



Full wwPDB X-ray Structure Validation Report i

Nov 22, 2023 – 11:34 PM JST

PDB ID : 7XXC
Title : Orf1-glycine-glycylthricin complex
Authors : Wang, Y.L.; Li, T.L.
Deposited on : 2022-05-29
Resolution : 1.99 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
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

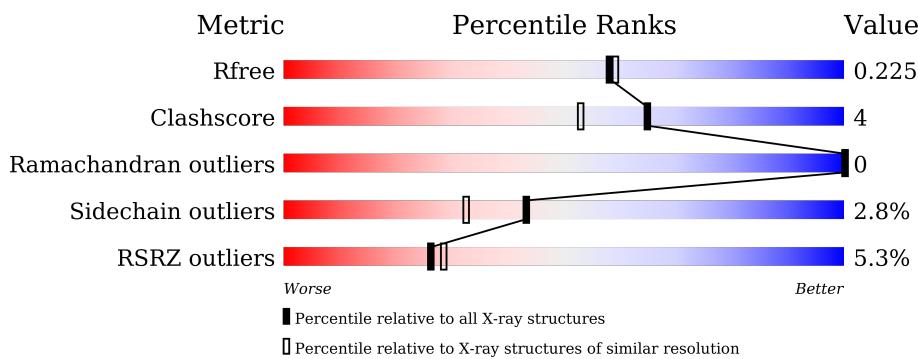
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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.



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Mol	Chain	Length	Quality of chain			
1	G	512	4%	86%	7%	6%
1	H	512	18%	84%	9%	6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32355 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 N-formimidoyl fortimicin A synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3645	2288	658	687	12			
1	B	482	Total	C	N	O	S	0	1	0
			3662	2298	661	690	13			
1	C	482	Total	C	N	O	S	0	1	0
			3662	2298	661	690	13			
1	D	479	Total	C	N	O	S	0	1	0
			3638	2284	658	684	12			
1	E	482	Total	C	N	O	S	0	0	0
			3654	2293	660	689	12			
1	F	482	Total	C	N	O	S	0	0	0
			3654	2293	660	689	12			
1	G	481	Total	C	N	O	S	0	2	0
			3664	2299	663	689	13			
1	H	479	Total	C	N	O	S	0	2	0
			3646	2289	659	685	13			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A125Szc1
A	-19	GLY	-	expression tag	UNP A0A125Szc1
A	-18	SER	-	expression tag	UNP A0A125Szc1
A	-17	SER	-	expression tag	UNP A0A125Szc1
A	-16	HIS	-	expression tag	UNP A0A125Szc1
A	-15	HIS	-	expression tag	UNP A0A125Szc1
A	-14	HIS	-	expression tag	UNP A0A125Szc1
A	-13	HIS	-	expression tag	UNP A0A125Szc1
A	-12	HIS	-	expression tag	UNP A0A125Szc1
A	-11	HIS	-	expression tag	UNP A0A125Szc1
A	-10	SER	-	expression tag	UNP A0A125Szc1
A	-9	SER	-	expression tag	UNP A0A125Szc1
A	-8	GLY	-	expression tag	UNP A0A125Szc1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP A0A125S2C1
A	-6	VAL	-	expression tag	UNP A0A125S2C1
A	-5	PRO	-	expression tag	UNP A0A125S2C1
A	-4	ARG	-	expression tag	UNP A0A125S2C1
A	-3	GLY	-	expression tag	UNP A0A125S2C1
A	-2	SER	-	expression tag	UNP A0A125S2C1
A	-1	HIS	-	expression tag	UNP A0A125S2C1
A	0	MET	-	expression tag	UNP A0A125S2C1
B	-20	MET	-	initiating methionine	UNP A0A125S2C1
B	-19	GLY	-	expression tag	UNP A0A125S2C1
B	-18	SER	-	expression tag	UNP A0A125S2C1
B	-17	SER	-	expression tag	UNP A0A125S2C1
B	-16	HIS	-	expression tag	UNP A0A125S2C1
B	-15	HIS	-	expression tag	UNP A0A125S2C1
B	-14	HIS	-	expression tag	UNP A0A125S2C1
B	-13	HIS	-	expression tag	UNP A0A125S2C1
B	-12	HIS	-	expression tag	UNP A0A125S2C1
B	-11	HIS	-	expression tag	UNP A0A125S2C1
B	-10	SER	-	expression tag	UNP A0A125S2C1
B	-9	SER	-	expression tag	UNP A0A125S2C1
B	-8	GLY	-	expression tag	UNP A0A125S2C1
B	-7	LEU	-	expression tag	UNP A0A125S2C1
B	-6	VAL	-	expression tag	UNP A0A125S2C1
B	-5	PRO	-	expression tag	UNP A0A125S2C1
B	-4	ARG	-	expression tag	UNP A0A125S2C1
B	-3	GLY	-	expression tag	UNP A0A125S2C1
B	-2	SER	-	expression tag	UNP A0A125S2C1
B	-1	HIS	-	expression tag	UNP A0A125S2C1
B	0	MET	-	expression tag	UNP A0A125S2C1
C	-20	MET	-	initiating methionine	UNP A0A125S2C1
C	-19	GLY	-	expression tag	UNP A0A125S2C1
C	-18	SER	-	expression tag	UNP A0A125S2C1
C	-17	SER	-	expression tag	UNP A0A125S2C1
C	-16	HIS	-	expression tag	UNP A0A125S2C1
C	-15	HIS	-	expression tag	UNP A0A125S2C1
C	-14	HIS	-	expression tag	UNP A0A125S2C1
C	-13	HIS	-	expression tag	UNP A0A125S2C1
C	-12	HIS	-	expression tag	UNP A0A125S2C1
C	-11	HIS	-	expression tag	UNP A0A125S2C1
C	-10	SER	-	expression tag	UNP A0A125S2C1
C	-9	SER	-	expression tag	UNP A0A125S2C1
C	-8	GLY	-	expression tag	UNP A0A125S2C1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	expression tag	UNP A0A125S2C1
C	-6	VAL	-	expression tag	UNP A0A125S2C1
C	-5	PRO	-	expression tag	UNP A0A125S2C1
C	-4	ARG	-	expression tag	UNP A0A125S2C1
C	-3	GLY	-	expression tag	UNP A0A125S2C1
C	-2	SER	-	expression tag	UNP A0A125S2C1
C	-1	HIS	-	expression tag	UNP A0A125S2C1
C	0	MET	-	expression tag	UNP A0A125S2C1
D	-20	MET	-	initiating methionine	UNP A0A125S2C1
D	-19	GLY	-	expression tag	UNP A0A125S2C1
D	-18	SER	-	expression tag	UNP A0A125S2C1
D	-17	SER	-	expression tag	UNP A0A125S2C1
D	-16	HIS	-	expression tag	UNP A0A125S2C1
D	-15	HIS	-	expression tag	UNP A0A125S2C1
D	-14	HIS	-	expression tag	UNP A0A125S2C1
D	-13	HIS	-	expression tag	UNP A0A125S2C1
D	-12	HIS	-	expression tag	UNP A0A125S2C1
D	-11	HIS	-	expression tag	UNP A0A125S2C1
D	-10	SER	-	expression tag	UNP A0A125S2C1
D	-9	SER	-	expression tag	UNP A0A125S2C1
D	-8	GLY	-	expression tag	UNP A0A125S2C1
D	-7	LEU	-	expression tag	UNP A0A125S2C1
D	-6	VAL	-	expression tag	UNP A0A125S2C1
D	-5	PRO	-	expression tag	UNP A0A125S2C1
D	-4	ARG	-	expression tag	UNP A0A125S2C1
D	-3	GLY	-	expression tag	UNP A0A125S2C1
D	-2	SER	-	expression tag	UNP A0A125S2C1
D	-1	HIS	-	expression tag	UNP A0A125S2C1
D	0	MET	-	expression tag	UNP A0A125S2C1
E	-20	MET	-	initiating methionine	UNP A0A125S2C1
E	-19	GLY	-	expression tag	UNP A0A125S2C1
E	-18	SER	-	expression tag	UNP A0A125S2C1
E	-17	SER	-	expression tag	UNP A0A125S2C1
E	-16	HIS	-	expression tag	UNP A0A125S2C1
E	-15	HIS	-	expression tag	UNP A0A125S2C1
E	-14	HIS	-	expression tag	UNP A0A125S2C1
E	-13	HIS	-	expression tag	UNP A0A125S2C1
E	-12	HIS	-	expression tag	UNP A0A125S2C1
E	-11	HIS	-	expression tag	UNP A0A125S2C1
E	-10	SER	-	expression tag	UNP A0A125S2C1
E	-9	SER	-	expression tag	UNP A0A125S2C1
E	-8	GLY	-	expression tag	UNP A0A125S2C1

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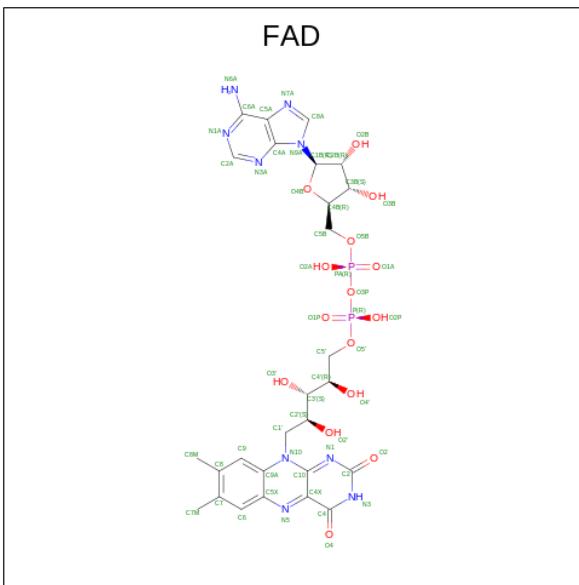
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E	-7	LEU	-	expression tag	UNP A0A125S2C1
E	-6	VAL	-	expression tag	UNP A0A125S2C1
E	-5	PRO	-	expression tag	UNP A0A125S2C1
E	-4	ARG	-	expression tag	UNP A0A125S2C1
E	-3	GLY	-	expression tag	UNP A0A125S2C1
E	-2	SER	-	expression tag	UNP A0A125S2C1
E	-1	HIS	-	expression tag	UNP A0A125S2C1
E	0	MET	-	expression tag	UNP A0A125S2C1
F	-20	MET	-	initiating methionine	UNP A0A125S2C1
F	-19	GLY	-	expression tag	UNP A0A125S2C1
F	-18	SER	-	expression tag	UNP A0A125S2C1
F	-17	SER	-	expression tag	UNP A0A125S2C1
F	-16	HIS	-	expression tag	UNP A0A125S2C1
F	-15	HIS	-	expression tag	UNP A0A125S2C1
F	-14	HIS	-	expression tag	UNP A0A125S2C1
F	-13	HIS	-	expression tag	UNP A0A125S2C1
F	-12	HIS	-	expression tag	UNP A0A125S2C1
F	-11	HIS	-	expression tag	UNP A0A125S2C1
F	-10	SER	-	expression tag	UNP A0A125S2C1
F	-9	SER	-	expression tag	UNP A0A125S2C1
F	-8	GLY	-	expression tag	UNP A0A125S2C1
F	-7	LEU	-	expression tag	UNP A0A125S2C1
F	-6	VAL	-	expression tag	UNP A0A125S2C1
F	-5	PRO	-	expression tag	UNP A0A125S2C1
F	-4	ARG	-	expression tag	UNP A0A125S2C1
F	-3	GLY	-	expression tag	UNP A0A125S2C1
F	-2	SER	-	expression tag	UNP A0A125S2C1
F	-1	HIS	-	expression tag	UNP A0A125S2C1
F	0	MET	-	expression tag	UNP A0A125S2C1
G	-20	MET	-	initiating methionine	UNP A0A125S2C1
G	-19	GLY	-	expression tag	UNP A0A125S2C1
G	-18	SER	-	expression tag	UNP A0A125S2C1
G	-17	SER	-	expression tag	UNP A0A125S2C1
G	-16	HIS	-	expression tag	UNP A0A125S2C1
G	-15	HIS	-	expression tag	UNP A0A125S2C1
G	-14	HIS	-	expression tag	UNP A0A125S2C1
G	-13	HIS	-	expression tag	UNP A0A125S2C1
G	-12	HIS	-	expression tag	UNP A0A125S2C1
G	-11	HIS	-	expression tag	UNP A0A125S2C1
G	-10	SER	-	expression tag	UNP A0A125S2C1
G	-9	SER	-	expression tag	UNP A0A125S2C1
G	-8	GLY	-	expression tag	UNP A0A125S2C1

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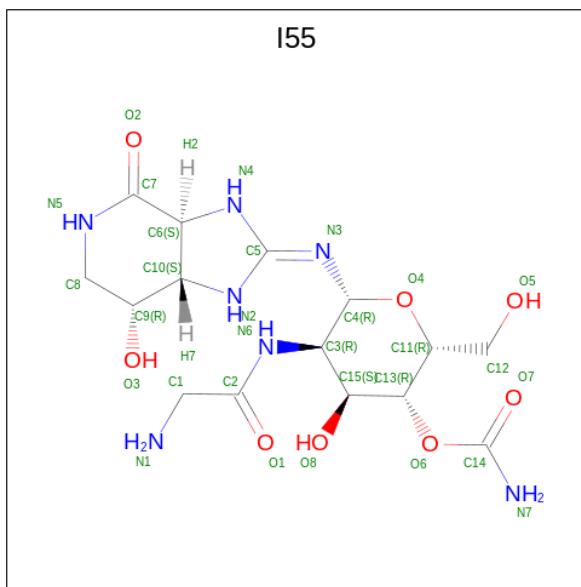
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	LEU	-	expression tag	UNP A0A125S2C1
G	-6	VAL	-	expression tag	UNP A0A125S2C1
G	-5	PRO	-	expression tag	UNP A0A125S2C1
G	-4	ARG	-	expression tag	UNP A0A125S2C1
G	-3	GLY	-	expression tag	UNP A0A125S2C1
G	-2	SER	-	expression tag	UNP A0A125S2C1
G	-1	HIS	-	expression tag	UNP A0A125S2C1
G	0	MET	-	expression tag	UNP A0A125S2C1
H	-20	MET	-	initiating methionine	UNP A0A125S2C1
H	-19	GLY	-	expression tag	UNP A0A125S2C1
H	-18	SER	-	expression tag	UNP A0A125S2C1
H	-17	SER	-	expression tag	UNP A0A125S2C1
H	-16	HIS	-	expression tag	UNP A0A125S2C1
H	-15	HIS	-	expression tag	UNP A0A125S2C1
H	-14	HIS	-	expression tag	UNP A0A125S2C1
H	-13	HIS	-	expression tag	UNP A0A125S2C1
H	-12	HIS	-	expression tag	UNP A0A125S2C1
H	-11	HIS	-	expression tag	UNP A0A125S2C1
H	-10	SER	-	expression tag	UNP A0A125S2C1
H	-9	SER	-	expression tag	UNP A0A125S2C1
H	-8	GLY	-	expression tag	UNP A0A125S2C1
H	-7	LEU	-	expression tag	UNP A0A125S2C1
H	-6	VAL	-	expression tag	UNP A0A125S2C1
H	-5	PRO	-	expression tag	UNP A0A125S2C1
H	-4	ARG	-	expression tag	UNP A0A125S2C1
H	-3	GLY	-	expression tag	UNP A0A125S2C1
H	-2	SER	-	expression tag	UNP A0A125S2C1
H	-1	HIS	-	expression tag	UNP A0A125S2C1
H	0	MET	-	expression tag	UNP A0A125S2C1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



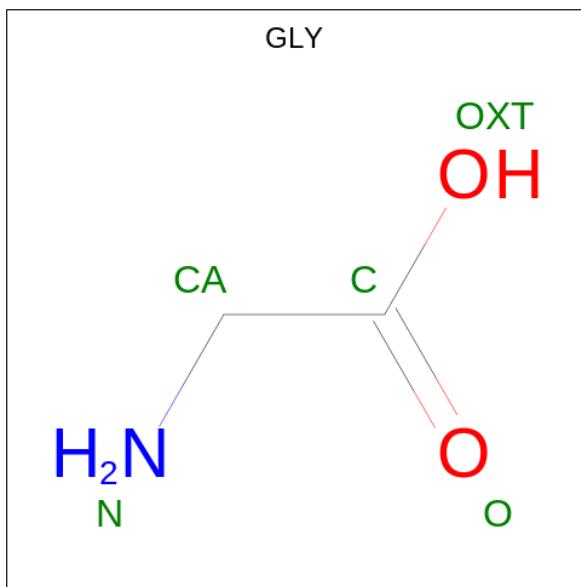
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	B	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	C	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	D	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	E	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	F	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	G	1	Total		C	N	O	P	
			53	27	9	15	2	0	0
2	H	1	Total		C	N	O	P	
			53	27	9	15	2	0	0

- Molecule 3 is [(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[({E})-[(3 {a} {S},7 {R},7 {a} {S})-7-oxidanyl-4-oxidanylidene-3,3 {a},5,6,7,7 {a}-hexahydro-1 {H}-imidazo[4,5-c]pyridin-2-ylidene]amino]-5-(2-azanylethanoylamino)-2-(hydroxymethyl)-4-oxidanyl-oxan-3-yl] carbamate (three-letter code: I55) (formula: C₁₅H₂₅N₇O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	O	
			30	15	7	8	0
3	B	1	Total	C	N	O	
			30	15	7	8	0
3	C	1	Total	C	N	O	
			30	15	7	8	0
3	D	1	Total	C	N	O	
			30	15	7	8	0
3	E	1	Total	C	N	O	
			30	15	7	8	0
3	F	1	Total	C	N	O	
			30	15	7	8	0
3	G	1	Total	C	N	O	
			30	15	7	8	0
3	H	1	Total	C	N	O	
			30	15	7	8	0

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 5 2 1 2	0	0
4	B	1	Total C N O 5 2 1 2	0	0
4	C	1	Total C N O 5 2 1 2	0	0
4	D	1	Total C N O 5 2 1 2	0	0
4	E	1	Total C N O 5 2 1 2	0	0
4	F	1	Total C N O 5 2 1 2	0	0
4	G	1	Total C N O 5 2 1 2	0	0
4	H	1	Total C N O 5 2 1 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	325	Total O 325 325	0	0
5	B	349	Total O 349 349	0	0
5	C	336	Total O 336 336	0	0
5	D	213	Total O 213 213	0	0

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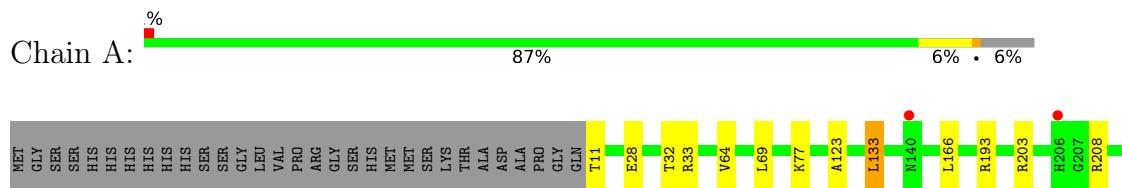
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	319	Total O 319 319	0	0
5	F	358	Total O 358 358	0	0
5	G	328	Total O 328 328	0	0
5	H	198	Total O 198 198	0	0

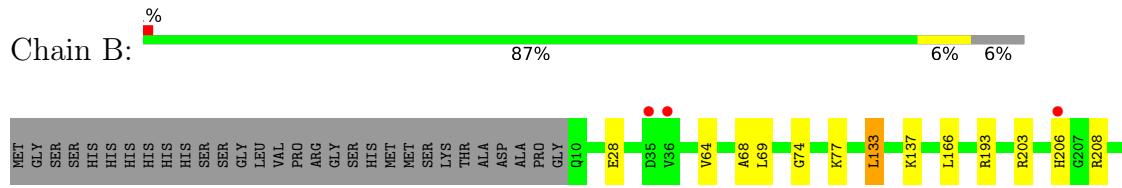
3 Residue-property plots

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.

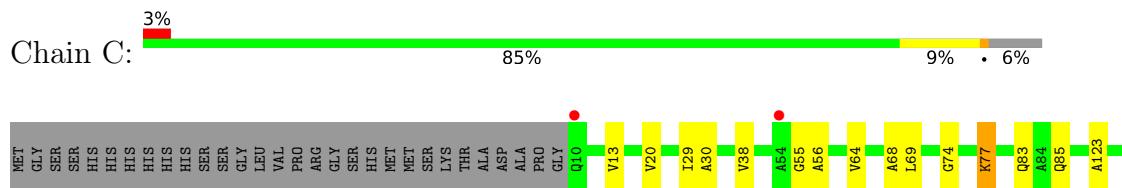
- Molecule 1: N-formimidoyl fortimicin A synthase



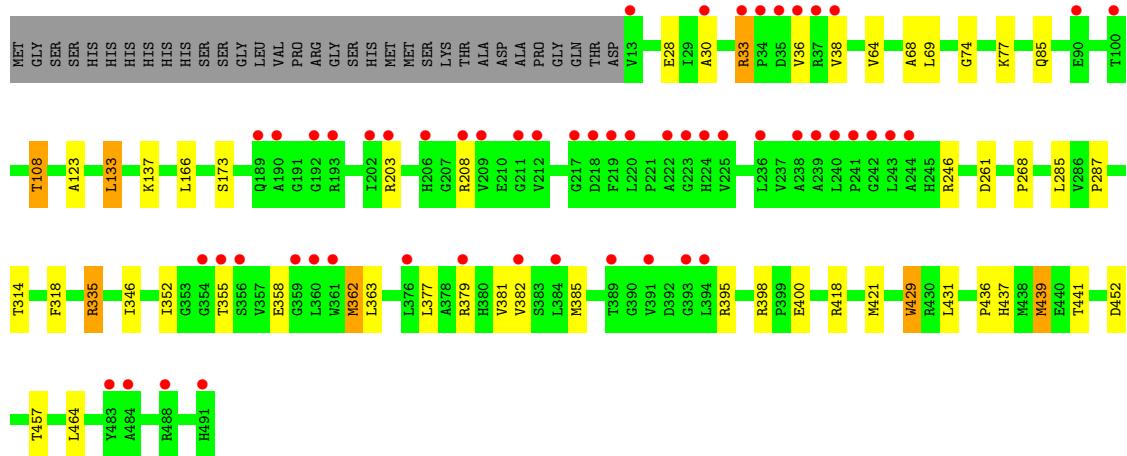
- Molecule 1: N-formimidoyl fortimicin A synthase



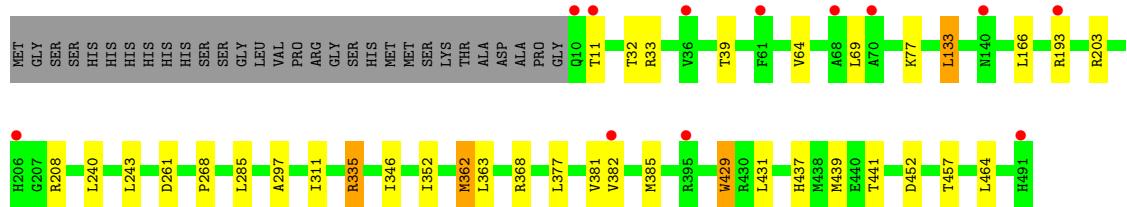
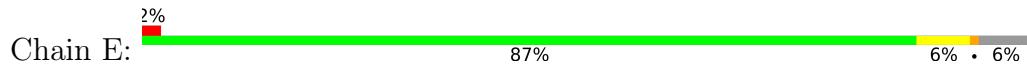
- Molecule 1: N-formimidoyl fortimicin A synthase



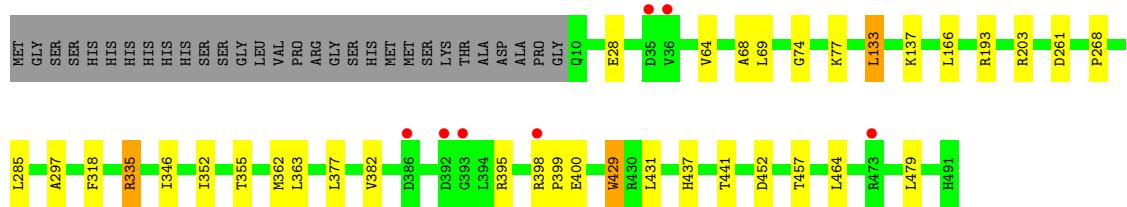
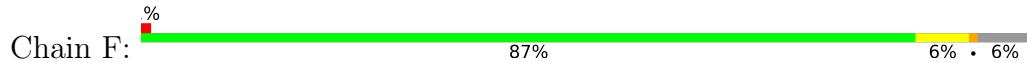
- Molecule 1: N-formimidoyl fortimicin A synthase



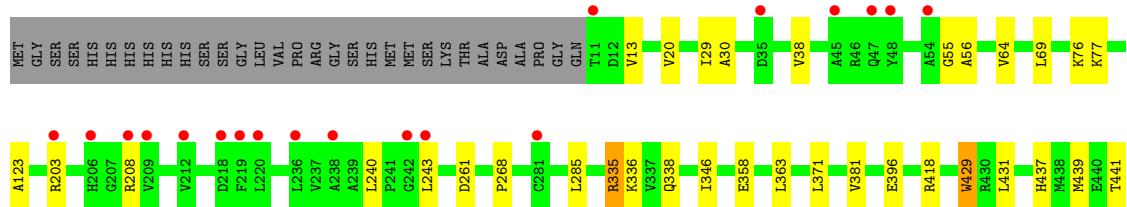
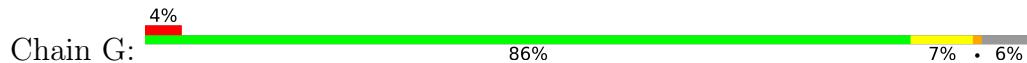
- Molecule 1: N-formimidoyl fortimicin A synthase

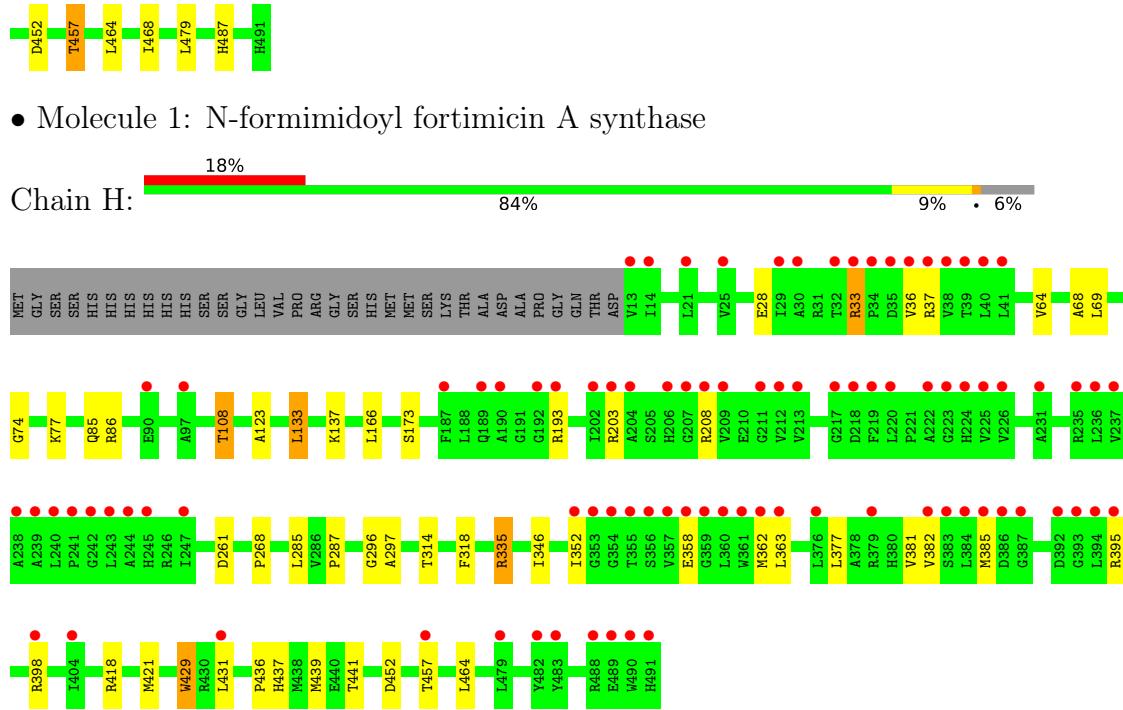


- Molecule 1: N-formimidoyl fortimicin A synthase



- Molecule 1: N-formimidoyl fortimicin A synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.47 Å 108.06 Å 134.56 Å 89.75° 90.08° 96.50°	Depositor
Resolution (Å)	27.82 – 1.99 27.81 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.5 (27.82-1.99) 96.5 (27.81-1.99)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	5.34 (at 1.99 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.221 0.204 , 0.225	Depositor DCC
R_{free} test set	18798 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{\text{sol}}(\text{e}/\text{\AA}^3)$, $B_{\text{sol}}(\text{\AA}^2)$	0.37 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.440 for -h,-k,l 0.008 for -k,-h,-l 0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32355	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: I55, FAD

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	0.67	0/3728	0.79	1/5080 (0.0%)
1	B	0.68	0/3745	0.78	0/5102
1	C	0.70	0/3745	0.80	0/5102
1	D	0.64	0/3721	0.77	0/5070
1	E	0.67	0/3737	0.79	0/5092
1	F	0.67	0/3737	0.78	0/5092
1	G	0.70	0/3747	0.79	0/5104
1	H	0.65	0/3729	0.77	0/5080
All	All	0.67	0/29889	0.78	1/40722 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	335	ARG	CG-CD-NE	-5.21	100.85	111.80

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	3645	0	3576	22	0
1	B	3662	0	3592	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3662	0	3592	31	0
1	D	3638	0	3570	49	0
1	E	3654	0	3584	24	0
1	F	3654	0	3584	23	0
1	G	3664	0	3596	28	0
1	H	3646	0	3578	42	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	2	0
2	F	53	0	31	2	0
2	G	53	0	31	1	0
2	H	53	0	31	1	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
3	E	30	0	0	0	0
3	F	30	0	0	0	0
3	G	30	0	0	0	0
3	H	30	0	0	0	0
4	A	5	0	2	0	0
4	B	5	0	2	1	0
4	C	5	0	2	1	0
4	D	5	0	2	0	0
4	E	5	0	2	1	0
4	F	5	0	2	1	0
4	G	5	0	2	0	0
4	H	5	0	2	0	0
5	A	325	0	0	5	0
5	B	349	0	0	3	0
5	C	336	0	0	3	0
5	D	213	0	0	2	0
5	E	319	0	0	1	0
5	F	358	0	0	5	0
5	G	328	0	0	0	0
5	H	198	0	0	1	0
All	All	32355	0	28936	241	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 4.

