-	expression tag	UNP A0A068Q5Q5
A	-9	SER	-	expression tag	UNP A0A068Q5Q5
A	-8	SER	-	expression tag	UNP A0A068Q5Q5
A	-7	GLY	-	expression tag	UNP A0A068Q5Q5
A	-6	LEU	-	expression tag	UNP A0A068Q5Q5
A	-5	VAL	-	expression tag	UNP A0A068Q5Q5
A	-4	PRO	-	expression tag	UNP A0A068Q5Q5
A	-3	ARG	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A068Q5Q5
A	-1	SER	-	expression tag	UNP A0A068Q5Q5
A	0	HIS	-	expression tag	UNP A0A068Q5Q5
A	213	THR	ALA	conflict	UNP A0A068Q5Q5
A	256	ILE	SER	conflict	UNP A0A068Q5Q5
A	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
A	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
B	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
B	-18	GLY	-	expression tag	UNP A0A068Q5Q5
B	-17	SER	-	expression tag	UNP A0A068Q5Q5
B	-16	SER	-	expression tag	UNP A0A068Q5Q5
B	-15	HIS	-	expression tag	UNP A0A068Q5Q5
B	-14	HIS	-	expression tag	UNP A0A068Q5Q5
B	-13	HIS	-	expression tag	UNP A0A068Q5Q5
B	-12	HIS	-	expression tag	UNP A0A068Q5Q5
B	-11	HIS	-	expression tag	UNP A0A068Q5Q5
B	-10	HIS	-	expression tag	UNP A0A068Q5Q5
B	-9	SER	-	expression tag	UNP A0A068Q5Q5
B	-8	SER	-	expression tag	UNP A0A068Q5Q5
B	-7	GLY	-	expression tag	UNP A0A068Q5Q5
B	-6	LEU	-	expression tag	UNP A0A068Q5Q5
B	-5	VAL	-	expression tag	UNP A0A068Q5Q5
B	-4	PRO	-	expression tag	UNP A0A068Q5Q5
B	-3	ARG	-	expression tag	UNP A0A068Q5Q5
B	-2	GLY	-	expression tag	UNP A0A068Q5Q5
B	-1	SER	-	expression tag	UNP A0A068Q5Q5
B	0	HIS	-	expression tag	UNP A0A068Q5Q5
B	213	THR	ALA	conflict	UNP A0A068Q5Q5
B	256	ILE	SER	conflict	UNP A0A068Q5Q5
B	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
B	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
C	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
C	-18	GLY	-	expression tag	UNP A0A068Q5Q5
C	-17	SER	-	expression tag	UNP A0A068Q5Q5
C	-16	SER	-	expression tag	UNP A0A068Q5Q5
C	-15	HIS	-	expression tag	UNP A0A068Q5Q5
C	-14	HIS	-	expression tag	UNP A0A068Q5Q5
C	-13	HIS	-	expression tag	UNP A0A068Q5Q5
C	-12	HIS	-	expression tag	UNP A0A068Q5Q5
C	-11	HIS	-	expression tag	UNP A0A068Q5Q5
C	-10	HIS	-	expression tag	UNP A0A068Q5Q5
C	-9	SER	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP A0A068Q5Q5
C	-7	GLY	-	expression tag	UNP A0A068Q5Q5
C	-6	LEU	-	expression tag	UNP A0A068Q5Q5
C	-5	VAL	-	expression tag	UNP A0A068Q5Q5
C	-4	PRO	-	expression tag	UNP A0A068Q5Q5
C	-3	ARG	-	expression tag	UNP A0A068Q5Q5
C	-2	GLY	-	expression tag	UNP A0A068Q5Q5
C	-1	SER	-	expression tag	UNP A0A068Q5Q5
C	0	HIS	-	expression tag	UNP A0A068Q5Q5
C	213	THR	ALA	conflict	UNP A0A068Q5Q5
C	256	ILE	SER	conflict	UNP A0A068Q5Q5
C	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
C	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
D	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
D	-18	GLY	-	expression tag	UNP A0A068Q5Q5
D	-17	SER	-	expression tag	UNP A0A068Q5Q5
D	-16	SER	-	expression tag	UNP A0A068Q5Q5
D	-15	HIS	-	expression tag	UNP A0A068Q5Q5
D	-14	HIS	-	expression tag	UNP A0A068Q5Q5
D	-13	HIS	-	expression tag	UNP A0A068Q5Q5
D	-12	HIS	-	expression tag	UNP A0A068Q5Q5
D	-11	HIS	-	expression tag	UNP A0A068Q5Q5
D	-10	HIS	-	expression tag	UNP A0A068Q5Q5
D	-9	SER	-	expression tag	UNP A0A068Q5Q5
D	-8	SER	-	expression tag	UNP A0A068Q5Q5
D	-7	GLY	-	expression tag	UNP A0A068Q5Q5
D	-6	LEU	-	expression tag	UNP A0A068Q5Q5
D	-5	VAL	-	expression tag	UNP A0A068Q5Q5
D	-4	PRO	-	expression tag	UNP A0A068Q5Q5
D	-3	ARG	-	expression tag	UNP A0A068Q5Q5
D	-2	GLY	-	expression tag	UNP A0A068Q5Q5
D	-1	SER	-	expression tag	UNP A0A068Q5Q5
D	0	HIS	-	expression tag	UNP A0A068Q5Q5
D	213	THR	ALA	conflict	UNP A0A068Q5Q5
D	256	ILE	SER	conflict	UNP A0A068Q5Q5
D	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
D	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
E	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
E	-18	GLY	-	expression tag	UNP A0A068Q5Q5
E	-17	SER	-	expression tag	UNP A0A068Q5Q5
E	-16	SER	-	expression tag	UNP A0A068Q5Q5
E	-15	HIS	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP A0A068Q5Q5
E	-13	HIS	-	expression tag	UNP A0A068Q5Q5
E	-12	HIS	-	expression tag	UNP A0A068Q5Q5
E	-11	HIS	-	expression tag	UNP A0A068Q5Q5
E	-10	HIS	-	expression tag	UNP A0A068Q5Q5
E	-9	SER	-	expression tag	UNP A0A068Q5Q5
E	-8	SER	-	expression tag	UNP A0A068Q5Q5
E	-7	GLY	-	expression tag	UNP A0A068Q5Q5
E	-6	LEU	-	expression tag	UNP A0A068Q5Q5
E	-5	VAL	-	expression tag	UNP A0A068Q5Q5
E	-4	PRO	-	expression tag	UNP A0A068Q5Q5
E	-3	ARG	-	expression tag	UNP A0A068Q5Q5
E	-2	GLY	-	expression tag	UNP A0A068Q5Q5
E	-1	SER	-	expression tag	UNP A0A068Q5Q5
E	0	HIS	-	expression tag	UNP A0A068Q5Q5
E	213	THR	ALA	conflict	UNP A0A068Q5Q5
E	256	ILE	SER	conflict	UNP A0A068Q5Q5
E	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
E	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
F	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
F	-18	GLY	-	expression tag	UNP A0A068Q5Q5
F	-17	SER	-	expression tag	UNP A0A068Q5Q5
F	-16	SER	-	expression tag	UNP A0A068Q5Q5
F	-15	HIS	-	expression tag	UNP A0A068Q5Q5
F	-14	HIS	-	expression tag	UNP A0A068Q5Q5
F	-13	HIS	-	expression tag	UNP A0A068Q5Q5
F	-12	HIS	-	expression tag	UNP A0A068Q5Q5
F	-11	HIS	-	expression tag	UNP A0A068Q5Q5
F	-10	HIS	-	expression tag	UNP A0A068Q5Q5
F	-9	SER	-	expression tag	UNP A0A068Q5Q5
F	-8	SER	-	expression tag	UNP A0A068Q5Q5
F	-7	GLY	-	expression tag	UNP A0A068Q5Q5
F	-6	LEU	-	expression tag	UNP A0A068Q5Q5
F	-5	VAL	-	expression tag	UNP A0A068Q5Q5
F	-4	PRO	-	expression tag	UNP A0A068Q5Q5
F	-3	ARG	-	expression tag	UNP A0A068Q5Q5
F	-2	GLY	-	expression tag	UNP A0A068Q5Q5
F	-1	SER	-	expression tag	UNP A0A068Q5Q5
F	0	HIS	-	expression tag	UNP A0A068Q5Q5
F	213	THR	ALA	conflict	UNP A0A068Q5Q5
F	256	ILE	SER	conflict	UNP A0A068Q5Q5
F	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

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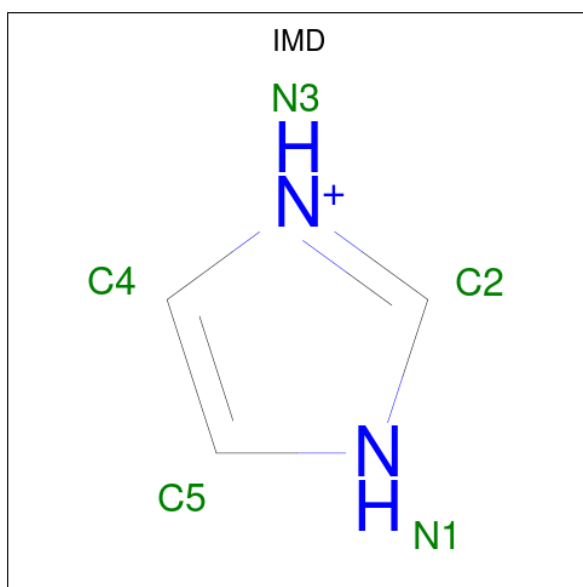
Chain	Residue	Modelled	Actual	Comment	Reference
F	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

- Molecule 2 is an oligosaccharide called 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			25	14	11			
2	H	2	Total	C	O	0	0	0
			25	14	11			
2	I	2	Total	C	O	0	0	0
			25	14	11			
2	J	2	Total	C	O	0	0	0
			25	14	11			
2	K	2	Total	C	O	0	0	0
			25	14	11			
2	L	2	Total	C	O	0	0	0
			25	14	11			
2	M	2	Total	C	O	0	0	0
			25	14	11			
2	N	2	Total	C	O	0	0	0
			25	14	11			
2	O	2	Total	C	O	0	0	0
			25	14	11			
2	P	2	Total	C	O	0	0	0
			25	14	11			

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂) (labeled as "Ligand of Interest" by depositor).



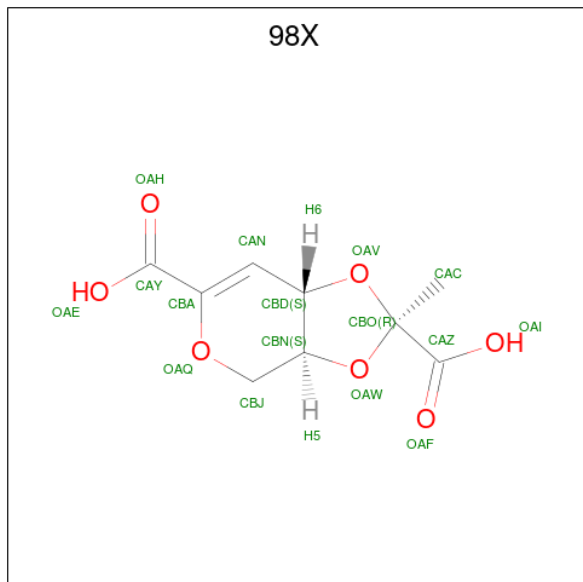
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		
3	E	1	Total	C	N	0	0
			5	3	2		
3	E	1	Total	C	N	0	0
			5	3	2		
3	F	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2,6-anhydro-4,5-O-[(1R)-1-carboxyethylidene]-3-deoxy-L-threo-hex-2-enonic acid (CCD ID: 98X) (formula: C₉H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	9	7		
5	A	1	Total	C	O	0	0
			16	9	7		
5	A	1	Total	C	O	0	0
			16	9	7		
5	B	1	Total	C	O	0	0
			16	9	7		
5	C	1	Total	C	O	0	0
			16	9	7		
5	D	1	Total	C	O	0	0
			16	9	7		
5	D	1	Total	C	O	0	0
			16	9	7		
5	E	1	Total	C	O	0	0
			16	9	7		
5	E	1	Total	C	O	0	0
			16	9	7		
5	F	1	Total	C	O	0	0
			16	9	7		

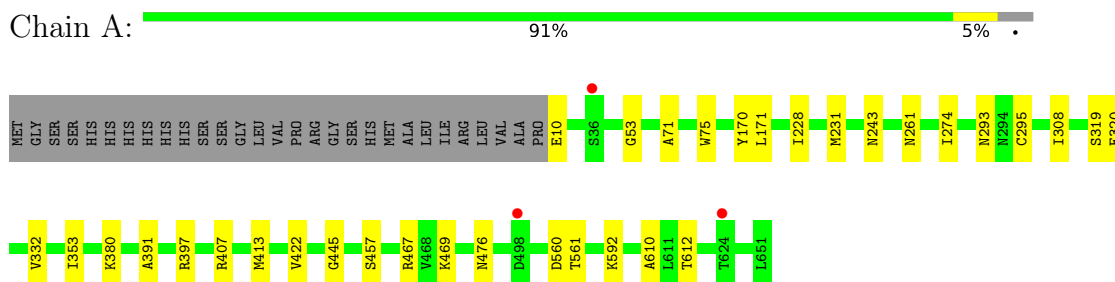
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	878	Total 878	O 878	0	0
6	B	786	Total 786	O 786	0	0
6	C	717	Total 717	O 717	0	0
6	D	863	Total 863	O 863	0	0
6	E	835	Total 835	O 835	0	0
6	F	808	Total 808	O 808	0	0

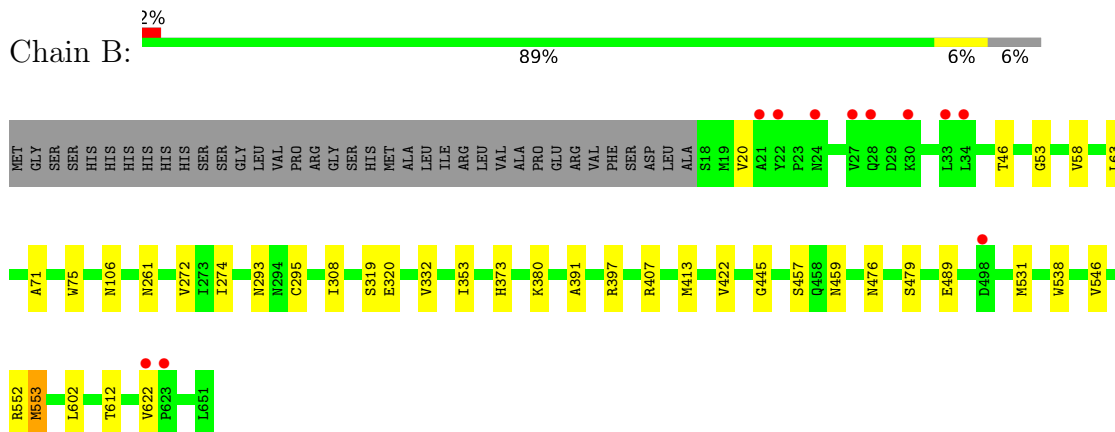
3 Residue-property plots [i](#)

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.

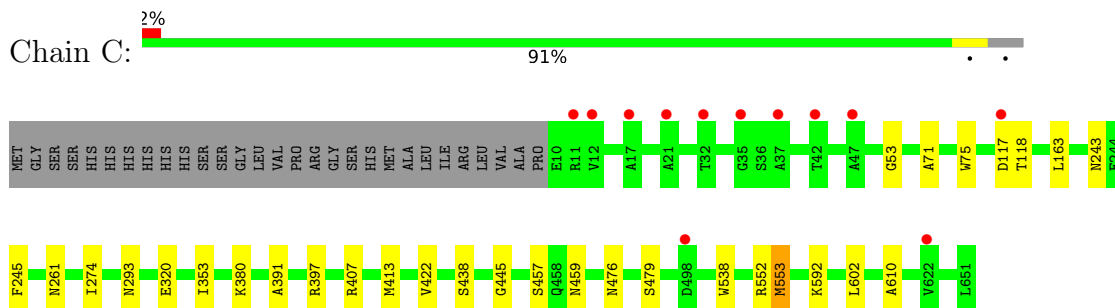
- Molecule 1: K1 LYASE



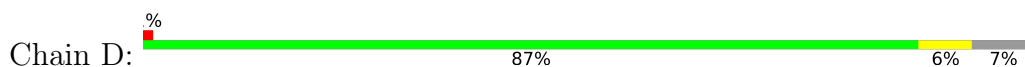
- Molecule 1: K1 LYASE

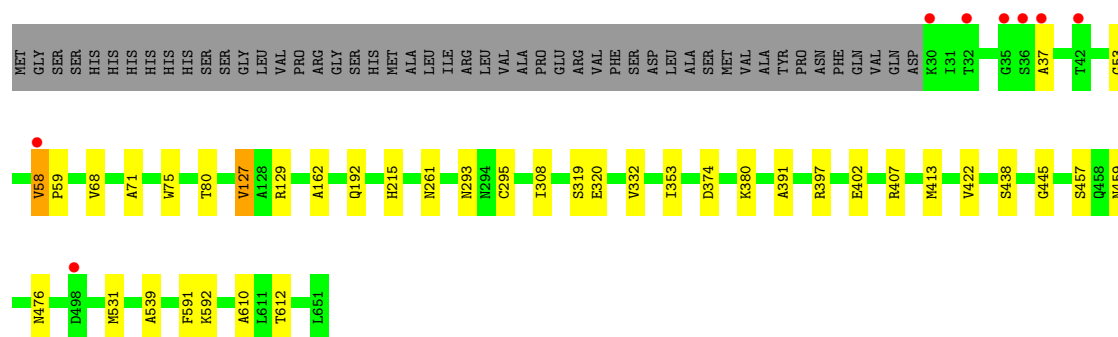


- Molecule 1: K1 LYASE

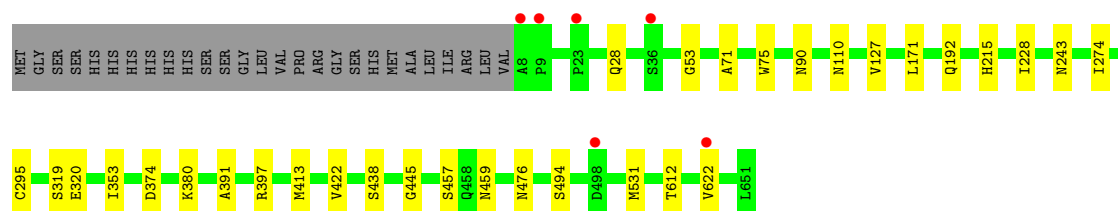


- Molecule 1: K1 LYASE

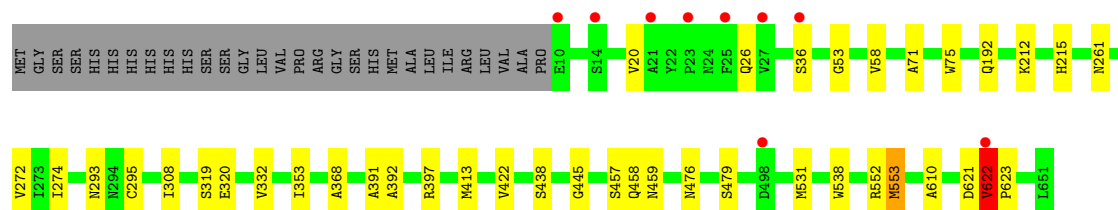




• Molecule 1: K1 LYASE



• Molecule 1: K1 LYASE



• Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose



• Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose



• Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose



BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain J:  100%BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain K:  50%  50%BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain L:  100%BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain M:  100%BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain N:  100%BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain O:  100%BGC1
9802

- Molecule 2: 3-O-acetyl-6-deoxy-alpha-L-galactopyranose-(1-3)-beta-D-glucopyranose

Chain P:  100%BGC1
9802

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.63Å 100.99Å 125.38Å 80.40° 70.48° 83.99°	Depositor
Resolution (Å)	30.00 – 1.46 30.00 – 1.46	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-1.46) 94.2 (30.00-1.46)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.114 , 0.148 (Not available) , 0.161	Depositor DCC
R_{free} test set	33731 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	34447	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: IMD, BGC, GOL, 98U, 98X

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	0.55	0/4993	0.75	0/6797
1	B	0.58	0/4917	0.76	2/6694 (0.0%)
1	C	0.55	0/4970	0.77	2/6766 (0.0%)
1	D	0.57	0/4810	0.77	2/6548 (0.0%)
1	E	0.54	0/5003	0.76	1/6812 (0.0%)
1	F	0.56	0/4977	0.79	5/6775 (0.1%)
All	All	0.56	0/29670	0.77	12/40392 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	553	MET	CG-SD-CE	-8.84	81.45	100.90
1	C	553	MET	CG-SD-CE	-8.84	81.45	100.90
1	B	553	MET	CG-SD-CE	-7.90	83.51	100.90
1	E	531	MET	CG-SD-CE	-7.72	83.92	100.90
1	F	622	VAL	CA-C-N	-7.63	110.30	119.84

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	4880	0	4739	23	0
1	B	4814	0	4663	20	0
1	C	4863	0	4723	20	0
1	D	4704	0	4573	22	0
1	E	4895	0	4753	17	0
1	F	4870	0	4722	22	0
2	G	25	0	11	1	0
2	H	25	0	11	0	0
2	I	25	0	11	1	0
2	J	25	0	11	0	0
2	K	25	0	10	2	0
2	L	25	0	11	0	0
2	M	25	0	11	0	0
2	N	25	0	11	0	0
2	O	25	0	11	0	0
2	P	25	0	10	0	0
3	A	10	0	10	0	0
3	B	5	0	5	1	0
3	C	5	0	5	0	0
3	D	5	0	5	0	0
3	E	10	0	10	1	0
3	F	5	0	5	1	0
4	A	18	0	24	4	0
4	B	12	0	16	1	0
4	C	12	0	16	2	0
4	D	12	0	16	4	0
4	E	12	0	16	0	0
4	F	18	0	24	0	0
5	A	48	0	0	0	0
5	B	16	0	0	0	0
5	C	16	0	0	0	0
5	D	32	0	0	0	0
5	E	32	0	0	0	0
5	F	16	0	0	0	0
6	A	878	0	0	3	0
6	B	786	0	0	2	0
6	C	717	0	0	5	0
6	D	863	0	0	3	0
6	E	835	0	0	3	0
6	F	808	0	0	3	0
All	All	34447	0	28433	124	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.

The worst 5 of 124 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)
6:C:1234:HOH:O	2:I:1:BGC:O6	1.95	0.84
1:D:539:ALA:HB3	4:D:703:GOL:H2	1.68	0.73
1:E:192:GLN:HE22	1:E:215:HIS:H	1.38	0.70
1:D:192:GLN:HE22	1:D:215:HIS:H	1.39	0.69
1:A:397:ARG:HH12	4:A:702:GOL:C3	2.06	0.68

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	644/671 (96%)	622 (97%)	20 (3%)	2 (0%)	36	16
1	B	635/671 (95%)	609 (96%)	24 (4%)	2 (0%)	36	16
1	C	641/671 (96%)	618 (96%)	21 (3%)	2 (0%)	36	16
1	D	622/671 (93%)	596 (96%)	23 (4%)	3 (0%)	24	7
1	E	646/671 (96%)	624 (97%)	20 (3%)	2 (0%)	36	16
1	F	642/671 (96%)	620 (97%)	19 (3%)	3 (0%)	24	7
All	All	3830/4026 (95%)	3689 (96%)	127 (3%)	14 (0%)	30	11

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	622	VAL
1	A	53	GLY
1	B	53	GLY
1	C	53	GLY
1	D	53	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	524/544 (96%)	523 (100%)	1 (0%)	87	76
1	B	516/544 (95%)	512 (99%)	4 (1%)	73	50
1	C	521/544 (96%)	520 (100%)	1 (0%)	87	76
1	D	504/544 (93%)	501 (99%)	3 (1%)	78	58
1	E	525/544 (96%)	522 (99%)	3 (1%)	78	58
1	F	522/544 (96%)	521 (100%)	1 (0%)	87	76
All	All	3112/3264 (95%)	3099 (100%)	13 (0%)	84	70

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	127	VAL
1	D	592	LYS
1	F	26	GLN
1	E	127	VAL
1	E	622	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	28	GLN
1	F	24	ASN
1	E	100	GLN
1	E	261	ASN
1	F	192	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

20 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	BGC	G	1	2	12,12,12	0.84	0	17,17,17	1.33	2 (11%)
2	98U	G	2	5,2	13,13,14	1.84	2 (15%)	17,18,20	1.81	2 (11%)
2	BGC	H	1	2	12,12,12	1.28	3 (25%)	17,17,17	1.31	2 (11%)
2	98U	H	2	5,2	13,13,14	1.65	3 (23%)	17,18,20	1.69	2 (11%)
2	BGC	I	1	2	12,12,12	1.07	1 (8%)	17,17,17	1.98	3 (17%)
2	98U	I	2	5,2	13,13,14	1.24	2 (15%)	17,18,20	1.44	2 (11%)
2	BGC	J	1	2	12,12,12	1.03	1 (8%)	17,17,17	1.44	4 (23%)
2	98U	J	2	5,2	13,13,14	1.40	2 (15%)	17,18,20	1.65	3 (17%)
2	BGC	K	1	2	12,12,12	1.42	1 (8%)	17,17,17	1.99	5 (29%)
2	98U	K	2	5,2	13,13,14	1.55	4 (30%)	17,18,20	1.51	2 (11%)
2	BGC	L	1	2	12,12,12	0.60	0	17,17,17	1.30	2 (11%)
2	98U	L	2	5,2	13,13,14	1.45	2 (15%)	17,18,20	2.03	3 (17%)
2	BGC	M	1	2	12,12,12	1.33	1 (8%)	17,17,17	1.18	2 (11%)
2	98U	M	2	5,2	13,13,14	1.60	3 (23%)	17,18,20	1.41	3 (17%)
2	BGC	N	1	2	12,12,12	0.63	0	17,17,17	1.42	3 (17%)
2	98U	N	2	5,2	13,13,14	1.59	2 (15%)	17,18,20	1.82	3 (17%)
2	BGC	O	1	2	12,12,12	1.35	2 (16%)	17,17,17	1.23	2 (11%)
2	98U	O	2	5,2	13,13,14	1.66	4 (30%)	17,18,20	1.42	2 (11%)
2	BGC	P	1	2	12,12,12	1.19	1 (8%)	17,17,17	2.02	2 (11%)
2	98U	P	2	5,2	13,13,14	1.32	2 (15%)	17,18,20	1.57	3 (17%)

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	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	98U	G	2	5,2	-	1/4/21/24	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	98U	H	2	5,2	-	2/4/21/24	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	98U	I	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	98U	J	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	K	1	2	-	1/2/22/22	0/1/1/1
2	98U	K	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	L	1	2	-	0/2/22/22	0/1/1/1
2	98U	L	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	M	1	2	-	2/2/22/22	0/1/1/1
2	98U	M	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	N	1	2	-	0/2/22/22	0/1/1/1
2	98U	N	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	O	1	2	-	0/2/22/22	0/1/1/1
2	98U	O	2	5,2	-	0/4/21/24	0/1/1/1
2	BGC	P	1	2	-	0/2/22/22	0/1/1/1
2	98U	P	2	5,2	-	0/4/21/24	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	98U	O3-C3	-5.16	1.37	1.44
2	H	2	98U	O7-C7	4.17	1.36	1.21
2	N	2	98U	O7-C7	3.77	1.34	1.21
2	O	2	98U	O2-C2	-3.53	1.35	1.43
2	G	2	98U	O7-C7	3.48	1.33	1.21

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	BGC	C1-O5-C5	-7.37	99.39	113.65
2	I	1	BGC	C1-O5-C5	-7.02	100.07	113.65
2	L	2	98U	C2-C3-C4	-5.87	105.80	110.91
2	H	2	98U	O3-C7-C8	5.29	120.53	111.09
2	G	2	98U	C2-C3-C4	-4.48	107.01	110.91

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

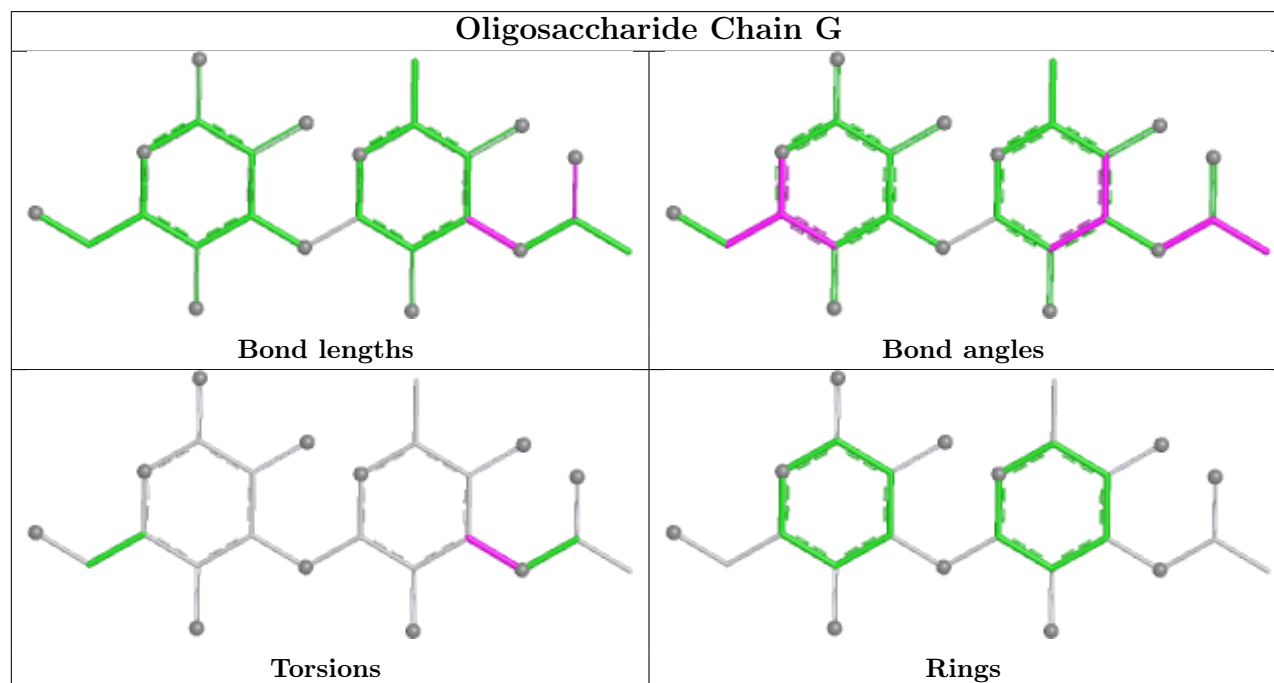
Mol	Chain	Res	Type	Atoms
2	H	2	98U	C8-C7-O3-C3
2	H	2	98U	O7-C7-O3-C3
2	M	1	BGC	O5-C5-C6-O6
2	M	1	BGC	C4-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6

There are no ring outliers.

