



# Full wwPDB X-ray Structure Validation Report i

Nov 23, 2023 – 12:41 AM JST

PDB ID : 7XXD  
Title : Orf1-sarcosine complex  
Authors : Wang, Y.L.; Li, T.L.  
Deposited on : 2022-05-29  
Resolution : 1.98 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) 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

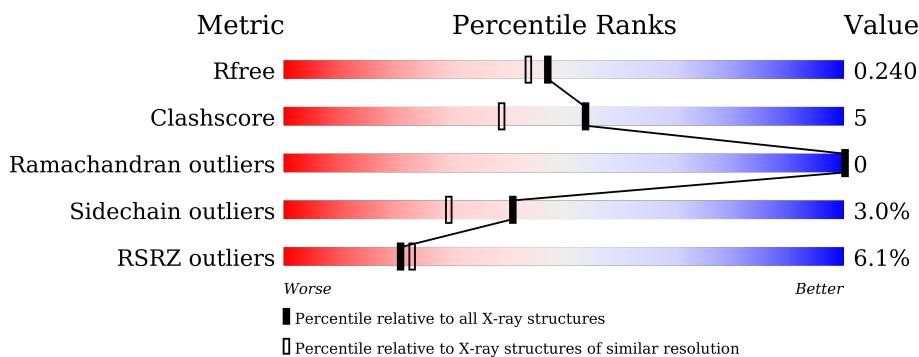
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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 <=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	5%	86%	7%	6%
1	H	512	17%	86%	7%	6%

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32439 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 3654	N 2293	O 660	S 689	12	0	0
1	B	482	Total	C 3662	N 2298	O 661	S 690	13	0	1
1	C	482	Total	C 3662	N 2298	O 661	S 690	13	0	1
1	D	479	Total	C 3630	N 2280	O 656	S 682	12	0	0
1	E	482	Total	C 3654	N 2293	O 660	S 689	12	0	0
1	F	482	Total	C 3662	N 2298	O 661	S 690	13	0	1
1	G	482	Total	C 3654	N 2293	O 660	S 689	12	0	0
1	H	479	Total	C 3630	N 2280	O 656	S 682	12	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A125SXC1
A	-19	GLY	-	expression tag	UNP A0A125SXC1
A	-18	SER	-	expression tag	UNP A0A125SXC1
A	-17	SER	-	expression tag	UNP A0A125SXC1
A	-16	HIS	-	expression tag	UNP A0A125SXC1
A	-15	HIS	-	expression tag	UNP A0A125SXC1
A	-14	HIS	-	expression tag	UNP A0A125SXC1
A	-13	HIS	-	expression tag	UNP A0A125SXC1
A	-12	HIS	-	expression tag	UNP A0A125SXC1
A	-11	HIS	-	expression tag	UNP A0A125SXC1
A	-10	SER	-	expression tag	UNP A0A125SXC1
A	-9	SER	-	expression tag	UNP A0A125SXC1
A	-8	GLY	-	expression tag	UNP A0A125SXC1

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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
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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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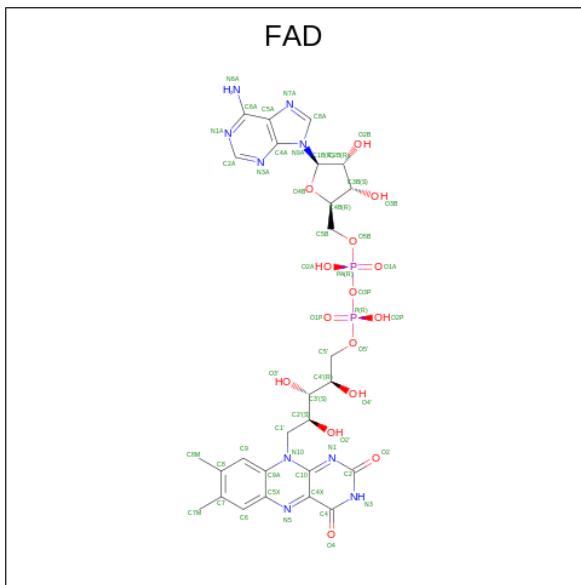
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E	-7	LEU	-	expression tag	UNP A0A125S2C1
E	-6	VAL	-	expression tag	UNP A0A125S2C1
E	-5	PRO	-	expression tag	UNP A0A125S2C1
E	-4	ARG	-	expression tag	UNP A0A125S2C1
E	-3	GLY	-	expression tag	UNP A0A125S2C1
E	-2	SER	-	expression tag	UNP A0A125S2C1
E	-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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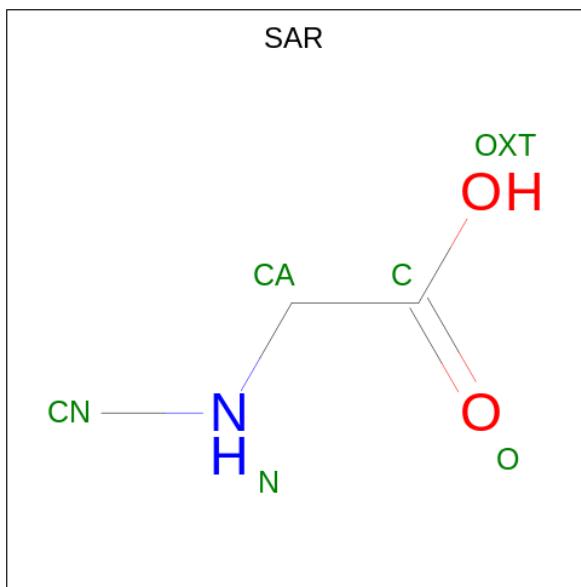
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	LEU	-	expression tag	UNP A0A125S2C1
G	-6	VAL	-	expression tag	UNP A0A125S2C1
G	-5	PRO	-	expression tag	UNP A0A125S2C1
G	-4	ARG	-	expression tag	UNP A0A125S2C1
G	-3	GLY	-	expression tag	UNP A0A125S2C1
G	-2	SER	-	expression tag	UNP A0A125S2C1
G	-1	HIS	-	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:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SARCOSINE (three-letter code: SAR) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 6 3 1 2	0	0
3	B	1	Total C N O 6 3 1 2	0	0
3	C	1	Total C N O 6 3 1 2	0	0
3	D	1	Total C N O 6 3 1 2	0	0
3	E	1	Total C N O 6 3 1 2	0	0
3	F	1	Total C N O 6 3 1 2	0	0
3	G	1	Total C N O 6 3 1 2	0	0
3	H	1	Total C N O 6 3 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	399	Total O 399 399	0	0
4	B	409	Total O 409 409	0	0
4	C	344	Total O 344 344	0	0
4	D	250	Total O 250 250	0	0

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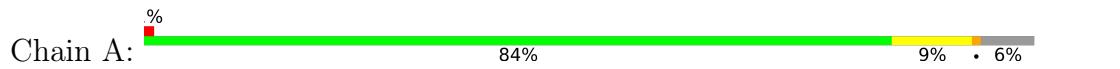
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	385	Total O 385 385	0	0
4	F	421	Total O 421 421	0	0
4	G	322	Total O 322 322	0	0
4	H	229	Total O 229 229	0	0

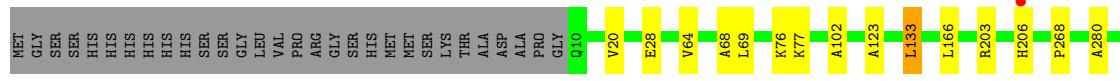
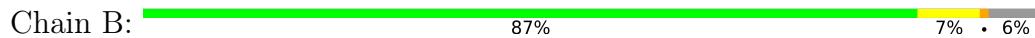
### 3 Residue-property plots

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.

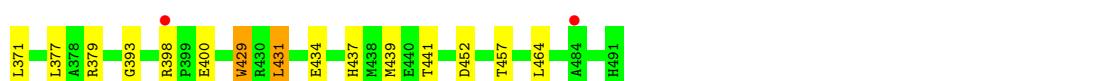
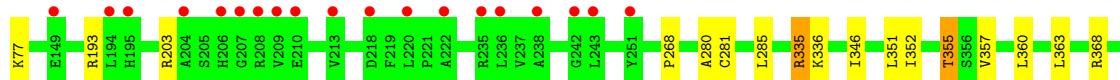
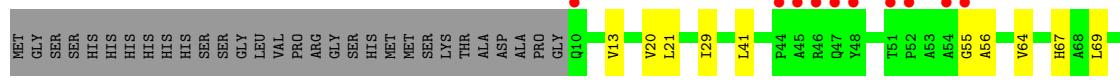
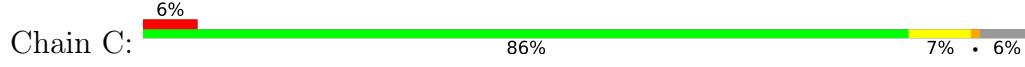
- Molecule 1: N-formimidoyl fortimicin A synthase



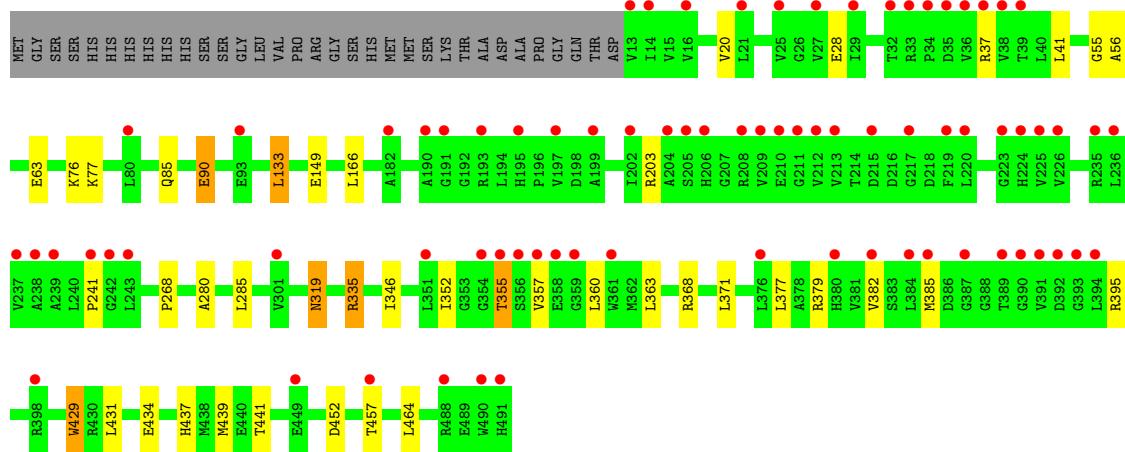
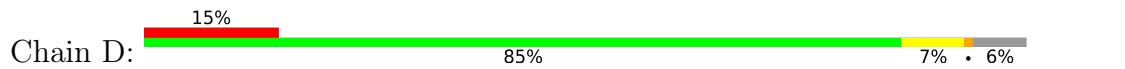
- Molecule 1: N-formimidoyl fortimicin A synthase



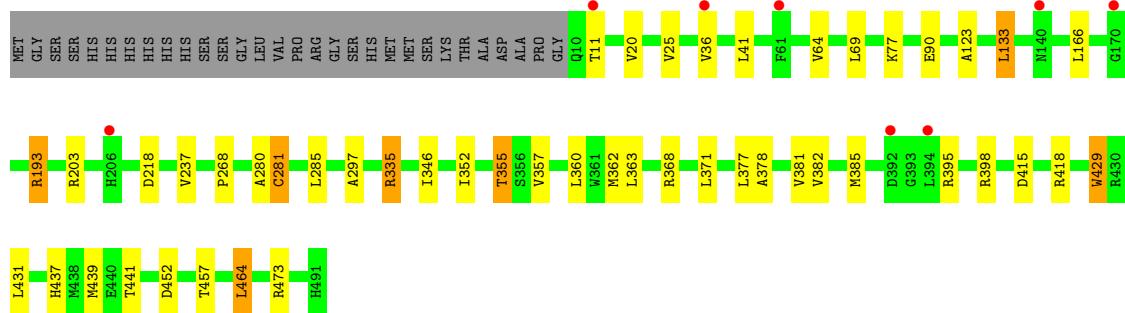
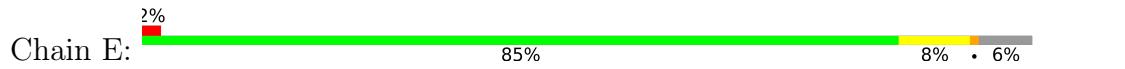
- Molecule 1: N-formimidoyl fortimicin A synthase



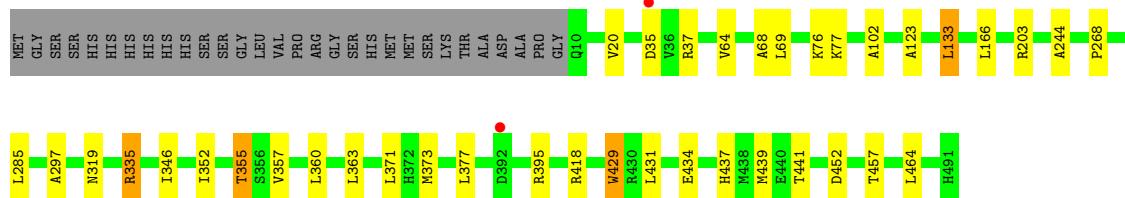
- Molecule 1: N-formimidoyl fortimicin A synthase



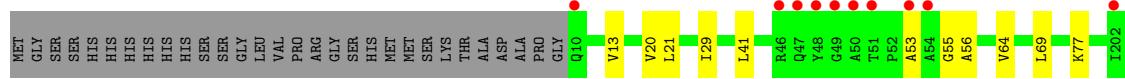
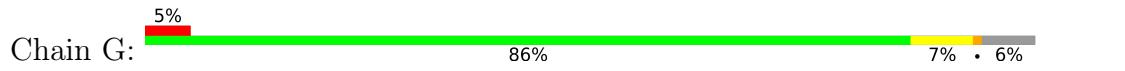
- Molecule 1: N-formimidoyl fortimicin A synthase

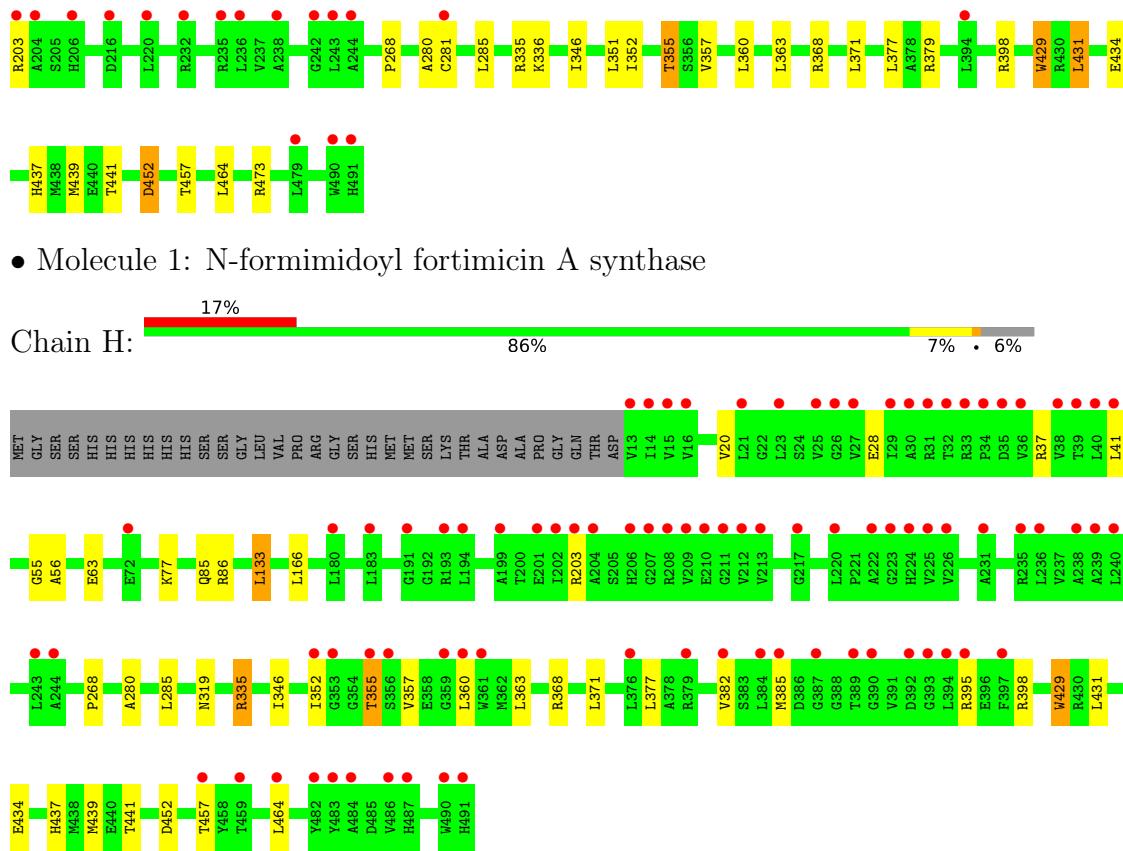


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## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.94Å 108.87Å 134.73Å 90.02° 90.00° 83.30°	Depositor
Resolution (Å)	28.73 – 1.98 28.71 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.73-1.98) 93.2 (28.71-1.98)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.62 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
$R$ , $R_{free}$	0.211 , 0.235 0.217 , 0.240	Depositor DCC
$R_{free}$ test set	18447 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.2	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l 0.012 for -k,-h,-l 0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  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, SAR

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	0/3737	0.81	1/5092 (0.0%)
1	B	0.68	0/3745	0.79	0/5102
1	C	0.70	1/3745 (0.0%)	0.80	0/5102
1	D	0.64	0/3713	0.77	0/5059
1	E	0.67	0/3737	0.80	0/5092
1	F	0.68	0/3745	0.79	0/5102
1	G	0.70	0/3737	0.80	0/5092
1	H	0.64	0/3713	0.77	0/5059
All	All	0.67	1/29872 (0.0%)	0.79	1/40700 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	400	GLU	CD-OE2	5.22	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH2	-5.56	117.52	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	3654	0	3584	55	0
1	B	3662	0	3592	38	0
1	C	3662	0	3592	40	0
1	D	3630	0	3565	42	0
1	E	3654	0	3584	51	0
1	F	3662	0	3592	40	0
1	G	3654	0	3584	38	0
1	H	3630	0	3565	35	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	1	0
2	G	53	0	31	0	0
2	H	53	0	31	3	0
3	A	6	0	6	1	0
3	B	6	0	6	0	0
3	C	6	0	6	0	0
3	D	6	0	6	1	0
3	E	6	0	6	1	0
3	F	6	0	6	0	0
3	G	6	0	6	0	0
3	H	6	0	6	1	0
4	A	399	0	0	19	0
4	B	409	0	0	8	0
4	C	344	0	0	11	0
4	D	250	0	0	9	0
4	E	385	0	0	15	0
4	F	421	0	0	12	0
4	G	322	0	0	7	0
4	H	229	0	0	3	0
All	All	32439	0	28954	311	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 5.

