



Full wwPDB X-ray Structure Validation Report i

Nov 22, 2023 – 11:03 PM JST

PDB ID : 7XXR
Title : Orf1 R342A-glycylthricin complex
Authors : Wang, Y.L.; Li, T.L.
Deposited on : 2022-05-30
Resolution : 2.40 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

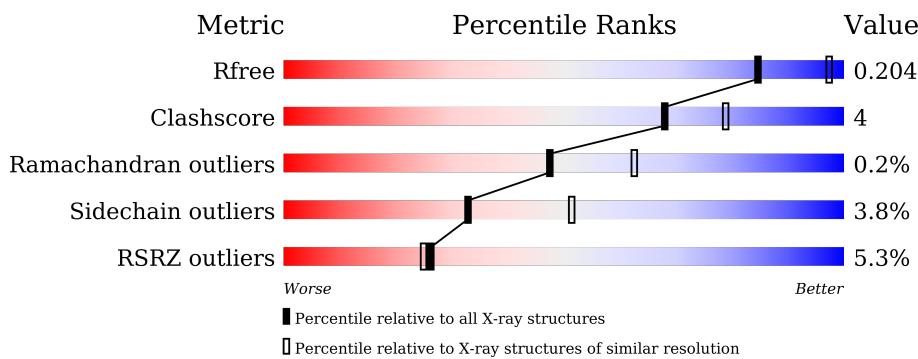
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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%	83%	10%	• 6%
1	H	512	13%	84%	9%	• 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30395 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	482	Total	C 3648	N 2290	O 657	S 689	12	0	0
1	B	482	Total	C 3648	N 2290	O 657	S 689	12	0	0
1	C	482	Total	C 3656	N 2295	O 658	S 690	13	0	1
1	D	480	Total	C 3640	N 2286	O 655	S 686	13	0	1
1	E	482	Total	C 3648	N 2290	O 657	S 689	12	0	0
1	F	482	Total	C 3648	N 2290	O 657	S 689	12	0	0
1	G	482	Total	C 3648	N 2290	O 657	S 689	12	0	0
1	H	480	Total	C 3640	N 2286	O 655	S 686	13	0	1

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A125S2C1
A	-19	GLY	-	expression tag	UNP A0A125S2C1
A	-18	SER	-	expression tag	UNP A0A125S2C1
A	-17	SER	-	expression tag	UNP A0A125S2C1
A	-16	HIS	-	expression tag	UNP A0A125S2C1
A	-15	HIS	-	expression tag	UNP A0A125S2C1
A	-14	HIS	-	expression tag	UNP A0A125S2C1
A	-13	HIS	-	expression tag	UNP A0A125S2C1
A	-12	HIS	-	expression tag	UNP A0A125S2C1
A	-11	HIS	-	expression tag	UNP A0A125S2C1
A	-10	SER	-	expression tag	UNP A0A125S2C1
A	-9	SER	-	expression tag	UNP A0A125S2C1
A	-8	GLY	-	expression tag	UNP A0A125S2C1

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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
A	342	ALA	ARG	engineered mutation	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
B	342	ALA	ARG	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	SER	-	expression tag	UNP A0A125S2C1
C	-8	GLY	-	expression tag	UNP A0A125S2C1
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
C	342	ALA	ARG	engineered mutation	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
D	342	ALA	ARG	engineered mutation	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

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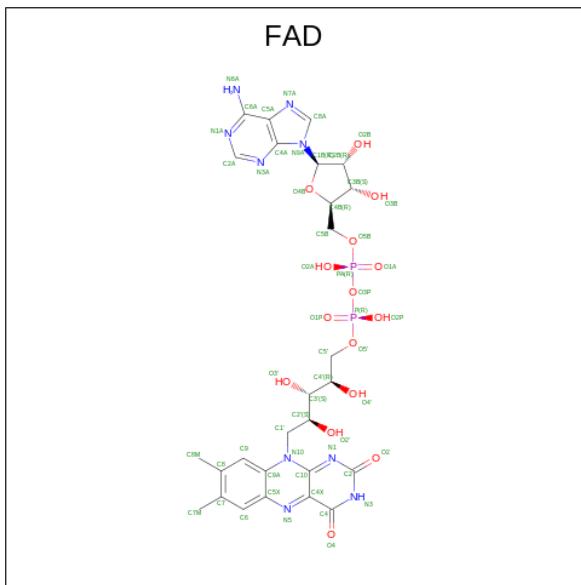
Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP A0A125S2C1
E	-10	SER	-	expression tag	UNP A0A125S2C1
E	-9	SER	-	expression tag	UNP A0A125S2C1
E	-8	GLY	-	expression tag	UNP A0A125S2C1
E	-7	LEU	-	expression tag	UNP A0A125S2C1
E	-6	VAL	-	expression tag	UNP A0A125S2C1
E	-5	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
E	342	ALA	ARG	engineered mutation	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
F	342	ALA	ARG	engineered mutation	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

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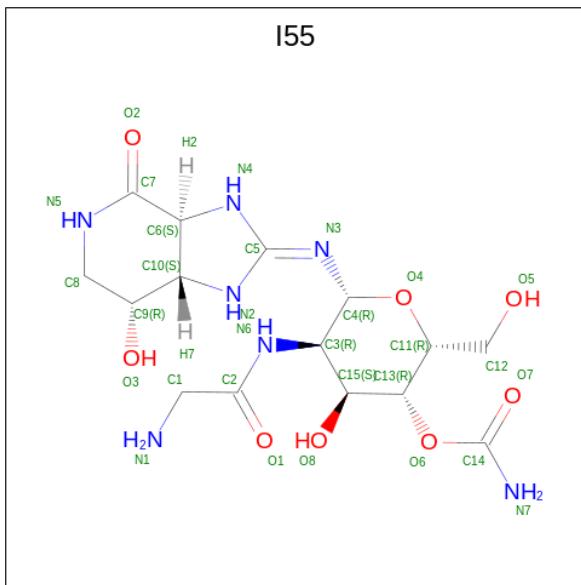
Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP A0A125S2C1
G	-12	HIS	-	expression tag	UNP A0A125S2C1
G	-11	HIS	-	expression tag	UNP A0A125S2C1
G	-10	SER	-	expression tag	UNP A0A125S2C1
G	-9	SER	-	expression tag	UNP A0A125S2C1
G	-8	GLY	-	expression tag	UNP A0A125S2C1
G	-7	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
G	342	ALA	ARG	engineered mutation	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
H	342	ALA	ARG	engineered mutation	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 30	C 15	N 7	O 8	0	0
3	B	1	Total 30	C 15	N 7	O 8	0	0
3	C	1	Total 30	C 15	N 7	O 8	0	0
3	D	1	Total 30	C 15	N 7	O 8	0	0
3	E	1	Total 30	C 15	N 7	O 8	0	0
3	F	1	Total 30	C 15	N 7	O 8	0	0
3	G	1	Total 30	C 15	N 7	O 8	0	0
3	H	1	Total 30	C 15	N 7	O 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	85	Total 85	O 85	0	0
4	C	80	Total 80	O 80	0	0
4	D	34	Total 34	O 34	0	0

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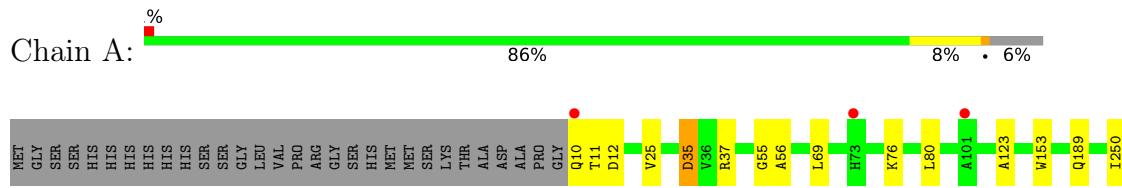
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	83	Total O 83 83	0	0
4	F	85	Total O 85 85	0	0
4	G	74	Total O 74 74	0	0
4	H	29	Total O 29 29	0	0

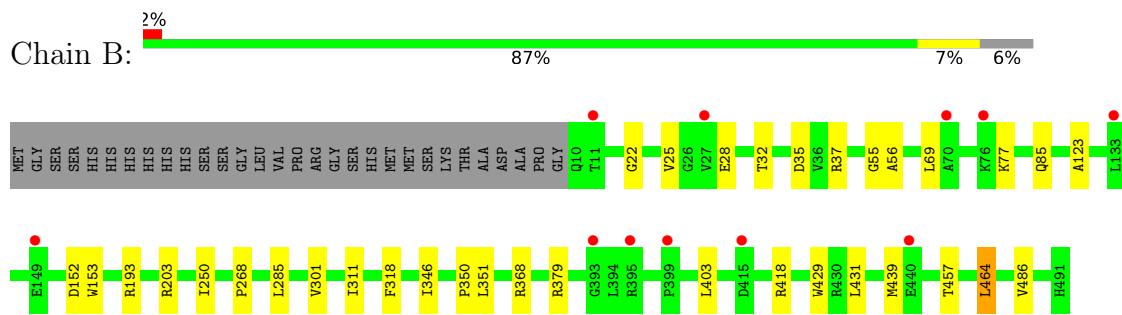
3 Residue-property plots

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.

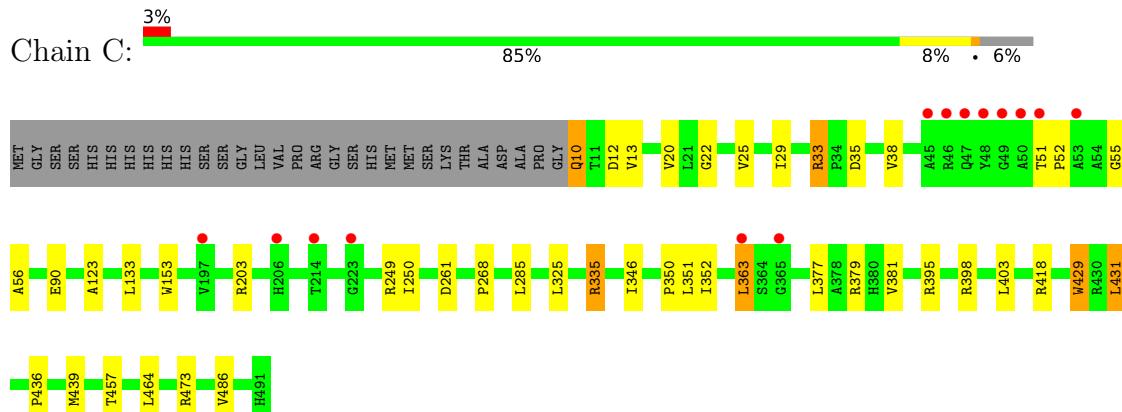
- Molecule 1: N-formimidoyl fortimicin A synthase



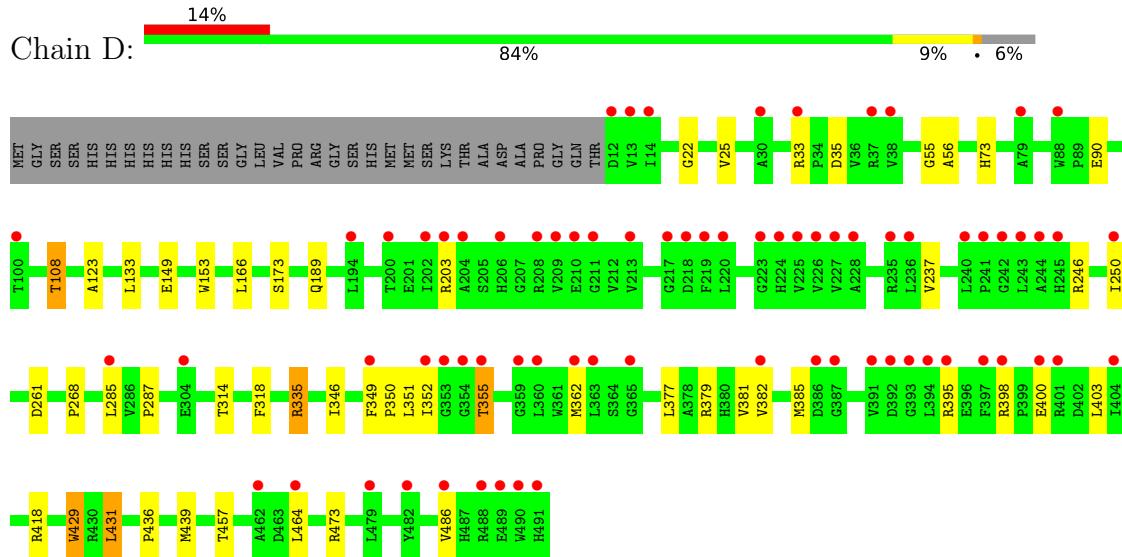
- Molecule 1: N-formimidoyl fortimicin A synthase



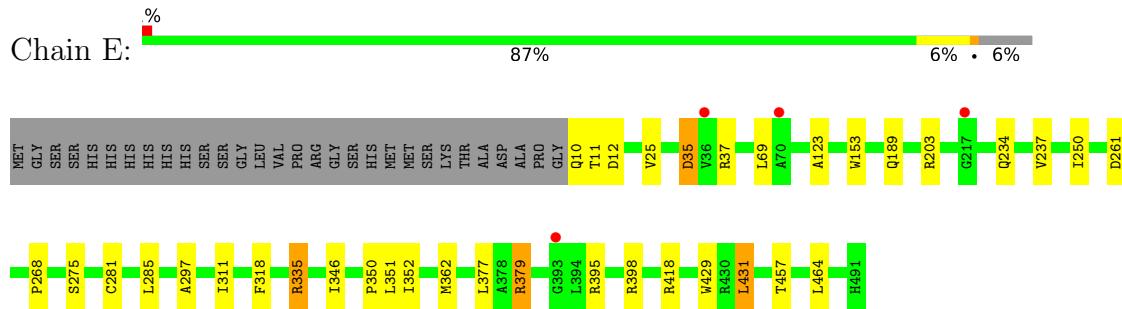
- Molecule 1: N-formimidoyl fortimicin A synthase



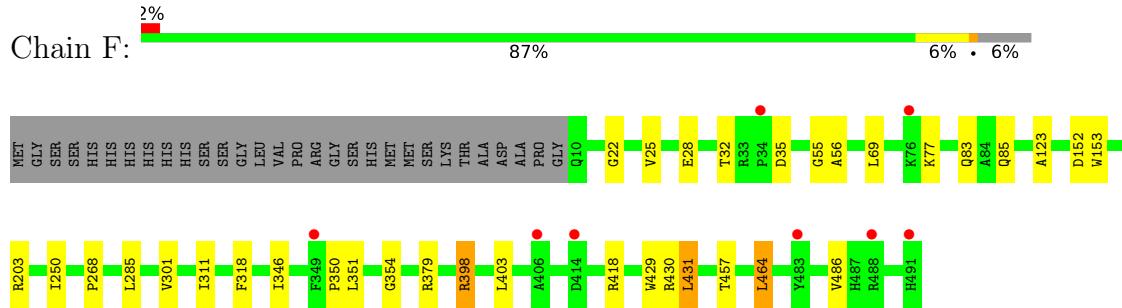
- Molecule 1: N-formimidoyl fortimicin A synthase



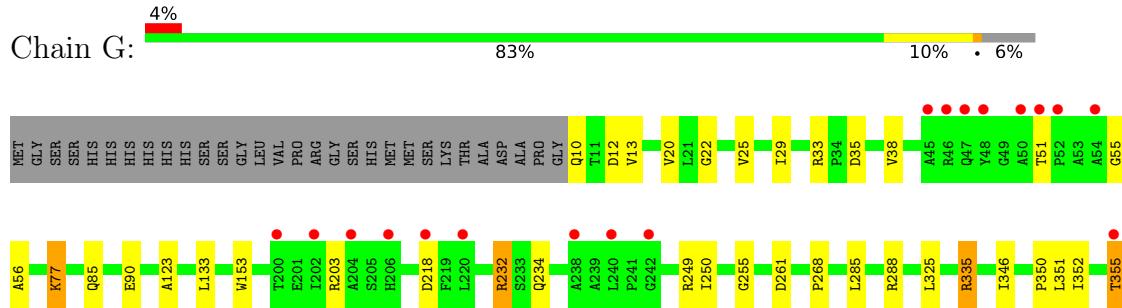
- Molecule 1: N-formimidoyl fortimicin A synthase



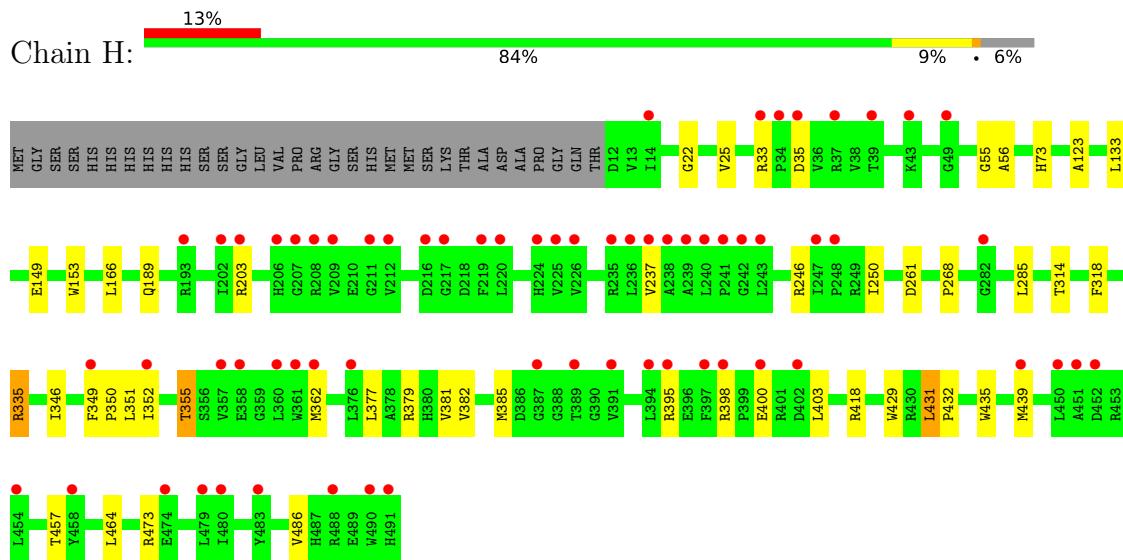
- Molecule 1: N-formimidoyl fortimicin A synthase



- Molecule 1: N-formimidoyl fortimicin A synthase



- 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	103.42Å 107.93Å 133.42Å 90.08° 90.01° 96.30°	Depositor
Resolution (Å)	28.62 – 2.40 28.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (28.62-2.40) 94.8 (28.60-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	3.20 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R , R_{free}	0.200 , 0.220 0.204 , 0.204	Depositor DCC
R_{free} test set	10662 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.0	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.460 for -h,-k,l 0.008 for k,h,-l 0.007 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30395	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, I55