All (241) 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:G:363:LEU:HD13	1:G:381:VAL:HG21	1.52	0.92
1:H:108:THR:HG21	1:H:287:PRO:O	1.89	0.73
1:A:32:THR:CG2	5:A:1101:HOH:O	2.36	0.72
1:G:429:TRP:CH2	1:G:439[B]:MET:HE1	2.25	0.72
1:D:108:THR:HG21	1:D:287:PRO:O	1.89	0.71
1:H:108:THR:HG22	1:H:173:SER:OG	1.93	0.69
1:E:382:VAL:HA	1:E:385:MET:CE	2.23	0.69
1:G:429:TRP:CH2	1:G:439[B]:MET:CE	2.76	0.69
1:D:108:THR:HG22	1:D:173:SER:OG	1.92	0.68
1:H:436:PRO:HA	1:H:439[B]:MET:HE2	1.75	0.68
1:D:382:VAL:HA	1:D:385:MET:CE	2.24	0.68
1:H:382:VAL:HA	1:H:385:MET:CE	2.24	0.68
1:A:355:THR:HG23	1:A:400:GLU:OE2	1.94	0.67
1:D:355:THR:HG23	1:D:400:GLU:OE2	1.95	0.67
1:H:436:PRO:HA	1:H:439[B]:MET:CE	2.25	0.67
1:C:355:THR:HG23	1:C:400:GLU:OE2	1.95	0.67
1:A:487:HIS:NE2	5:A:802:HOH:O	2.28	0.66
1:F:355:THR:HG23	1:F:400:GLU:OE2	1.94	0.66
1:E:382:VAL:HA	1:E:385:MET:HE2	1.77	0.66
1:D:436:PRO:HA	1:D:439:MET:CE	2.26	0.65
1:C:363:LEU:HD11	1:C:377:LEU:HB3	1.78	0.65
1:H:382:VAL:HA	1:H:385:MET:HE2	1.78	0.65
1:C:436:PRO:HA	1:C:439[B]:MET:CE	2.27	0.65
1:C:421:MET:CE	1:C:439[B]:MET:CE	2.76	0.64
1:D:246:ARG:NH1	1:D:400:GLU:OE1	2.31	0.64
1:D:421:MET:CE	1:D:439:MET:CE	2.76	0.63
1:A:32:THR:HG21	5:A:1101:HOH:O	1.97	0.63
1:F:346:ILE:HG13	1:F:464:LEU:CD2	2.29	0.63
1:B:439[A]:MET:HE1	1:D:439:MET:HA	1.81	0.63
1:D:382:VAL:HA	1:D:385:MET:HE2	1.80	0.63
1:D:436:PRO:HA	1:D:439:MET:HE2	1.80	0.63
1:E:346:ILE:HG13	1:E:464:LEU:CD2	2.28	0.62
1:H:346:ILE:HG13	1:H:464:LEU:CD2	2.30	0.62
1:A:346:ILE:HG13	1:A:464:LEU:CD2	2.29	0.62
1:D:346:ILE:HG13	1:D:464:LEU:CD2	2.30	0.62
1:F:479:LEU:CD2	5:F:881:HOH:O	2.47	0.62
1:B:346:ILE:HG13	1:B:464:LEU:CD2	2.29	0.62
1:G:363:LEU:CD1	1:G:381:VAL:HG21	2.28	0.61
1:D:363:LEU:HD11	1:D:377:LEU:HB3	1.83	0.61
1:H:363:LEU:HD11	1:H:377:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:HG22	5:A:1101:HOH:O	2.01	0.60
1:H:421:MET:CE	1:H:439[B]:MET:CE	2.79	0.60
1:G:429:TRP:HH2	1:G:439[B]:MET:CE	2.13	0.60
1:H:123:ALA:HB1	1:H:418:ARG:HD2	1.83	0.60
1:C:346:ILE:HG13	1:C:464:LEU:CD2	2.32	0.59
1:B:479:LEU:CD2	5:B:885:HOH:O	2.51	0.58
1:G:346:ILE:HG13	1:G:464:LEU:CD2	2.33	0.58
1:H:108:THR:CG2	1:H:287:PRO:O	2.52	0.58
1:G:123:ALA:HB1	1:G:418:ARG:HD2	1.87	0.57
1:C:436:PRO:HA	1:C:439[B]:MET:HE2	1.86	0.57
1:F:363:LEU:HD11	1:F:377:LEU:HB3	1.86	0.57
1:A:123:ALA:HB1	1:A:418:ARG:HD2	1.86	0.57
1:G:429:TRP:HH2	1:G:439[B]:MET:HE3	1.69	0.57
1:B:363:LEU:HD11	1:B:377:LEU:HB3	1.86	0.57
1:D:108:THR:CG2	1:D:287:PRO:O	2.51	0.57
1:E:363:LEU:HD11	1:E:377:LEU:HB3	1.87	0.56
1:D:429:TRP:CH2	1:D:439:MET:CE	2.88	0.56
1:A:363:LEU:HD11	1:A:377:LEU:HB3	1.87	0.56
1:C:429:TRP:CH2	1:C:439[B]:MET:CE	2.89	0.56
1:C:421:MET:HE1	1:C:439[B]:MET:CE	2.37	0.55
1:A:64:VAL:HG13	1:A:69:LEU:HD22	1.90	0.54
1:E:64:VAL:HG13	1:E:69:LEU:HD22	1.89	0.54
1:D:379:ARG:NH2	5:D:802:HOH:O	2.41	0.54
4:C:703:GLY:N	5:C:803:HOH:O	2.41	0.54
1:C:421:MET:HE1	1:C:439[B]:MET:HE2	1.89	0.53
1:D:429:TRP:HH2	1:D:439:MET:HE3	1.73	0.53
1:G:363:LEU:HD13	1:G:381:VAL:CG2	2.34	0.53
1:H:429:TRP:CG	1:H:431:LEU:HD13	2.44	0.53
1:F:335:ARG:HG2	5:F:999:HOH:O	2.09	0.52
1:C:429:TRP:HH2	1:C:439[B]:MET:HE3	1.73	0.52
1:F:429:TRP:CG	1:F:431:LEU:HD13	2.44	0.52
1:B:133:LEU:HD13	1:B:166:LEU:HD22	1.92	0.52
1:F:64:VAL:HG13	1:F:69:LEU:HD22	1.91	0.52
1:B:64:VAL:HG13	1:B:69:LEU:HD22	1.92	0.52
1:A:133:LEU:HD13	1:A:166:LEU:HD22	1.92	0.51
1:D:421:MET:HE3	1:D:439:MET:CE	2.40	0.51
1:C:429:TRP:HH2	1:C:439[B]:MET:CE	2.23	0.51
1:D:429:TRP:CG	1:D:431:LEU:HD13	2.45	0.51
1:H:64:VAL:HG13	1:H:69:LEU:HD22	1.92	0.51
1:D:429:TRP:HH2	1:D:439:MET:CE	2.23	0.51
1:E:133:LEU:HD13	1:E:166:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:LYS:HE2	1:G:396:GLU:HG3	1.93	0.51
1:A:429:TRP:CG	1:A:431:LEU:HD13	2.46	0.51
1:E:429:TRP:CG	1:E:431:LEU:HD13	2.46	0.51
1:F:133:LEU:HD13	1:F:166:LEU:HD22	1.92	0.51
1:H:429:TRP:CH2	1:H:439[B]:MET:CE	2.94	0.51
1:B:429:TRP:CG	1:B:431:LEU:HD13	2.45	0.50
1:G:429:TRP:CH2	1:G:439[B]:MET:HE3	2.45	0.50
1:D:335:ARG:HG2	5:D:976:HOH:O	2.11	0.50
1:E:352:ILE:HG23	1:E:363:LEU:HD13	1.94	0.50
1:A:352:ILE:HG23	1:A:363:LEU:HD13	1.94	0.50
1:C:468:ILE:HD13	1:C:479:LEU:CD2	2.41	0.50
1:G:64:VAL:HG13	1:G:69:LEU:HD22	1.95	0.49
1:G:468:ILE:HD13	1:G:479:LEU:CD2	2.42	0.49
1:D:64:VAL:HG13	1:D:69:LEU:HD22	1.94	0.49
1:F:352:ILE:HG23	1:F:363:LEU:HD13	1.95	0.49
1:D:429:TRP:CH2	1:D:439:MET:HE1	2.48	0.49
1:C:123:ALA:HB1	1:C:418:ARG:HD3	1.94	0.49
1:E:32:THR:HG22	1:E:33:ARG:HG2	1.95	0.49
1:B:206:HIS:O	1:H:86:ARG:HD2	2.12	0.49
1:H:421:MET:HE1	1:H:439[B]:MET:HE2	1.95	0.49
1:H:421:MET:HE1	1:H:439[B]:MET:CE	2.42	0.48
1:D:382:VAL:HA	1:D:385:MET:HE3	1.94	0.48
1:E:208:ARG:HG2	5:E:816:HOH:O	2.12	0.48
1:D:133:LEU:HD13	1:D:166:LEU:HD22	1.96	0.48
1:D:352:ILE:HD13	1:D:377:LEU:HD22	1.95	0.48
1:G:261:ASP:OD2	1:G:335:ARG:HD3	2.14	0.48
1:H:429:TRP:CH2	1:H:439[B]:MET:HE1	2.48	0.48
1:D:261:ASP:OD2	1:D:335:ARG:HD3	2.13	0.48
1:H:261:ASP:OD2	1:H:335:ARG:HD3	2.14	0.48
1:E:439:MET:HE2	1:G:439[B]:MET:SD	2.53	0.48
1:C:261:ASP:OD2	1:C:335:ARG:HD3	2.14	0.48
1:G:336:LYS:HE3	1:G:338:GLN:HG2	1.96	0.48
1:H:133:LEU:HD13	1:H:166:LEU:HD22	1.96	0.48
1:C:64:VAL:HG13	1:C:69:LEU:HD22	1.95	0.47
1:E:261:ASP:OD2	1:E:335:ARG:HD3	2.15	0.47
1:C:336:LYS:HE3	1:C:338:GLN:HG2	1.97	0.47
1:E:297:ALA:HB1	2:E:701:FAD:HM73	1.96	0.47
1:F:261:ASP:OD2	1:F:335:ARG:HD3	2.14	0.47
1:G:363:LEU:CD1	1:G:381:VAL:CG2	2.92	0.47
1:B:352:ILE:HG23	1:B:363:LEU:HD13	1.96	0.47
1:D:421:MET:HE1	1:D:439:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439[A]:MET:HE2	1:D:439:MET:HG2	1.96	0.47
1:A:268:PRO:HG3	1:A:285:LEU:HD22	1.97	0.46
1:F:352:ILE:HD13	1:F:377:LEU:HD22	1.97	0.46
1:H:352:ILE:HD13	1:H:377:LEU:HD22	1.96	0.46
1:B:268:PRO:HG3	1:B:285:LEU:HD22	1.98	0.46
1:H:314:THR:CG2	1:H:318:PHE:CE2	2.98	0.46
1:B:431:LEU:HD11	1:D:431:LEU:CD1	2.46	0.46
4:F:703:GLY:N	5:F:816:HOH:O	2.49	0.46
1:C:13:VAL:HG11	1:C:29:ILE:HD13	1.98	0.46
1:G:437:HIS:O	1:G:441:THR:HG23	2.16	0.46
1:B:352:ILE:HD13	1:B:377:LEU:HD22	1.97	0.46
1:F:268:PRO:HG3	1:F:285:LEU:HD22	1.97	0.46
1:C:429:TRP:CH2	1:C:439[B]:MET:HE1	2.51	0.46
1:B:379:ARG:HD3	5:B:1004:HOH:O	2.15	0.46
1:E:437:HIS:O	1:E:441:THR:HG23	2.16	0.45
1:H:382:VAL:HA	1:H:385:MET:HE3	1.97	0.45
1:D:314:THR:CG2	1:D:318:PHE:CE2	3.00	0.45
1:B:431:LEU:CD1	1:D:431:LEU:HD11	2.46	0.45
1:H:314:THR:HG22	1:H:318:PHE:CE2	2.52	0.45
2:H:701:FAD:H1'2	2:H:701:FAD:H9	1.78	0.45
1:E:268:PRO:HG3	1:E:285:LEU:HD22	1.98	0.45
1:A:32:THR:HG22	1:A:33:ARG:HG2	1.98	0.45
1:D:268:PRO:HG3	1:D:285:LEU:HD22	1.99	0.45
1:E:311:ILE:HG23	1:F:318:PHE:HB3	1.99	0.45
1:G:13:VAL:HG11	1:G:29:ILE:HD13	1.99	0.45
1:D:381:VAL:O	1:D:385:MET:HE2	2.17	0.45
1:E:381:VAL:O	1:E:385:MET:HE2	2.17	0.45
1:F:431:LEU:CD1	1:H:431:LEU:HD11	2.47	0.45
1:F:28:GLU:HB3	1:F:382:VAL:HG21	1.99	0.44
1:F:431:LEU:HD11	1:H:431:LEU:CD1	2.48	0.44
1:H:37:ARG:NH2	5:H:808:HOH:O	2.50	0.44
1:H:381:VAL:O	1:H:385:MET:HE2	2.17	0.44
1:C:208:ARG:HG3	1:C:358:GLU:HB3	2.00	0.44
1:C:437:HIS:O	1:C:441:THR:HG23	2.17	0.44
1:D:395:ARG:O	1:D:398:ARG:HG3	2.18	0.44
1:D:421:MET:HE1	1:D:439:MET:CE	2.48	0.44
1:H:268:PRO:HG3	1:H:285:LEU:HD22	1.99	0.44
1:H:395:ARG:O	1:H:398:ARG:HG3	2.18	0.44
1:C:83:GLN:NE2	5:C:801:HOH:O	2.31	0.44
1:D:28:GLU:HB3	1:D:382:VAL:HG21	2.00	0.44
1:E:382:VAL:HA	1:E:385:MET:HE3	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:HB3	1:B:382:VAL:HG21	1.99	0.44
1:F:464:LEU:HB2	5:F:1105:HOH:O	2.17	0.44
4:B:703:GLY:N	5:B:814:HOH:O	2.51	0.44
1:C:30:ALA:HB2	1:C:38:VAL:HG11	2.00	0.44
1:D:314:THR:HG22	1:D:318:PHE:CE2	2.53	0.44
1:F:479:LEU:HD22	5:F:881:HOH:O	2.16	0.44
1:G:208:ARG:HG3	1:G:358:GLU:HB3	2.00	0.44
1:C:268:PRO:HG3	1:C:285:LEU:HD22	2.00	0.44
1:D:33:ARG:HB3	1:D:36:VAL:HG22	2.00	0.43
1:D:208:ARG:HG3	1:D:358:GLU:HB3	1.99	0.43
1:F:437:HIS:O	1:F:441:THR:HG23	2.18	0.43
1:H:33:ARG:HB3	1:H:36:VAL:HG22	2.00	0.43
1:C:55:GLY:N	1:C:56:ALA:HA	2.33	0.43
1:E:39:THR:OG1	1:E:193:ARG:NH1	2.50	0.43
1:H:429:TRP:HH2	1:H:439[B]:MET:CE	2.31	0.43
2:E:701:FAD:H9	2:E:701:FAD:H1'2	1.74	0.43
1:H:28:GLU:HB3	1:H:382:VAL:HG21	2.00	0.43
1:A:346:ILE:HG13	1:A:464:LEU:HD21	2.01	0.43
1:H:439[B]:MET:HE2	1:H:439[B]:MET:HB2	1.50	0.43
1:E:346:ILE:HG13	1:E:464:LEU:HD21	2.01	0.43
1:A:297:ALA:HB1	2:A:701:FAD:HM73	2.00	0.43
1:G:439[B]:MET:HE2	1:G:439[B]:MET:HB2	1.59	0.43
1:D:352:ILE:HG23	1:D:363:LEU:HD13	2.01	0.43
1:H:208:ARG:HG3	1:H:358:GLU:HB3	1.99	0.43
1:A:429:TRP:HB2	1:A:431:LEU:CD1	2.49	0.42
1:G:55:GLY:N	1:G:56:ALA:HA	2.34	0.42
1:G:268:PRO:HG3	1:G:285:LEU:HD22	2.00	0.42
1:A:261:ASP:OD2	1:A:335:ARG:HD3	2.19	0.42
1:F:429:TRP:HB2	1:F:431:LEU:CD1	2.49	0.42
1:H:352:ILE:HG23	1:H:363:LEU:HD13	2.01	0.42
1:G:30:ALA:HB2	1:G:38:VAL:HG11	2.01	0.42
1:E:368:ARG:NH2	4:E:703:GLY:HA2	2.35	0.42
1:B:429:TRP:HB2	1:B:431:LEU:CD1	2.49	0.42
1:C:439[B]:MET:HE2	1:C:439[B]:MET:HB2	1.57	0.42
1:D:437:HIS:O	1:D:441:THR:HG23	2.19	0.42
1:E:429:TRP:HB2	1:E:431:LEU:CD1	2.50	0.42
2:F:701:FAD:H9	2:F:701:FAD:H1'2	1.79	0.42
1:H:437:HIS:O	1:H:441:THR:HG23	2.19	0.42
1:D:429:TRP:HB2	1:D:431:LEU:CD1	2.50	0.42
1:B:297:ALA:HB1	2:B:701:FAD:HM73	2.01	0.42
1:A:28:GLU:HB3	1:A:382:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LYS:HE3	5:C:891:HOH:O	2.20	0.41
1:F:398:ARG:HG3	1:F:399:PRO:HD2	2.01	0.41
1:B:398:ARG:HG3	1:B:399:PRO:HD2	2.02	0.41
1:D:362:MET:HE2	1:D:362:MET:HB2	2.00	0.41
1:G:20:VAL:HG11	1:G:371:LEU:HA	2.02	0.41
1:G:240:LEU:HB2	1:G:243:LEU:HD22	2.02	0.41
1:E:362:MET:HE2	1:E:362:MET:HB2	1.90	0.41
1:H:429:TRP:HB2	1:H:431:LEU:CD1	2.49	0.41
1:D:68:ALA:O	1:D:74:GLY:HA3	2.20	0.41
1:C:457:THR:HG21	1:C:487:HIS:CE1	2.56	0.41
1:F:68:ALA:O	1:F:74:GLY:HA3	2.20	0.41
1:A:240:LEU:HB2	1:A:243:LEU:HD22	2.02	0.41
1:B:208:ARG:HG3	1:B:358:GLU:HB3	2.03	0.41
1:H:68:ALA:O	1:H:74:GLY:HA3	2.20	0.41
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.93	0.41
1:B:68:ALA:O	1:B:74:GLY:HA3	2.21	0.41
1:D:133:LEU:HD12	1:D:133:LEU:HA	1.93	0.41
2:A:701:FAD:H9	2:A:701:FAD:H1'2	1.76	0.41
1:E:240:LEU:HB2	1:E:243:LEU:HD22	2.02	0.41
1:F:297:ALA:HB1	2:F:701:FAD:HM73	2.03	0.41
2:G:701:FAD:H9	2:G:701:FAD:H1'2	1.82	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.94	0.40
1:C:20:VAL:HG11	1:C:371:LEU:HA	2.02	0.40
1:C:436:PRO:HA	1:C:439[B]:MET:HE1	2.00	0.40
1:A:208:ARG:HG2	5:A:828:HOH:O	2.21	0.40
1:B:439[A]:MET:CE	1:D:439:MET:HA	2.49	0.40
1:G:457:THR:HG21	1:G:487:HIS:CE1	2.56	0.40
1:C:240:LEU:HB2	1:C:243:LEU:HD22	2.02	0.40
1:H:421:MET:HE3	1:H:439[B]:MET:CE	2.50	0.40
1:B:346:ILE:HG13	1:B:464:LEU:HD21	2.03	0.40
1:H:296:GLY:HA3	1:H:297:ALA:HB2	2.03	0.40
1:C:68:ALA:O	1:C:74:GLY:HA3	2.21	0.40
1:D:30:ALA:HB2	1:D:38:VAL:HG11	2.04	0.40
1:D:123:ALA:HB1	1:D:418:ARG:HD2	2.03	0.40
1:D:381:VAL:HG12	1:D:385:MET:CE	2.51	0.40
1:G:468:ILE:CD1	1:G:479:LEU:CD2	3.00	0.40
1:H:381:VAL:HG12	1:H:385:MET:CE	2.51	0.40

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	479/512 (94%)	470 (98%)	9 (2%)	0	100 100
1	B	481/512 (94%)	472 (98%)	9 (2%)	0	100 100
1	C	481/512 (94%)	470 (98%)	11 (2%)	0	100 100
1	D	478/512 (93%)	467 (98%)	11 (2%)	0	100 100
1	E	480/512 (94%)	471 (98%)	9 (2%)	0	100 100
1	F	480/512 (94%)	470 (98%)	10 (2%)	0	100 100
1	G	481/512 (94%)	470 (98%)	11 (2%)	0	100 100
1	H	479/512 (94%)	468 (98%)	11 (2%)	0	100 100
All	All	3839/4096 (94%)	3758 (98%)	81 (2%)	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	375/400 (94%)	365 (97%)	10 (3%)	44 35
1	B	377/400 (94%)	366 (97%)	11 (3%)	42 31
1	C	377/400 (94%)	367 (97%)	10 (3%)	44 35
1	D	374/400 (94%)	361 (96%)	13 (4%)	36 24
1	E	376/400 (94%)	367 (98%)	9 (2%)	49 41
1	F	376/400 (94%)	365 (97%)	11 (3%)	42 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	377/400 (94%)	370 (98%)	7 (2%)	57 50
1	H	375/400 (94%)	362 (96%)	13 (4%)	36 24
All	All	3007/3200 (94%)	2923 (97%)	84 (3%)	43 32

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	77	LYS
1	A	133	LEU
1	A	193	ARG
1	A	203	ARG
1	A	362	MET
1	A	395	ARG
1	A	429	TRP
1	A	452	ASP
1	A	457	THR
1	B	77	LYS
1	B	133	LEU
1	B	137	LYS
1	B	193	ARG
1	B	203	ARG
1	B	335	ARG
1	B	362	MET
1	B	395	ARG
1	B	429	TRP
1	B	452	ASP
1	B	457	THR
1	C	77	LYS
1	C	85	GLN
1	C	203	ARG
1	C	335	ARG
1	C	386	ASP
1	C	429	TRP
1	C	431	LEU
1	C	452	ASP
1	C	457	THR
1	C	473	ARG
1	D	33	ARG
1	D	77	LYS
1	D	85	GLN

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Mol	Chain	Res	Type
1	D	108	THR
1	D	133	LEU
1	D	137	LYS
1	D	203	ARG
1	D	335	ARG
1	D	362	MET
1	D	429	TRP
1	D	439	MET
1	D	452	ASP
1	D	457	THR
1	E	11	THR
1	E	77	LYS
1	E	133	LEU
1	E	203	ARG
1	E	335	ARG
1	E	362	MET
1	E	429	TRP
1	E	452	ASP
1	E	457	THR
1	F	77	LYS
1	F	133	LEU
1	F	137	LYS
1	F	193	ARG
1	F	203	ARG
1	F	335	ARG
1	F	362	MET
1	F	395	ARG
1	F	429	TRP
1	F	452	ASP
1	F	457	THR
1	G	77	LYS
1	G	203	ARG
1	G	335	ARG
1	G	429	TRP
1	G	431	LEU
1	G	452	ASP
1	G	457	THR
1	H	33	ARG
1	H	77	LYS
1	H	85	GLN
1	H	108	THR
1	H	133	LEU

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Mol	Chain	Res	Type
1	H	137	LYS
1	H	193	ARG
1	H	203	ARG
1	H	335	ARG
1	H	362	MET
1	H	429	TRP
1	H	452	ASP
1	H	457	THR

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	487	HIS
1	B	10	GLN
1	B	83	GLN
1	F	10	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	GLY	E	703	-	4,4,4	1.01	0	3,4,4	1.04	0
2	FAD	G	701	-	53,58,58	0.65	0	68,89,89	0.84	3 (4%)
4	GLY	B	703	-	4,4,4	0.61	0	3,4,4	1.35	0
2	FAD	C	701	-	53,58,58	0.66	0	68,89,89	0.87	4 (5%)
4	GLY	G	703	-	4,4,4	0.76	0	3,4,4	1.44	0
3	I55	G	702	-	28,32,32	0.79	1 (3%)	31,46,46	1.23	3 (9%)
3	I55	F	702	-	28,32,32	1.09	1 (3%)	31,46,46	1.09	2 (6%)
3	I55	H	702	-	28,32,32	0.71	1 (3%)	31,46,46	0.94	1 (3%)
3	I55	D	702	-	28,32,32	0.62	1 (3%)	31,46,46	0.95	1 (3%)
3	I55	A	702	-	28,32,32	1.05	1 (3%)	31,46,46	1.07	1 (3%)
2	FAD	F	701	-	53,58,58	0.72	0	68,89,89	0.85	2 (2%)
2	FAD	H	701	-	53,58,58	0.64	0	68,89,89	0.81	3 (4%)
4	GLY	C	703	-	4,4,4	0.70	0	3,4,4	1.23	0
4	GLY	F	703	-	4,4,4	0.58	0	3,4,4	1.38	0
2	FAD	D	701	-	53,58,58	0.62	0	68,89,89	0.81	3 (4%)
4	GLY	D	703	-	4,4,4	1.12	0	3,4,4	0.79	0
4	GLY	A	703	-	4,4,4	1.06	0	3,4,4	0.73	0
2	FAD	B	701	-	53,58,58	0.72	0	68,89,89	0.84	2 (2%)
2	FAD	E	701	-	53,58,58	0.72	0	68,89,89	0.97	5 (7%)
4	GLY	H	703	-	4,4,4	0.97	0	3,4,4	1.00	0
3	I55	E	702	-	28,32,32	1.13	2 (7%)	31,46,46	1.17	1 (3%)
2	FAD	A	701	-	53,58,58	0.67	0	68,89,89	0.92	4 (5%)
3	I55	B	702	-	28,32,32	1.22	1 (3%)	31,46,46	1.08	4 (12%)
3	I55	C	702	-	28,32,32	0.64	0	31,46,46	1.18	3 (9%)