All (311) 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:B:102:ALA:HB1	4:B:972:HOH:O	1.61	0.99
1:A:398:ARG:HG2	4:A:903:HOH:O	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:ARG:HG2	4:E:897:HOH:O	1.62	0.98
1:E:415:ASP:HB2	4:E:886:HOH:O	1.62	0.97
1:E:281:CYS:SG	4:E:1103:HOH:O	2.22	0.96
1:F:441:THR:HB	4:F:807:HOH:O	1.71	0.91
1:E:439:MET:CE	1:G:439:MET:CE	2.50	0.90
1:A:439:MET:CE	1:C:439[A]:MET:CE	2.50	0.89
1:D:319:ASN:HB3	4:D:984:HOH:O	1.73	0.88
1:E:335:ARG:HG2	4:E:1116:HOH:O	1.74	0.87
1:A:335:ARG:HG2	4:A:1116:HOH:O	1.75	0.86
1:A:355:THR:HG22	1:A:357:VAL:H	1.42	0.85
1:F:439[A]:MET:CE	1:H:439:MET:CE	2.55	0.85
1:B:355:THR:HG22	1:B:357:VAL:H	1.42	0.84
1:C:355:THR:HG22	1:C:357:VAL:H	1.42	0.84
1:D:241:PRO:HA	4:D:1012:HOH:O	1.77	0.84
1:D:355:THR:HG22	1:D:357:VAL:H	1.42	0.84
1:E:439:MET:HE3	1:G:439:MET:CE	2.08	0.84
1:F:439[A]:MET:CE	1:H:439:MET:HE2	2.08	0.84
1:E:439:MET:CE	1:G:439:MET:HE3	2.08	0.83
1:E:355:THR:HG22	1:E:357:VAL:H	1.41	0.83
1:G:355:THR:HG22	1:G:357:VAL:H	1.42	0.83
1:B:439[A]:MET:CE	1:D:439:MET:CE	2.55	0.82
1:B:441:THR:HB	4:B:835:HOH:O	1.76	0.82
1:H:355:THR:HG22	1:H:357:VAL:H	1.42	0.82
1:F:355:THR:HG22	1:F:357:VAL:H	1.42	0.82
4:A:819:HOH:O	1:C:434:GLU:HG2	1.78	0.82
1:A:439:MET:CE	1:C:439[A]:MET:HE2	2.10	0.81
1:A:439:MET:HE2	1:C:439[A]:MET:CE	2.11	0.81
1:C:398:ARG:HD2	4:C:1092:HOH:O	1.80	0.80
1:C:335:ARG:HG2	4:C:1096:HOH:O	1.82	0.79
4:F:870:HOH:O	1:H:434:GLU:HG2	1.83	0.79
1:A:439:MET:CE	1:C:439[A]:MET:HE3	2.14	0.78
1:B:439[A]:MET:HE2	1:D:439:MET:CE	2.13	0.77
4:B:858:HOH:O	1:D:434:GLU:HG2	1.84	0.77
1:A:415:ASP:HB2	4:A:936:HOH:O	1.82	0.77
1:A:439:MET:HE3	1:C:439[A]:MET:CE	2.15	0.77
1:B:439[A]:MET:CE	1:D:439:MET:HE3	2.14	0.77
1:A:439:MET:HE2	1:C:439[A]:MET:HE2	1.66	0.76
1:E:439:MET:CE	1:G:439:MET:HE2	2.15	0.76
1:F:439[A]:MET:HE3	1:H:439:MET:CE	2.14	0.76
1:F:439[A]:MET:HE2	1:H:439:MET:HE2	1.66	0.76
1:F:434:GLU:HG2	4:H:807:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:809:HOH:O	1:G:434:GLU:HG2	1.88	0.74
1:C:363:LEU:HD11	1:C:377:LEU:HB3	1.70	0.74
1:E:439:MET:HE2	1:G:439:MET:CE	2.17	0.73
1:F:441:THR:CB	4:F:807:HOH:O	2.34	0.72
1:D:382:VAL:HA	1:D:385:MET:HE2	1.71	0.71
1:B:439[A]:MET:CE	1:D:439:MET:HE2	2.20	0.71
1:F:102:ALA:HB1	4:F:941:HOH:O	1.90	0.71
1:E:382:VAL:HA	1:E:385:MET:CE	2.21	0.71
1:G:363:LEU:HD11	1:G:377:LEU:HB3	1.70	0.71
1:A:382:VAL:HA	1:A:385:MET:HE2	1.72	0.71
1:D:382:VAL:HA	1:D:385:MET:CE	2.21	0.70
1:A:382:VAL:HA	1:A:385:MET:CE	2.21	0.70
1:H:382:VAL:HA	1:H:385:MET:CE	2.21	0.70
1:G:452:ASP:HB3	4:G:820:HOH:O	1.91	0.70
1:F:335:ARG:HG2	4:F:1167:HOH:O	1.91	0.69
1:H:382:VAL:HA	1:H:385:MET:HE2	1.73	0.69
1:A:449:GLU:HB3	4:A:1131:HOH:O	1.92	0.69
1:F:352:ILE:HD13	1:F:377:LEU:HD22	1.75	0.68
1:F:439[A]:MET:HE2	1:H:439:MET:CE	2.20	0.68
1:C:429:TRP:CD1	1:C:431:LEU:HD11	2.29	0.68
1:B:439[A]:MET:HE3	1:D:439:MET:CE	2.22	0.68
1:G:429:TRP:CD1	1:G:431:LEU:HD11	2.28	0.68
1:B:319:ASN:HB3	4:B:980:HOH:O	1.94	0.67
1:F:35:ASP:HB3	4:F:1155:HOH:O	1.95	0.67
1:B:439[A]:MET:HE2	1:D:439:MET:HE2	1.74	0.66
1:H:352:ILE:HD13	1:H:377:LEU:HD22	1.77	0.66
1:D:352:ILE:HD13	1:D:377:LEU:HD22	1.77	0.66
1:B:441:THR:CB	4:B:835:HOH:O	2.41	0.66
1:E:382:VAL:HA	1:E:385:MET:HE2	1.77	0.65
1:E:415:ASP:CB	4:E:886:HOH:O	2.32	0.65
1:G:355:THR:HG21	1:G:360:LEU:HD23	1.78	0.65
1:B:355:THR:HG21	1:B:360:LEU:HD23	1.78	0.65
1:B:352:ILE:HD13	1:B:377:LEU:HD22	1.80	0.64
1:E:439:MET:HE3	1:G:439:MET:HE2	1.75	0.64
1:F:439[A]:MET:CE	1:H:439:MET:HE3	2.27	0.64
1:G:53:ALA:HB1	4:G:850:HOH:O	1.97	0.63
1:B:434:GLU:HG2	4:D:836:HOH:O	1.97	0.63
1:C:355:THR:HG21	1:C:360:LEU:HD23	1.79	0.63
1:E:355:THR:HG21	1:E:360:LEU:HD23	1.80	0.63
1:B:439[A]:MET:HE2	1:D:439:MET:HE3	1.78	0.63
1:F:355:THR:HG21	1:F:360:LEU:HD23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:THR:HG21	1:D:360:LEU:HD23	1.80	0.62
1:A:355:THR:HG21	1:A:360:LEU:HD23	1.80	0.62
1:H:355:THR:HG21	1:H:360:LEU:HD23	1.81	0.62
1:A:352:ILE:HD13	1:A:377:LEU:HD22	1.82	0.61
1:F:346:ILE:HG13	1:F:464:LEU:CD2	2.30	0.61
1:G:429:TRP:NE1	1:G:431:LEU:HD11	2.15	0.61
1:C:429:TRP:NE1	1:C:431:LEU:HD11	2.15	0.61
1:A:335:ARG:CD	4:A:1113:HOH:O	2.49	0.60
1:D:346:ILE:HG13	1:D:464:LEU:CD2	2.32	0.60
1:E:346:ILE:HG13	1:E:464:LEU:CD2	2.32	0.60
1:H:346:ILE:HG13	1:H:464:LEU:CD2	2.32	0.60
1:G:429:TRP:CE2	1:G:431:LEU:HD11	2.37	0.60
1:C:429:TRP:CE2	1:C:431:LEU:HD11	2.37	0.59
1:D:363:LEU:HD11	1:D:377:LEU:HB3	1.84	0.59
1:E:395:ARG:N	4:E:803:HOH:O	2.35	0.59
1:H:363:LEU:HD11	1:H:377:LEU:HB3	1.85	0.59
1:E:439:MET:HE2	1:G:439:MET:HE3	1.78	0.59
1:E:352:ILE:HD13	1:E:377:LEU:HD22	1.84	0.58
1:G:346:ILE:HG13	1:G:464:LEU:CD2	2.34	0.58
1:E:363:LEU:HD11	1:E:377:LEU:HB3	1.86	0.58
1:C:346:ILE:HG13	1:C:464:LEU:CD2	2.34	0.58
1:E:335:ARG:CD	4:E:1114:HOH:O	2.51	0.57
1:B:206:HIS:O	1:H:86:ARG:HD2	2.03	0.57
1:F:439[A]:MET:HE3	1:H:439:MET:HE2	1.76	0.57
1:E:441:THR:HG22	4:E:1084:HOH:O	2.05	0.57
1:A:189:GLN:HG2	4:A:1119:HOH:O	2.03	0.57
1:F:363:LEU:HD11	1:F:377:LEU:HB3	1.87	0.56
1:H:355:THR:CG2	1:H:357:VAL:H	2.17	0.56
1:B:363:LEU:HD11	1:B:377:LEU:HB3	1.87	0.56
1:E:335:ARG:HD2	4:E:1114:HOH:O	2.05	0.56
1:D:335:ARG:HG2	4:D:925:HOH:O	2.06	0.56
1:E:346:ILE:HG13	1:E:464:LEU:HD21	1.86	0.56
1:G:473:ARG:HB2	4:G:1047:HOH:O	2.04	0.56
1:E:439:MET:HE2	1:G:439:MET:HE2	1.82	0.56
1:C:398:ARG:HG2	4:C:802:HOH:O	2.05	0.55
1:C:398:ARG:CG	4:C:802:HOH:O	2.54	0.55
1:A:335:ARG:HD3	4:A:1113:HOH:O	2.07	0.55
1:A:363:LEU:HD11	1:A:377:LEU:HB3	1.88	0.55
1:E:355:THR:CG2	1:E:357:VAL:H	2.17	0.55
1:A:90:GLU:HG3	4:A:1118:HOH:O	2.07	0.54
1:A:439:MET:HE2	1:C:439[A]:MET:HE3	1.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:ILE:HD12	1:G:363:LEU:HD12	1.89	0.54
1:C:352:ILE:HD12	1:C:363:LEU:HD12	1.90	0.54
1:G:355:THR:CG2	1:G:357:VAL:H	2.18	0.54
1:A:346:ILE:HG13	1:A:464:LEU:CD1	2.37	0.54
1:A:352:ILE:HG23	1:A:363:LEU:HD13	1.90	0.54
1:A:335:ARG:HD2	4:A:1113:HOH:O	2.07	0.54
1:E:352:ILE:HG23	1:E:363:LEU:HD13	1.89	0.54
1:A:355:THR:CG2	1:A:357:VAL:H	2.17	0.54
1:C:393:GLY:N	4:C:804:HOH:O	2.42	0.53
1:H:335:ARG:HG2	4:H:904:HOH:O	2.08	0.53
1:F:68:ALA:HA	4:F:990:HOH:O	2.09	0.53
1:F:355:THR:CG2	1:F:357:VAL:H	2.17	0.52
1:A:457:THR:HG23	4:A:1159:HOH:O	2.08	0.52
1:E:90:GLU:HG3	4:E:1115:HOH:O	2.09	0.52
1:B:68:ALA:HA	4:B:987:HOH:O	2.10	0.51
1:B:355:THR:CG2	1:B:357:VAL:H	2.17	0.51
1:D:355:THR:CG2	1:D:357:VAL:H	2.17	0.51
1:B:352:ILE:HG23	1:B:363:LEU:HD13	1.92	0.51
1:C:355:THR:CG2	1:C:357:VAL:H	2.18	0.51
1:A:439:MET:HE3	1:C:439[A]:MET:HE2	1.82	0.51
1:E:268:PRO:HG3	1:E:285:LEU:HD22	1.93	0.51
1:F:268:PRO:HG3	1:F:285:LEU:HD22	1.93	0.50
1:C:268:PRO:HG3	1:C:285:LEU:HD22	1.94	0.50
1:E:193:ARG:HG2	1:E:193:ARG:HH11	1.77	0.50
1:G:398:ARG:HG2	4:G:802:HOH:O	2.11	0.50
1:B:133:LEU:HD13	1:B:166:LEU:HD22	1.93	0.50
1:A:133:LEU:HD13	1:A:166:LEU:HD22	1.93	0.50
1:D:268:PRO:HG3	1:D:285:LEU:HD22	1.94	0.49
1:F:133:LEU:HD13	1:F:166:LEU:HD22	1.93	0.49
1:A:268:PRO:HG3	1:A:285:LEU:HD22	1.94	0.49
1:B:268:PRO:HG3	1:B:285:LEU:HD22	1.94	0.49
1:G:398:ARG:CG	4:G:802:HOH:O	2.60	0.49
1:F:352:ILE:HG23	1:F:363:LEU:HD13	1.93	0.49
1:C:398:ARG:HB2	4:C:1092:HOH:O	2.13	0.49
1:H:63:GLU:OE1	3:H:702:SAR:HN2	2.13	0.49
1:E:335:ARG:HD3	4:E:1114:HOH:O	2.13	0.48
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.79	0.48
1:F:319:ASN:HB3	4:F:1074:HOH:O	2.13	0.48
1:H:268:PRO:HG3	1:H:285:LEU:HD22	1.94	0.48
1:F:373:MET:HE1	4:F:880:HOH:O	2.14	0.48
1:G:55:GLY:N	1:G:56:ALA:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:HB1	1:A:418:ARG:HD2	1.96	0.48
1:B:431:LEU:HD11	1:D:431:LEU:CD1	2.44	0.48
1:E:25:VAL:HG22	1:E:378:ALA:HA	1.96	0.48
1:C:55:GLY:N	1:C:56:ALA:HA	2.28	0.48
1:E:123:ALA:HB1	1:E:418:ARG:HD2	1.96	0.48
1:H:133:LEU:HD13	1:H:166:LEU:HD22	1.95	0.48
2:H:701:FAD:H1'1	2:H:701:FAD:O4'	2.14	0.47
1:D:133:LEU:HD13	1:D:166:LEU:HD22	1.96	0.47
1:F:431:LEU:HD11	1:H:431:LEU:CD1	2.44	0.47
1:A:25:VAL:HG22	1:A:378:ALA:HA	1.95	0.47
1:G:268:PRO:HG3	1:G:285:LEU:HD22	1.95	0.47
1:B:355:THR:HG22	1:B:357:VAL:N	2.22	0.47
1:A:346:ILE:HG13	1:A:464:LEU:HD12	1.96	0.47
1:D:335:ARG:HD2	4:D:1035:HOH:O	2.13	0.47
1:E:133:LEU:HD13	1:E:166:LEU:HD22	1.95	0.47
1:E:382:VAL:HA	1:E:385:MET:HE3	1.96	0.47
1:H:429:TRP:CZ3	1:H:439:MET:HE1	2.50	0.47
1:A:64:VAL:HG13	1:A:69:LEU:HD22	1.96	0.47
1:A:429:TRP:CZ3	1:A:439:MET:HE1	2.50	0.47
1:C:379:ARG:HD3	4:C:915:HOH:O	2.15	0.47
1:A:291:GLY:N	4:A:802:HOH:O	2.35	0.47
2:D:701:FAD:H9	2:D:701:FAD:H1'2	1.74	0.47
1:A:355:THR:HG22	1:A:357:VAL:N	2.22	0.46
1:C:67:HIS:HD2	4:C:1112:HOH:O	1.98	0.46
1:D:63:GLU:OE1	3:D:702:SAR:HN2	2.16	0.46
1:A:72:GLU:HG3	4:A:1037:HOH:O	2.14	0.46
1:B:431:LEU:CD1	1:D:431:LEU:HD11	2.46	0.46
1:C:429:TRP:CZ3	1:C:439[A]:MET:HE1	2.50	0.46
1:B:429:TRP:CZ3	1:B:439[A]:MET:HE1	2.51	0.46
1:E:64:VAL:HG13	1:E:69:LEU:HD22	1.97	0.46
1:B:352:ILE:HG23	1:B:363:LEU:CD1	2.46	0.46
2:D:701:FAD:H1'1	2:D:701:FAD:O4'	2.15	0.46
1:A:415:ASP:CB	4:A:936:HOH:O	2.51	0.46
1:B:64:VAL:HG13	1:B:69:LEU:HD22	1.98	0.46
1:D:355:THR:HG22	1:D:357:VAL:N	2.22	0.46
1:E:429:TRP:CZ3	1:E:439:MET:HE1	2.51	0.46
1:G:355:THR:HG22	1:G:357:VAL:N	2.22	0.45
1:F:431:LEU:CD1	1:H:431:LEU:HD11	2.46	0.45
1:G:352:ILE:HG23	1:G:363:LEU:CD1	2.46	0.45
1:H:352:ILE:HG23	1:H:363:LEU:CD1	2.47	0.45
1:D:429:TRP:CZ3	1:D:439:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ILE:HG23	1:C:363:LEU:CD1	2.46	0.45
1:C:20:VAL:HG11	1:C:371:LEU:HA	1.99	0.45
1:D:352:ILE:HG23	1:D:363:LEU:CD1	2.47	0.45
1:D:76:LYS:HE2	4:D:966:HOH:O	2.17	0.45
1:F:64:VAL:HG13	1:F:69:LEU:HD22	1.98	0.45
1:F:429:TRP:CZ3	1:F:439[A]:MET:HE1	2.52	0.45
1:E:437:HIS:O	1:E:441:THR:HG23	2.17	0.45
1:E:368:ARG:NH2	3:E:702:SAR:HA3	2.32	0.44
1:F:352:ILE:HG23	1:F:363:LEU:CD1	2.47	0.44
1:H:352:ILE:HG23	1:H:363:LEU:HD13	2.00	0.44
1:A:437:HIS:O	1:A:441:THR:HG23	2.17	0.44
1:A:453:ARG:CG	4:A:1078:HOH:O	2.65	0.44
1:E:473:ARG:HD3	4:E:1091:HOH:O	2.17	0.44
1:G:336:LYS:HG3	4:G:1079:HOH:O	2.17	0.44
1:D:352:ILE:HG23	1:D:363:LEU:HD13	2.00	0.44
1:E:218:ASP:CB	4:E:1087:HOH:O	2.66	0.44
1:E:218:ASP:HB2	4:E:1087:HOH:O	2.17	0.44
1:G:437:HIS:O	1:G:441:THR:HG23	2.18	0.44
2:B:701:FAD:H9	2:B:701:FAD:H1'2	1.75	0.44
1:G:429:TRP:CZ3	1:G:439:MET:HE1	2.52	0.44
1:C:437:HIS:O	1:C:441:THR:HG23	2.18	0.44
1:F:244:ALA:CB	4:F:1039:HOH:O	2.66	0.44
1:D:149:GLU:HG3	4:D:863:HOH:O	2.17	0.43
1:G:379:ARG:HD3	4:G:951:HOH:O	2.18	0.43
2:H:701:FAD:H1'2	2:H:701:FAD:H9	1.74	0.43
1:G:351:LEU:O	1:G:352:ILE:HD13	2.19	0.43
1:C:351:LEU:O	1:C:352:ILE:HD13	2.18	0.43
1:G:363:LEU:HD12	1:G:363:LEU:HA	1.84	0.43
1:C:13:VAL:HG11	1:C:29:ILE:HD13	2.01	0.43
1:D:90:GLU:HG3	4:D:825:HOH:O	2.17	0.43
1:F:437:HIS:O	1:F:441:THR:HG23	2.19	0.43
1:E:352:ILE:HG23	1:E:363:LEU:CD1	2.48	0.43
1:G:64:VAL:HG13	1:G:69:LEU:HD22	2.01	0.43
1:H:355:THR:HG22	1:H:357:VAL:N	2.22	0.43
1:B:76:LYS:HE3	4:B:1118:HOH:O	2.18	0.42
1:D:280:ALA:HB1	1:D:368:ARG:HD2	2.00	0.42
2:D:701:FAD:O4'	2:D:701:FAD:C1'	2.66	0.42
1:E:193:ARG:HH11	1:E:193:ARG:CG	2.32	0.42
1:E:297:ALA:HB1	2:E:701:FAD:HM73	2.00	0.42
1:G:20:VAL:HG11	1:G:371:LEU:HA	2.00	0.42
1:A:473:ARG:HD3	4:A:1093:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:HIS:O	1:B:441:THR:HG23	2.19	0.42
1:B:123:ALA:HB1	1:B:418:ARG:HD2	2.01	0.42
2:E:701:FAD:H1'2	2:E:701:FAD:H9	1.73	0.42
1:G:13:VAL:HG11	1:G:29:ILE:HD13	2.02	0.42
1:A:297:ALA:HB1	2:A:701:FAD:HM73	2.01	0.42
1:A:382:VAL:HA	1:A:385:MET:HE3	2.01	0.42
1:A:193:ARG:HH11	1:A:193:ARG:CG	2.32	0.42
1:A:352:ILE:HG23	1:A:363:LEU:CD1	2.48	0.42
1:F:123:ALA:HB1	1:F:418:ARG:HD2	2.02	0.42
1:C:336:LYS:HG3	4:C:1114:HOH:O	2.19	0.42
1:D:379:ARG:HD3	4:D:993:HOH:O	2.19	0.42
1:H:280:ALA:HB1	1:H:368:ARG:HD2	2.00	0.42
1:D:437:HIS:O	1:D:441:THR:HG23	2.19	0.42
1:F:297:ALA:HB1	2:F:701:FAD:HM73	2.00	0.42
1:E:381:VAL:O	1:E:385:MET:HE2	2.20	0.42
1:B:20:VAL:HG11	1:B:371:LEU:HA	2.01	0.42
1:C:64:VAL:HG13	1:C:69:LEU:HD22	2.01	0.42
1:A:280:ALA:HB1	1:A:368:ARG:HD2	2.02	0.41
1:B:431:LEU:CD1	1:D:431:LEU:CD1	2.98	0.41
1:E:11:THR:O	1:E:36:VAL:HG22	2.20	0.41
1:D:28:GLU:HB3	1:D:382:VAL:HG21	2.02	0.41
1:H:437:HIS:O	1:H:441:THR:HG23	2.19	0.41
2:A:701:FAD:C4	3:A:702:SAR:HN3	2.50	0.41
1:B:280:ALA:HB1	1:B:368:ARG:HD2	2.02	0.41
1:F:20:VAL:HG11	1:F:371:LEU:HA	2.01	0.41
2:H:701:FAD:O4'	2:H:701:FAD:C1'	2.69	0.41
2:A:701:FAD:H1'2	2:A:701:FAD:H9	1.72	0.41
1:F:76:LYS:HE3	4:F:1146:HOH:O	2.20	0.41
1:F:431:LEU:CD1	1:H:431:LEU:CD1	2.98	0.41
1:G:280:ALA:HB1	1:G:368:ARG:HD2	2.02	0.41
1:A:105:ARG:HD3	4:A:842:HOH:O	2.19	0.41
1:B:429:TRP:CG	1:B:431:LEU:HD13	2.55	0.41
1:C:280:ALA:HB1	1:C:368:ARG:HD2	2.02	0.41
1:D:55:GLY:N	1:D:56:ALA:HA	2.35	0.41
1:D:363:LEU:HD12	1:D:363:LEU:HA	1.89	0.41
1:E:20:VAL:HG11	1:E:371:LEU:HA	2.01	0.41
1:F:37:ARG:NH1	4:F:836:HOH:O	2.54	0.41
1:H:28:GLU:HB3	1:H:382:VAL:HG21	2.03	0.41
1:H:55:GLY:N	1:H:56:ALA:HA	2.34	0.41
1:A:373:MET:HE1	4:A:991:HOH:O	2.19	0.41
1:E:237:VAL:HG21	1:E:362:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:429:TRP:CG	1:H:431:LEU:HD13	2.56	0.41
1:A:453:ARG:HD2	4:A:1078:HOH:O	2.20	0.41
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.90	0.41
1:E:280:ALA:HB1	1:E:368:ARG:HD2	2.02	0.41
1:F:363:LEU:HD12	1:F:363:LEU:HA	1.93	0.41
1:H:20:VAL:HG11	1:H:371:LEU:HA	2.03	0.41
1:A:381:VAL:O	1:A:385:MET:HE2	2.21	0.41
1:D:429:TRP:CG	1:D:431:LEU:HD13	2.56	0.41
1:C:69:LEU:HD23	4:C:920:HOH:O	2.21	0.40
1:D:20:VAL:HG11	1:D:371:LEU:HA	2.03	0.40
1:F:429:TRP:CG	1:F:431:LEU:HD13	2.56	0.40
1:A:11:THR:O	1:A:36:VAL:HG22	2.21	0.40
1:A:20:VAL:HG11	1:A:371:LEU:HA	2.02	0.40
1:A:237:VAL:HG21	1:A:362:MET:HE1	2.03	0.40
1:B:28:GLU:HB3	1:B:382:VAL:HG21	2.04	0.40
1:E:429:TRP:CG	1:E:431:LEU:HD13	2.57	0.40
1:C:193:ARG:HA	4:C:965:HOH:O	2.20	0.40
1:G:21:LEU:HD23	1:G:21:LEU:HA	1.91	0.40
1:A:429:TRP:CG	1:A:431:LEU:HD13	2.56	0.40
1:B:431:LEU:HD11	1:D:431:LEU:HD11	2.03	0.40
1:B:479:LEU:HD22	4:B:872:HOH:O	2.22	0.40
1:H:398:ARG:HB2	4:H:1001:HOH:O	2.21	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	480/512 (94%)	470 (98%)	10 (2%)	0	100 100
1	B	481/512 (94%)	470 (98%)	11 (2%)	0	100 100
1	C	481/512 (94%)	470 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	477/512 (93%)	466 (98%)	11 (2%)	0	100	100
1	E	480/512 (94%)	469 (98%)	11 (2%)	0	100	100
1	F	481/512 (94%)	471 (98%)	10 (2%)	0	100	100
1	G	480/512 (94%)	469 (98%)	11 (2%)	0	100	100
1	H	477/512 (93%)	466 (98%)	11 (2%)	0	100	100
All	All	3837/4096 (94%)	3751 (98%)	86 (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	376/400 (94%)	365 (97%)	11 (3%)	42	31
1	B	377/400 (94%)	367 (97%)	10 (3%)	44	35
1	C	377/400 (94%)	367 (97%)	10 (3%)	44	35
1	D	373/400 (93%)	359 (96%)	14 (4%)	33	21
1	E	376/400 (94%)	364 (97%)	12 (3%)	39	28
1	F	377/400 (94%)	368 (98%)	9 (2%)	49	41
1	G	376/400 (94%)	366 (97%)	10 (3%)	44	35
1	H	373/400 (93%)	360 (96%)	13 (4%)	36	24
All	All	3005/3200 (94%)	2916 (97%)	89 (3%)	41	29