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	0.68	0/3731	0.82	1/5085 (0.0%)
1	B	0.68	0/3731	0.83	1/5085 (0.0%)
1	C	0.71	0/3739	0.83	0/5095
1	D	0.66	0/3723	0.80	0/5073
1	E	0.68	0/3731	0.82	0/5085
1	F	0.68	0/3731	0.82	1/5085 (0.0%)
1	G	0.70	0/3731	0.83	0/5085
1	H	0.66	0/3723	0.80	0/5073
All	All	0.68	0/29840	0.82	3/40666 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	430	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	431	LEU	CB-CA-C	-5.27	100.19	110.20
1	A	368	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	3648	0	3576	22	0
1	B	3648	0	3576	19	0
1	C	3656	0	3584	38	0
1	D	3640	0	3569	39	0
1	E	3648	0	3576	18	0
1	F	3648	0	3576	22	0
1	G	3648	0	3576	36	0
1	H	3640	0	3569	38	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	1	0
2	F	53	0	31	0	0
2	G	53	0	31	0	0
2	H	53	0	31	0	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	85	0	0	0	0
4	B	85	0	0	2	0
4	C	80	0	0	1	0
4	D	34	0	0	1	0
4	E	83	0	0	1	0
4	F	85	0	0	3	0
4	G	74	0	0	2	0
4	H	29	0	0	1	0
All	All	30395	0	28850	222	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 (222) 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:D:436:PRO:HA	1:D:439[A]:MET:HE2	1.25	1.15
1:C:436:PRO:HA	1:C:439[B]:MET:HE2	1.28	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:VAL:HG23	1:C:51:THR:CG2	1.89	1.02
1:G:20:VAL:HG23	1:G:51:THR:HG21	1.42	1.01
1:G:20:VAL:HG23	1:G:51:THR:CG2	1.89	1.00
1:D:436:PRO:HA	1:D:439[A]:MET:CE	1.92	0.99
1:C:20:VAL:HG23	1:C:51:THR:HG21	1.42	0.98
1:C:436:PRO:HA	1:C:439[B]:MET:CE	1.95	0.97
1:H:352:ILE:HD13	1:H:377:LEU:HD22	1.61	0.83
1:D:352:ILE:HD13	1:D:377:LEU:HD22	1.61	0.81
1:G:352:ILE:HD13	1:G:377:LEU:HD22	1.62	0.81
1:B:85:GLN:HG2	4:B:858:HOH:O	1.80	0.81
1:H:431:LEU:H	1:H:431:LEU:HD23	1.45	0.80
1:C:352:ILE:HD13	1:C:377:LEU:HD22	1.62	0.78
1:H:431:LEU:HD23	1:H:431:LEU:N	1.96	0.78
1:G:355:THR:HG22	1:G:400:GLU:OE2	1.86	0.76
1:E:379:ARG:HD3	4:E:863:HOH:O	1.86	0.75
1:D:108:THR:HG21	1:D:287:PRO:O	1.87	0.75
1:D:436:PRO:CA	1:D:439[A]:MET:HE2	2.13	0.75
1:G:20:VAL:HG23	1:G:51:THR:HG23	1.69	0.74
1:C:436:PRO:CA	1:C:439[B]:MET:HE2	2.16	0.73
1:C:20:VAL:HG23	1:C:51:THR:HG23	1.70	0.72
1:G:288:ARG:HD3	4:G:810:HOH:O	1.91	0.71
1:H:431:LEU:N	1:H:431:LEU:CD2	2.54	0.70
1:F:77:LYS:NZ	4:F:801:HOH:O	2.24	0.69
1:C:123:ALA:HB1	1:C:418:ARG:HD3	1.74	0.69
1:H:355:THR:HG22	1:H:400:GLU:OE2	1.92	0.69
1:H:246:ARG:NH1	1:H:400:GLU:OE1	2.26	0.69
1:D:355:THR:HG22	1:D:400:GLU:OE2	1.92	0.69
1:D:246:ARG:NH1	1:D:400:GLU:OE1	2.26	0.68
1:C:33:ARG:HD2	4:C:854:HOH:O	1.93	0.68
1:D:108:THR:HG22	1:D:173:SER:OG	1.95	0.67
1:G:123:ALA:HB1	1:G:418:ARG:HD3	1.75	0.67
1:H:261:ASP:OD2	1:H:335:ARG:NE	2.24	0.65
1:H:382:VAL:HA	1:H:385:MET:CE	2.26	0.65
1:D:382:VAL:HA	1:D:385:MET:CE	2.27	0.65
1:A:439:MET:HE2	1:C:439[B]:MET:SD	2.37	0.64
1:F:85:GLN:HG2	4:F:846:HOH:O	2.00	0.62
1:B:439:MET:HE2	1:D:439[A]:MET:SD	2.39	0.61
1:F:301:VAL:HG11	1:F:464:LEU:HD12	1.83	0.60
1:D:382:VAL:HA	1:D:385:MET:HE2	1.83	0.59
1:C:20:VAL:CG2	1:C:51:THR:HG23	2.33	0.59
1:D:261:ASP:OD2	1:D:335:ARG:NE	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:O	1:B:32:THR:HG23	2.03	0.58
1:C:352:ILE:HD13	1:C:377:LEU:CD2	2.34	0.58
1:H:382:VAL:HA	1:H:385:MET:HE2	1.86	0.58
1:G:20:VAL:CG2	1:G:51:THR:HG23	2.33	0.57
1:D:436:PRO:CA	1:D:439[A]:MET:CE	2.75	0.57
1:C:20:VAL:CG2	1:C:51:THR:CG2	2.76	0.57
1:F:28:GLU:O	1:F:32:THR:HG23	2.04	0.57
1:G:352:ILE:HD13	1:G:377:LEU:CD2	2.35	0.57
1:H:431:LEU:HD12	1:H:439[A]:MET:HE1	1.88	0.56
1:B:301:VAL:HG11	1:B:464:LEU:HD12	1.86	0.56
1:H:431:LEU:HD12	1:H:439[A]:MET:CE	2.36	0.56
1:B:77:LYS:NZ	4:B:801:HOH:O	2.38	0.55
1:C:363:LEU:HG	1:C:381:VAL:HG21	1.89	0.54
1:E:12:ASP:OD1	1:E:37:ARG:HB3	2.07	0.54
1:G:255:GLY:HA3	1:G:368:ARG:HH22	1.72	0.54
1:E:311:ILE:HG23	1:F:318:PHE:HB3	1.90	0.54
1:A:12:ASP:OD1	1:A:37:ARG:HB3	2.08	0.54
1:F:354:GLY:H	1:F:398:ARG:NH1	2.05	0.53
1:H:246:ARG:NH1	1:H:400:GLU:HG2	2.24	0.53
1:A:311:ILE:HG23	1:B:318:PHE:HB3	1.90	0.53
1:H:435:TRP:HB3	1:H:439[A]:MET:CE	2.38	0.53
1:C:363:LEU:HD21	1:C:377:LEU:HB3	1.89	0.53
1:G:363:LEU:HG	1:G:381:VAL:HG21	1.90	0.53
1:D:429:TRP:CH2	1:D:439[A]:MET:HE3	2.44	0.53
1:B:268:PRO:HG3	1:B:285:LEU:HD22	1.91	0.52
1:A:268:PRO:HG3	1:A:285:LEU:HD22	1.92	0.52
1:B:439:MET:CE	1:D:439[A]:MET:SD	2.98	0.52
1:D:246:ARG:NH1	1:D:400:GLU:HG2	2.24	0.52
1:G:363:LEU:HD21	1:G:377:LEU:HB3	1.90	0.52
1:C:436:PRO:CA	1:C:439[B]:MET:CE	2.78	0.52
1:E:268:PRO:HG3	1:E:285:LEU:HD22	1.91	0.52
1:G:355:THR:CG2	1:G:400:GLU:OE2	2.57	0.51
1:H:355:THR:CG2	1:H:400:GLU:OE2	2.56	0.51
1:F:268:PRO:HG3	1:F:285:LEU:HD22	1.91	0.51
1:H:381:VAL:O	1:H:385:MET:HE2	2.11	0.51
1:D:355:THR:CG2	1:D:400:GLU:OE2	2.57	0.51
1:C:429:TRP:CH2	1:C:439[B]:MET:HE3	2.46	0.51
1:G:20:VAL:CG2	1:G:51:THR:CG2	2.77	0.51
1:H:268:PRO:HG3	1:H:285:LEU:HD22	1.93	0.50
1:C:268:PRO:HG3	1:C:285:LEU:HD22	1.94	0.50
1:D:268:PRO:HG3	1:D:285:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:THR:CG2	1:D:287:PRO:O	2.56	0.50
1:G:288:ARG:CD	4:G:810:HOH:O	2.55	0.50
1:H:123:ALA:HB1	1:H:418:ARG:HD3	1.94	0.49
1:G:55:GLY:N	1:G:56:ALA:HA	2.27	0.49
1:H:149:GLU:HG3	4:H:828:HOH:O	2.13	0.49
1:C:55:GLY:N	1:C:56:ALA:HA	2.27	0.49
1:D:381:VAL:O	1:D:385:MET:HE2	2.11	0.49
1:G:268:PRO:HG3	1:G:285:LEU:HD22	1.94	0.49
1:H:382:VAL:HA	1:H:385:MET:HE3	1.94	0.49
1:H:431:LEU:CD1	1:H:439[A]:MET:HE1	2.43	0.49
1:H:435:TRP:HB3	1:H:439[A]:MET:HE2	1.95	0.49
1:F:354:GLY:H	1:F:398:ARG:HH11	1.61	0.48
1:D:381:VAL:HG12	1:D:385:MET:CE	2.42	0.48
1:A:429:TRP:HB2	1:A:431:LEU:CD1	2.43	0.48
1:H:381:VAL:HG12	1:H:385:MET:CE	2.43	0.48
1:G:77:LYS:HE3	1:G:369:ASP:OD2	2.13	0.48
1:B:346:ILE:HG13	1:B:464:LEU:HD21	1.97	0.47
1:F:346:ILE:HG13	1:F:464:LEU:HD21	1.96	0.47
1:H:314:THR:HG22	1:H:318:PHE:CE2	2.50	0.47
1:D:381:VAL:HG12	1:D:385:MET:HE1	1.96	0.47
1:F:350:PRO:C	1:F:351:LEU:HD12	2.35	0.47
1:A:352:ILE:HD13	1:A:377:LEU:HD22	1.95	0.47
1:B:350:PRO:C	1:B:351:LEU:HD12	2.35	0.47
1:E:318:PHE:HB3	1:F:311:ILE:HG23	1.97	0.47
1:E:350:PRO:C	1:E:351:LEU:HD12	2.35	0.47
1:A:350:PRO:C	1:A:351:LEU:HD12	2.35	0.47
1:D:123:ALA:HB1	1:D:418:ARG:HD3	1.96	0.47
1:A:123:ALA:HB1	1:A:418:ARG:HD3	1.98	0.46
1:A:318:PHE:HB3	1:B:311:ILE:HG23	1.97	0.46
1:B:123:ALA:HB1	1:B:418:ARG:HD3	1.98	0.46
1:G:352:ILE:HG23	1:G:363:LEU:CD2	2.46	0.46
1:D:382:VAL:HA	1:D:385:MET:HE3	1.97	0.46
1:H:350:PRO:C	1:H:351:LEU:HD12	2.36	0.46
1:E:351:LEU:HD12	1:E:351:LEU:N	2.31	0.46
1:A:351:LEU:HD12	1:A:351:LEU:N	2.31	0.46
1:F:123:ALA:HB1	1:F:418:ARG:HD3	1.98	0.46
1:C:403:LEU:HG	1:C:486:VAL:HG11	1.98	0.46
1:C:29:ILE:HG22	1:C:38:VAL:HG21	1.99	0.45
1:D:73:HIS:HB3	1:D:349:PHE:CZ	2.51	0.45
1:F:351:LEU:HD12	1:F:351:LEU:N	2.31	0.45
1:A:311:ILE:CG2	1:B:318:PHE:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD12	1:B:351:LEU:N	2.32	0.45
1:E:123:ALA:HB1	1:E:418:ARG:HD3	1.98	0.45
1:E:352:ILE:HG13	1:E:377:LEU:HD22	1.98	0.45
1:G:13:VAL:HG11	1:G:29:ILE:HD13	1.97	0.45
1:G:29:ILE:HG22	1:G:38:VAL:HG21	1.99	0.45
1:G:403:LEU:HG	1:G:486:VAL:HG11	1.97	0.45
1:G:431:LEU:N	1:G:431:LEU:HD12	2.32	0.45
1:C:13:VAL:HG11	1:C:29:ILE:HD13	1.98	0.45
1:C:350:PRO:C	1:C:351:LEU:HD12	2.37	0.45
1:D:431:LEU:HD12	1:D:431:LEU:H	1.82	0.45
1:D:431:LEU:HD12	1:D:431:LEU:N	2.31	0.45
1:E:346:ILE:HG13	1:E:464:LEU:CD2	2.47	0.45
1:F:346:ILE:HG13	1:F:464:LEU:CD2	2.46	0.45
1:A:346:ILE:HG13	1:A:464:LEU:CD2	2.46	0.45
1:A:430:ARG:C	1:A:431:LEU:HD12	2.37	0.45
1:D:22:GLY:O	1:D:25:VAL:HG12	2.17	0.45
1:D:55:GLY:N	1:D:56:ALA:HA	2.32	0.45
1:D:350:PRO:C	1:D:351:LEU:HD12	2.37	0.45
1:A:439:MET:CE	1:C:439[B]:MET:SD	3.04	0.45
1:F:431:LEU:N	1:F:431:LEU:HD12	2.31	0.45
1:G:352:ILE:HG23	1:G:363:LEU:HD23	1.99	0.45
1:E:431:LEU:HD12	1:E:431:LEU:N	2.32	0.44
1:E:311:ILE:CG2	1:F:318:PHE:HB3	2.47	0.44
1:B:346:ILE:HG13	1:B:464:LEU:CD2	2.47	0.44
1:C:352:ILE:HG23	1:C:363:LEU:HD23	1.99	0.44
1:F:83:GLN:HG3	4:F:834:HOH:O	2.17	0.44
1:B:250:ILE:HD11	1:B:351:LEU:HD22	2.00	0.44
1:C:363:LEU:HD23	1:C:363:LEU:HA	1.87	0.44
1:D:346:ILE:HG13	1:D:464:LEU:CD2	2.48	0.44
1:H:22:GLY:O	1:H:25:VAL:HG12	2.17	0.44
1:A:250:ILE:HD11	1:A:351:LEU:HD22	2.00	0.44
1:F:431:LEU:HD12	1:F:431:LEU:H	1.83	0.44
1:G:346:ILE:HG13	1:G:464:LEU:CD2	2.48	0.44
1:C:352:ILE:HG23	1:C:363:LEU:CD2	2.47	0.44
1:E:250:ILE:HD11	1:E:351:LEU:HD22	2.00	0.44
1:F:22:GLY:O	1:F:25:VAL:HG12	2.17	0.44
1:C:431:LEU:HD12	1:C:431:LEU:N	2.32	0.43
1:D:133:LEU:HD13	1:D:166:LEU:HD22	1.99	0.43
1:G:351:LEU:N	1:G:351:LEU:HD12	2.33	0.43
1:H:55:GLY:N	1:H:56:ALA:HA	2.32	0.43
1:H:346:ILE:HG13	1:H:464:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLY:O	1:B:25:VAL:HG12	2.18	0.43
1:C:346:ILE:HG13	1:C:464:LEU:CD2	2.48	0.43
1:G:22:GLY:O	1:G:25:VAL:HG12	2.18	0.43
1:E:237:VAL:HG11	1:E:362:MET:HE1	2.00	0.43
1:G:350:PRO:C	1:G:351:LEU:HD12	2.37	0.43
1:D:351:LEU:HD12	1:D:351:LEU:N	2.33	0.43
1:C:22:GLY:O	1:C:25:VAL:HG12	2.18	0.43
1:D:314:THR:HG22	1:D:318:PHE:CE2	2.53	0.43
1:E:431:LEU:HD12	1:E:431:LEU:H	1.83	0.43
1:H:431:LEU:HB2	1:H:432:PRO:HD2	1.99	0.43
1:C:351:LEU:HD12	1:C:351:LEU:N	2.33	0.43
1:H:250:ILE:HD11	1:H:351:LEU:HD22	2.01	0.43
1:H:431:LEU:HB2	1:H:432:PRO:CD	2.48	0.43
1:H:73:HIS:HB3	1:H:349:PHE:CZ	2.54	0.43
1:F:250:ILE:HD11	1:F:351:LEU:HD22	2.00	0.43
1:H:381:VAL:C	1:H:385:MET:HE2	2.39	0.43
1:D:250:ILE:HD11	1:D:351:LEU:HD22	2.01	0.43
1:H:351:LEU:HD12	1:H:351:LEU:N	2.33	0.43
1:A:429:TRP:CG	1:A:431:LEU:HD13	2.53	0.42
1:A:80:LEU:HB3	1:A:373:MET:HE2	2.00	0.42
1:C:10:GLN:HB3	1:C:12:ASP:HB2	2.02	0.42
1:H:381:VAL:HG12	1:H:385:MET:HE1	2.00	0.42
1:A:10:GLN:HA	1:A:35:ASP:O	2.20	0.42
1:B:55:GLY:N	1:B:56:ALA:HA	2.35	0.42
1:D:149:GLU:HG3	4:D:829:HOH:O	2.19	0.42
1:C:431:LEU:HD12	1:C:431:LEU:H	1.84	0.42
1:D:237:VAL:HG11	1:D:362:MET:HE1	2.02	0.42
1:G:133:LEU:HD23	1:G:133:LEU:HA	1.89	0.42
1:G:250:ILE:HD11	1:G:351:LEU:HD22	2.02	0.42
1:H:237:VAL:HG11	1:H:362:MET:HE1	2.02	0.42
1:C:250:ILE:HD11	1:C:351:LEU:HD22	2.02	0.42
1:D:403:LEU:HG	1:D:486:VAL:HG11	2.02	0.42
1:G:261:ASP:OD1	1:G:335:ARG:NH1	2.53	0.42
1:A:403:LEU:HG	1:A:486:VAL:HG11	2.02	0.41
1:D:381:VAL:C	1:D:385:MET:HE2	2.40	0.41
1:E:10:GLN:HA	1:E:35:ASP:O	2.20	0.41
1:E:297:ALA:HB1	2:E:701:FAD:HM73	2.02	0.41
1:G:431:LEU:HD12	1:G:431:LEU:H	1.84	0.41
1:H:403:LEU:HG	1:H:486:VAL:HG11	2.03	0.41
1:C:51:THR:HB	1:C:52:PRO:HD3	2.03	0.41
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:GLN:HB3	1:G:12:ASP:HB2	2.03	0.41
1:B:403:LEU:HG	1:B:486:VAL:HG11	2.03	0.40
1:E:261:ASP:OD1	1:E:335:ARG:NH1	2.54	0.40
1:A:427:PHE:N	1:A:428:PRO:HA	2.37	0.40
1:F:55:GLY:N	1:F:56:ALA:HA	2.35	0.40
1:C:285:LEU:HB2	1:C:325:LEU:HD13	2.03	0.40
1:F:403:LEU:HG	1:F:486:VAL:HG11	2.02	0.40
1:A:55:GLY:N	1:A:56:ALA:HA	2.36	0.40
1:C:261:ASP:OD1	1:C:335:ARG:NH1	2.54	0.40
1:G:232:ARG:HD3	1:G:232:ARG:HA	1.96	0.40
1:G:285:LEU:HB2	1:G:325:LEU:HD13	2.04	0.40
1:G:374:SER:N	1:G:375:PRO:HD2	2.37	0.40
1:H:133:LEU:HD13	1:H:166:LEU:HD22	2.02	0.40
1:A:374:SER:N	1:A:375:PRO:HD2	2.36	0.40
1:H:431:LEU:CD1	1:H:439[A]:MET:CE	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	480/512 (94%)	467 (97%)	12 (2%)	1 (0%)	47 62
1	B	480/512 (94%)	467 (97%)	12 (2%)	1 (0%)	47 62
1	C	481/512 (94%)	467 (97%)	13 (3%)	1 (0%)	47 62
1	D	479/512 (94%)	466 (97%)	12 (2%)	1 (0%)	47 62
1	E	480/512 (94%)	467 (97%)	12 (2%)	1 (0%)	47 62
1	F	480/512 (94%)	467 (97%)	12 (2%)	1 (0%)	47 62
1	G	480/512 (94%)	465 (97%)	14 (3%)	1 (0%)	47 62
1	H	479/512 (94%)	465 (97%)	13 (3%)	1 (0%)	47 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3839/4096 (94%)	3731 (97%)	100 (3%)	8 (0%)	47 62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	TRP
1	G	153	TRP
1	H	153	TRP
1	A	153	TRP
1	D	153	TRP
1	E	153	TRP
1	F	153	TRP
1	B	153	TRP

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	375/399 (94%)	363 (97%)	12 (3%)	39 59
1	B	375/399 (94%)	364 (97%)	11 (3%)	42 62
1	C	376/399 (94%)	361 (96%)	15 (4%)	31 49
1	D	374/399 (94%)	359 (96%)	15 (4%)	31 49
1	E	375/399 (94%)	359 (96%)	16 (4%)	29 46
1	F	375/399 (94%)	365 (97%)	10 (3%)	44 65
1	G	375/399 (94%)	353 (94%)	22 (6%)	19 32
1	H	374/399 (94%)	361 (96%)	13 (4%)	36 55
All	All	2999/3192 (94%)	2885 (96%)	114 (4%)	33 51

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	25	VAL

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Mol	Chain	Res	Type
1	A	35	ASP
1	A	69	LEU
1	A	76	LYS
1	A	189	GLN
1	A	275	SER
1	A	281	CYS
1	A	368	ARG
1	A	379	ARG
1	A	429	TRP
1	A	457	THR
1	B	35	ASP
1	B	37	ARG
1	B	69	LEU
1	B	152	ASP
1	B	193	ARG
1	B	203	ARG
1	B	368	ARG
1	B	379	ARG
1	B	429	TRP
1	B	457	THR
1	B	464	LEU
1	C	10	GLN
1	C	33	ARG
1	C	35	ASP
1	C	90	GLU
1	C	203	ARG
1	C	249	ARG
1	C	335	ARG
1	C	363	LEU
1	C	379	ARG
1	C	395	ARG
1	C	398	ARG
1	C	429	TRP
1	C	431	LEU
1	C	457	THR
1	C	473	ARG
1	D	33	ARG
1	D	35	ASP
1	D	90	GLU
1	D	108	THR
1	D	189	GLN
1	D	203	ARG

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Mol	Chain	Res	Type
1	D	335	ARG
1	D	355	THR
1	D	379	ARG
1	D	395	ARG
1	D	398	ARG
1	D	429	TRP
1	D	431	LEU
1	D	457	THR
1	D	473	ARG
1	E	11	THR
1	E	25	VAL
1	E	35	ASP
1	E	69	LEU
1	E	189	GLN
1	E	203	ARG
1	E	234	GLN
1	E	275	SER
1	E	281	CYS
1	E	335	ARG
1	E	379	ARG
1	E	395	ARG
1	E	398	ARG
1	E	429	TRP
1	E	431	LEU
1	E	457	THR
1	F	35	ASP
1	F	69	LEU
1	F	152	ASP
1	F	203	ARG
1	F	379	ARG
1	F	398	ARG
1	F	429	TRP
1	F	431	LEU
1	F	457	THR
1	F	464	LEU
1	G	33	ARG
1	G	35	ASP
1	G	77	LYS
1	G	85	GLN
1	G	90	GLU
1	G	203	ARG
1	G	218	ASP

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Mol	Chain	Res	Type
1	G	232	ARG
1	G	234	GLN
1	G	249	ARG
1	G	335	ARG
1	G	355	THR
1	G	363	LEU
1	G	368	ARG
1	G	379	ARG
1	G	386	ASP
1	G	395	ARG
1	G	398	ARG
1	G	429	TRP
1	G	431	LEU
1	G	457	THR
1	G	473	ARG
1	H	33	ARG
1	H	35	ASP
1	H	189	GLN
1	H	203	ARG
1	H	335	ARG
1	H	355	THR
1	H	379	ARG
1	H	395	ARG
1	H	398	ARG
1	H	429	TRP
1	H	431	LEU
1	H	457	THR
1	H	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	234	GLN
1	G	234	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 [\(i\)](#)