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	GLY	E	703	-	-	0/2/2/2	-
2	FAD	G	701	-	-	2/30/50/50	0/6/6/6
4	GLY	B	703	-	-	0/2/2/2	-
2	FAD	C	701	-	-	3/30/50/50	0/6/6/6
4	GLY	G	703	-	-	0/2/2/2	-
3	I55	G	702	-	-	1/14/61/61	0/3/3/3
3	I55	F	702	-	-	2/14/61/61	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I55	H	702	-	-	2/14/61/61	0/3/3/3
3	I55	D	702	-	-	2/14/61/61	0/3/3/3
3	I55	A	702	-	-	1/14/61/61	0/3/3/3
2	FAD	F	701	-	-	1/30/50/50	0/6/6/6
2	FAD	H	701	-	-	3/30/50/50	0/6/6/6
4	GLY	C	703	-	-	0/2/2/2	-
4	GLY	F	703	-	-	0/2/2/2	-
2	FAD	D	701	-	-	2/30/50/50	0/6/6/6
4	GLY	D	703	-	-	0/2/2/2	-
4	GLY	A	703	-	-	0/2/2/2	-
2	FAD	B	701	-	-	1/30/50/50	0/6/6/6
2	FAD	E	701	-	-	1/30/50/50	0/6/6/6
4	GLY	H	703	-	-	0/2/2/2	-
3	I55	E	702	-	-	1/14/61/61	0/3/3/3
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6
3	I55	B	702	-	-	2/14/61/61	0/3/3/3
3	I55	C	702	-	-	1/14/61/61	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	I55	C4-C3	-5.59	1.49	1.53
3	E	702	I55	C4-C3	-4.81	1.50	1.53
3	F	702	I55	C4-C3	-4.64	1.50	1.53
3	A	702	I55	C4-C3	-4.48	1.50	1.53
3	G	702	I55	C4-C3	-3.13	1.51	1.53
3	H	702	I55	C4-C3	-2.95	1.51	1.53
3	D	702	I55	C4-C3	-2.35	1.51	1.53
3	E	702	I55	C8-C9	2.30	1.54	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	702	I55	C10-N6-C5	-5.15	107.62	112.56
3	G	702	I55	C10-N6-C5	-4.71	108.04	112.56
3	C	702	I55	C10-N6-C5	-4.29	108.45	112.56
3	A	702	I55	C10-N6-C5	-4.25	108.49	112.56
3	F	702	I55	C10-N6-C5	-4.13	108.60	112.56
3	H	702	I55	C10-N6-C5	-3.79	108.93	112.56
3	B	702	I55	C10-N6-C5	-3.30	109.40	112.56
3	D	702	I55	C10-N6-C5	-3.25	109.44	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	FAD	C5A-C6A-N6A	3.03	124.96	120.35
2	A	701	FAD	C5A-C6A-N6A	2.87	124.71	120.35
2	E	701	FAD	C4'-C3'-C2'	2.71	119.01	113.36
2	A	701	FAD	C4'-C3'-C2'	2.62	118.80	113.36
2	F	701	FAD	O2A-PA-O1A	2.59	125.06	112.24
2	G	701	FAD	O2P-P-O1P	2.50	124.62	112.24
2	A	701	FAD	O2A-PA-O1A	2.49	124.54	112.24
2	F	701	FAD	C4'-C3'-C2'	2.42	118.39	113.36
2	E	701	FAD	O4'-C4'-C3'	2.38	114.89	109.10
2	B	701	FAD	O2A-PA-O1A	2.37	123.95	112.24
2	G	701	FAD	C5A-C6A-N6A	2.34	123.91	120.35
3	C	702	I55	C6-C7-N5	-2.31	115.34	118.19
3	F	702	I55	C9-C8-N5	2.30	112.21	109.83
2	E	701	FAD	O2A-PA-O1A	2.29	123.56	112.24
2	C	701	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	B	701	FAD	C4'-C3'-C2'	2.27	118.09	113.36
3	B	702	I55	C9-C8-N5	2.25	112.16	109.83
2	C	701	FAD	O2P-P-O1P	2.22	123.21	112.24
2	C	701	FAD	C4-N3-C2	-2.22	121.55	125.64
3	B	702	I55	O4-C4-C3	2.20	113.32	111.20
2	H	701	FAD	C5A-C6A-N6A	2.18	123.67	120.35
2	D	701	FAD	C5A-C6A-N6A	2.17	123.66	120.35
2	E	701	FAD	C4-N3-C2	-2.17	121.64	125.64
3	G	702	I55	C6-C7-N5	-2.16	115.52	118.19
3	C	702	I55	O3-C9-C10	2.11	114.62	109.77
3	B	702	I55	C6-C7-N5	-2.10	115.60	118.19
2	C	701	FAD	O4-C4-C4X	-2.06	121.12	126.60
2	G	701	FAD	C4-N3-C2	-2.03	121.89	125.64
2	H	701	FAD	O2P-P-O1P	2.03	122.27	112.24
2	D	701	FAD	O2P-P-O1P	2.02	122.21	112.24
2	D	701	FAD	C4-N3-C2	-2.02	121.92	125.64
3	G	702	I55	C9-C8-N5	2.02	111.92	109.83
2	H	701	FAD	C4-N3-C2	-2.01	121.92	125.64
2	A	701	FAD	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	702	I55	C11-C13-O6-C14
3	F	702	I55	C15-C13-O6-C14
2	C	701	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	701	FAD	C2'-C1'-N10-C10
2	H	701	FAD	C2'-C1'-N10-C10
2	G	701	FAD	O4B-C4B-C5B-O5B
3	A	702	I55	C15-C13-O6-C14
3	B	702	I55	C11-C13-O6-C14
3	B	702	I55	C15-C13-O6-C14
3	C	702	I55	C15-C13-O6-C14
3	D	702	I55	C11-C13-O6-C14
3	D	702	I55	C15-C13-O6-C14
3	E	702	I55	C15-C13-O6-C14
3	G	702	I55	C15-C13-O6-C14
3	H	702	I55	C11-C13-O6-C14
3	H	702	I55	C15-C13-O6-C14
2	A	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C2'-C1'-N10-C10
2	G	701	FAD	C2'-C1'-N10-C10
2	C	701	FAD	C3B-C4B-C5B-O5B
2	H	701	FAD	O4B-C4B-C5B-O5B
2	H	701	FAD	O4'-C4'-C5'-O5'

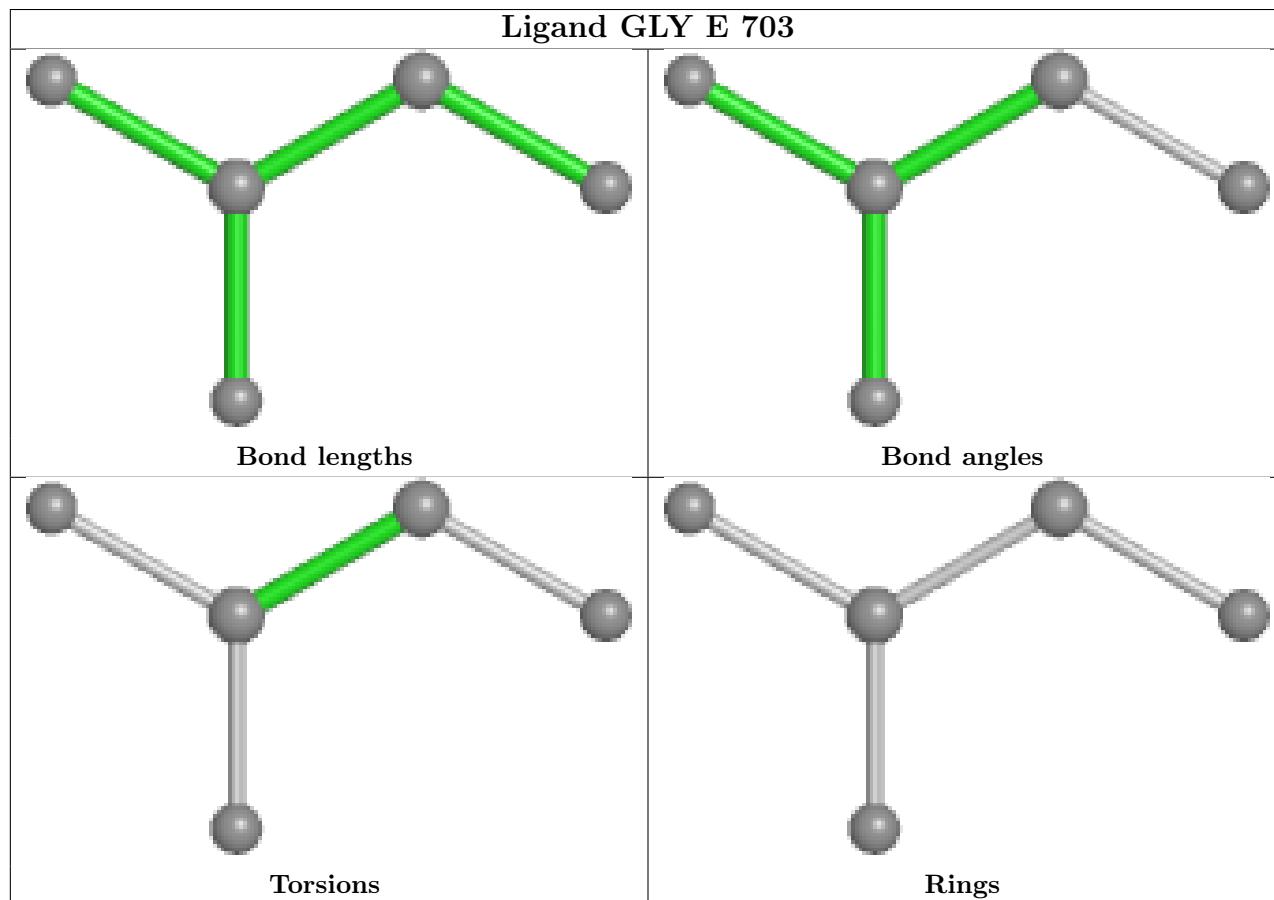
There are no ring outliers.

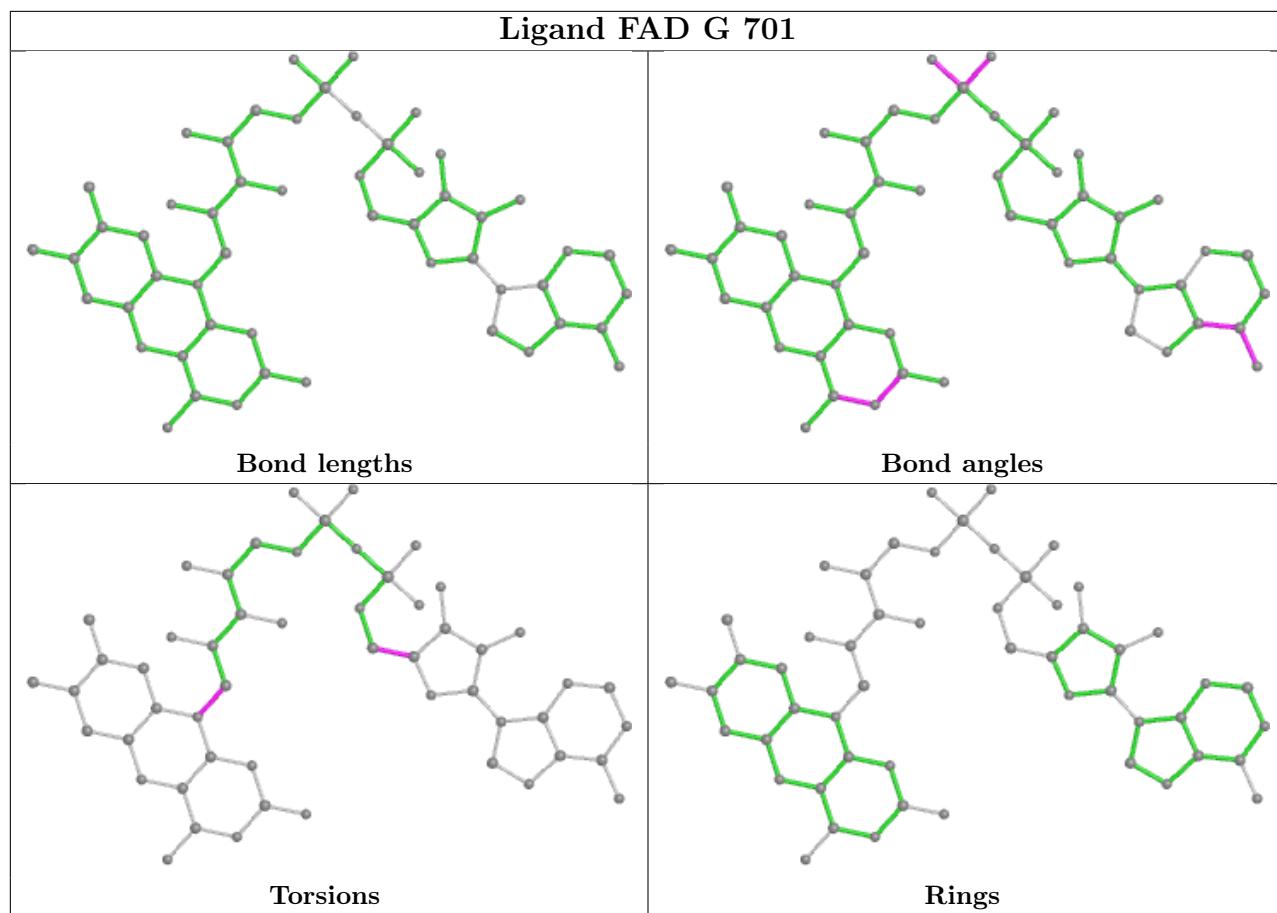
10 monomers are involved in 13 short contacts:

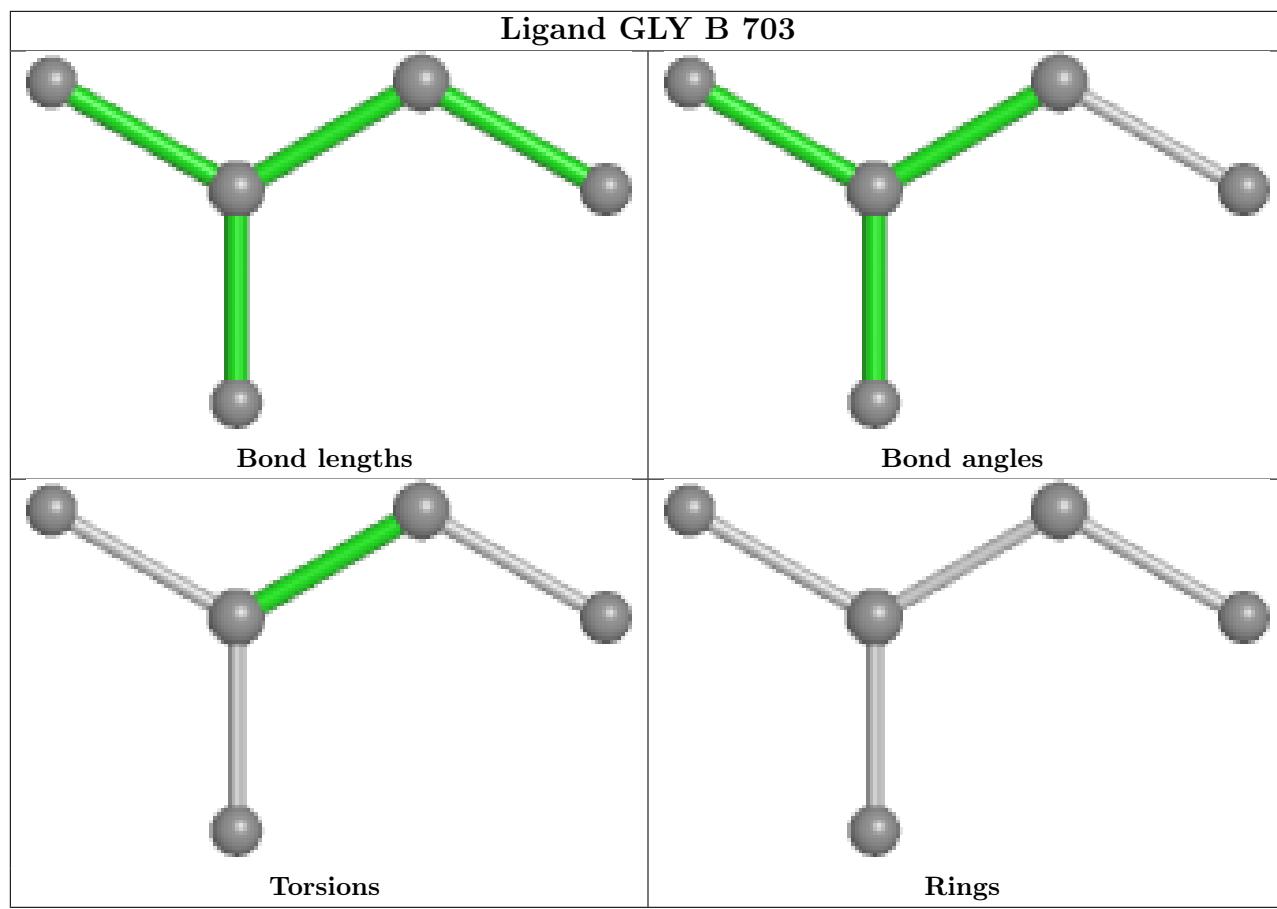
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	703	GLY	1	0
2	G	701	FAD	1	0
4	B	703	GLY	1	0
2	F	701	FAD	2	0
2	H	701	FAD	1	0
4	C	703	GLY	1	0
4	F	703	GLY	1	0
2	B	701	FAD	1	0
2	E	701	FAD	2	0
2	A	701	FAD	2	0

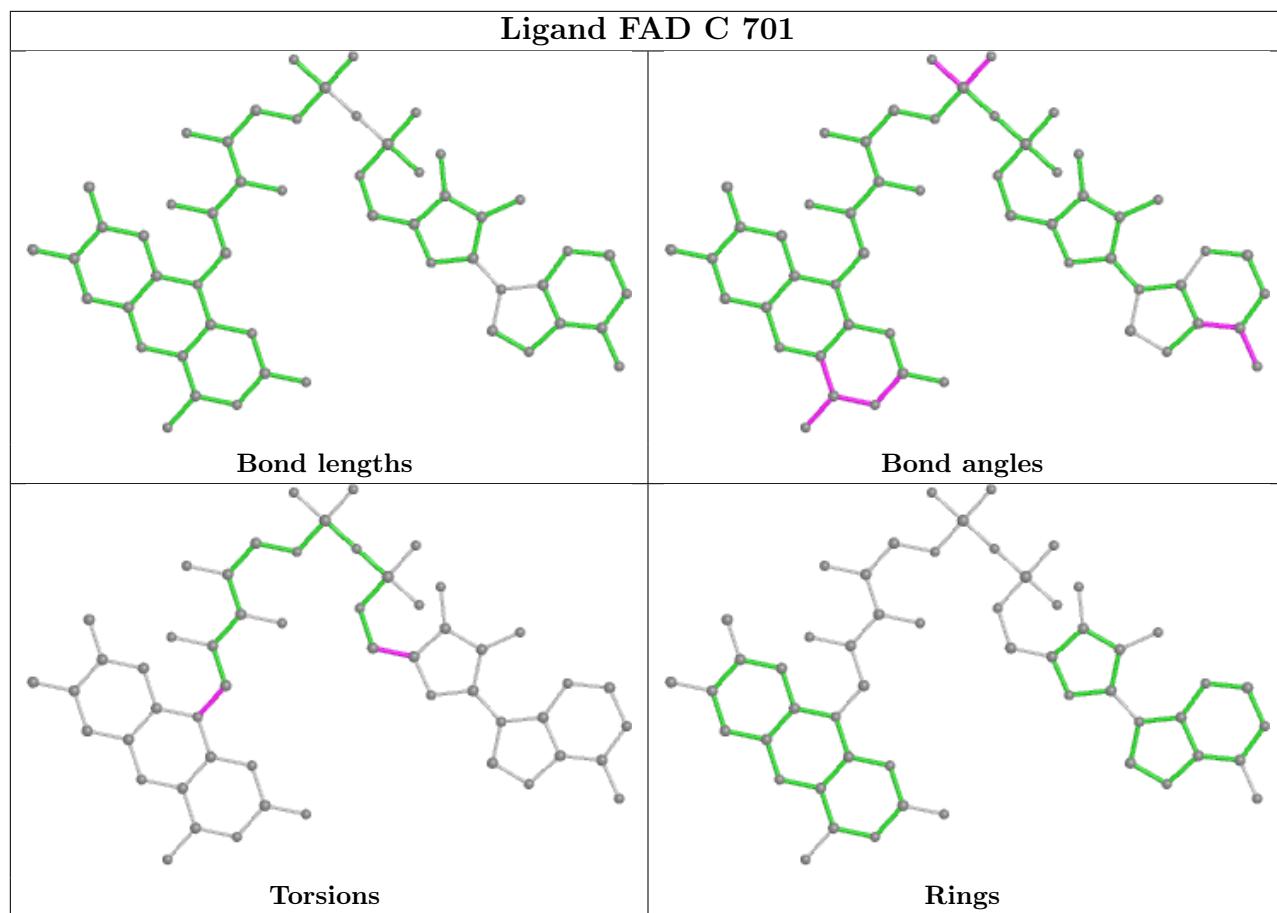
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

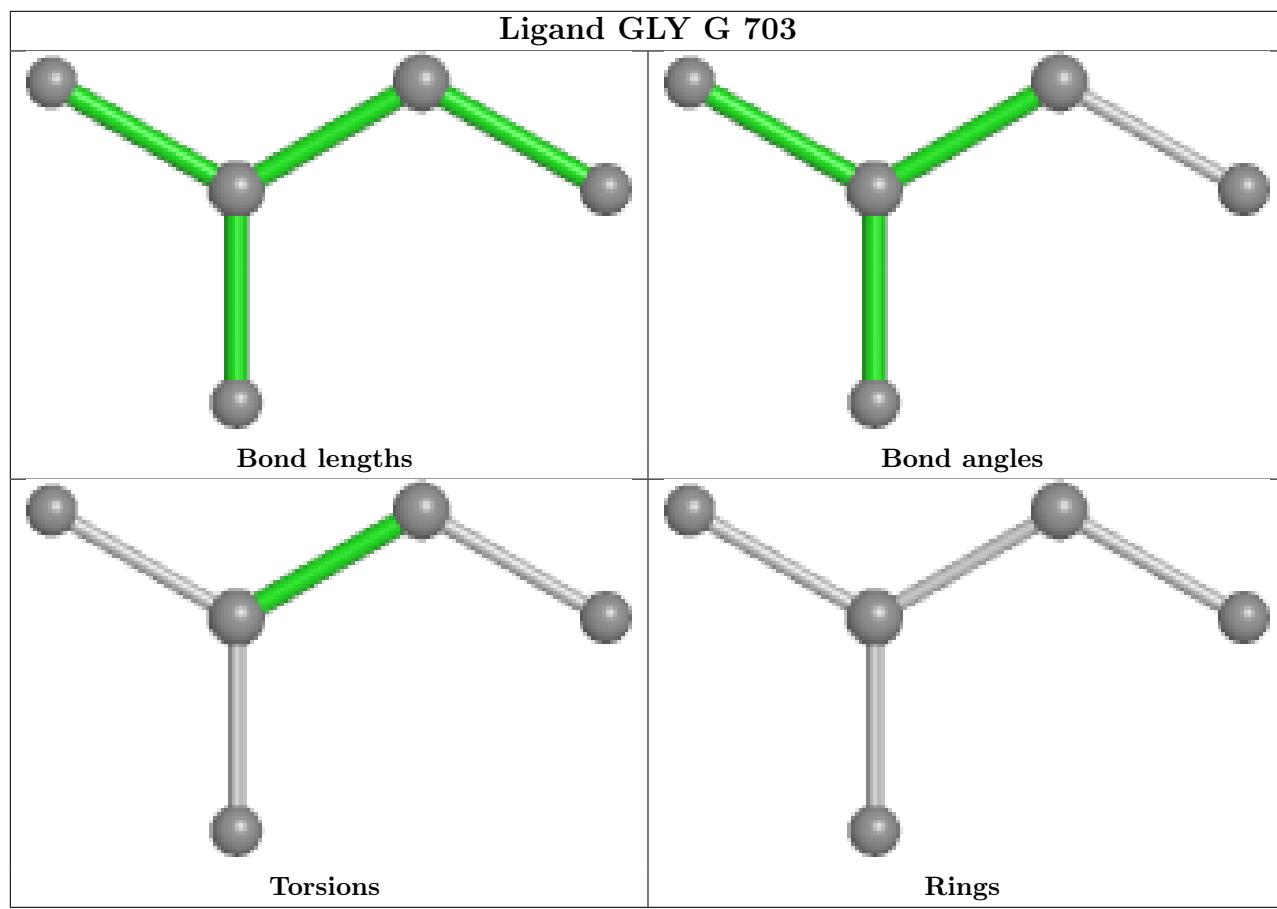
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