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	77	LYS
1	A	133	LEU
1	A	193	ARG
1	A	203	ARG

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	355	THR
1	A	429	TRP
1	A	452	ASP
1	A	457	THR
1	A	464	LEU
1	B	77	LYS
1	B	133	LEU
1	B	203	ARG
1	B	335	ARG
1	B	355	THR
1	B	395	ARG
1	B	429	TRP
1	B	452	ASP
1	B	457	THR
1	B	464	LEU
1	C	41	LEU
1	C	77	LYS
1	C	203	ARG
1	C	281	CYS
1	C	335	ARG
1	C	355	THR
1	C	429	TRP
1	C	431	LEU
1	C	452	ASP
1	C	457	THR
1	D	37	ARG
1	D	41	LEU
1	D	77	LYS
1	D	85	GLN
1	D	90	GLU
1	D	133	LEU
1	D	203	ARG
1	D	319	ASN
1	D	335	ARG
1	D	355	THR
1	D	395	ARG
1	D	429	TRP
1	D	452	ASP
1	D	457	THR
1	E	41	LEU
1	E	77	LYS

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Mol	Chain	Res	Type
1	E	133	LEU
1	E	193	ARG
1	E	203	ARG
1	E	281	CYS
1	E	335	ARG
1	E	355	THR
1	E	429	TRP
1	E	452	ASP
1	E	457	THR
1	E	464	LEU
1	F	77	LYS
1	F	133	LEU
1	F	203	ARG
1	F	335	ARG
1	F	355	THR
1	F	395	ARG
1	F	429	TRP
1	F	452	ASP
1	F	457	THR
1	G	41	LEU
1	G	77	LYS
1	G	203	ARG
1	G	281	CYS
1	G	335	ARG
1	G	355	THR
1	G	429	TRP
1	G	431	LEU
1	G	452	ASP
1	G	457	THR
1	H	37	ARG
1	H	41	LEU
1	H	77	LYS
1	H	85	GLN
1	H	133	LEU
1	H	203	ARG
1	H	319	ASN
1	H	335	ARG
1	H	355	THR
1	H	395	ARG
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	B	10	GLN
1	C	10	GLN
1	F	10	GLN
1	G	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 [\(i\)](#)

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	SAR	D	702	-	5,5,5	0.86	0	3,5,5	2.17	1 (33%)
2	FAD	A	701	-	53,58,58	0.74	0	68,89,89	0.96	5 (7%)
2	FAD	E	701	-	53,58,58	0.78	1 (1%)	68,89,89	0.96	3 (4%)
2	FAD	B	701	-	53,58,58	0.78	1 (1%)	68,89,89	0.87	1 (1%)
2	FAD	H	701	-	53,58,58	0.69	0	68,89,89	0.77	2 (2%)
2	FAD	F	701	-	53,58,58	0.73	1 (1%)	68,89,89	0.88	2 (2%)
2	FAD	C	701	-	53,58,58	0.64	0	68,89,89	0.86	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SAR	B	702	-	5,5,5	1.19	0	3,5,5	0.57	0
3	SAR	H	702	-	5,5,5	0.86	0	3,5,5	1.88	1 (33%)
3	SAR	F	702	-	5,5,5	1.18	0	3,5,5	0.43	0
3	SAR	E	702	-	5,5,5	0.81	0	3,5,5	1.29	0
2	FAD	G	701	-	53,58,58	0.65	0	68,89,89	0.87	2 (2%)
3	SAR	A	702	-	5,5,5	0.77	0	3,5,5	1.42	1 (33%)
3	SAR	G	702	-	5,5,5	1.09	0	3,5,5	1.70	2 (66%)
3	SAR	C	702	-	5,5,5	1.05	0	3,5,5	1.86	2 (66%)
2	FAD	D	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	SAR	D	702	-	-	0/2/3/3	-
2	FAD	A	701	-	-	2/30/50/50	0/6/6/6
2	FAD	E	701	-	-	2/30/50/50	0/6/6/6
2	FAD	B	701	-	-	2/30/50/50	0/6/6/6
2	FAD	H	701	-	-	2/30/50/50	0/6/6/6
2	FAD	F	701	-	-	2/30/50/50	0/6/6/6
2	FAD	C	701	-	-	1/30/50/50	0/6/6/6
3	SAR	B	702	-	-	0/2/3/3	-
3	SAR	H	702	-	-	0/2/3/3	-
3	SAR	F	702	-	-	0/2/3/3	-
3	SAR	E	702	-	-	0/2/3/3	-
2	FAD	G	701	-	-	3/30/50/50	0/6/6/6
3	SAR	A	702	-	-	0/2/3/3	-
3	SAR	G	702	-	-	0/2/3/3	-
3	SAR	C	702	-	-	0/2/3/3	-
2	FAD	D	701	-	-	2/30/50/50	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C9-C8	-2.26	1.36	1.39
2	F	701	FAD	C9-C8	-2.25	1.36	1.39
2	E	701	FAD	C9-C8	-2.18	1.36	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FAD	O2A-PA-O1A	3.15	127.82	112.24
2	E	701	FAD	O2A-PA-O1A	3.13	127.71	112.24
2	E	701	FAD	C4'-C3'-C2'	3.05	119.71	113.36
3	D	702	SAR	OXT-C-CA	3.03	123.27	112.74
2	F	701	FAD	O2A-PA-O1A	2.88	126.50	112.24
2	B	701	FAD	O2A-PA-O1A	2.85	126.32	112.24
3	H	702	SAR	OXT-C-CA	2.64	121.92	112.74
2	A	701	FAD	C4'-C3'-C2'	2.61	118.80	113.36
2	E	701	FAD	C5A-C6A-N6A	2.47	124.10	120.35
2	A	701	FAD	C5A-C6A-N6A	2.43	124.04	120.35
2	G	701	FAD	C5A-C6A-N6A	2.37	123.96	120.35
2	C	701	FAD	C5A-C6A-N6A	2.35	123.92	120.35
3	C	702	SAR	OXT-C-CA	2.35	120.90	112.74
2	D	701	FAD	O2P-P-O1P	2.35	123.85	112.24
2	H	701	FAD	O2P-P-O1P	2.20	123.12	112.24
3	C	702	SAR	OXT-C-O	-2.16	117.92	123.30
2	H	701	FAD	C5A-C6A-N6A	2.12	123.57	120.35
3	G	702	SAR	OXT-C-CA	2.12	120.10	112.74
2	D	701	FAD	C5A-C6A-N6A	2.11	123.55	120.35
3	A	702	SAR	OXT-C-CA	2.10	120.05	112.74
2	A	701	FAD	C1B-N9A-C4A	-2.09	122.98	126.64
2	F	701	FAD	C4'-C3'-C2'	2.06	117.64	113.36
2	G	701	FAD	C4-N3-C2	-2.04	121.87	125.64
3	G	702	SAR	OXT-C-O	-2.04	118.22	123.30
2	C	701	FAD	C4-N3-C2	-2.01	121.94	125.64
2	A	701	FAD	O4'-C4'-C3'	2.00	113.96	109.10
2	C	701	FAD	O2P-P-O1P	2.00	122.13	112.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

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	P-O3P-PA-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C2'-C1'-N10-C10

