



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:26 AM BST

PDB ID : 6TJR  
Title : Structure of HdrA-like subunit from *Hyphomicrobium denitrificans*  
Authors : Kayastha, K.; Ermler, U.; Dahl, C.  
Deposited on : 2019-11-26  
Resolution : 1.43 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

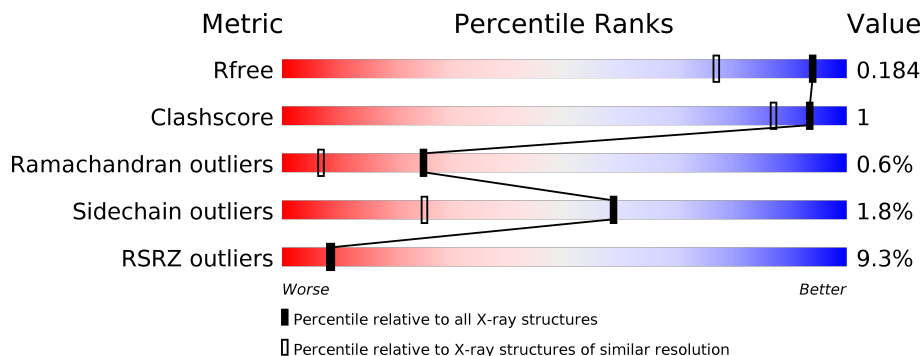
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	A	403	-	-	-	X
4	MES	A	405	-	-	-	X

## 2 Entry composition [i](#)

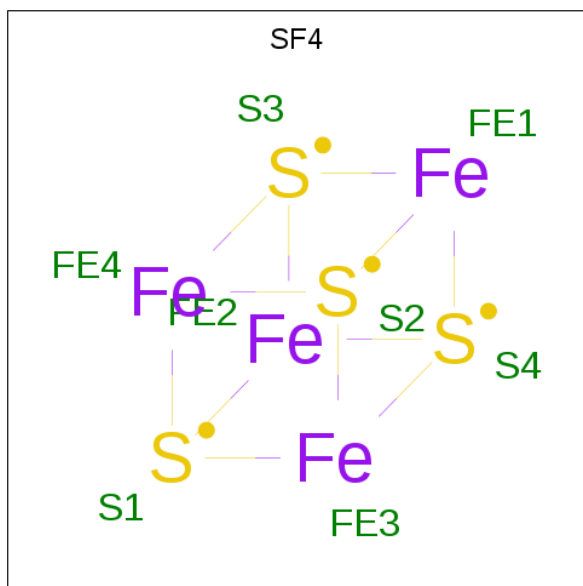
There are 5 unique types of molecules in this entry. The entry contains 6076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fumarate reductase/succinate dehydrogenase flavoprotein domain protein.

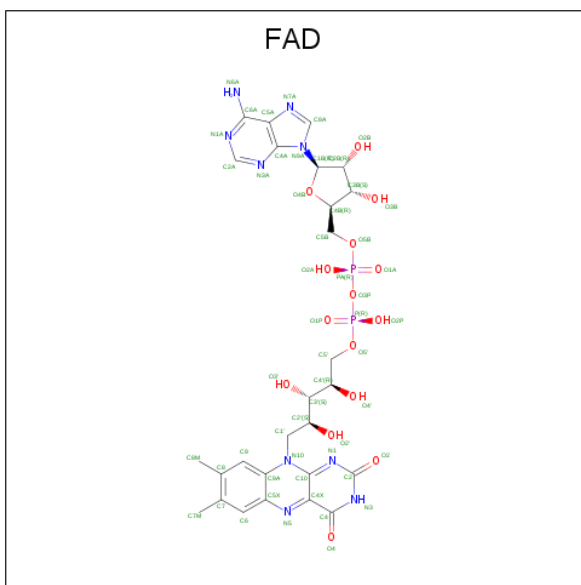
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	Total 2663	C 1684	N 459	O 500	S 20	0	10	0
1	B	340	Total 2628	C 1658	N 454	O 496	S 20	0	6	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by author).