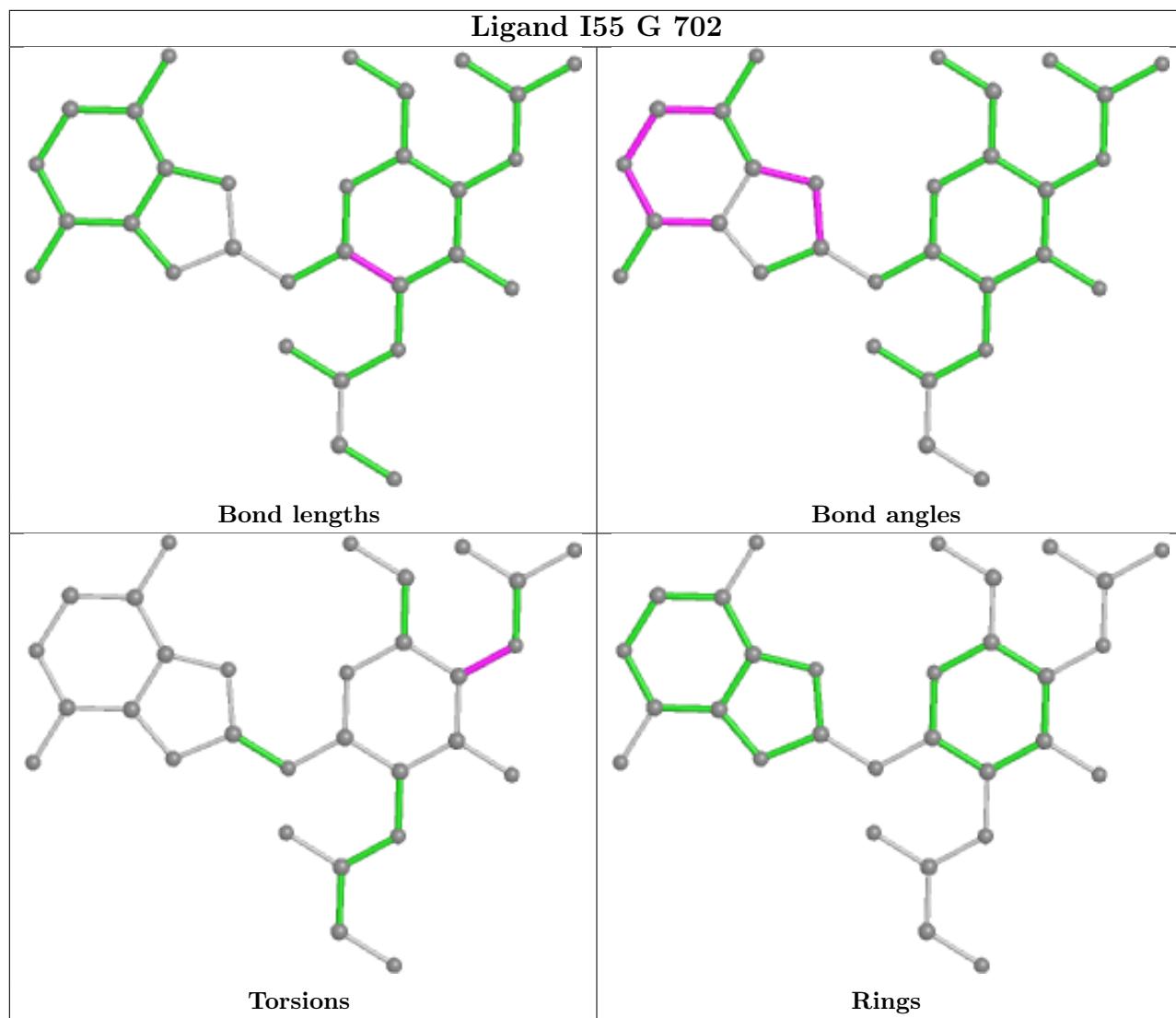


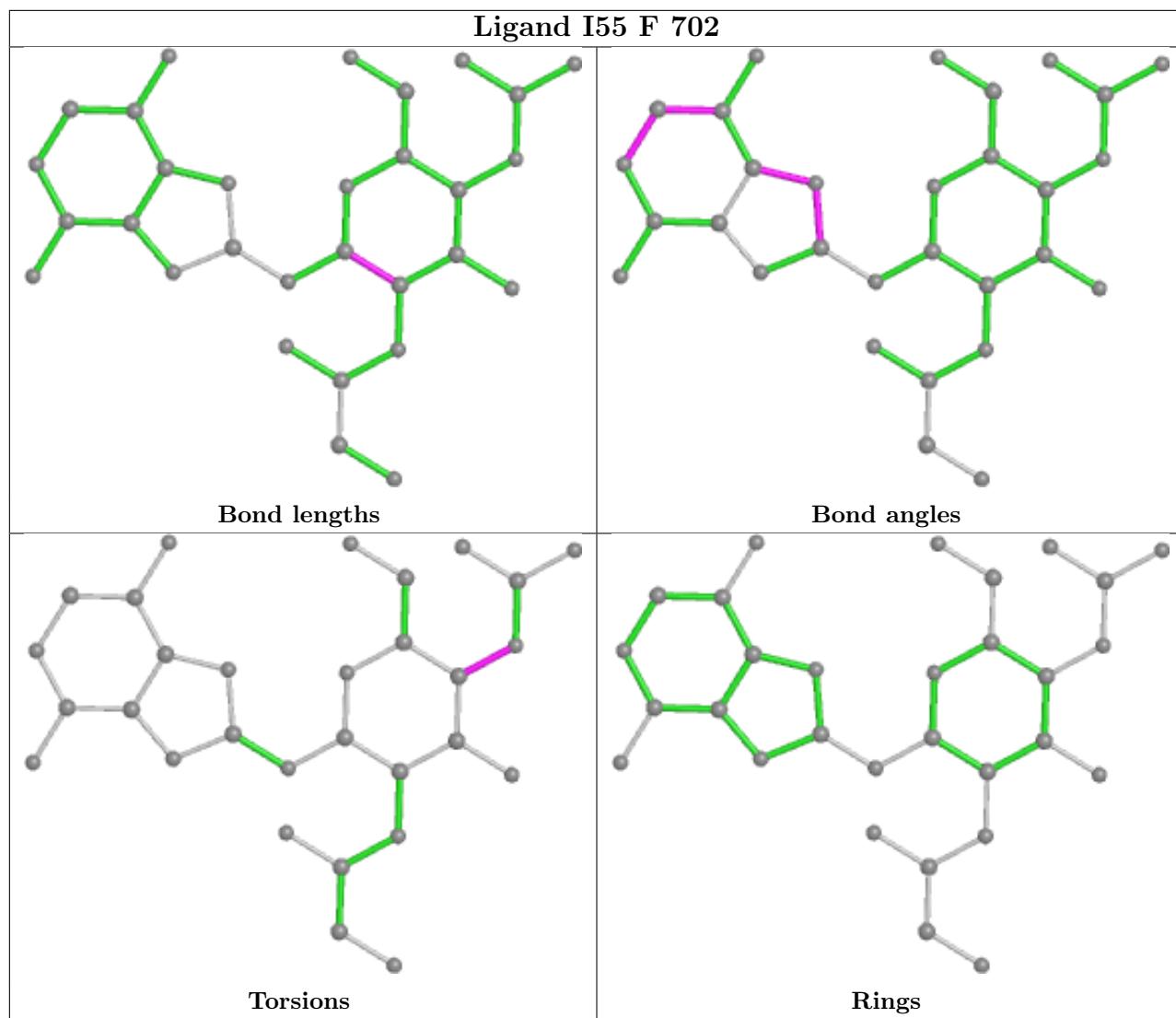


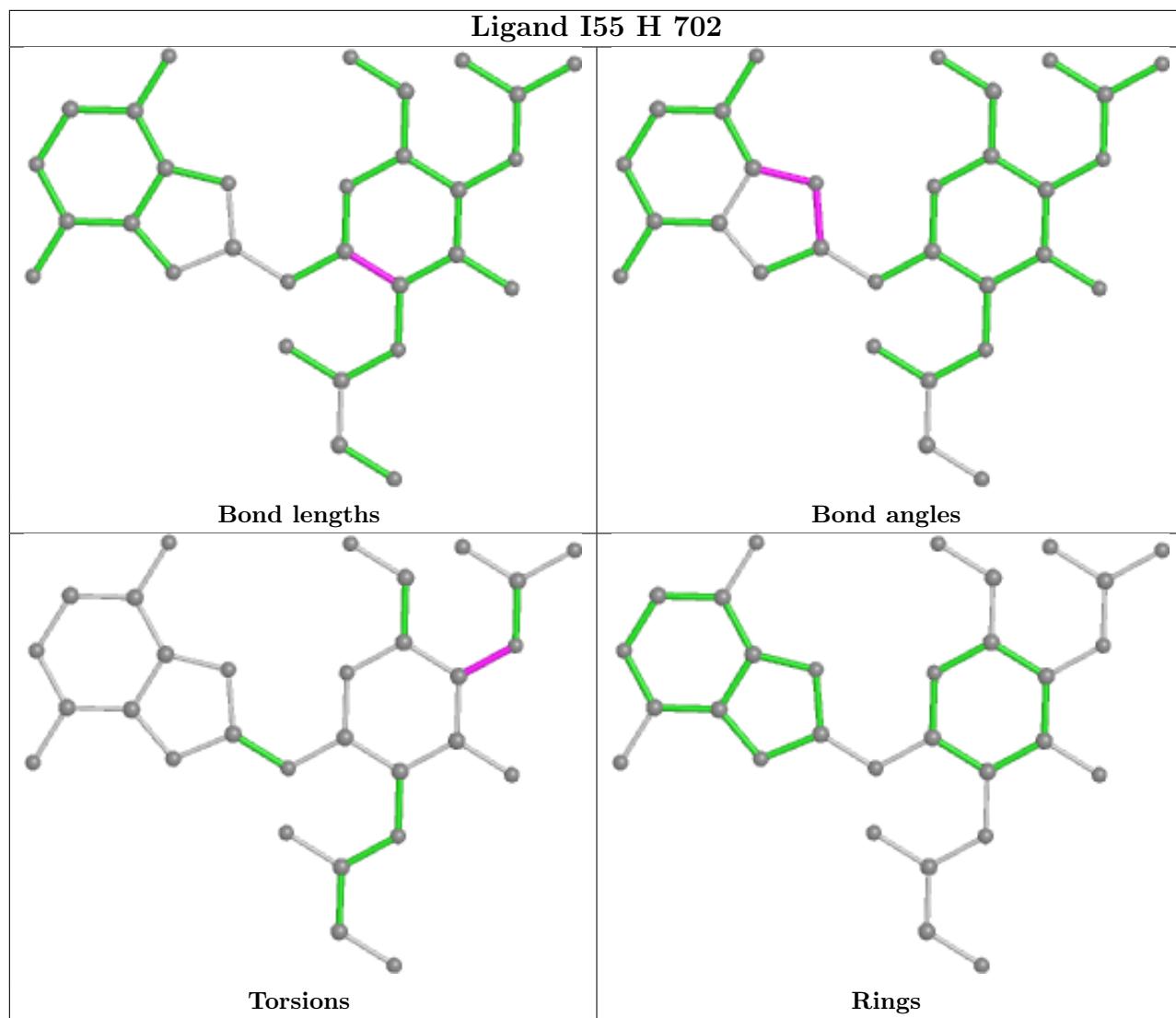


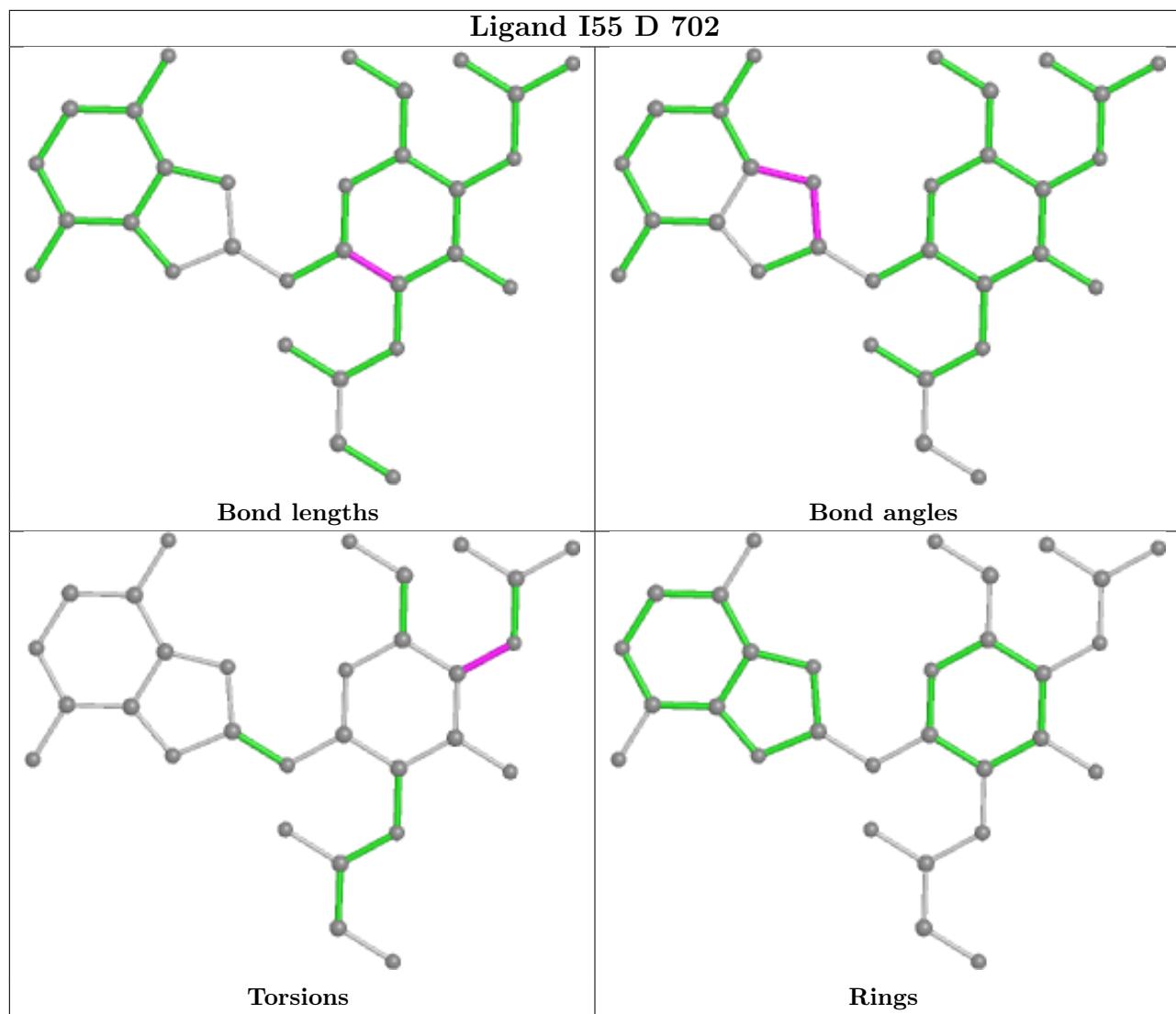


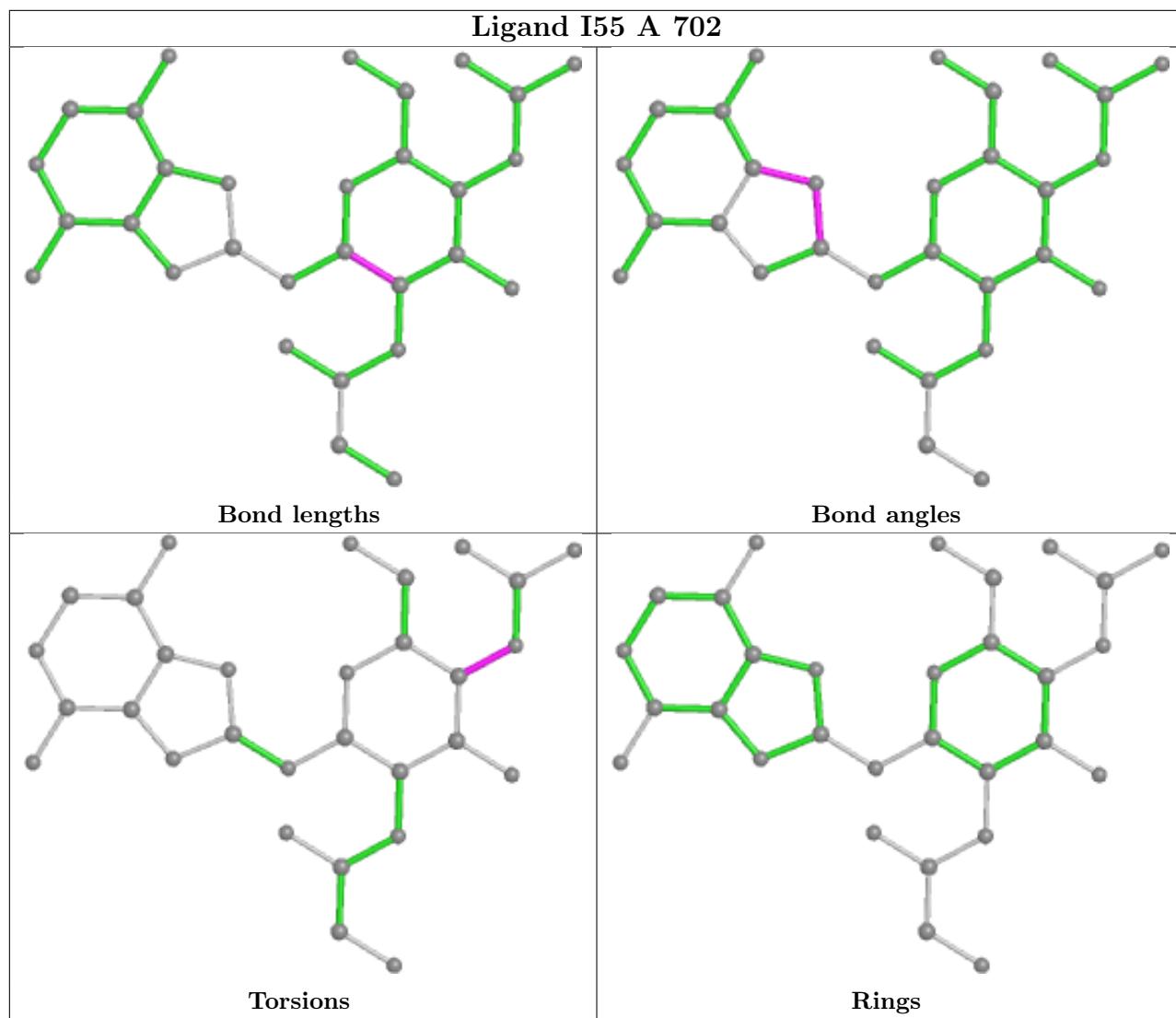


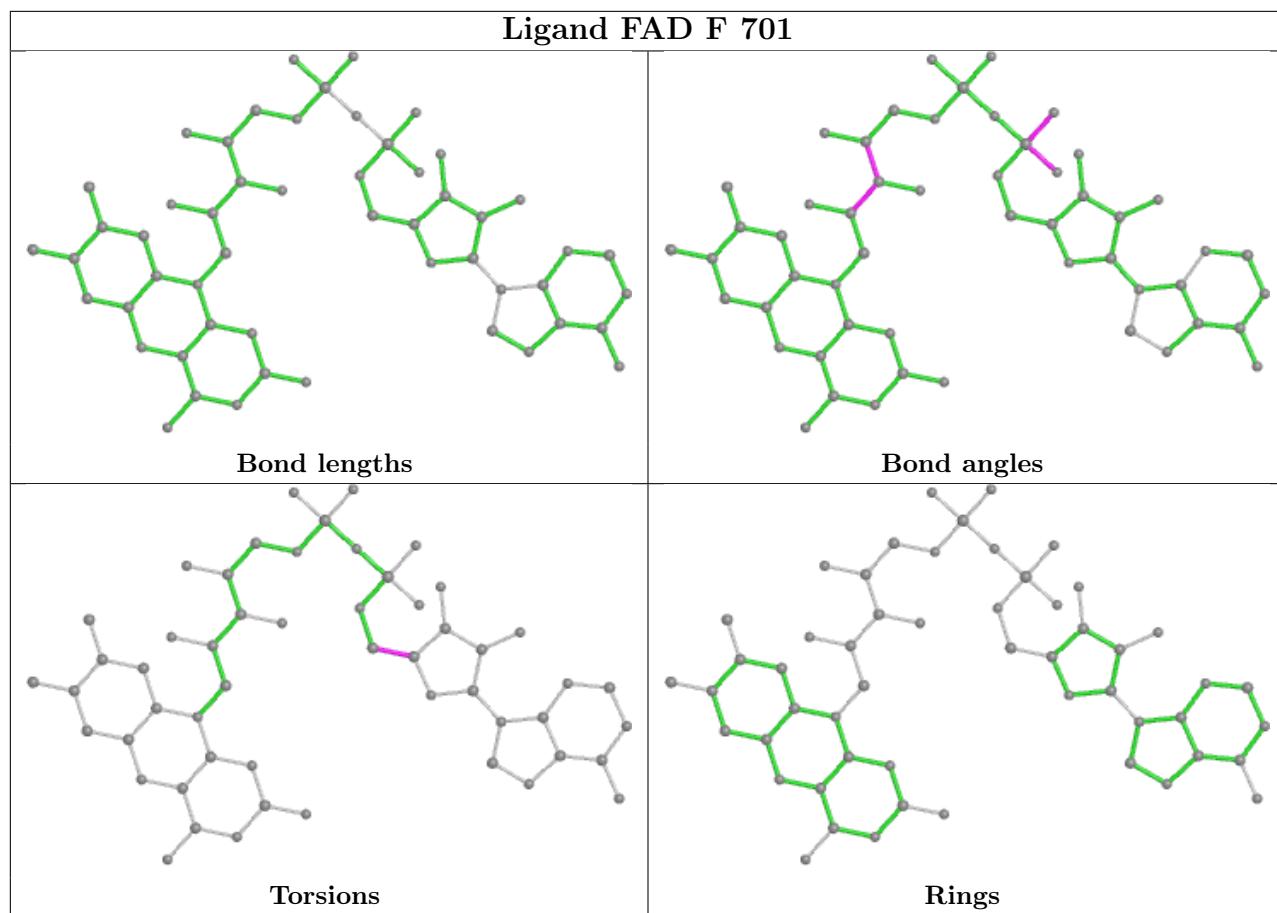


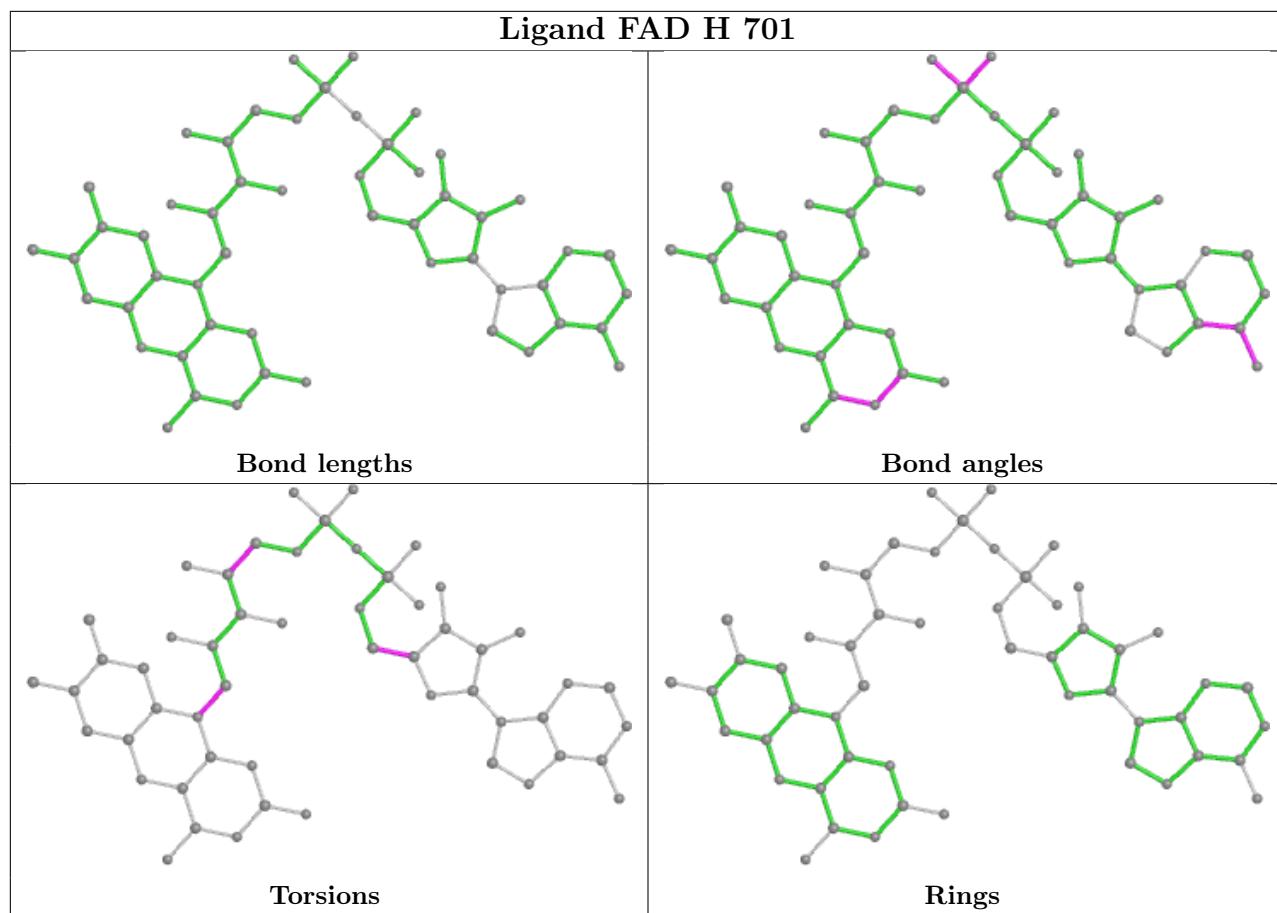


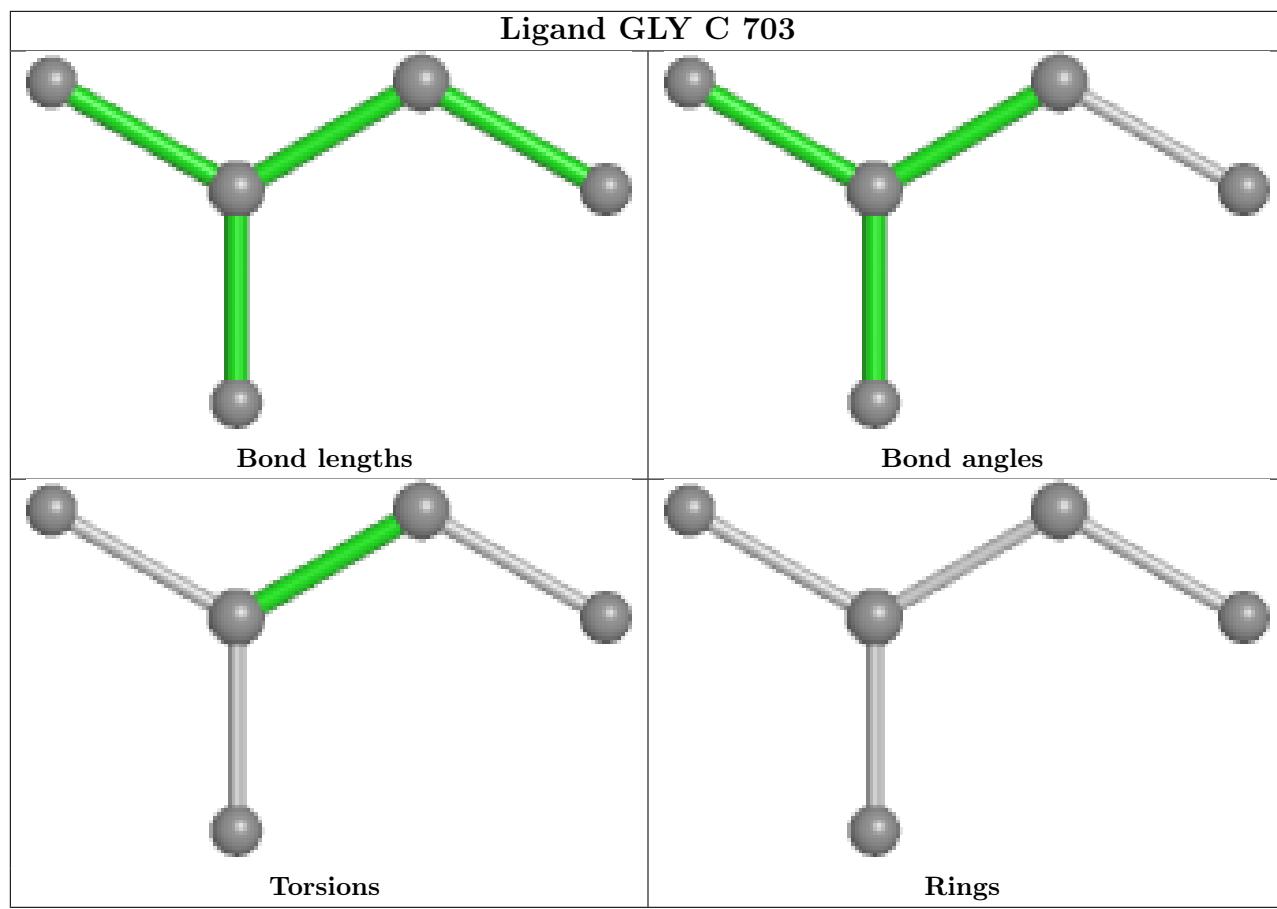


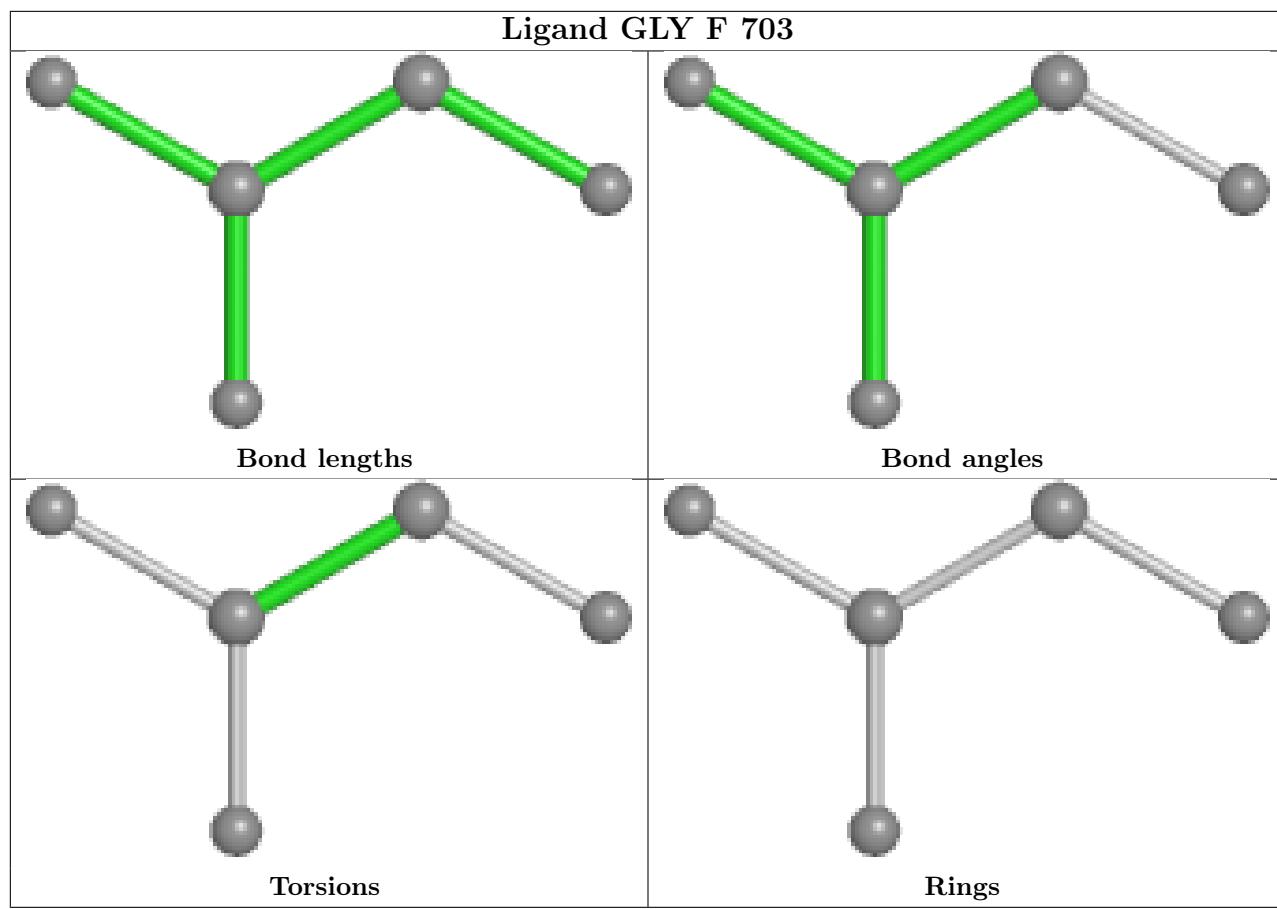


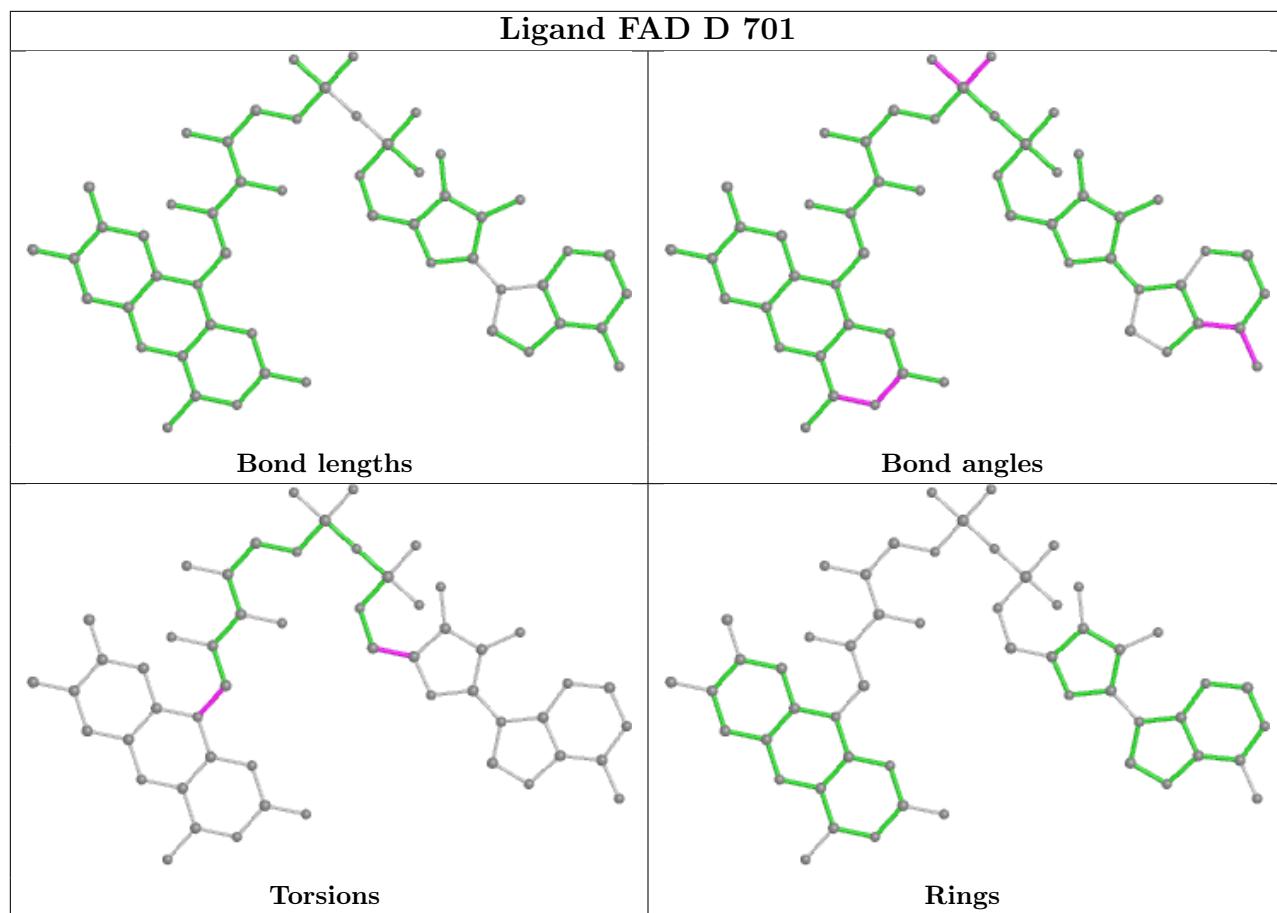


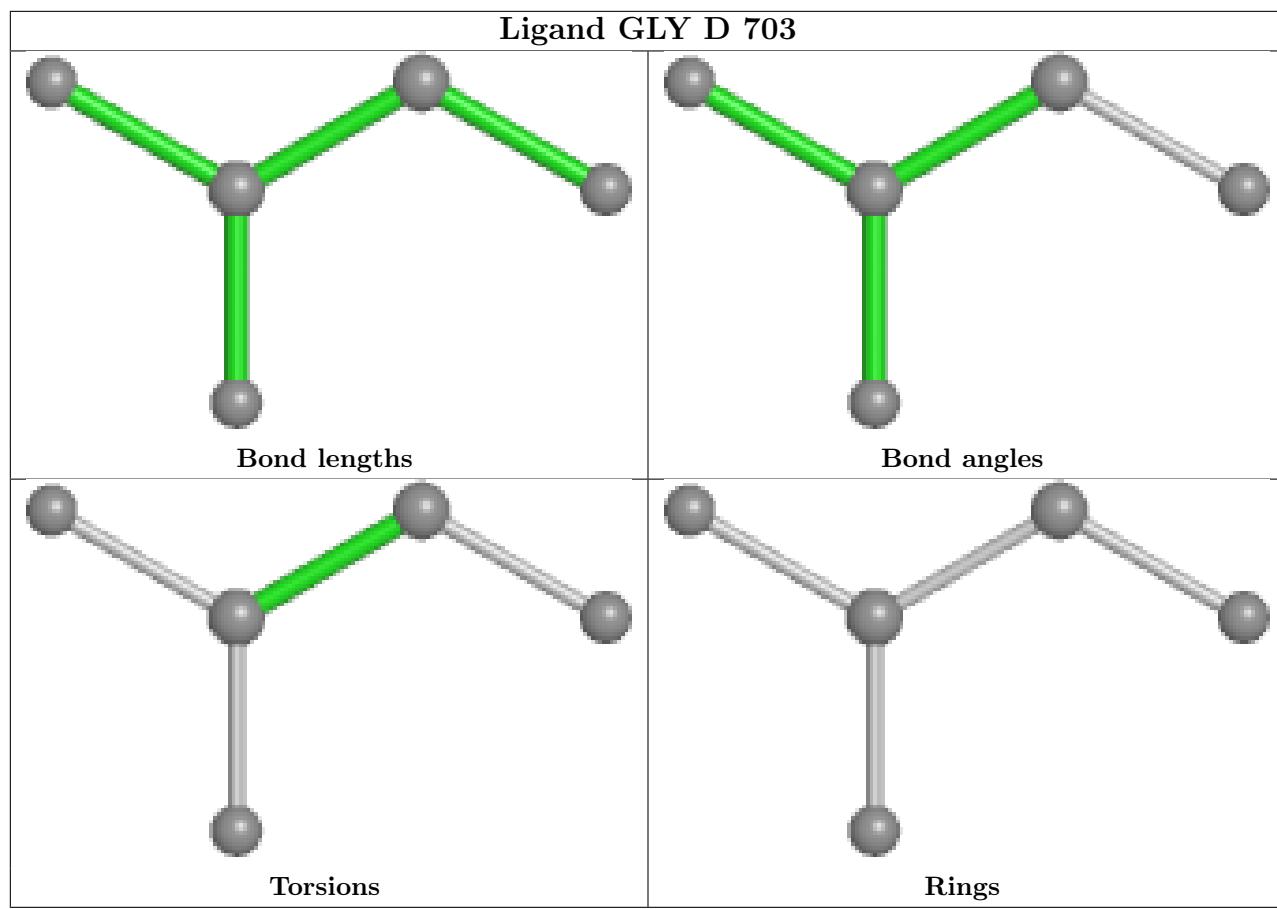


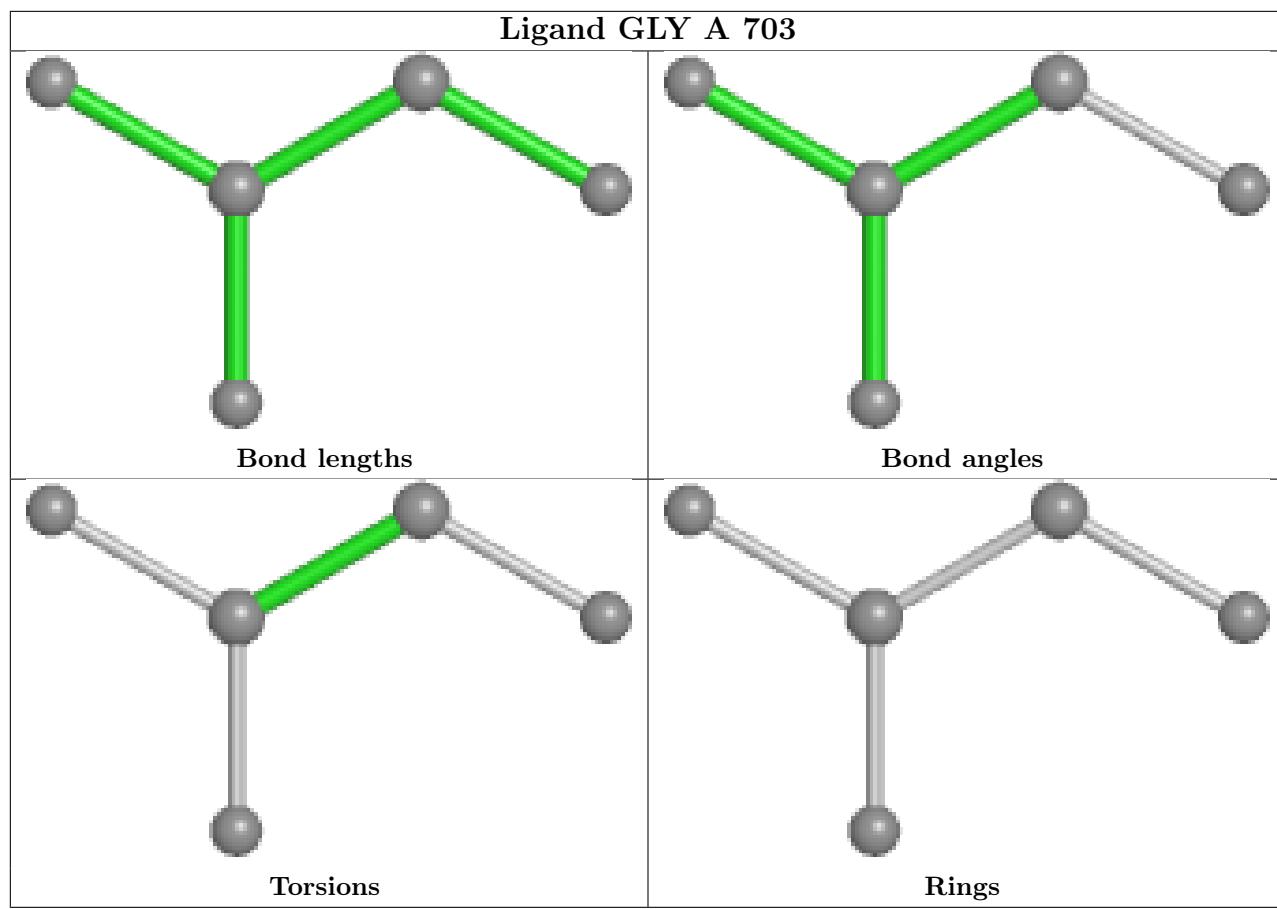


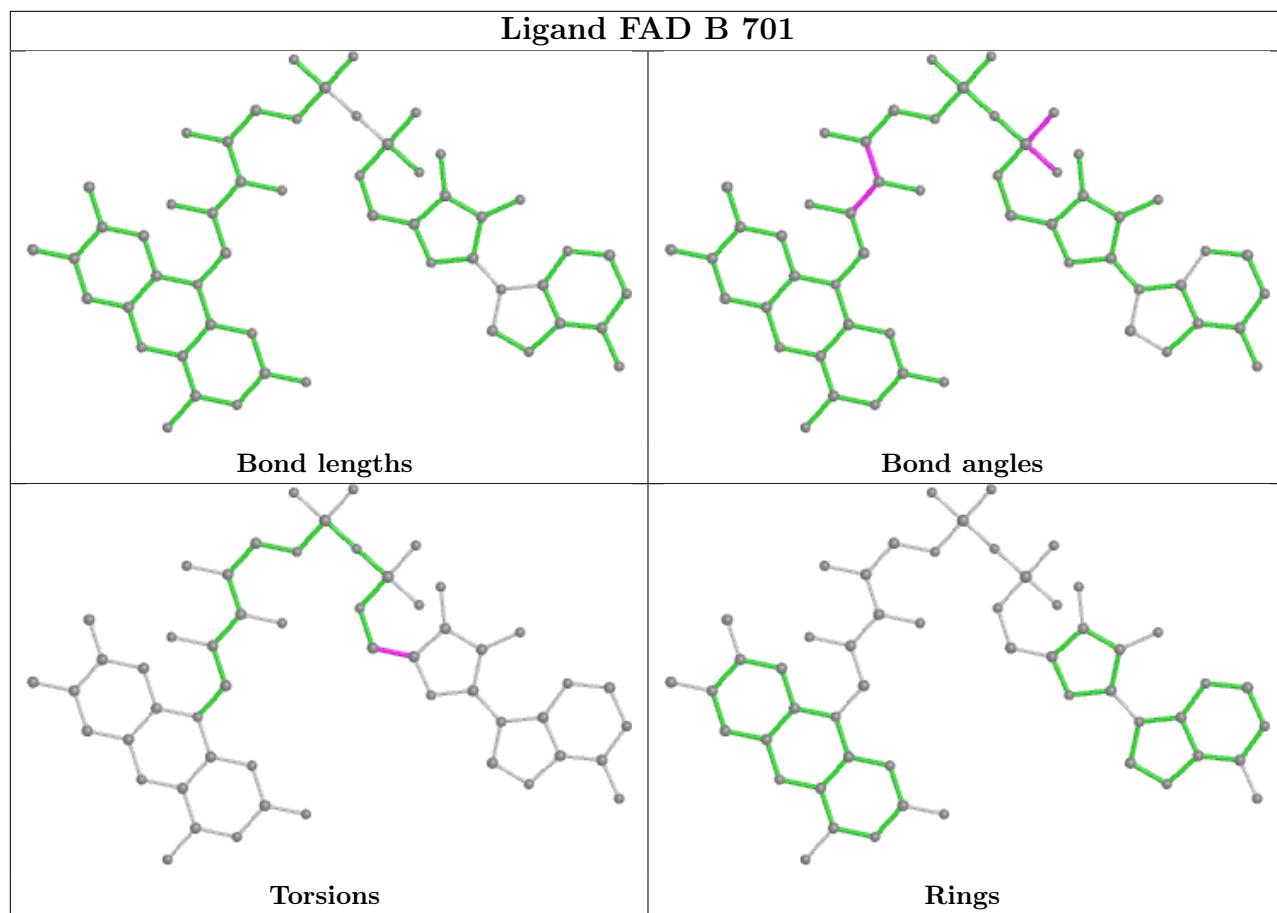


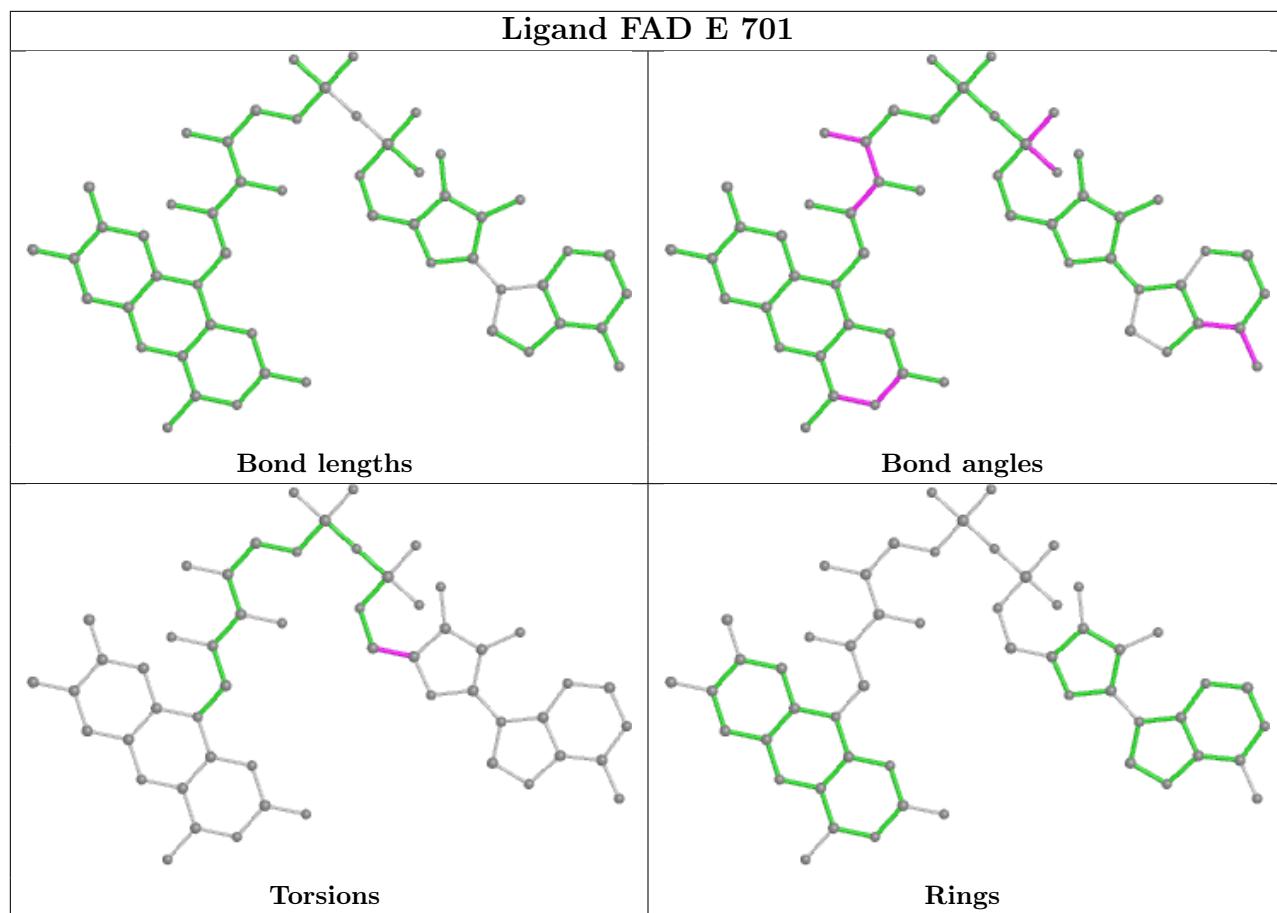


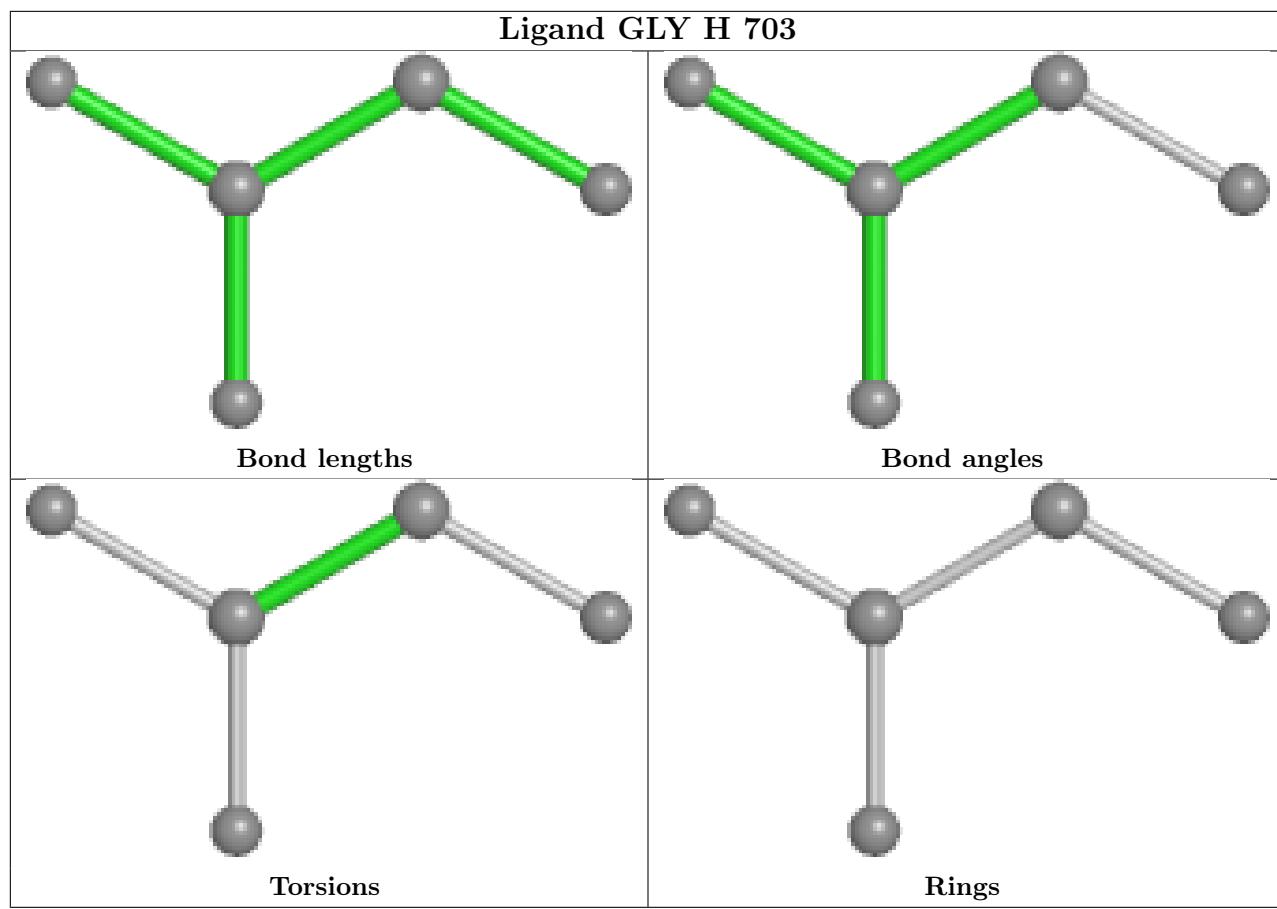


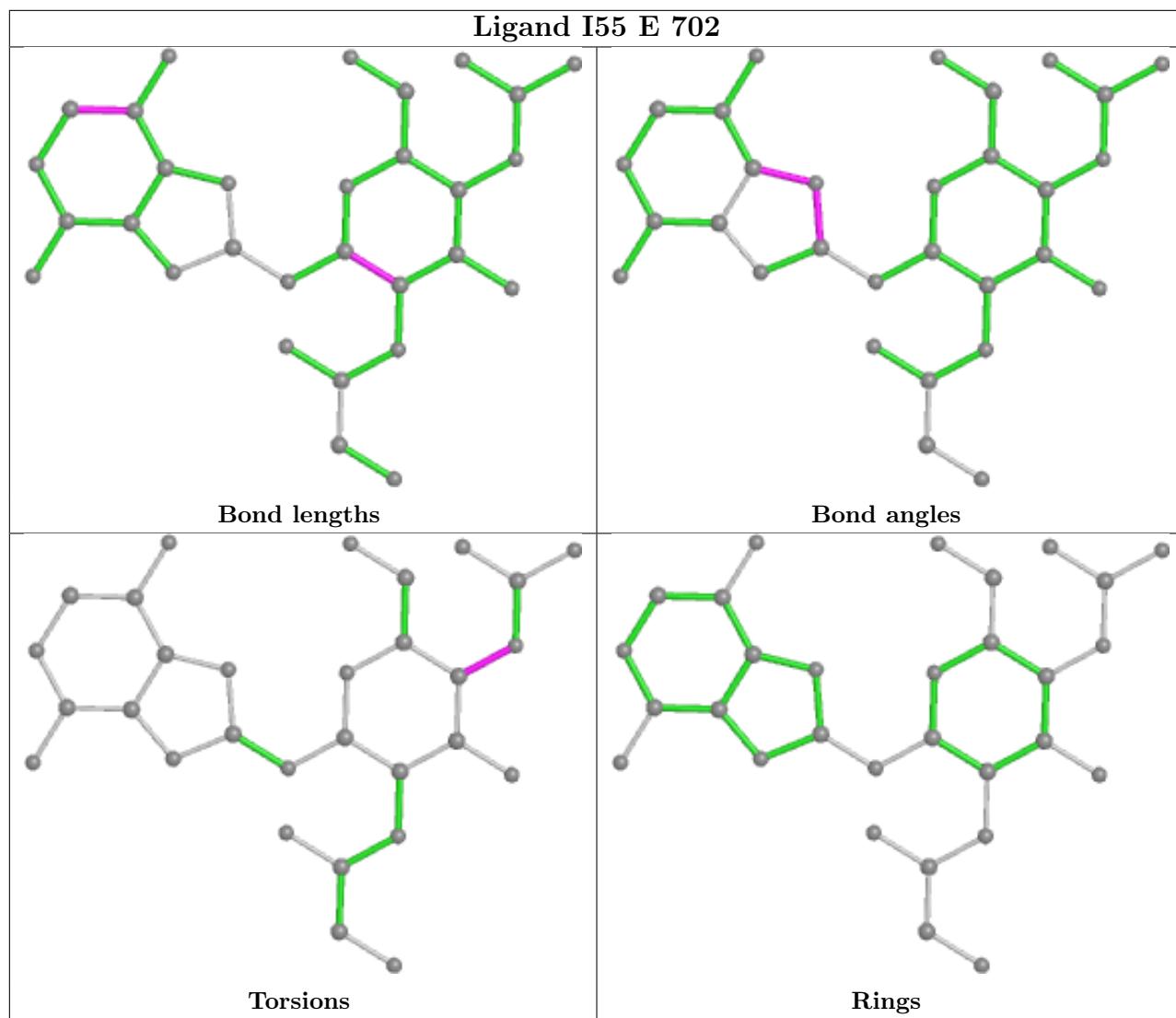


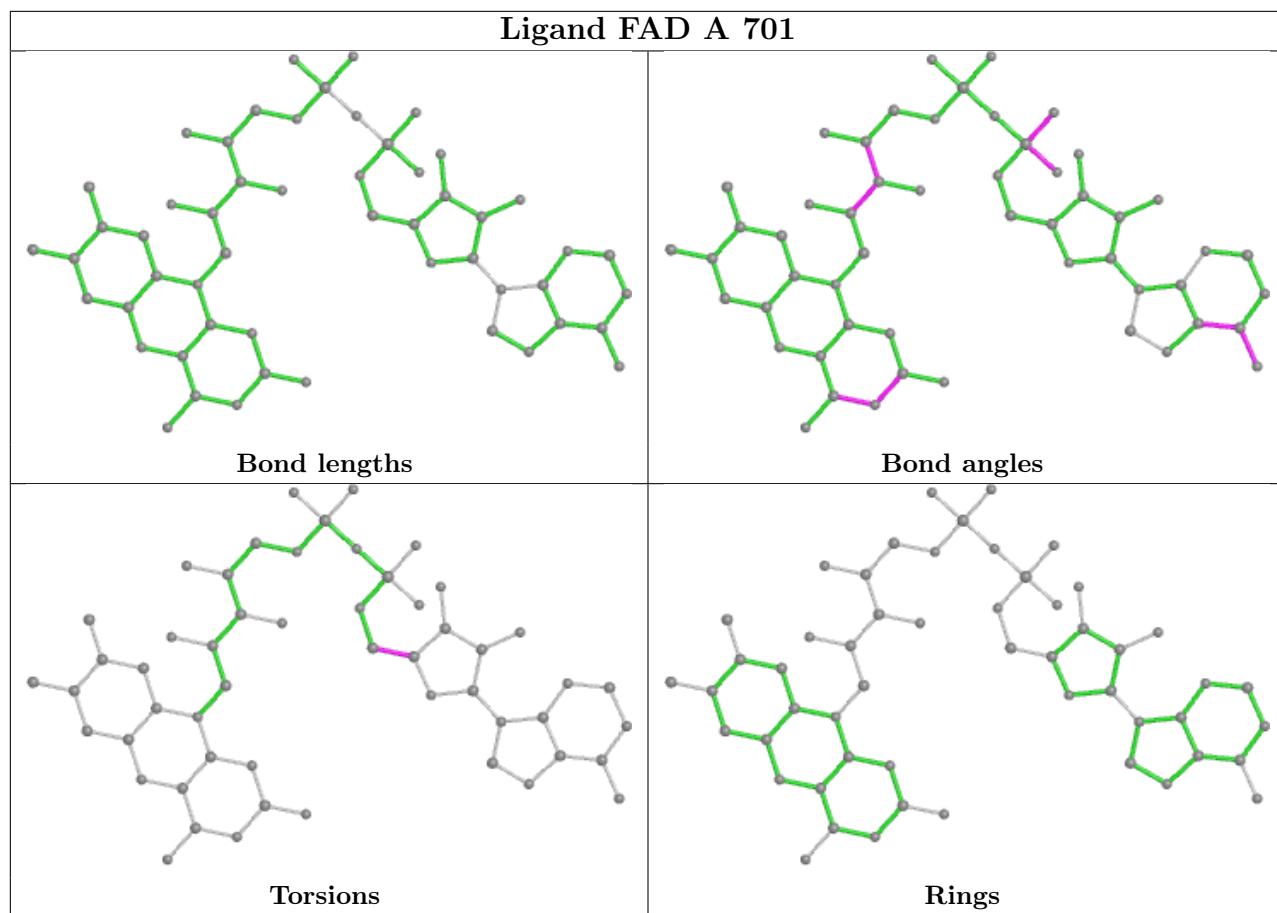


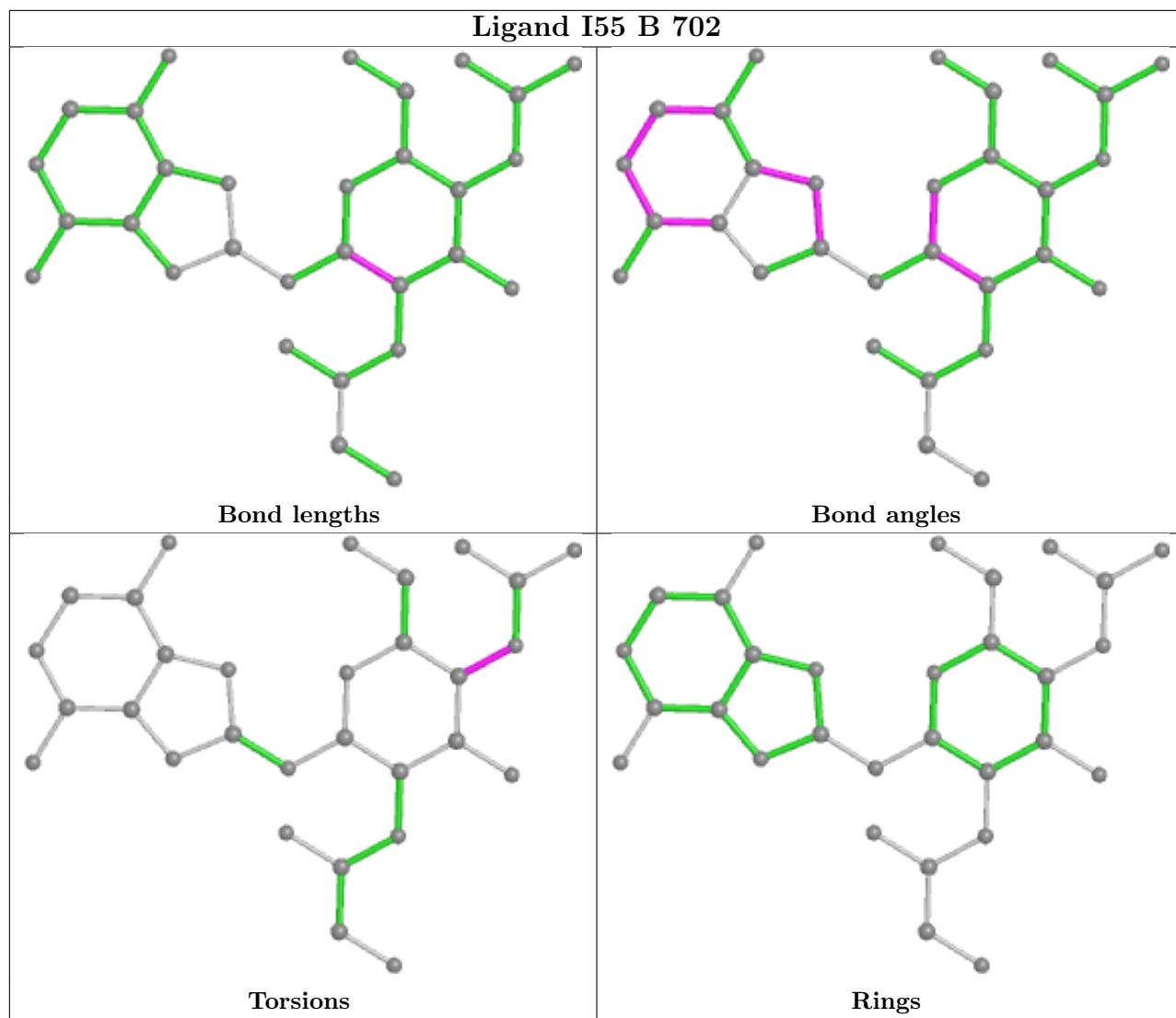


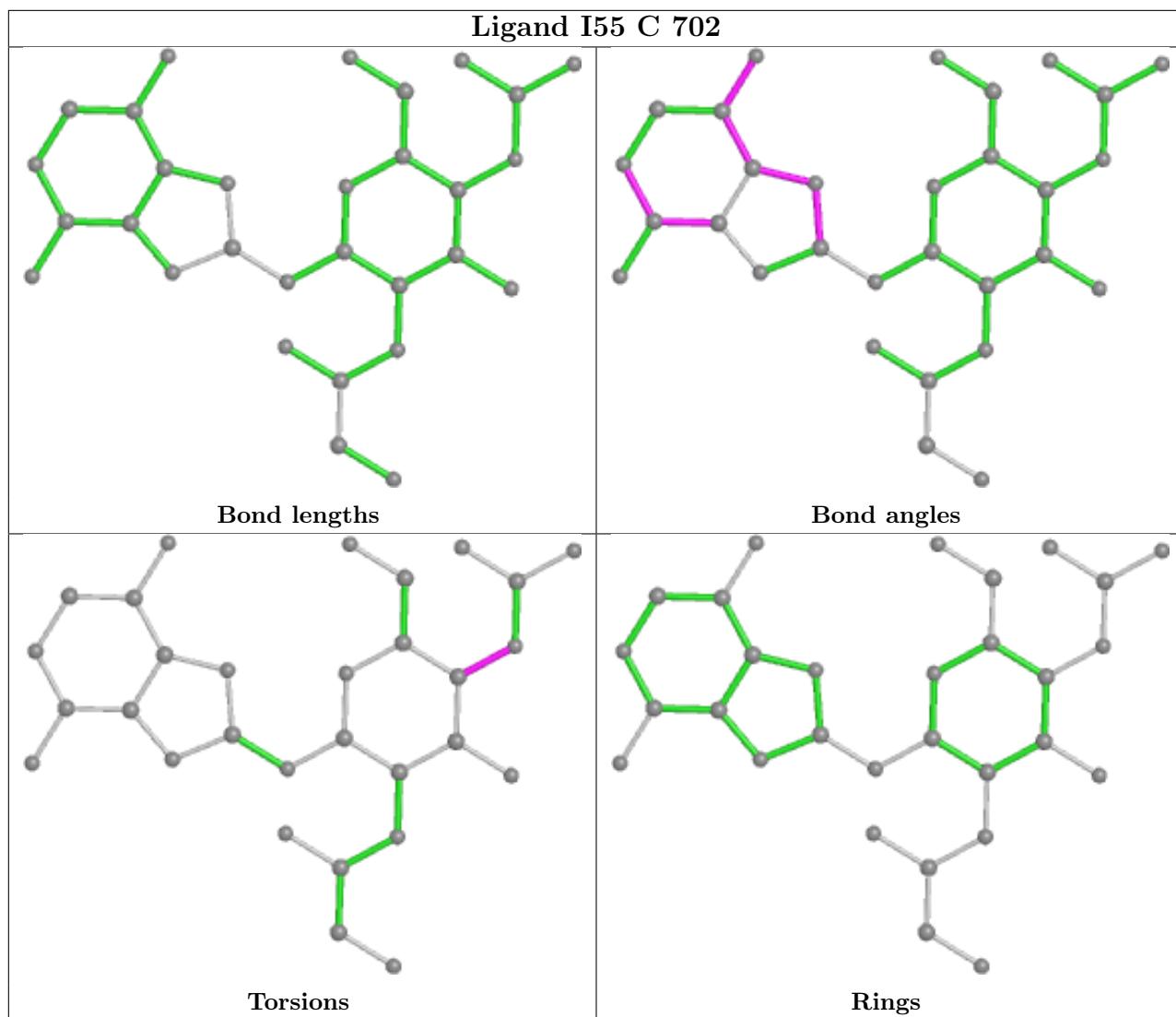












5.7 Other polymers [\(i\)](#)

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, 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	481/512 (93%)	0.30	3 (0%)	89	90	13, 25, 46, 64
1	B	482/512 (94%)	0.21	5 (1%)	82	83	11, 23, 43, 65
1	C	482/512 (94%)	0.40	14 (2%)	51	54	11, 25, 54, 80
1	D	479/512 (93%)	0.75	55 (11%)	4	5	16, 38, 80, 98
1	E	482/512 (94%)	0.35	12 (2%)	57	59	14, 25, 46, 69
1	F	482/512 (94%)	0.21	7 (1%)	73	75	11, 23, 44, 68
1	G	481/512 (93%)	0.41	19 (3%)	38	40	11, 25, 55, 76
1	H	479/512 (93%)	0.99	90 (18%)	1	1	16, 39, 83, 103
All	All	3848/4096 (93%)	0.45	205 (5%)	26	28	11, 27, 64, 103
							0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	220	LEU	7.1
1	H	202	ILE	7.0
1	H	36	VAL	6.8
1	H	34	PRO	6.7
1	D	36	VAL	6.7
1	D	34	PRO	6.6
1	H	243	LEU	6.1
1	H	206	HIS	5.3
1	H	361	TRP	5.1
1	H	224	HIS	5.1
1	H	219	PHE	4.9
1	D	202	ILE	4.9
1	H	241	PRO	4.8
1	H	384	LEU	4.8
1	H	223	GLY	4.7
1	H	38	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	243	LEU	4.6
1	D	33	ARG	4.6
1	H	13	VAL	4.6
1	H	192	GLY	4.6
1	H	211	GLY	4.5
1	C	242	GLY	4.5
1	H	240	LEU	4.4
1	D	219	PHE	4.3
1	D	38	VAL	4.3
1	D	361	TRP	4.1
1	H	382	VAL	4.1
1	H	193	ARG	4.1
1	H	33	ARG	4.1
1	H	217	GLY	4.0
1	D	13	VAL	4.0
1	H	225	VAL	4.0
1	H	209	VAL	4.0
1	H	239	ALA	3.9
1	H	208	ARG	3.8
1	D	242	GLY	3.8
1	D	240	LEU	3.8
1	H	203	ARG	3.8
1	H	352	ILE	3.7
1	H	242	GLY	3.7
1	H	190	ALA	3.6