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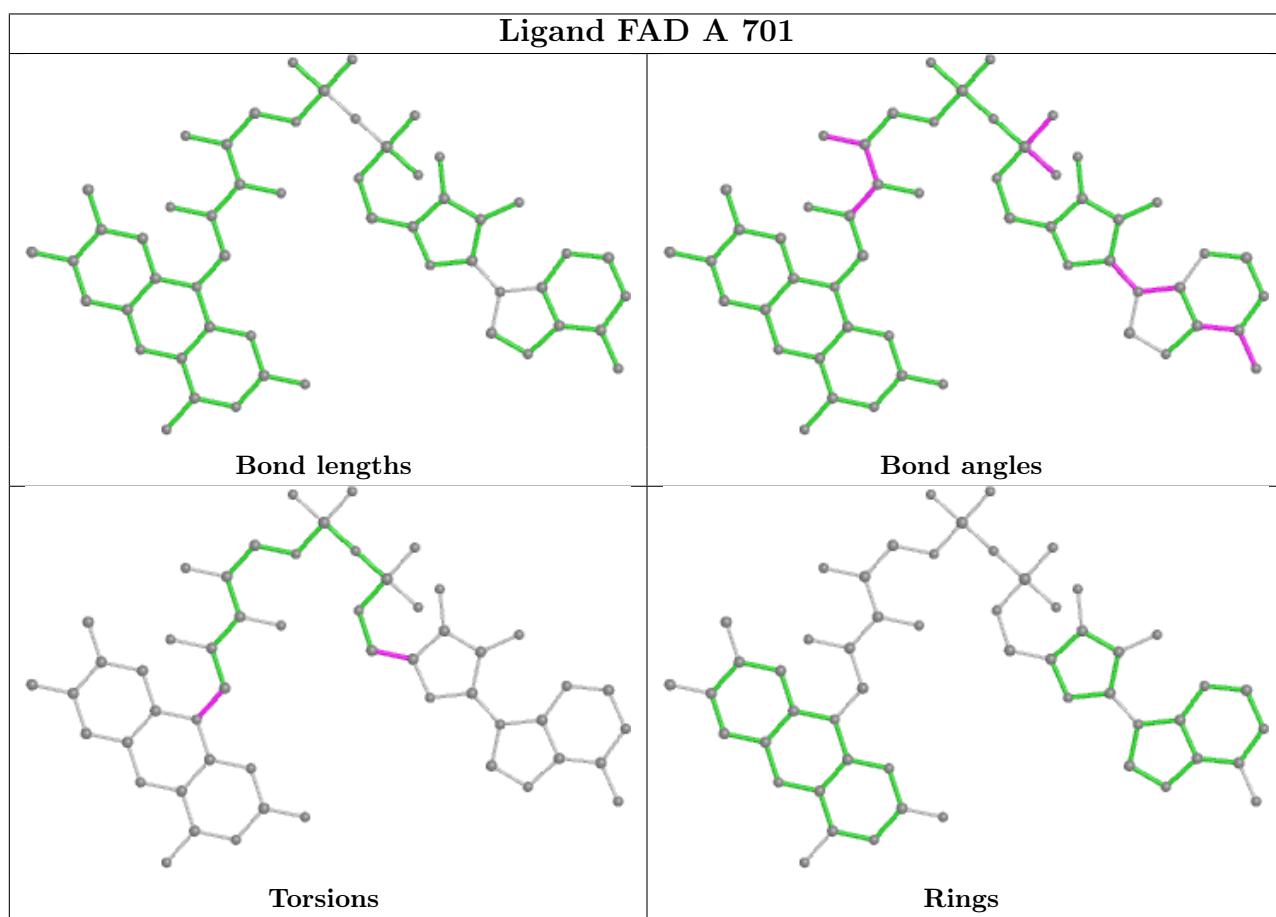
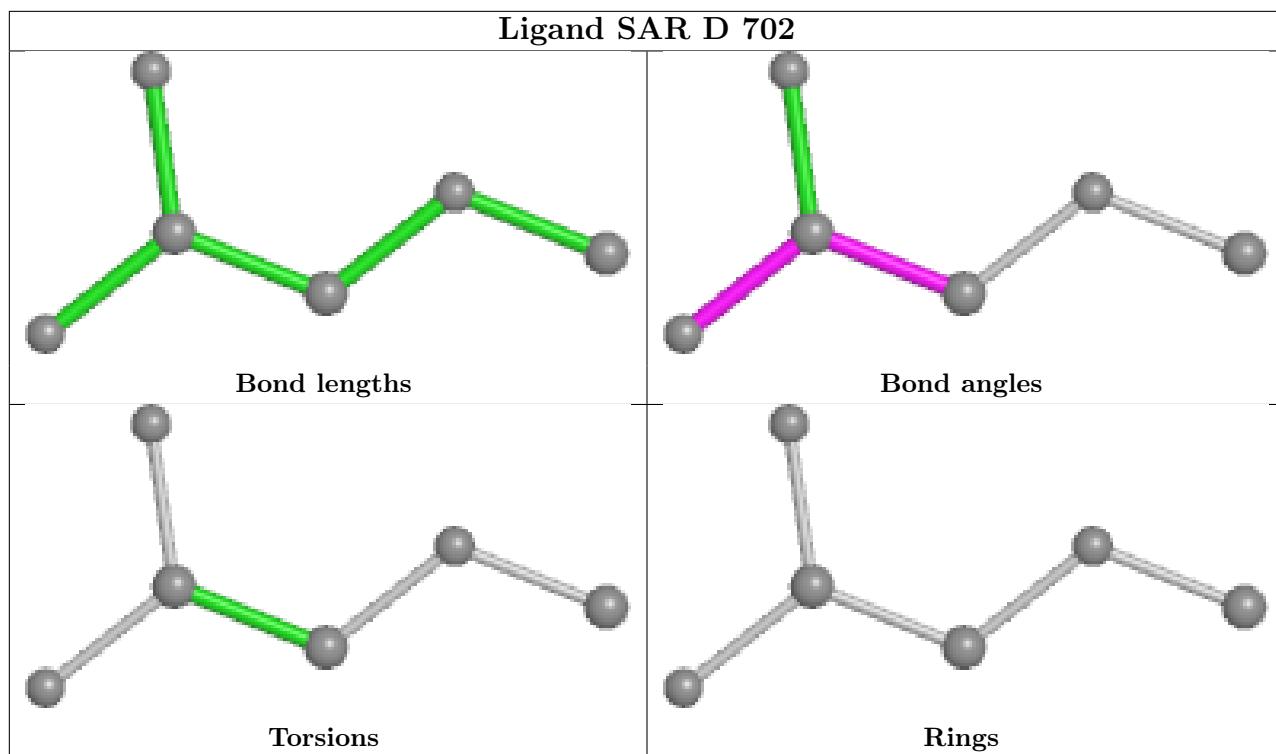
Mol	Chain	Res	Type	Atoms
2	E	701	FAD	C2'-C1'-N10-C10
2	C	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	C3B-C4B-C5B-O5B
2	G	701	FAD	O4B-C4B-C5B-O5B
2	H	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	N10-C1'-C2'-O2'

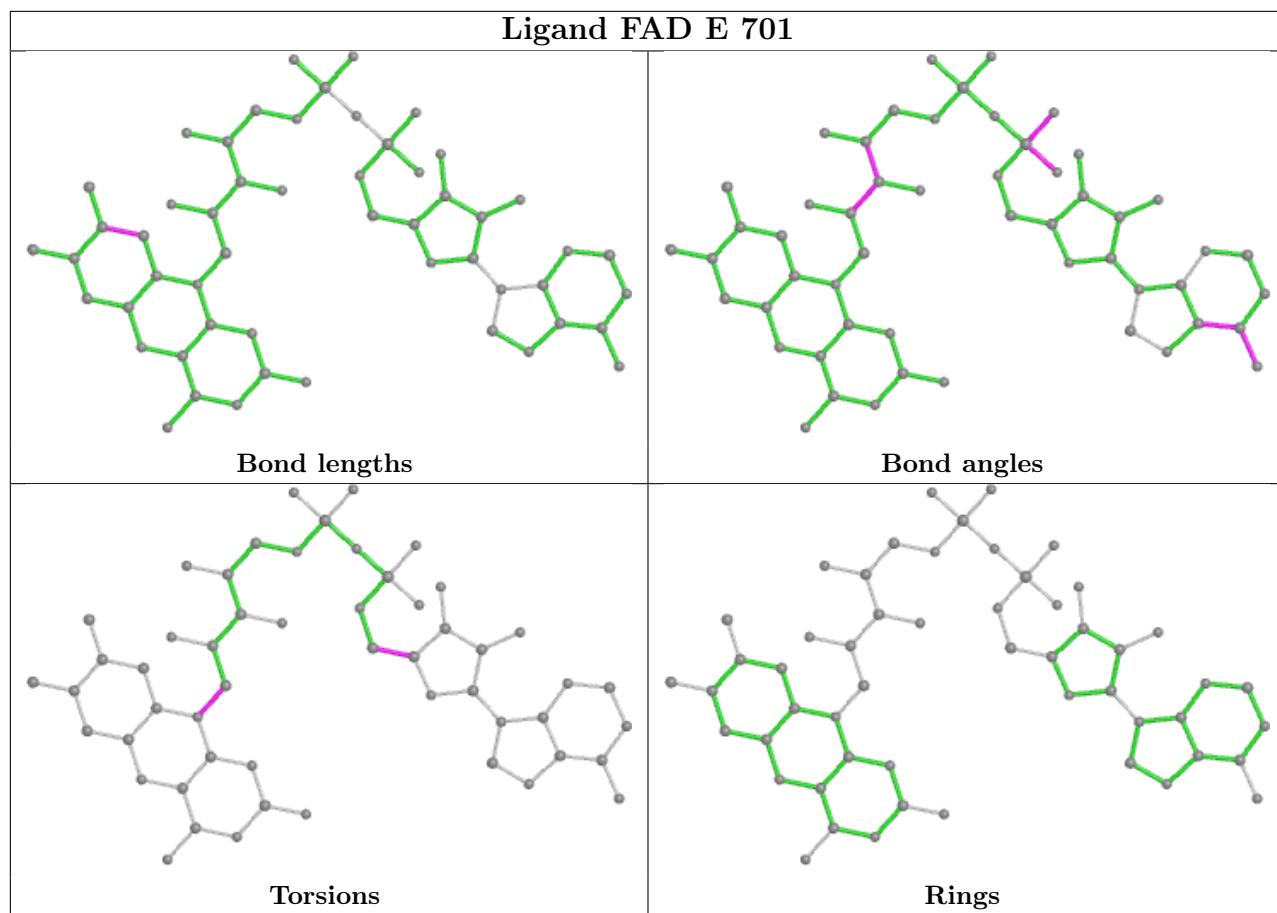
There are no ring outliers.

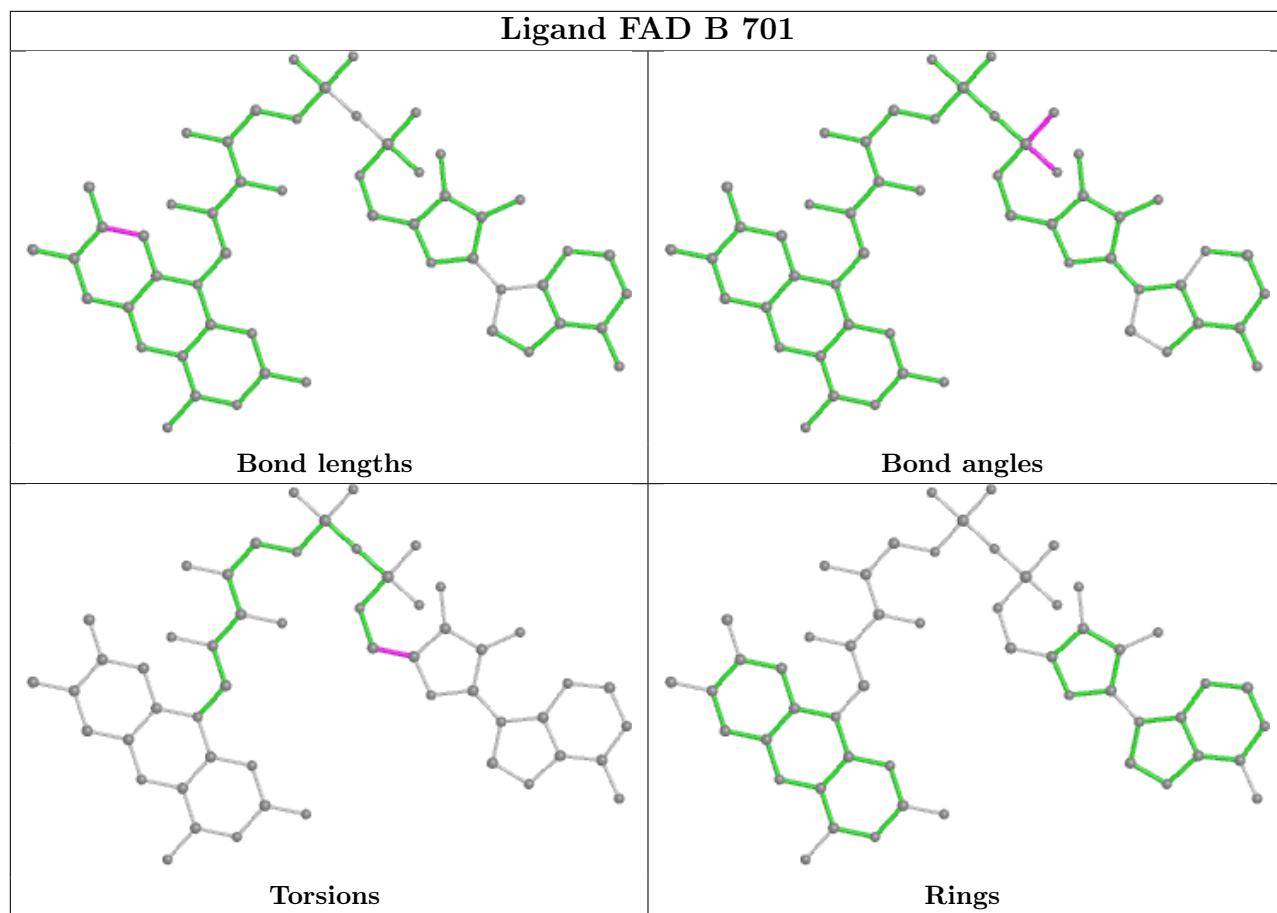
10 monomers are involved in 16 short contacts:

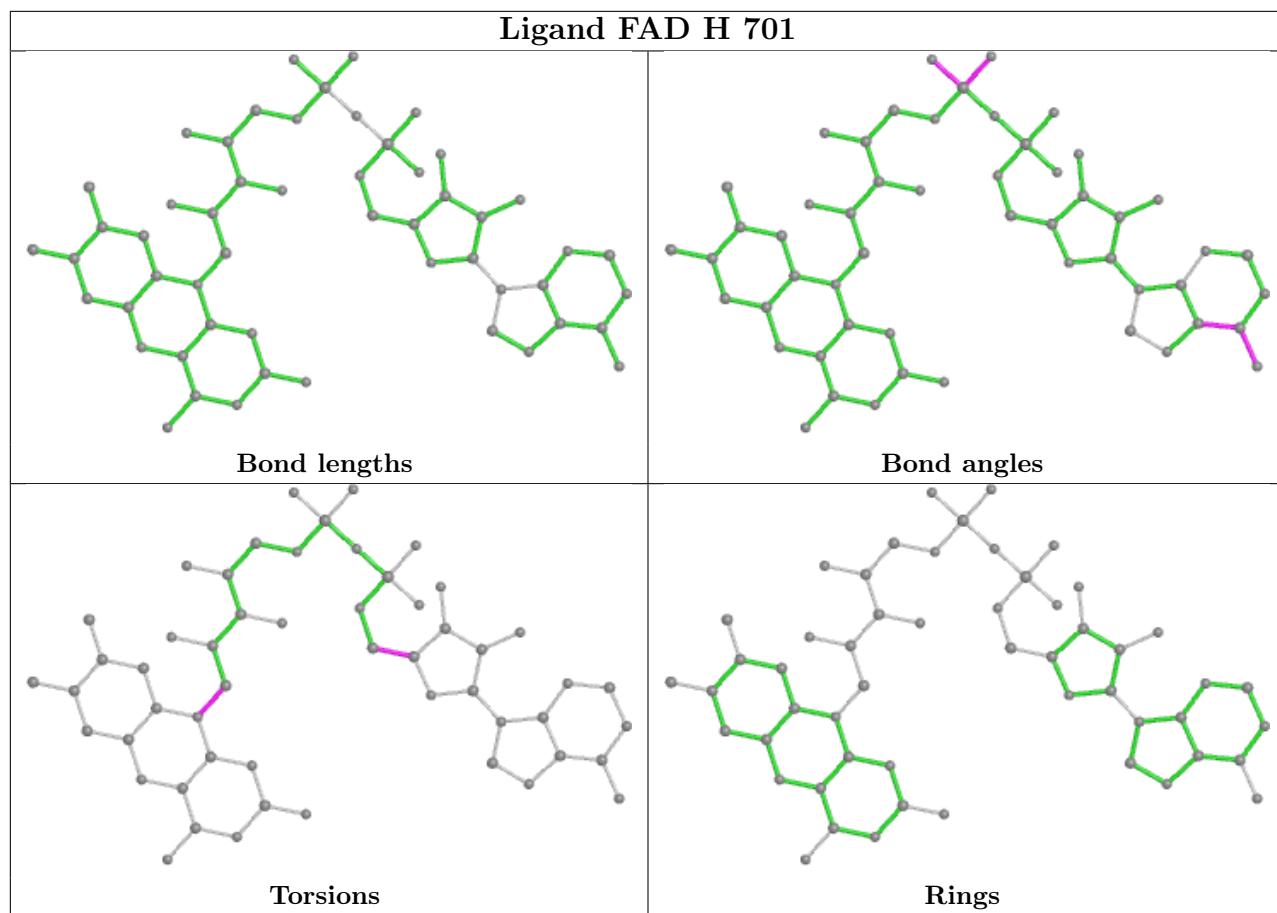
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	702	SAR	1	0
2	A	701	FAD	3	0
2	E	701	FAD	2	0
2	B	701	FAD	1	0
2	H	701	FAD	3	0
2	F	701	FAD	1	0
3	H	702	SAR	1	0
3	E	702	SAR	1	0
3	A	702	SAR	1	0
2	D	701	FAD	3	0