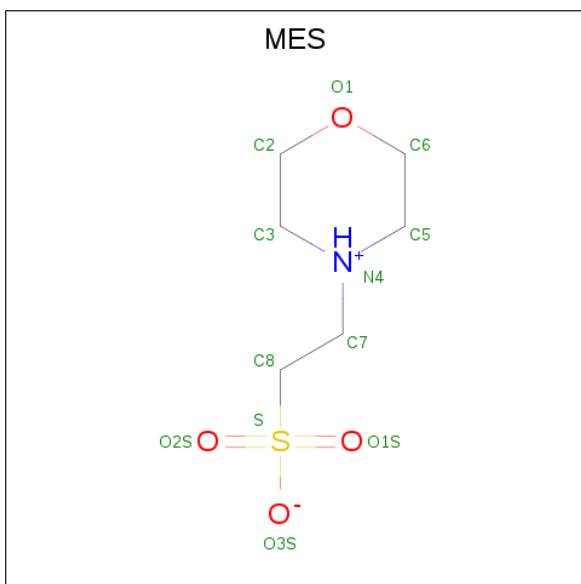
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	12	6	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

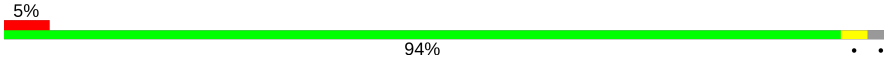
- Molecule 5 is water.

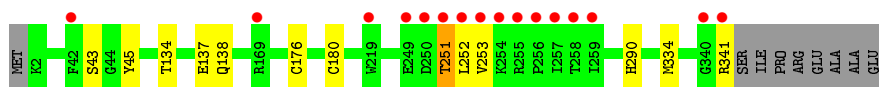
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	333	Total	O	0	3
			336	336		
5	B	265	Total	O	0	2
			267	267		

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

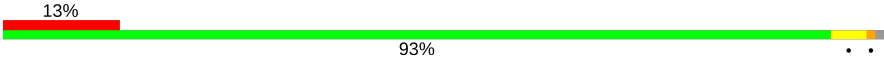
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

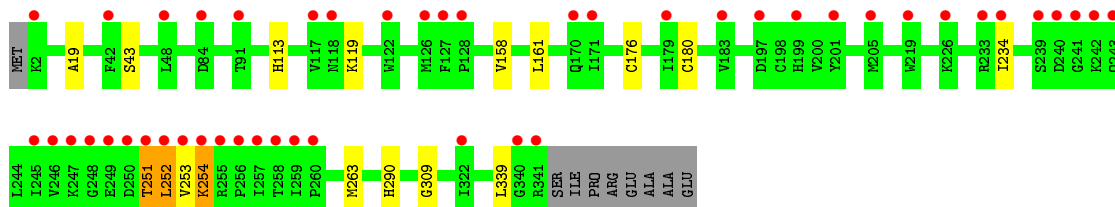
- Molecule 1: Fumarate reductase/succinate dehydrogenase flavoprotein domain protein

Chain A: 



- Molecule 1: Fumarate reductase/succinate dehydrogenase flavoprotein domain protein

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.62Å 145.62Å 64.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.67 – 1.43 47.67 – 1.43	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.67-1.43) 96.7 (47.67-1.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.43Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.163 , 0.179 0.165 , 0.184	Depositor DCC
$R_{free}$ test set	6799 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FAD, MES

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	0.52	0/2720	0.64	0/3680
1	B	0.49	0/2680	0.62	0/3625
All	All	0.51	0/5400	0.63	0/7305

There are no bond length outliers.

There are no bond angle outliers.

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	2663	0	2657	8	0
1	B	2628	0	2619	9	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	36	0	39	2	0
4	B	24	0	26	0	0
5	A	336	0	0	1	0
5	B	267	0	0	2	0
All	All	6076	0	5403	15	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 1.