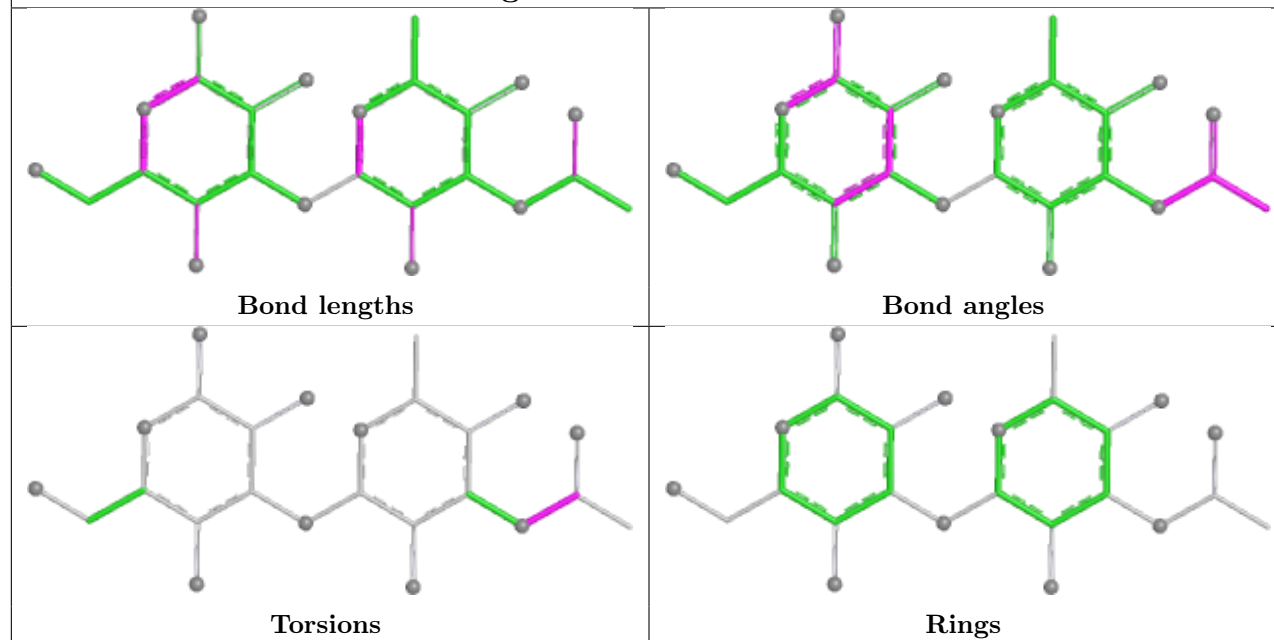
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	BGC	2	0
2	I	1	BGC	1	0
2	G	1	BGC	1	0

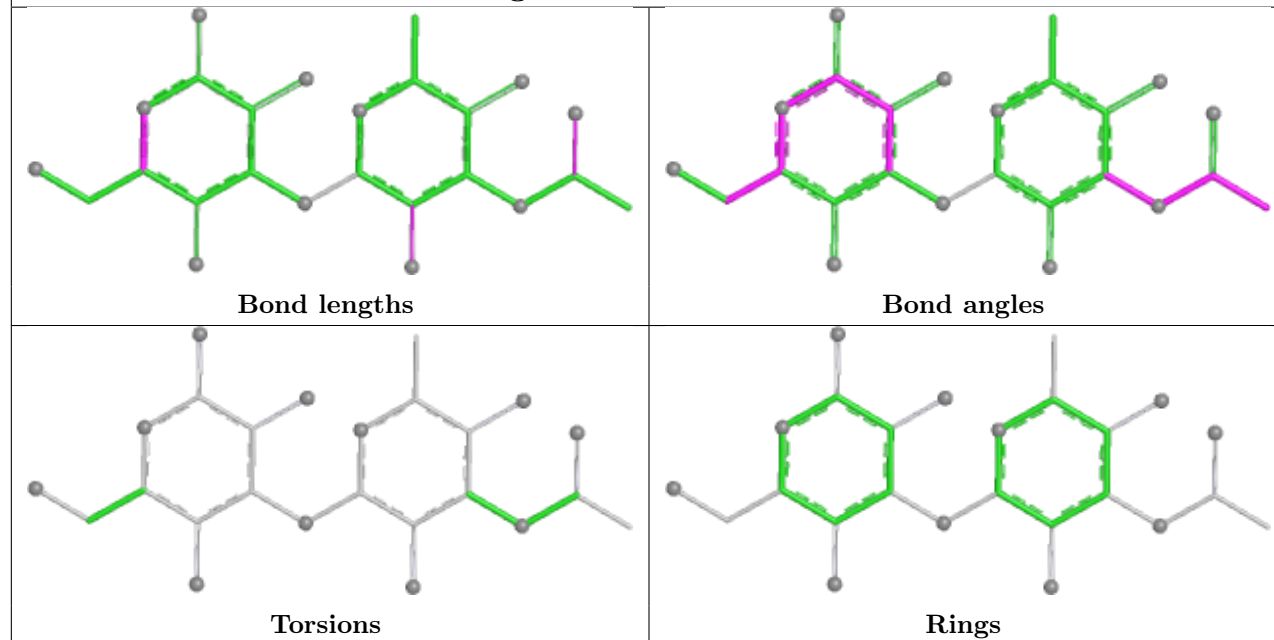
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

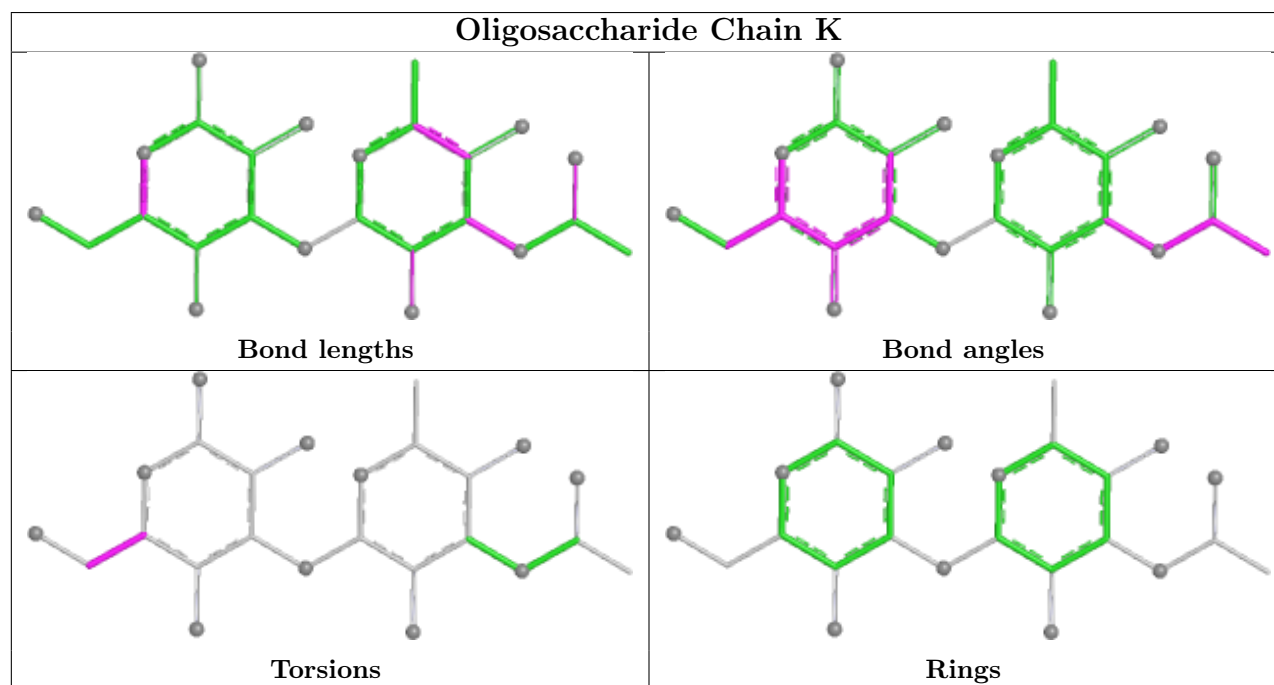
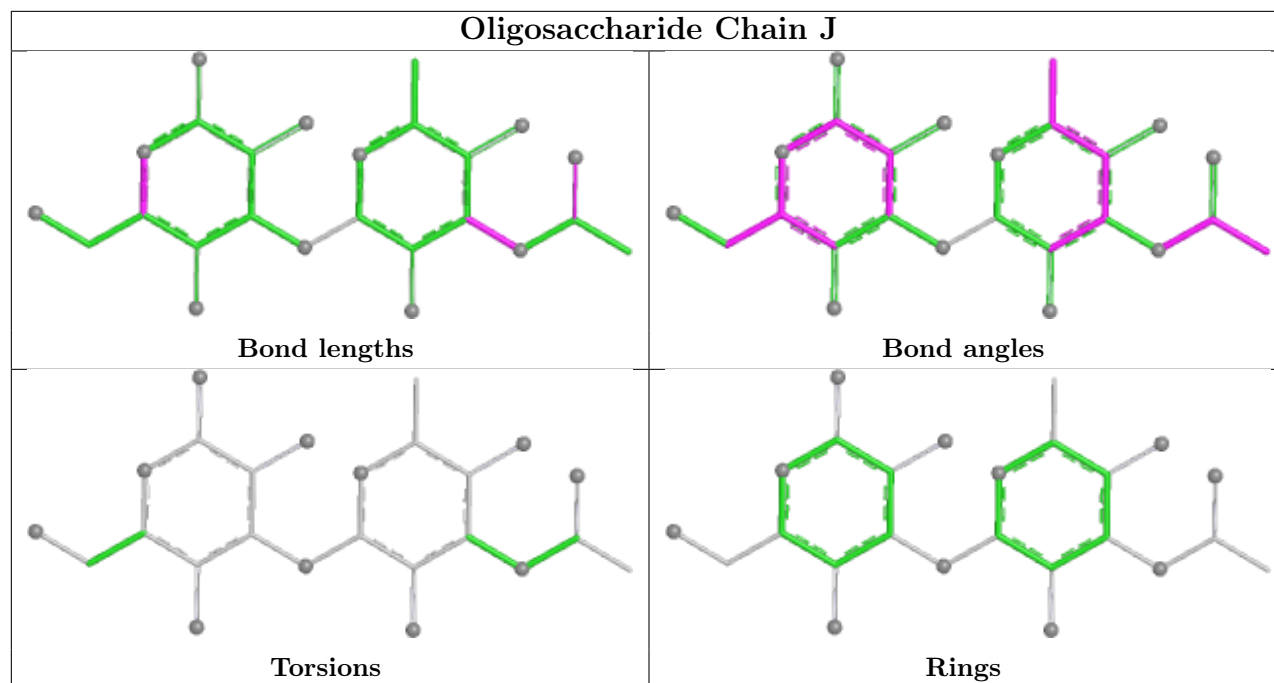


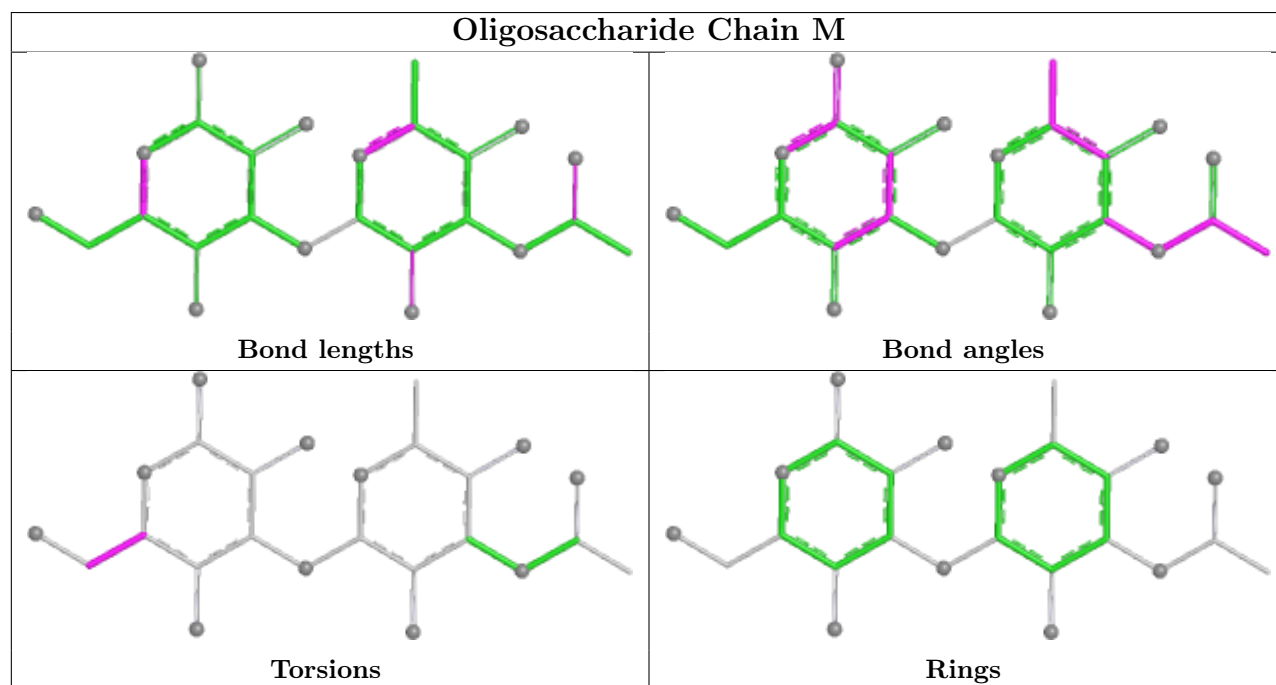
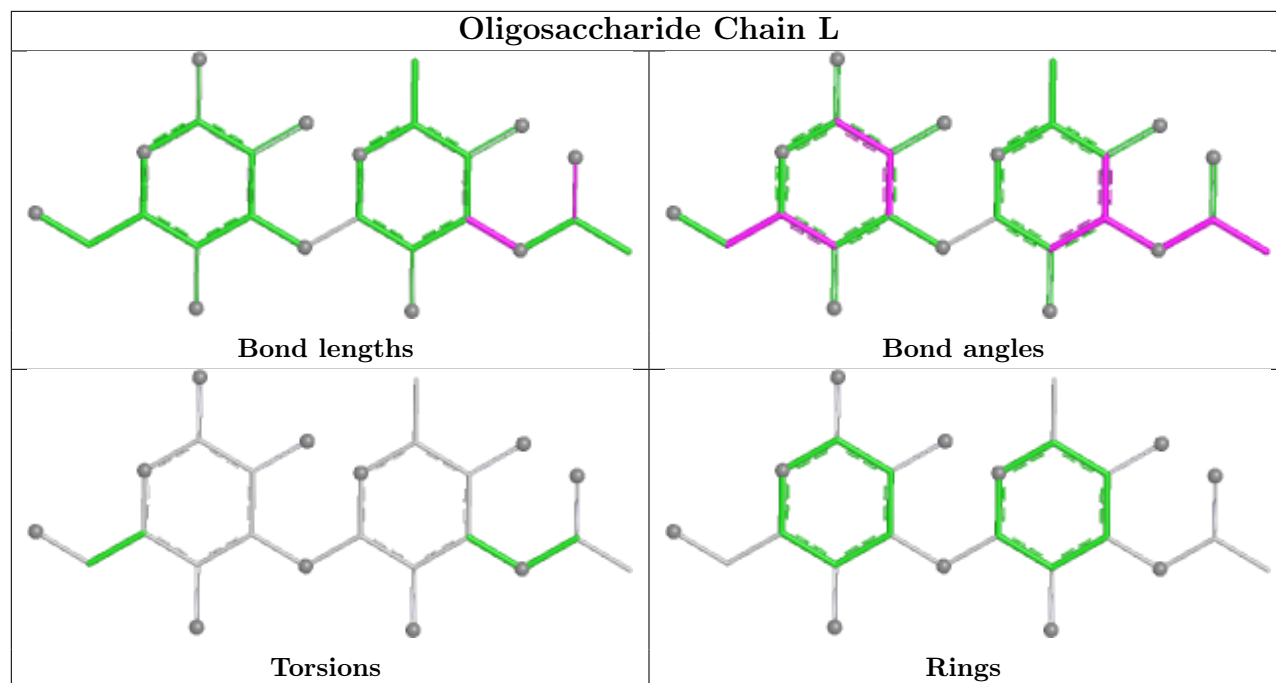
Oligosaccharide Chain H

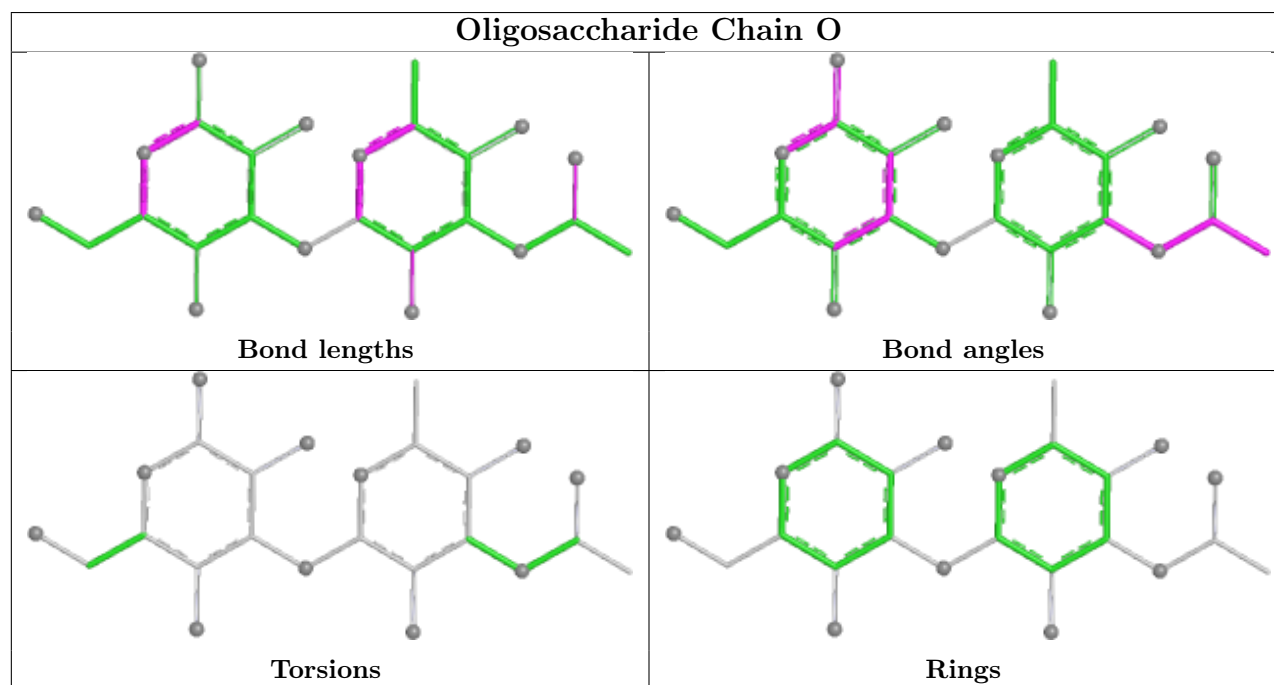
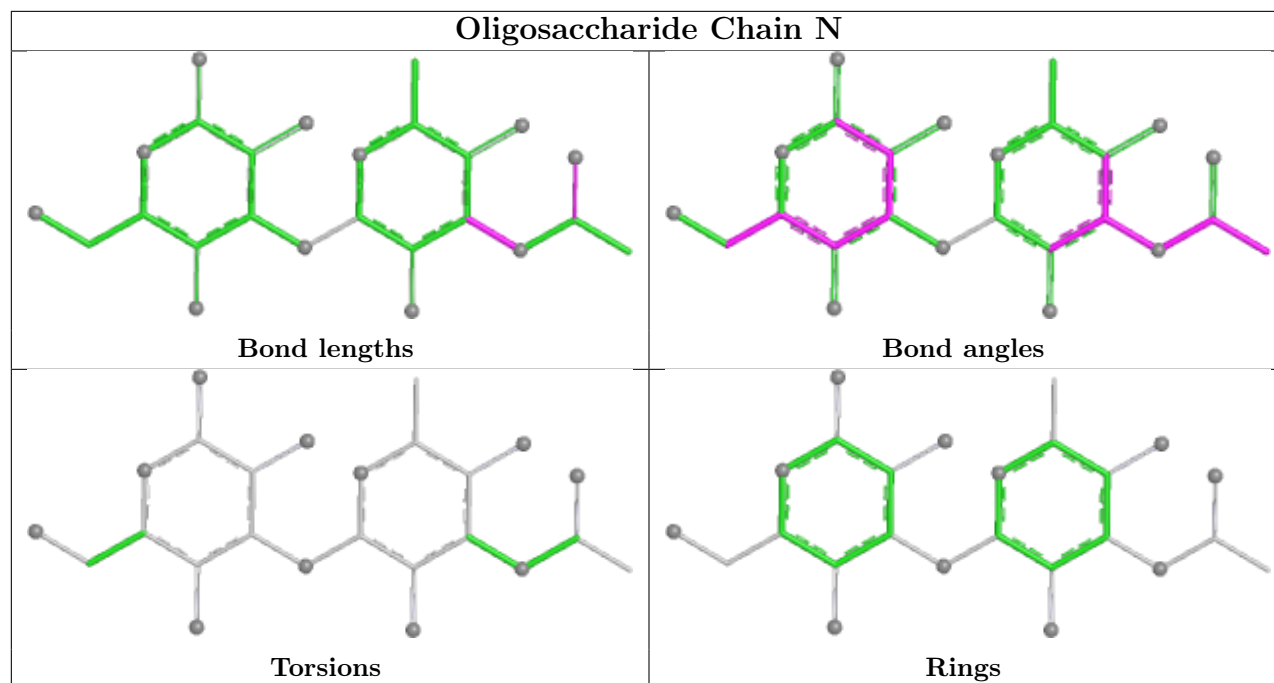


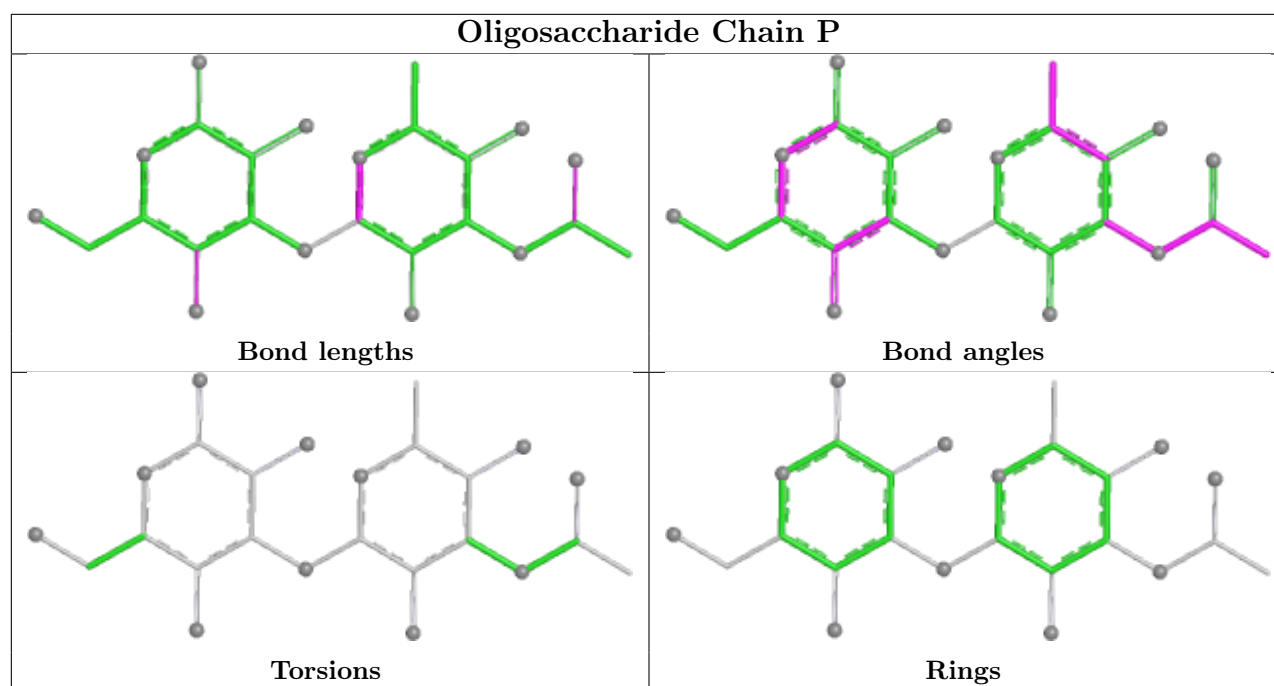
Oligosaccharide Chain I











5.6 Ligand geometry [i](#)

32 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	GOL	E	701	-	5,5,5	0.53	0	5,5,5	0.52	0
4	GOL	E	704	-	5,5,5	0.97	0	5,5,5	1.05	0
4	GOL	B	703	-	5,5,5	0.93	0	5,5,5	1.20	0
3	IMD	A	701	-	5,5,5	0.62	0	5,5,5	0.43	0
4	GOL	D	703	-	5,5,5	1.19	0	5,5,5	1.89	2 (40%)
5	98X	A	706	2	16,17,17	2.95	7 (43%)	15,26,26	2.93	8 (53%)
5	98X	F	705	2	16,17,17	2.21	7 (43%)	15,26,26	2.27	7 (46%)
3	IMD	B	702	-	5,5,5	0.62	0	5,5,5	0.31	0
5	98X	A	707	2	16,17,17	2.62	8 (50%)	15,26,26	2.55	7 (46%)
4	GOL	B	701	-	5,5,5	0.18	0	5,5,5	0.42	0
3	IMD	E	702	-	5,5,5	0.66	0	5,5,5	0.43	0
5	98X	E	705	2	16,17,17	2.40	7 (43%)	15,26,26	2.68	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	98X	C	704	2	16,17,17	2.59	7 (43%)	15,26,26	2.75	8 (53%)
4	GOL	C	701	-	5,5,5	0.65	0	5,5,5	0.58	0
4	GOL	A	702	-	5,5,5	0.63	0	5,5,5	1.09	0
4	GOL	F	701	-	5,5,5	0.19	0	5,5,5	0.44	0
4	GOL	F	702	-	5,5,5	1.08	1 (20%)	5,5,5	0.28	0
3	IMD	C	703	-	5,5,5	0.49	0	5,5,5	0.29	0
4	GOL	C	702	-	5,5,5	0.72	0	5,5,5	0.43	0
3	IMD	E	703	-	5,5,5	0.57	0	5,5,5	0.58	0
3	IMD	F	703	-	5,5,5	0.56	0	5,5,5	0.51	0
4	GOL	F	704	-	5,5,5	1.00	0	5,5,5	0.78	0
5	98X	D	705	2	16,17,17	2.51	6 (37%)	15,26,26	2.30	7 (46%)
3	IMD	D	701	-	5,5,5	0.62	0	5,5,5	0.37	0
3	IMD	A	704	-	5,5,5	0.56	0	5,5,5	0.56	0
5	98X	B	704	2	16,17,17	2.45	8 (50%)	15,26,26	2.45	7 (46%)
5	98X	A	708	2	16,17,17	2.30	5 (31%)	15,26,26	2.19	7 (46%)
5	98X	D	704	2	16,17,17	2.68	6 (37%)	15,26,26	2.78	8 (53%)
4	GOL	D	702	-	5,5,5	1.22	0	5,5,5	1.65	2 (40%)
4	GOL	A	703	-	5,5,5	0.61	0	5,5,5	0.71	0
5	98X	E	706	2	16,17,17	2.92	7 (43%)	15,26,26	2.87	8 (53%)
4	GOL	A	705	-	5,5,5	0.31	0	5,5,5	0.45	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
4	GOL	E	701	-	-	3/4/4/4	-
4	GOL	E	704	-	-	2/4/4/4	-
4	GOL	B	703	-	-	2/4/4/4	-
3	IMD	A	701	-	-	-	0/1/1/1
4	GOL	D	703	-	-	1/4/4/4	-
5	98X	F	705	2	-	1/9/33/33	0/2/2/2
3	IMD	B	702	-	-	-	0/1/1/1
5	98X	A	707	2	-	1/9/33/33	0/2/2/2
4	GOL	B	701	-	-	0/4/4/4	-
5	98X	E	705	2	-	1/9/33/33	0/2/2/2
3	IMD	E	702	-	-	-	0/1/1/1
5	98X	C	704	2	-	0/9/33/33	0/2/2/2
4	GOL	C	701	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	702	-	-	2/4/4/4	-
4	GOL	F	701	-	-	2/4/4/4	-
4	GOL	F	702	-	-	0/4/4/4	-
3	IMD	C	703	-	-	-	0/1/1/1
4	GOL	C	702	-	-	3/4/4/4	-
3	IMD	E	703	-	-	-	0/1/1/1
3	IMD	F	703	-	-	-	0/1/1/1
4	GOL	F	704	-	-	2/4/4/4	-
5	98X	D	705	2	-	2/9/33/33	0/2/2/2
4	GOL	A	703	-	-	4/4/4/4	-
3	IMD	D	701	-	-	-	0/1/1/1
3	IMD	A	704	-	-	-	0/1/1/1
5	98X	B	704	2	-	0/9/33/33	0/2/2/2
5	98X	A	708	2	-	1/9/33/33	0/2/2/2
5	98X	D	704	2	-	3/9/33/33	0/2/2/2
4	GOL	D	702	-	-	2/4/4/4	-
5	98X	A	706	2	-	3/9/33/33	0/2/2/2
5	98X	E	706	2	-	1/9/33/33	0/2/2/2
4	GOL	A	705	-	-	2/4/4/4	-

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	98X	CBD-CAN	-8.61	1.37	1.50
5	E	706	98X	CBD-CAN	-8.26	1.37	1.50
5	D	704	98X	CBD-CAN	-7.77	1.38	1.50
5	C	704	98X	CBD-CAN	-7.43	1.39	1.50
5	A	707	98X	CBD-CAN	-5.31	1.42	1.50

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	704	98X	CBJ-CBN-CBD	-6.62	104.15	114.80
5	D	704	98X	CBJ-CBN-CBD	-6.44	104.44	114.80
5	A	706	98X	CBJ-CBN-CBD	-6.22	104.79	114.80
5	E	706	98X	CBJ-CBN-CBD	-6.16	104.89	114.80
5	A	706	98X	OAQ-CBJ-CBN	-5.92	104.71	111.10

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

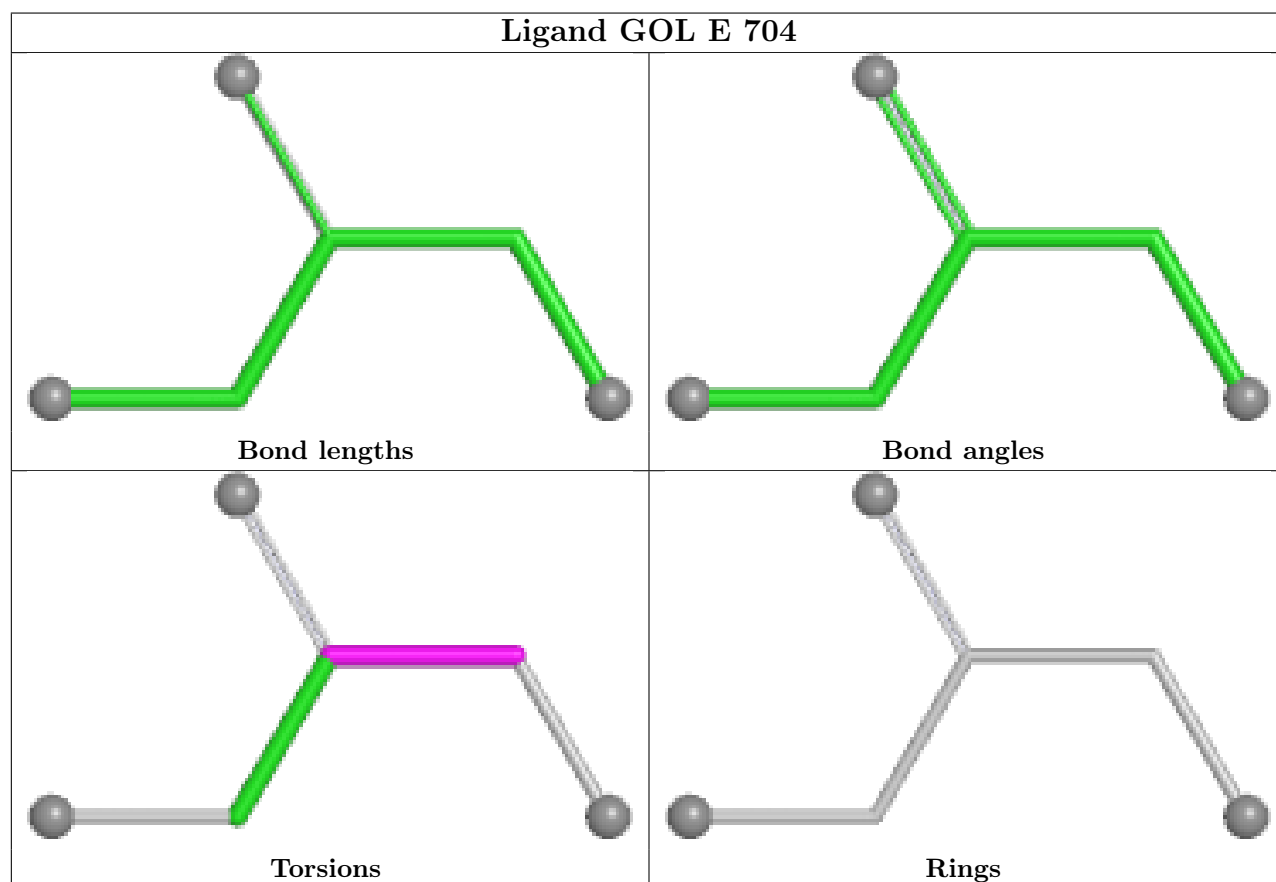
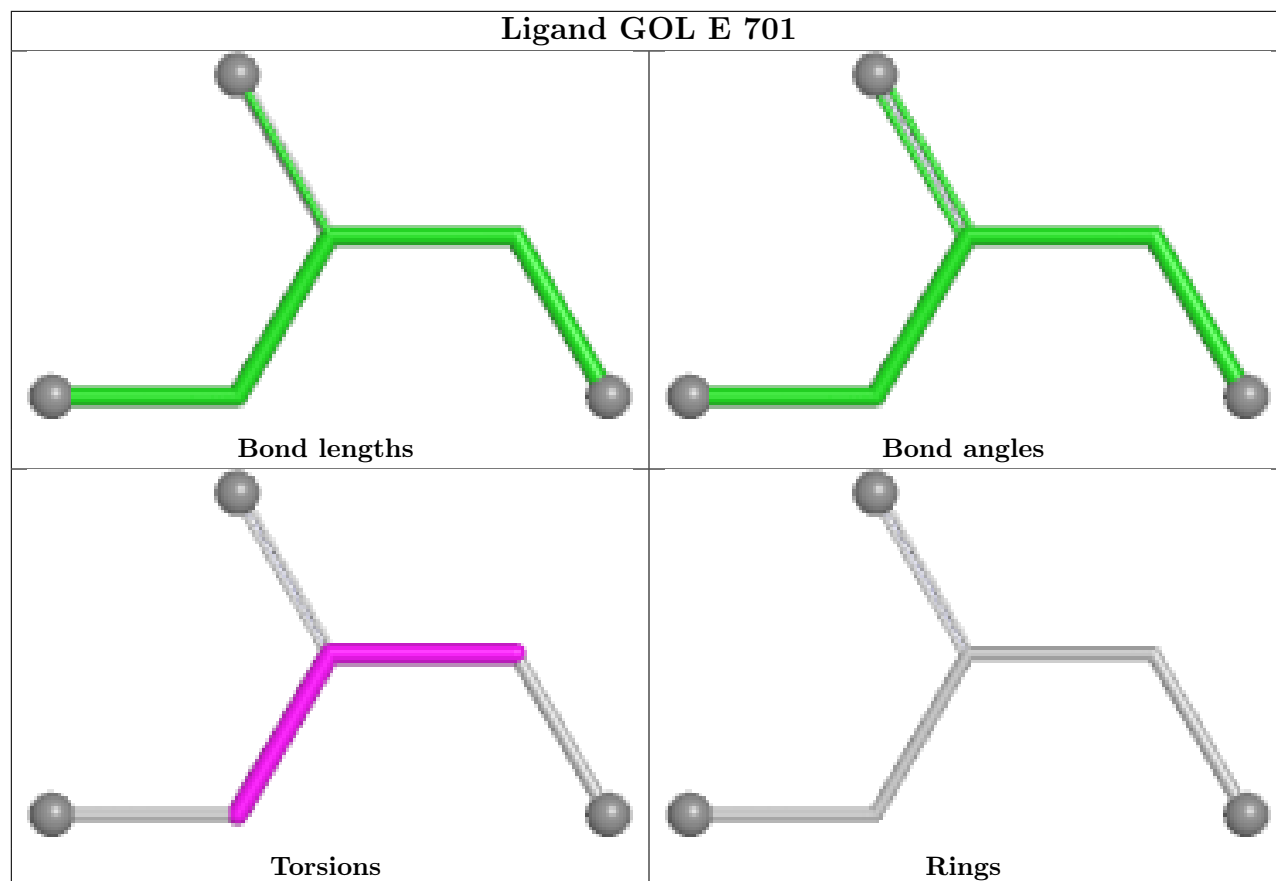
Mol	Chain	Res	Type	Atoms
4	A	702	GOL	C1-C2-C3-O3
4	A	703	GOL	C1-C2-C3-O3
4	A	705	GOL	C1-C2-C3-O3
4	C	702	GOL	O1-C1-C2-C3
4	D	702	GOL	C1-C2-C3-O3

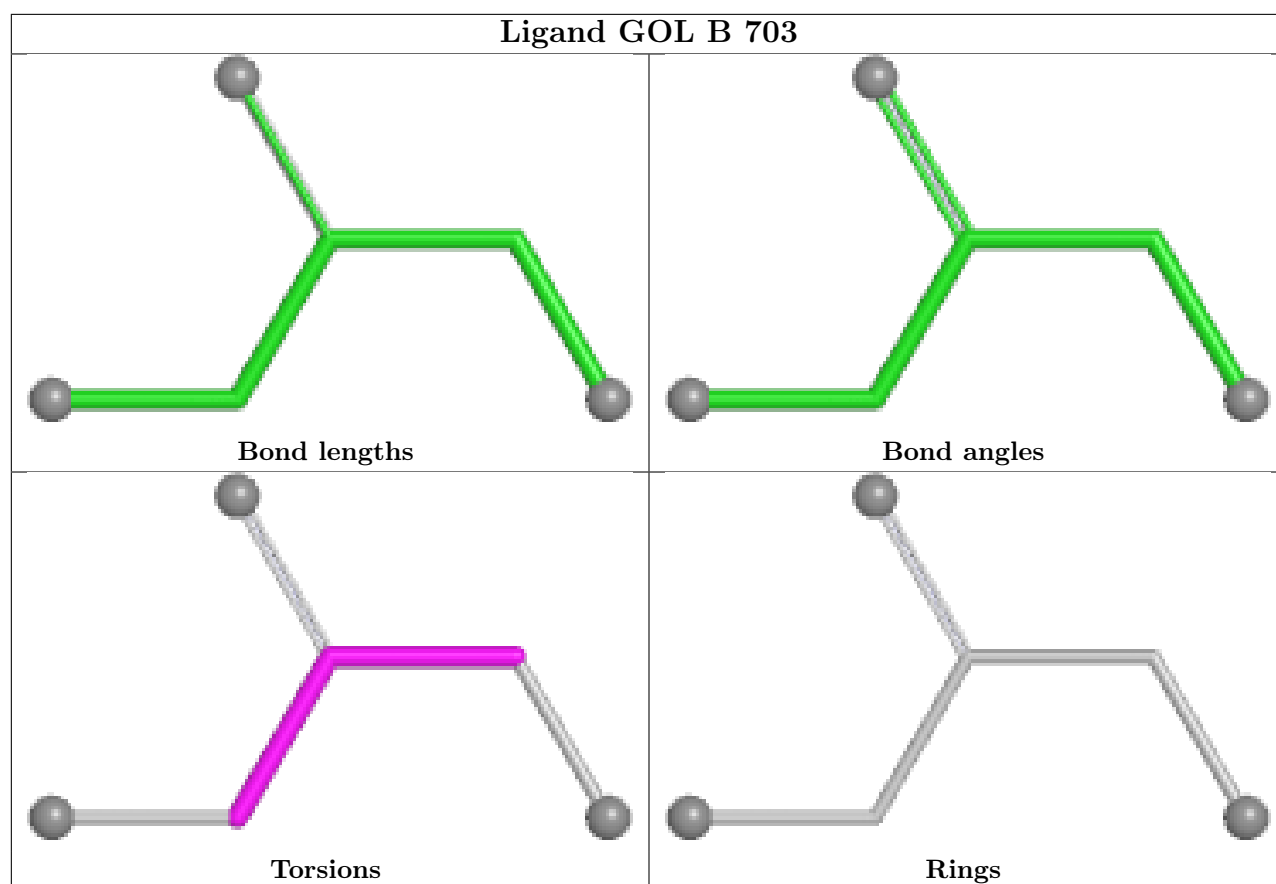
There are no ring outliers.