1	H	387	GLY	3.6
1	C	204	ALA	3.6
1	G	242	GLY	3.5
1	H	491	HIS	3.5
1	H	236	LEU	3.5
1	D	379	ARG	3.5
1	D	211	GLY	3.4
1	H	244	ALA	3.4
1	D	394	LEU	3.4
1	D	209	VAL	3.4
1	D	223	GLY	3.4
1	A	395	ARG	3.4
1	D	488	ARG	3.4
1	H	483	TYR	3.4
1	D	208	ARG	3.3
1	G	243	LEU	3.3
1	C	223	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	220	LEU	3.3
1	D	384	LEU	3.3
1	D	189	GLN	3.2
1	D	30	ALA	3.2
1	H	376	LEU	3.2
1	H	392	ASP	3.1
1	D	241	PRO	3.1
1	D	37	ARG	3.1
1	H	393	GLY	3.1
1	C	243	LEU	3.1
1	H	360	LEU	3.1
1	E	140	ASN	3.1
1	F	35	ASP	3.0
1	H	358	GLU	3.0
1	H	356	SER	3.0
1	E	395	ARG	3.0
1	D	222	ALA	3.0
1	H	37	ARG	3.0
1	A	140	ASN	3.0
1	C	236	LEU	3.0
1	H	204	ALA	3.0
1	D	90	GLU	2.9
1	C	10	GLN	2.9
1	D	206	HIS	2.9
1	D	224	HIS	2.9
1	H	385	MET	2.9
1	D	359	GLY	2.9
1	H	383	SER	2.8
1	H	212	VAL	2.8
1	C	206	HIS	2.8
1	H	35	ASP	2.8
1	H	39	THR	2.8
1	H	398	ARG	2.8
1	H	394	LEU	2.8
1	B	392	ASP	2.7
1	D	239	ALA	2.7
1	F	36	VAL	2.7
1	D	192	GLY	2.7
1	D	217	GLY	2.7
1	E	61	PHE	2.7
1	C	238	ALA	2.7
1	H	226	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	484	ALA	2.7
1	H	245	HIS	2.7
1	E	11	THR	2.7
1	H	386	ASP	2.6
1	H	379	ARG	2.6
1	G	218	ASP	2.6
1	E	10	GLN	2.6
1	G	236	LEU	2.6
1	H	90	GLU	2.6
1	G	45	ALA	2.6
1	D	203	ARG	2.6
1	E	382	VAL	2.6
1	H	41	LEU	2.6
1	G	238	ALA	2.6
1	H	457	THR	2.6
1	D	225	VAL	2.6
1	D	354	GLY	2.6
1	B	395	ARG	2.5
1	G	54	ALA	2.5
1	G	203	ARG	2.5
1	G	11	THR	2.5
1	G	212	VAL	2.5
1	H	357	VAL	2.5
1	H	355	THR	2.5
1	C	222	ALA	2.5
1	D	244	ALA	2.5
1	H	213	VAL	2.5
1	D	483	TYR	2.5
1	H	353	GLY	2.5
1	G	208	ARG	2.5
1	E	70	ALA	2.5
1	H	222	ALA	2.5
1	D	389	THR	2.5
1	H	363	LEU	2.5
1	H	489	GLU	2.5
1	F	398	ARG	2.5
1	G	206	HIS	2.4
1	E	36	VAL	2.4
1	D	35	ASP	2.4
1	D	193	ARG	2.4
1	H	235	ARG	2.4
1	H	488	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	237	VAL	2.4
1	D	360	LEU	2.4
1	E	206	HIS	2.4
1	D	190	ALA	2.4
1	B	35	ASP	2.4
1	H	14	ILE	2.4
1	H	479	LEU	2.4
1	F	386	ASP	2.3
1	F	393	GLY	2.3
1	H	359	GLY	2.3
1	H	490	TRP	2.3
1	H	362	MET	2.3
1	D	376	LEU	2.3
1	A	206	HIS	2.3
1	D	391	VAL	2.3
1	C	220	LEU	2.3
1	D	212	VAL	2.3
1	D	355	THR	2.3
1	H	32	THR	2.3
1	H	21	LEU	2.3
1	F	392	ASP	2.3
1	H	25	VAL	2.2
1	D	491	HIS	2.2
1	G	220	LEU	2.2
1	H	207	GLY	2.2
1	C	212	VAL	2.2
1	H	29	ILE	2.2
1	H	247	ILE	2.2