16 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
3	I55	B	702	-	28,32,32	1.34	1 (3%)	31,46,46	1.38	3 (9%)
2	FAD	E	701	-	53,58,58	0.64	0	68,89,89	0.87	2 (2%)
3	I55	F	702	-	28,32,32	1.61	2 (7%)	31,46,46	1.24	3 (9%)
3	I55	G	702	-	28,32,32	0.67	0	31,46,46	1.16	3 (9%)
2	FAD	D	701	-	53,58,58	0.57	0	68,89,89	0.74	1 (1%)
2	FAD	H	701	-	53,58,58	0.57	0	68,89,89	0.76	2 (2%)
2	FAD	B	701	-	53,58,58	0.63	0	68,89,89	0.95	5 (7%)
3	I55	E	702	-	28,32,32	1.50	1 (3%)	31,46,46	1.15	2 (6%)
3	I55	D	702	-	28,32,32	0.73	1 (3%)	31,46,46	1.30	3 (9%)
3	I55	C	702	-	28,32,32	0.72	1 (3%)	31,46,46	1.26	5 (16%)
3	I55	H	702	-	28,32,32	0.74	1 (3%)	31,46,46	1.13	1 (3%)
2	FAD	C	701	-	53,58,58	0.64	0	68,89,89	0.89	3 (4%)
2	FAD	F	701	-	53,58,58	0.67	1 (1%)	68,89,89	0.93	4 (5%)
2	FAD	G	701	-	53,58,58	0.65	0	68,89,89	0.92	3 (4%)
3	I55	A	702	-	28,32,32	1.61	2 (7%)	31,46,46	0.94	1 (3%)
2	FAD	A	701	-	53,58,58	0.67	0	68,89,89	0.80	2 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I55	B	702	-	-	1/14/61/61	0/3/3/3
2	FAD	E	701	-	-	1/30/50/50	0/6/6/6
3	I55	F	702	-	-	1/14/61/61	0/3/3/3
3	I55	G	702	-	-	1/14/61/61	0/3/3/3
2	FAD	D	701	-	-	1/30/50/50	0/6/6/6
2	FAD	H	701	-	-	1/30/50/50	0/6/6/6
2	FAD	B	701	-	-	3/30/50/50	0/6/6/6
3	I55	E	702	-	-	2/14/61/61	0/3/3/3
3	I55	D	702	-	-	1/14/61/61	0/3/3/3
3	I55	C	702	-	-	1/14/61/61	0/3/3/3
3	I55	H	702	-	-	1/14/61/61	0/3/3/3
2	FAD	C	701	-	-	9/30/50/50	0/6/6/6
2	FAD	F	701	-	-	3/30/50/50	0/6/6/6
2	FAD	G	701	-	-	8/30/50/50	0/6/6/6
3	I55	A	702	-	-	2/14/61/61	0/3/3/3
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	702	I55	C4-C3	-7.70	1.48	1.53
3	A	702	I55	C4-C3	-7.69	1.48	1.53
3	E	702	I55	C4-C3	-7.08	1.48	1.53
3	B	702	I55	C4-C3	-6.36	1.49	1.53
3	D	702	I55	C4-C3	-2.97	1.51	1.53
3	H	702	I55	C4-C3	-2.82	1.51	1.53
2	F	701	FAD	C1'-C2'	-2.69	1.48	1.52
3	F	702	I55	C8-C9	2.43	1.54	1.52
3	C	702	I55	C8-C9	2.32	1.54	1.52
3	A	702	I55	C14-N7	2.28	1.37	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	I55	C10-N6-C5	-5.29	107.49	112.56
3	B	702	I55	C10-N6-C5	-5.14	107.63	112.56
3	H	702	I55	C10-N6-C5	-4.74	108.01	112.56
3	E	702	I55	C10-N6-C5	-4.26	108.48	112.56
3	C	702	I55	C10-N6-C5	-4.17	108.56	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	702	I55	C10-N6-C5	-4.11	108.62	112.56
3	F	702	I55	C10-N6-C5	-4.04	108.69	112.56
2	F	701	FAD	O2A-PA-O1A	3.04	127.26	112.24
3	A	702	I55	C10-N6-C5	-3.03	109.66	112.56
3	B	702	I55	C6-C7-N5	-3.01	114.47	118.19
2	B	701	FAD	O2A-PA-O1A	3.00	127.05	112.24
3	F	702	I55	C6-C7-N5	-2.82	114.71	118.19
2	B	701	FAD	O5'-P-O1P	-2.75	98.32	109.07
2	C	701	FAD	P-O3P-PA	2.62	141.82	132.83
3	B	702	I55	C9-C8-N5	2.43	112.35	109.83
3	C	702	I55	C9-C8-N5	2.43	112.35	109.83
2	F	701	FAD	C5A-C6A-N6A	2.43	124.04	120.35
2	F	701	FAD	O2P-P-O1P	2.43	124.24	112.24
2	B	701	FAD	O2P-P-O1P	2.33	123.74	112.24
2	B	701	FAD	C5A-C6A-N6A	2.31	123.86	120.35
2	F	701	FAD	O5'-P-O1P	-2.28	100.15	109.07
2	E	701	FAD	O2A-PA-O1A	2.27	123.48	112.24
3	G	702	I55	C9-C8-N5	2.27	112.18	109.83
2	A	701	FAD	O2A-PA-O1A	2.27	123.47	112.24
2	G	701	FAD	C4'-C3'-C2'	2.27	118.08	113.36
2	E	701	FAD	O2P-P-O1P	2.21	123.19	112.24
3	F	702	I55	C9-C8-N5	2.21	112.11	109.83
2	G	701	FAD	P-O3P-PA	2.21	140.39	132.83
2	H	701	FAD	C5A-C6A-N6A	2.20	123.69	120.35
3	E	702	I55	C4-C3-N2	-2.19	107.90	111.08
2	H	701	FAD	O2P-P-O1P	2.18	123.00	112.24
3	C	702	I55	C4-C3-N2	2.16	114.22	111.08
3	C	702	I55	C6-C7-N5	-2.15	115.54	118.19
2	A	701	FAD	O2P-P-O1P	2.13	122.75	112.24
3	D	702	I55	C4-C3-N2	2.12	114.16	111.08
2	B	701	FAD	C4-N3-C2	-2.10	121.77	125.64
3	D	702	I55	O4-C4-N3	-2.07	103.47	109.13
2	C	701	FAD	C4'-C3'-C2'	2.06	117.64	113.36
2	C	701	FAD	C4-N3-C2	-2.04	121.87	125.64
2	D	701	FAD	C5A-C6A-N6A	2.04	123.45	120.35
3	C	702	I55	C15-C3-N2	-2.03	106.78	110.62
2	G	701	FAD	C4-N3-C2	-2.02	121.90	125.64
3	G	702	I55	C6-C7-N5	-2.00	115.72	118.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

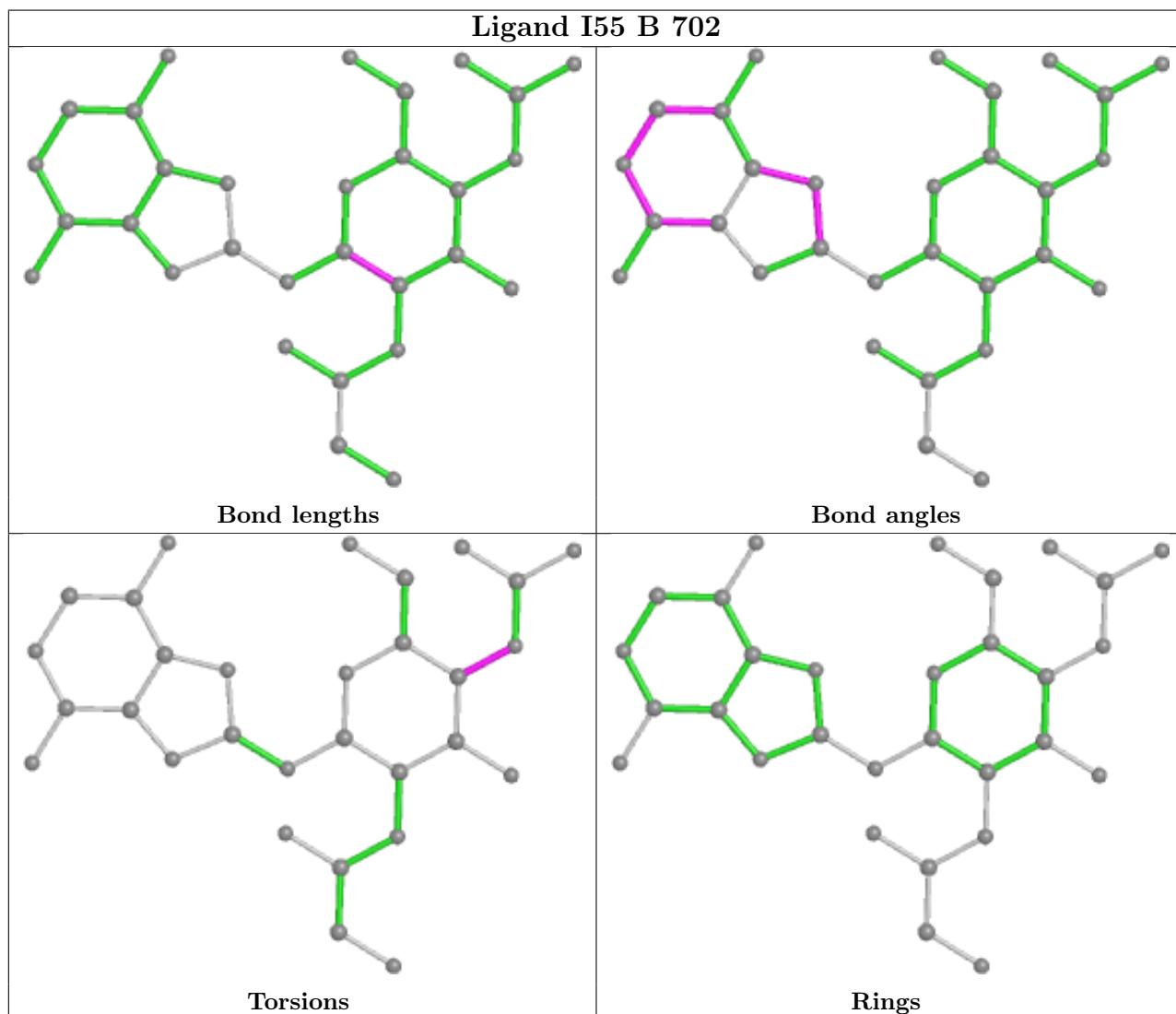
Mol	Chain	Res	Type	Atoms
2	C	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5B-O5B-PA-O2A
2	C	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	O4'-C4'-C5'-O5'
2	F	701	FAD	C5B-O5B-PA-O2A
2	F	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	C5B-O5B-PA-O1A
2	G	701	FAD	C5B-O5B-PA-O2A
2	G	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	C3B-C4B-C5B-O5B
2	G	701	FAD	C3B-C4B-C5B-O5B
2	G	701	FAD	C4B-C5B-O5B-PA
2	C	701	FAD	P-O3P-PA-O5B
2	G	701	FAD	P-O3P-PA-O5B
2	C	701	FAD	C4B-C5B-O5B-PA
3	A	702	I55	C11-C13-O6-C14
3	A	702	I55	C15-C13-O6-C14
3	B	702	I55	C15-C13-O6-C14
3	C	702	I55	C15-C13-O6-C14
3	D	702	I55	C15-C13-O6-C14
3	E	702	I55	C11-C13-O6-C14
3	E	702	I55	C15-C13-O6-C14
3	F	702	I55	C15-C13-O6-C14
3	G	702	I55	C15-C13-O6-C14
3	H	702	I55	C15-C13-O6-C14
2	A	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C3'-C4'-C5'-O5'
2	H	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C5B-O5B-PA-O3P
2	G	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	O4B-C4B-C5B-O5B

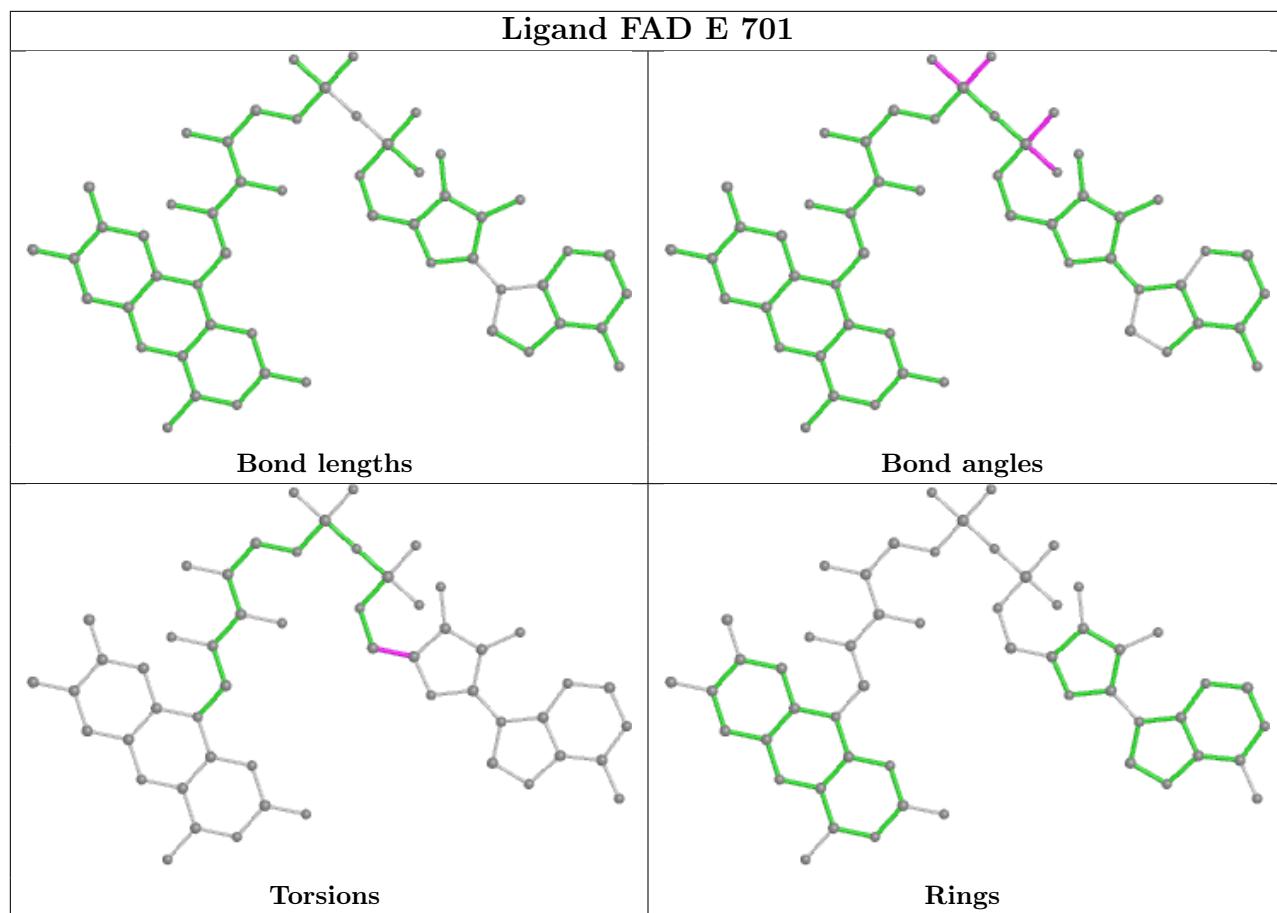
There are no ring outliers.

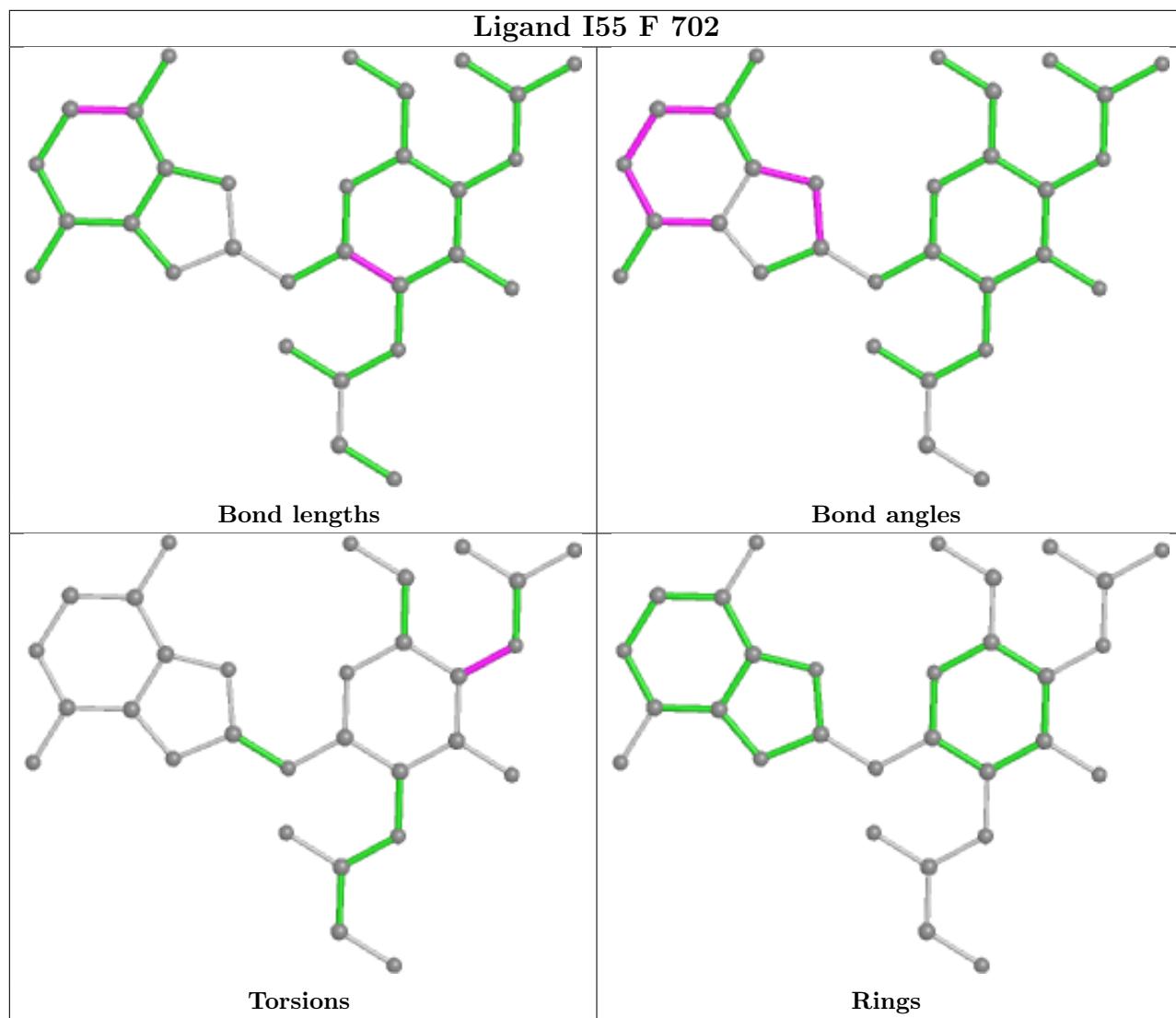
1 monomer is involved in 1 short contact:

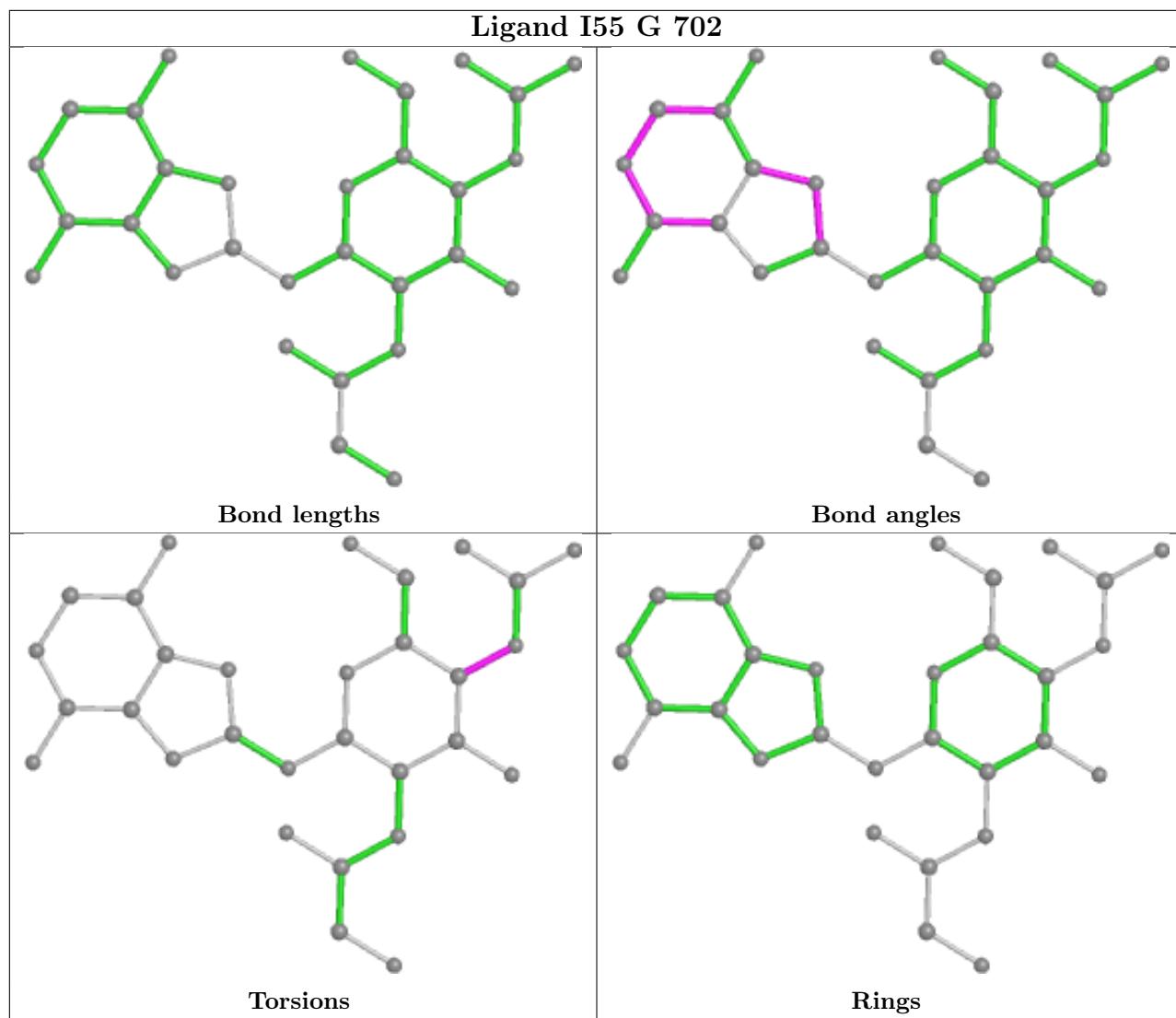
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	FAD	1	0