8 monomers are involved in 14 short contacts:

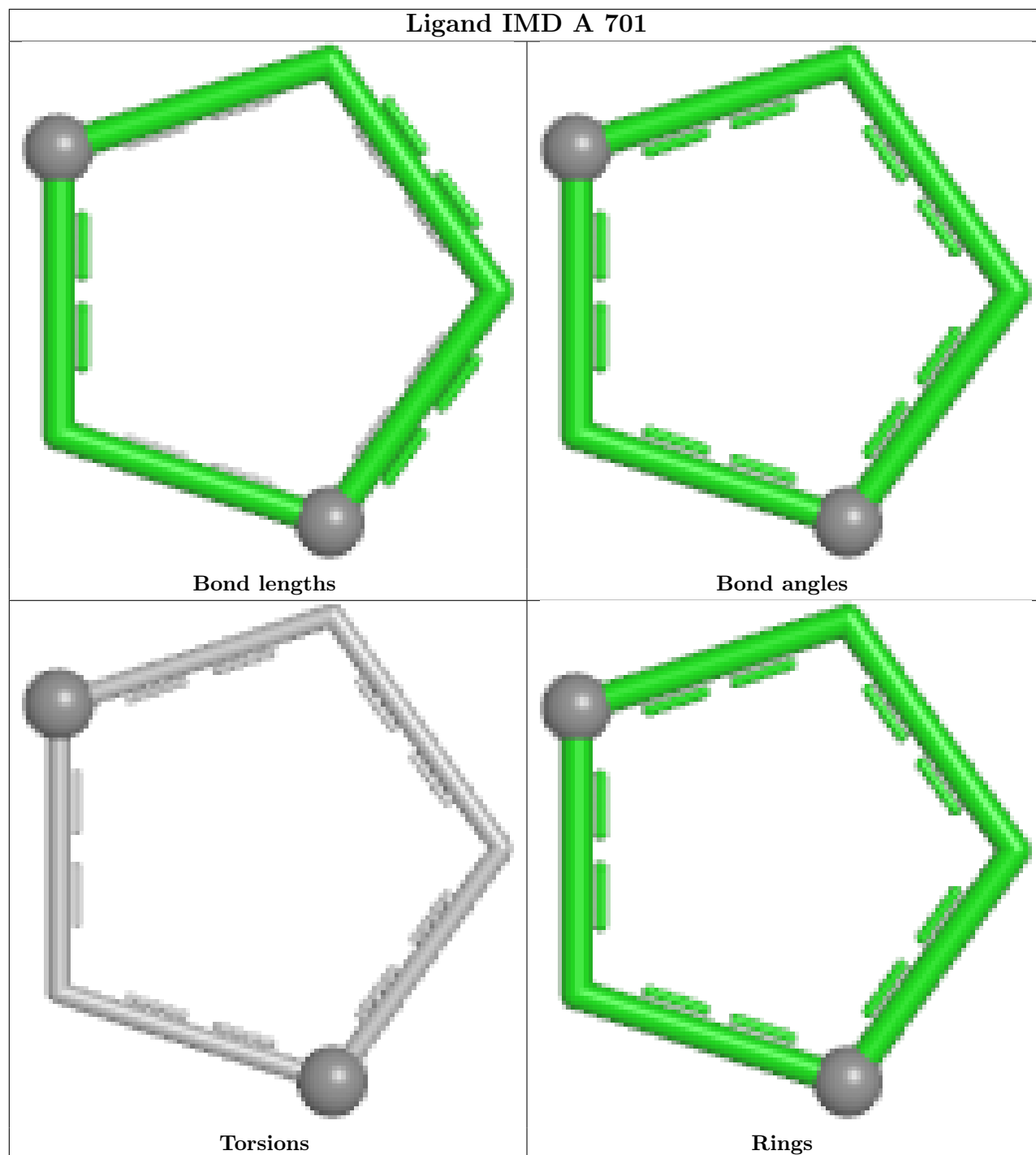
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	GOL	1	0
4	D	703	GOL	3	0
3	B	702	IMD	1	0
4	A	702	GOL	4	0
4	C	702	GOL	2	0
3	E	703	IMD	1	0
3	F	703	IMD	1	0
4	D	702	GOL	1	0

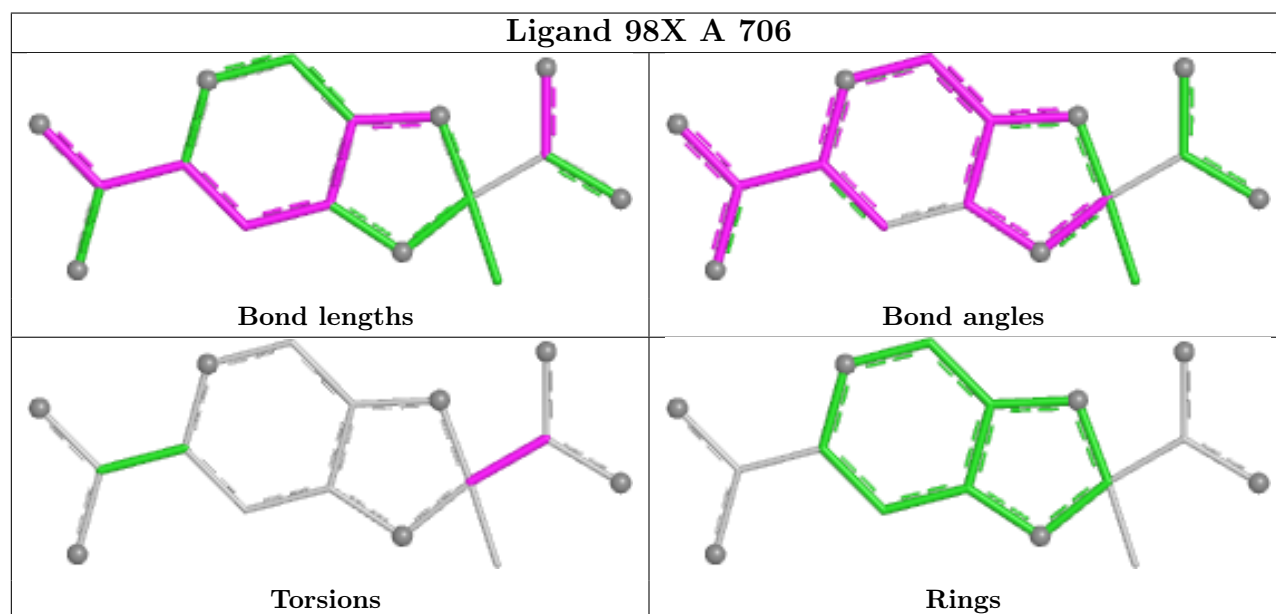
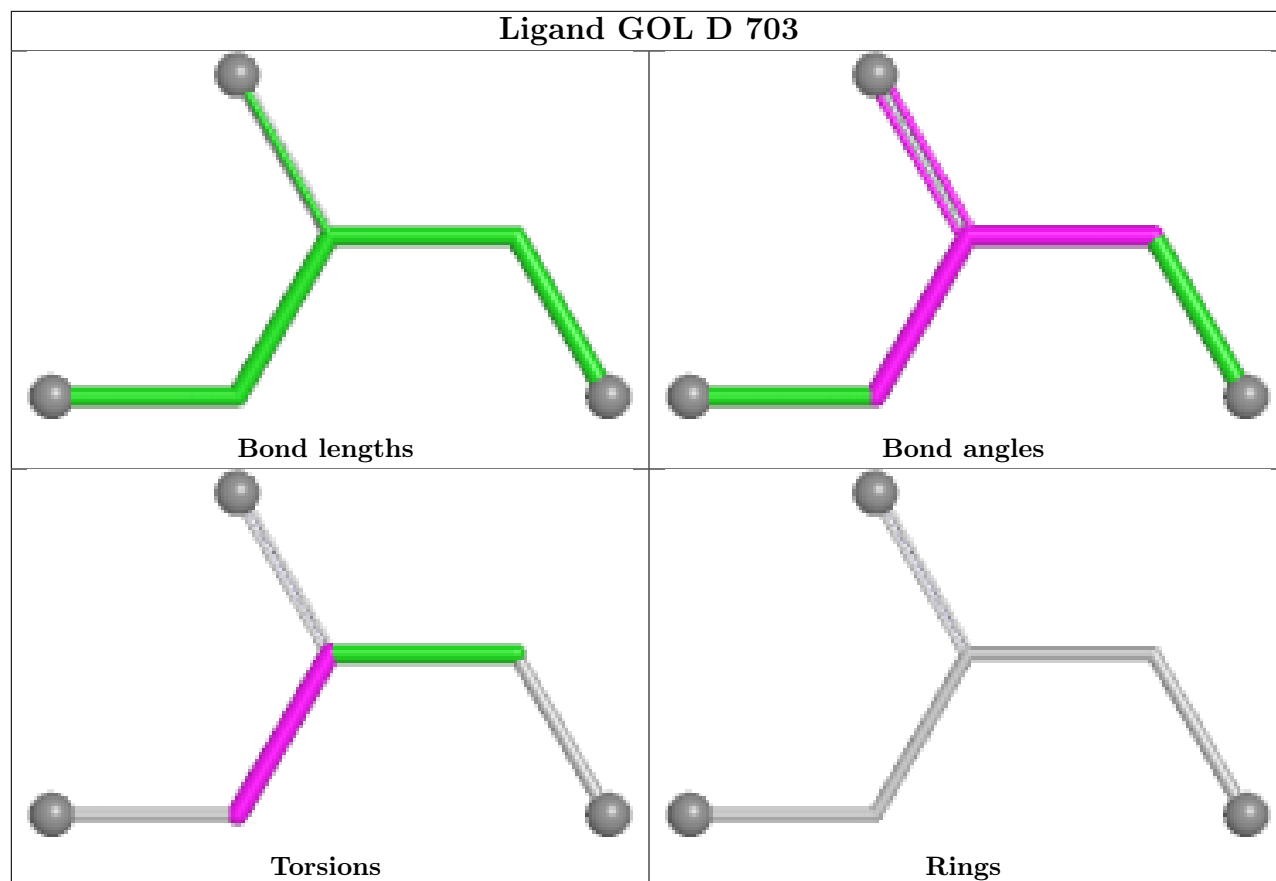
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