1	H	189	GLN	2.2
1	B	206	HIS	2.2
1	E	193	ARG	2.2
1	G	209	VAL	2.2
1	D	236	LEU	2.1
1	H	30	ALA	2.1
1	D	356	SER	2.1
1	B	36	VAL	2.1
1	F	473	ARG	2.1
1	D	218	ASP	2.1
1	D	393	GLY	2.1
1	H	218	ASP	2.1
1	H	97	ALA	2.1
1	E	68	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	47	GLN	2.1
1	G	48	TYR	2.1
1	H	354	GLY	2.1
1	H	395	ARG	2.1
1	C	54	ALA	2.1
1	H	238	ALA	2.1
1	H	404	ILE	2.1
1	H	40	LEU	2.1
1	G	35	ASP	2.1
1	D	382	VAL	2.1
1	D	238	ALA	2.1
1	H	231	ALA	2.1
1	H	431	LEU	2.1
1	H	482	TYR	2.0
1	G	219	PHE	2.0
1	H	187	PHE	2.0
1	C	244	ALA	2.0
1	G	281	CYS	2.0
1	D	100	THR	2.0
1	C	488	ARG	2.0
1	E	491	HIS	2.0

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 [\(i\)](#)

There are no monosaccharides in this entry.

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, 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.

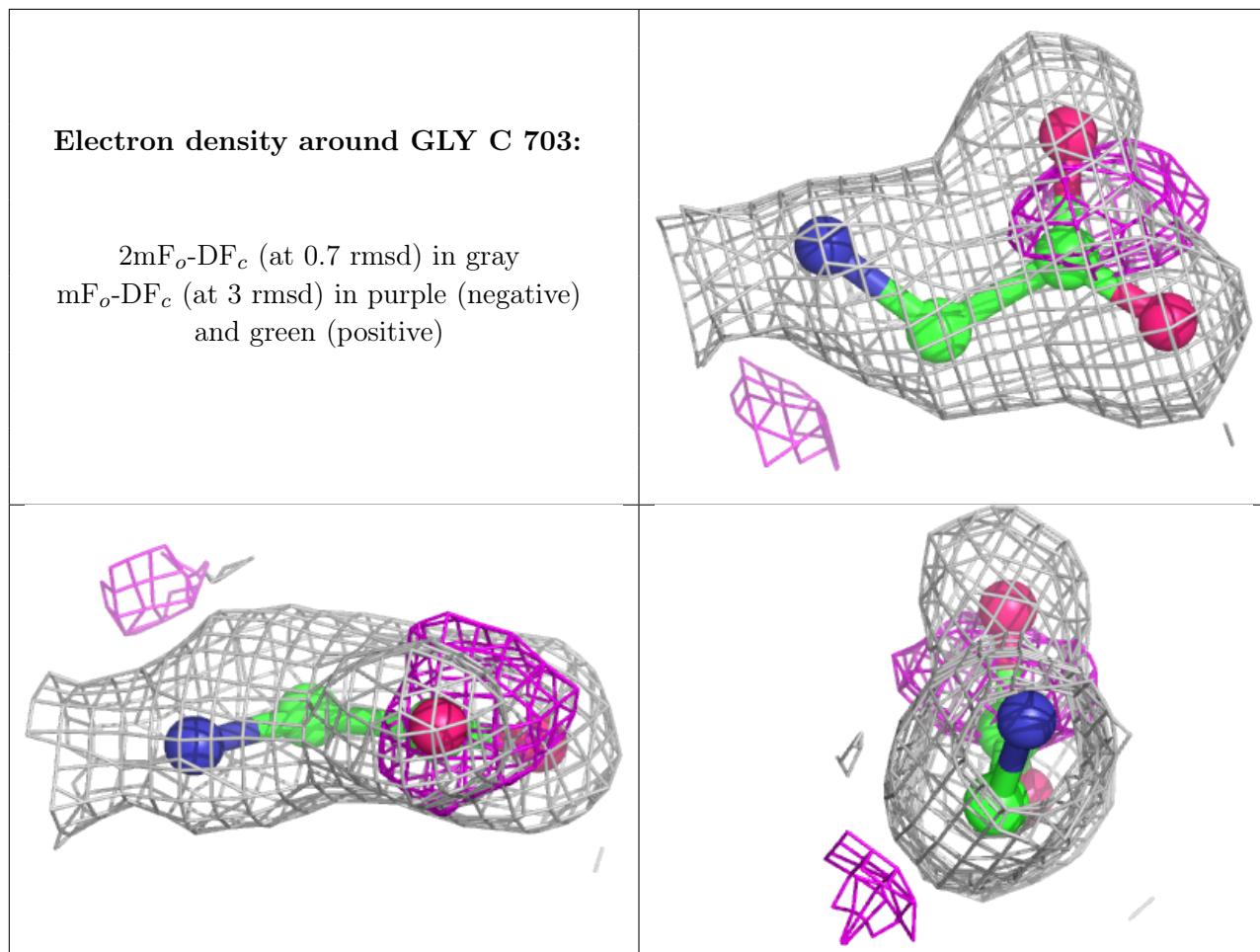
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLY	C	703	5/5	0.82	0.21	33,35,39,40	0
2	FAD	G	701	53/53	0.88	0.18	28,34,45,47	0

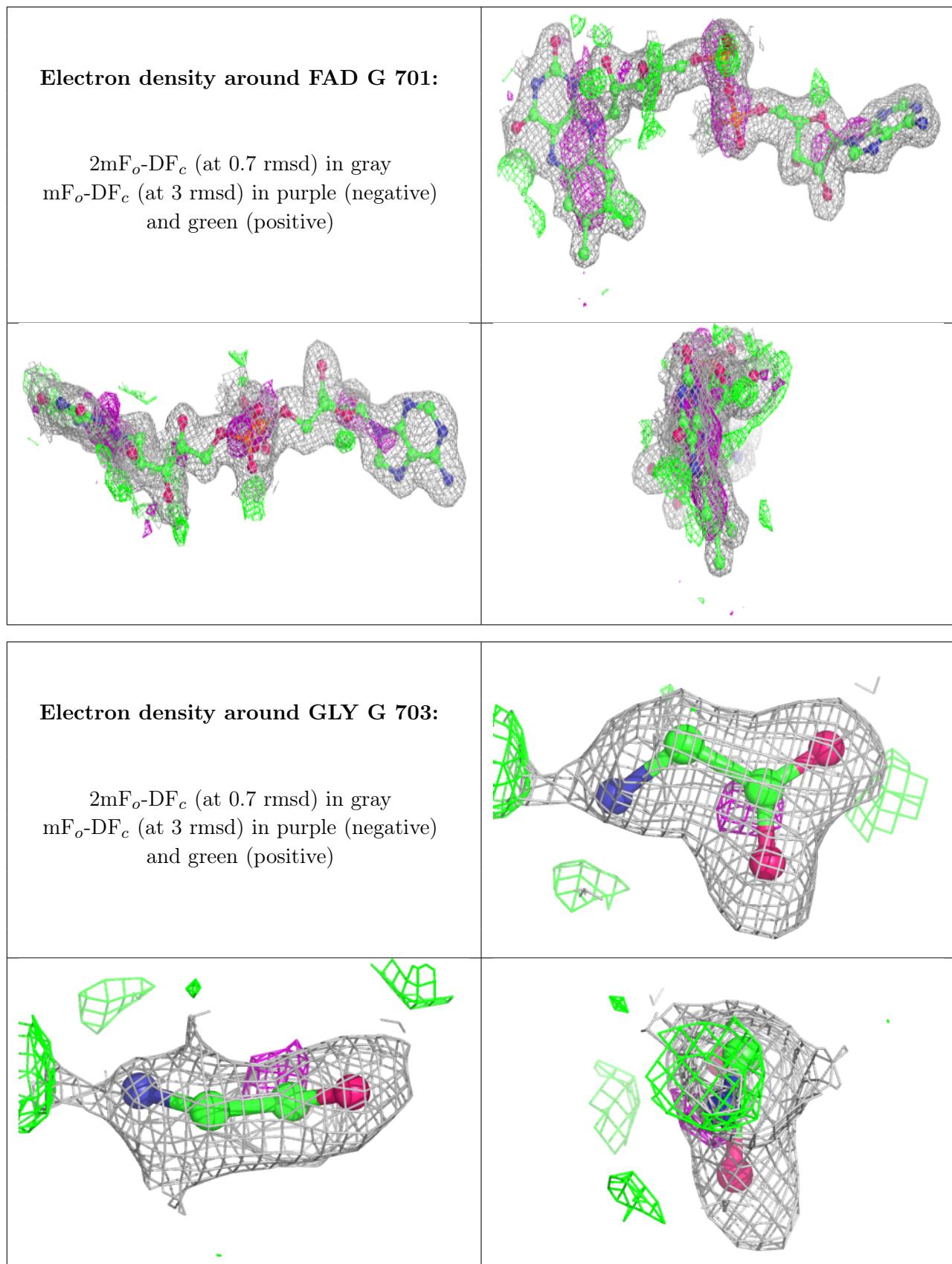
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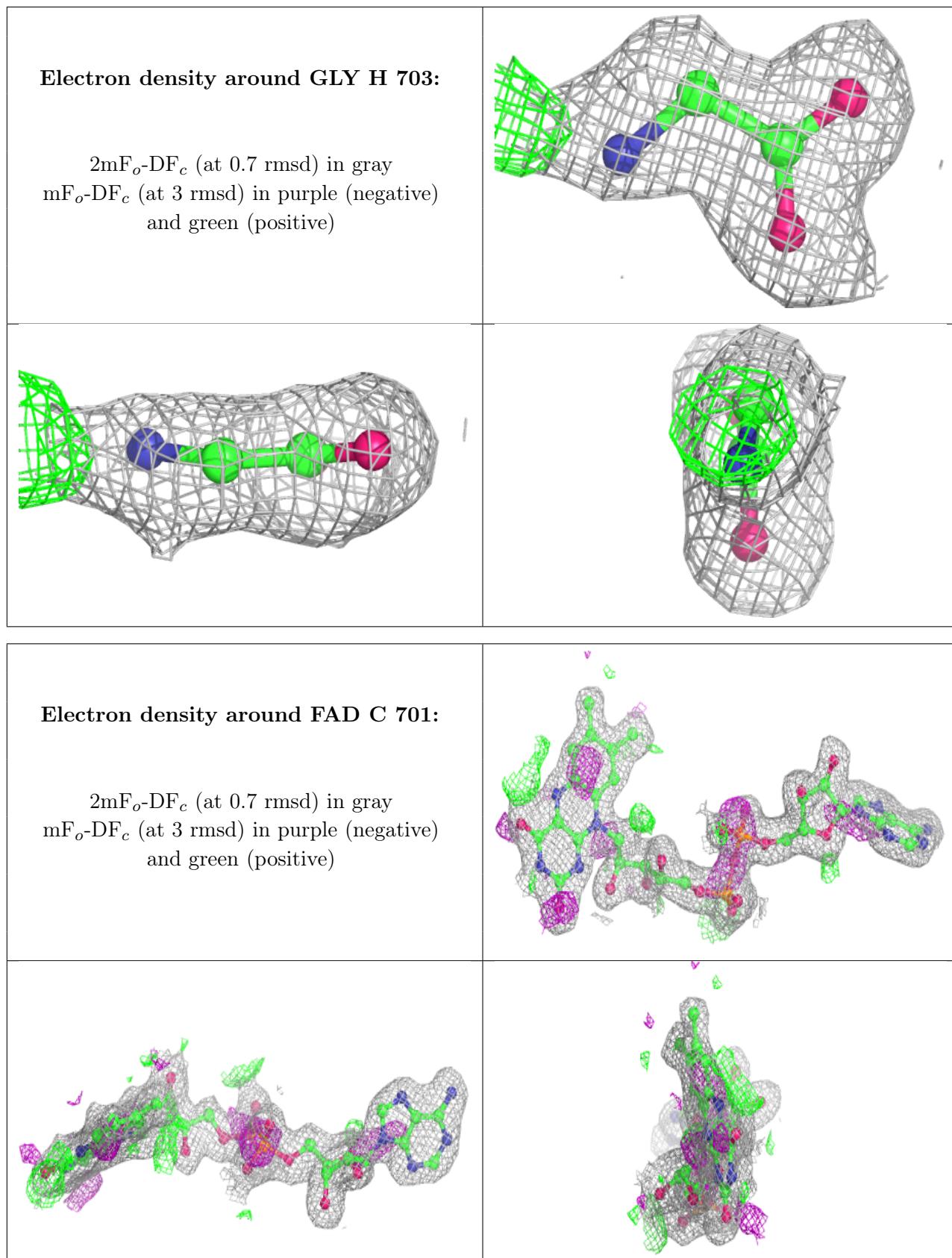
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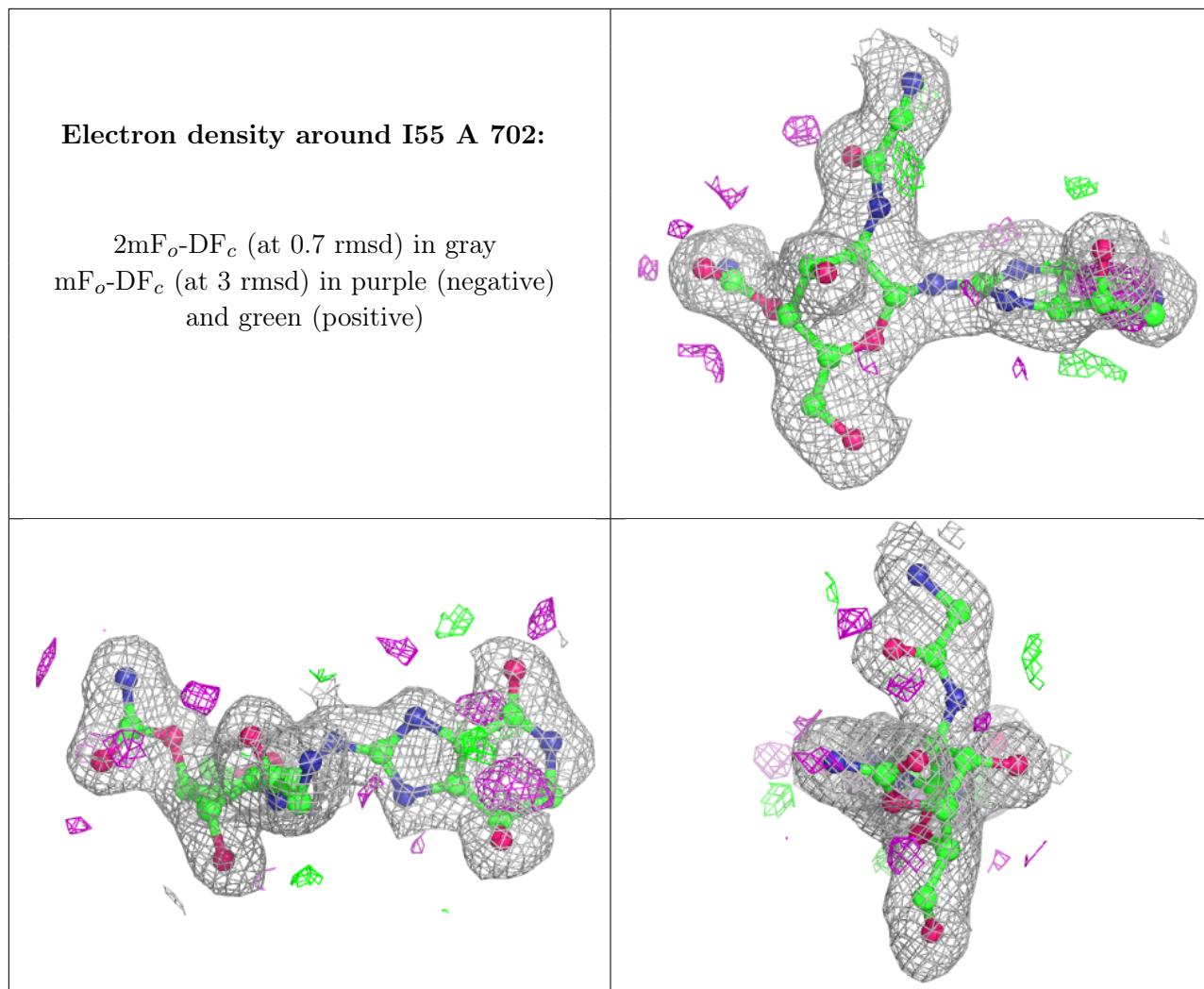
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLY	G	703	5/5	0.88	0.22	34,39,42,44	0
4	GLY	H	703	5/5	0.89	0.11	34,34,41,41	0
2	FAD	C	701	53/53	0.91	0.16	26,32,43,44	0
3	I55	A	702	30/30	0.92	0.13	17,24,32,34	0
2	FAD	H	701	53/53	0.92	0.14	30,42,62,63	0
3	I55	B	702	30/30	0.93	0.13	18,24,32,32	0
3	I55	C	702	30/30	0.93	0.12	17,27,39,39	0
3	I55	H	702	30/30	0.93	0.13	20,30,44,46	0
4	GLY	B	703	5/5	0.94	0.09	19,22,22,24	0
3	I55	D	702	30/30	0.94	0.13	20,30,43,44	0
4	GLY	D	703	5/5	0.94	0.13	32,34,40,40	0
4	GLY	F	703	5/5	0.94	0.13	19,22,22,23	0
3	I55	F	702	30/30	0.94	0.12	19,26,33,34	0
2	FAD	D	701	53/53	0.94	0.12	28,40,58,60	0
4	GLY	E	703	5/5	0.95	0.11	21,21,25,26	0
3	I55	G	702	30/30	0.95	0.12	18,28,40,41	0
3	I55	E	702	30/30	0.95	0.11	17,25,31,33	0
4	GLY	A	703	5/5	0.95	0.09	22,22,26,26	0
2	FAD	A	701	53/53	0.96	0.10	15,19,21,23	0
2	FAD	E	701	53/53	0.96	0.10	15,19,22,24	0
2	FAD	B	701	53/53	0.97	0.10	12,15,19,21	0
2	FAD	F	701	53/53	0.98	0.09	12,15,18,21	0