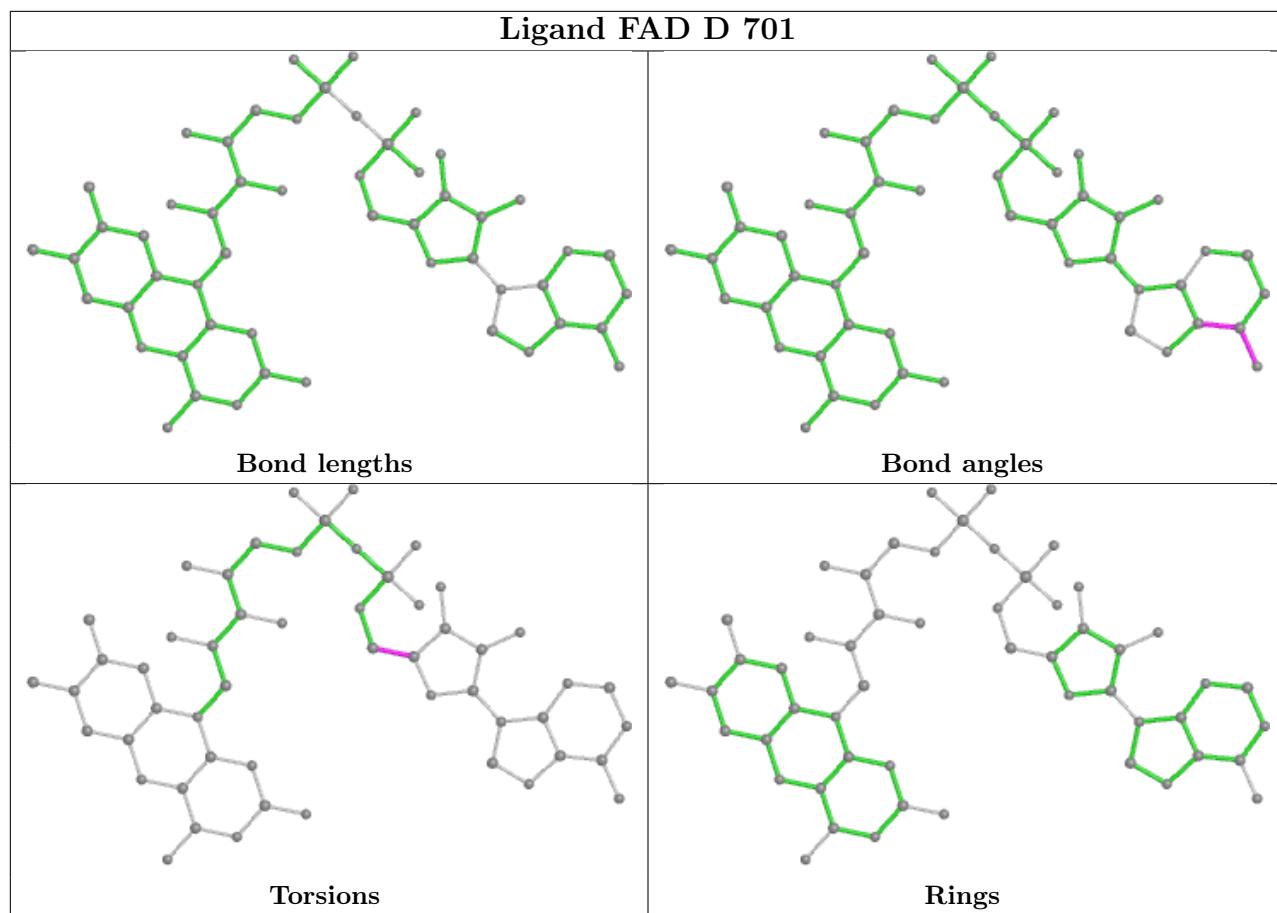
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