All (15) 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)
5:A:609:HOH:O	1:B:290:HIS:HD2	1.85	0.59
1:A:290:HIS:HD2	5:B:585:HOH:O	1.87	0.58
1:A:134[B]:THR:HG21	4:A:404:MES:O1S	2.04	0.57
1:B:251:THR:O	1:B:252:LEU:HB2	2.10	0.52
1:A:134[B]:THR:HG22	1:A:138:GLN:NE2	2.28	0.49
1:B:43:SER:OG	1:B:113:HIS:HE1	1.99	0.46
1:A:334[B]:MET:HG2	1:B:19:ALA:HB1	1.99	0.44
1:A:251:THR:HB	1:B:252:LEU:HG	2.00	0.42
1:B:113:HIS:HD2	5:B:505:HOH:O	2.01	0.42
1:B:161:LEU:HD22	1:B:234:ILE:HG13	2.02	0.42
1:B:309:GLY:HA2	1:B:339:LEU:HD11	2.01	0.41
1:A:43:SER:HB3	1:A:134[B]:THR:HG23	2.03	0.41
1:B:158:VAL:HG22	1:B:263[B]:MET:HB3	2.02	0.41
1:A:134[B]:THR:CG2	4:A:404:MES:O1S	2.69	0.40
1:A:45:TYR:HA	1:A:137:GLU:HB3	2.03	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	348/349 (100%)	338 (97%)	8 (2%)	2 (1%)	25	7
1	B	344/349 (99%)	334 (97%)	8 (2%)	2 (1%)	25	7
All	All	692/698 (99%)	672 (97%)	16 (2%)	4 (1%)	25	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	254	LYS
1	A	251	THR
1	B	252	LEU
1	A	253	VAL

### 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	288/285 (101%)	284 (99%)	4 (1%)	67	37
1	B	284/285 (100%)	278 (98%)	6 (2%)	53	19
All	All	572/570 (100%)	562 (98%)	10 (2%)	59	28

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	CYS
1	A	180	CYS
1	A	252	LEU
1	A	341	ARG
1	B	119	LYS
1	B	176	CYS
1	B	180	CYS
1	B	251	THR
1	B	253	VAL
1	B	254	LYS

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

Mol	Chain	Res	Type
1	A	25	GLN
1	A	290	HIS
1	B	113	HIS
1	B	290	HIS

### 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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MES	A	405	-	12,12,12	0.64	0	14,16,16	1.15	1 (7%)
3	FAD	B	402	-	51,58,58	1.31	5 (9%)	60,89,89	2.18	7 (11%)
4	MES	B	403	-	12,12,12	0.87	0	14,16,16	0.55	0
2	SF4	A	401	1	0,12,12	0.00	-	-		
2	SF4	B	401	1	0,12,12	0.00	-	-		
4	MES	A	404	-	12,12,12	0.68	0	14,16,16	0.43	0
4	MES	A	403	-	12,12,12	1.15	2 (16%)	14,16,16	0.66	0
3	FAD	A	402	-	51,58,58	1.11	4 (7%)	60,89,89	2.33	7 (11%)
4	MES	B	404	-	12,12,12	0.82	0	14,16,16	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	405	-	-	1/6/14/14	0/1/1/1
3	FAD	B	402	-	-	2/30/50/50	0/6/6/6
4	MES	B	403	-	-	2/6/14/14	0/1/1/1
2	SF4	A	401	1	-	-	0/6/5/5
2	SF4	B	401	1	-	-	0/6/5/5
4	MES	A	404	-	-	1/6/14/14	0/1/1/1
4	MES	A	403	-	-	6/6/14/14	0/1/1/1
3	FAD	A	402	-	-	2/30/50/50	0/6/6/6
4	MES	B	404	-	-	2/6/14/14	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	FAD	C4X-C10	6.47	1.45	1.38
3	A	402	FAD	C4X-C10	4.02	1.42	1.38
3	A	402	FAD	C4-N3	3.63	1.39	1.33
3	B	402	FAD	C4-N3	3.58	1.39	1.33
3	A	402	FAD	C9A-N10	2.90	1.42	1.38
3	B	402	FAD	C4-C4X	2.61	1.45	1.41
3	B	402	FAD	C5X-N5	2.54	1.39	1.35
3	A	402	FAD	C5X-N5	2.50	1.39	1.35
3	B	402	FAD	C9A-N10	2.46	1.41	1.38
4	A	403	MES	O2S-S	-2.29	1.38	1.45
4	A	403	MES	O1S-S	-2.05	1.39	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	FAD	C4-N3-C2	12.63	125.80	115.14
3	B	402	FAD	C4-N3-C2	12.45	125.65	115.14
3	B	402	FAD	C4X-C4-N3	-6.58	114.44	123.43
3	A	402	FAD	C4X-C4-N3	-6.27	114.85	123.43
3	A	402	FAD	C1'-N10-C9A	6.07	123.07	118.29
3	A	402	FAD	C10-C4X-N5	4.51	124.38	121.26
3	A	402	FAD	C4-C4X-C10	-4.28	117.12	119.95
3	B	402	FAD	C10-C4X-N5	3.92	123.97	121.26
3	B	402	FAD	C1'-N10-C9A	3.54	121.08	118.29
3	B	402	FAD	C4-C4X-C10	-3.46	117.66	119.95
3	B	402	FAD	C4X-C10-N10	-3.43	116.78	120.30
3	A	402	FAD	C4X-C10-N10	-3.43	116.78	120.30
4	A	405	MES	O1S-S-C8	-3.31	102.92	106.92
3	A	402	FAD	C1'-N10-C10	-2.59	116.09	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	FAD	C5A-C6A-N6A	2.19	123.68	120.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