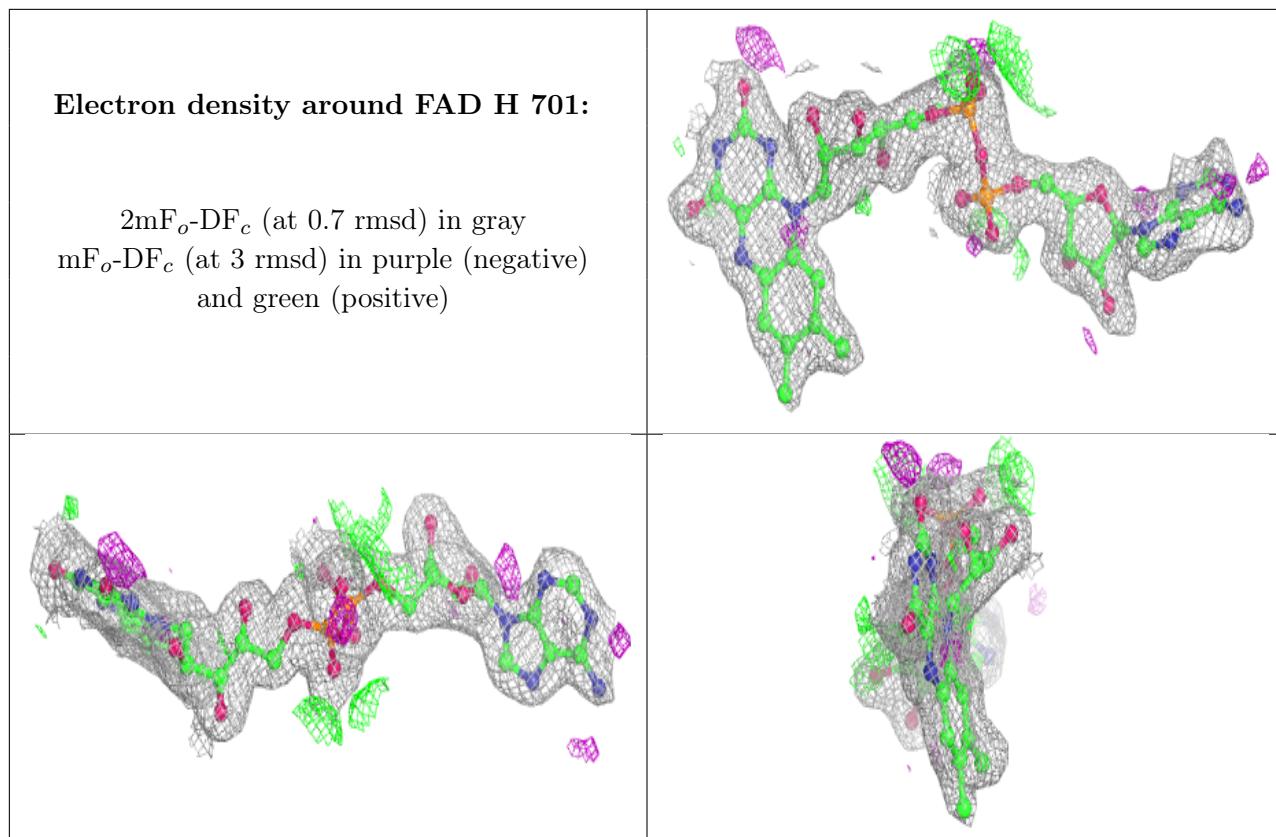
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