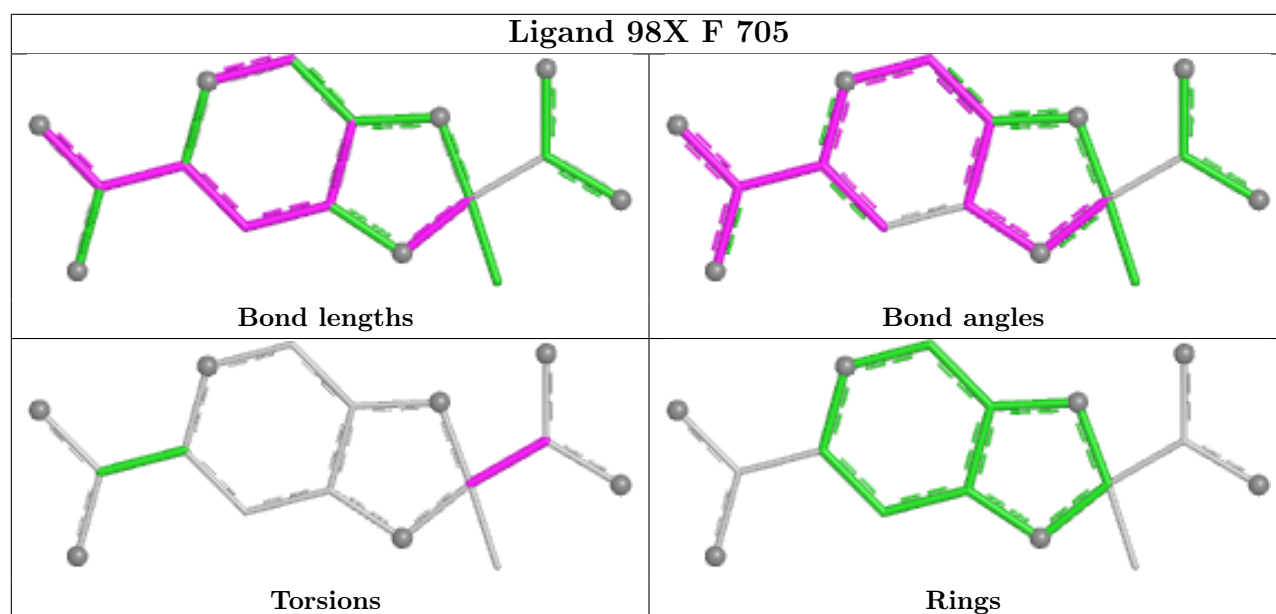




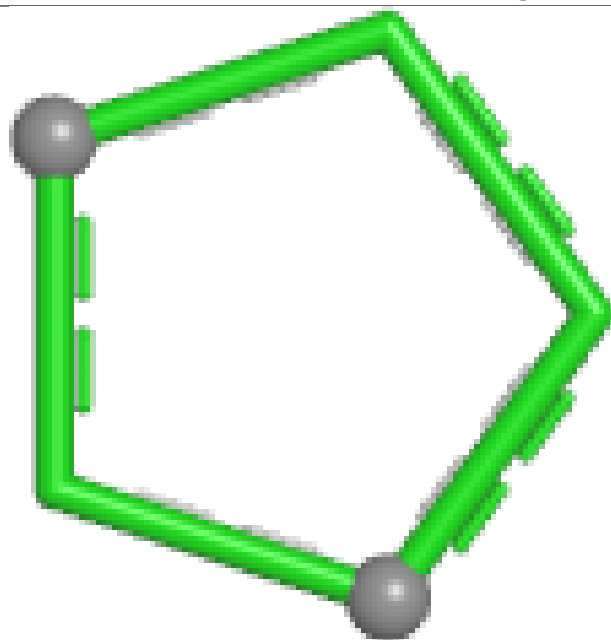
Ligand IMD A 701



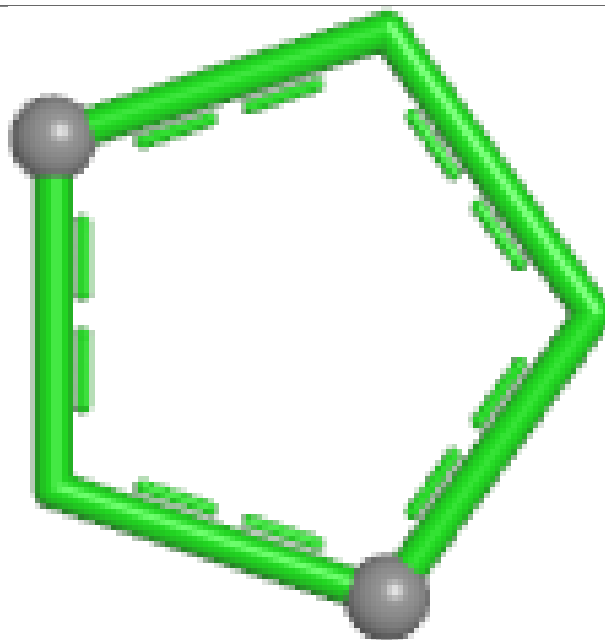




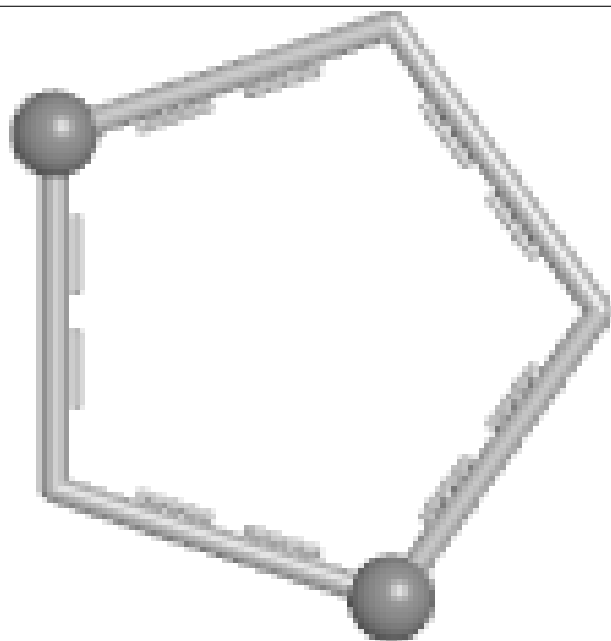
Ligand IMD B 702



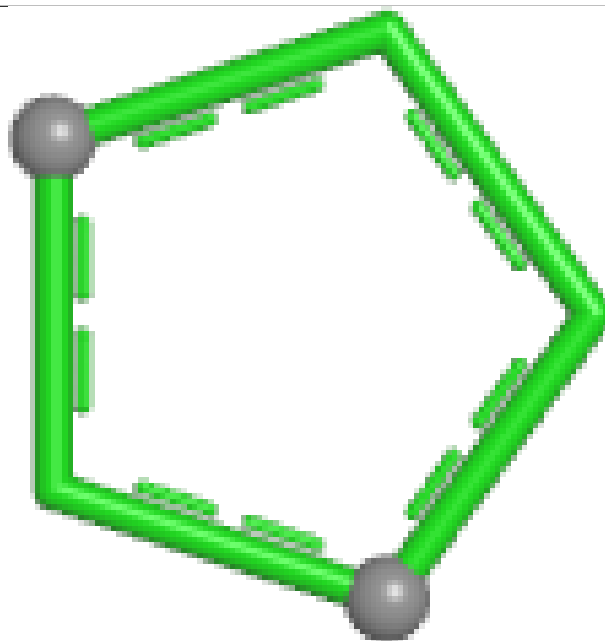
Bond lengths



Bond angles

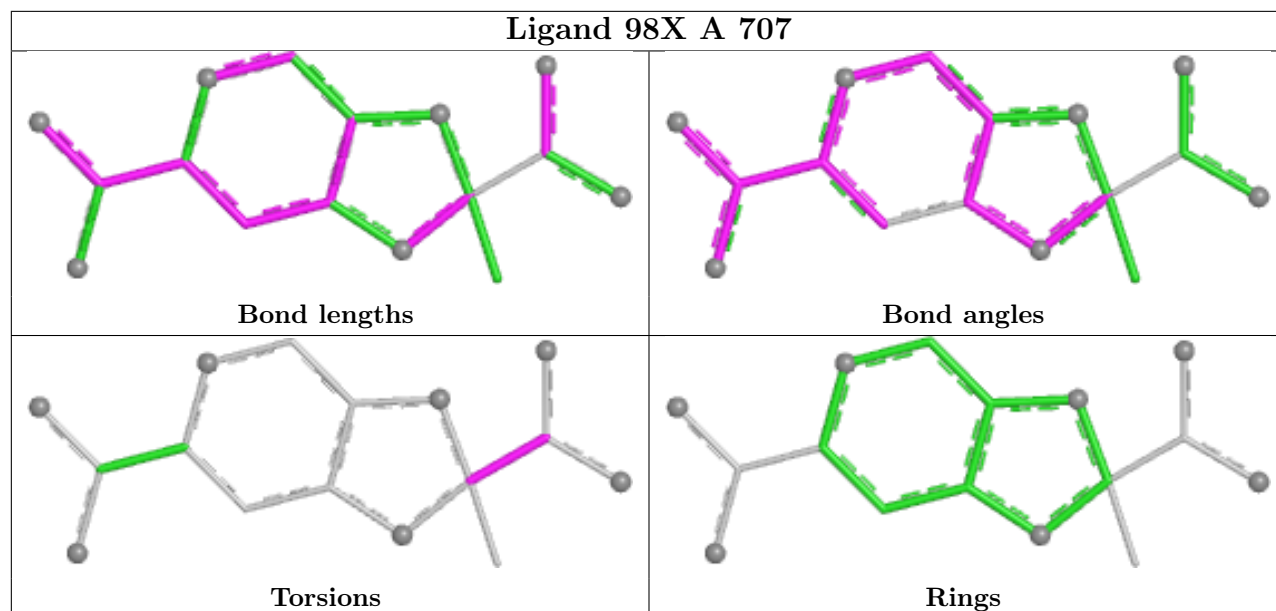


Torsions

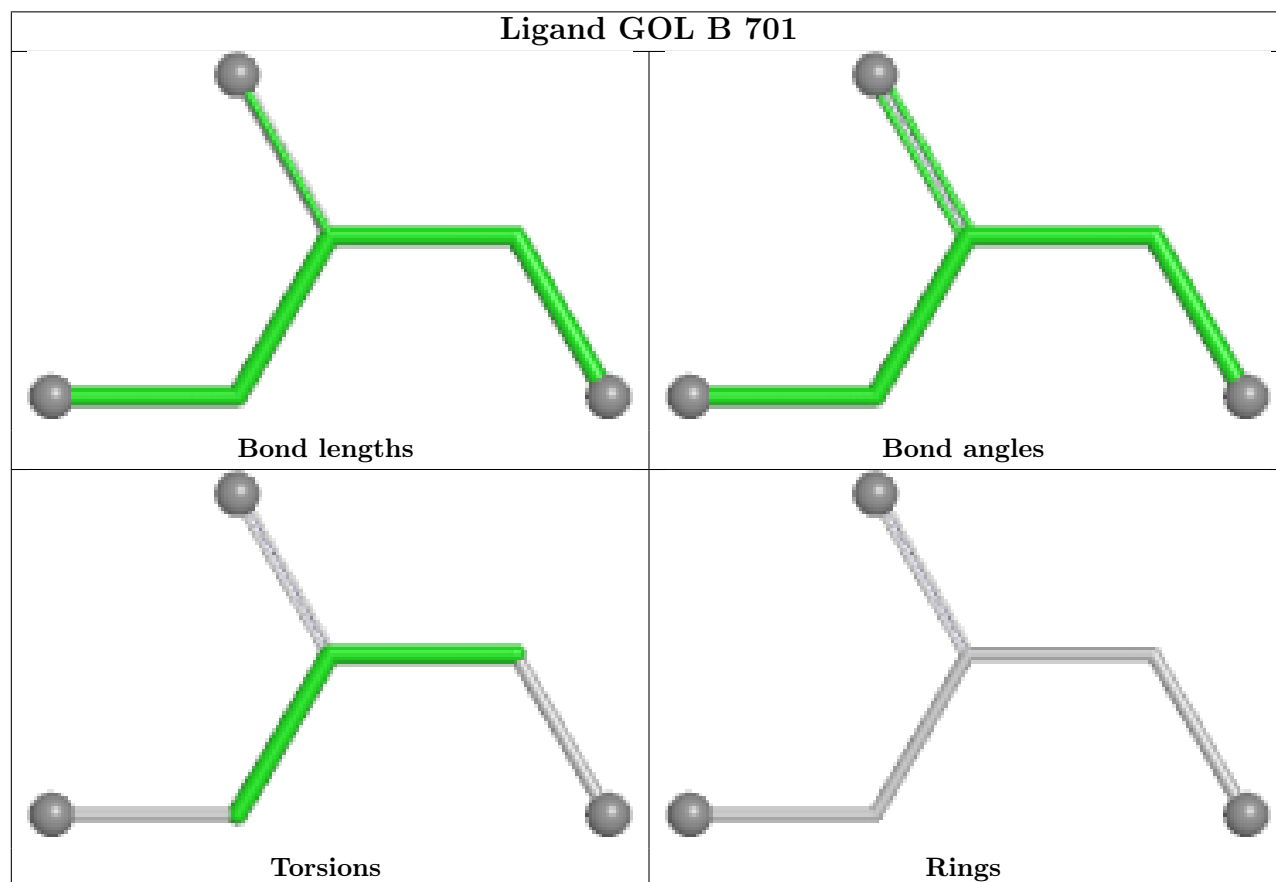


Rings

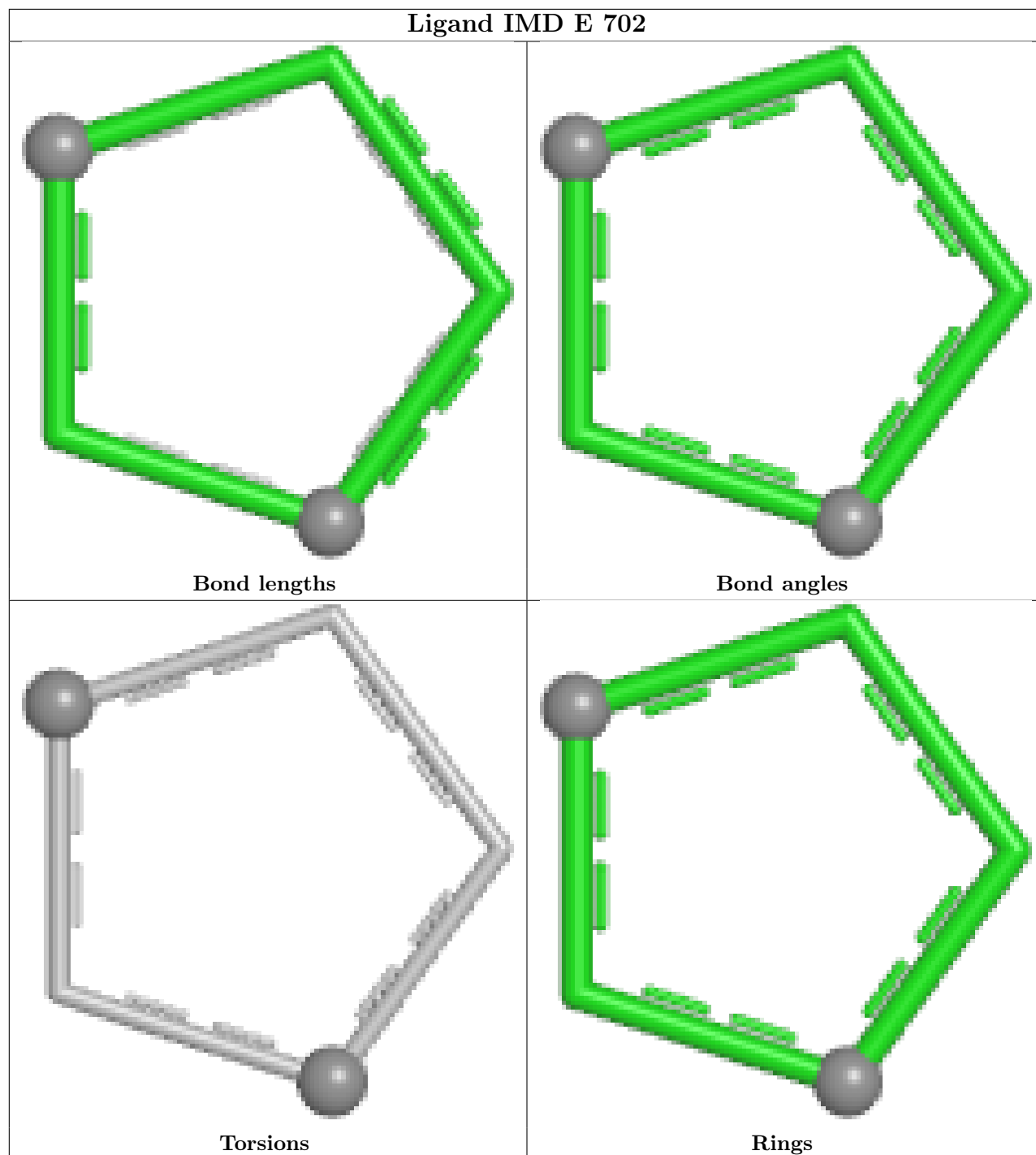
Ligand 98X A 707



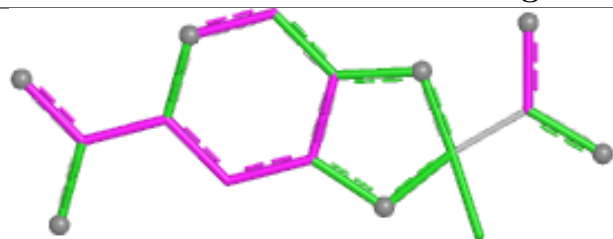
Ligand GOL B 701



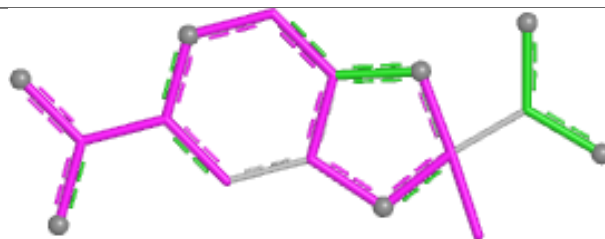
Ligand IMD E 702



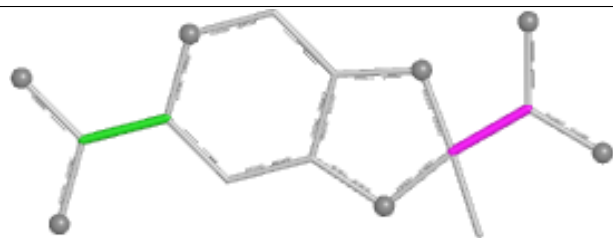
Ligand 98X E 705



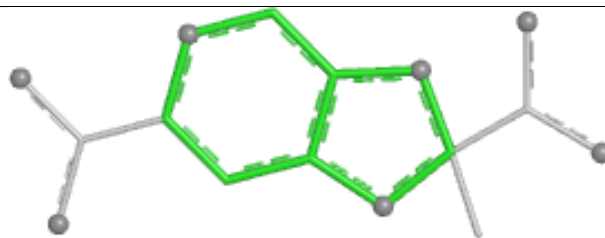
Bond lengths



Bond angles

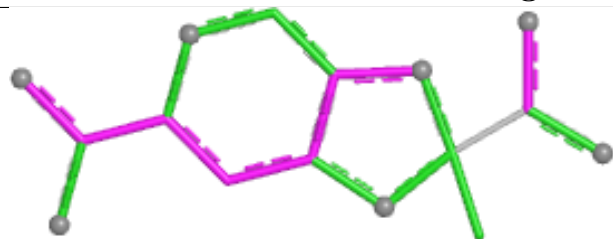


Torsions

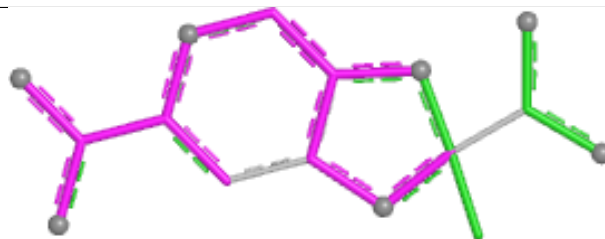


Rings

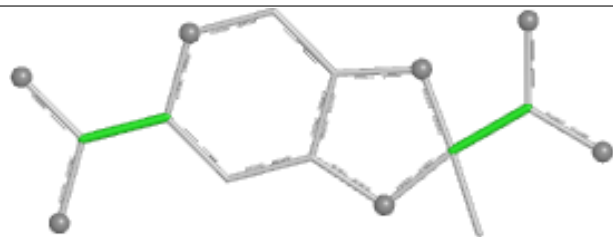
Ligand 98X C 704



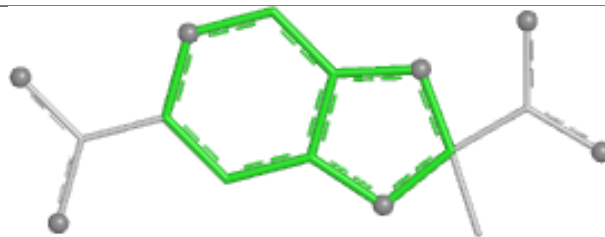
Bond lengths



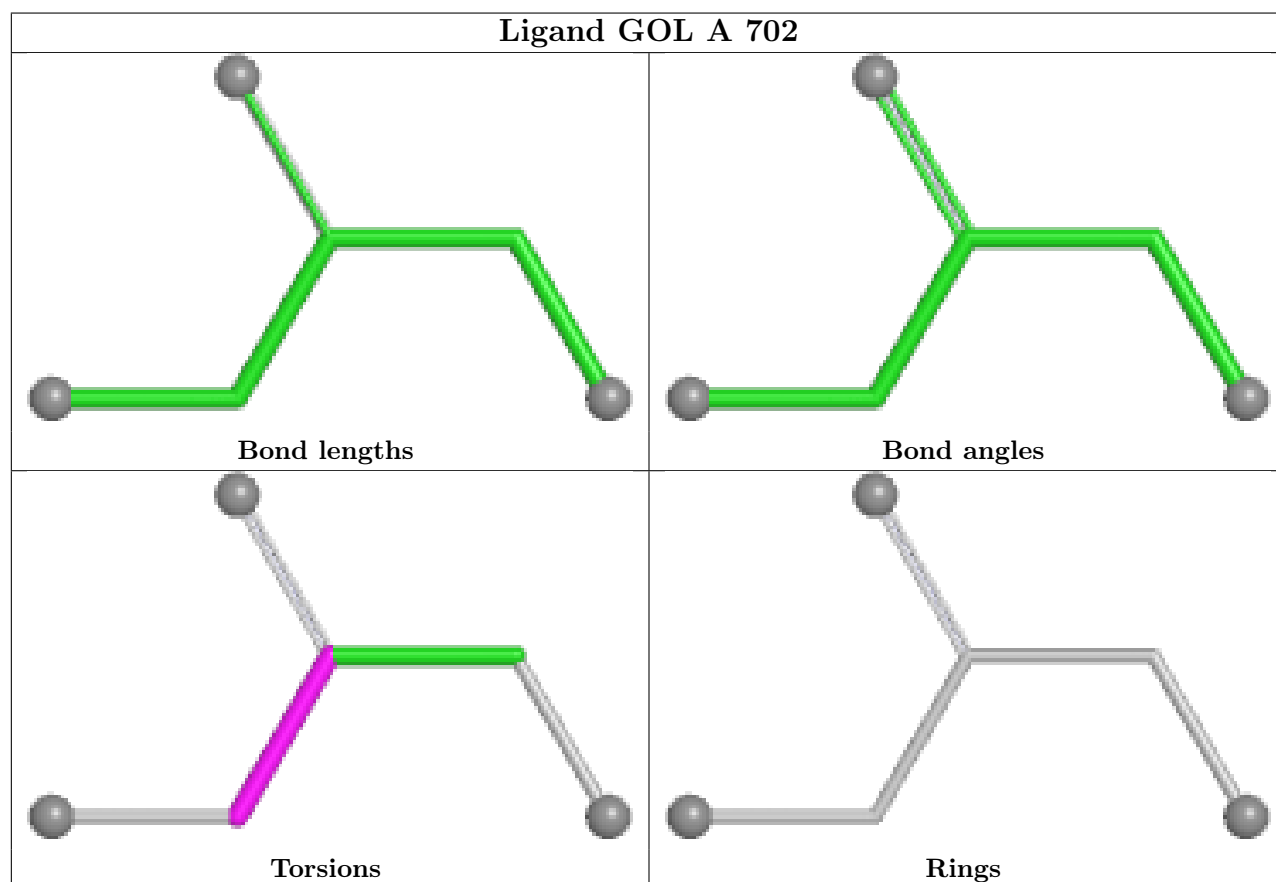
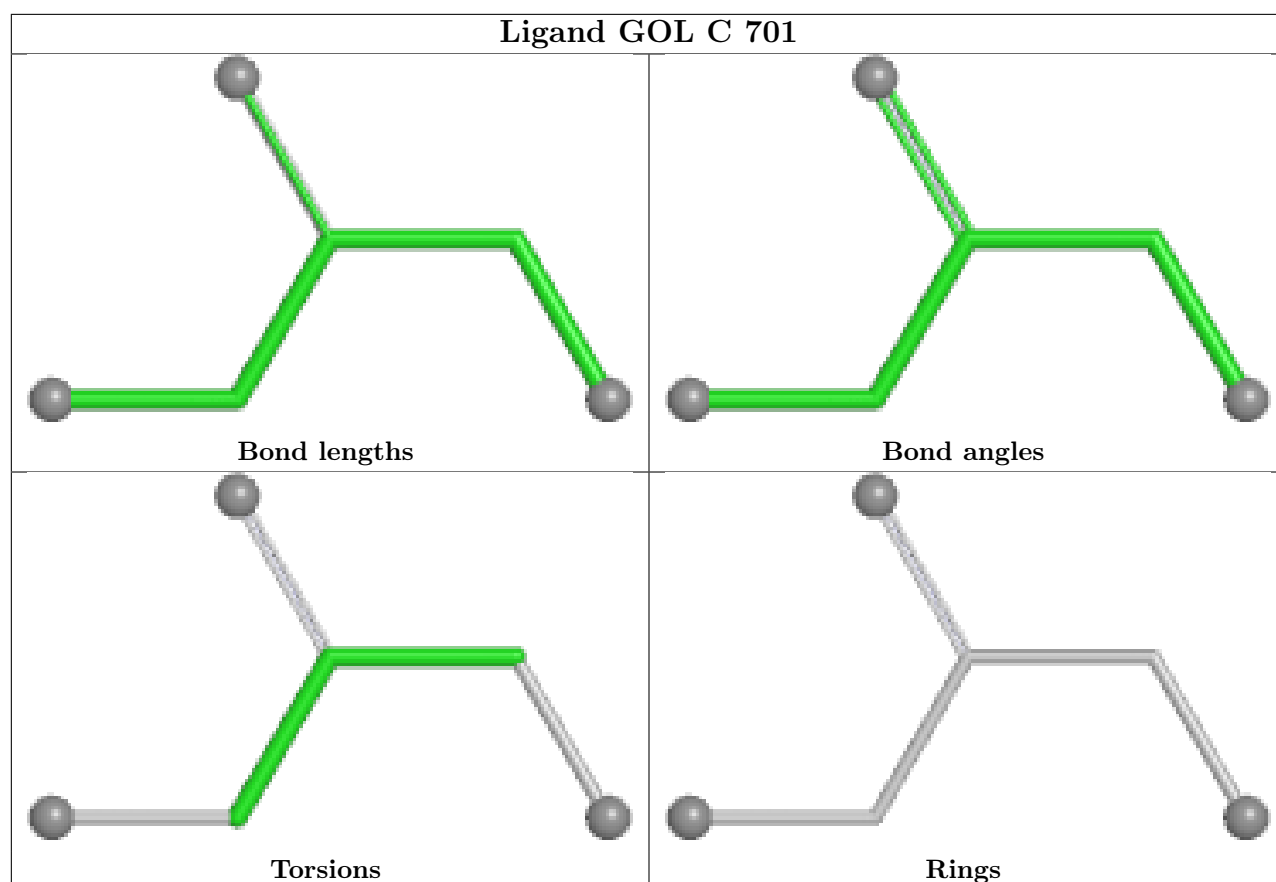
Bond angles

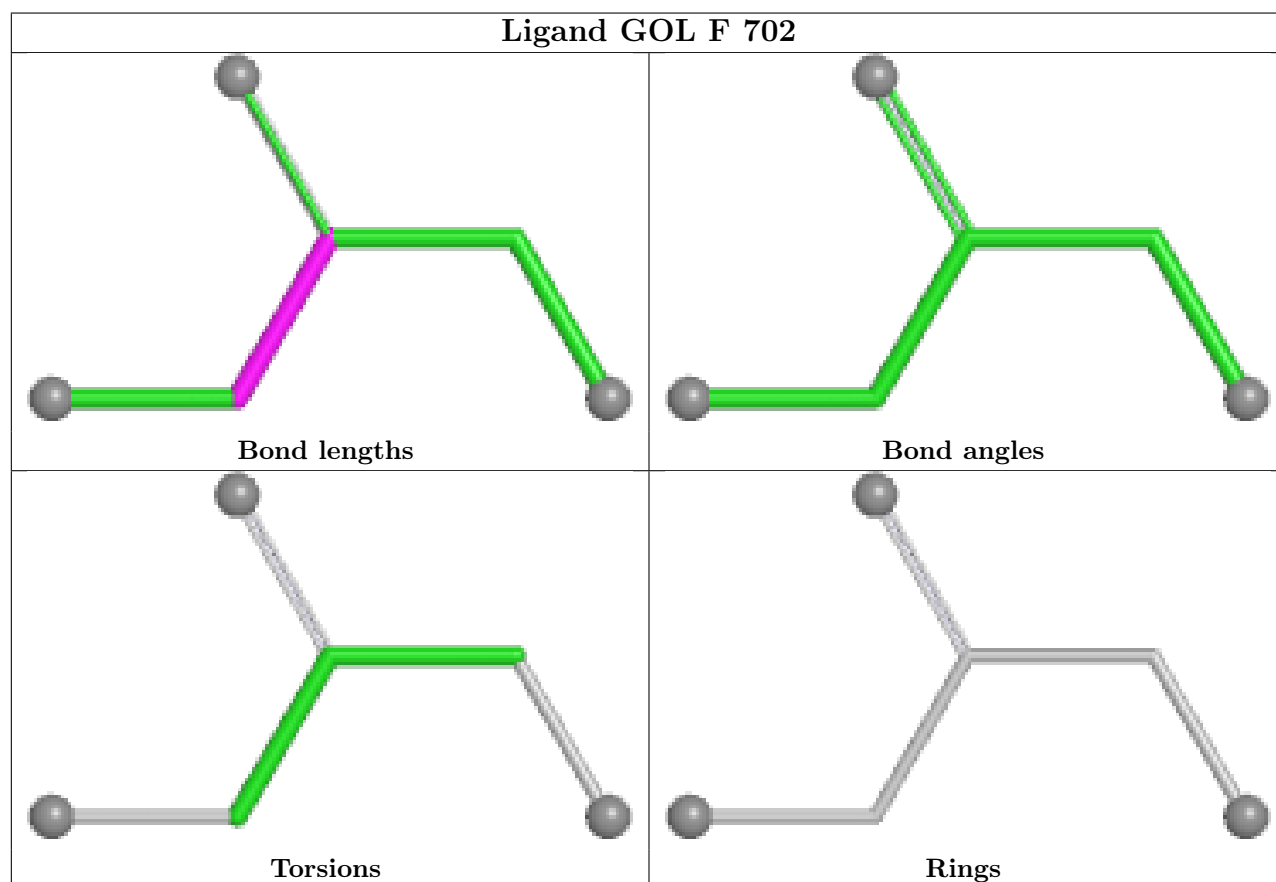
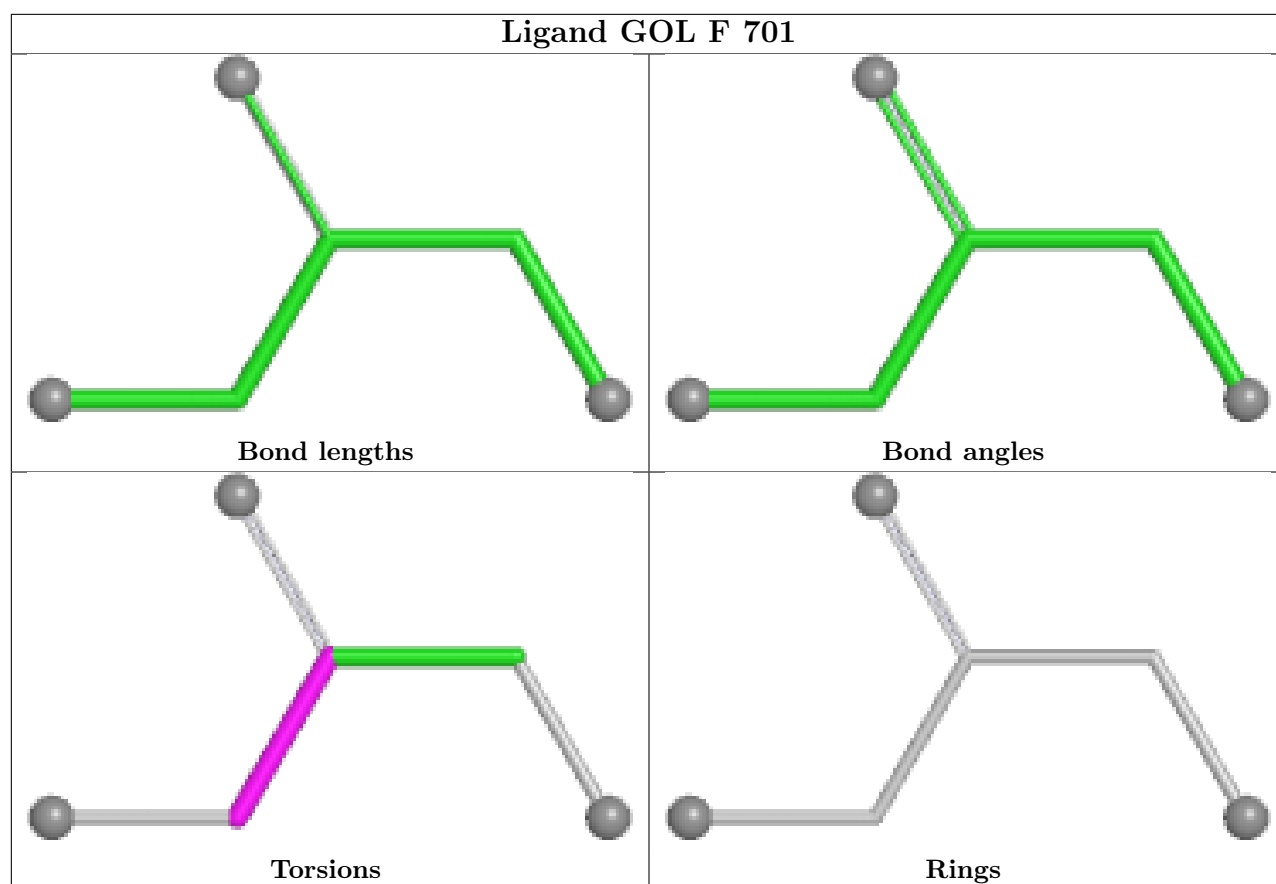


Torsions

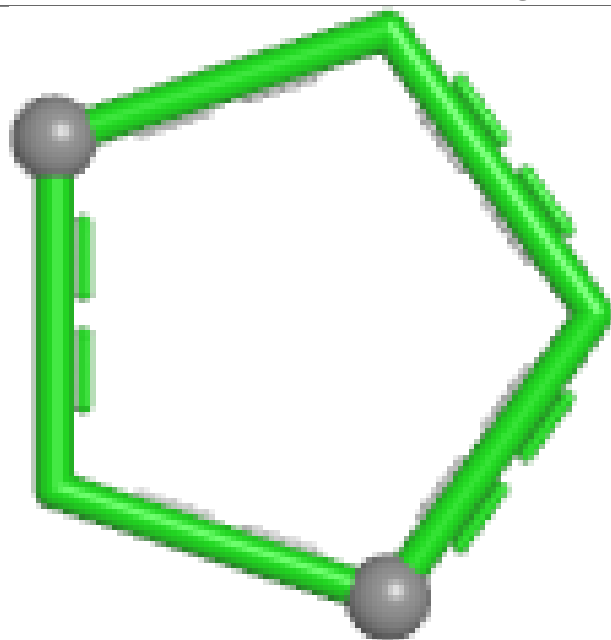


Rings

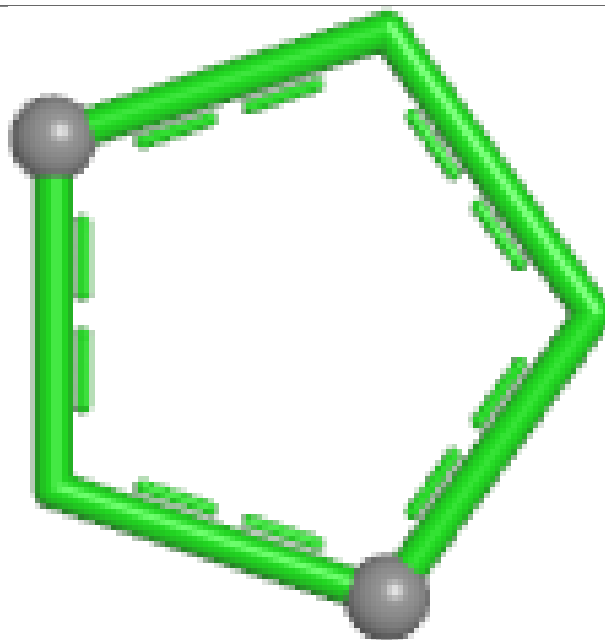




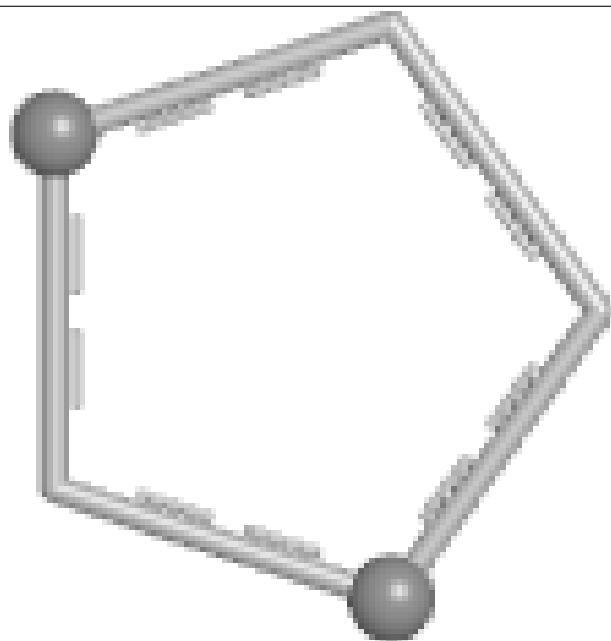
Ligand IMD C 703



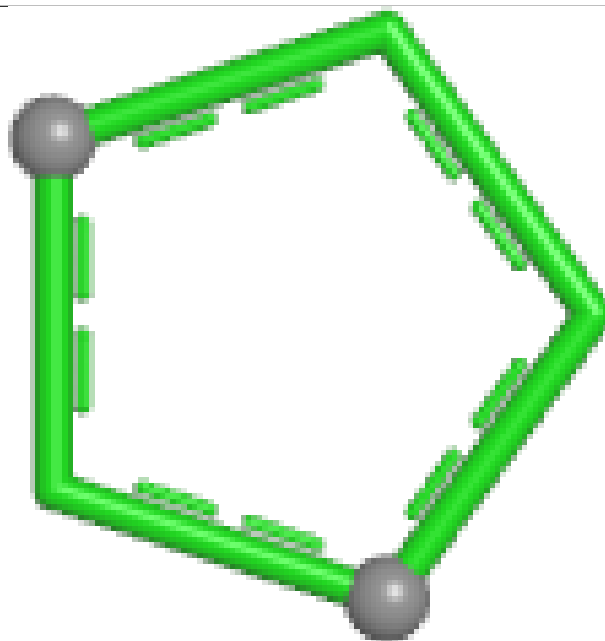
Bond lengths



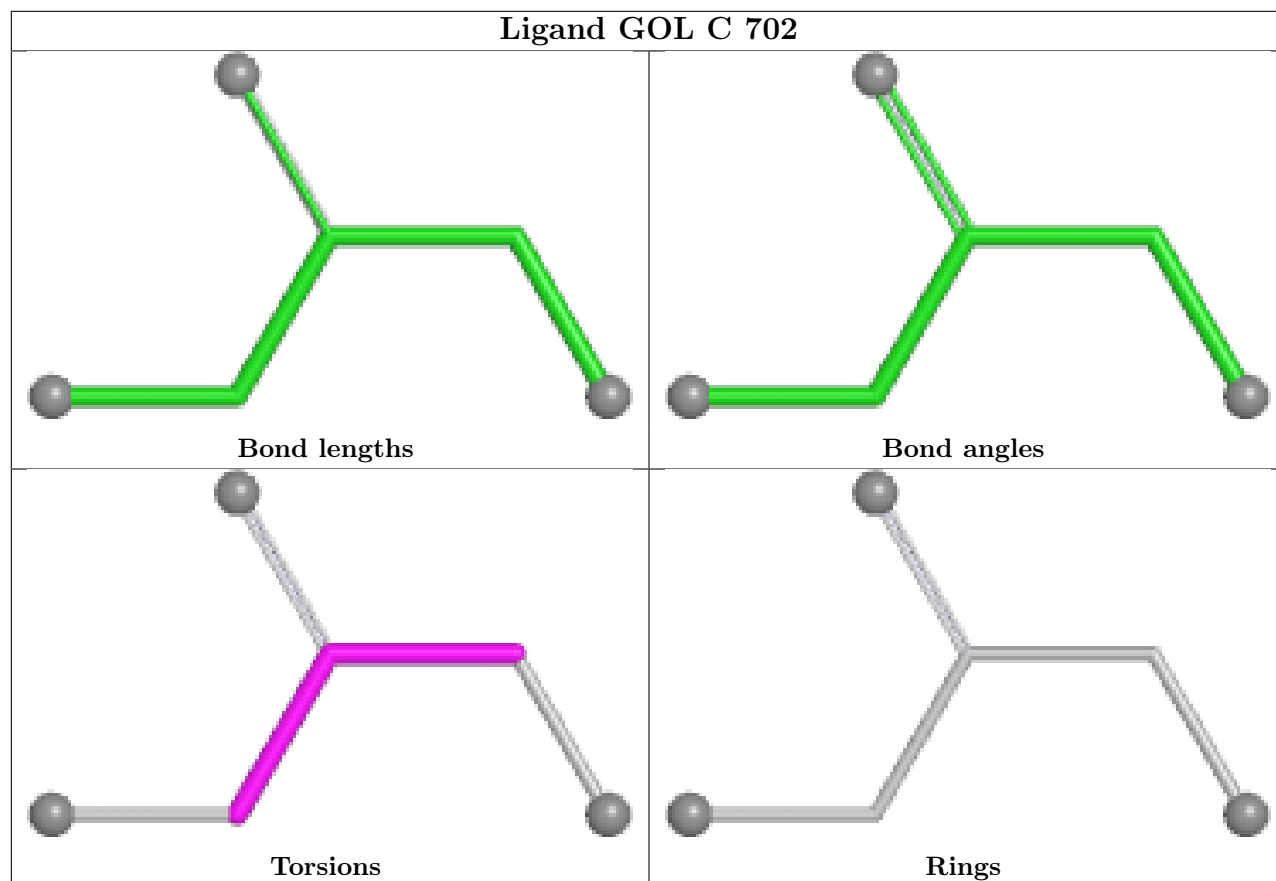
Bond angles



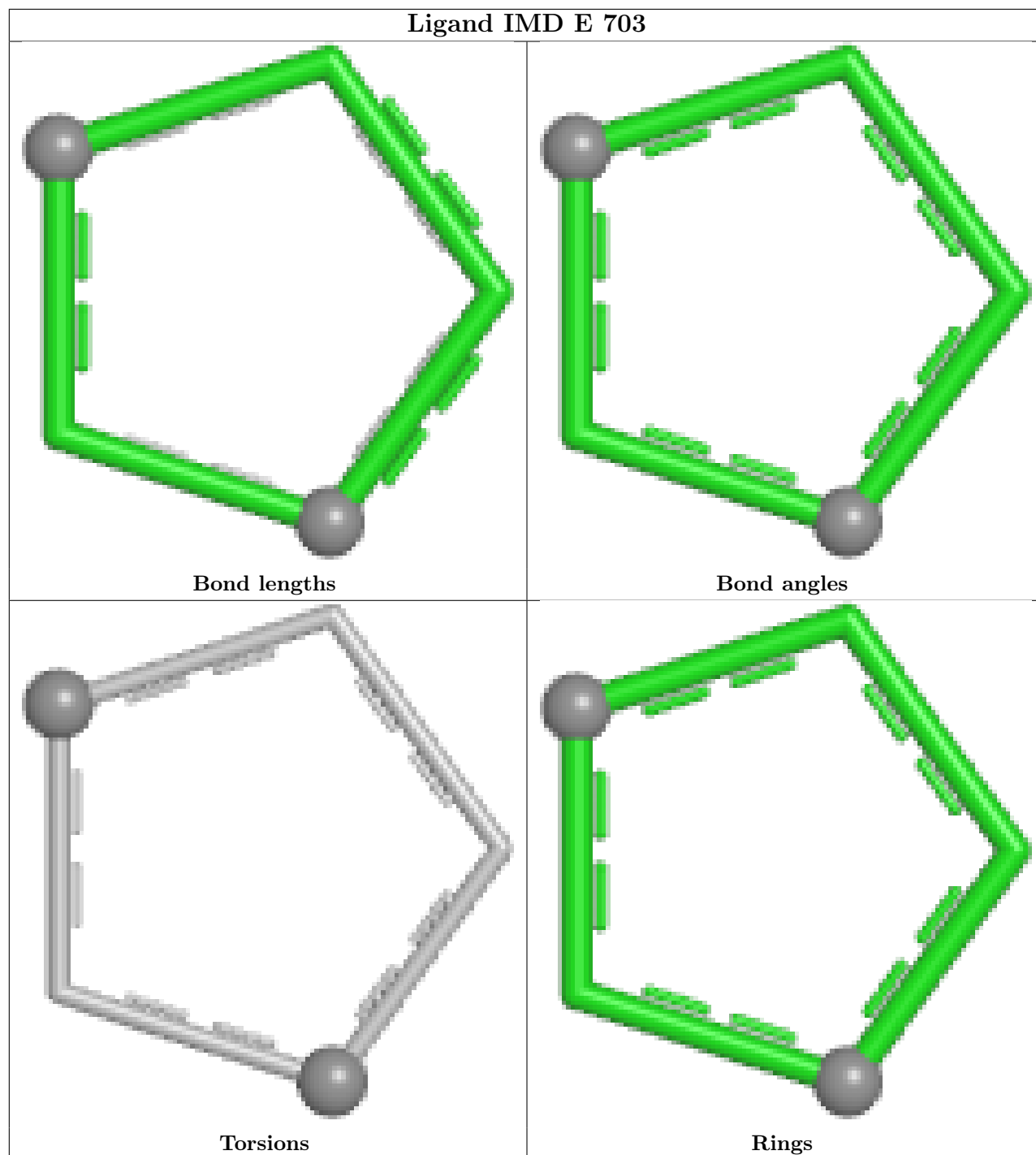
Torsions



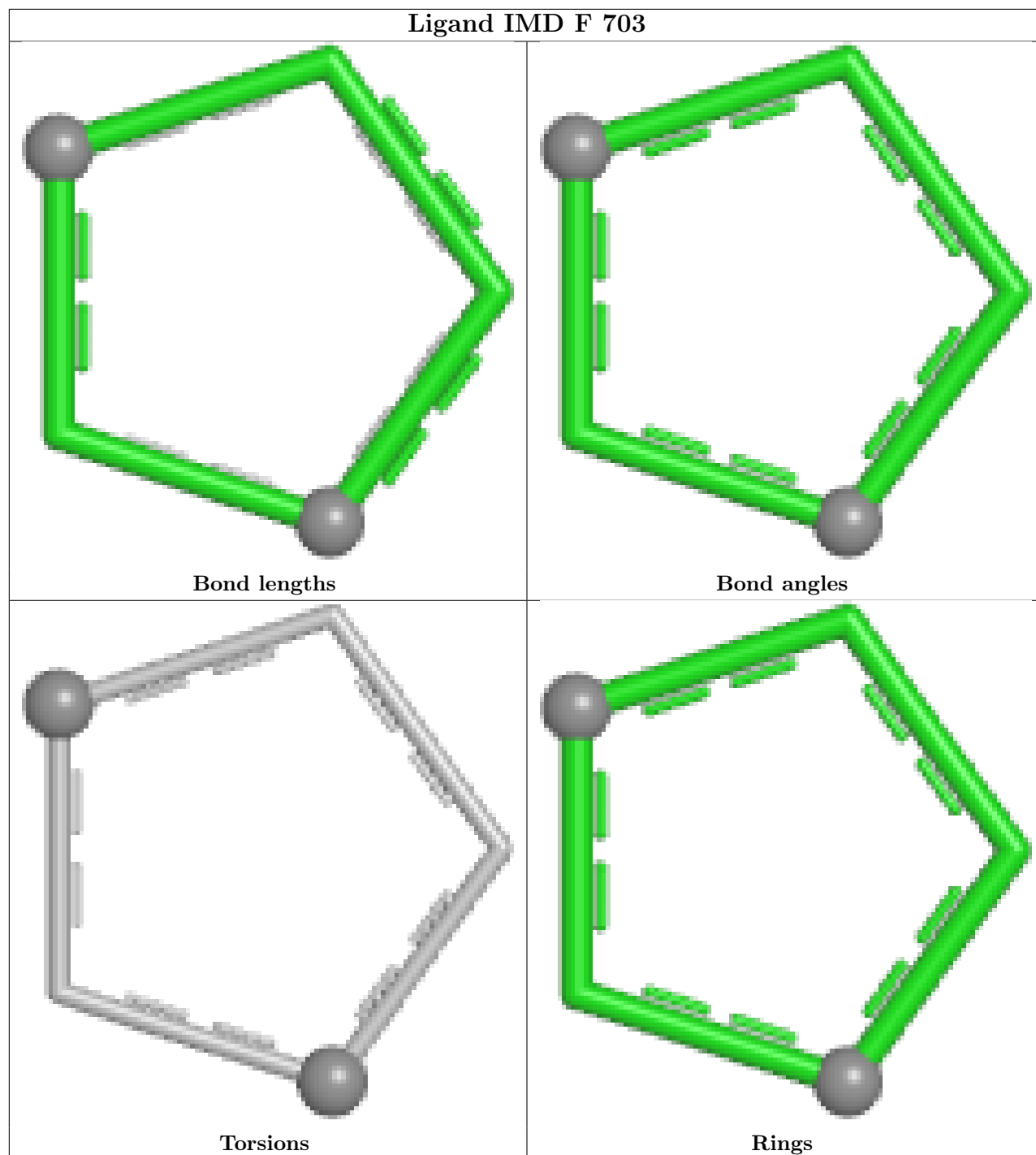
Rings

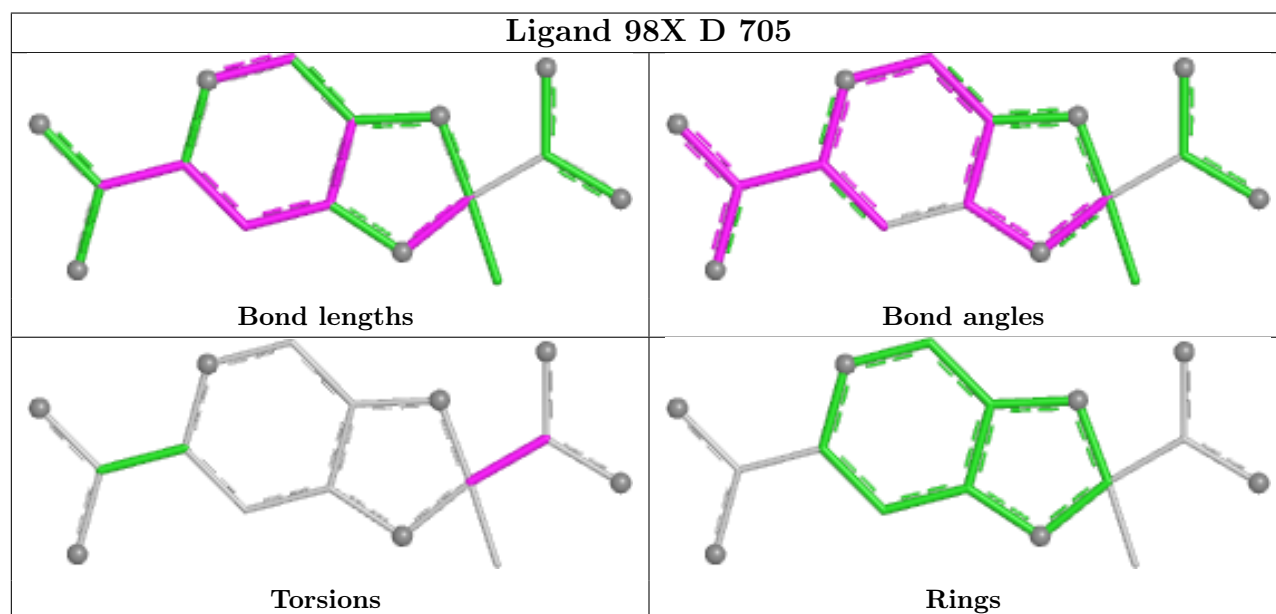
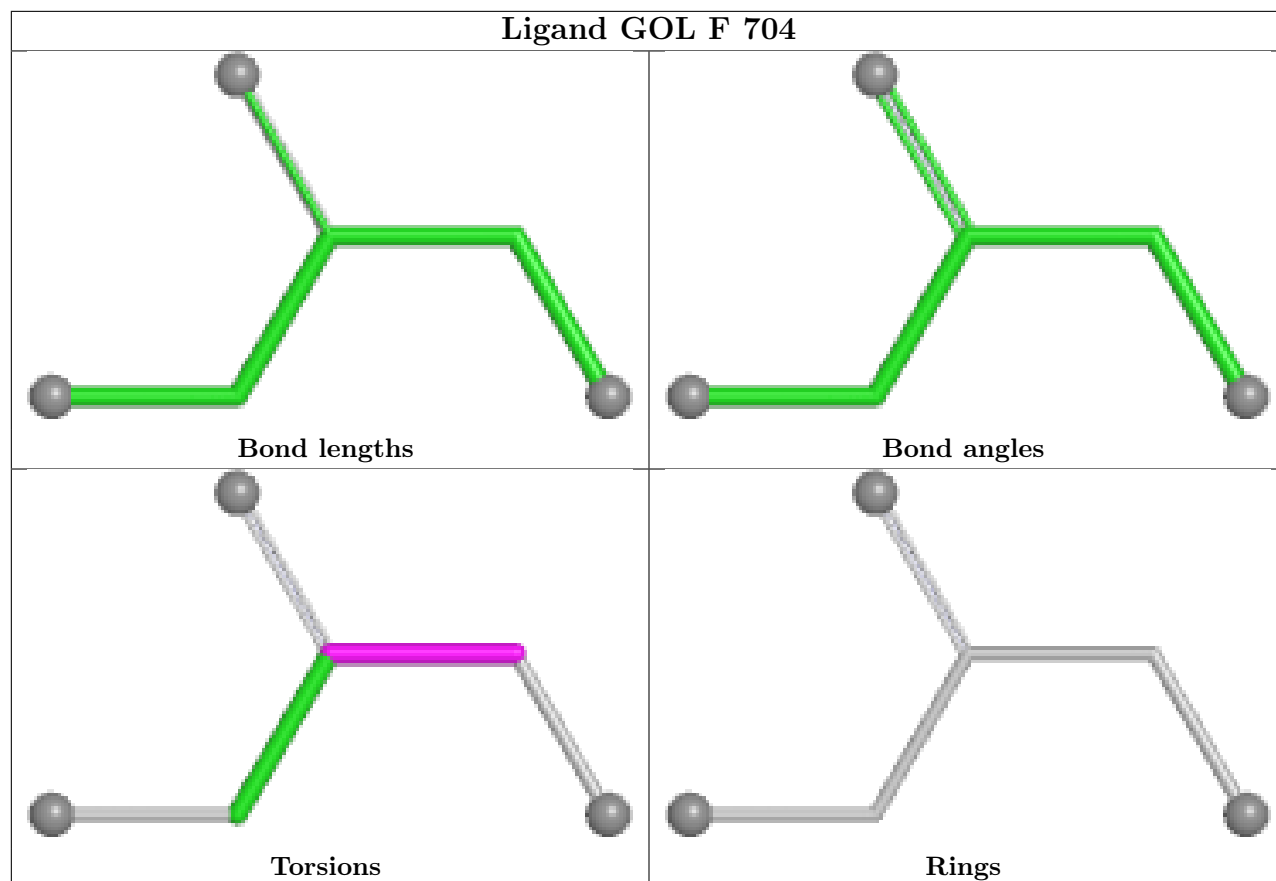