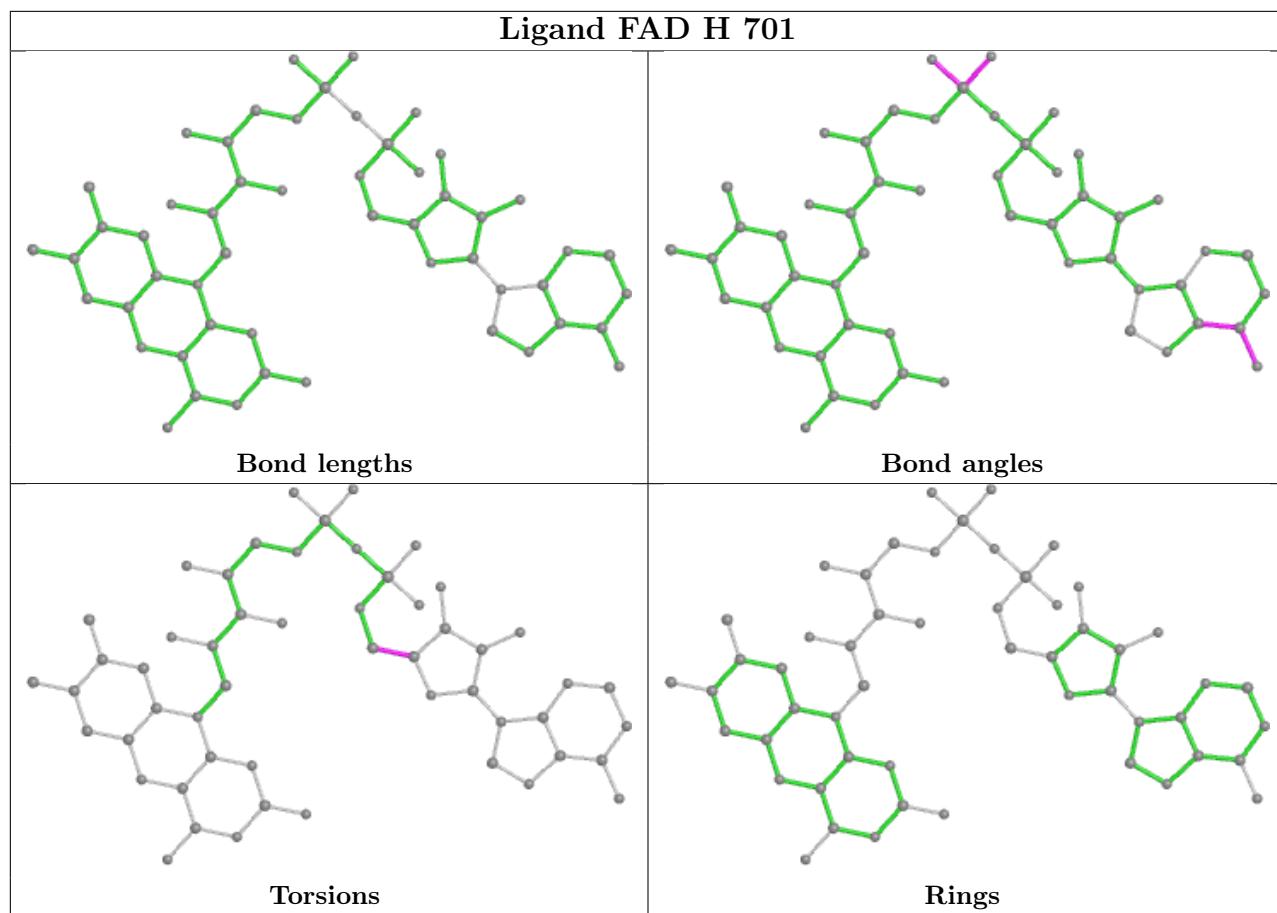


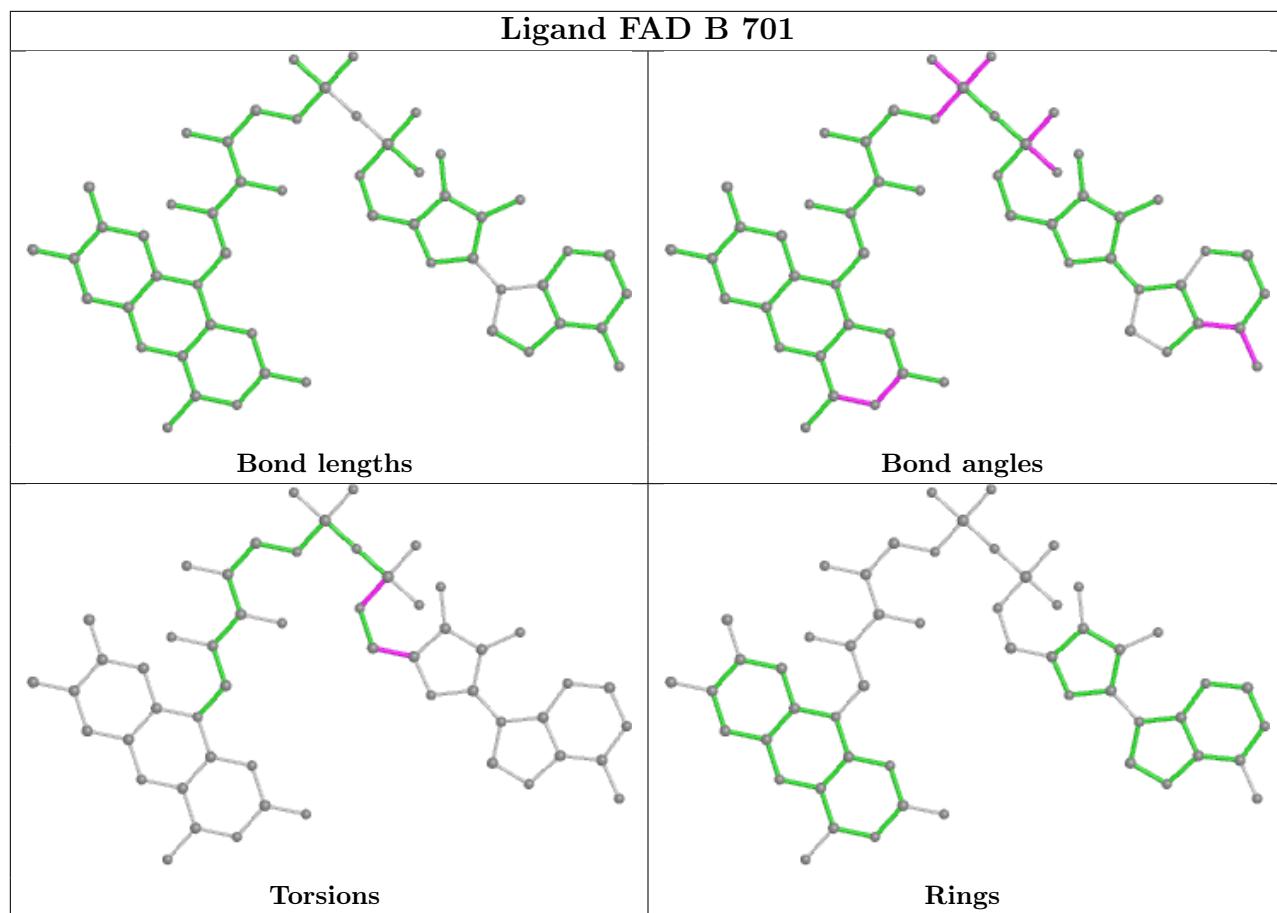


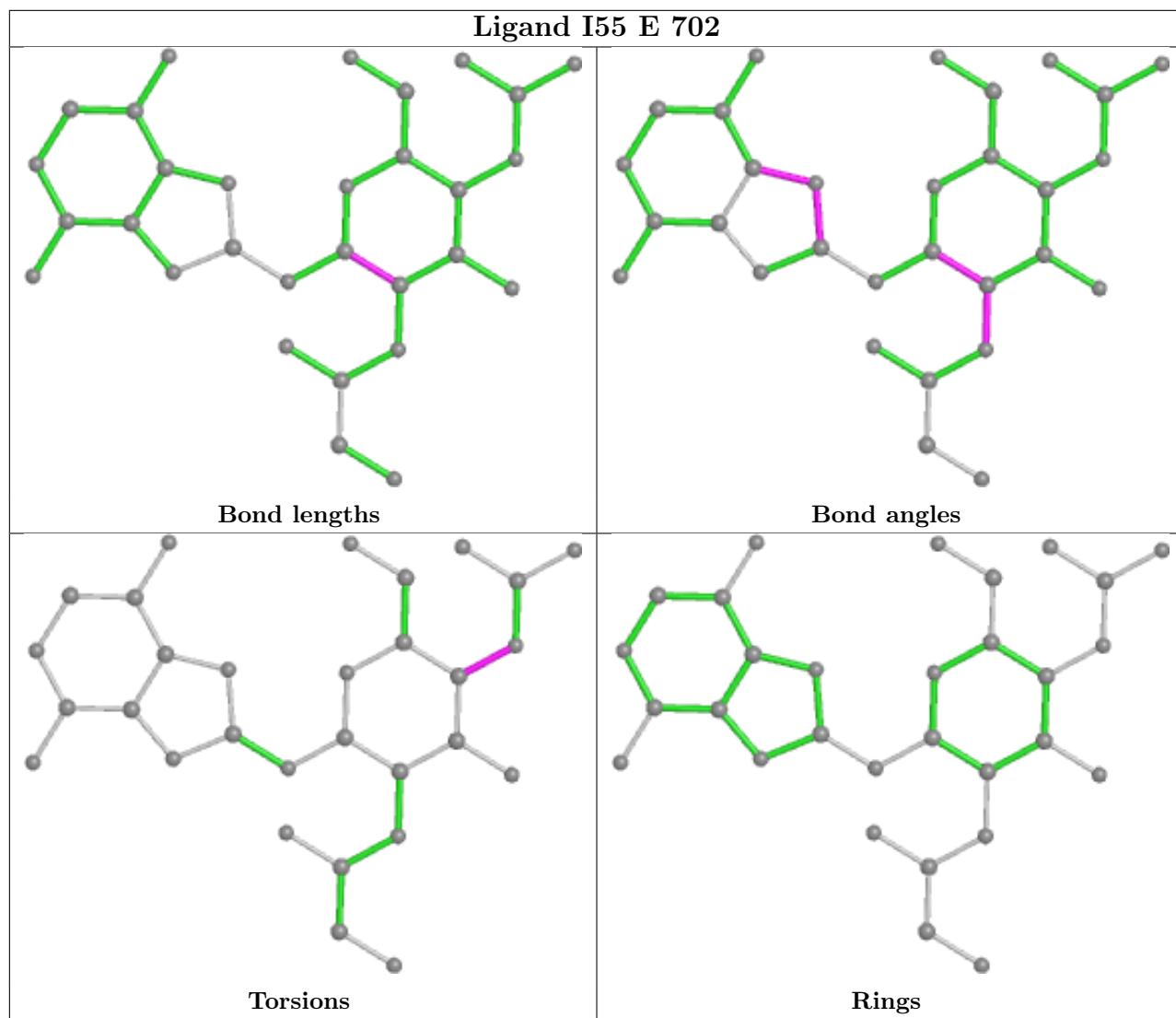


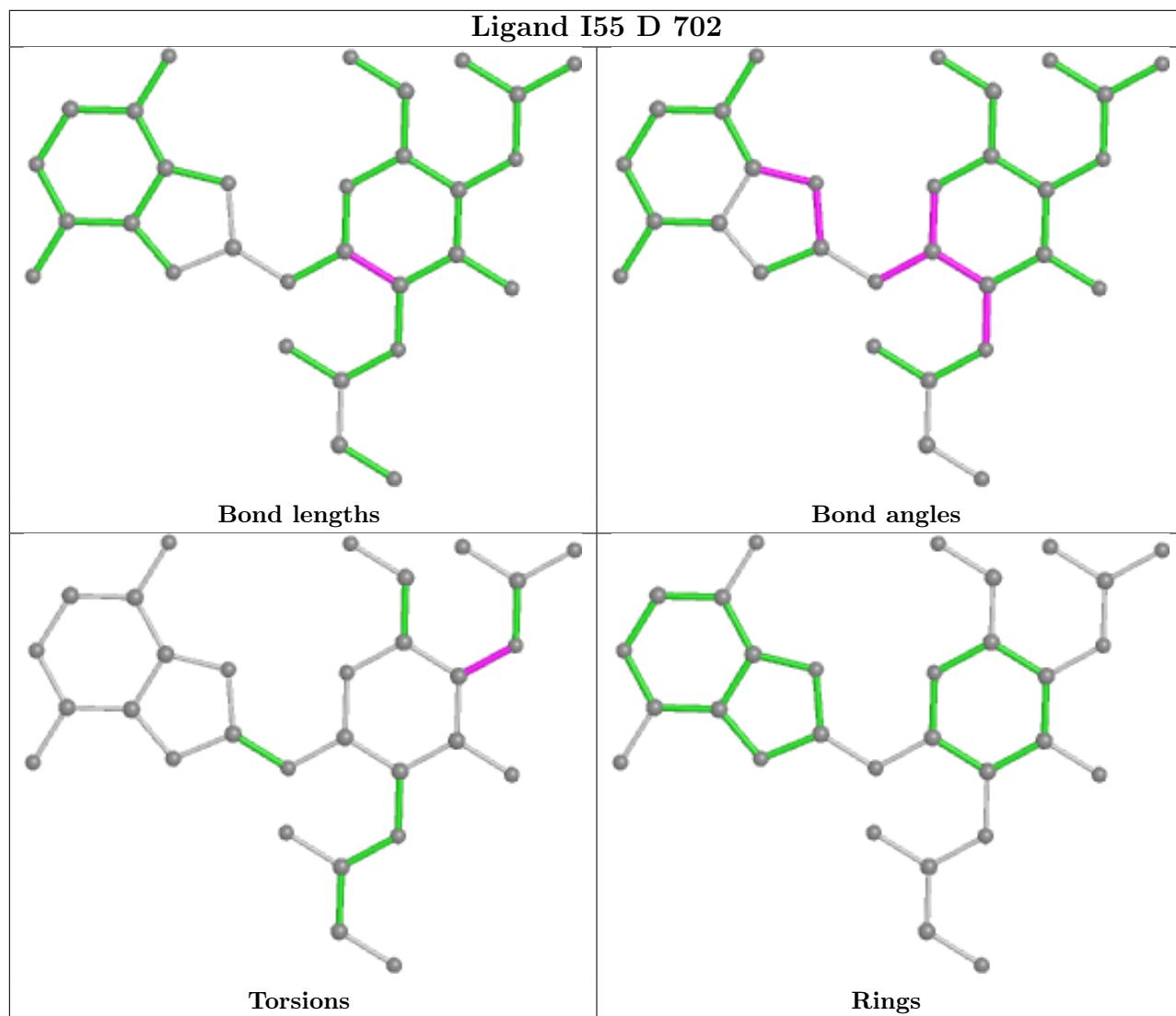


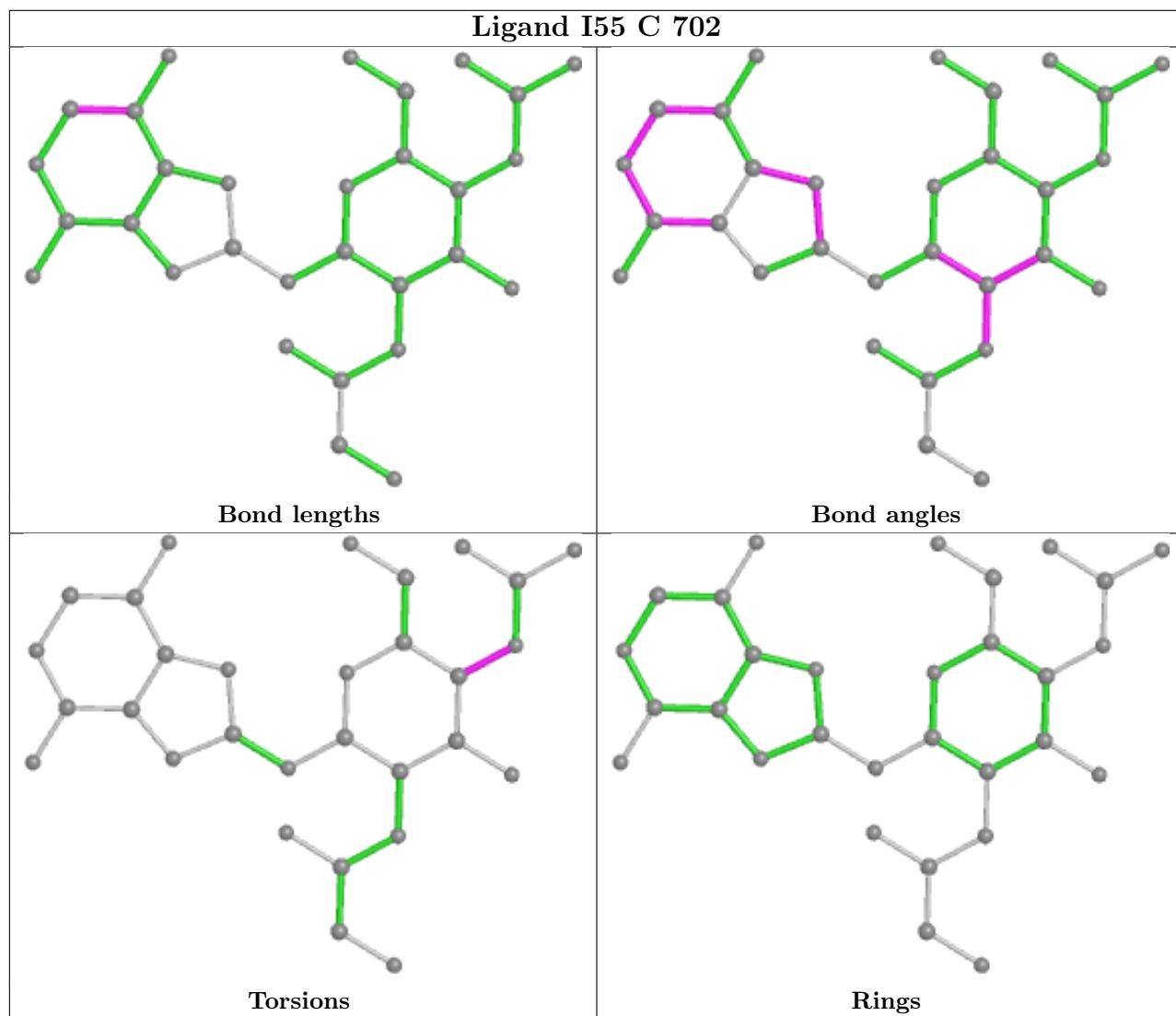


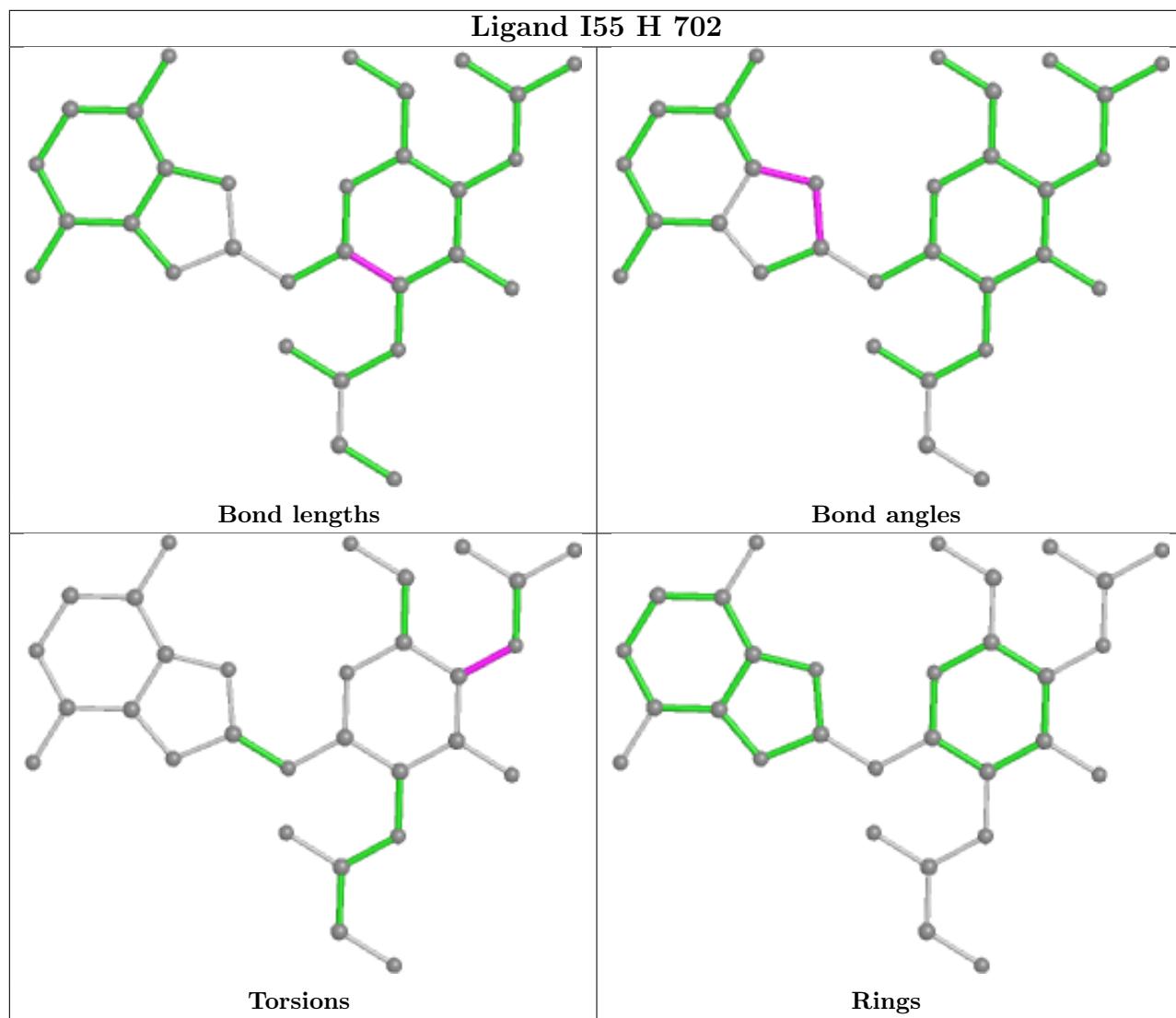


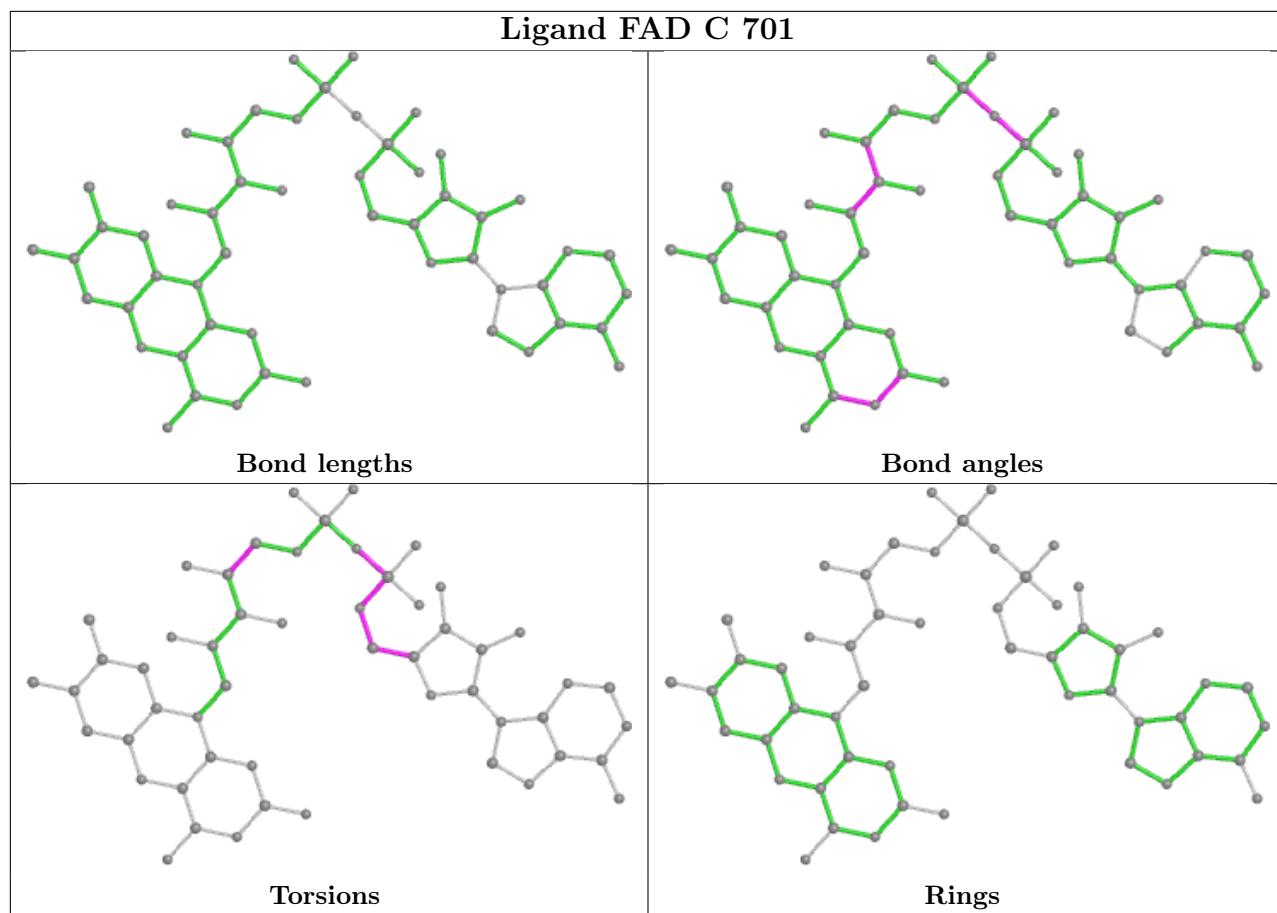


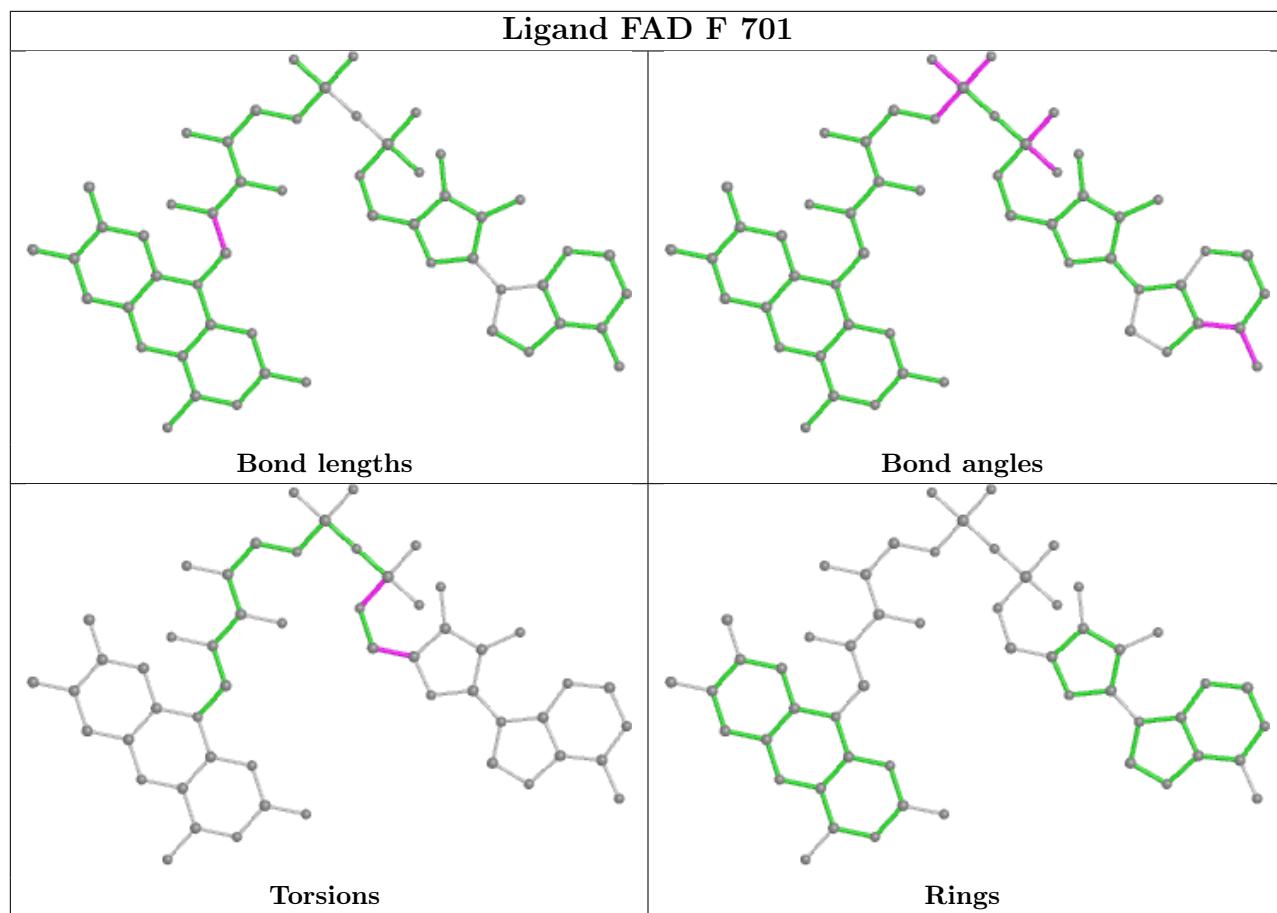


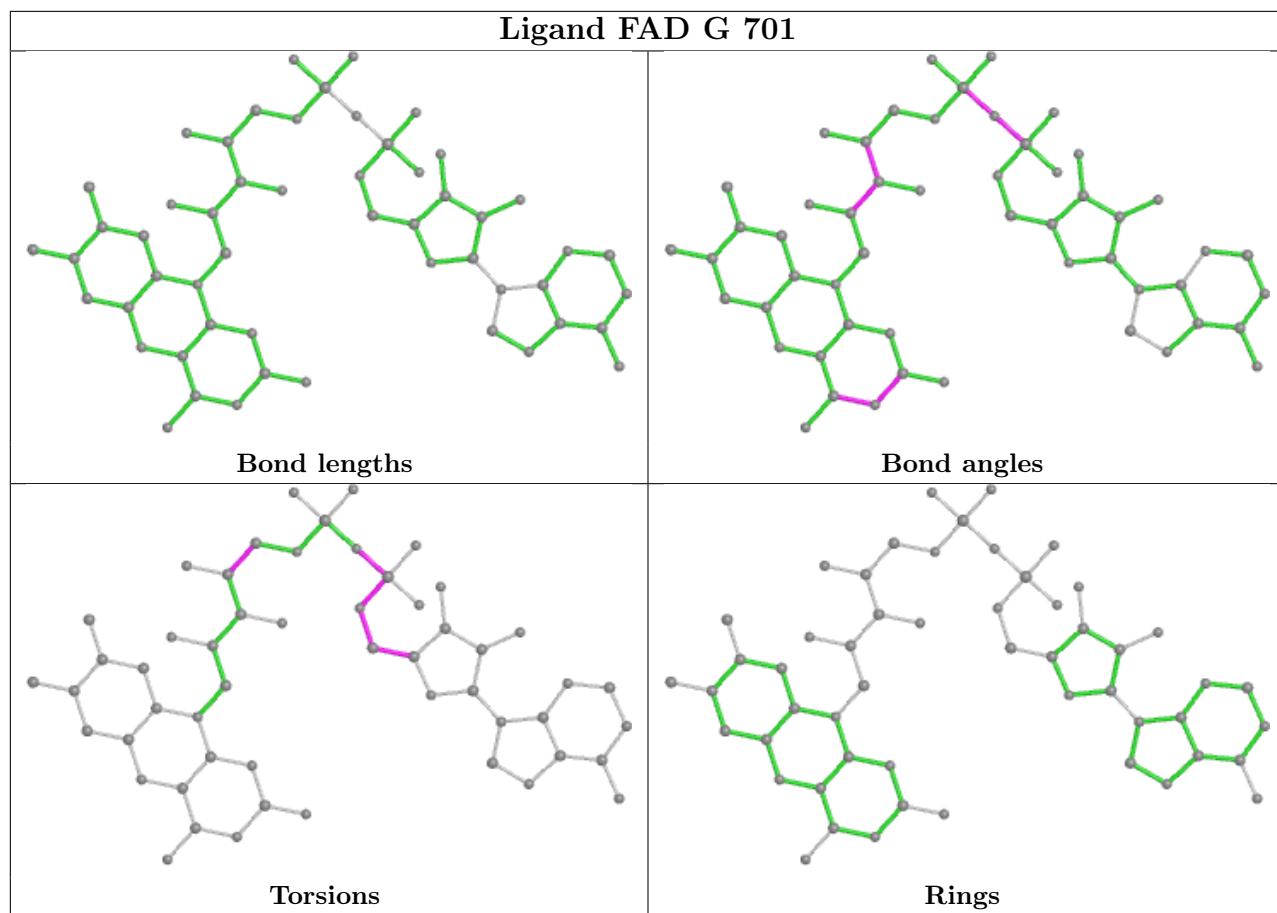


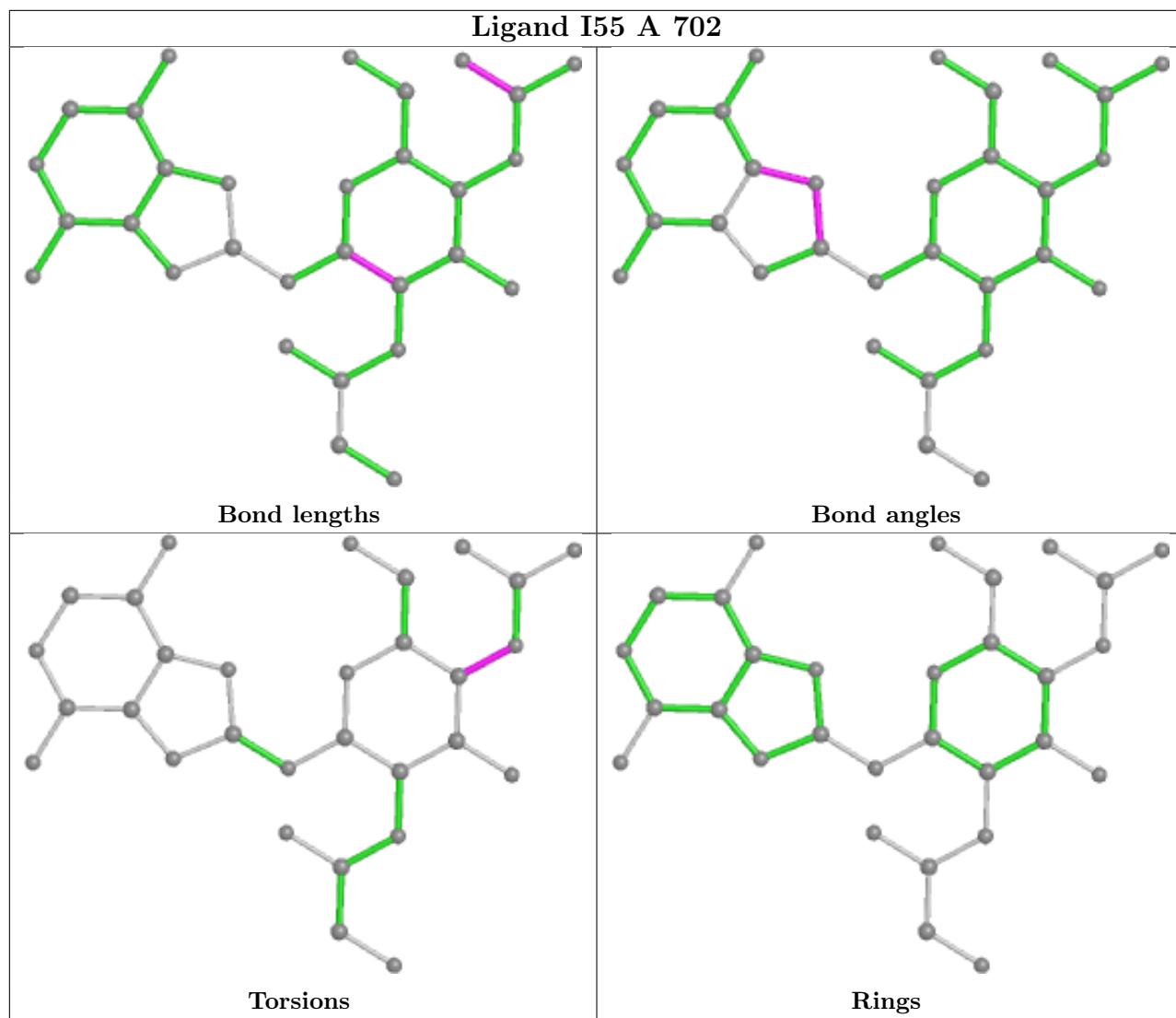


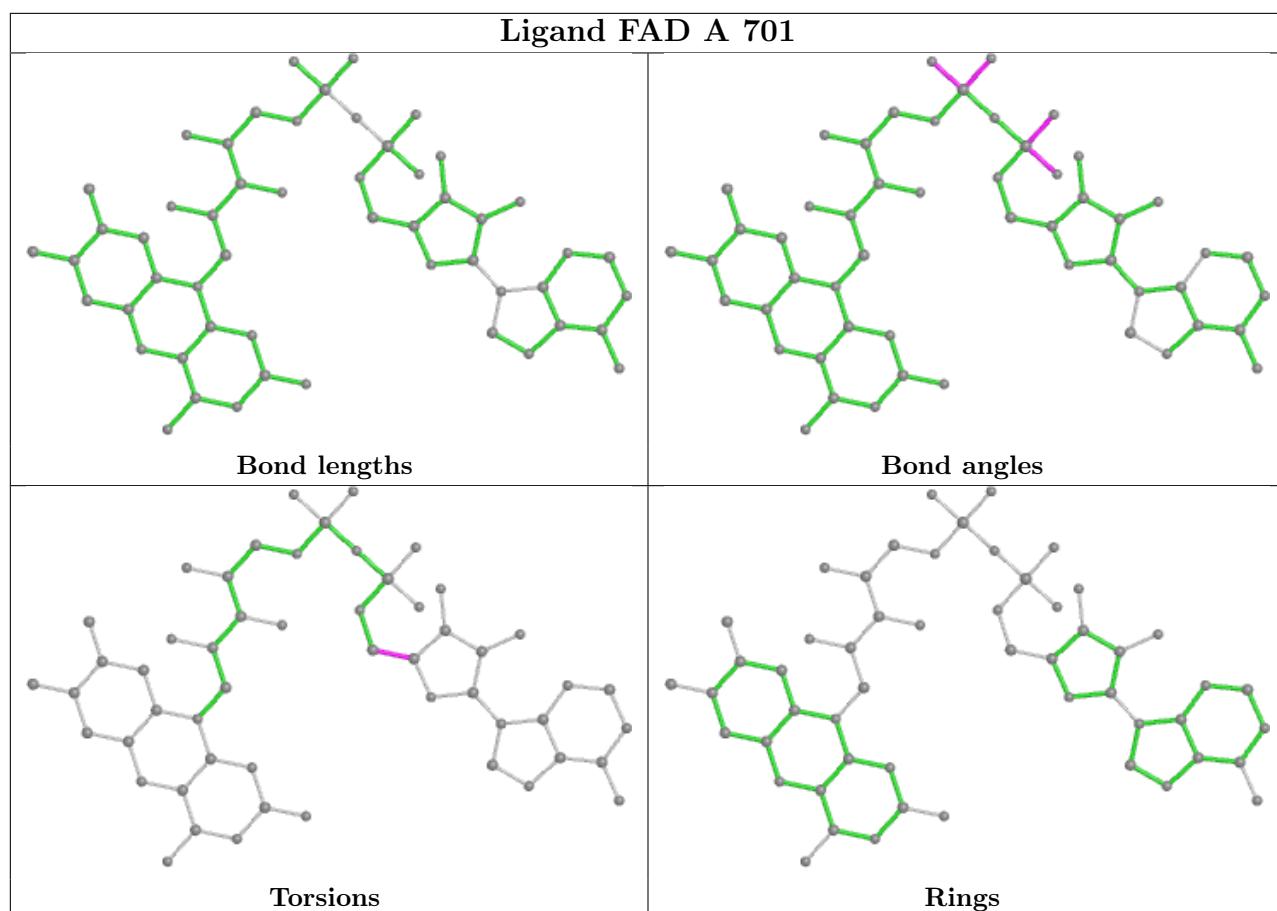












5.7 Other polymers i

There are no such residues in this entry.