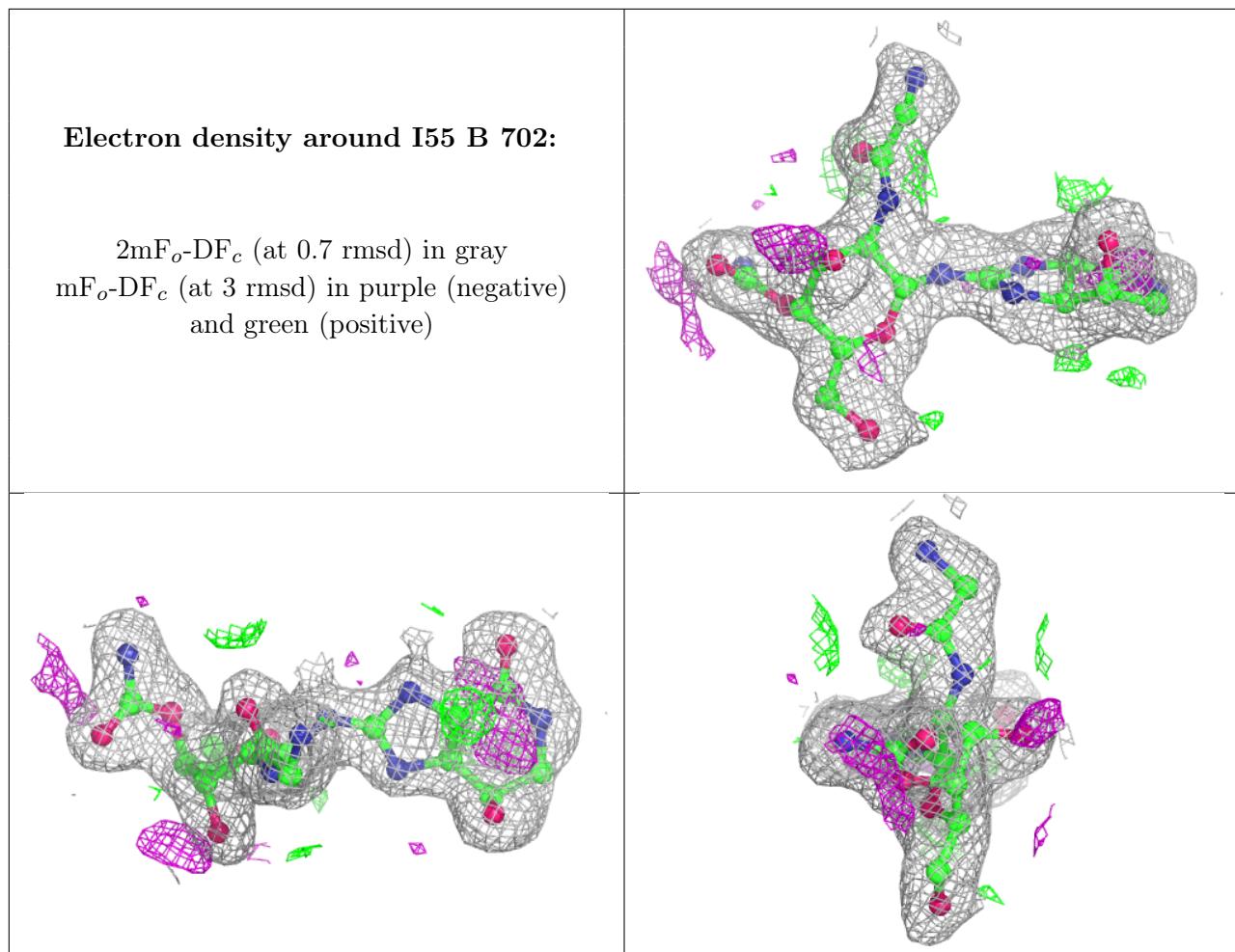


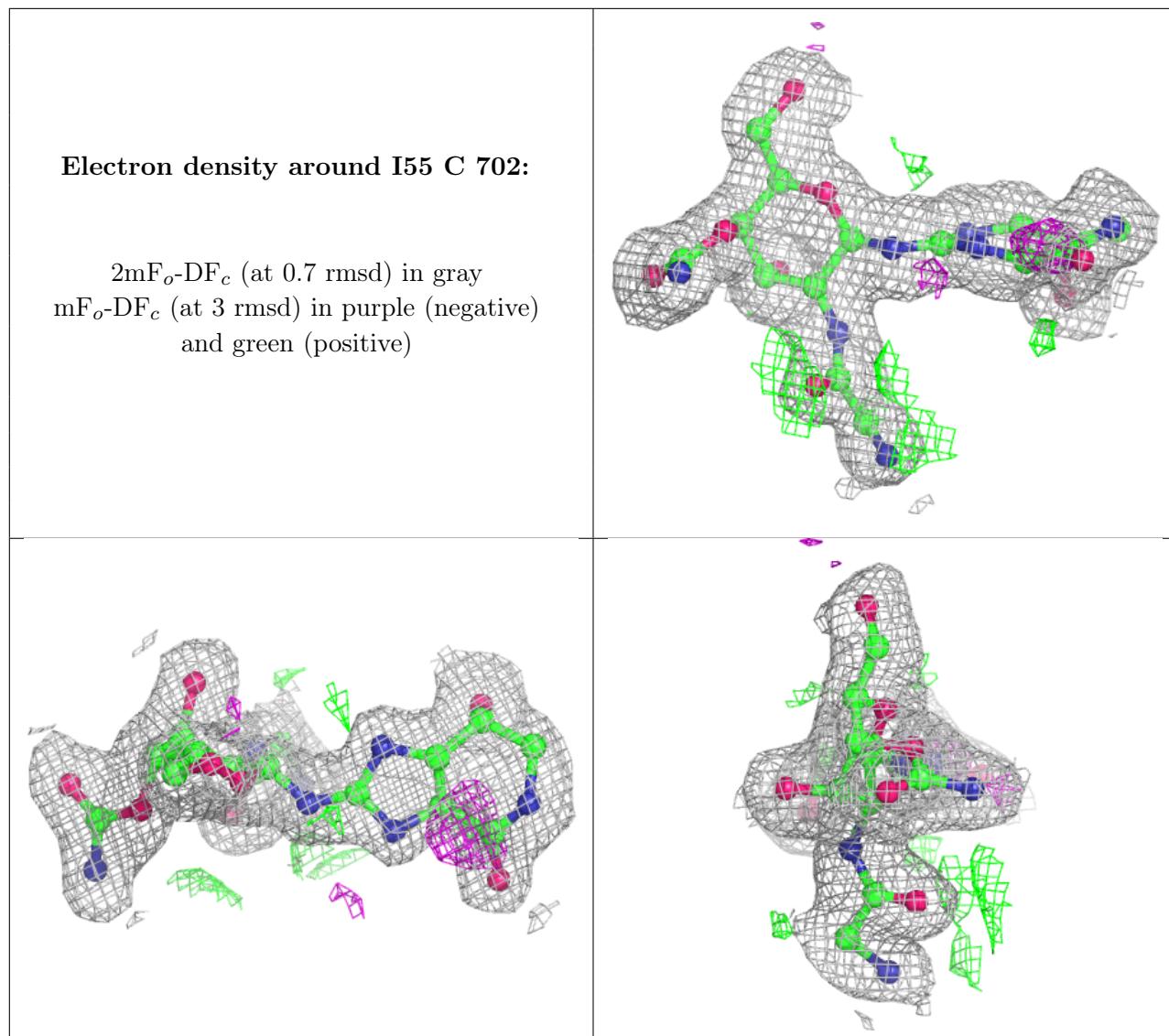


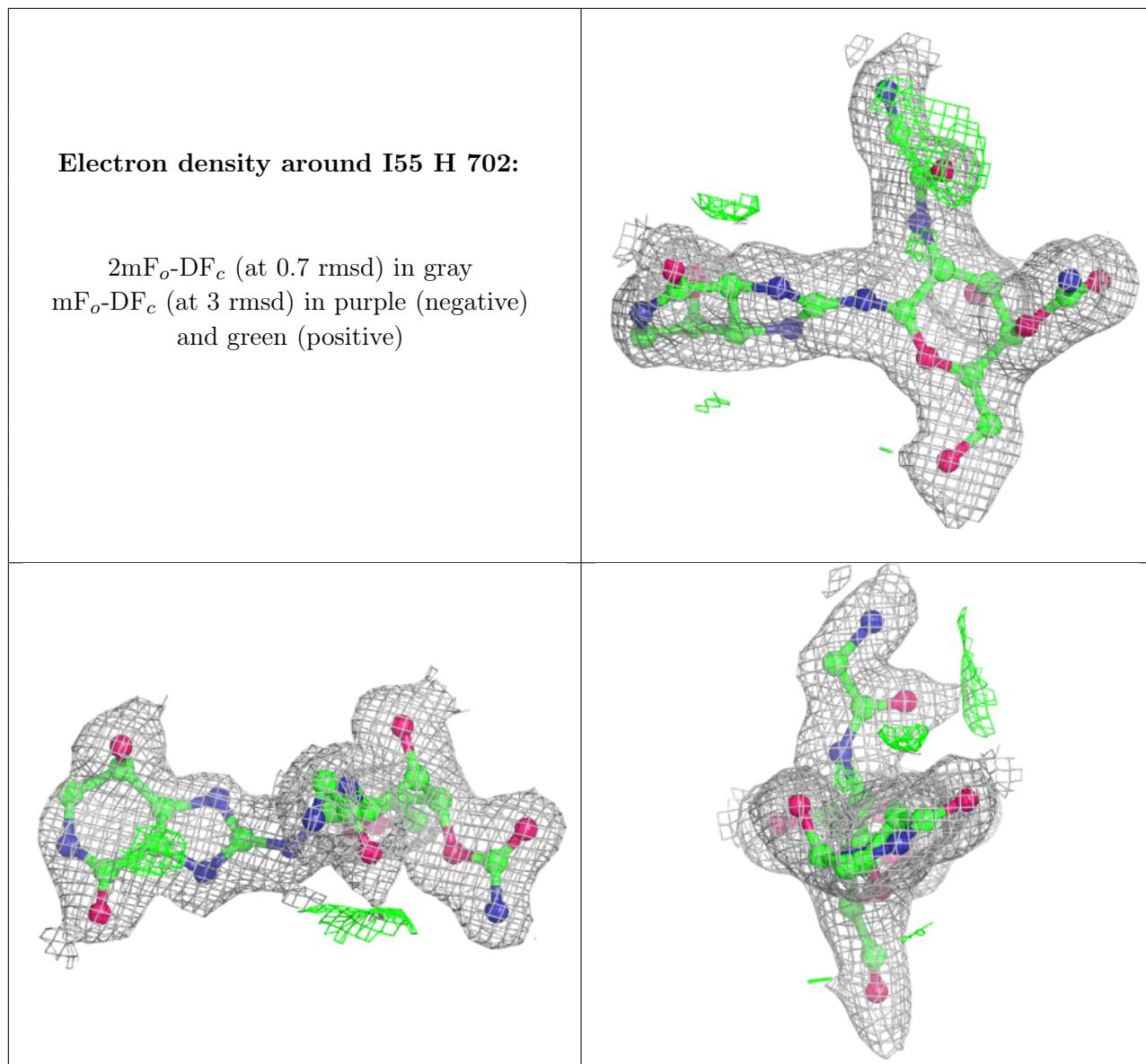


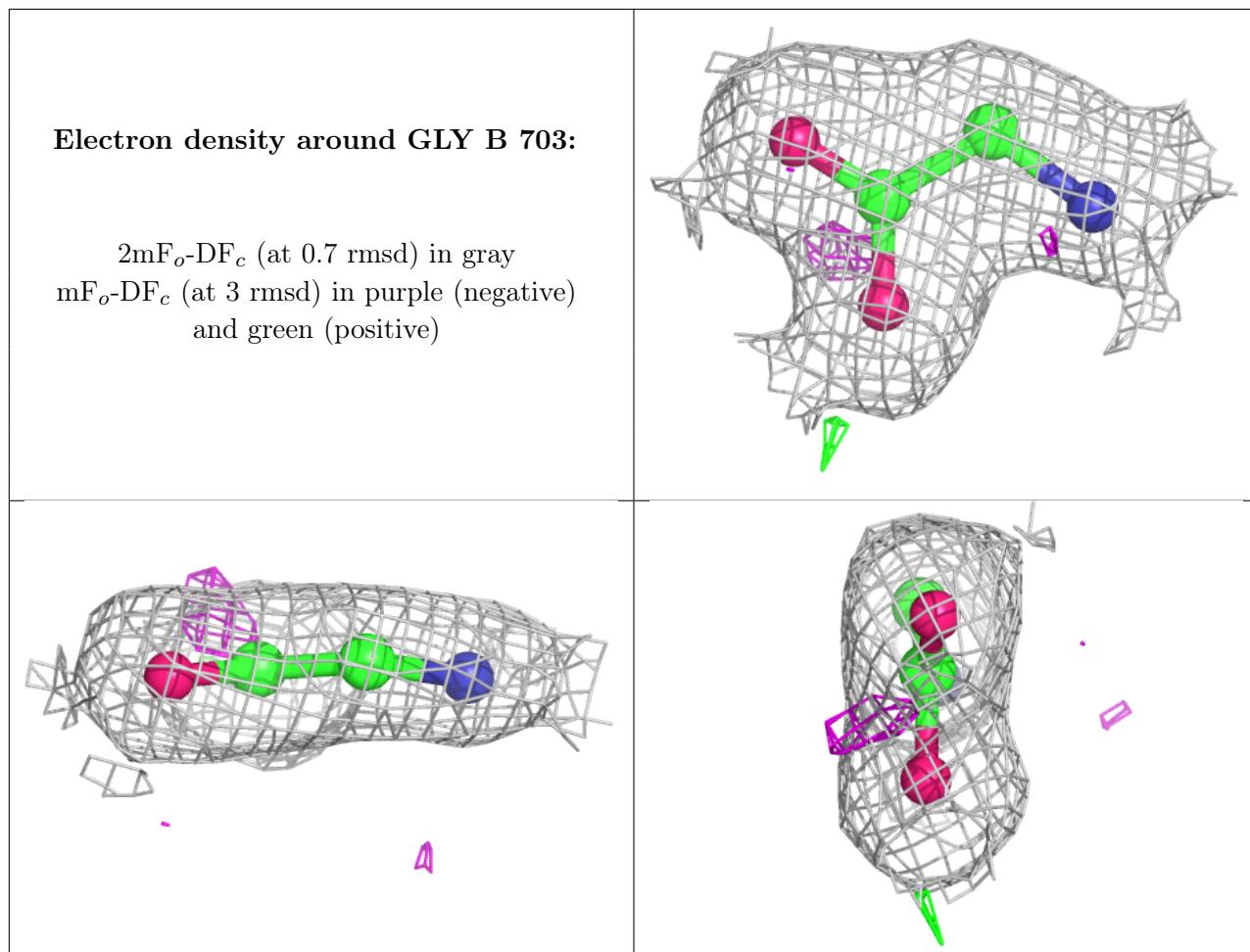


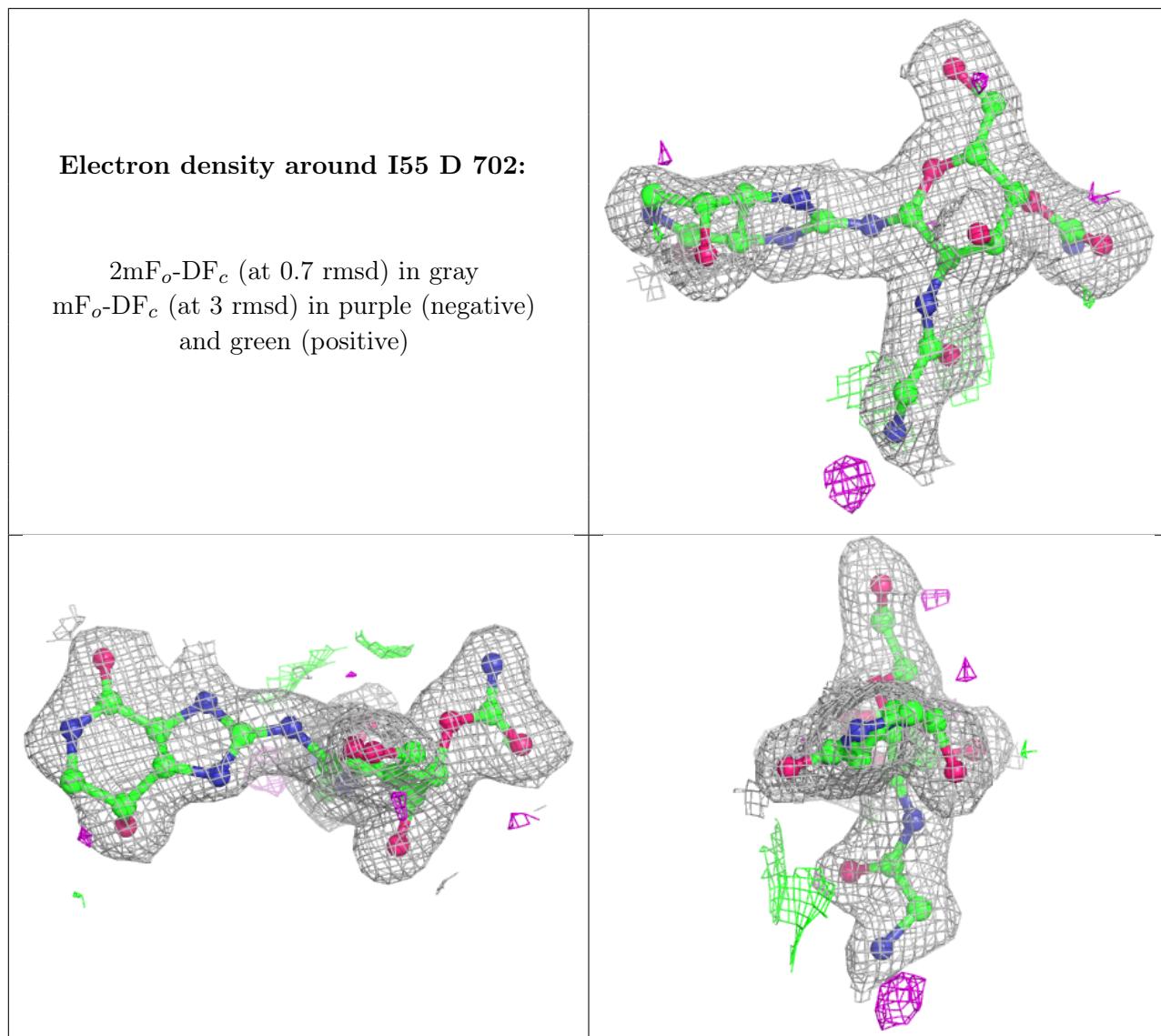


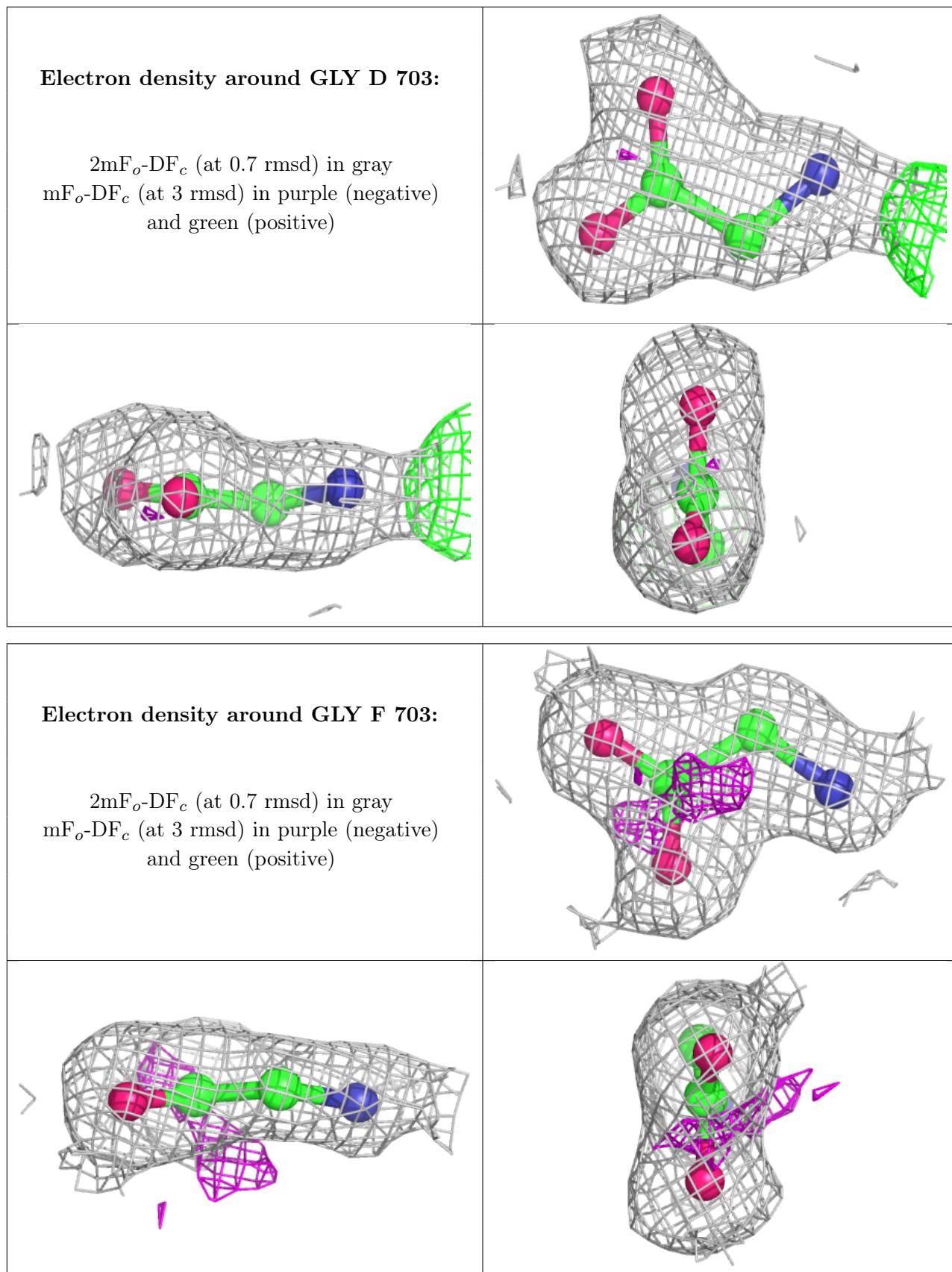


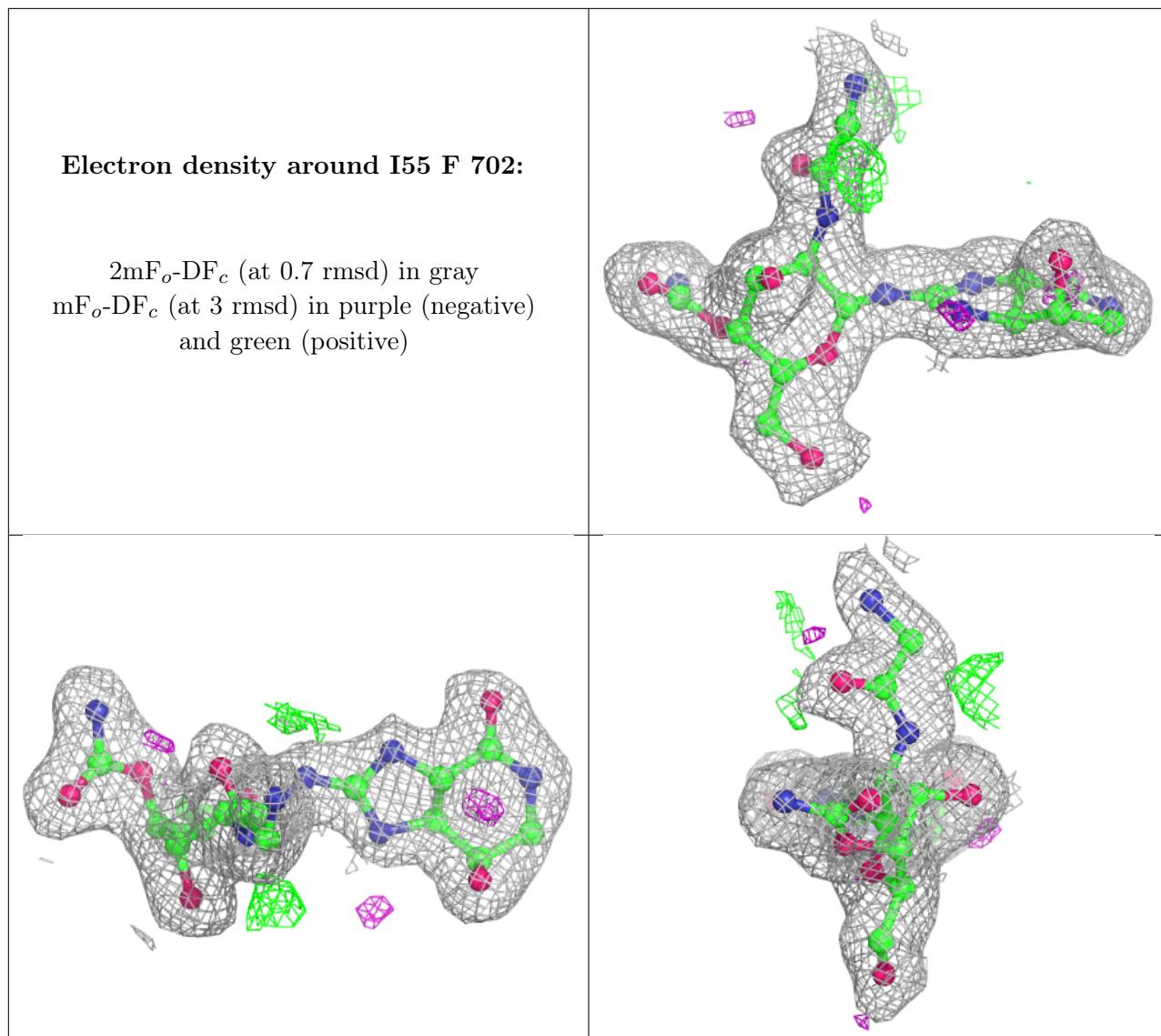


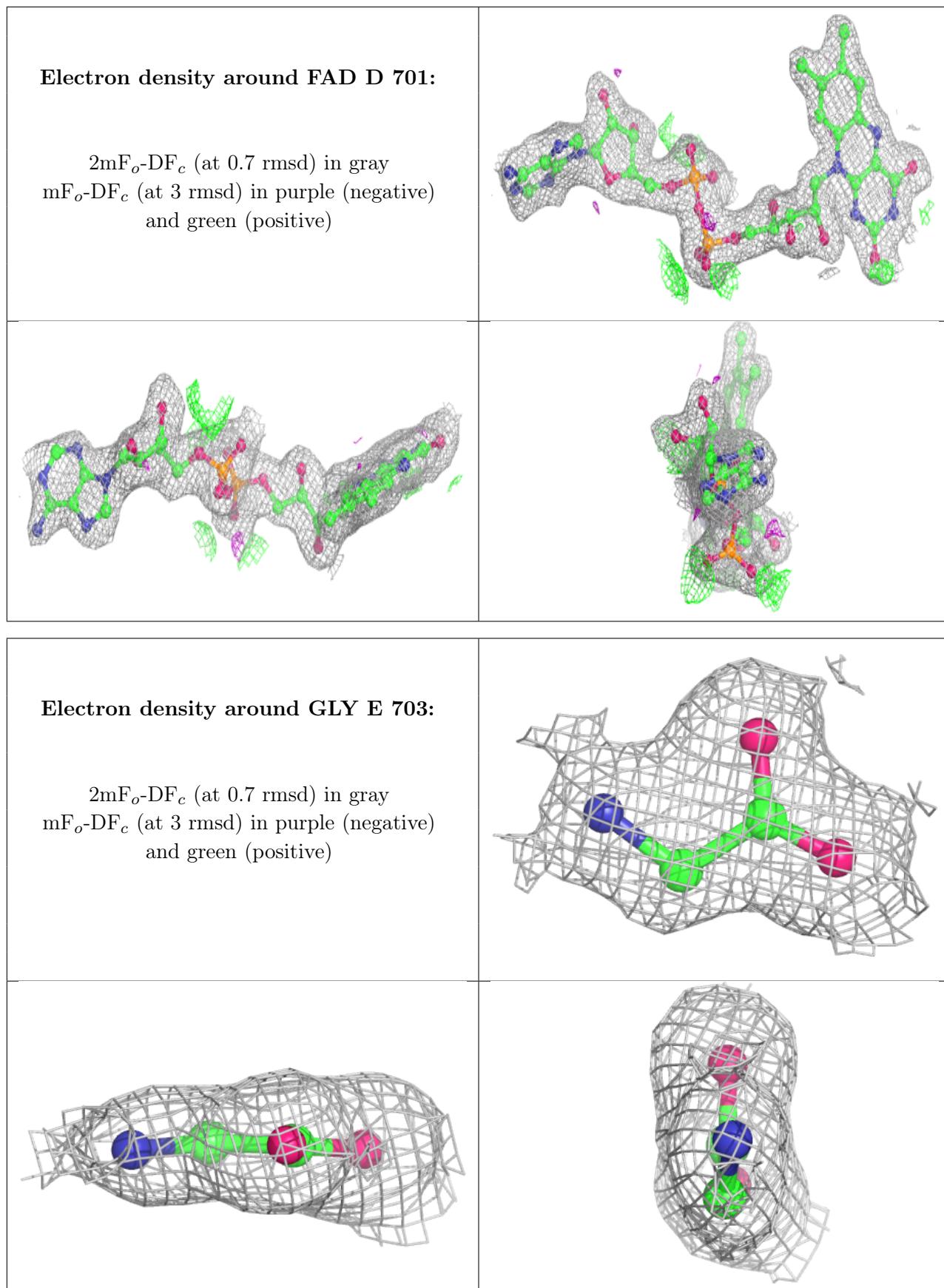


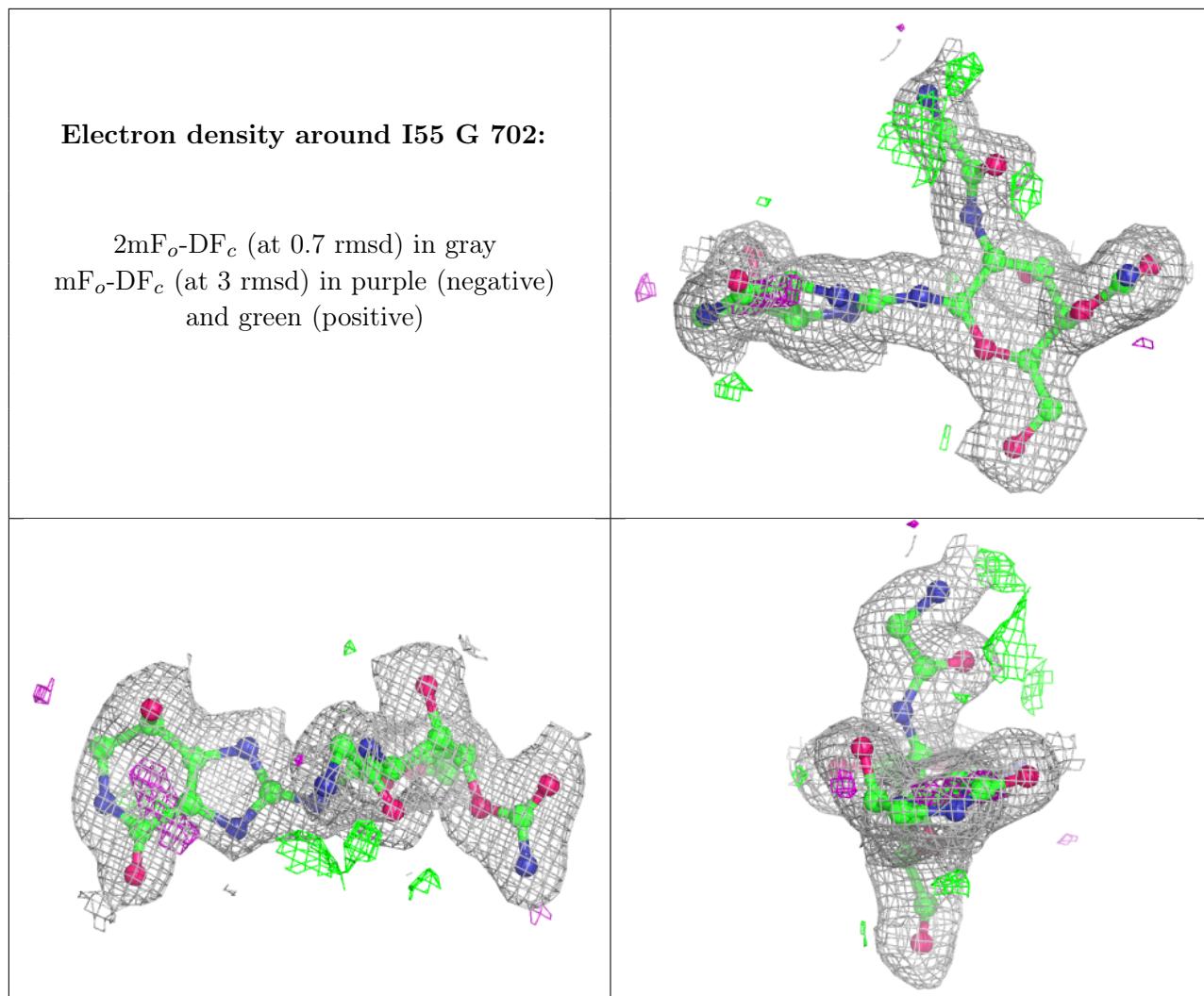


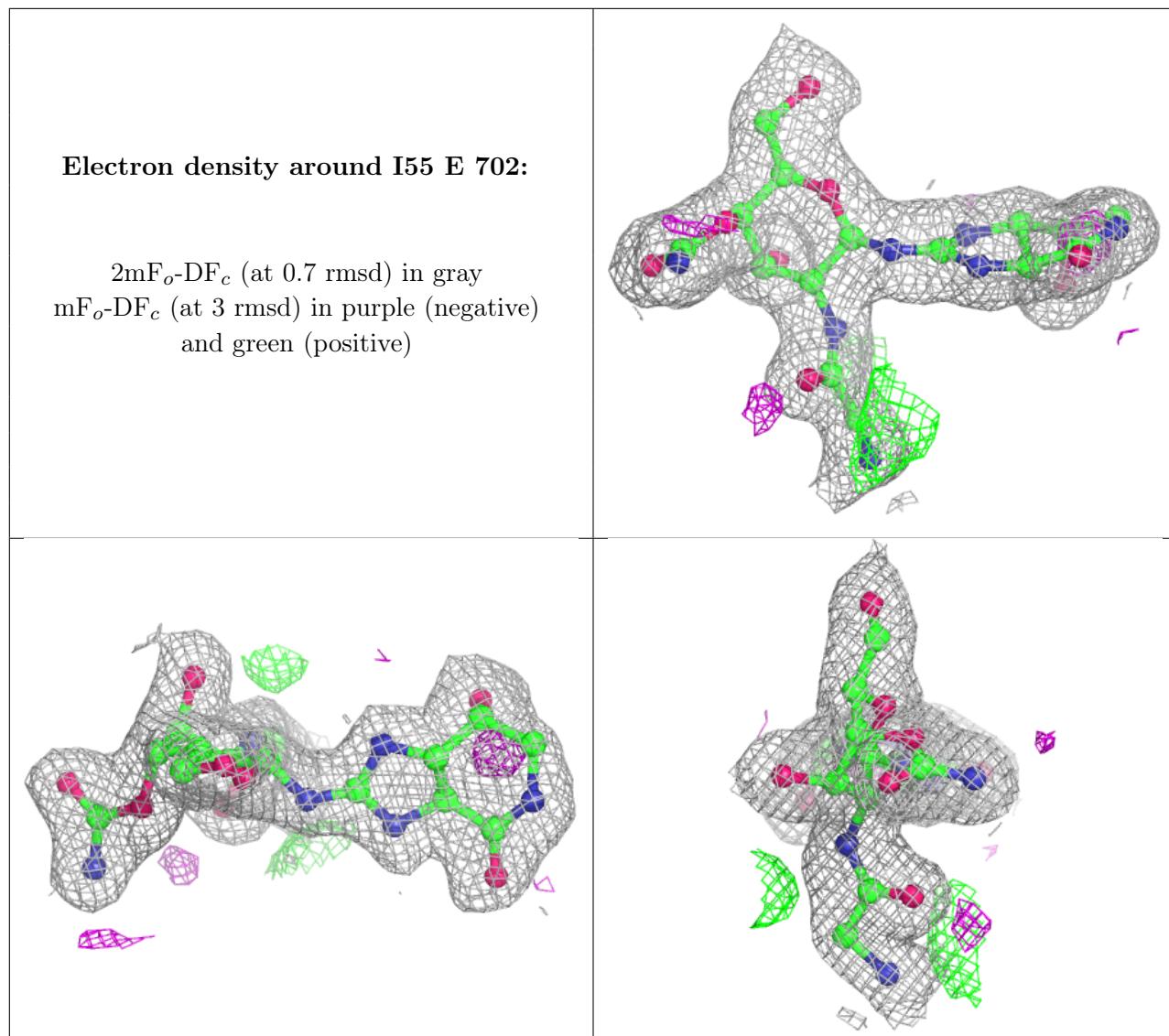


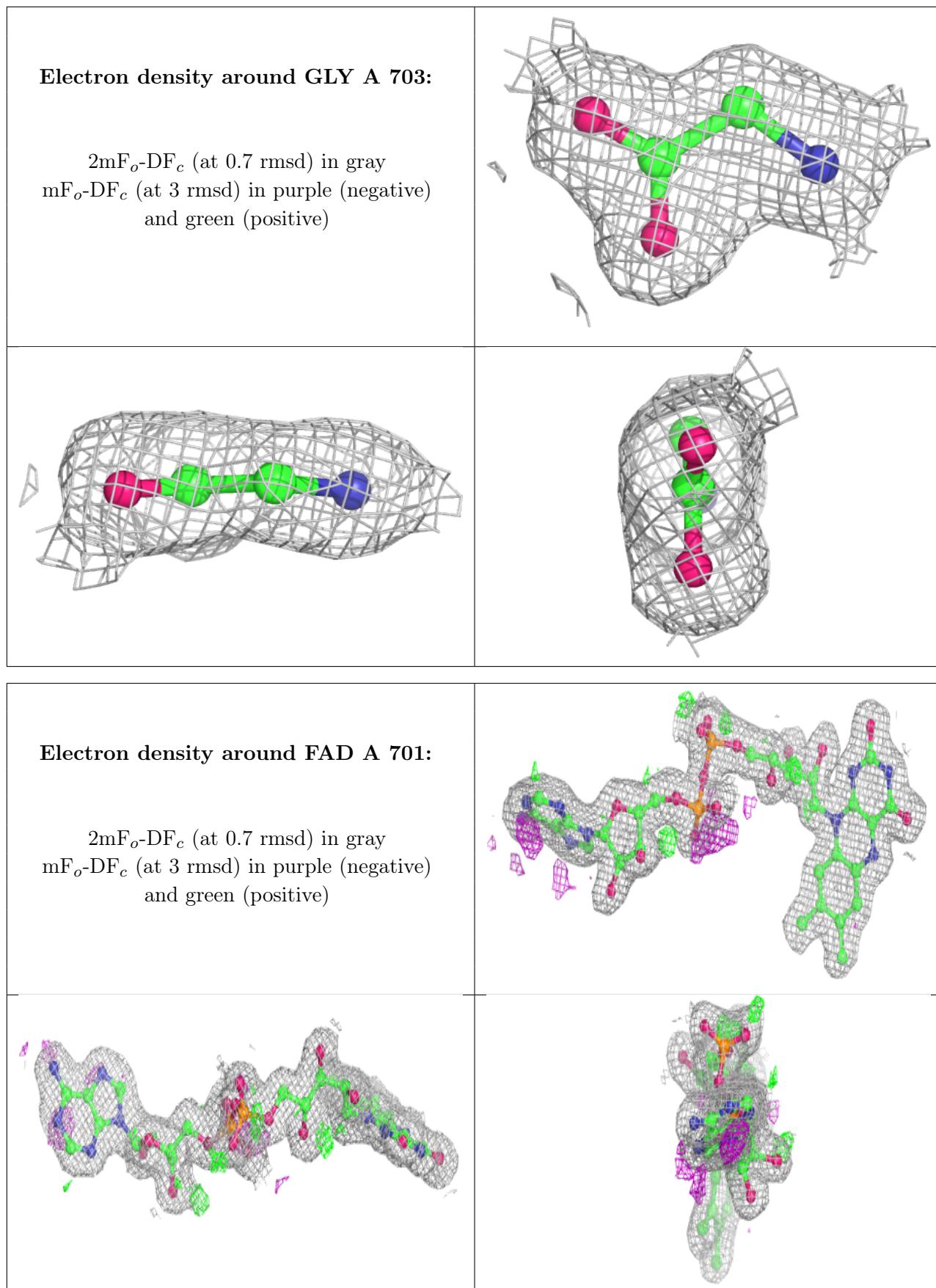


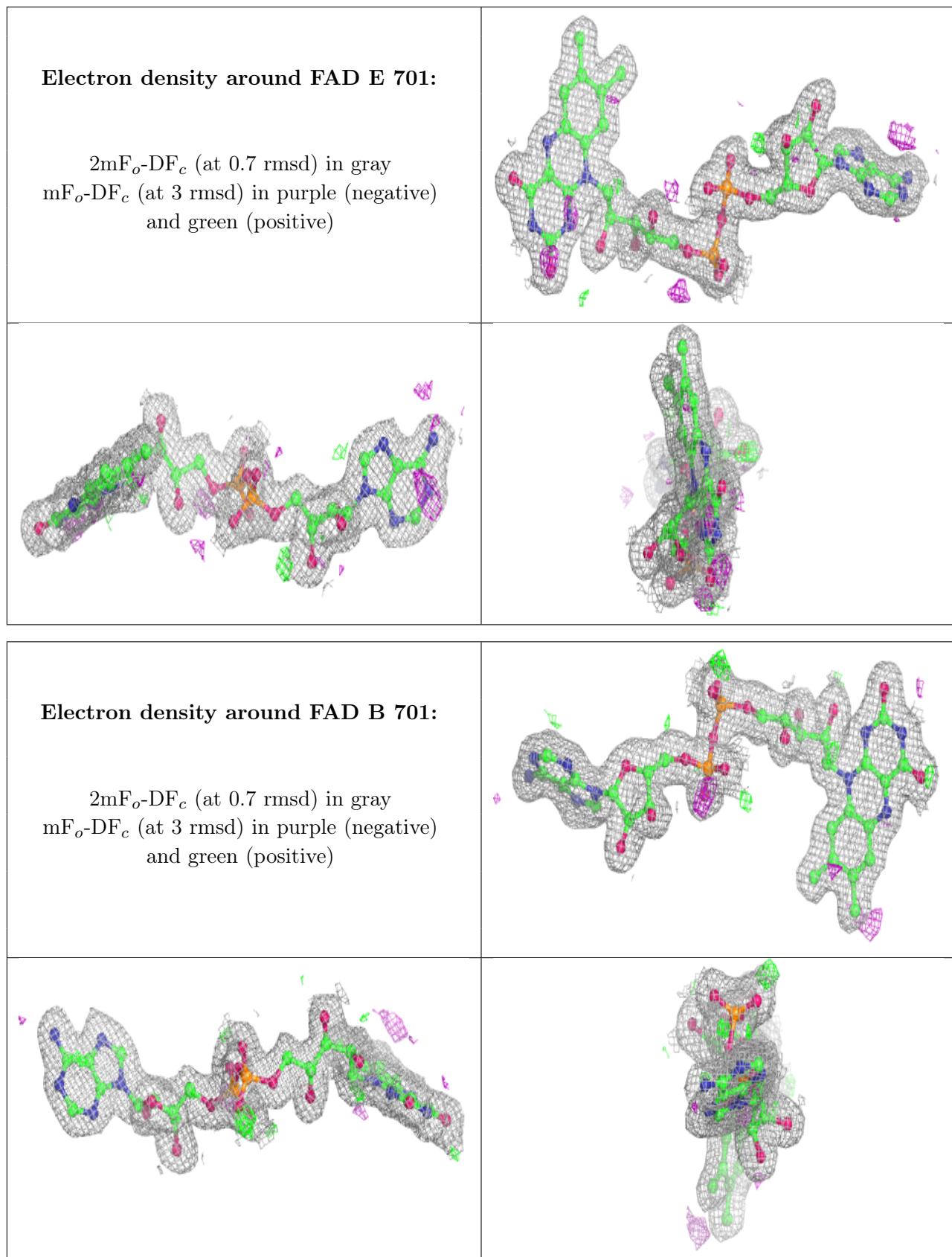


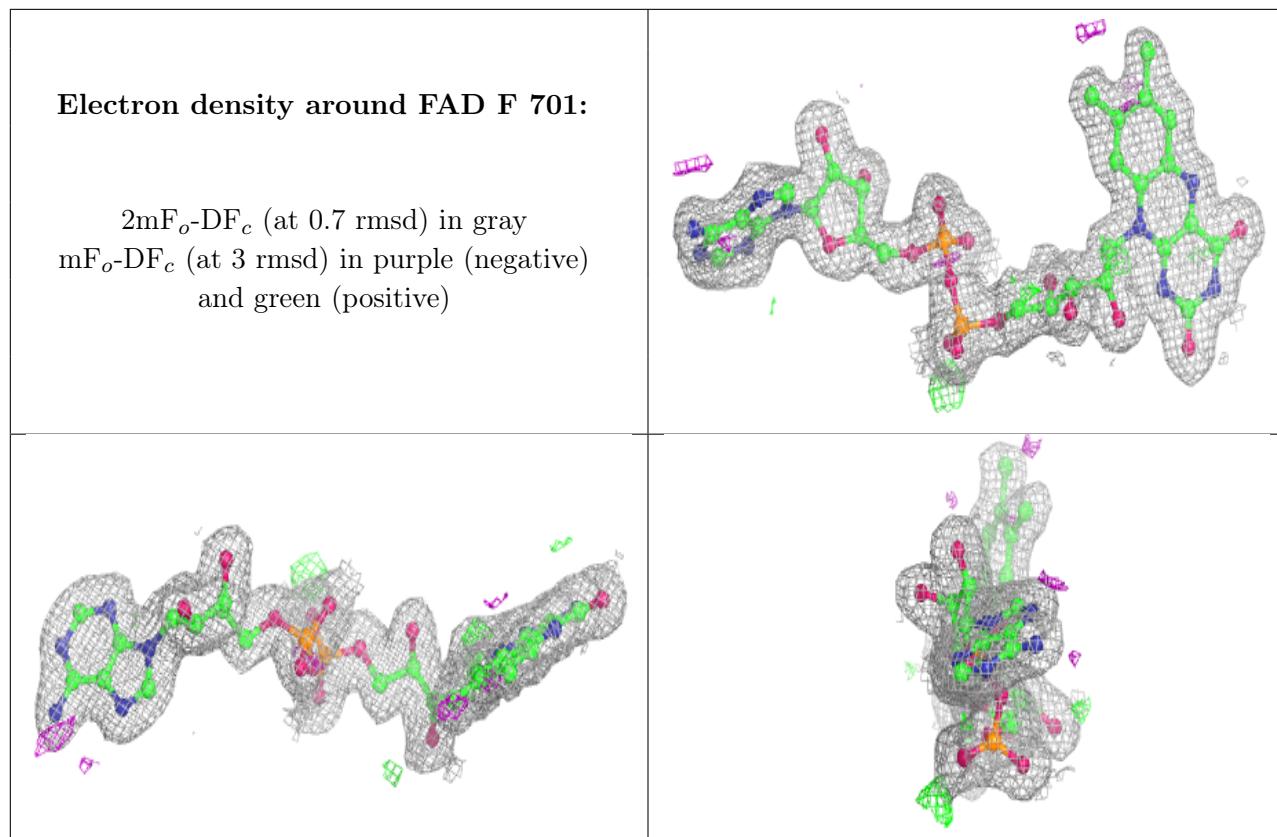












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.