Ligand IMD E 703

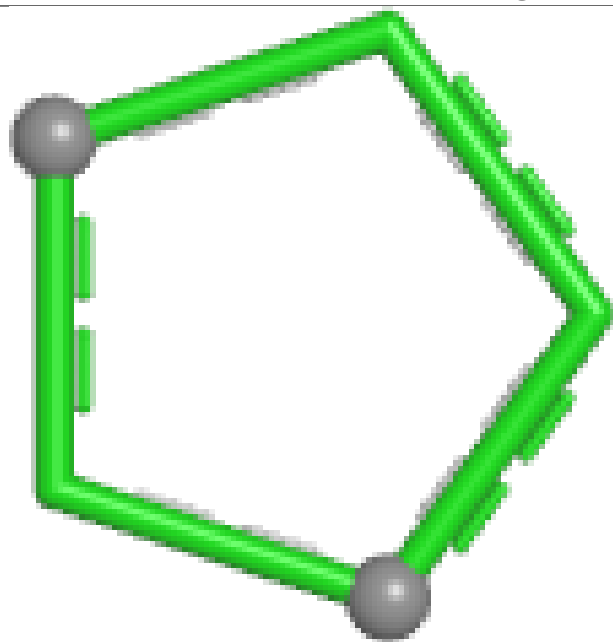


Ligand IMD F 703

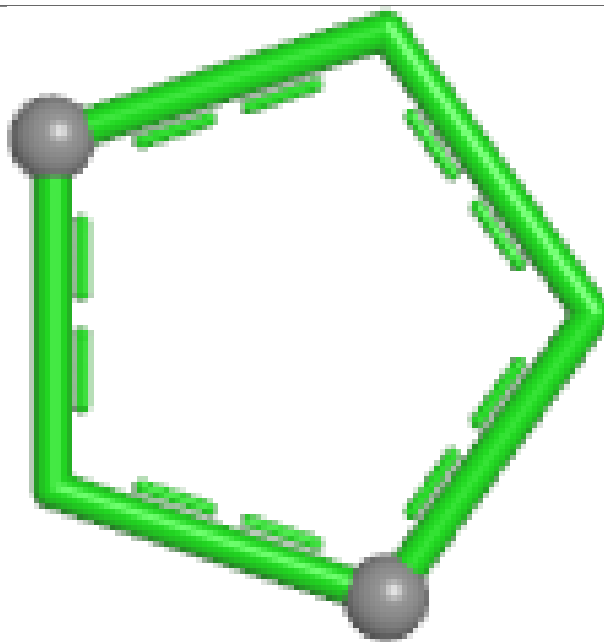




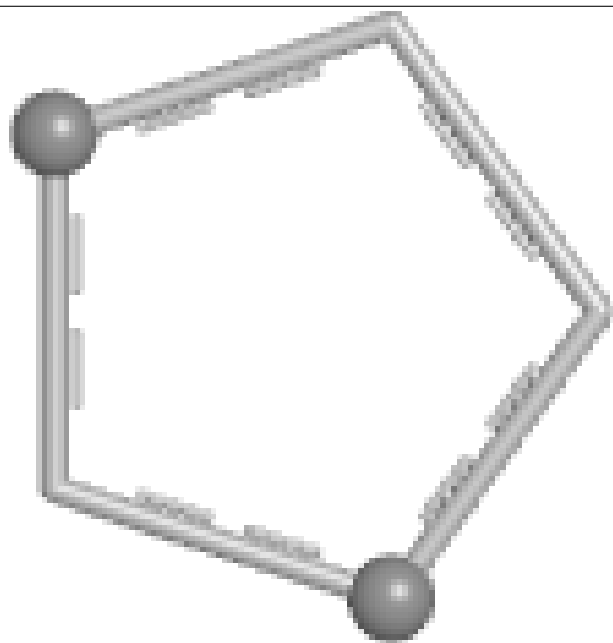
Ligand IMD D 701



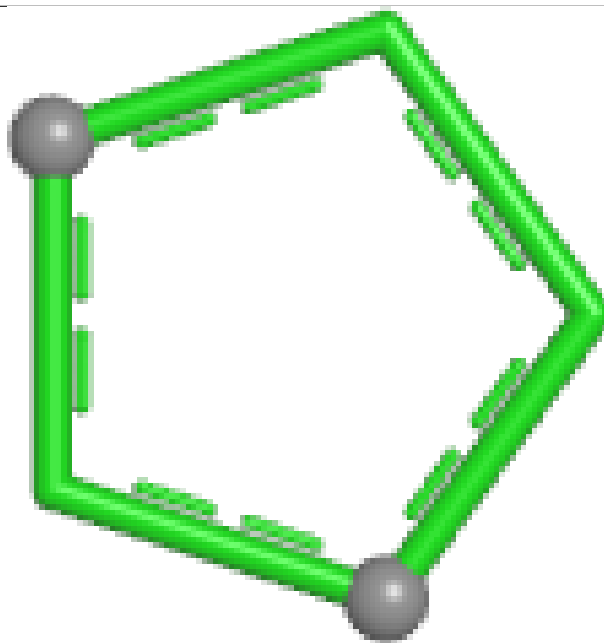
Bond lengths



Bond angles

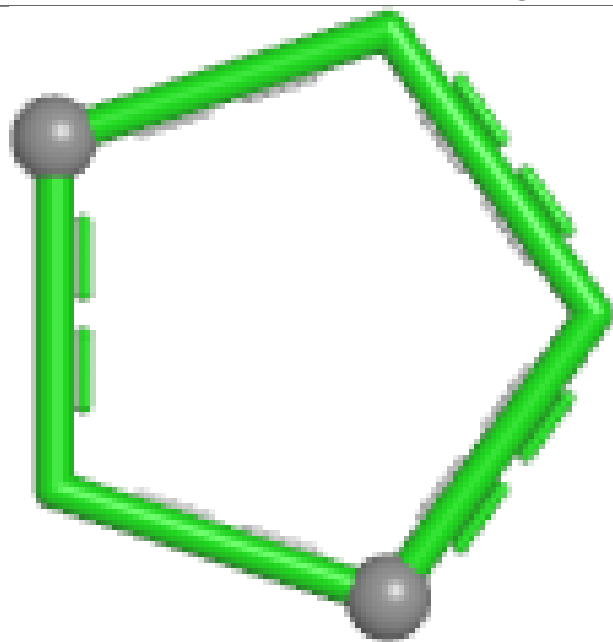


Torsions

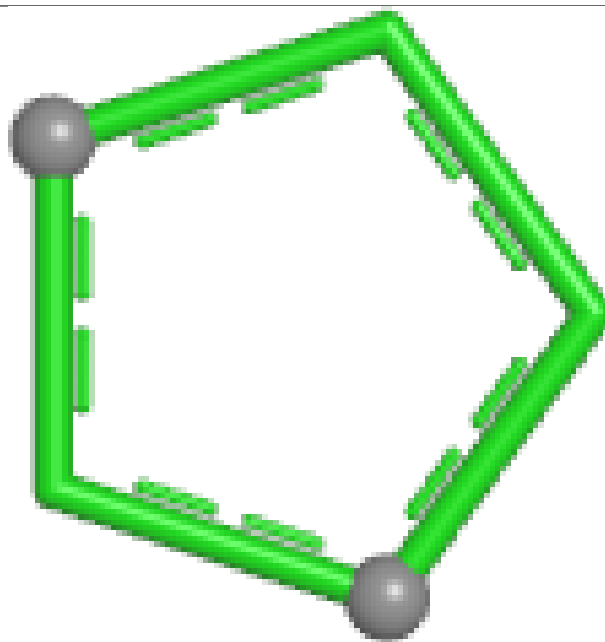


Rings

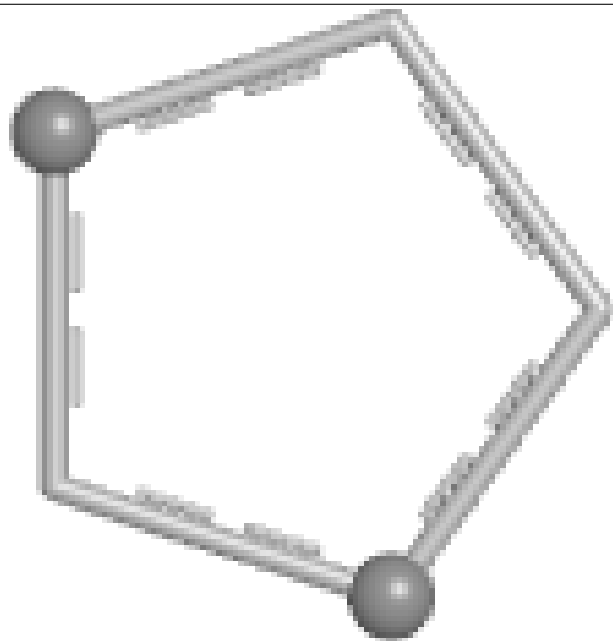
Ligand IMD A 704



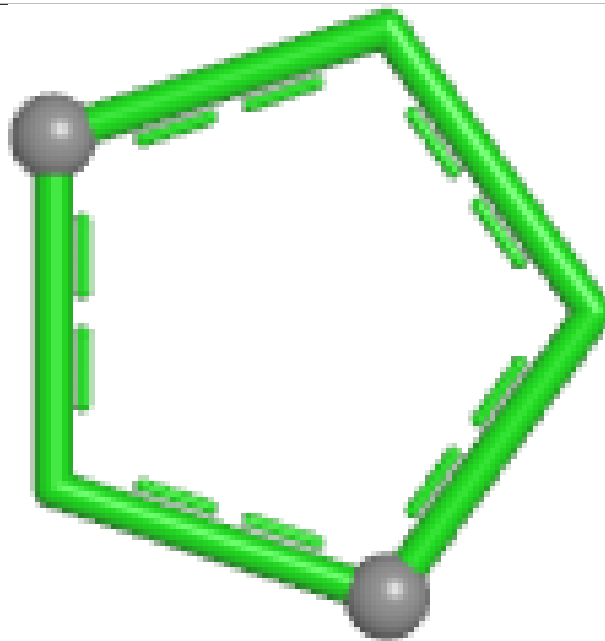
Bond lengths



Bond angles

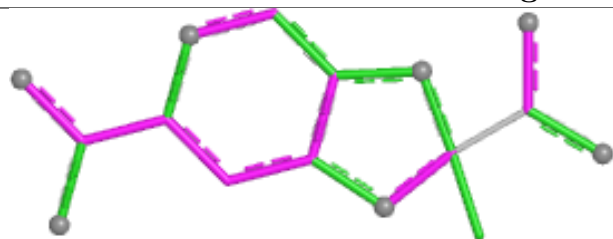


Torsions

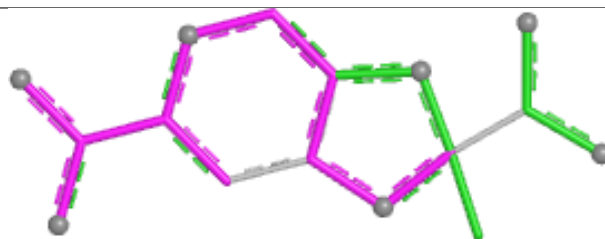


Rings

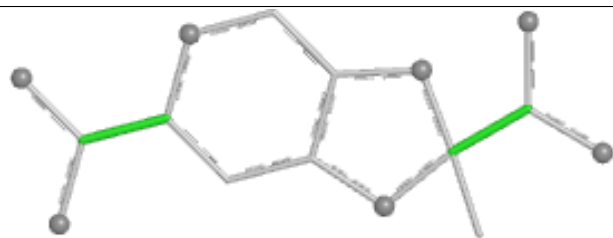
Ligand 98X B 704



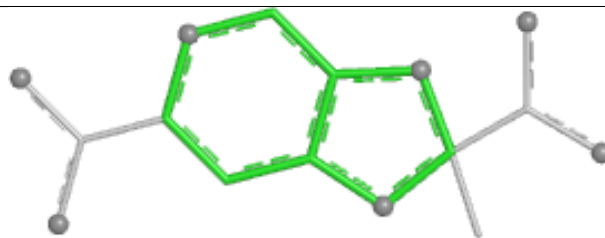
Bond lengths



Bond angles

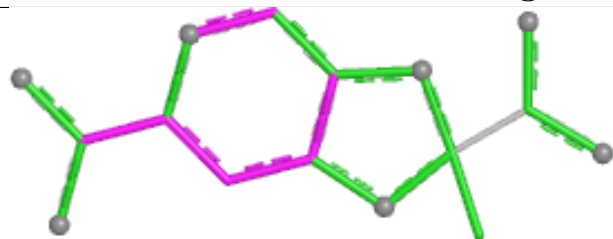


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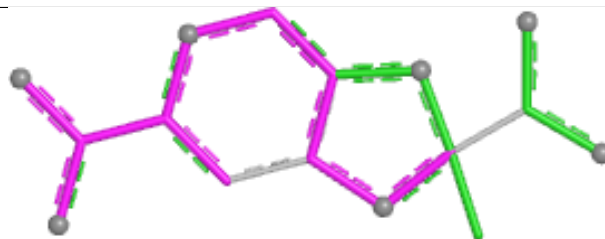


Rings

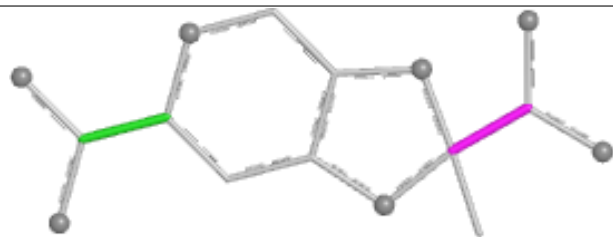
Ligand 98X A 708



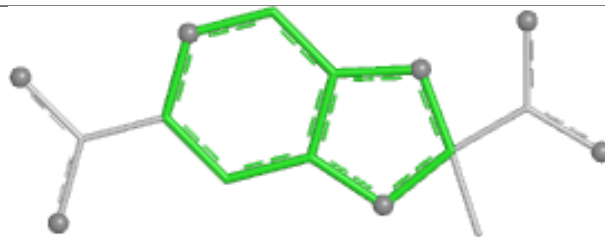
Bond lengths



Bond angles

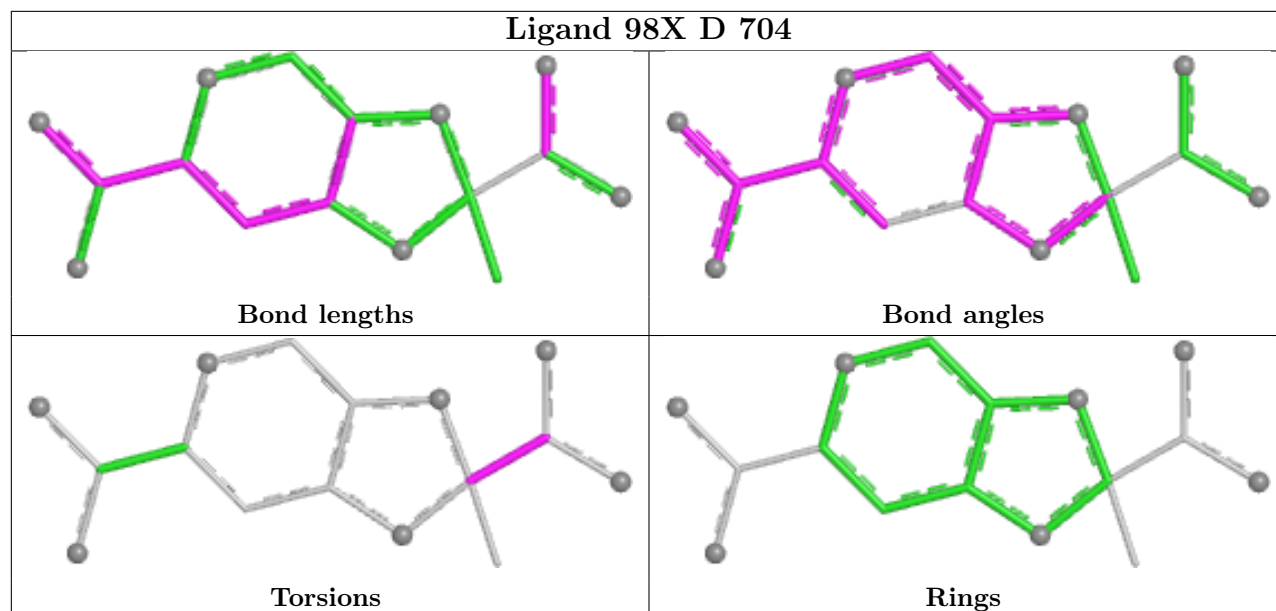


Torsions

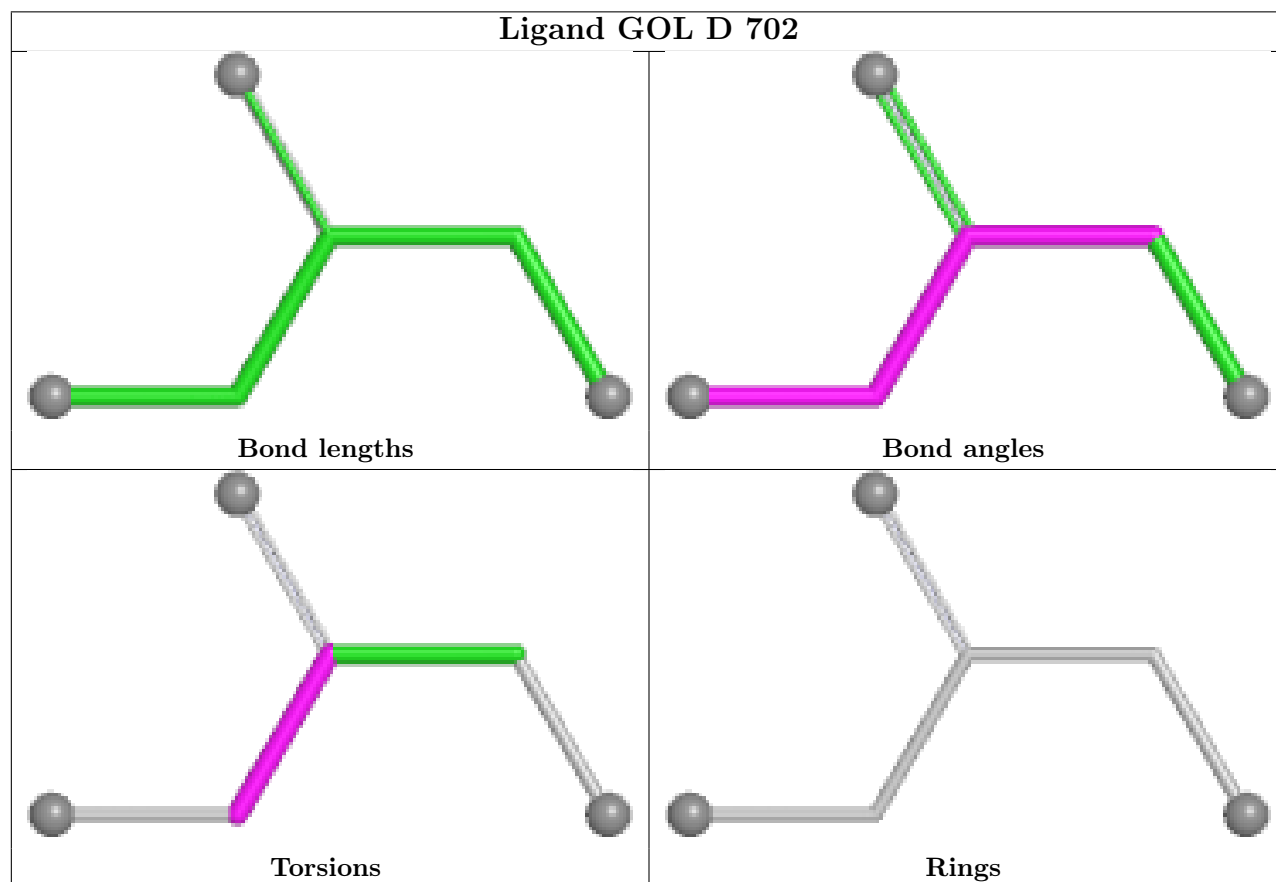


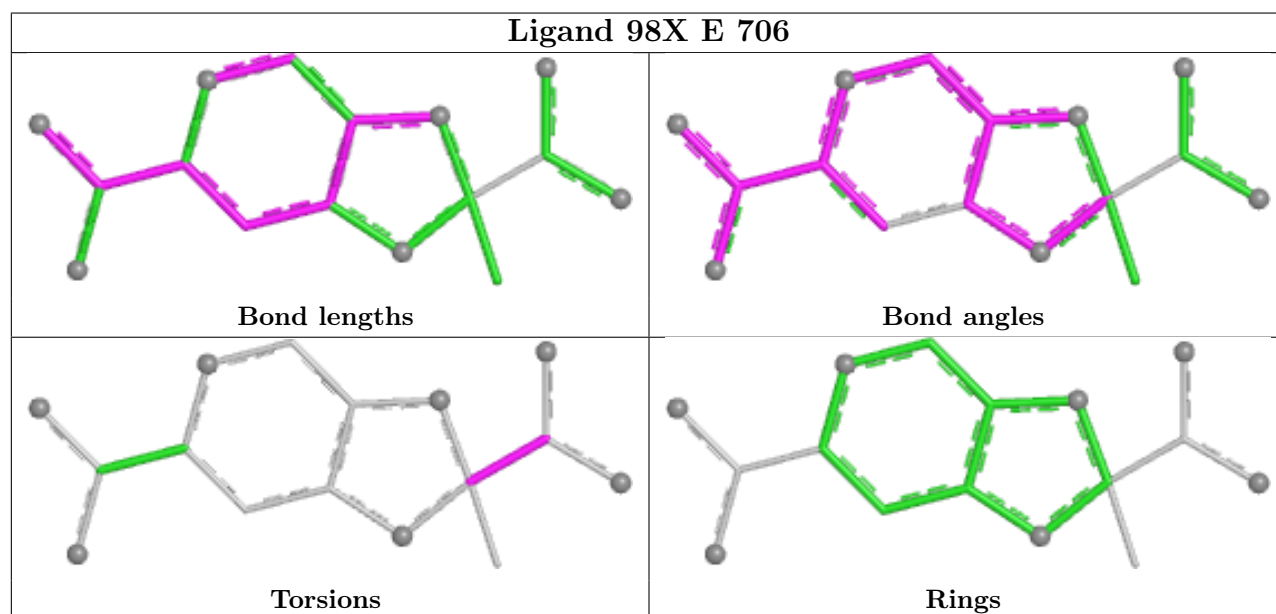
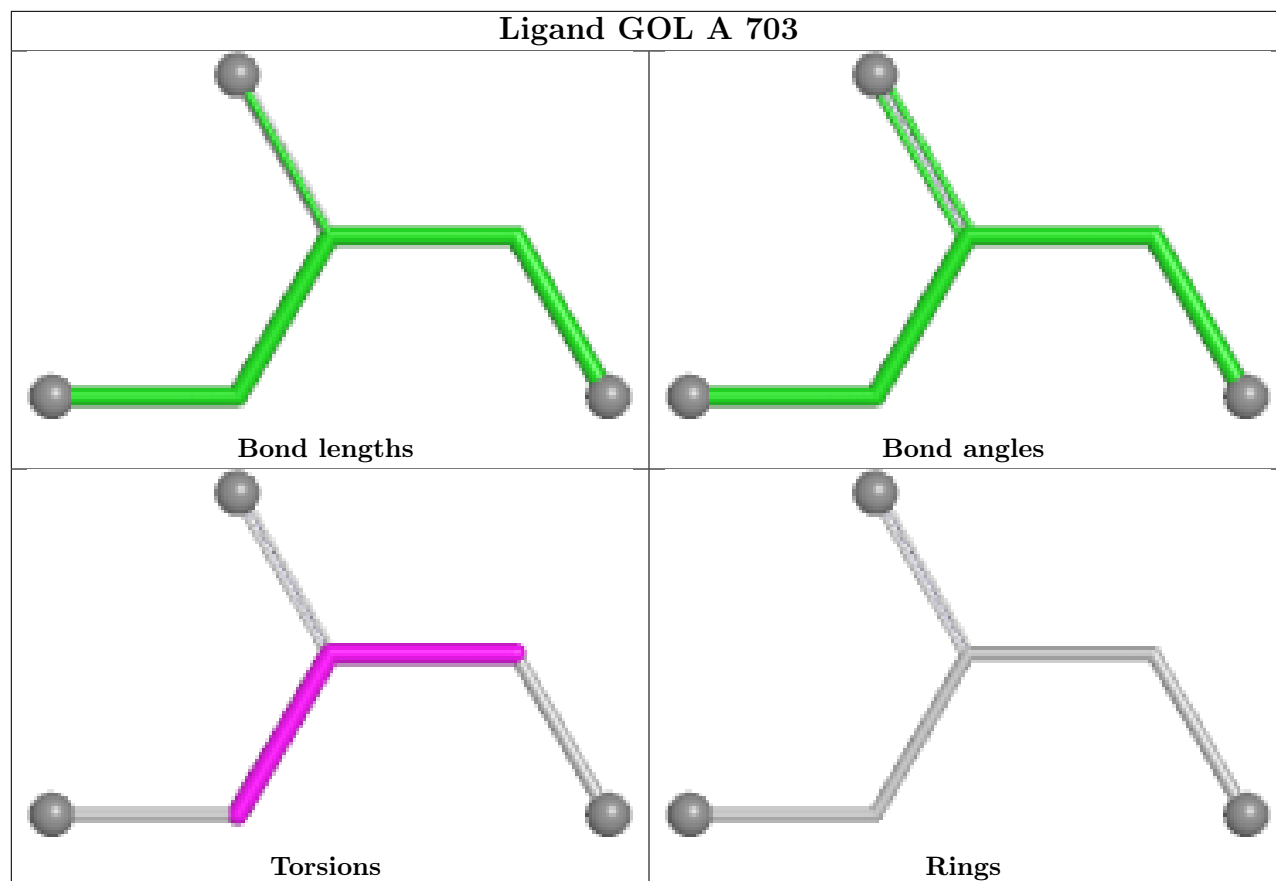
Rings

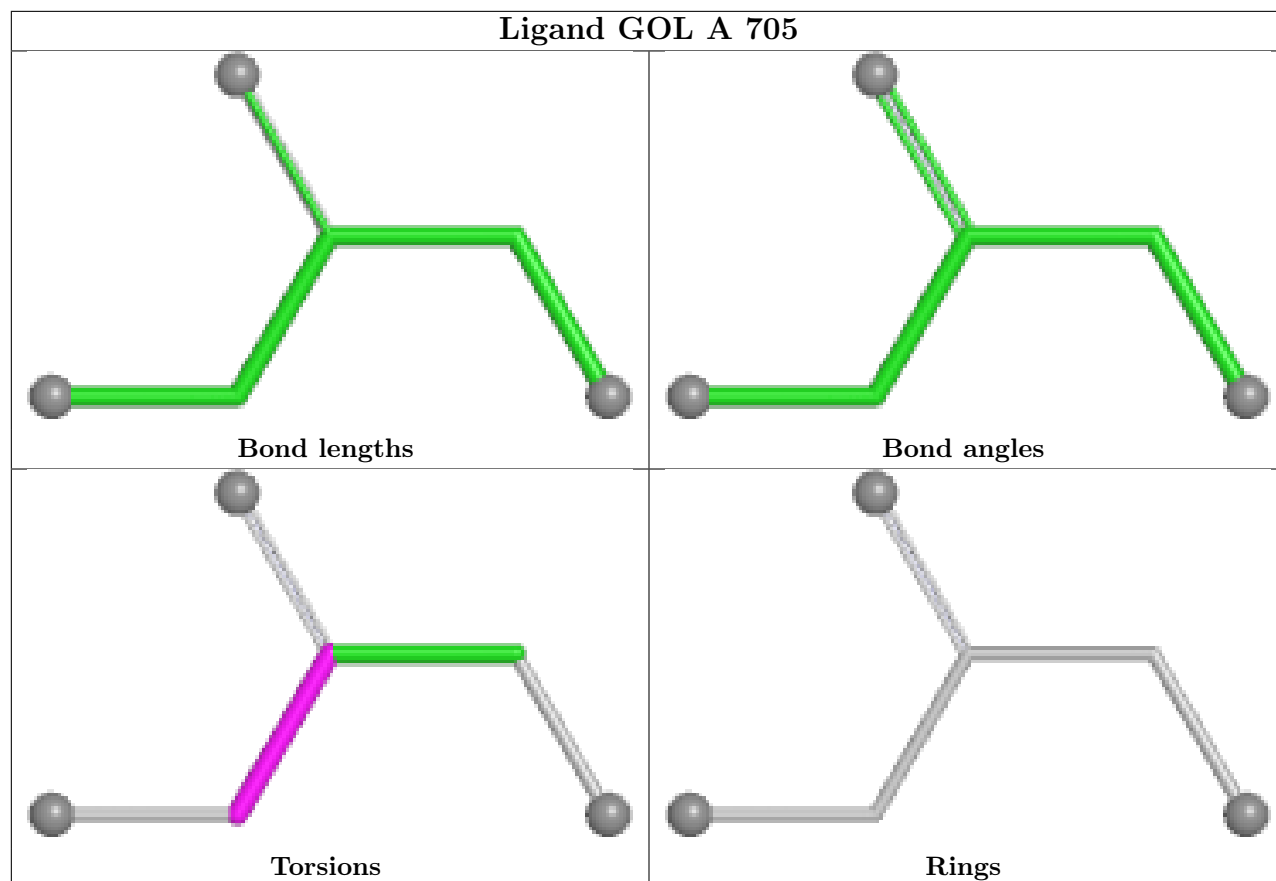
Ligand 98X D 704



Ligand GOL D 702







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, 95th 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 ²)	Q<0.9
1	A	642/671 (95%)	-0.52	3 (0%) 87 90	7, 15, 29, 68	4 (0%)
1	B	634/671 (94%)	-0.44	11 (1%) 69 72	9, 15, 40, 90	3 (0%)
1	C	642/671 (95%)	-0.41	12 (1%) 66 68	8, 16, 35, 63	1 (0%)
1	D	622/671 (92%)	-0.60	8 (1%) 75 78	7, 13, 28, 76	2 (0%)
1	E	644/671 (95%)	-0.58	6 (0%) 81 84	6, 14, 29, 71	4 (0%)
1	F	642/671 (95%)	-0.51	9 (1%) 73 77	7, 14, 41, 92	2 (0%)
All	All	3826/4026 (95%)	-0.51	49 (1%) 75 78	6, 14, 34, 92	16 (0%)

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	622	VAL	7.3
1	D	36	SER	5.7
1	B	622	VAL	4.5
1	D	35	GLY	4.5
1	E	8	ALA	4.2

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](#)

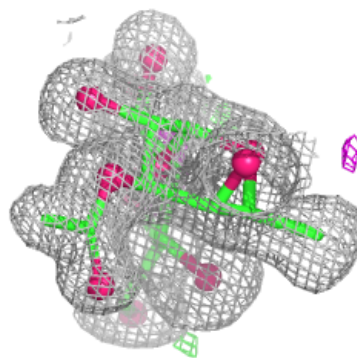
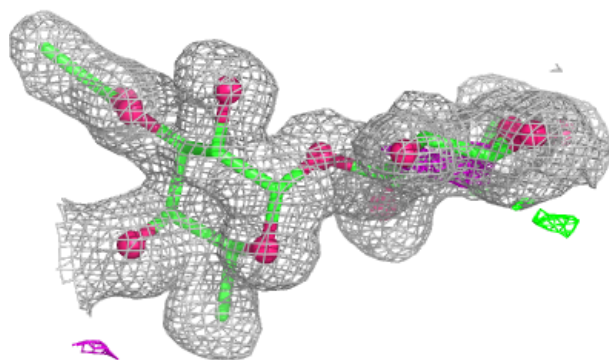
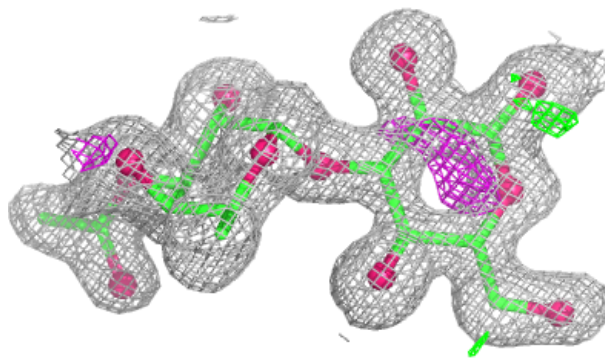
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	BGC	M	1	12/12	0.87	0.09	27,37,44,51	0
2	BGC	P	1	12/12	0.88	0.10	24,37,48,58	0
2	BGC	H	1	12/12	0.89	0.09	25,32,42,45	0
2	BGC	I	1	12/12	0.89	0.09	27,40,55,58	0
2	BGC	O	1	12/12	0.92	0.08	25,34,43,52	0
2	98U	I	2	13/14	0.93	0.09	21,23,28,29	0
2	98U	H	2	13/14	0.93	0.08	16,22,27,27	0
2	98U	P	2	13/14	0.93	0.09	18,20,25,26	0
2	98U	M	2	13/14	0.95	0.07	20,22,28,29	0
2	98U	J	2	13/14	0.95	0.07	18,21,26,29	0
2	98U	O	2	13/14	0.95	0.08	18,20,24,26	0
2	BGC	K	1	12/12	0.95	0.08	19,24,33,39	0
2	BGC	G	1	12/12	0.95	0.07	16,21,26,31	0
2	BGC	L	1	12/12	0.96	0.07	13,18,32,32	0
2	BGC	N	1	12/12	0.96	0.07	15,20,35,36	0
2	BGC	J	1	12/12	0.96	0.06	16,21,27,33	0
2	98U	G	2	13/14	0.97	0.06	16,19,23,27	0
2	98U	N	2	13/14	0.97	0.06	17,19,22,25	0
2	98U	L	2	13/14	0.97	0.06	14,16,22,22	0
2	98U	K	2	13/14	0.98	0.05	13,15,19,21	0