5.8 Polymer linkage issues i

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	482/512 (94%)	0.24	5 (1%)	82	80	18, 36, 65, 87
1	B	482/512 (94%)	0.27	11 (2%)	60	58	18, 35, 67, 88
1	C	482/512 (94%)	0.42	14 (2%)	51	50	18, 38, 81, 139
1	D	480/512 (93%)	0.87	74 (15%)	2	1	24, 58, 113, 149
1	E	482/512 (94%)	0.24	4 (0%)	86	84	19, 36, 67, 88
1	F	482/512 (94%)	0.30	8 (1%)	70	68	17, 35, 66, 85
1	G	482/512 (94%)	0.46	21 (4%)	34	33	18, 38, 81, 132
1	H	480/512 (93%)	0.83	66 (13%)	2	2	24, 57, 112, 145
All	All	3852/4096 (94%)	0.46	203 (5%)	26	25	17, 40, 90, 149

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	243	LEU	10.7
1	C	48	TYR	8.7
1	H	209	VAL	7.6
1	D	240	LEU	6.0
1	H	208	ARG	5.6
1	H	483	TYR	5.5
1	C	53	ALA	5.3
1	D	488	ARG	5.2
1	D	224	HIS	5.0
1	H	239	ALA	5.0
1	B	11	THR	5.0
1	G	51	THR	5.0
1	D	392	ASP	4.9
1	D	227	VAL	4.9
1	D	211	GLY	4.8
1	H	212	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	247	ILE	4.8
1	D	206	HIS	4.7
1	G	238	ALA	4.6
1	H	224	HIS	4.6
1	G	368	ARG	4.5
1	H	211	GLY	4.4
1	H	397	PHE	4.4
1	C	47	GLN	4.4
1	D	236	LEU	4.3
1	H	225	VAL	4.3
1	H	33	ARG	4.2
1	H	236	LEU	4.2
1	E	70	ALA	4.2
1	H	202	ILE	4.1
1	H	398	ARG	4.1
1	G	48	TYR	4.1
1	H	361	TRP	4.1
1	H	217	GLY	4.0
1	D	243	LEU	4.0
1	H	206	HIS	4.0
1	H	237	VAL	4.0
1	G	204	ALA	3.9
1	D	204	ALA	3.9
1	C	45	ALA	3.8
1	D	241	PRO	3.8
1	D	387	GLY	3.7
1	H	454	LEU	3.6
1	D	200	THR	3.6
1	H	240	LEU	3.6
1	H	479	LEU	3.6
1	D	30	ALA	3.6
1	D	490	TRP	3.6
1	D	225	VAL	3.6
1	G	50	ALA	3.5
1	H	34	PRO	3.5
1	H	207	GLY	3.5
1	G	240	LEU	3.5
1	D	33	ARG	3.5
1	D	394	LEU	3.4
1	G	47	GLN	3.4
1	G	46	ARG	3.4
1	D	355	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	394	LEU	3.3
1	D	397	PHE	3.2
1	D	217	GLY	3.2
1	D	210	GLU	3.2
1	D	404	ILE	3.2
1	C	46	ARG	3.2
1	H	458	TYR	3.2
1	H	358	GLU	3.1
1	D	242	GLY	3.1
1	D	203	ARG	3.1
1	C	363	LEU	3.1
1	H	389	THR	3.1
1	G	52	PRO	3.1
1	D	13	VAL	3.1
1	H	391	VAL	3.1
1	H	242	GLY	3.1
1	H	402	ASP	3.1
1	C	49	GLY	3.1
1	H	360	LEU	3.1
1	G	45	ALA	3.0
1	D	486	VAL	3.0
1	C	50	ALA	3.0
1	H	49	GLY	3.0
1	D	400	GLU	3.0
1	D	359	GLY	3.0
1	H	235	ARG	3.0
1	D	37	ARG	2.9
1	D	395	ARG	2.9
1	A	73	HIS	2.9
1	D	489	GLU	2.8
1	G	218	ASP	2.8
1	C	365	GLY	2.8
1	D	235	ARG	2.8
1	D	398	ARG	2.8
1	H	480	ILE	2.8
1	E	36	VAL	2.8
1	G	54	ALA	2.8
1	D	491	HIS	2.8
1	D	464	LEU	2.8
1	D	386	ASP	2.8
1	H	241	PRO	2.8
1	D	219	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	202	ILE	2.7
1	D	363	LEU	2.7
1	D	208	ARG	2.7
1	D	79	ALA	2.7
1	H	219	PHE	2.7
1	H	220	LEU	2.7
1	D	218	ASP	2.7
1	H	226	VAL	2.7
1	C	51	THR	2.7
1	B	395	ARG	2.7
1	H	395	ARG	2.7
1	E	217	GLY	2.7
1	D	352	ILE	2.6
1	H	357	VAL	2.6
1	C	223	GLY	2.6
1	H	37	ARG	2.6
1	E	393	GLY	2.6
1	F	491	HIS	2.6
1	A	488	ARG	2.5
1	D	228	ALA	2.5
1	D	391	VAL	2.5
1	D	362	MET	2.5
1	H	376	LEU	2.5
1	D	100	THR	2.5
1	F	406	ALA	2.5
1	G	220	LEU	2.5
1	H	193	ARG	2.5
1	H	491	HIS	2.5
1	G	202	ILE	2.5
1	G	399	PRO	2.4
1	H	450	LEU	2.4
1	D	353	GLY	2.4
1	B	76	LYS	2.4
1	H	14	ILE	2.4
1	B	415	ASP	2.4
1	D	479	LEU	2.4
1	D	245	HIS	2.3
1	D	209	VAL	2.3
1	F	34	PRO	2.3
1	H	362	MET	2.3
1	A	406	ALA	2.3
1	G	242	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	133	LEU	2.3
1	B	440	GLU	2.3
1	D	354	GLY	2.3
1	H	203	ARG	2.3
1	D	393	GLY	2.3
1	A	101	ALA	2.3
1	C	197	VAL	2.3
1	D	401	ARG	2.3
1	H	400	GLU	2.3
1	F	76	LYS	2.2
1	D	12	ASP	2.2
1	H	238	ALA	2.2
1	H	451	ALA	2.2
1	D	38	VAL	2.2
1	D	194	LEU	2.2
1	D	250	ILE	2.2
1	H	352	ILE	2.2
1	H	248	PRO	2.2
1	H	282	GLY	2.2
1	H	488	ARG	2.2
1	D	213	VAL	2.2
1	B	393	GLY	2.2
1	G	200	THR	2.2
1	H	39	THR	2.2
1	B	70	ALA	2.1
1	D	304	GLU	2.1
1	F	349	PHE	2.1
1	H	387	GLY	2.1
1	H	35	ASP	2.1
1	H	452	ASP	2.1
1	D	226	VAL	2.1
1	D	244	ALA	2.1
1	F	483	TYR	2.1
1	B	399	PRO	2.1
1	D	220	LEU	2.1
1	D	360	LEU	2.1
1	H	216	ASP	2.1
1	B	149	GLU	2.1
1	G	367	TYR	2.1
1	H	43	LYS	2.1
1	D	382	VAL	2.1
1	D	14	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	349	PHE	2.1
1	D	462	ALA	2.0
1	G	355	THR	2.0
1	G	206	HIS	2.0
1	A	10	GLN	2.0
1	D	365	GLY	2.0
1	H	349	PHE	2.0
1	D	88	TRP	2.0
1	C	206	HIS	2.0
1	D	285	LEU	2.0
1	F	488	ARG	2.0
1	F	414	ASP	2.0
1	H	439[A]	MET	2.0
1	H	474	GLU	2.0
1	H	490	TRP	2.0
1	C	214	THR	2.0
1	B	27	VAL	2.0
1	D	223	GLY	2.0
1	D	482	TYR	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.

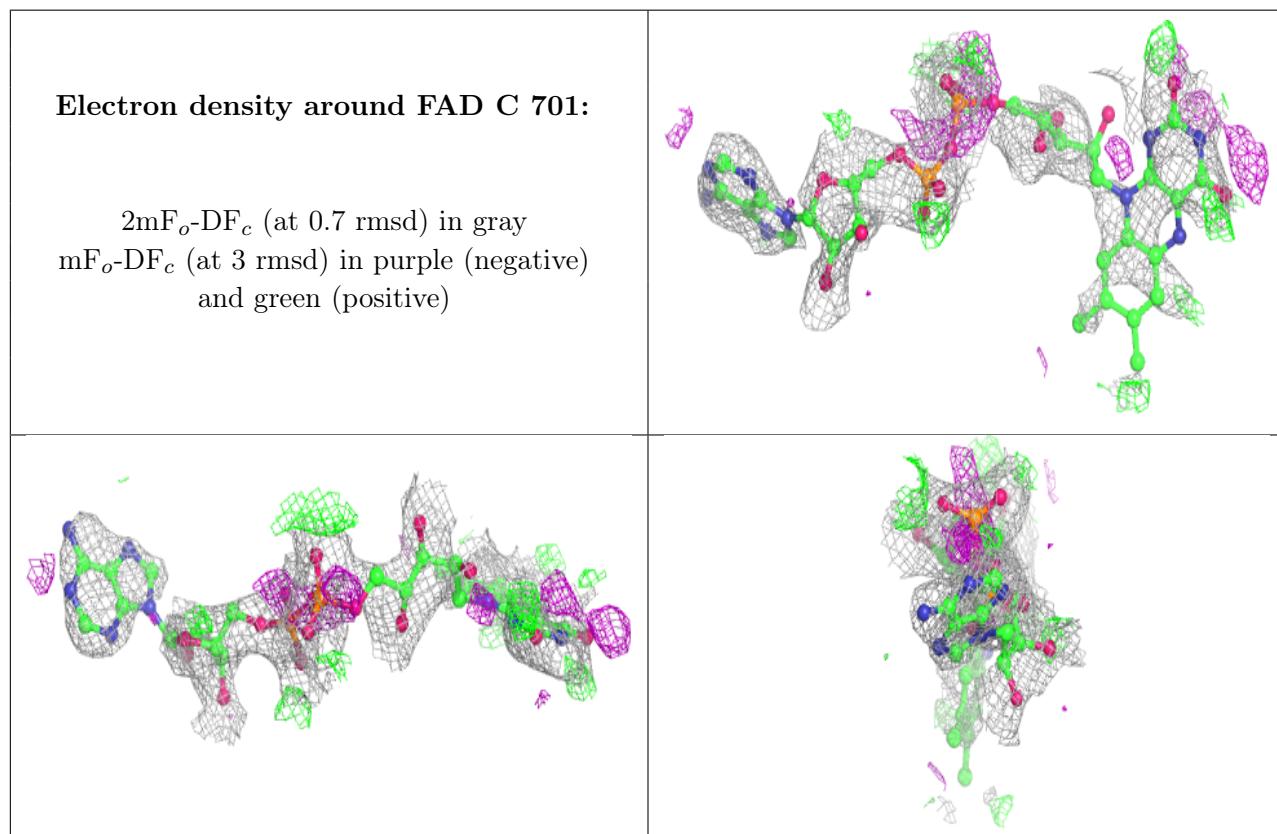
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	C	701	53/53	0.63	0.37	67,103,123,127	0
2	FAD	G	701	53/53	0.74	0.27	62,104,121,125	0
3	I55	A	702	30/30	0.87	0.18	25,35,49,50	0
3	I55	H	702	30/30	0.87	0.22	36,41,69,71	0

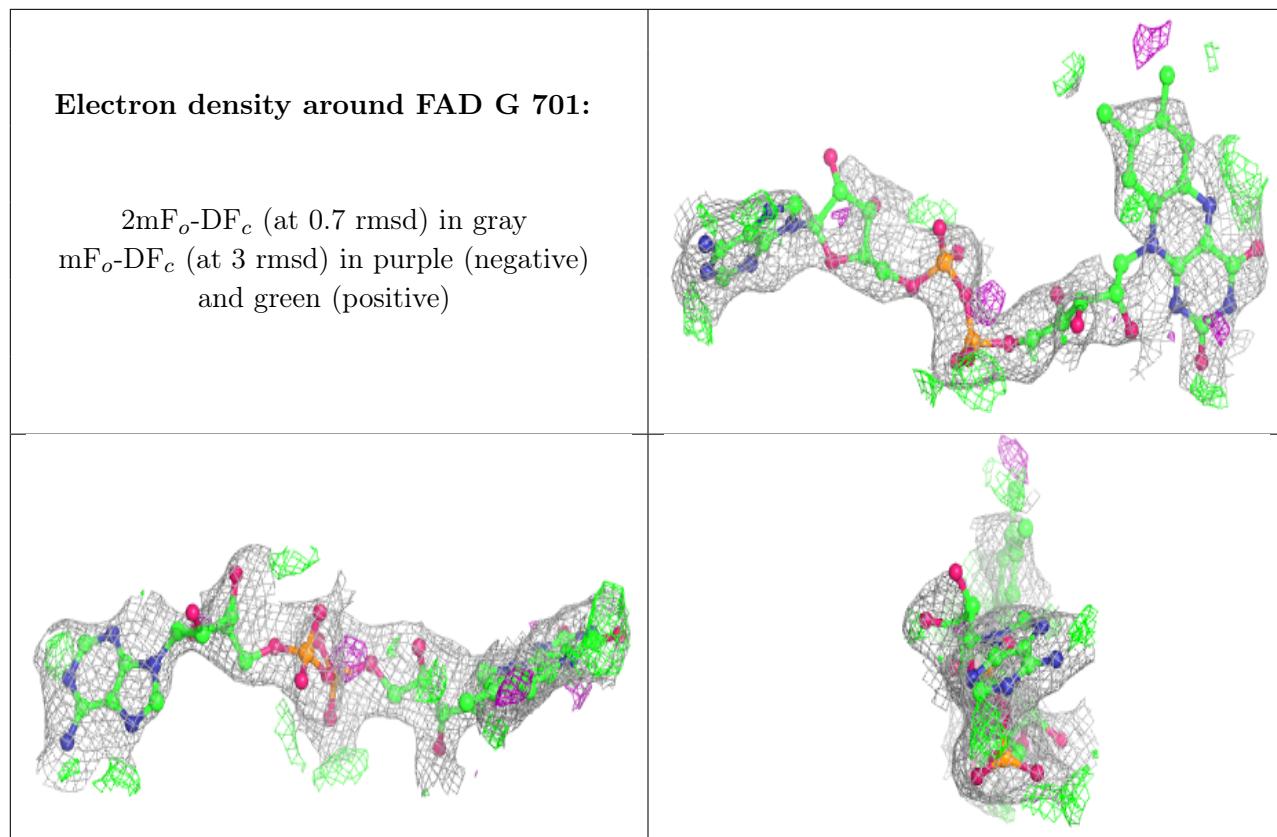
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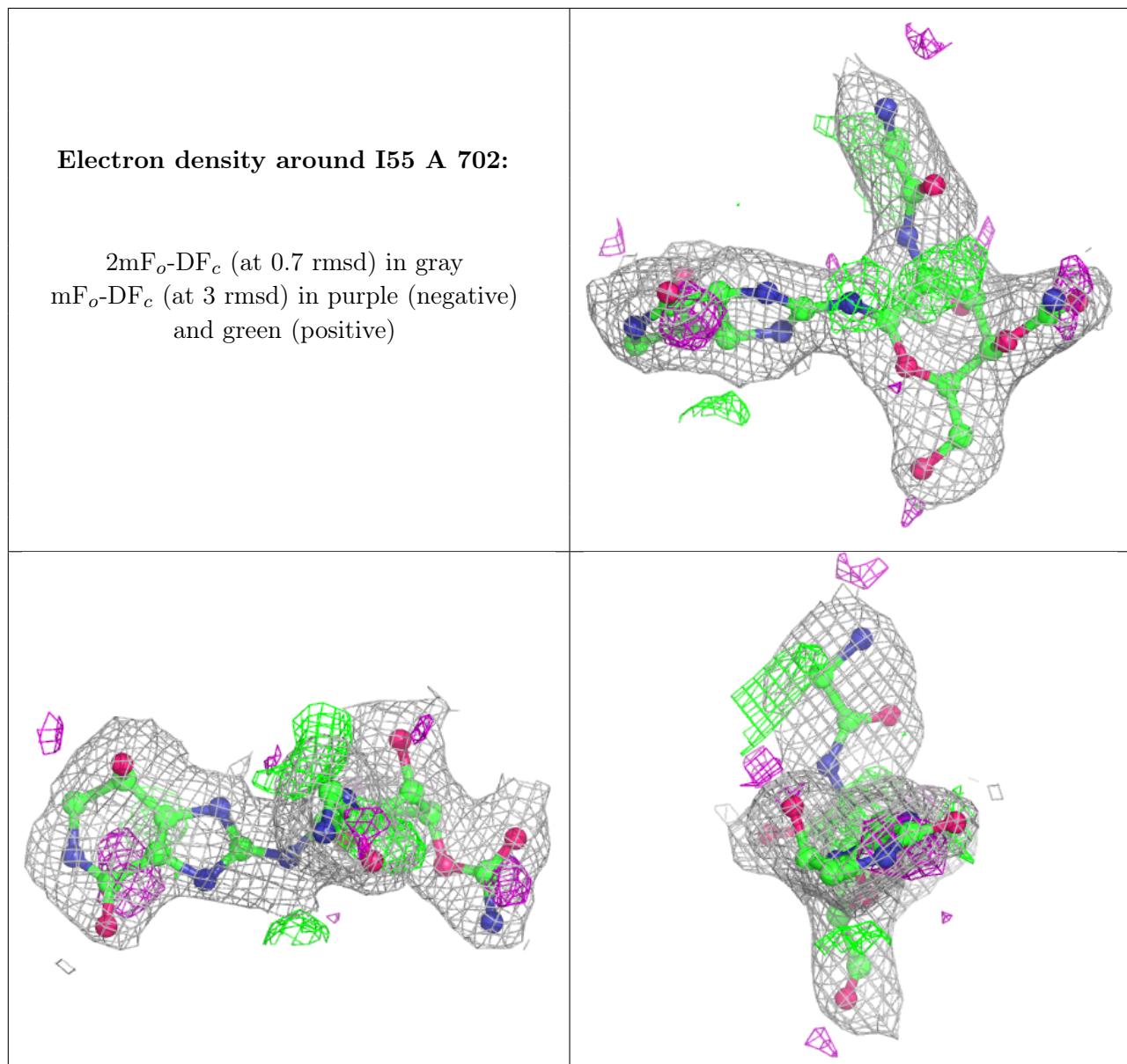
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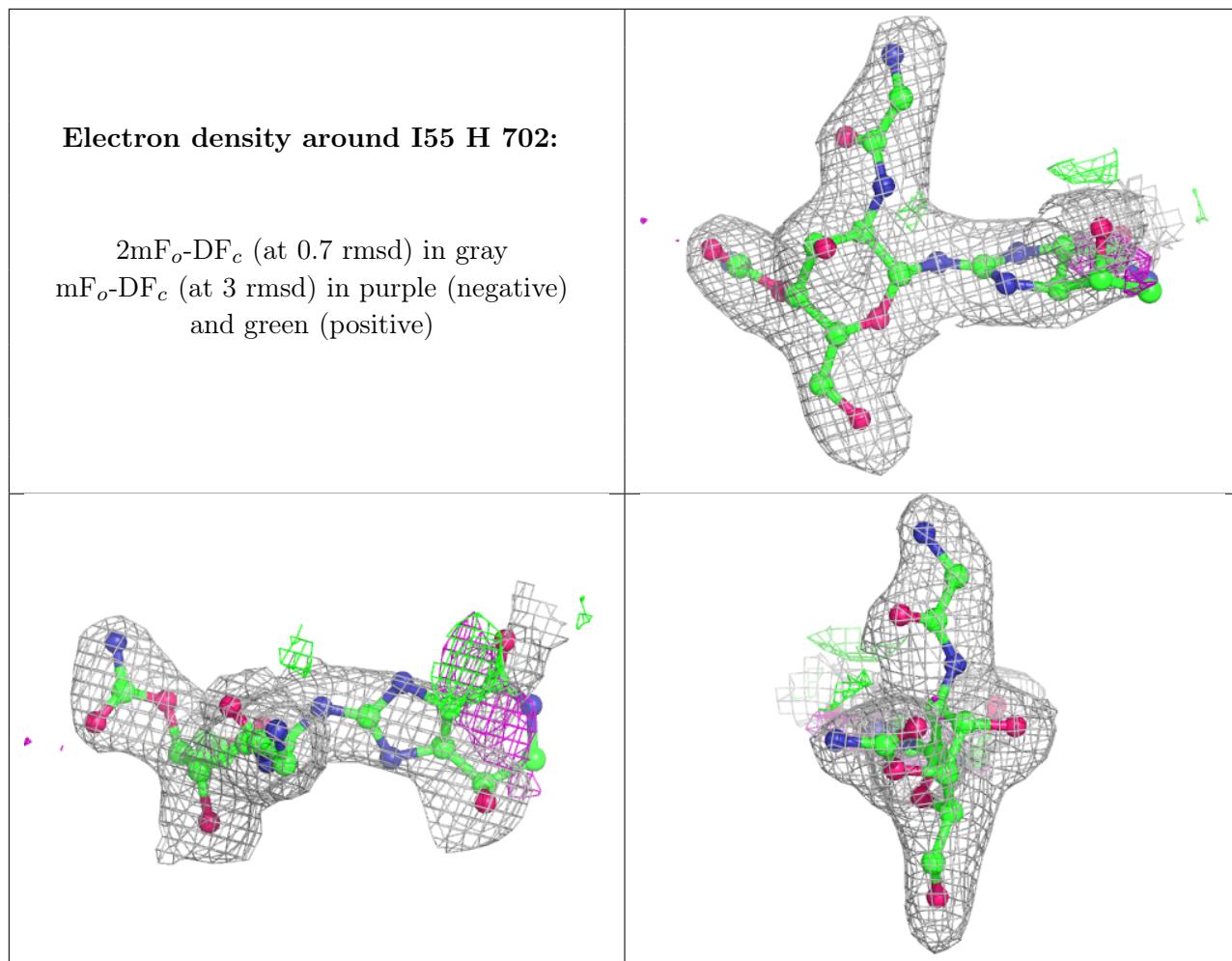
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	H	701	53/53	0.88	0.20	50,66,86,88	0
3	I55	C	702	30/30	0.90	0.18	31,40,64,66	0
2	FAD	D	701	53/53	0.90	0.15	51,68,80,83	0
3	I55	F	702	30/30	0.91	0.21	32,39,60,63	0
3	I55	B	702	30/30	0.92	0.16	30,39,58,59	0
3	I55	D	702	30/30	0.93	0.15	34,40,70,73	0
3	I55	E	702	30/30	0.93	0.18	25,33,49,50	0
2	FAD	F	701	53/53	0.94	0.14	23,27,32,34	0
2	FAD	B	701	53/53	0.94	0.16	23,28,34,35	0
2	FAD	A	701	53/53	0.95	0.14	25,28,32,35	0
3	I55	G	702	30/30	0.95	0.16	29,38,62,65	0
2	FAD	E	701	53/53	0.95	0.15	24,28,31,33	0