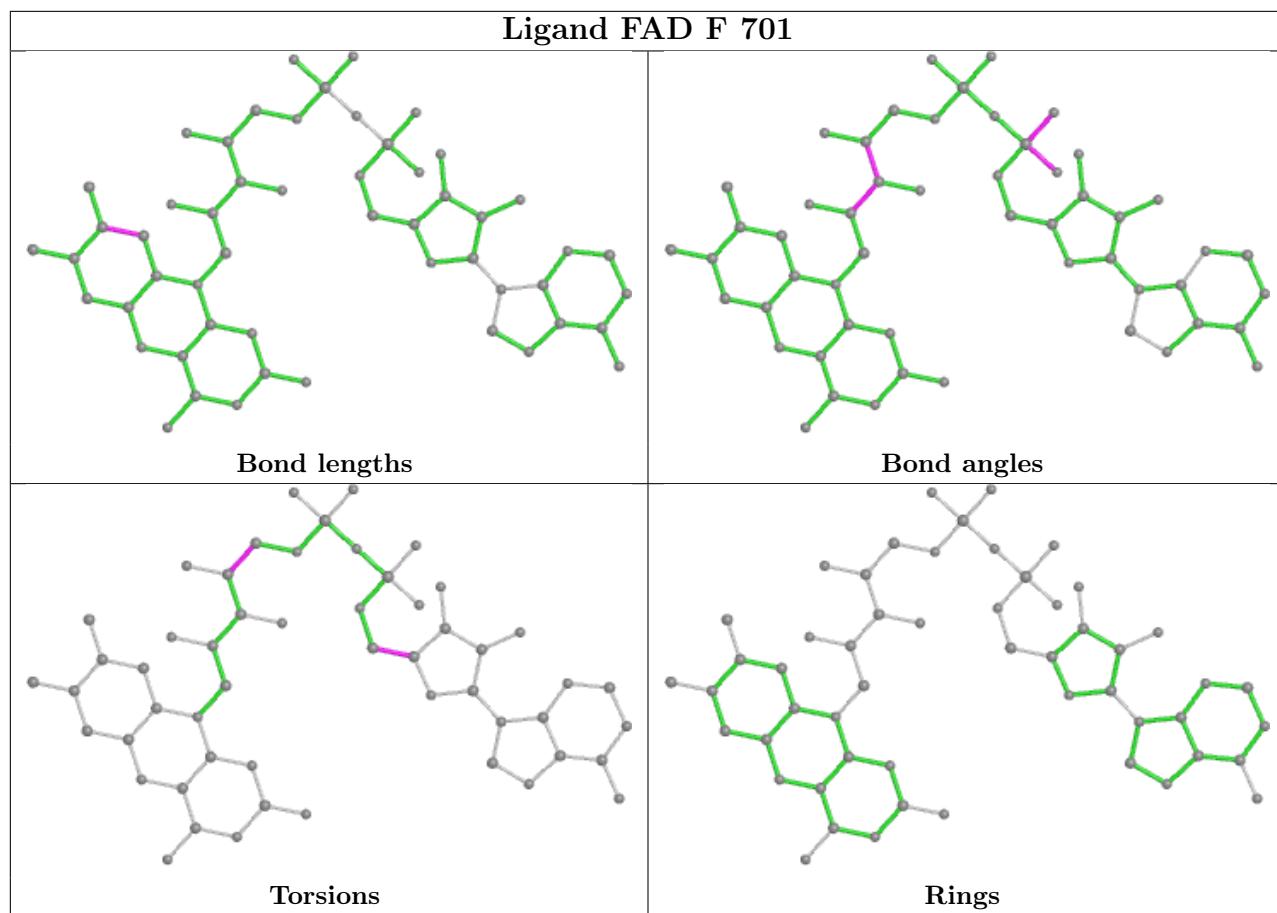
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

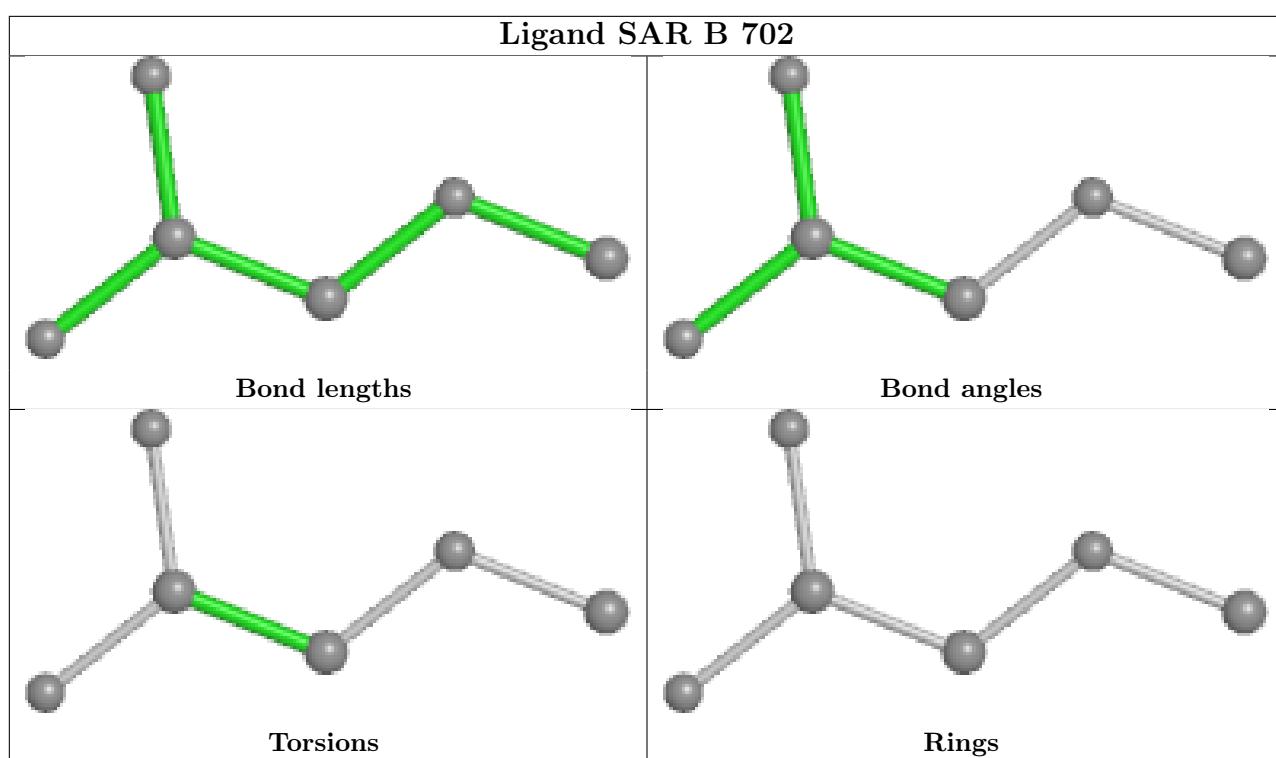
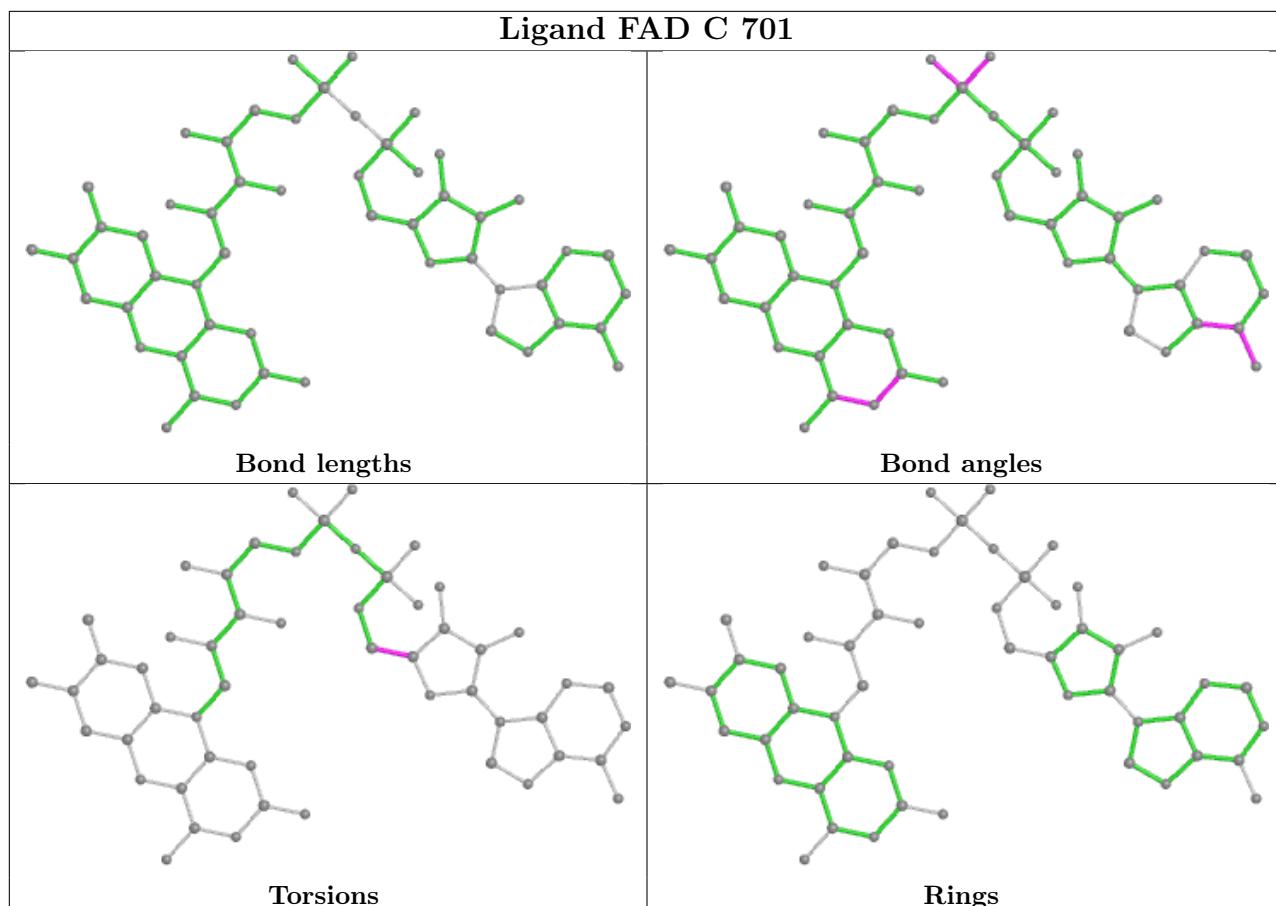


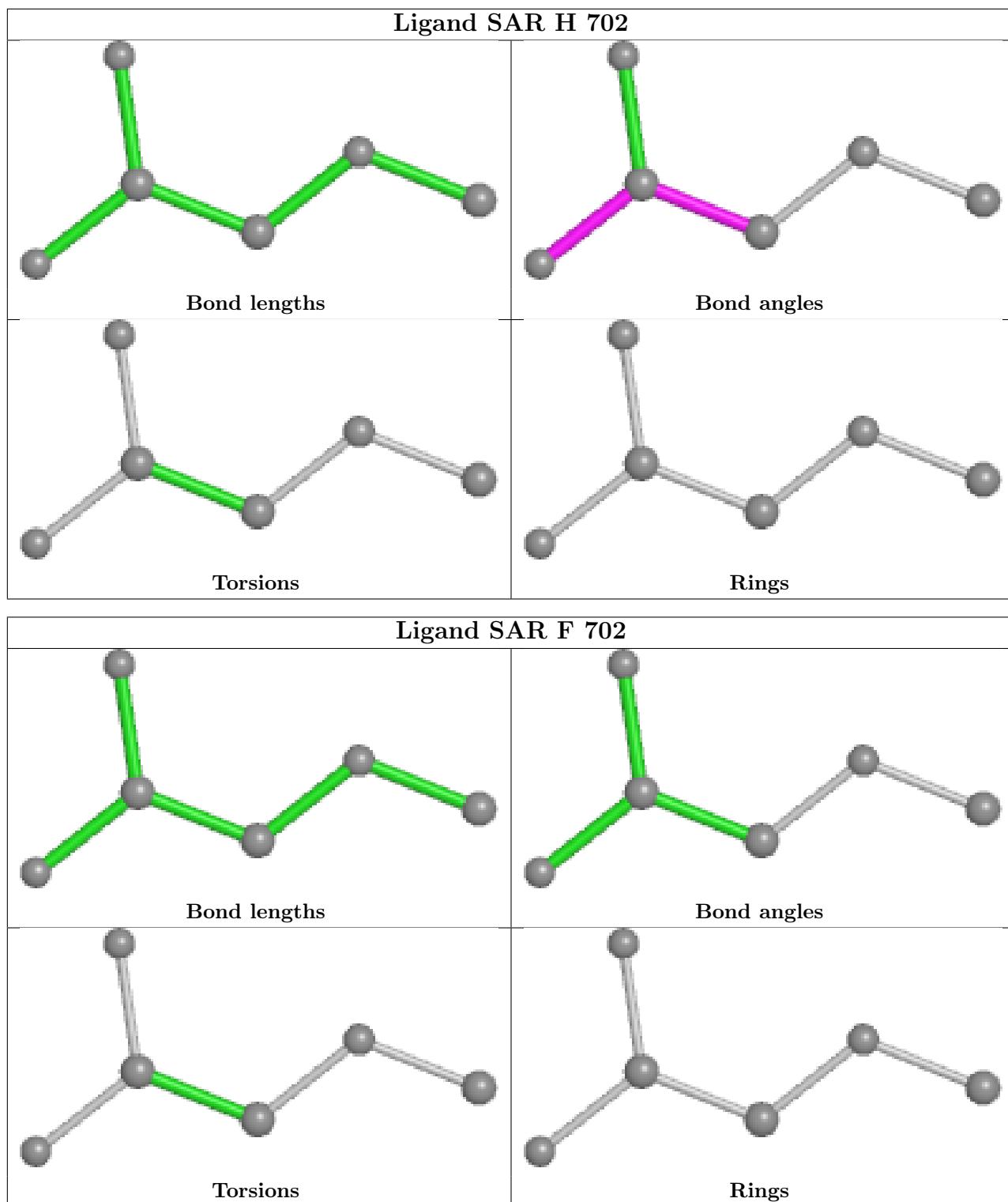


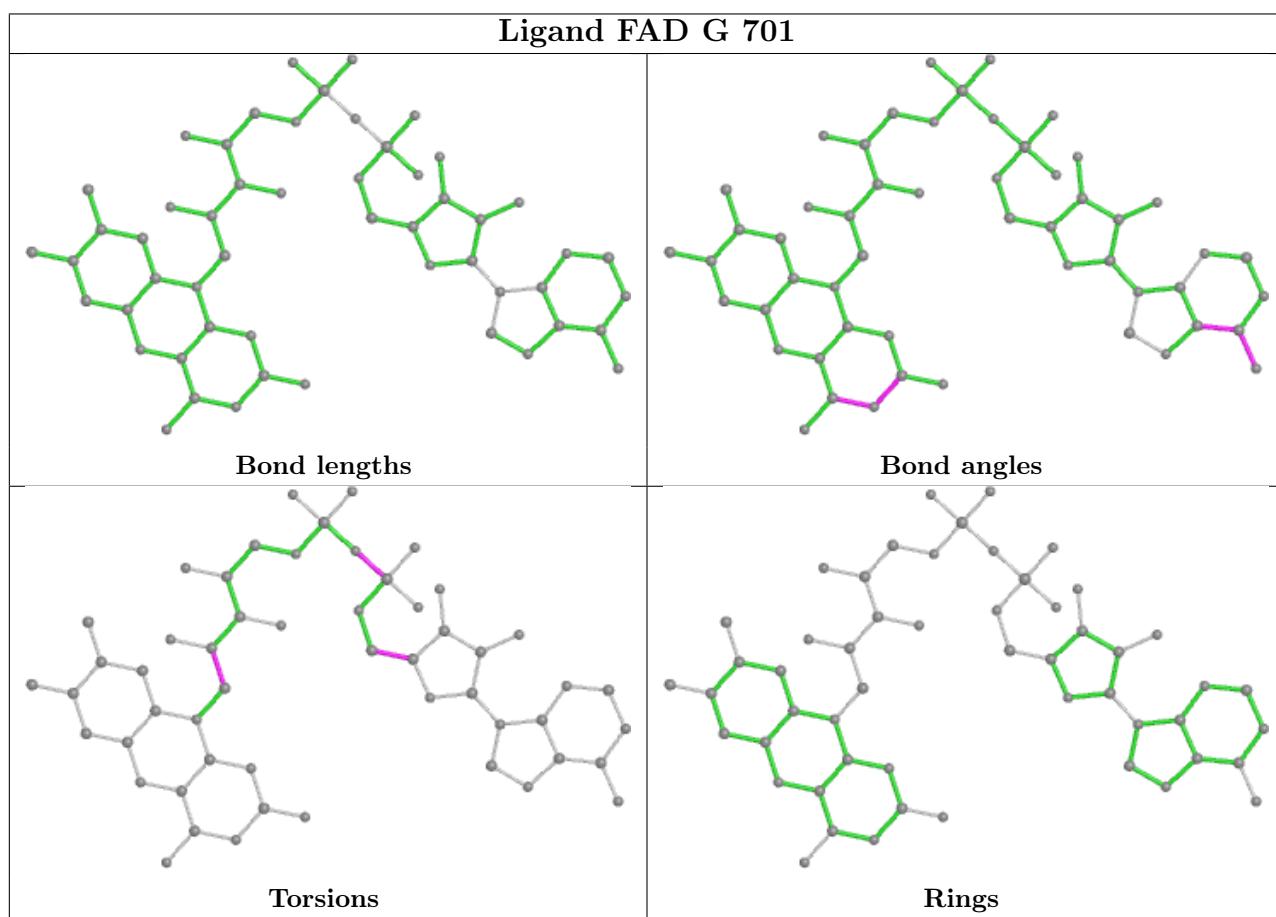
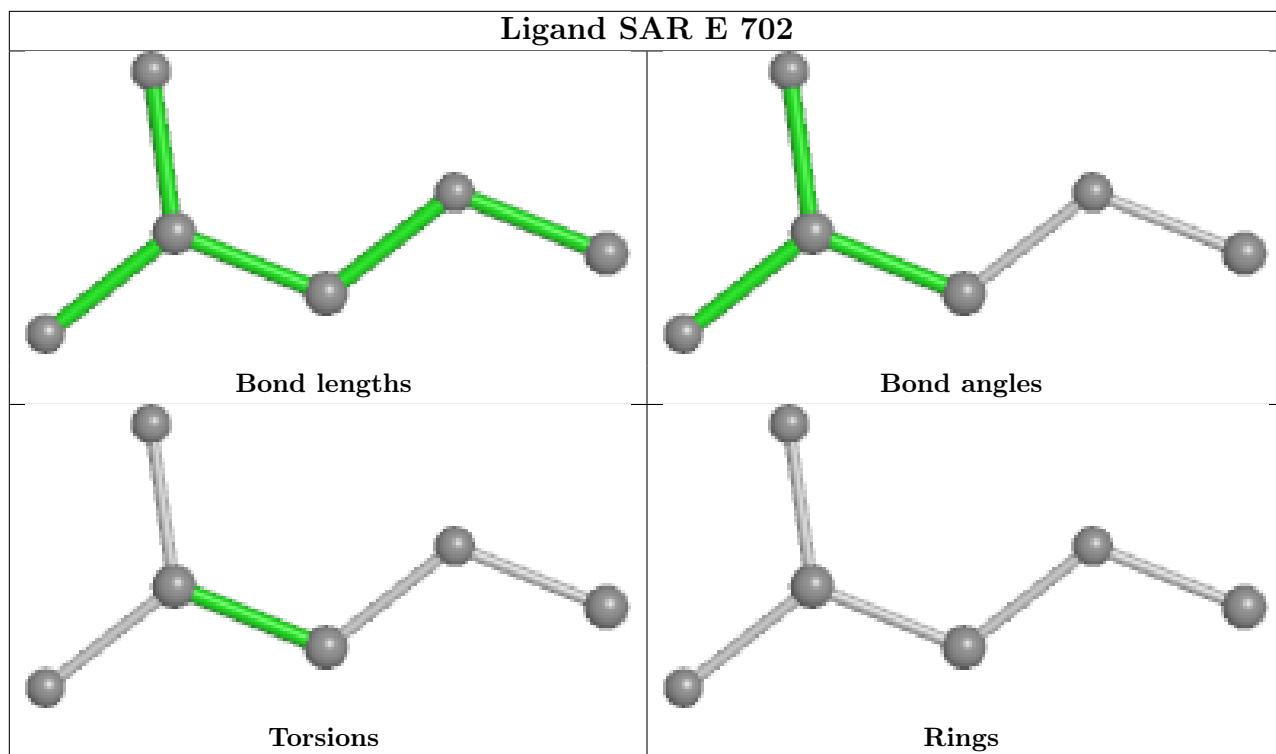