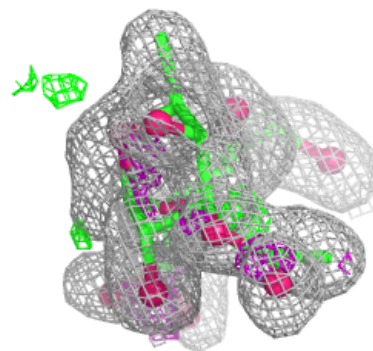
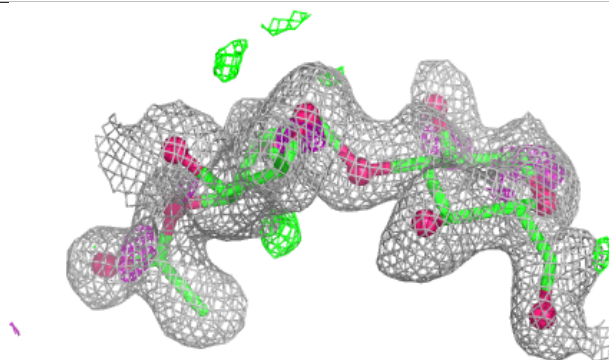
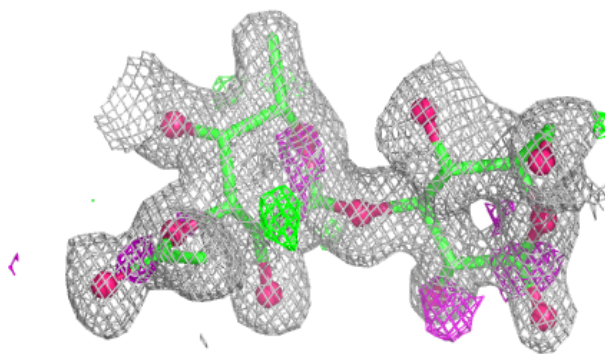
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

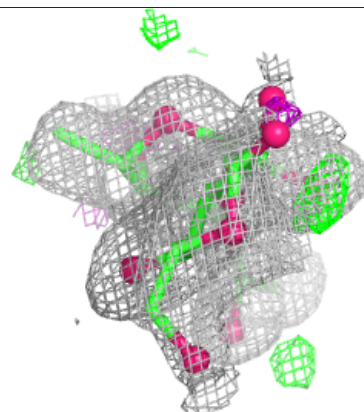
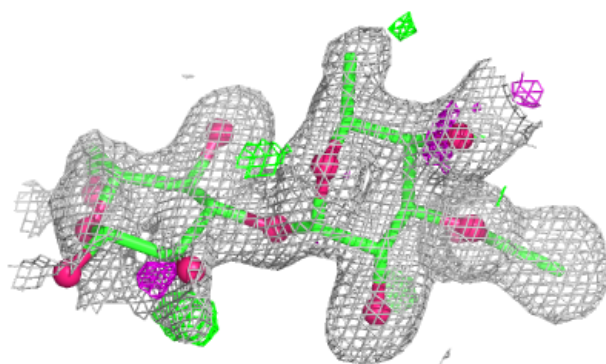
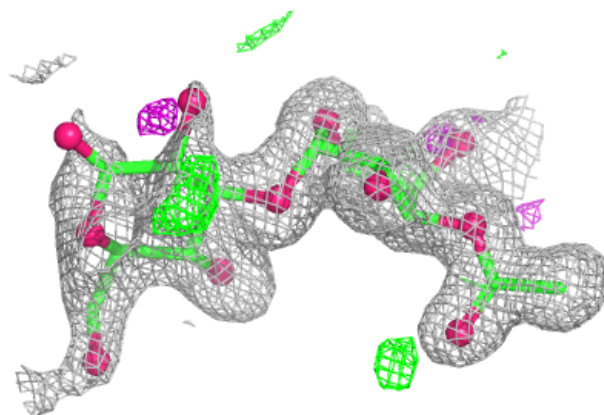
**Electron density around Chain H:**

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

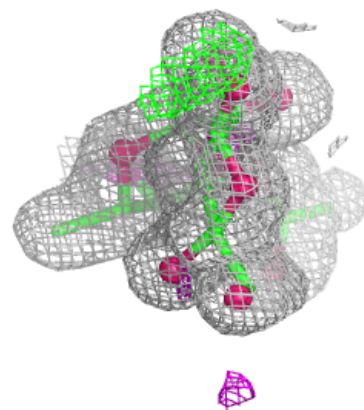
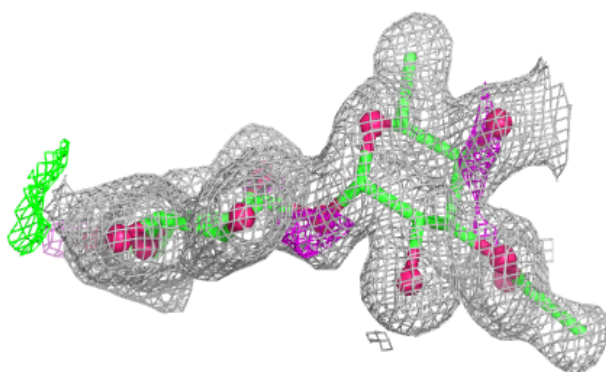
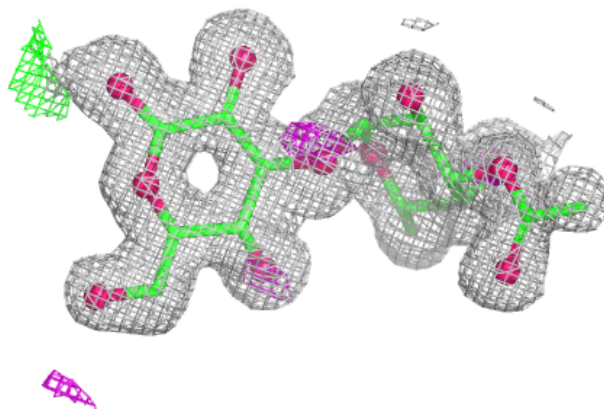


Electron density around Chain I:

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

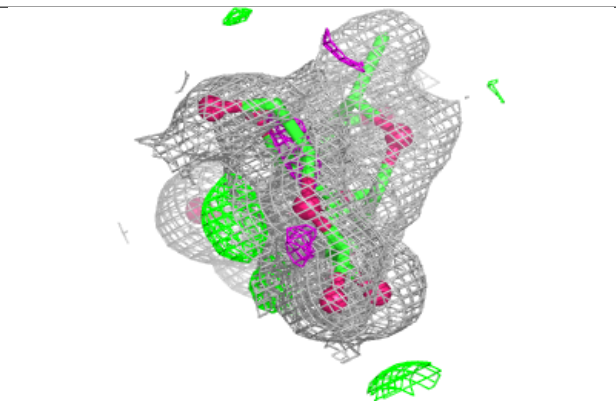
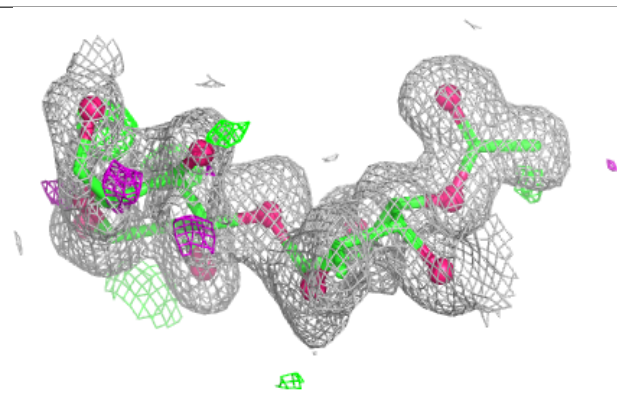
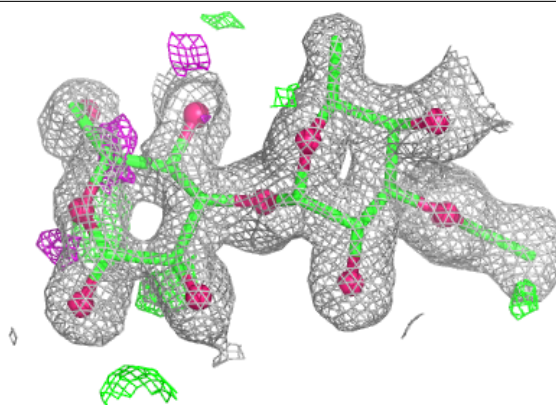
**Electron density around Chain J:**

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

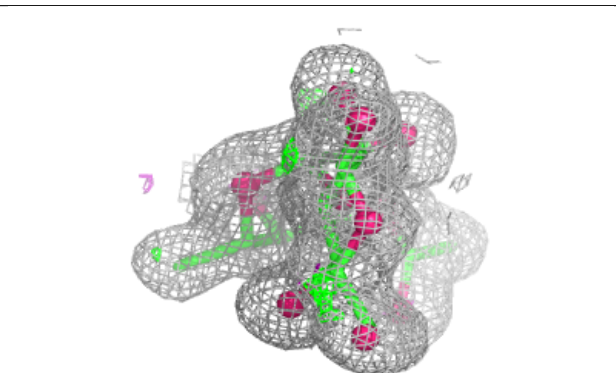
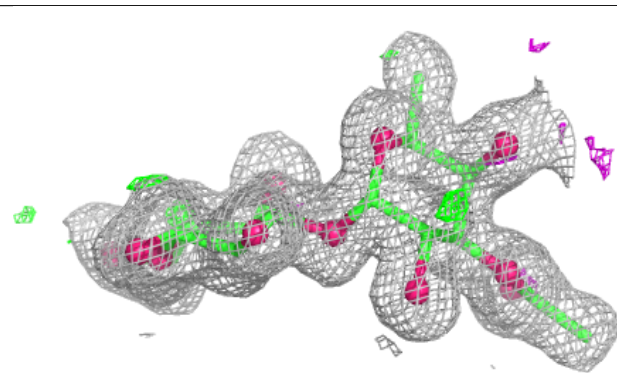
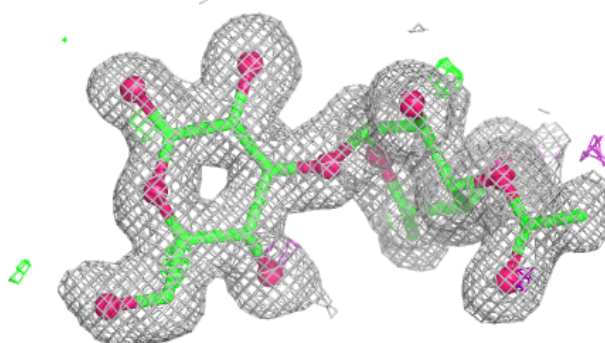


Electron density around Chain K:

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

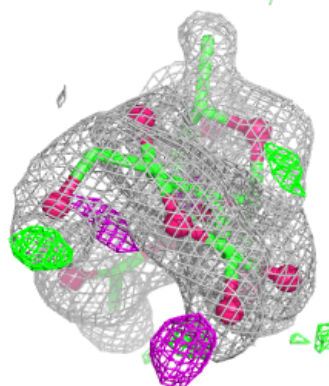
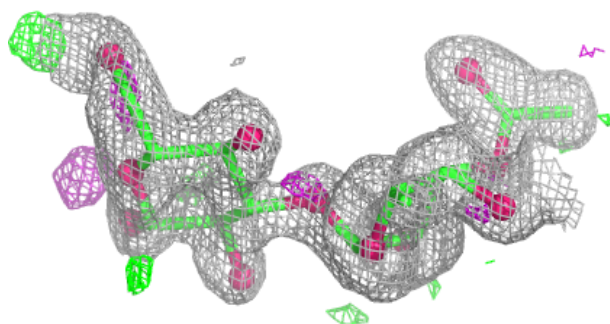
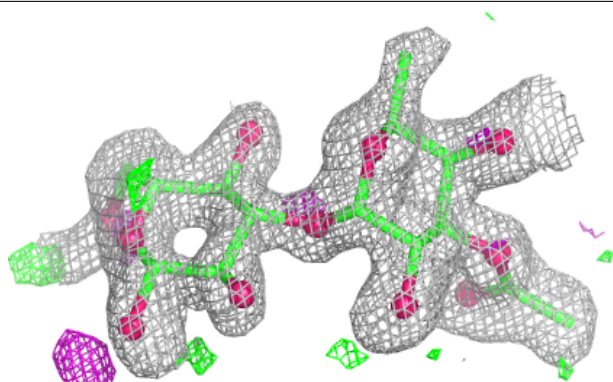
**Electron density around Chain L:**

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

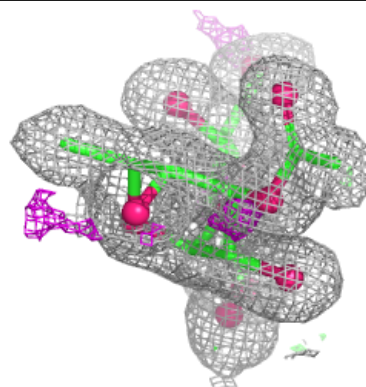
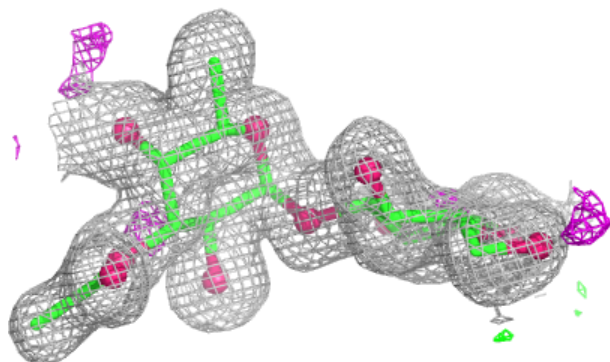
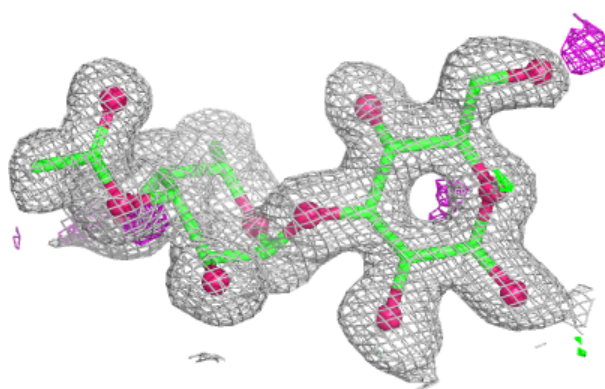


Electron density around Chain M:

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

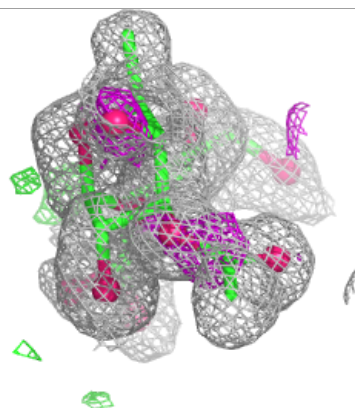
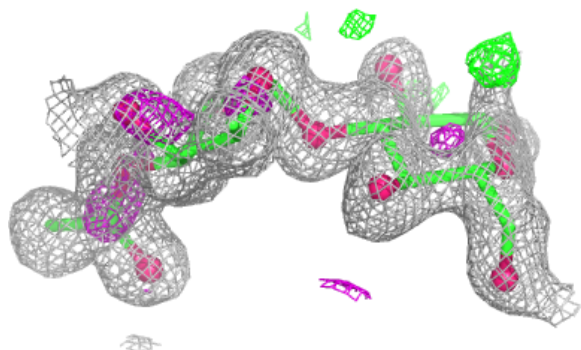
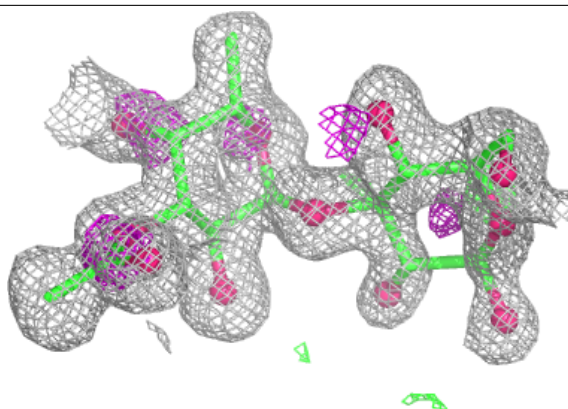
**Electron density around Chain N:**

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

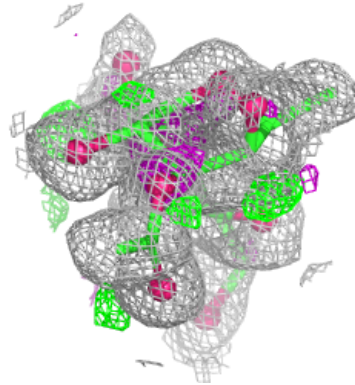
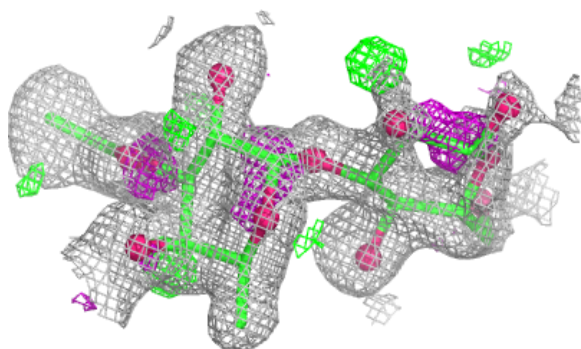
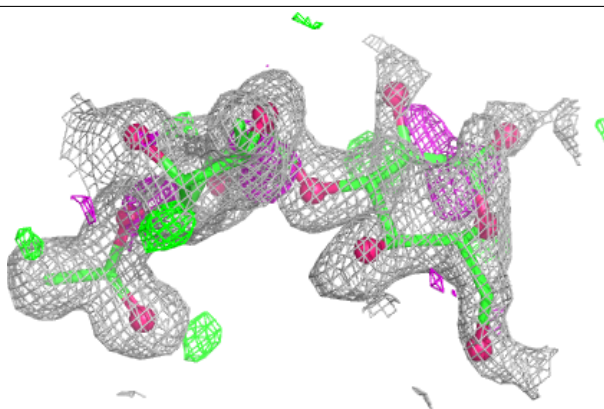


Electron density around Chain O:

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

**Electron density around Chain P:**

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



6.4 Ligands ⓘ

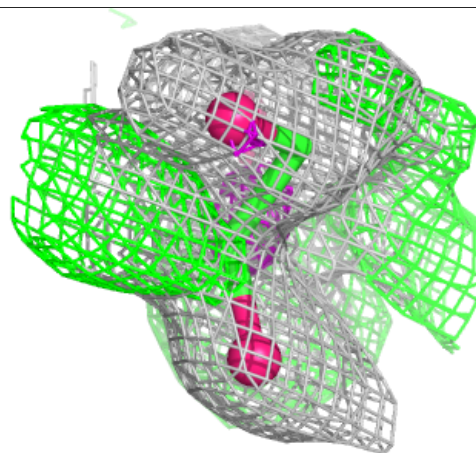
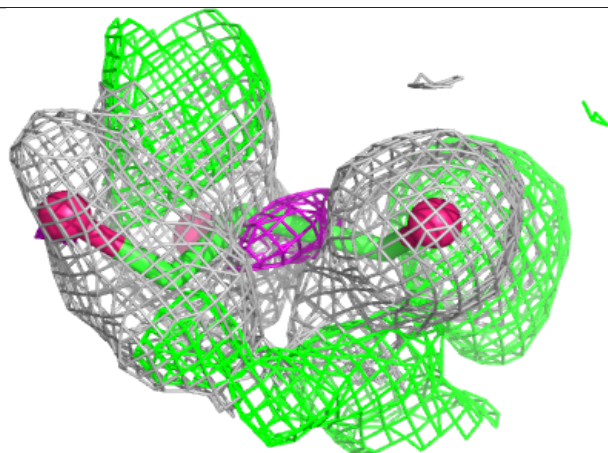
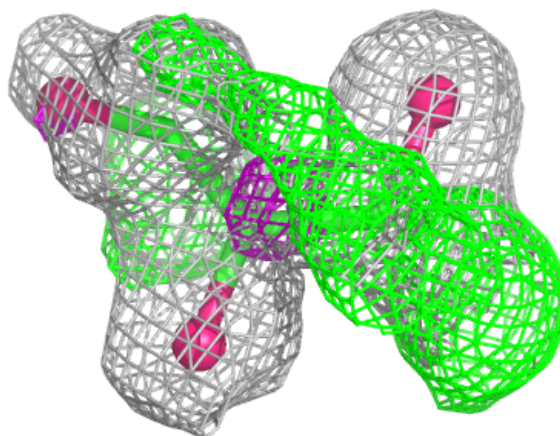
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	F	702	6/6	0.77	0.15	18,29,33,43	0
3	IMD	B	702	5/5	0.78	0.12	35,37,40,41	0
4	GOL	B	703	6/6	0.81	0.15	19,32,36,41	0
4	GOL	D	702	6/6	0.83	0.13	27,35,36,36	0
4	GOL	A	702	6/6	0.85	0.12	23,31,34,42	0
4	GOL	D	703	6/6	0.86	0.12	20,27,28,33	0
3	IMD	A	701	5/5	0.87	0.12	35,37,43,44	0
4	GOL	E	704	6/6	0.88	0.10	22,32,37,40	0
3	IMD	F	703	5/5	0.89	0.10	23,30,32,37	0
4	GOL	F	704	6/6	0.90	0.13	21,25,30,32	0
5	98X	A	706	16/16	0.90	0.09	20,25,38,39	0
4	GOL	C	701	6/6	0.91	0.11	20,32,34,36	0
4	GOL	A	705	6/6	0.91	0.10	20,27,29,34	0
4	GOL	F	701	6/6	0.91	0.09	17,23,24,30	0
5	98X	C	704	16/16	0.91	0.08	23,26,39,49	0
5	98X	E	706	16/16	0.92	0.08	20,24,36,41	0
3	IMD	E	702	5/5	0.93	0.08	26,26,29,32	0
3	IMD	A	704	5/5	0.93	0.09	32,37,43,44	0
3	IMD	C	703	5/5	0.93	0.09	22,25,31,35	0
4	GOL	E	701	6/6	0.94	0.09	18,23,27,34	0
3	IMD	D	701	5/5	0.94	0.09	19,24,33,36	0
4	GOL	B	701	6/6	0.94	0.09	21,27,28,41	0
5	98X	D	704	16/16	0.94	0.07	17,21,32,37	0
5	98X	E	705	16/16	0.94	0.07	21,23,28,30	0
4	GOL	A	703	6/6	0.94	0.09	22,25,29,31	0
3	IMD	E	703	5/5	0.95	0.08	20,26,32,33	0
4	GOL	C	702	6/6	0.95	0.08	22,27,30,30	0
5	98X	D	705	16/16	0.95	0.06	19,21,26,27	0
5	98X	A	707	16/16	0.95	0.06	21,24,28,29	0
5	98X	B	704	16/16	0.95	0.07	21,24,32,34	0
5	98X	F	705	16/16	0.95	0.06	18,22,25,26	0
5	98X	A	708	16/16	0.96	0.05	16,18,23,26	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.

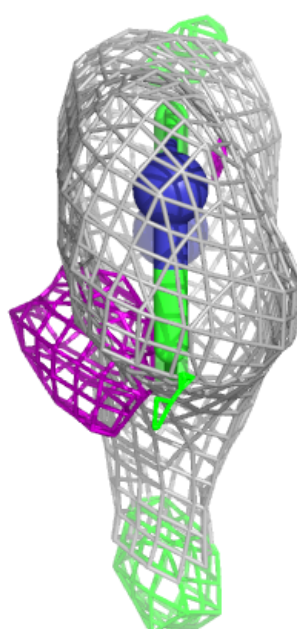
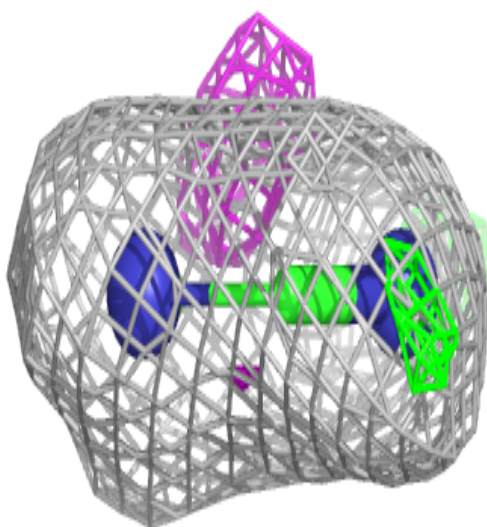
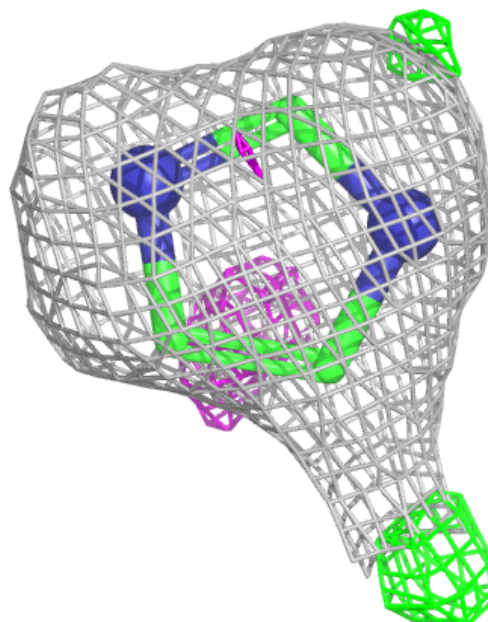
Electron density around GOL F 702:

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



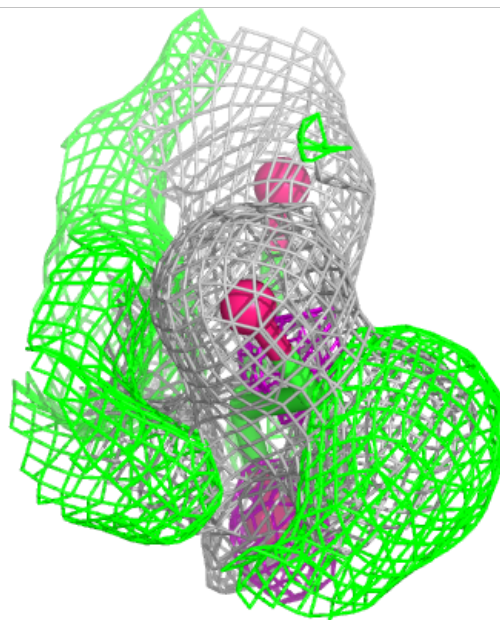
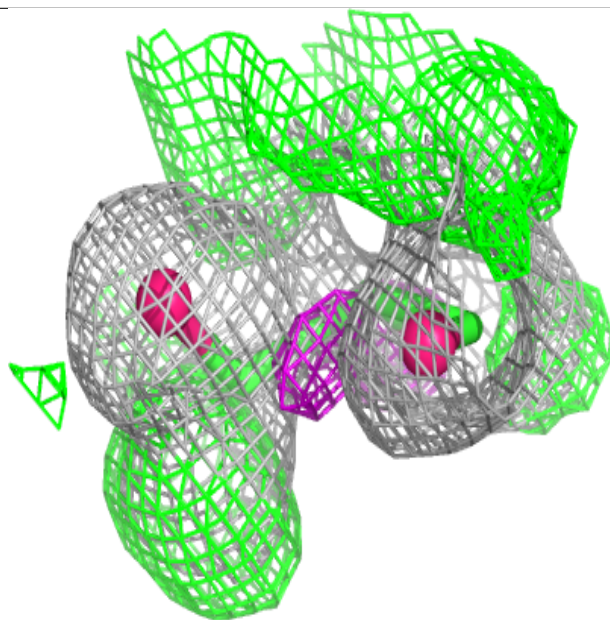
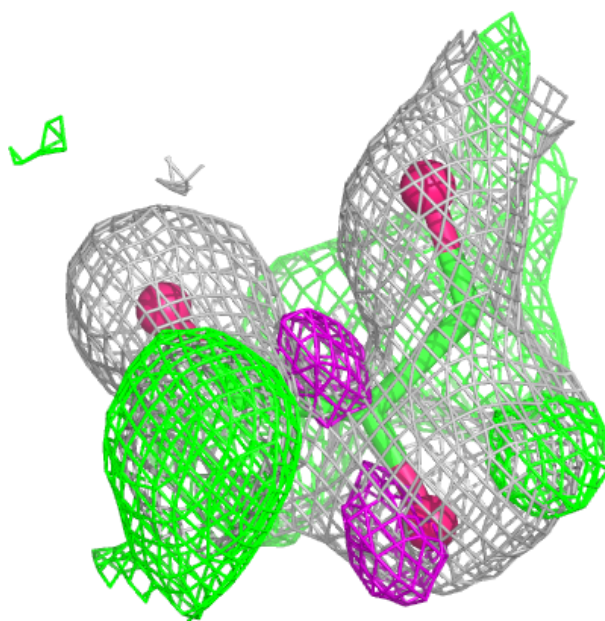
Electron density around IMD B 702:

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



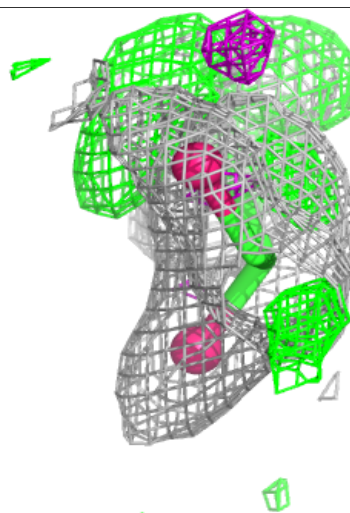
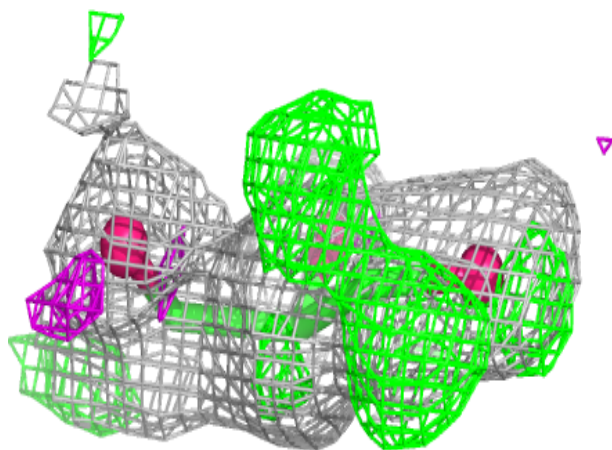
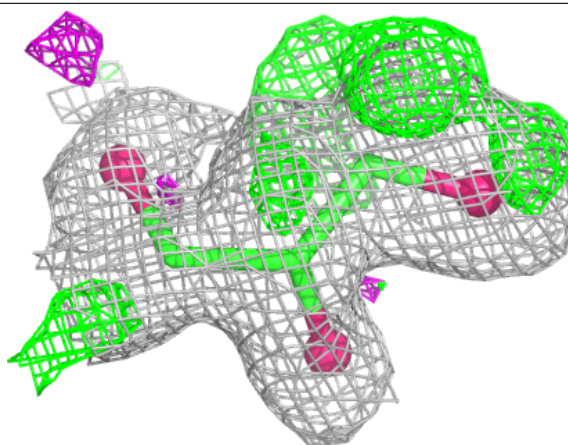
Electron density around GOL B 703:

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



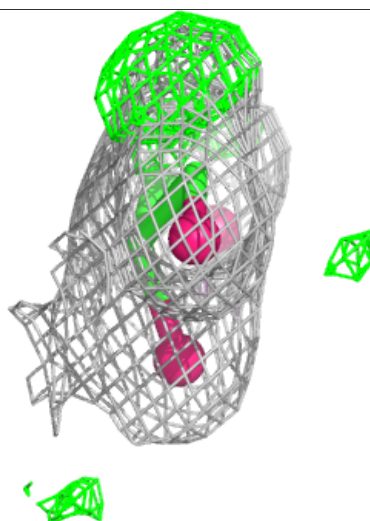
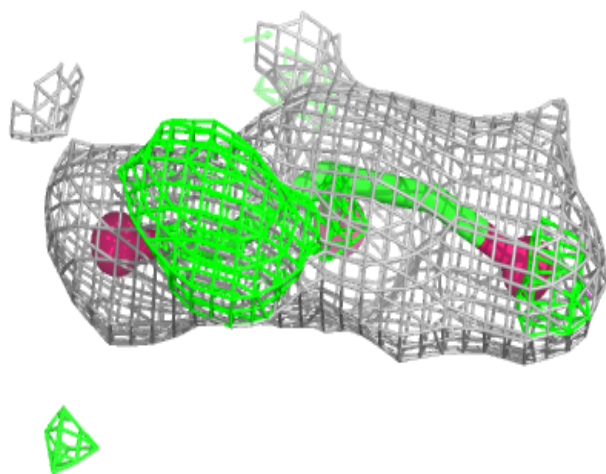
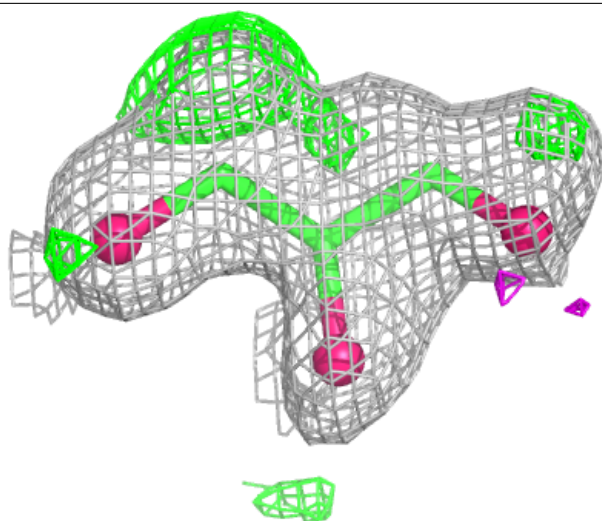
Electron density around GOL D 702:

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



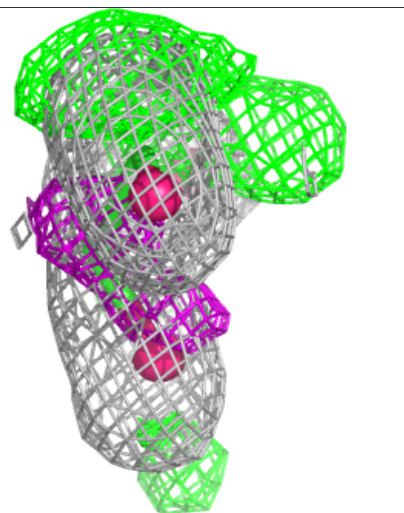
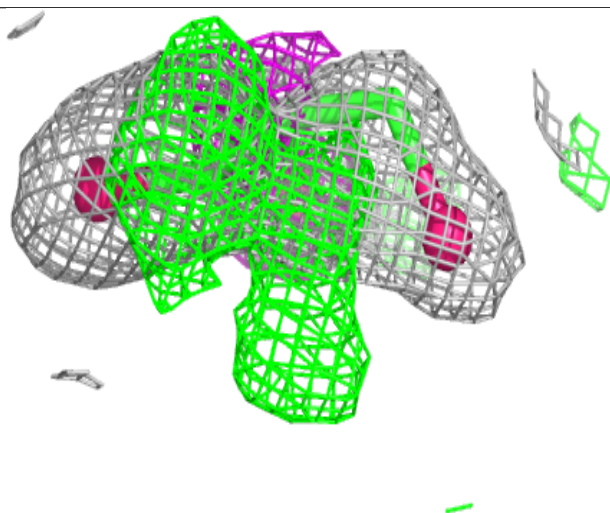
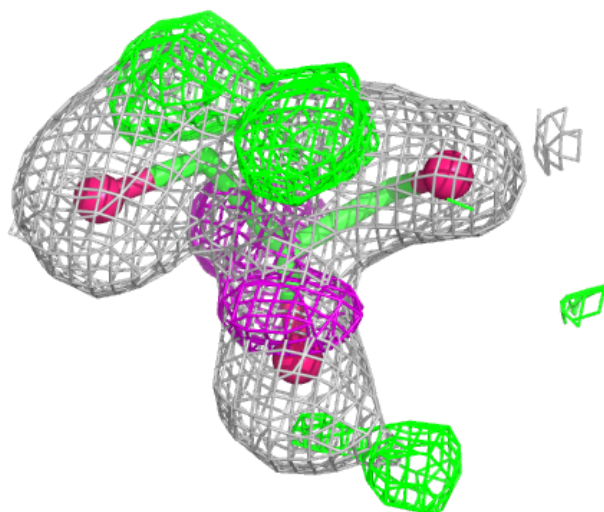
Electron density around GOL A 702:

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



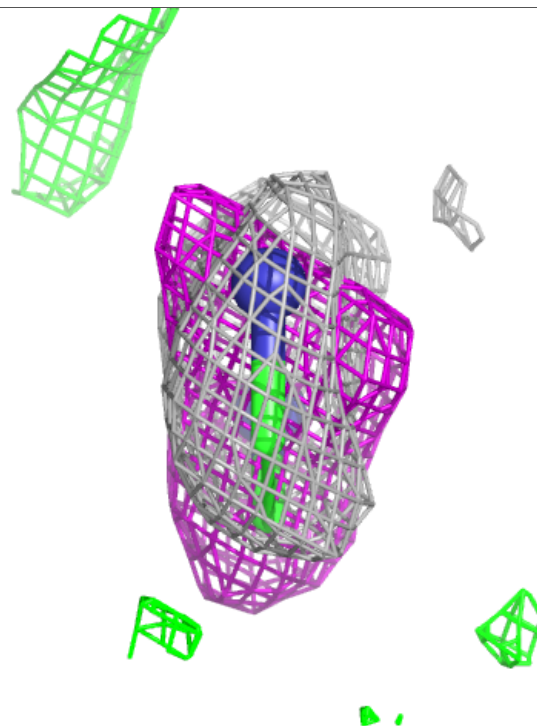
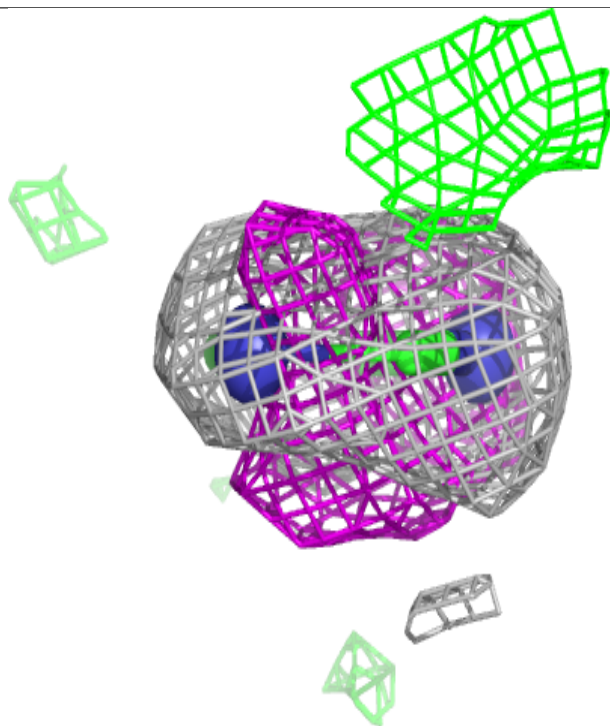
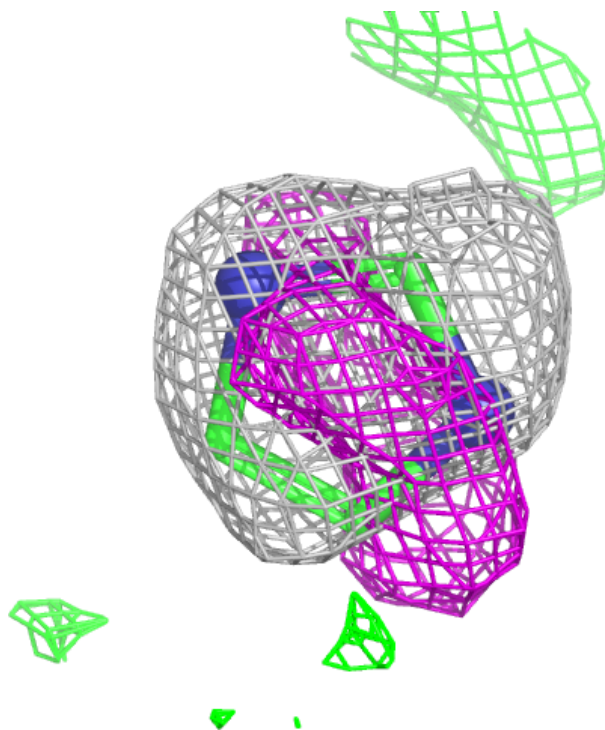
Electron density around GOL D 703:

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



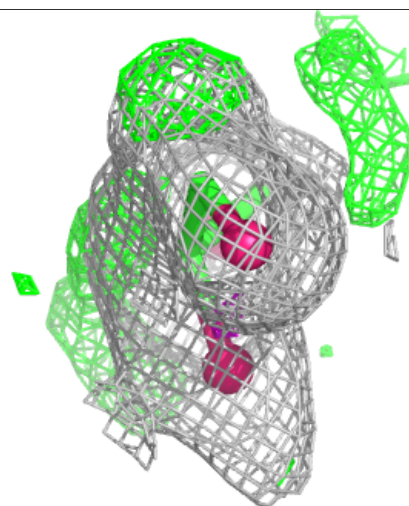
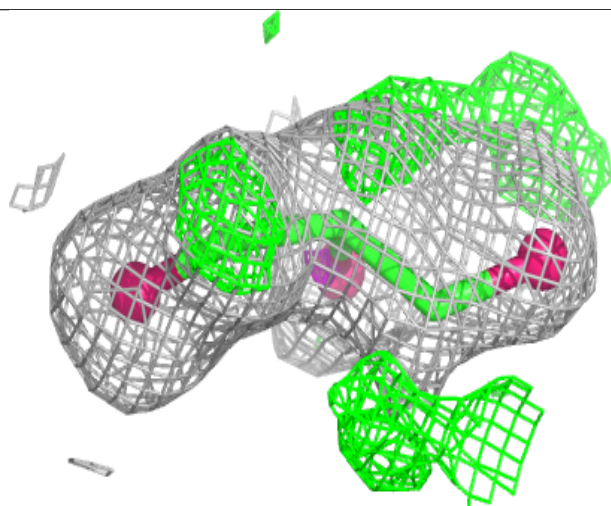
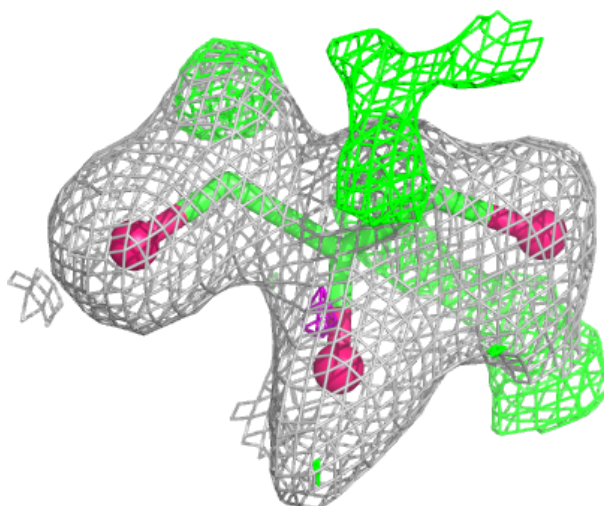
Electron density around IMD A 701:

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



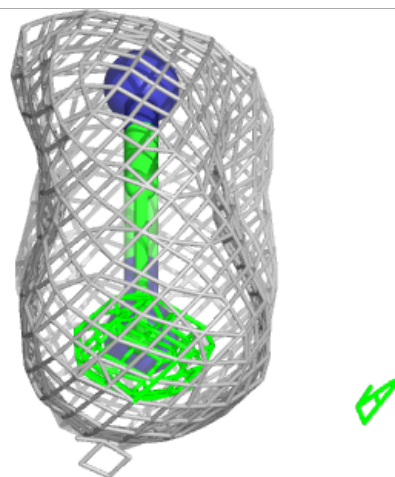
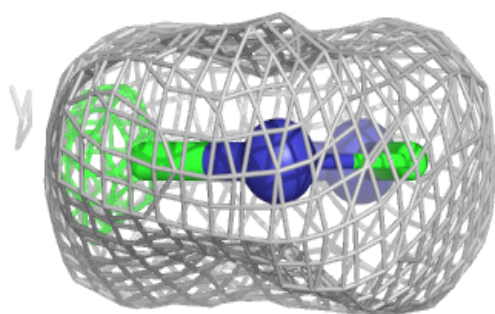
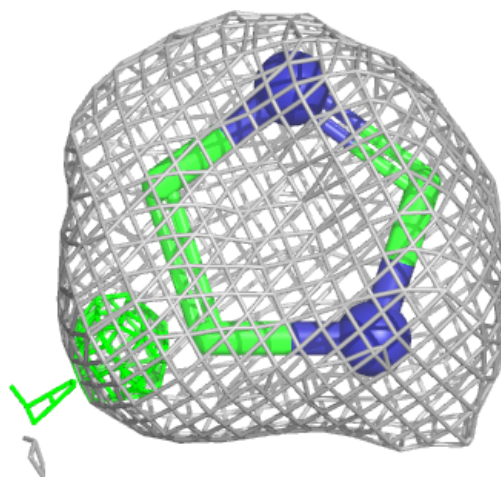
Electron density around GOL E 704:

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



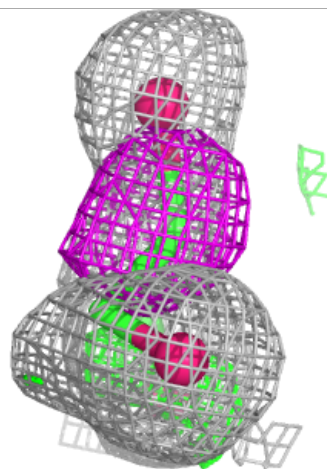
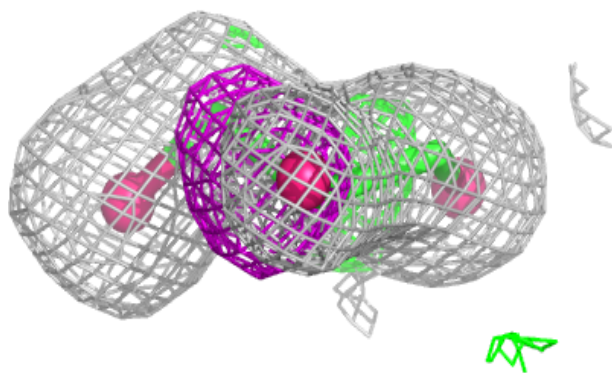
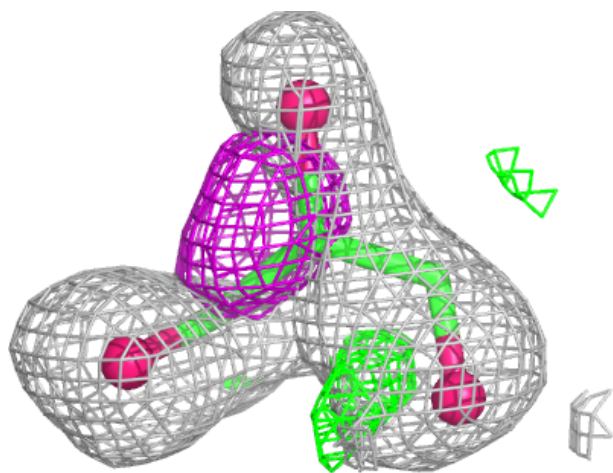
Electron density around IMD F 703:

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



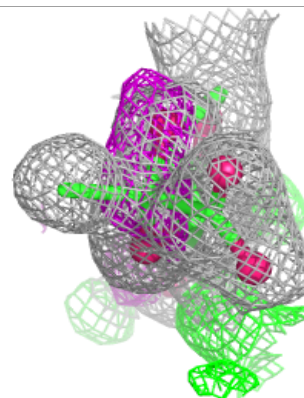
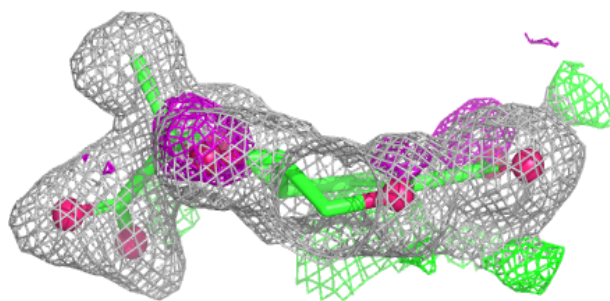
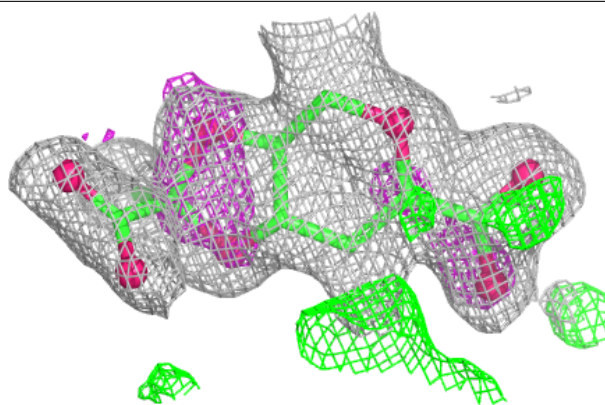
Electron density around GOL F 704:

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

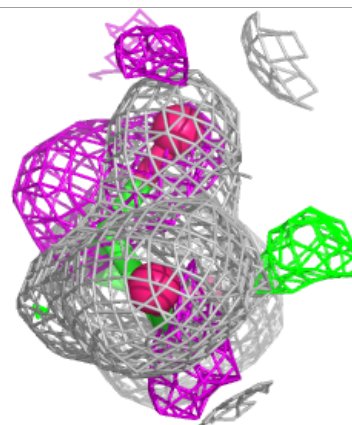
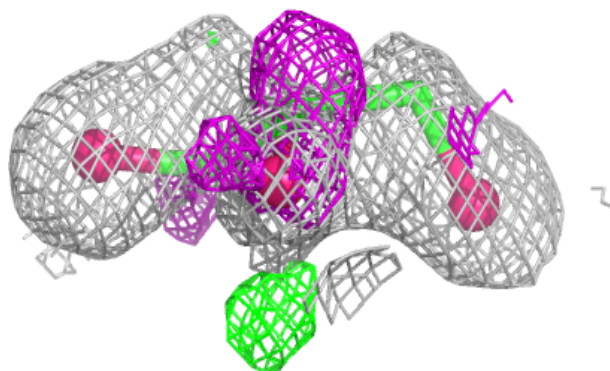
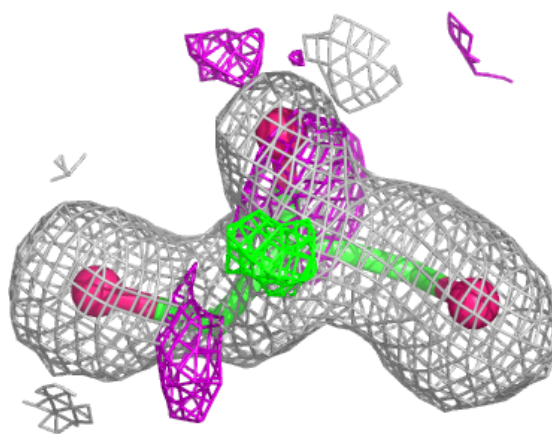


Electron density around 98X A 706:

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

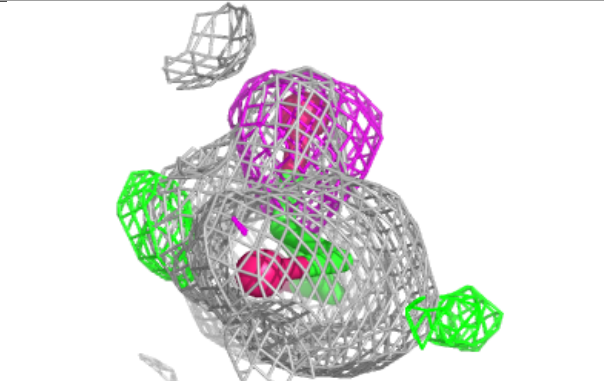
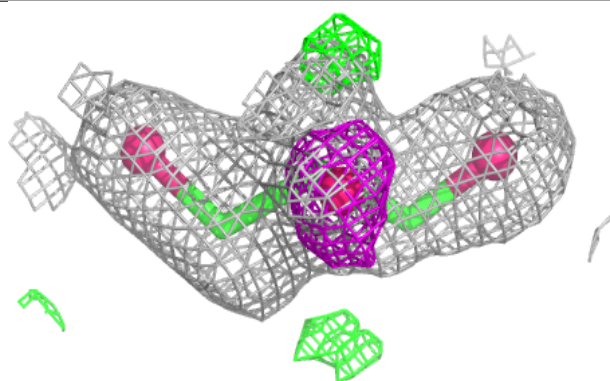
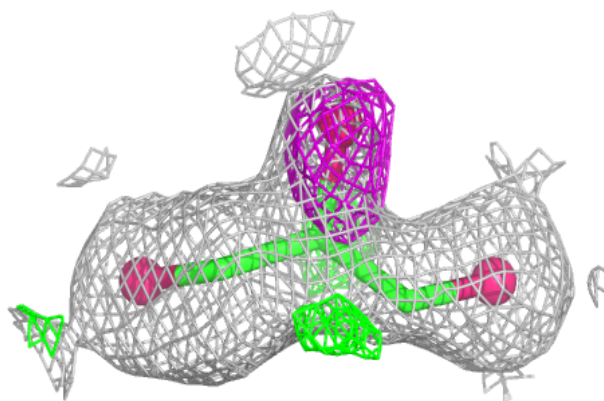
**Electron density around GOL C 701:**

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

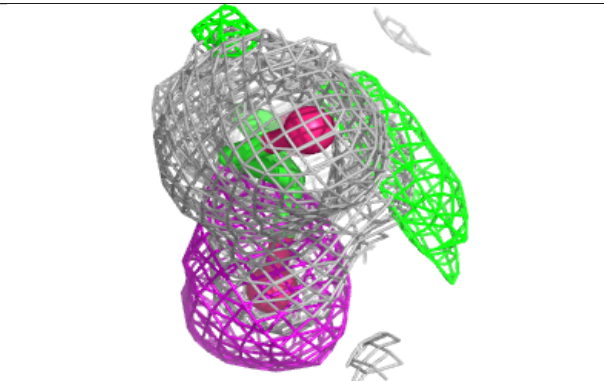
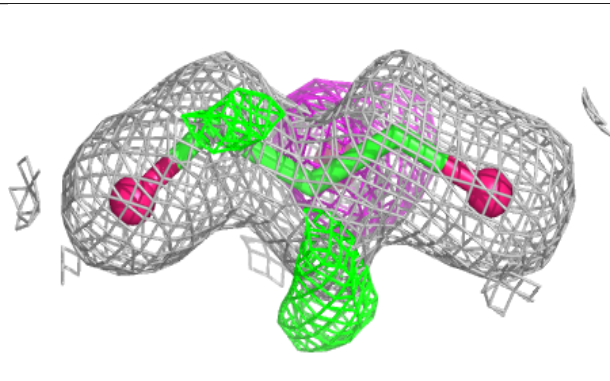
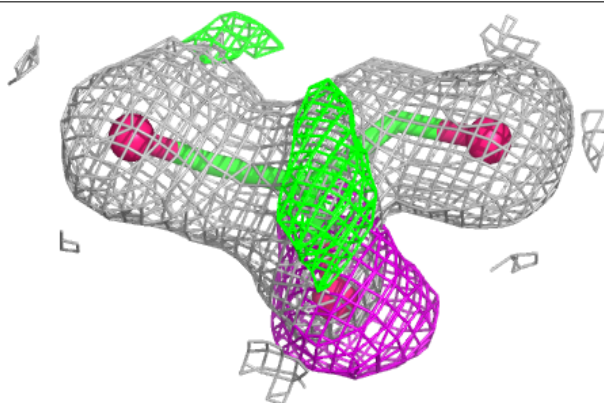


Electron density around GOL A 705:

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

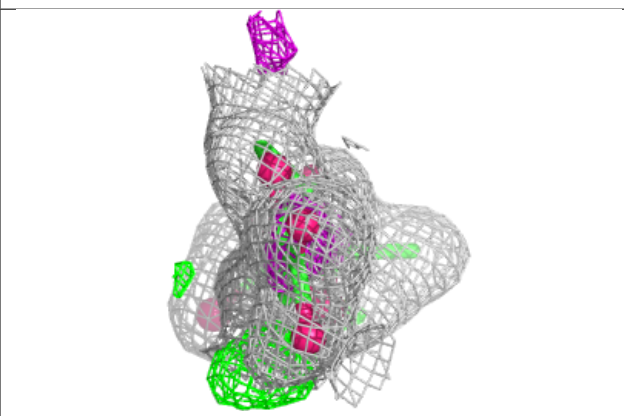
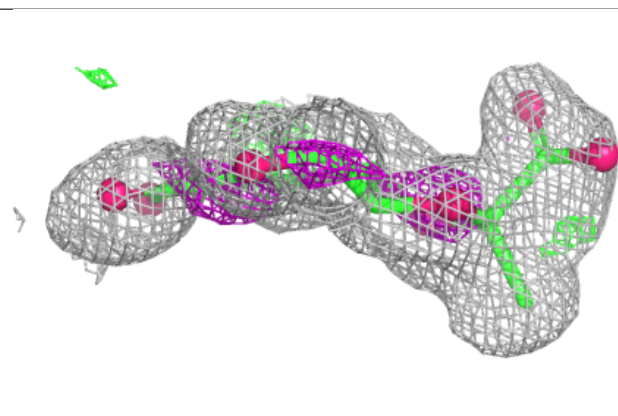
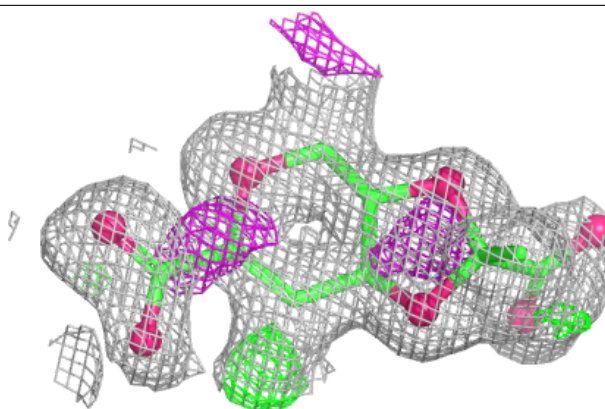
**Electron density around GOL F 701:**

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

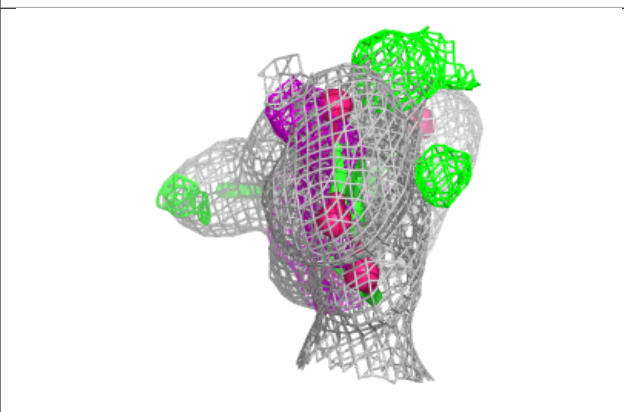
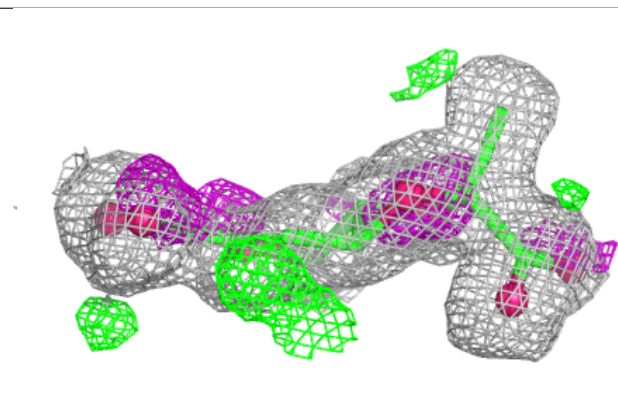
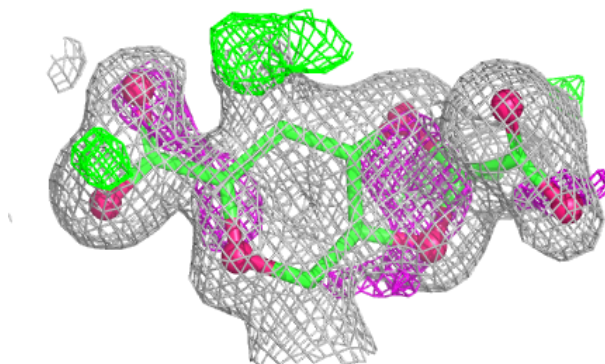


Electron density around 98X C 704:

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

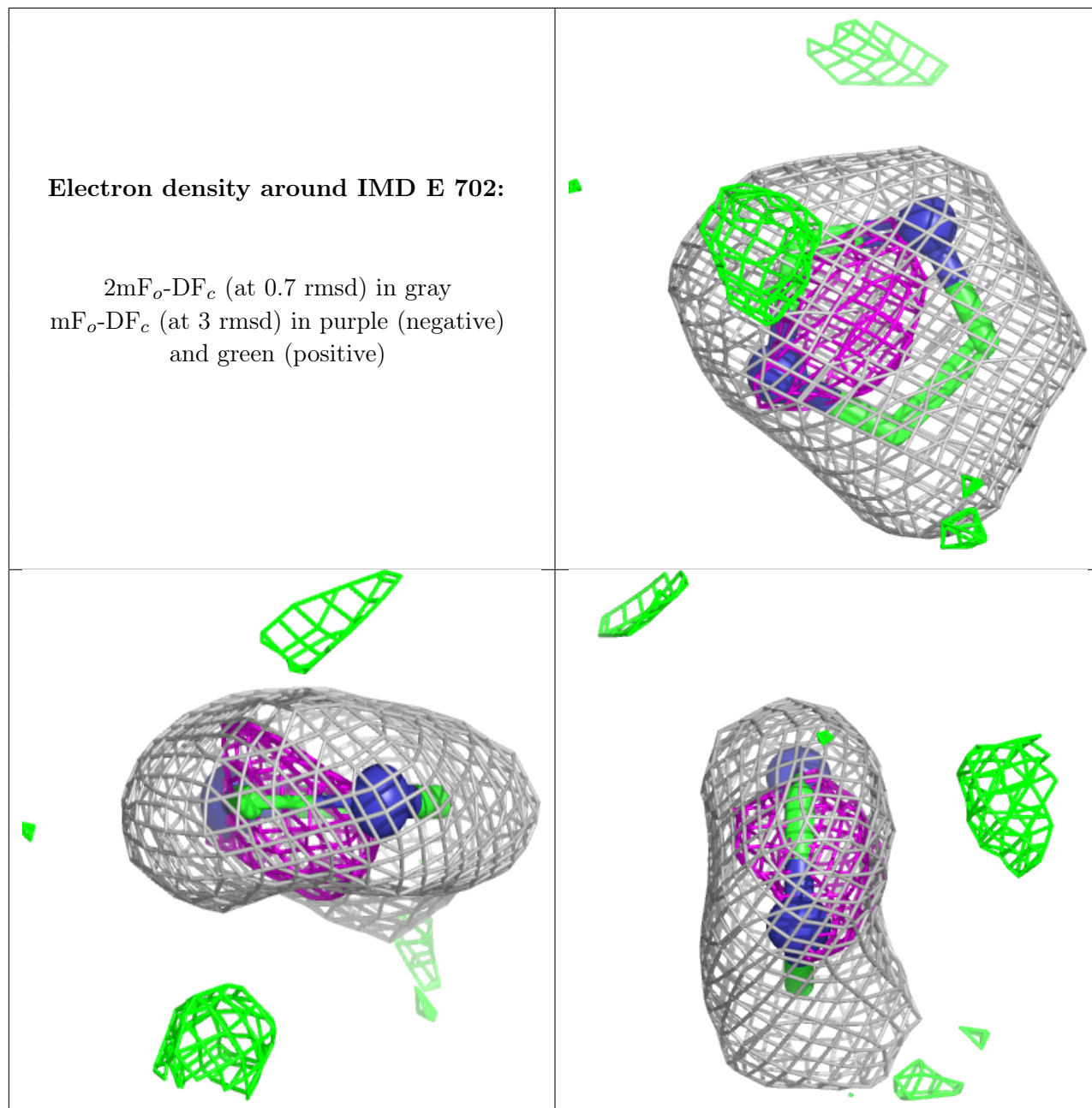
**Electron density around 98X E 706:**

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



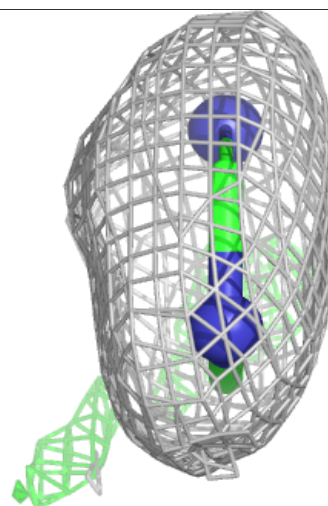
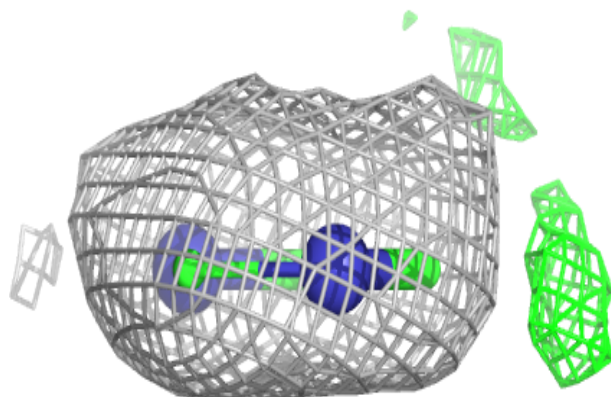
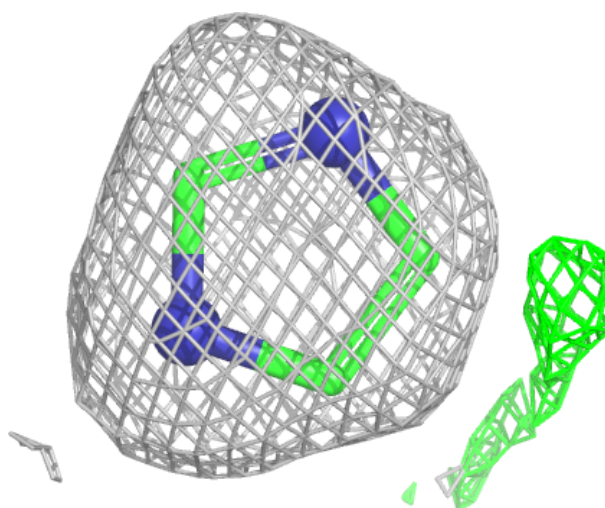
Electron density around IMD E 702:

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



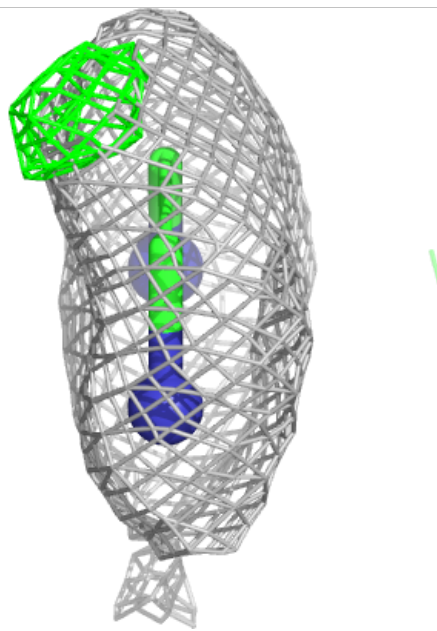
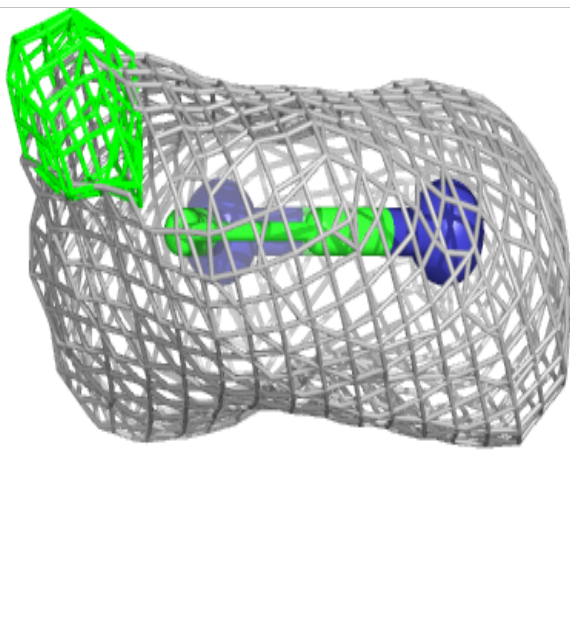
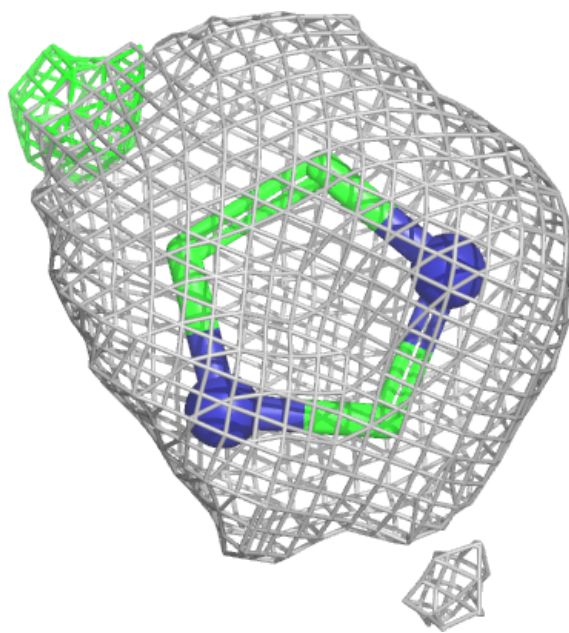
Electron density around IMD A 704:

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



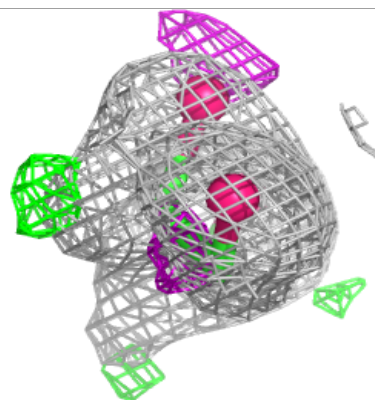
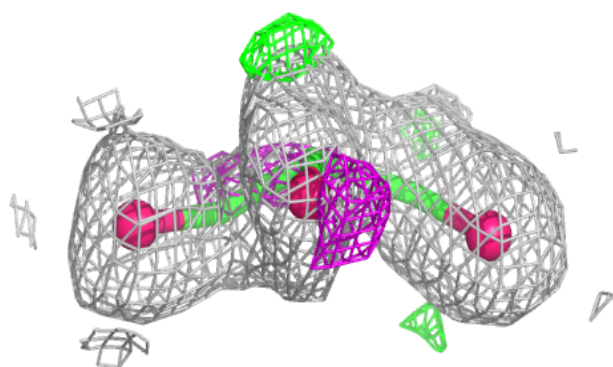
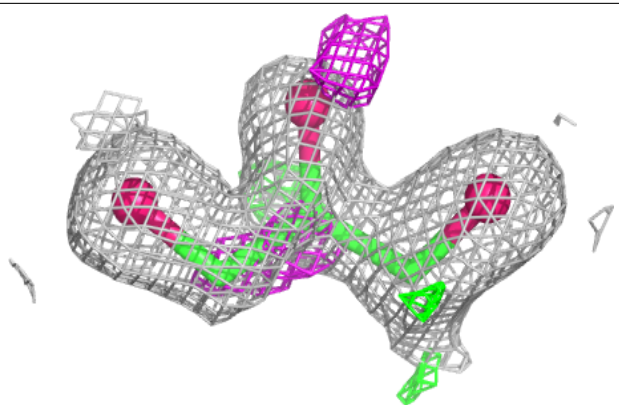
Electron density around IMD C 703:

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



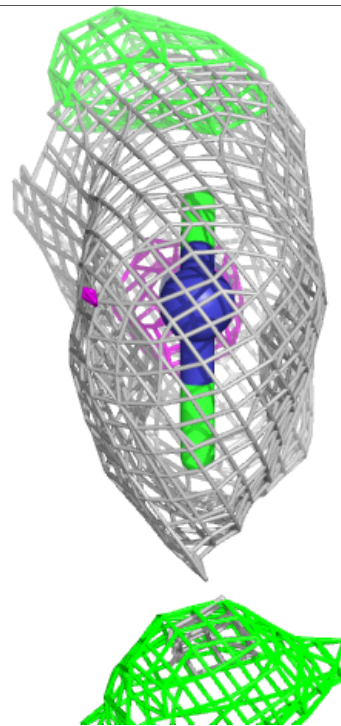
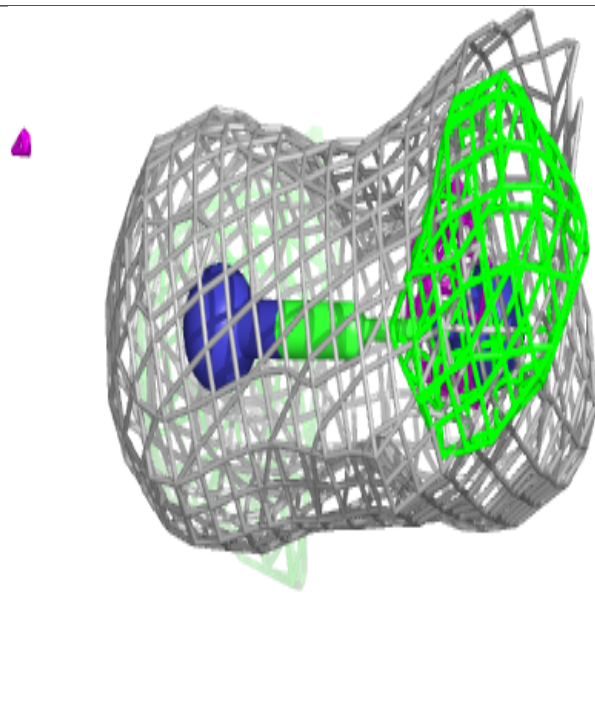
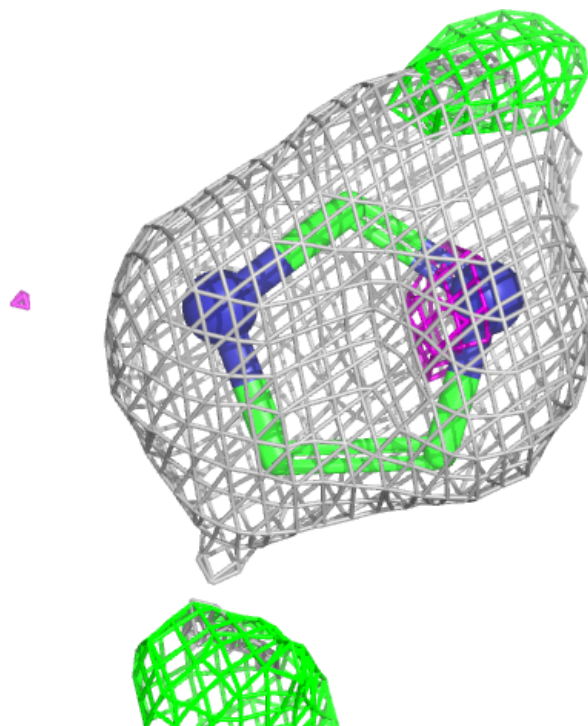
Electron density around GOL E 701:

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



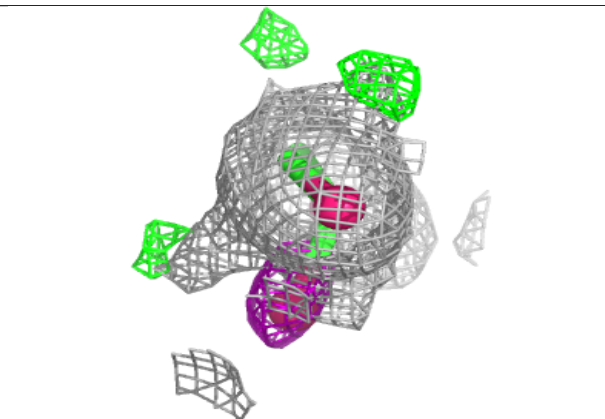
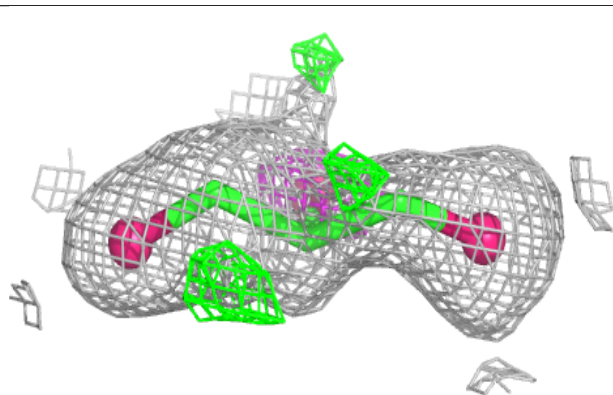
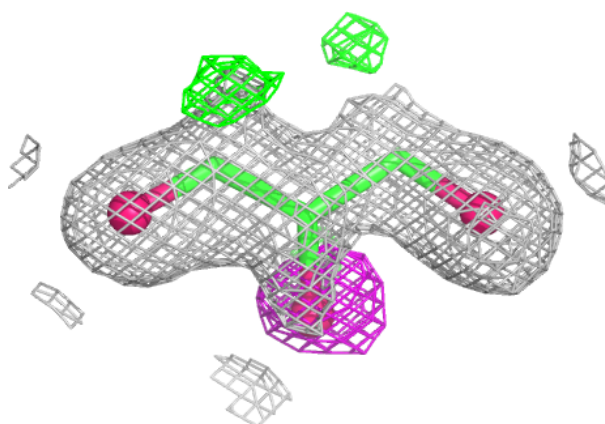
Electron density around IMD D 701:

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

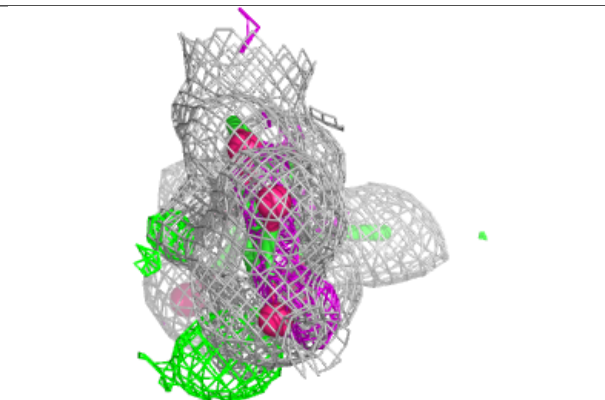
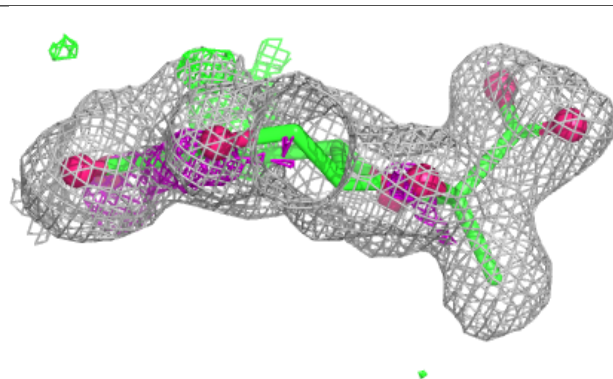
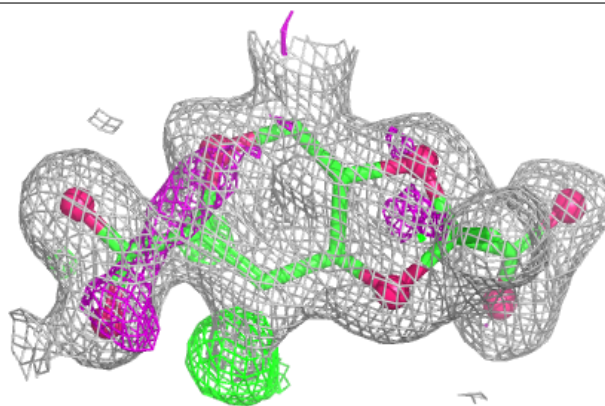


Electron density around GOL B 701:

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

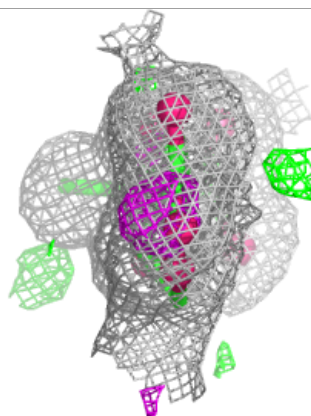
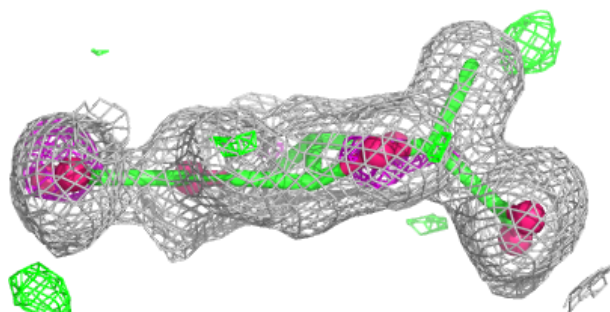
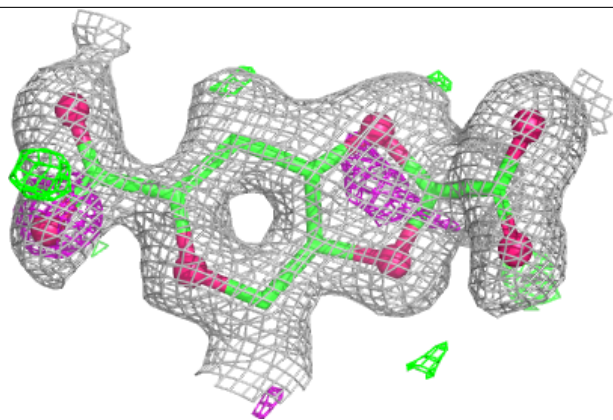
**Electron density around 98X D 704:**

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

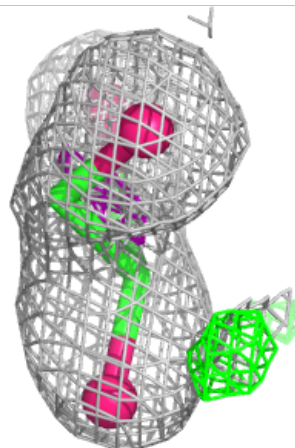
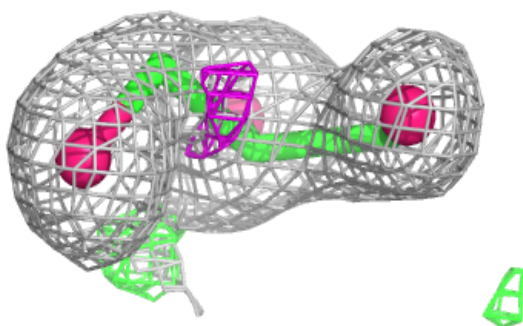
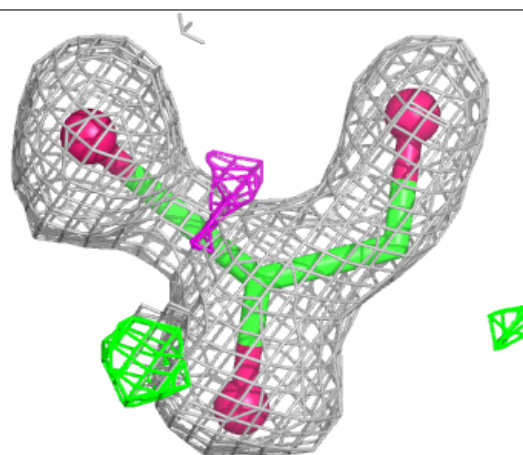


Electron density around 98X E 705:

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

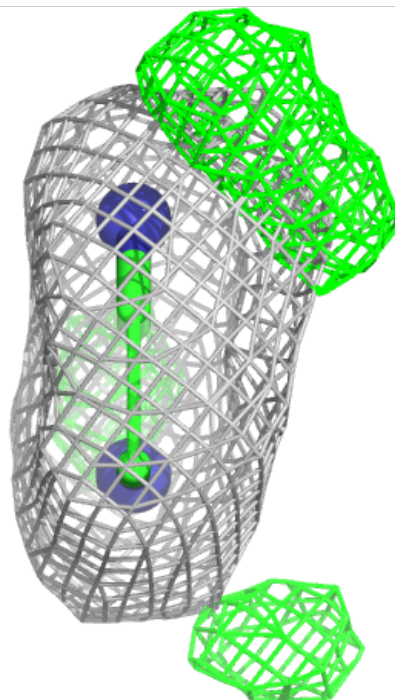
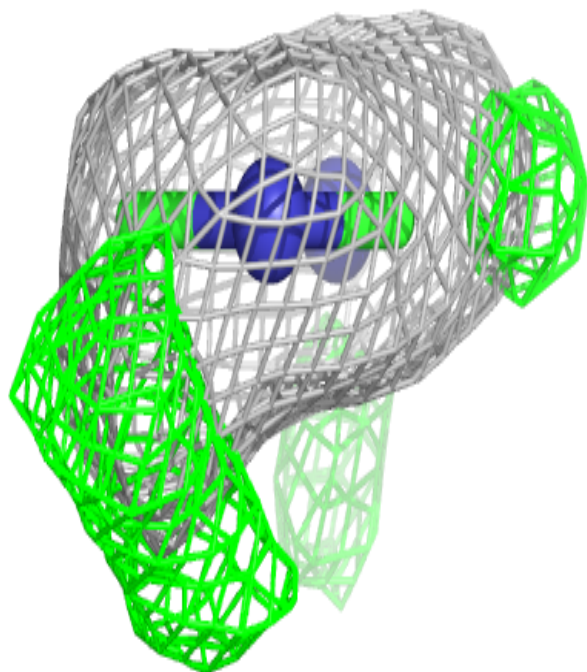
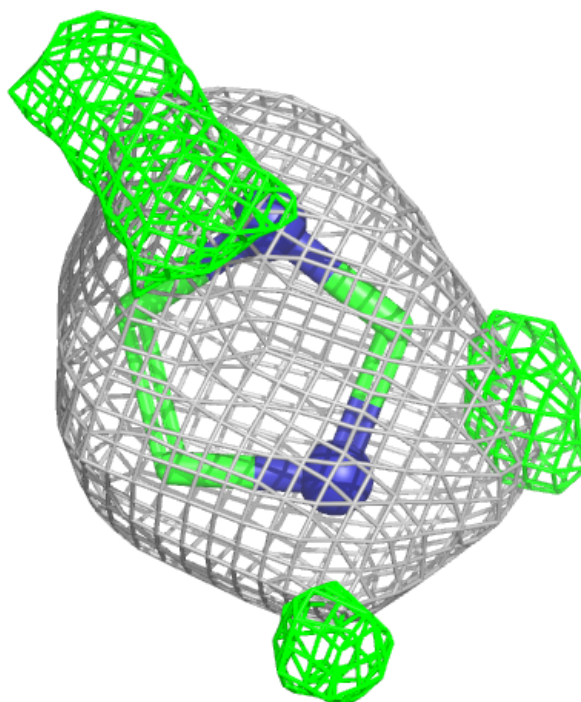
**Electron density around GOL A 703:**

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



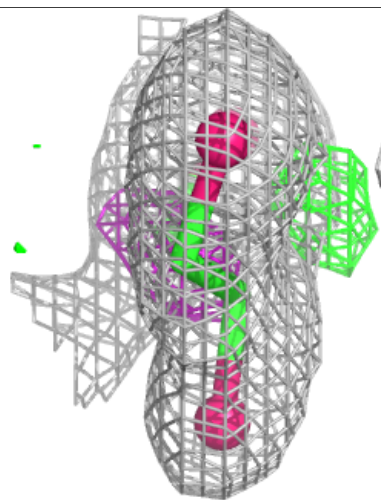
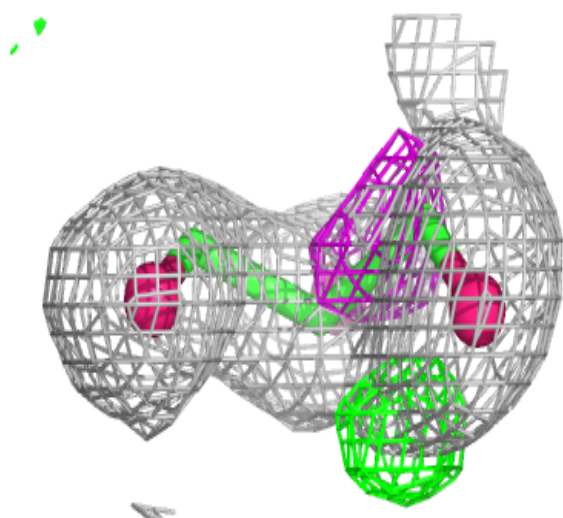
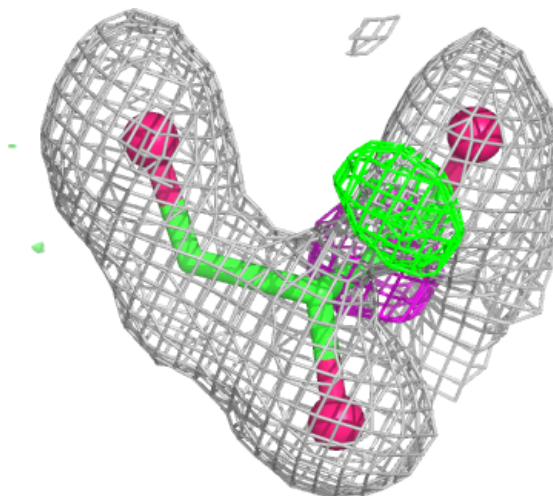
Electron density around IMD E 703:

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



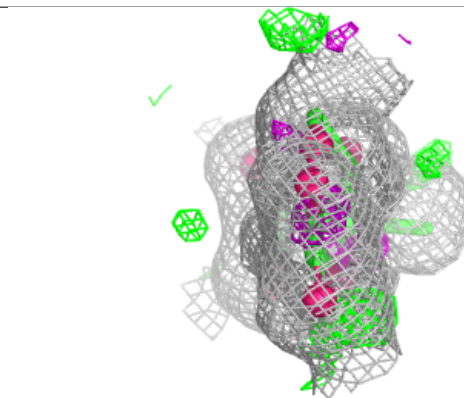
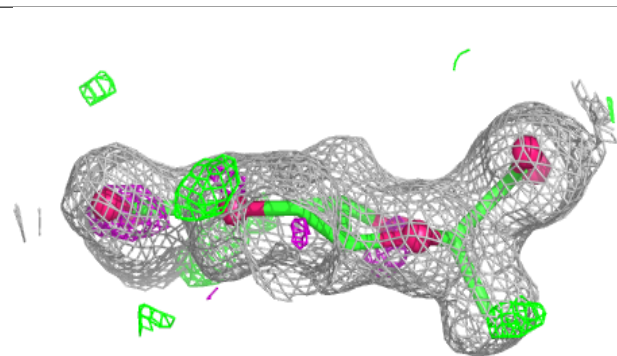
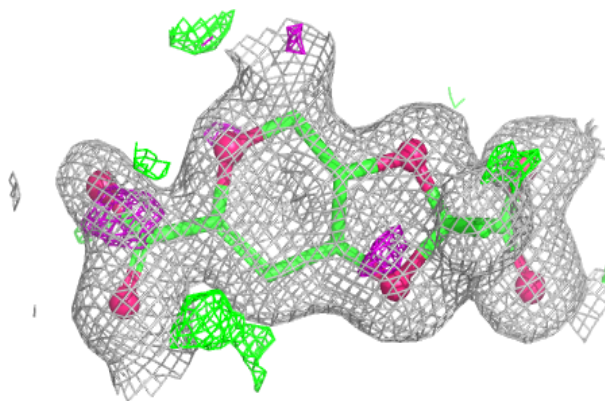
Electron density around GOL C 702:

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

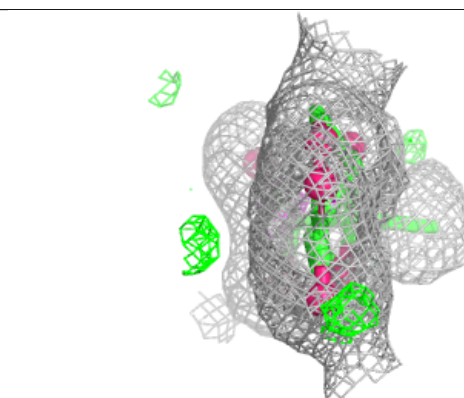
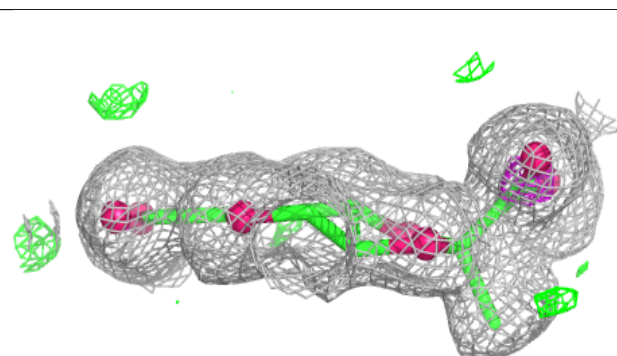
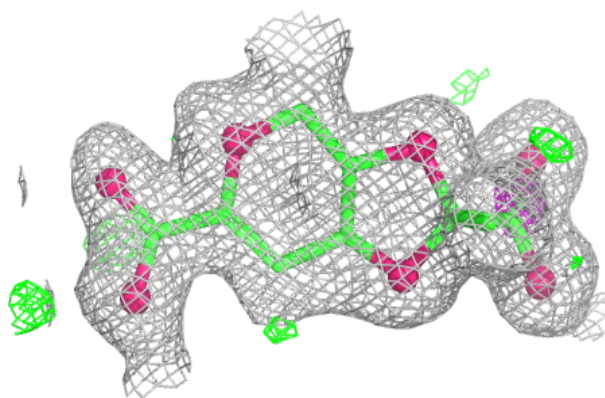


Electron density around 98X D 705:

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

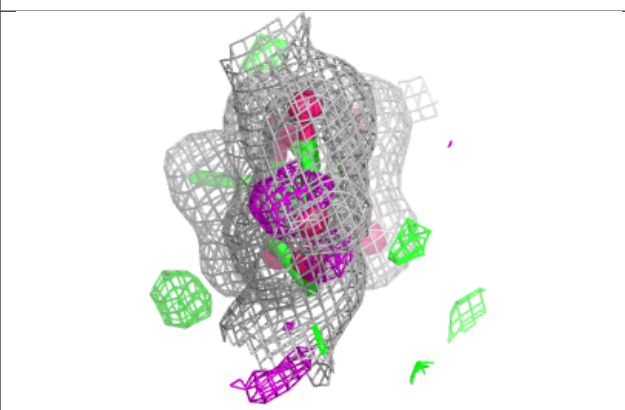
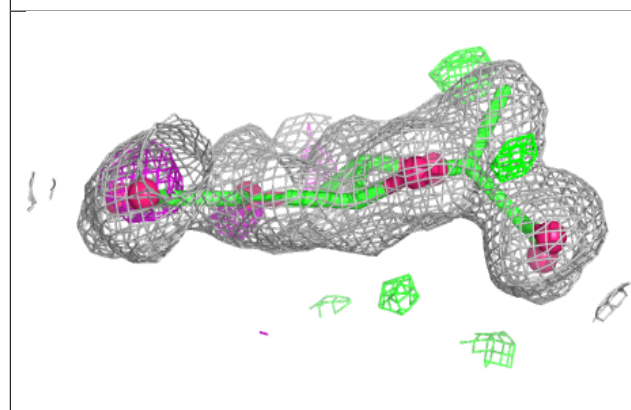
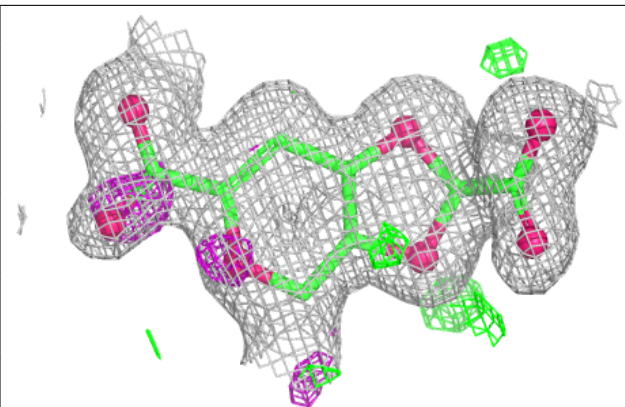
**Electron density around 98X A 707:**

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

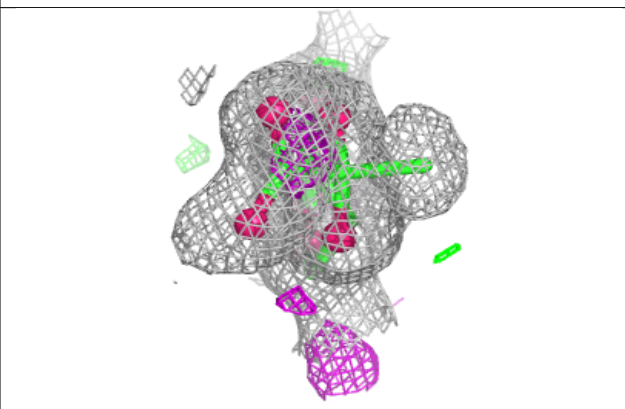
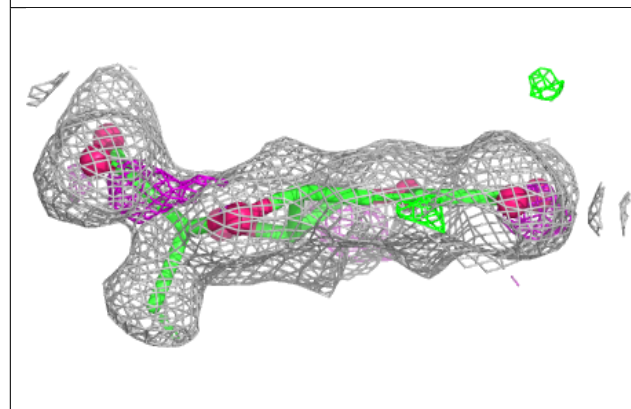
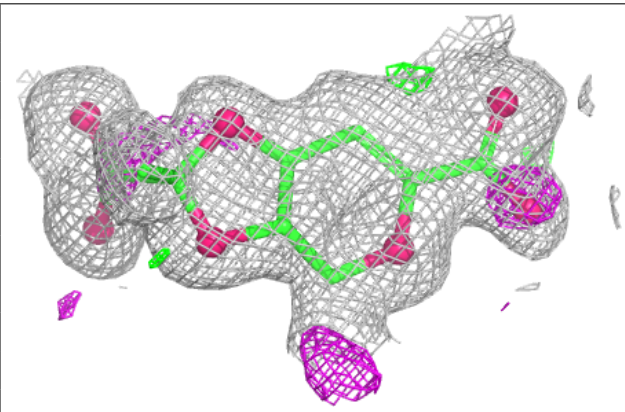


Electron density around 98X B 704:

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

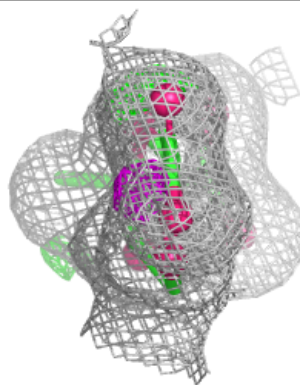
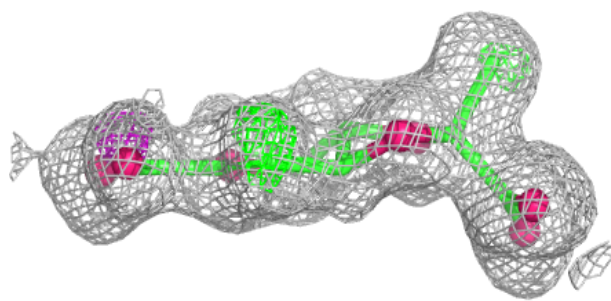
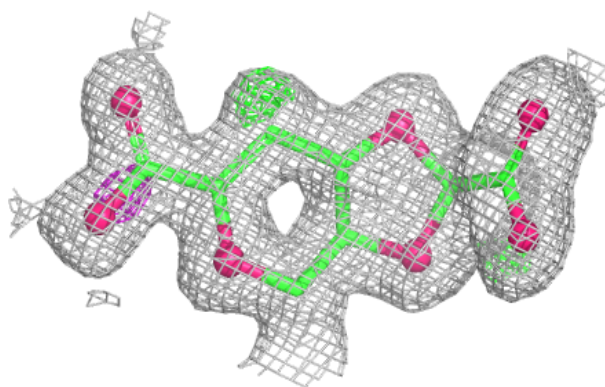
**Electron density around 98X F 705:**

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



Electron density around 98X A 708:

$2mF_o-DF_c$ (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.