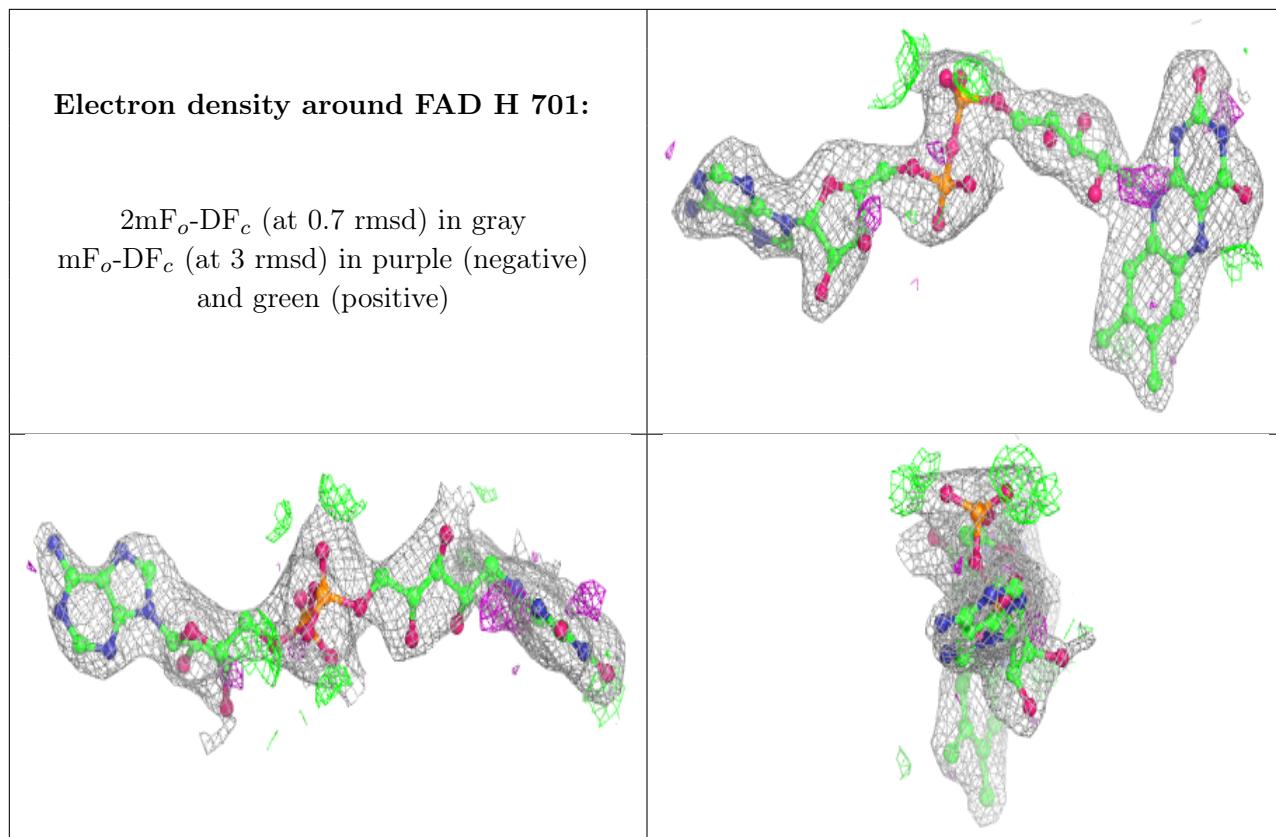
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