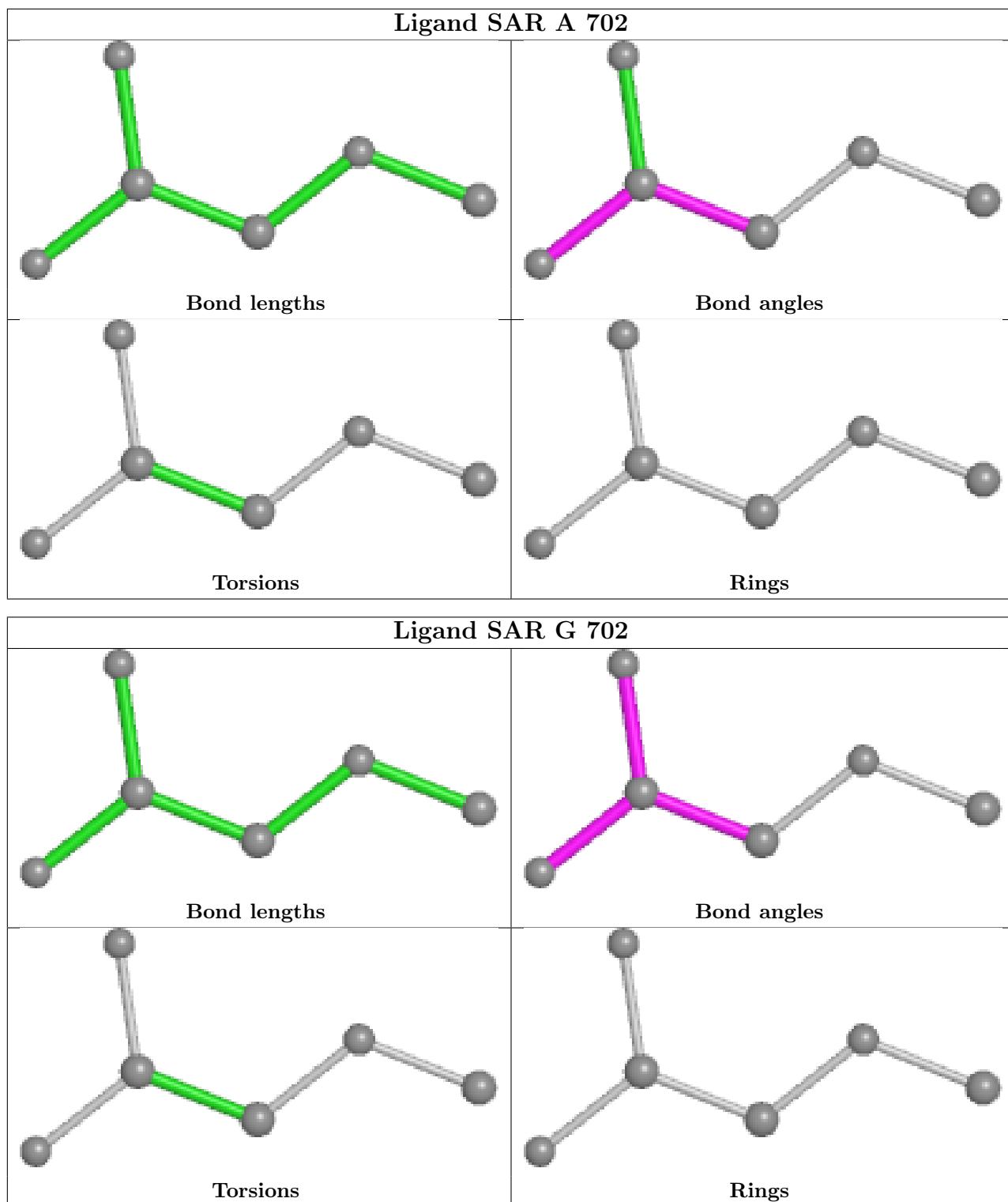


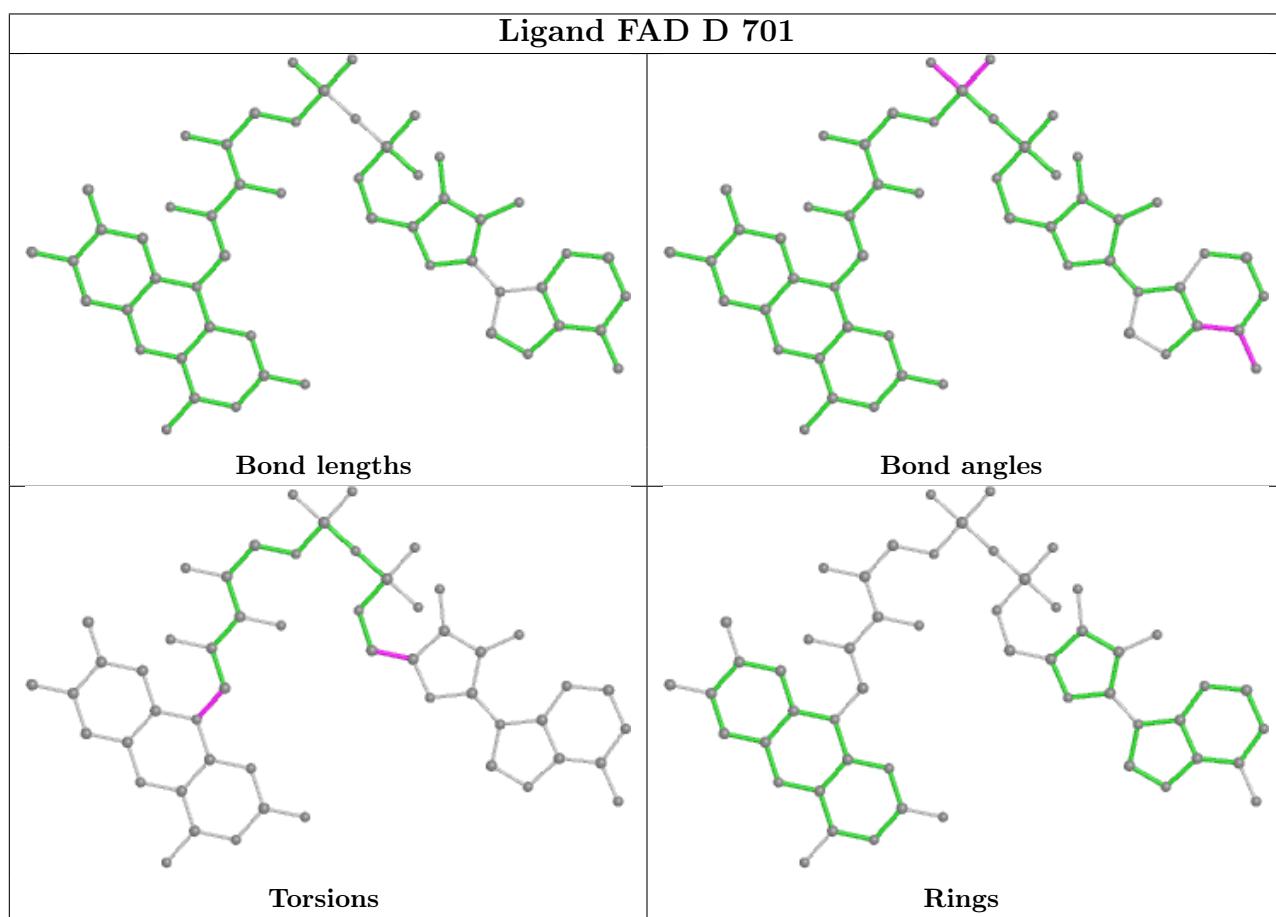
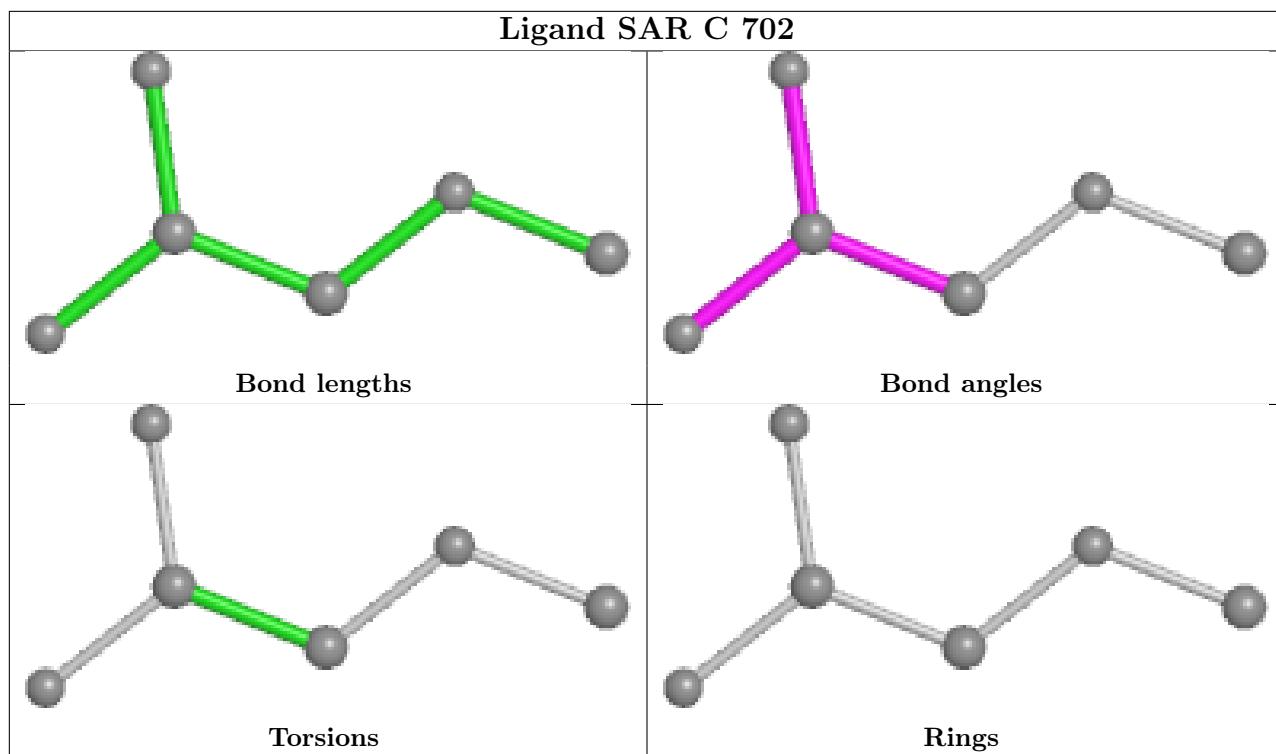












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	482/512 (94%)	0.31	5 (1%)	82	83	14, 27, 49, 80
1	B	482/512 (94%)	0.19	1 (0%)	95	95	12, 24, 46, 67
1	C	482/512 (94%)	0.52	31 (6%)	19	21	11, 29, 65, 87
1	D	479/512 (93%)	1.03	77 (16%)	1	1	16, 43, 96, 116
1	E	482/512 (94%)	0.31	8 (1%)	70	71	14, 27, 50, 75
1	F	482/512 (94%)	0.20	2 (0%)	92	93	11, 24, 47, 69
1	G	482/512 (94%)	0.55	27 (5%)	24	26	11, 29, 65, 88
1	H	479/512 (93%)	0.99	85 (17%)	1	1	16, 43, 97, 118
All	All	3850/4096 (93%)	0.51	236 (6%)	21	23	11, 29, 73, 118
							0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	34	PRO	7.5
1	D	211	GLY	7.2
1	H	206	HIS	7.0
1	G	243	LEU	6.5
1	H	211	GLY	6.4
1	H	202	ILE	6.2
1	D	361	TRP	6.0
1	D	223	GLY	5.9
1	D	190	ALA	5.8
1	D	242	GLY	5.6
1	D	202	ILE	5.6
1	G	47	GLN	5.6
1	D	238	ALA	5.5
1	H	238	ALA	5.5
1	G	48	TYR	5.5
1	D	219	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	13	VAL	5.4
1	H	41	LEU	5.3
1	H	209	VAL	5.2
1	D	193	ARG	5.2
1	D	358	GLU	5.2
1	H	243	LEU	5.1
1	D	217	GLY	5.1
1	D	206	HIS	5.0
1	H	361	TRP	4.9
1	D	239	ALA	4.9
1	D	224	HIS	4.9
1	D	393	GLY	4.8
1	D	394	LEU	4.7
1	H	36	VAL	4.7
1	D	220	LEU	4.6
1	H	212	VAL	4.6
1	D	204	ALA	4.6
1	D	38	VAL	4.5
1	H	208	ARG	4.5
1	H	222	ALA	4.5
1	D	236	LEU	4.5
1	D	491	HIS	4.4
1	C	54	ALA	4.3
1	H	225	VAL	4.3
1	A	11	THR	4.3
1	G	242	GLY	4.2
1	H	193	ARG	4.2
1	C	45	ALA	4.2
1	C	48	TYR	4.2
1	H	352	ILE	4.1
1	D	208	ARG	4.1
1	H	217	GLY	4.1
1	D	199	ALA	4.1
1	G	54	ALA	4.0
1	D	37	ARG	4.0
1	G	46	ARG	4.0
1	H	224	HIS	3.9
1	D	29	ILE	3.9
1	H	35	ASP	3.9
1	H	491	HIS	3.9
1	H	38	VAL	3.8
1	H	14	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	207	GLY	3.8
1	H	394	LEU	3.8
1	D	354	GLY	3.8
1	C	52	PRO	3.7
1	H	203	ARG	3.7
1	D	457	THR	3.7
1	H	25	VAL	3.7
1	G	281	CYS	3.6
1	D	191	GLY	3.6
1	G	49	GLY	3.6
1	H	384	LEU	3.6
1	H	392	ASP	3.5
1	H	220	LEU	3.5
1	H	244	ALA	3.5
1	D	384	LEU	3.5
1	H	40	LEU	3.5
1	A	10	GLN	3.4
1	D	16	VAL	3.4
1	D	34	PRO	3.4
1	D	209	VAL	3.4
1	H	359	GLY	3.4
1	D	389	THR	3.4
1	D	226	VAL	3.3
1	H	240	LEU	3.3
1	G	244	ALA	3.3
1	H	226	VAL	3.3
1	H	353	GLY	3.3
1	C	236	LEU	3.3
1	G	491	HIS	3.2
1	H	393	GLY	3.2
1	D	33	ARG	3.2
1	H	385	MET	3.2
1	D	210	GLU	3.2
1	H	15	VAL	3.2
1	G	235	ARG	3.1
1	H	223	GLY	3.1
1	D	27	VAL	3.1
1	D	225	VAL	3.1
1	A	395	ARG	3.1
1	H	210	GLU	3.0
1	H	395	ARG	3.0
1	D	351	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	464	LEU	3.0
1	E	11	THR	3.0
1	C	235	ARG	3.0
1	H	16	VAL	3.0
1	H	236	LEU	3.0
1	D	243	LEU	2.9
1	D	25	VAL	2.9
1	D	235	ARG	2.9
1	C	10	GLN	2.9
1	C	55	GLY	2.9
1	G	50	ALA	2.9
1	C	51	THR	2.9
1	H	33	ARG	2.9
1	C	220	LEU	2.9
1	H	13	VAL	2.8
1	H	387	GLY	2.8
1	H	397	PHE	2.8
1	D	356	SER	2.8
1	G	53	ALA	2.8
1	D	35	ASP	2.8
1	D	39	THR	2.8
1	H	194	LEU	2.8
1	H	204	ALA	2.8
1	D	359	GLY	2.7
1	E	36	VAL	2.7
1	C	398	ARG	2.7
1	H	376	LEU	2.7
1	H	487	HIS	2.7
1	D	212	VAL	2.7
1	H	32	THR	2.7
1	D	14	ILE	2.6
1	C	207	GLY	2.6
1	G	394	LEU	2.6
1	F	392	ASP	2.6
1	H	356	SER	2.6
1	H	457	THR	2.6
1	H	29	ILE	2.6
1	G	206	HIS	2.6
1	D	382	VAL	2.6
1	D	376	LEU	2.6
1	G	236	LEU	2.6
1	A	139	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	215	ASP	2.6
1	G	216	ASP	2.6
1	D	182	ALA	2.6
1	H	484	ALA	2.6
1	C	210	GLU	2.6
1	C	222	ALA	2.5
1	C	484	ALA	2.5
1	H	490	TRP	2.5
1	C	206	HIS	2.5
1	G	204	ALA	2.5
1	H	483	TYR	2.5
1	H	360	LEU	2.5
1	G	203	ARG	2.5
1	D	301	VAL	2.5
1	H	199	ALA	2.5
1	E	392	ASP	2.5
1	C	238	ALA	2.5
1	H	382	VAL	2.5
1	G	10	GLN	2.5
1	C	218	ASP	2.5
1	C	194	LEU	2.5
1	H	389	THR	2.5
1	A	68	ALA	2.4
1	C	242	GLY	2.4
1	D	355	THR	2.4
1	E	61	PHE	2.4
1	H	23	LEU	2.4
1	H	39	THR	2.4
1	H	183	LEU	2.4
1	H	239	ALA	2.4
1	D	488	ARG	2.4
1	H	482	TYR	2.4
1	D	357	VAL	2.4
1	D	32	THR	2.3
1	D	449	GLU	2.3
1	C	243	LEU	2.3
1	E	170	GLY	2.3
1	D	490	TRP	2.3
1	G	479	LEU	2.3
1	C	204	ALA	2.3
1	D	80	LEU	2.3
1	E	394	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	213	VAL	2.3
1	H	26	GLY	2.2
1	C	208	ARG	2.2
1	H	31	ARG	2.2
1	D	241	PRO	2.2
1	D	387	GLY	2.2
1	H	390	GLY	2.2
1	F	35	ASP	2.2
1	H	355	THR	2.2
1	H	30	ALA	2.2
1	C	195	HIS	2.2
1	E	140	ASN	2.2
1	C	44	PRO	2.2
1	H	459	THR	2.2
1	C	46	ARG	2.2
1	D	213	VAL	2.2
1	H	27	VAL	2.2
1	G	202	ILE	2.2
1	H	180	LEU	2.2
1	D	391	VAL	2.2
1	D	195	HIS	2.1
1	D	21	LEU	2.1
1	D	93	GLU	2.1
1	G	220	LEU	2.1
1	H	21	LEU	2.1
1	C	47	GLN	2.1
1	H	213	VAL	2.1
1	H	379	ARG	2.1
1	D	385	MET	2.1
1	H	201	GLU	2.1
1	D	205	SER	2.1
1	D	398	ARG	2.1
1	H	235	ARG	2.1
1	D	237	VAL	2.1
1	D	390	GLY	2.1
1	H	191	GLY	2.1
1	C	209	VAL	2.1
1	D	36	VAL	2.1
1	D	197	VAL	2.1
1	C	251	TYR	2.1
1	G	490	TRP	2.1
1	H	486	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	206	HIS	2.1
1	G	51	THR	2.0
1	C	149	GLU	2.0
1	H	72	GLU	2.0
1	B	206	HIS	2.0
1	D	380	HIS	2.0
1	G	238	ALA	2.0
1	H	231	ALA	2.0
1	D	392	ASP	2.0
1	G	232	ARG	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

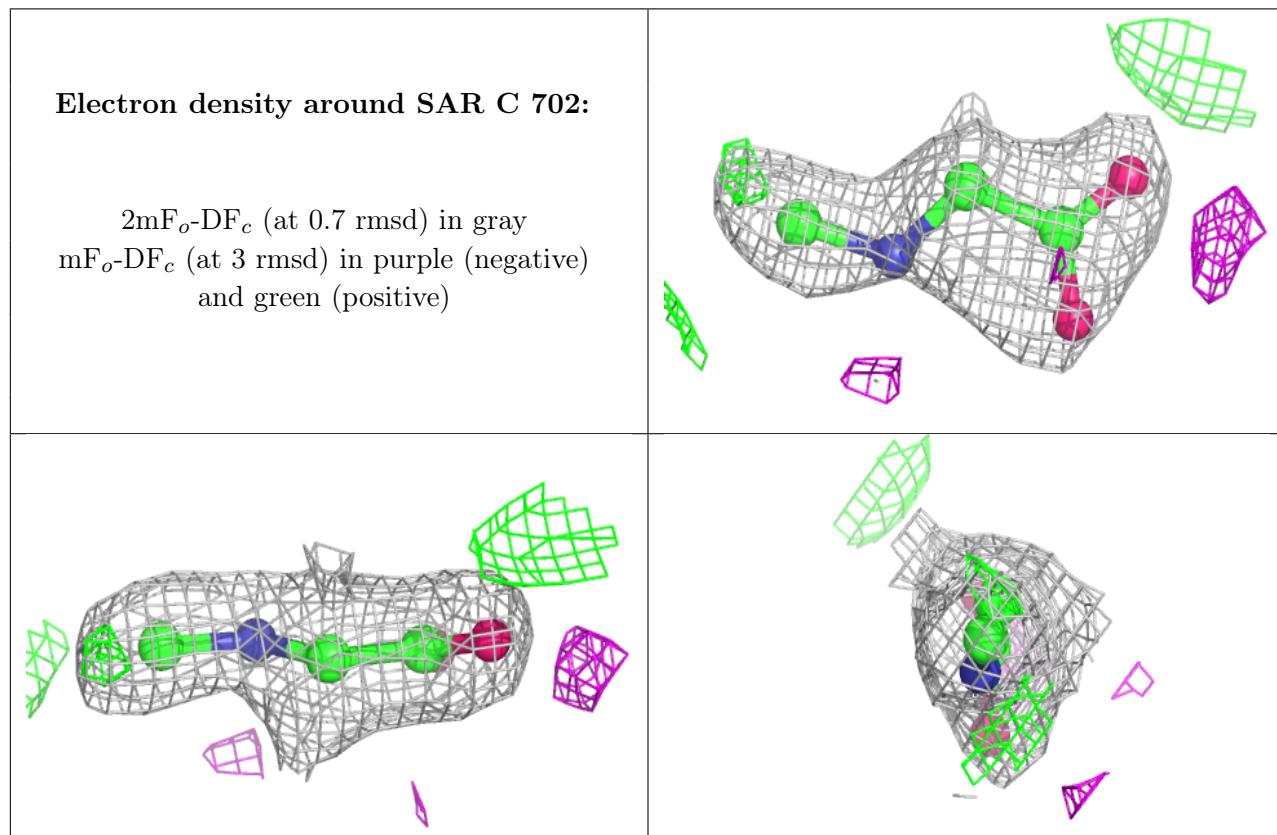
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SAR	C	702	6/6	0.77	0.22	48,51,57,57	0
3	SAR	G	702	6/6	0.77	0.23	48,50,52,54	0
2	FAD	G	701	53/53	0.79	0.23	35,51,67,68	0
3	SAR	H	702	6/6	0.80	0.29	42,43,48,49	0
2	FAD	C	701	53/53	0.86	0.20	32,49,66,67	0
2	FAD	H	701	53/53	0.89	0.15	38,47,77,81	0
2	FAD	D	701	53/53	0.92	0.14	35,46,74,79	0
3	SAR	D	702	6/6	0.95	0.11	41,45,46,47	0
3	SAR	F	702	6/6	0.95	0.12	19,22,25,27	0
2	FAD	E	701	53/53	0.96	0.11	15,20,23,24	0
3	SAR	A	702	6/6	0.97	0.12	24,28,31,34	0
2	FAD	A	701	53/53	0.97	0.11	15,21,23,24	0
2	FAD	F	701	53/53	0.97	0.10	12,16,18,20	0

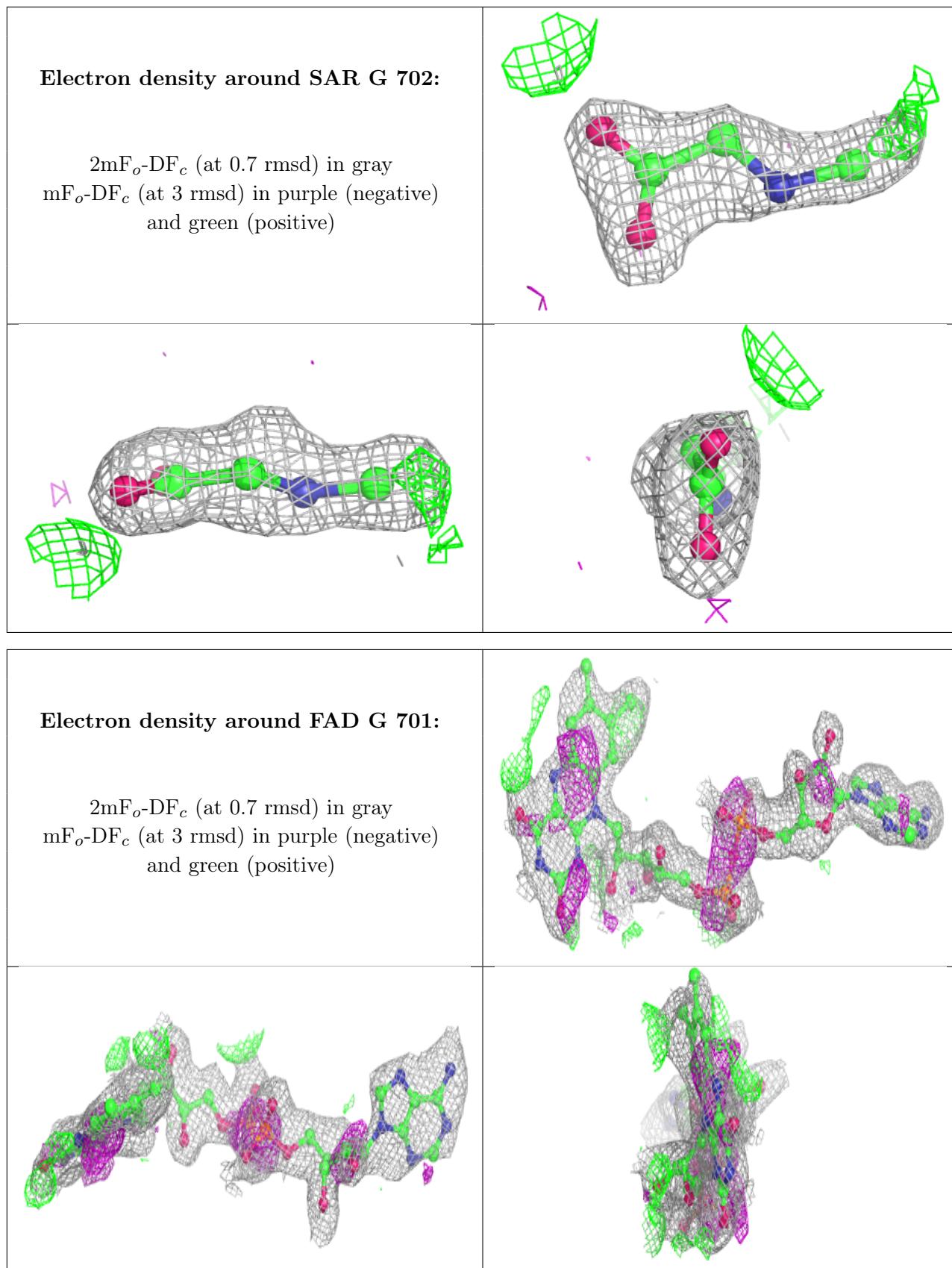
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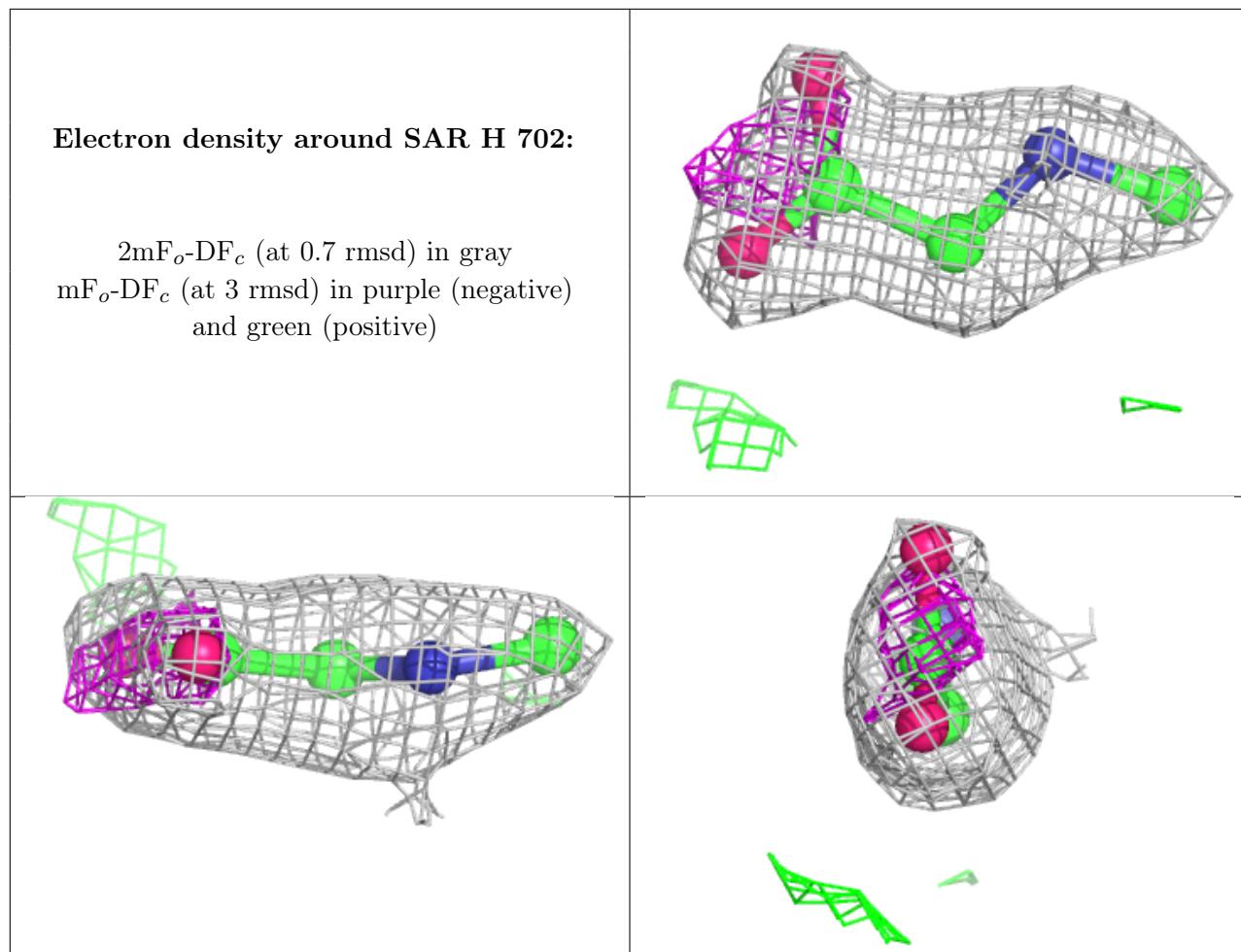
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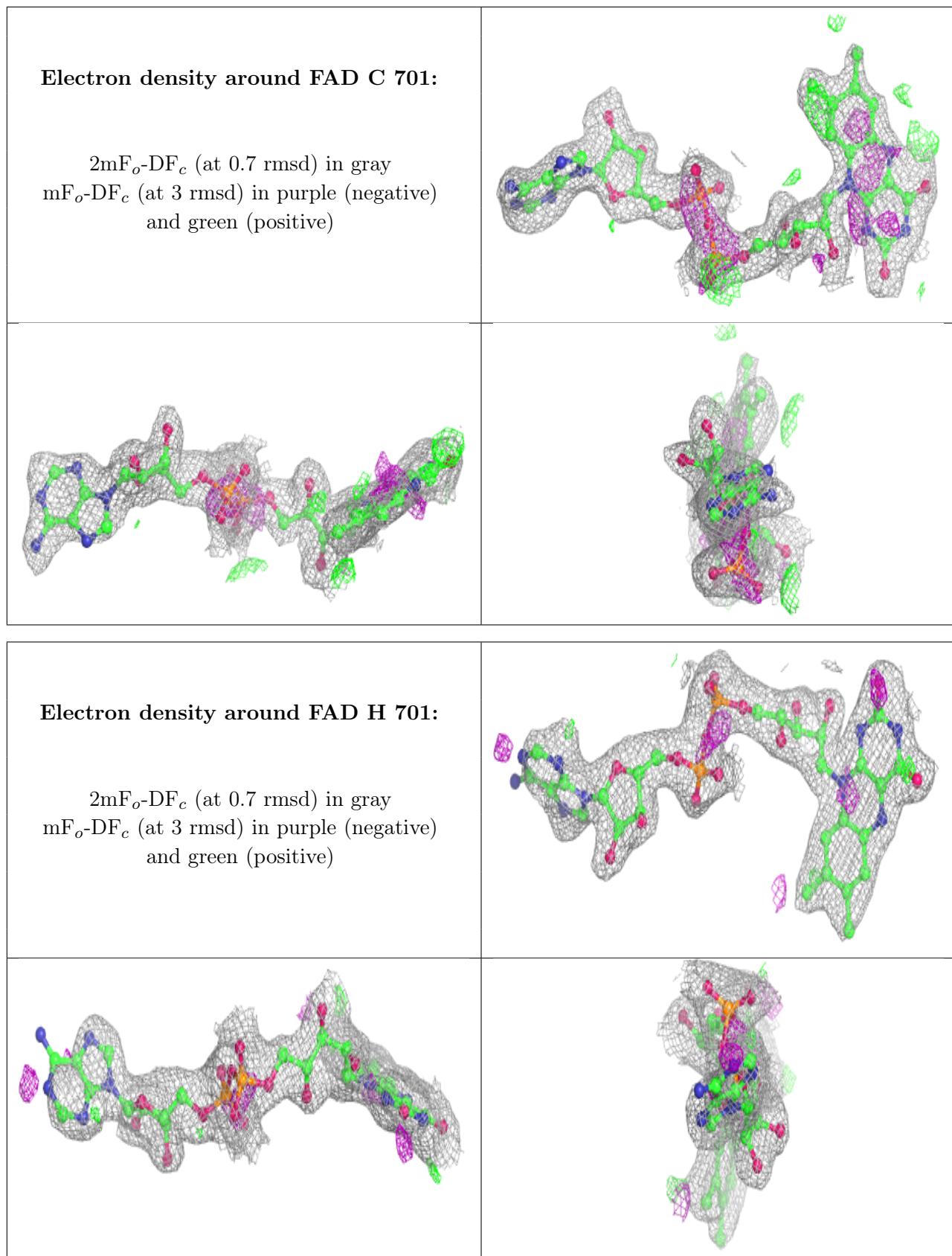
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	B	701	53/53	0.98	0.09	13,16,18,20	0
3	SAR	B	702	6/6	0.98	0.08	19,22,24,28	0
3	SAR	E	702	6/6	0.98	0.11	23,29,30,32	0