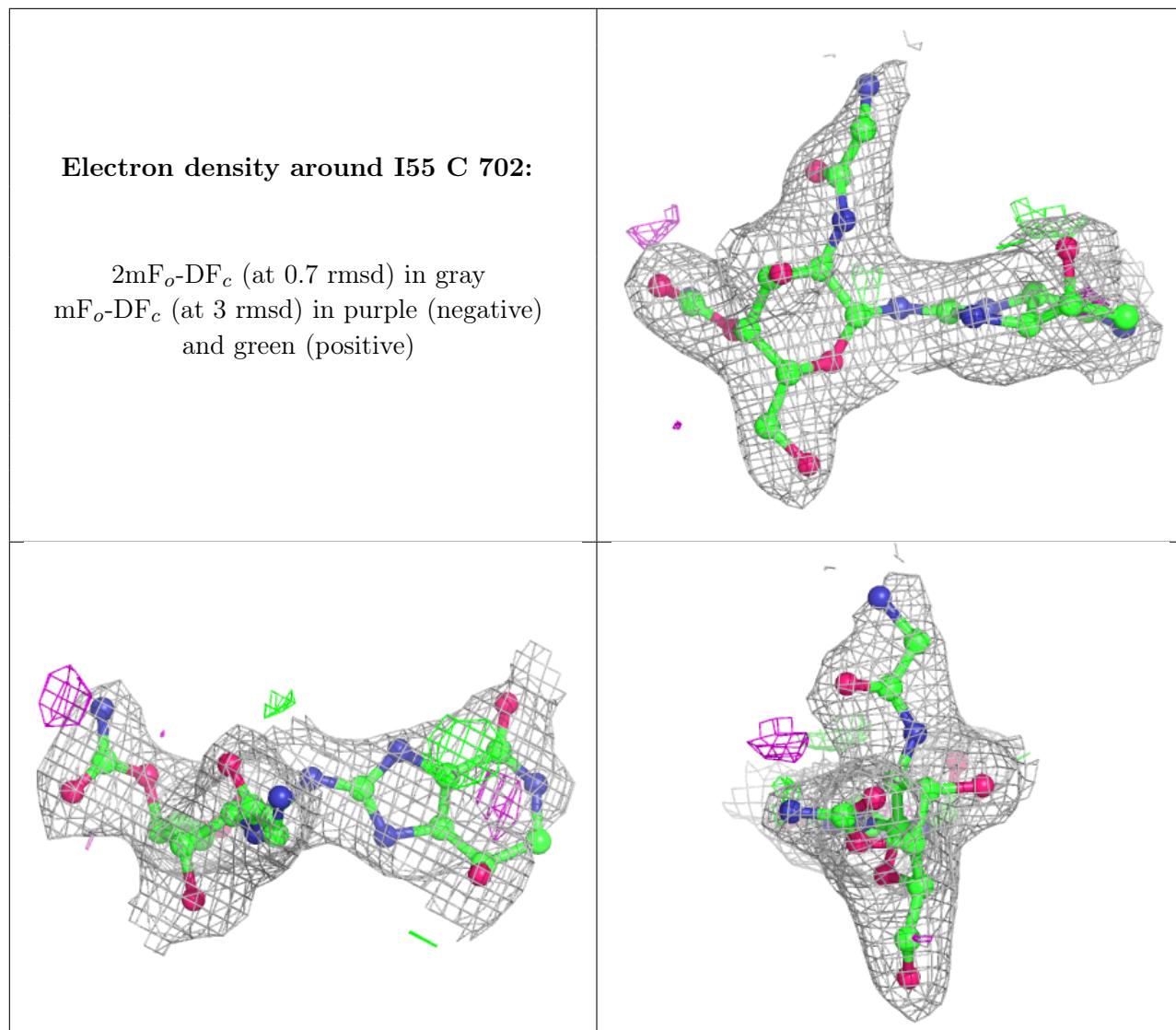


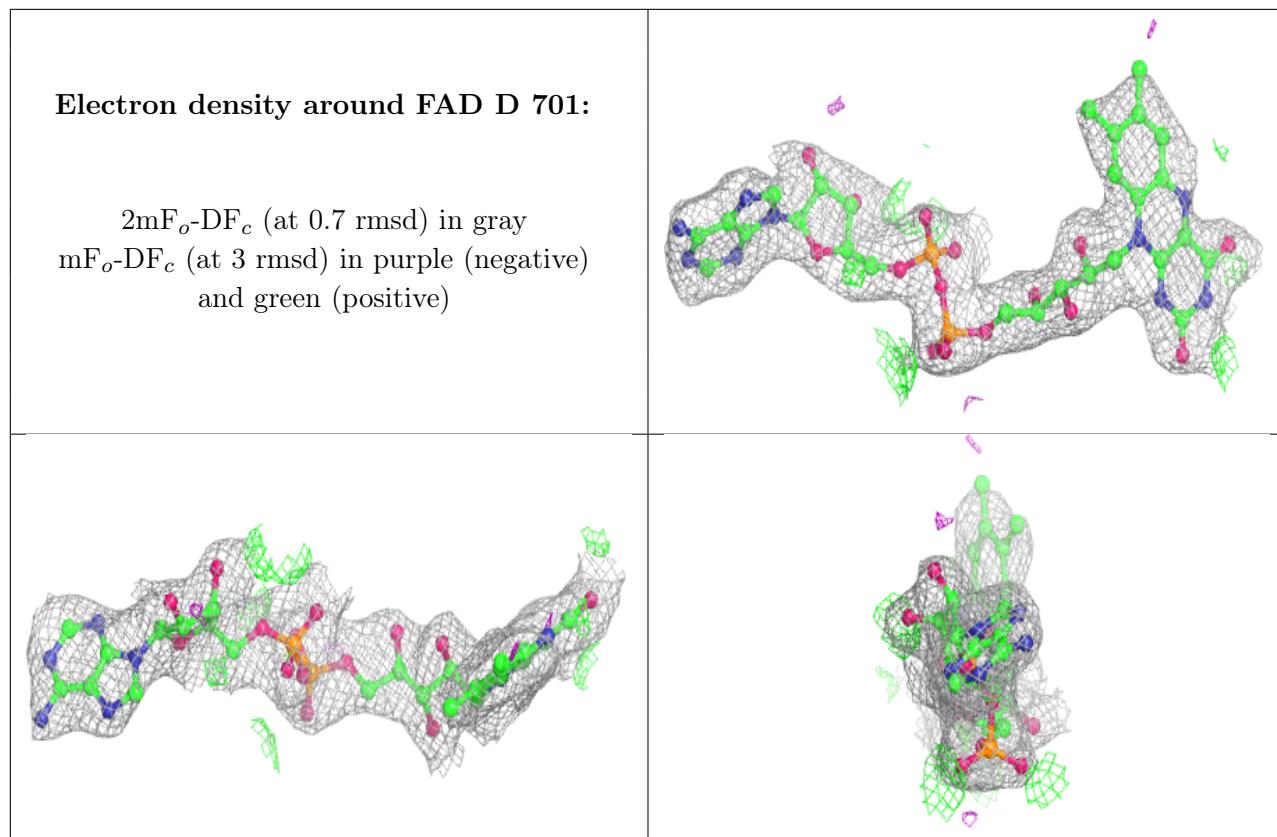


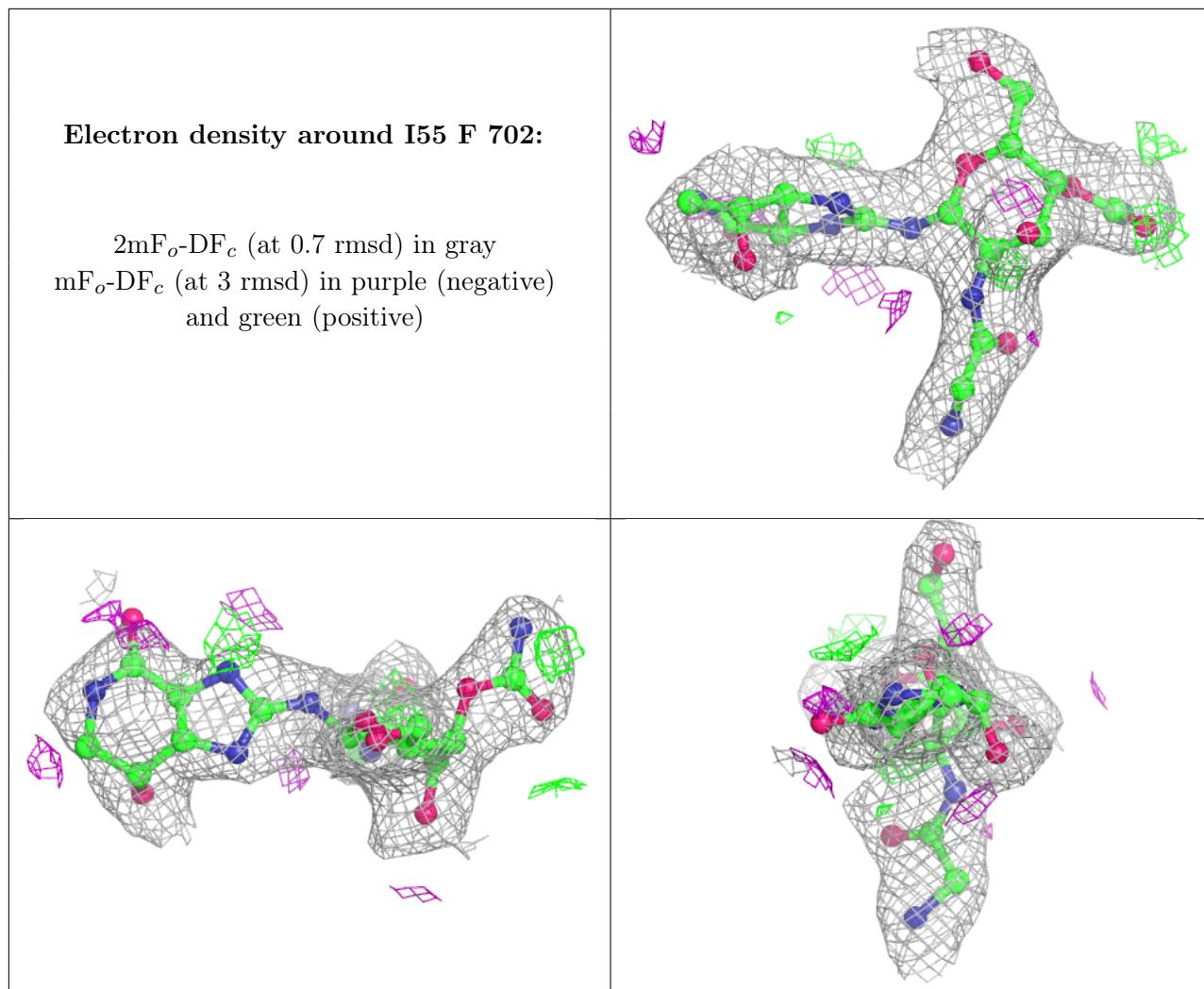


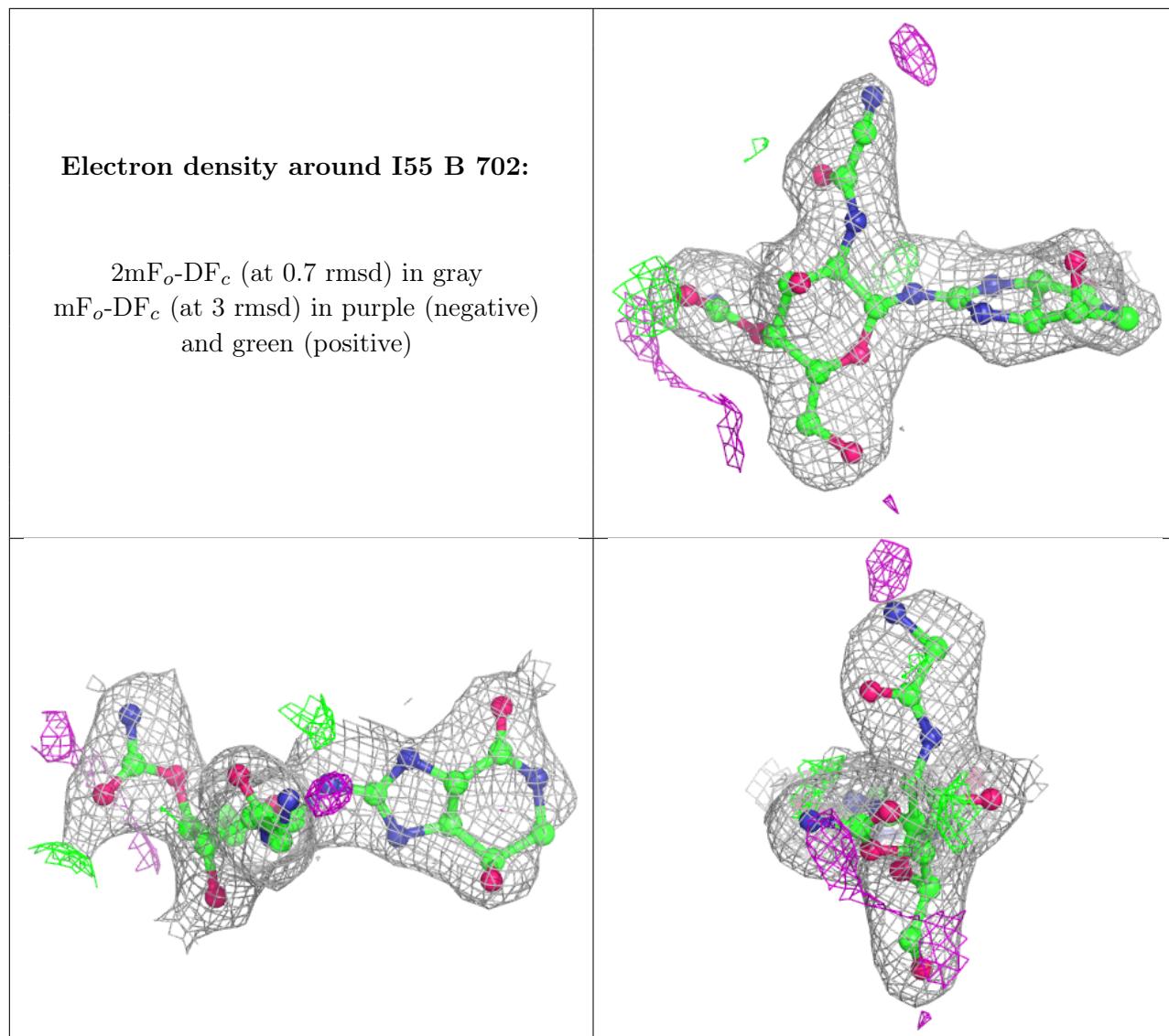


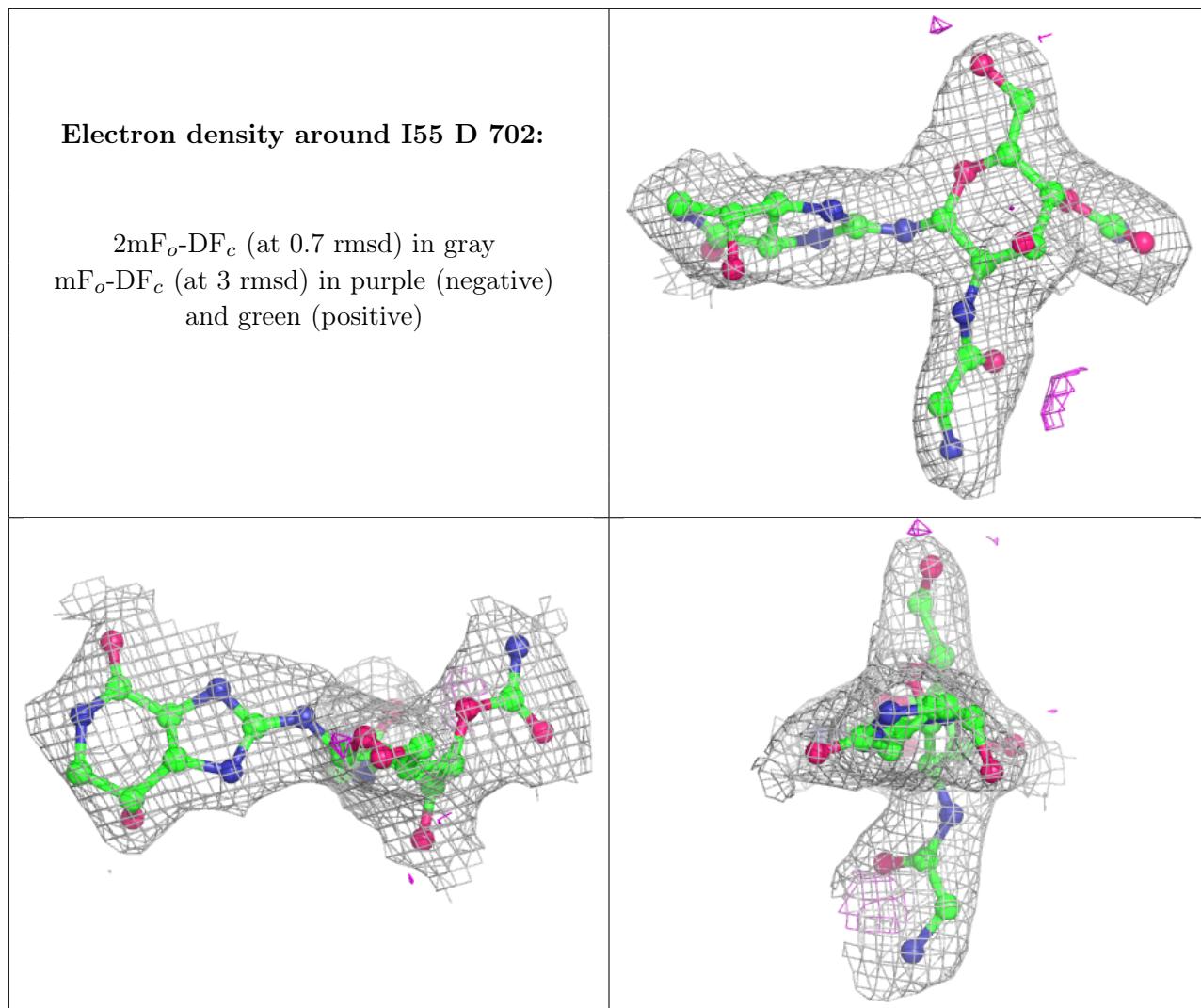


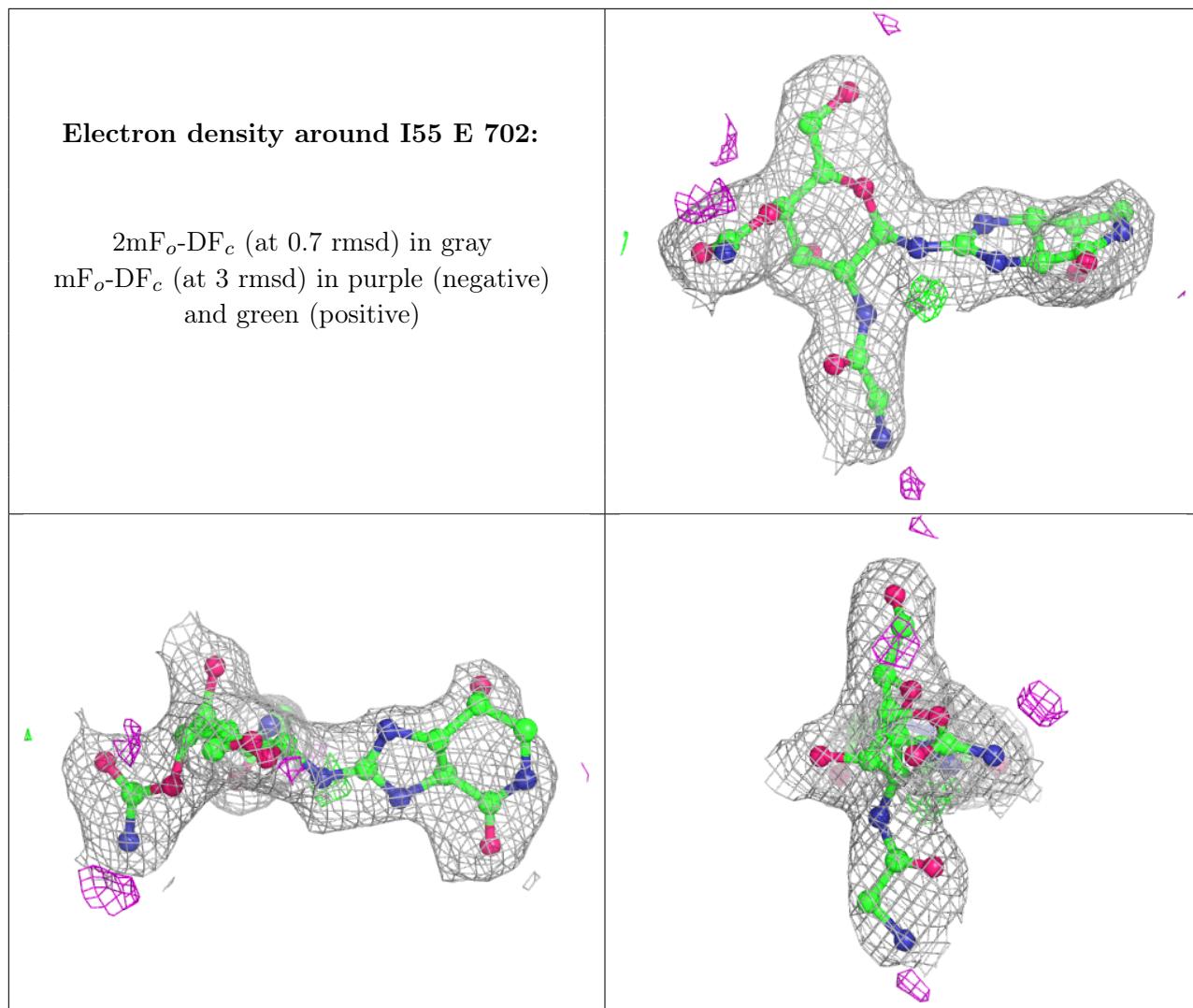


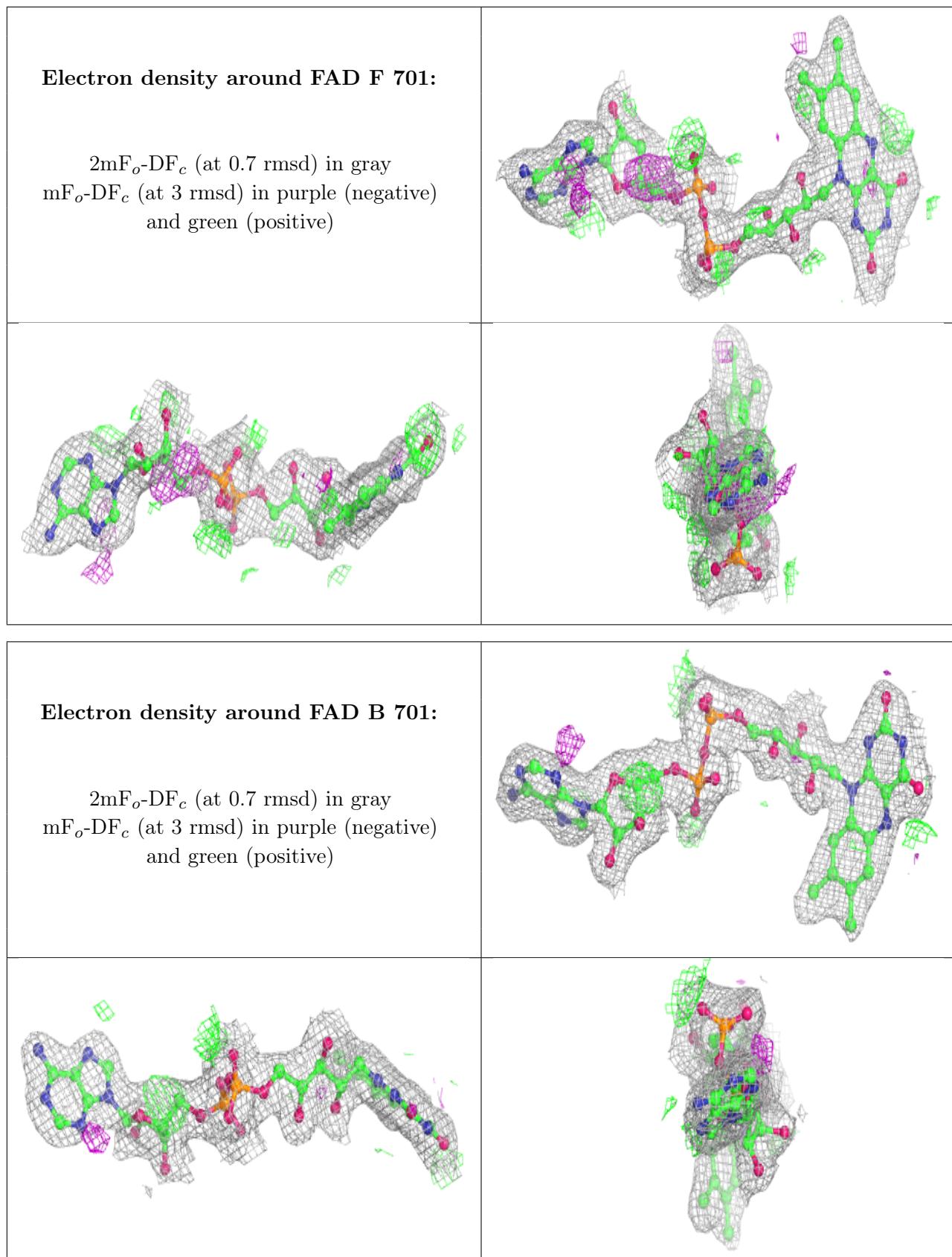


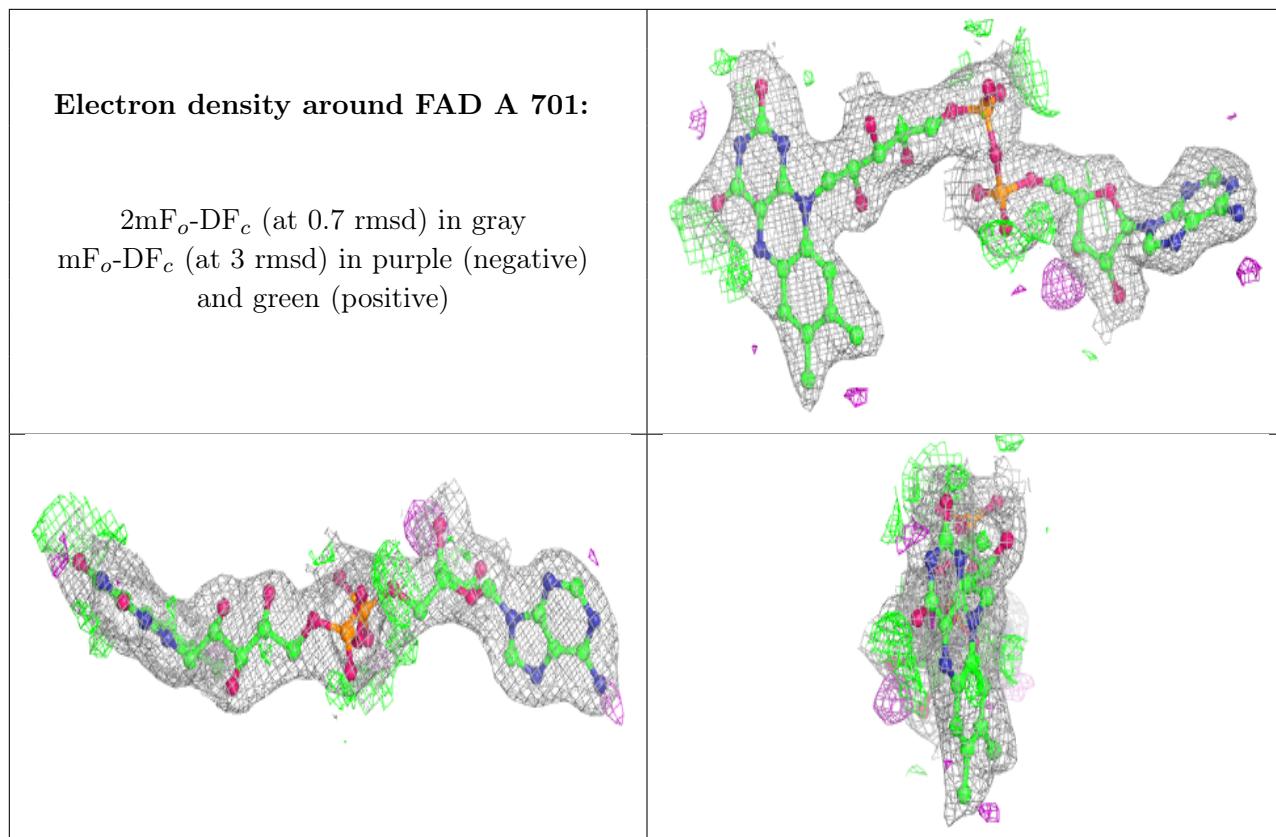


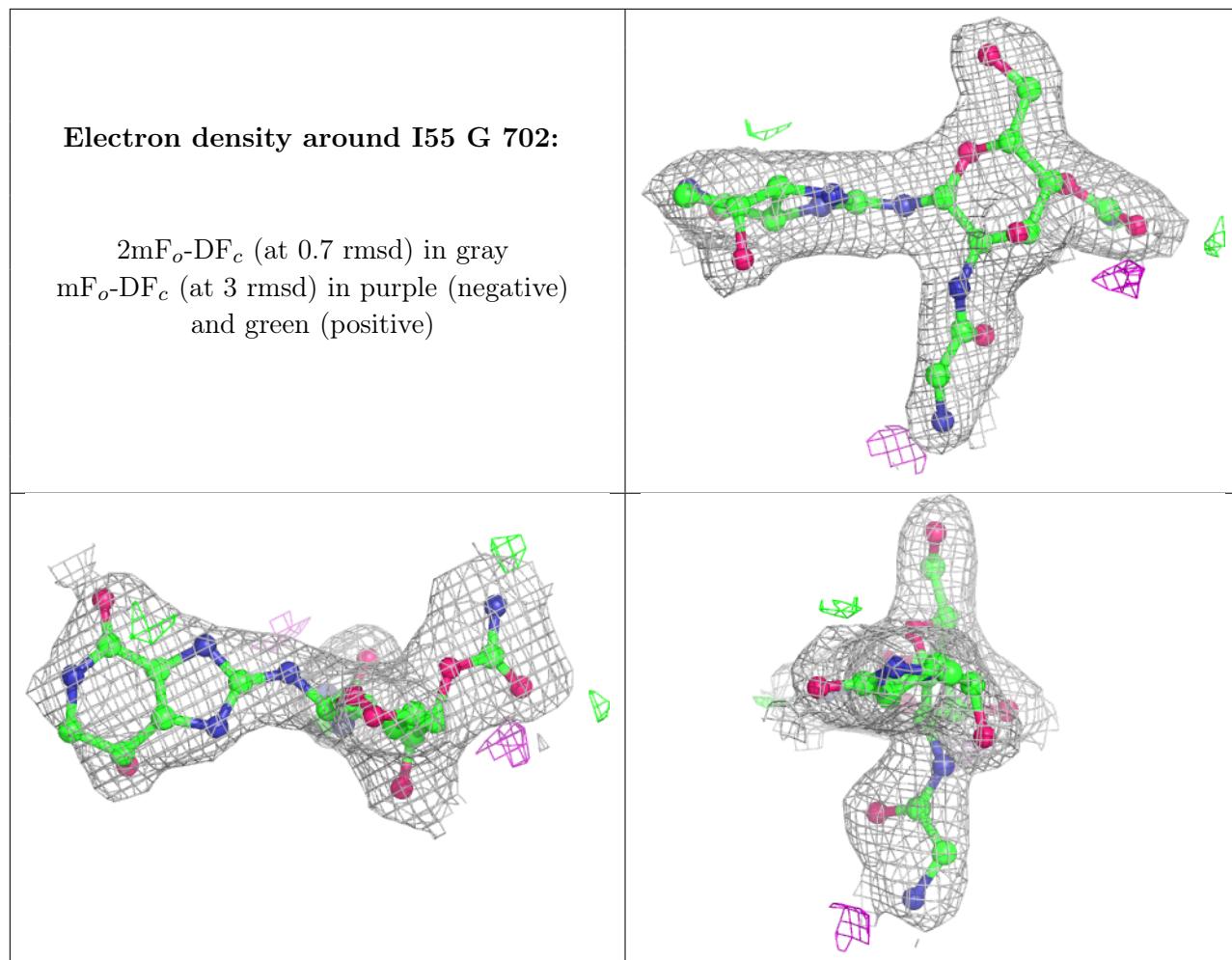


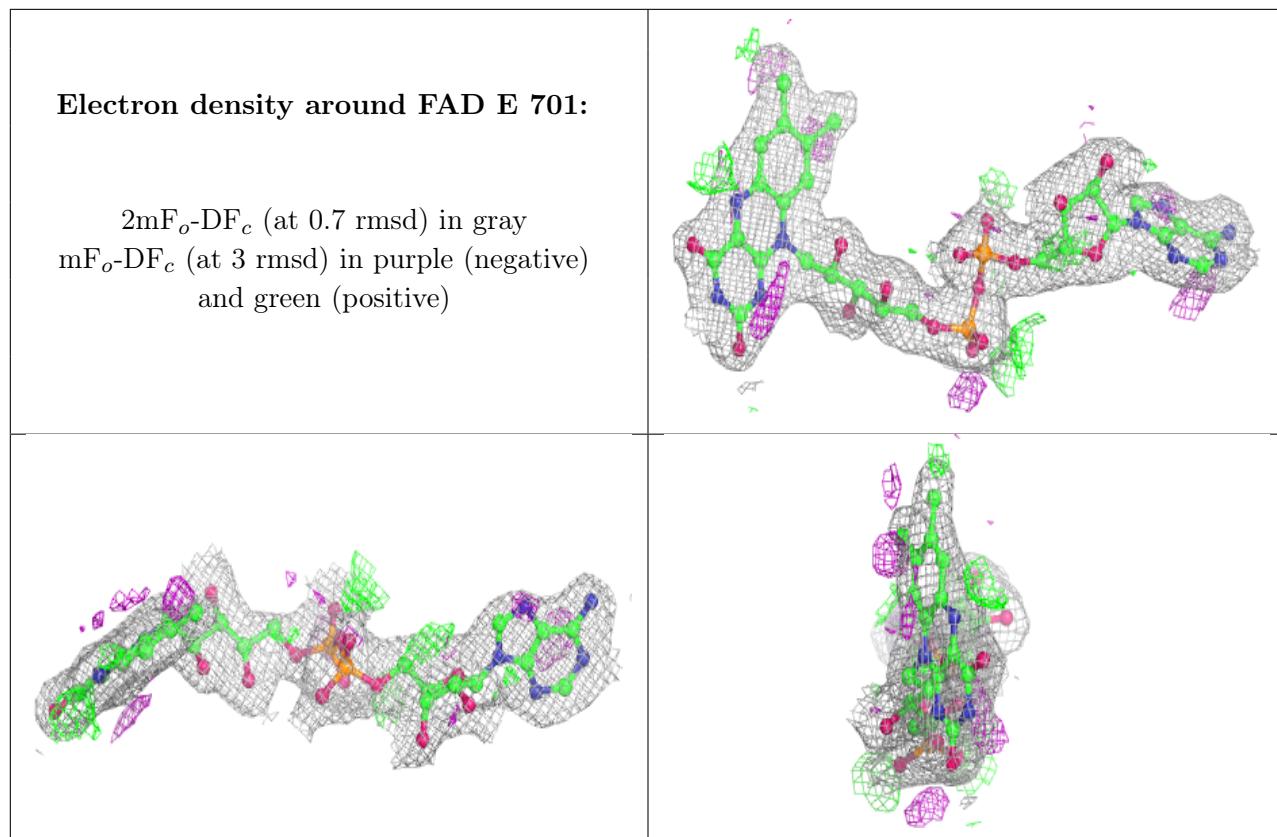












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.