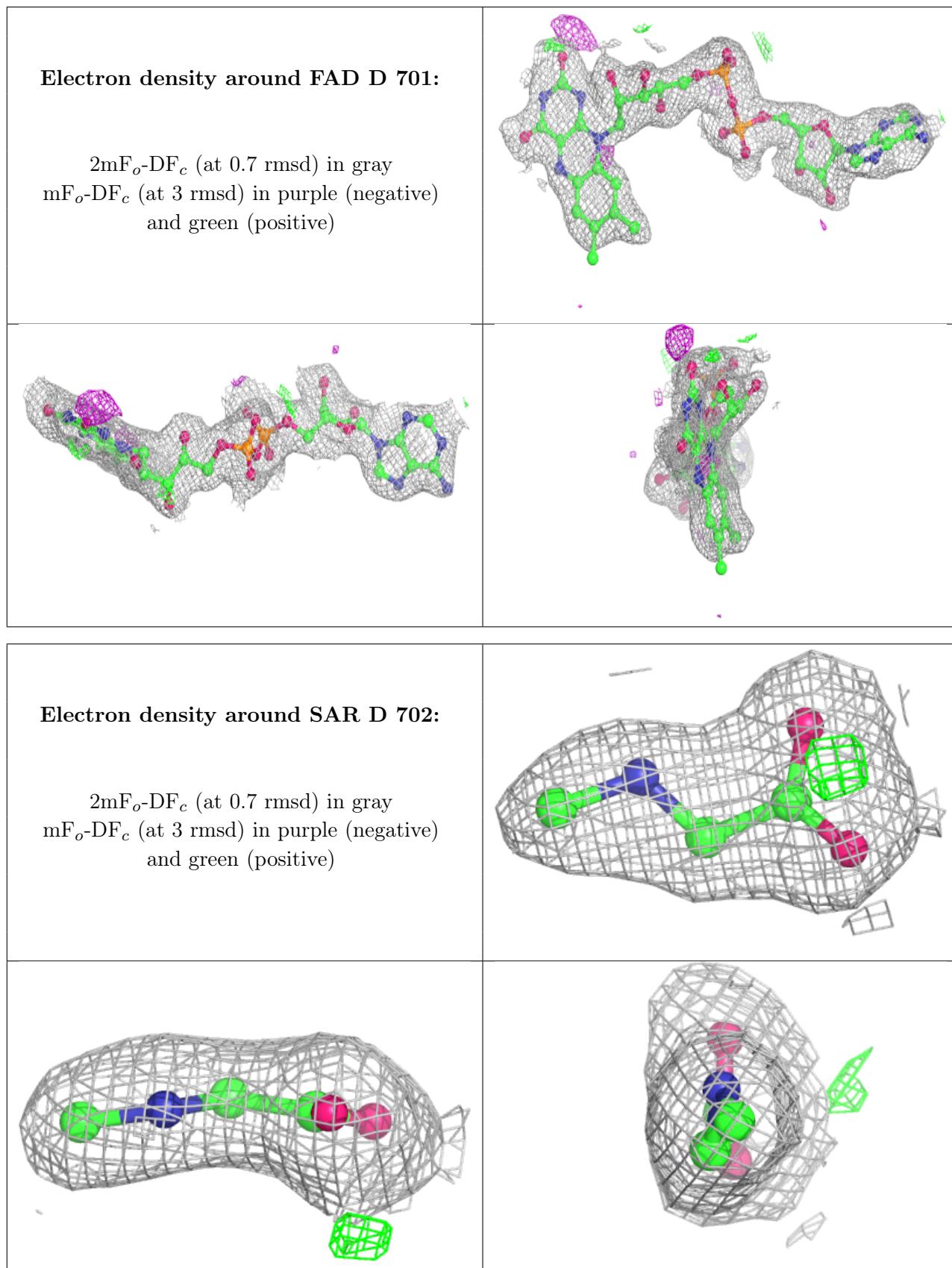
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

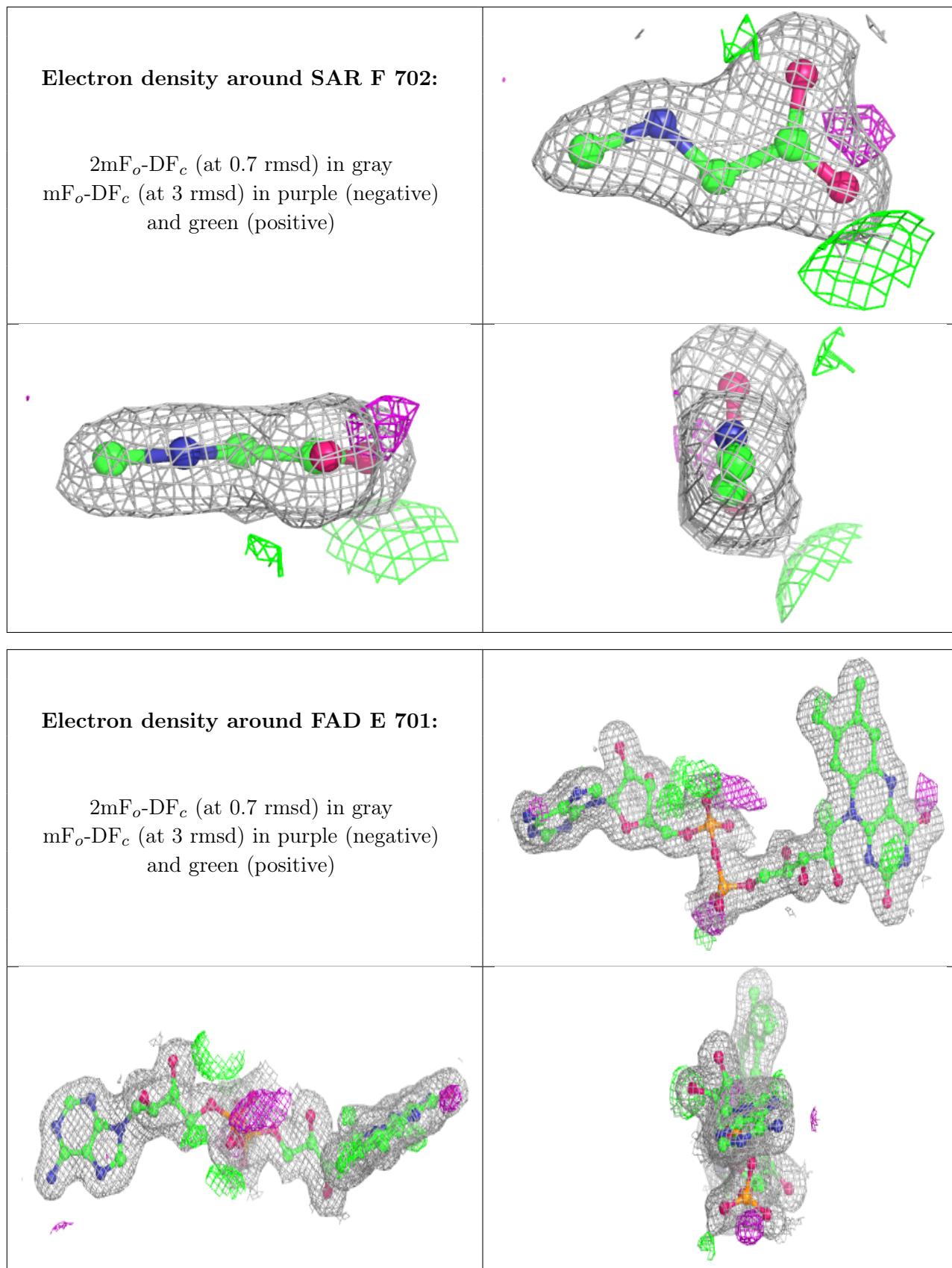


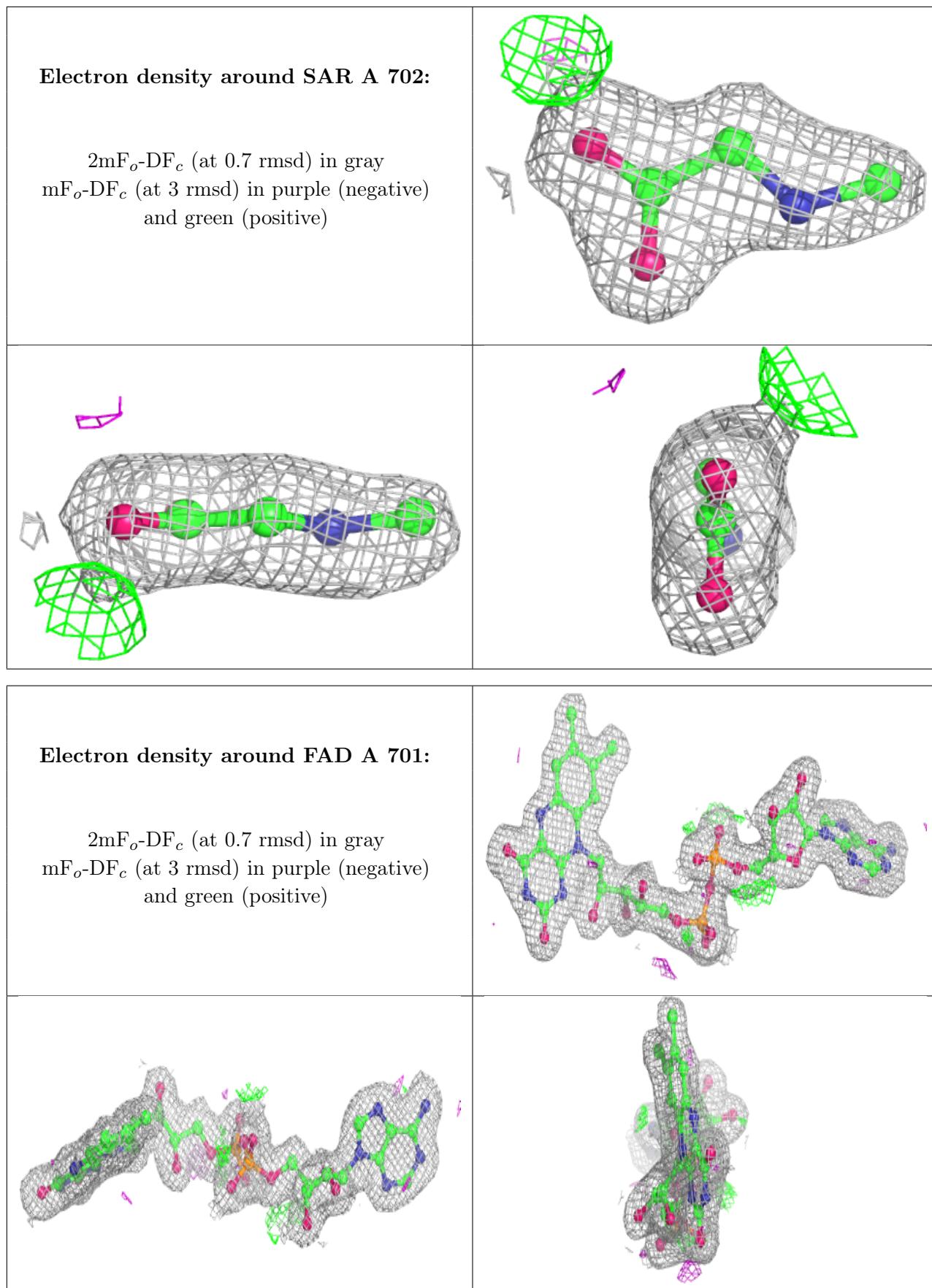


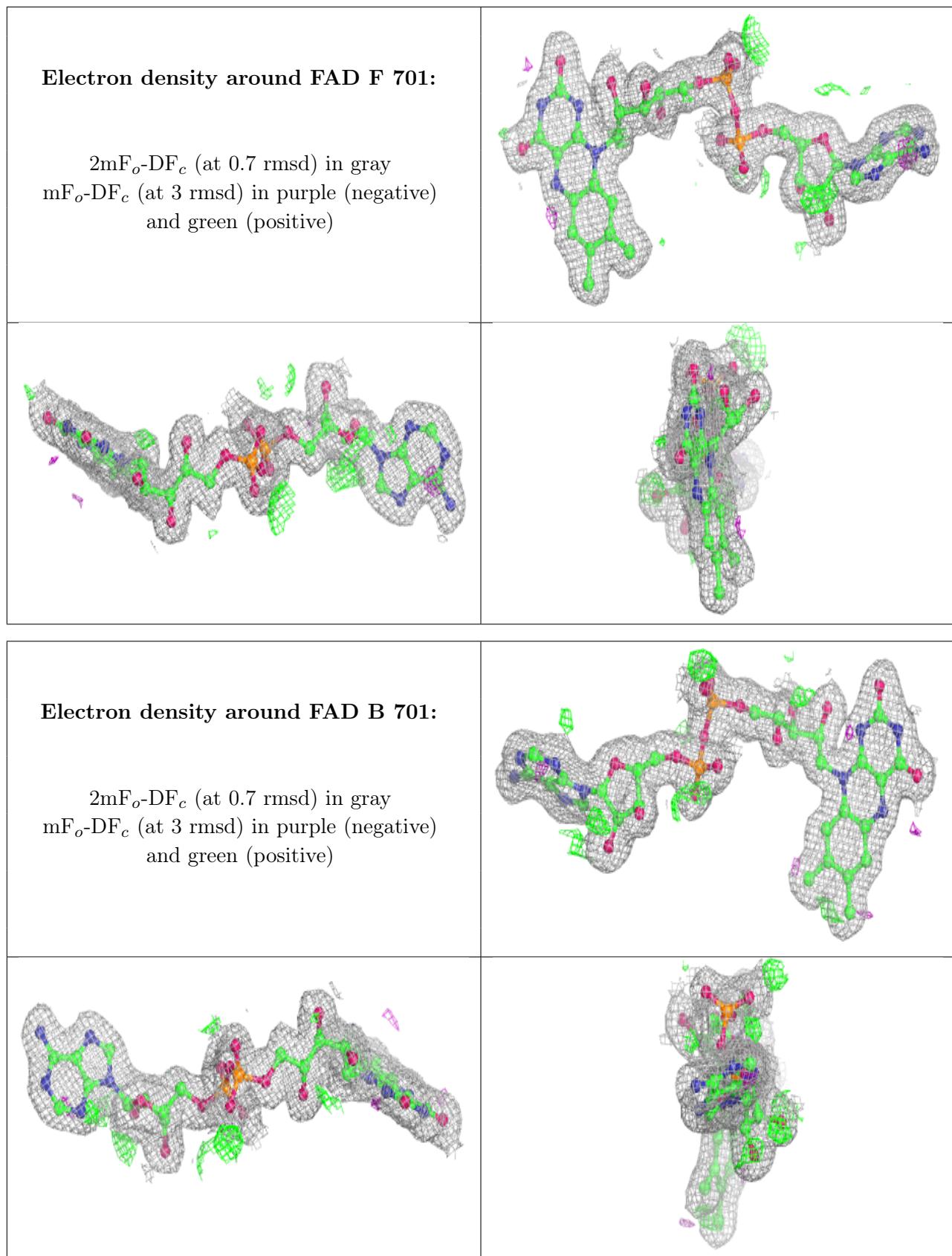


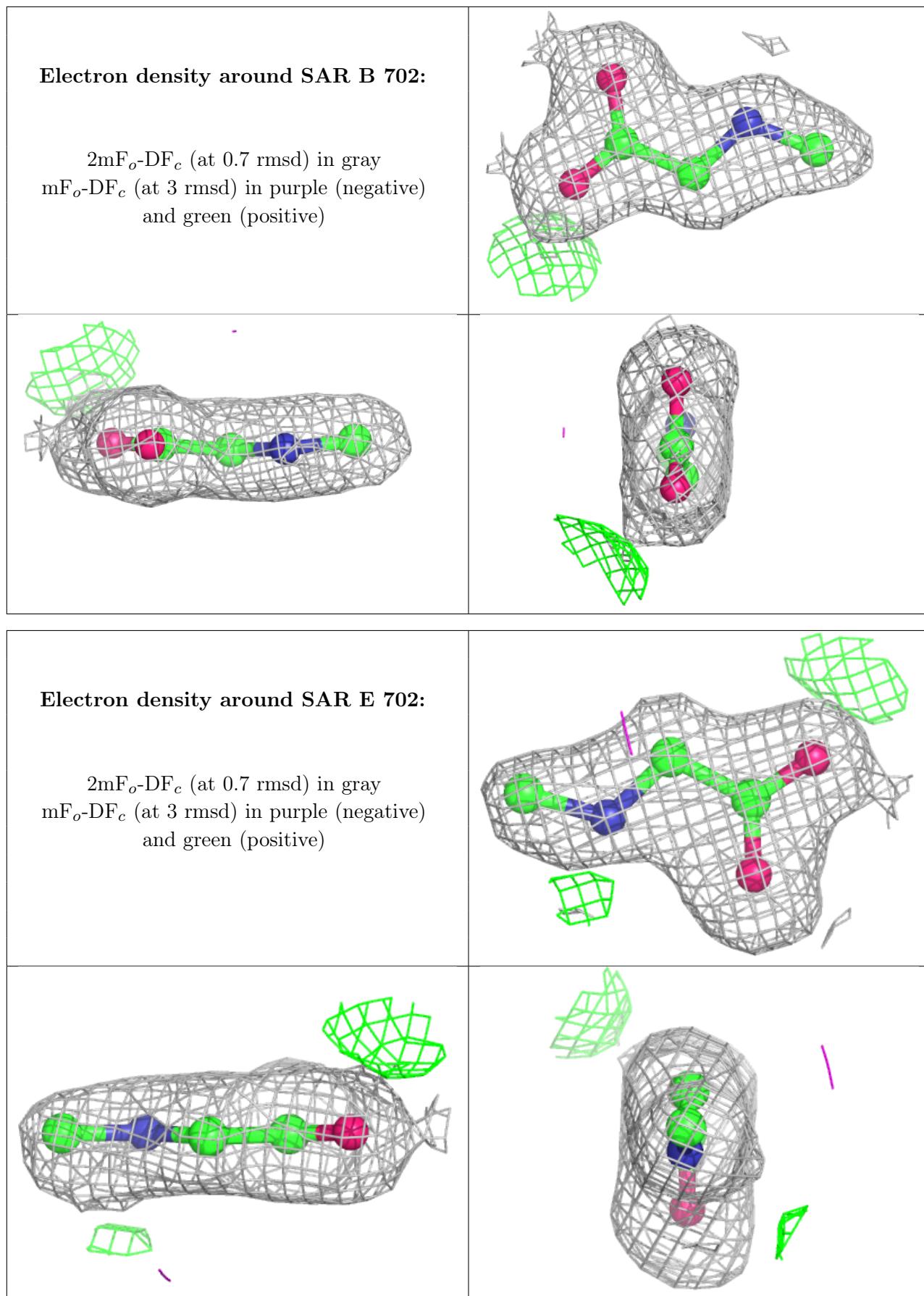












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.