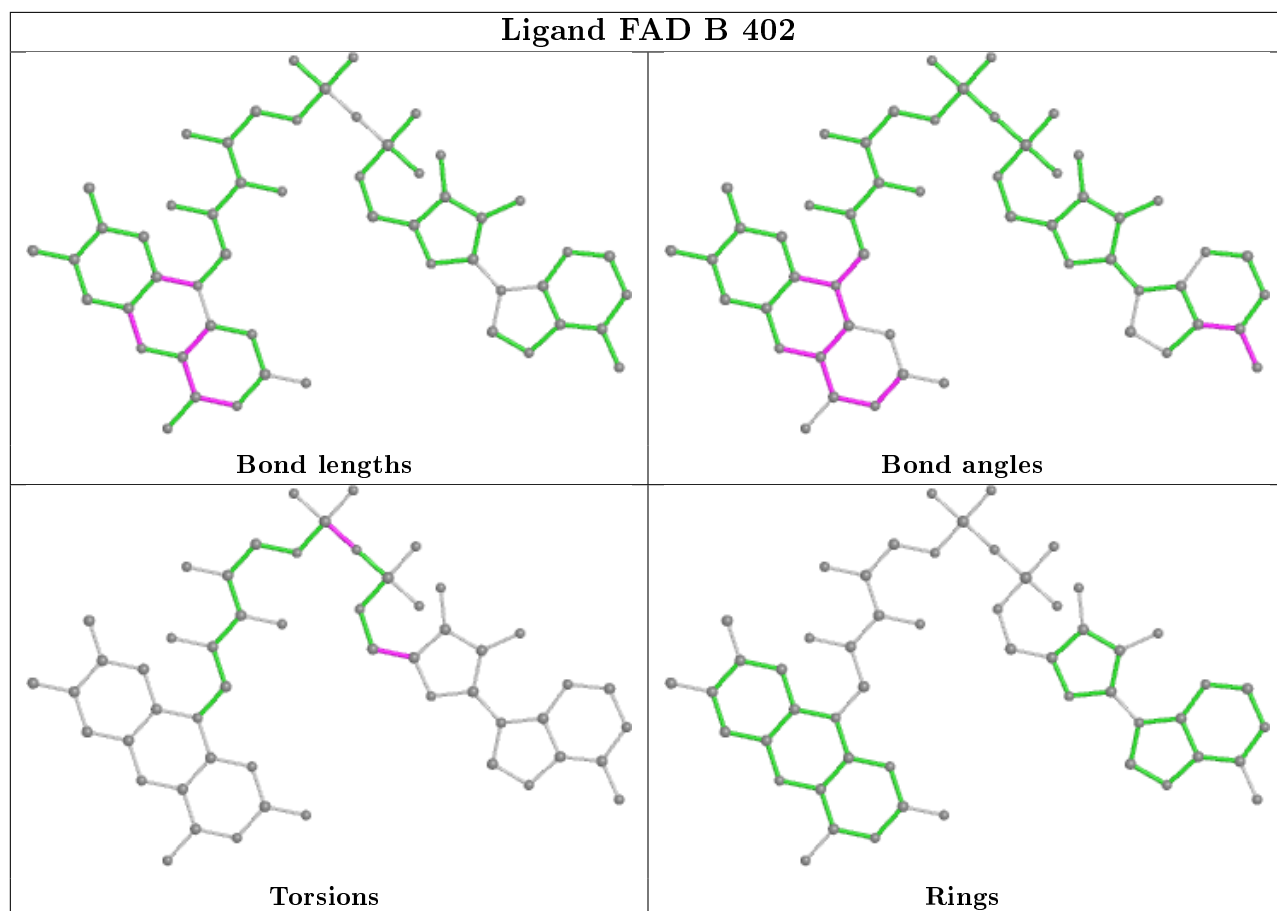
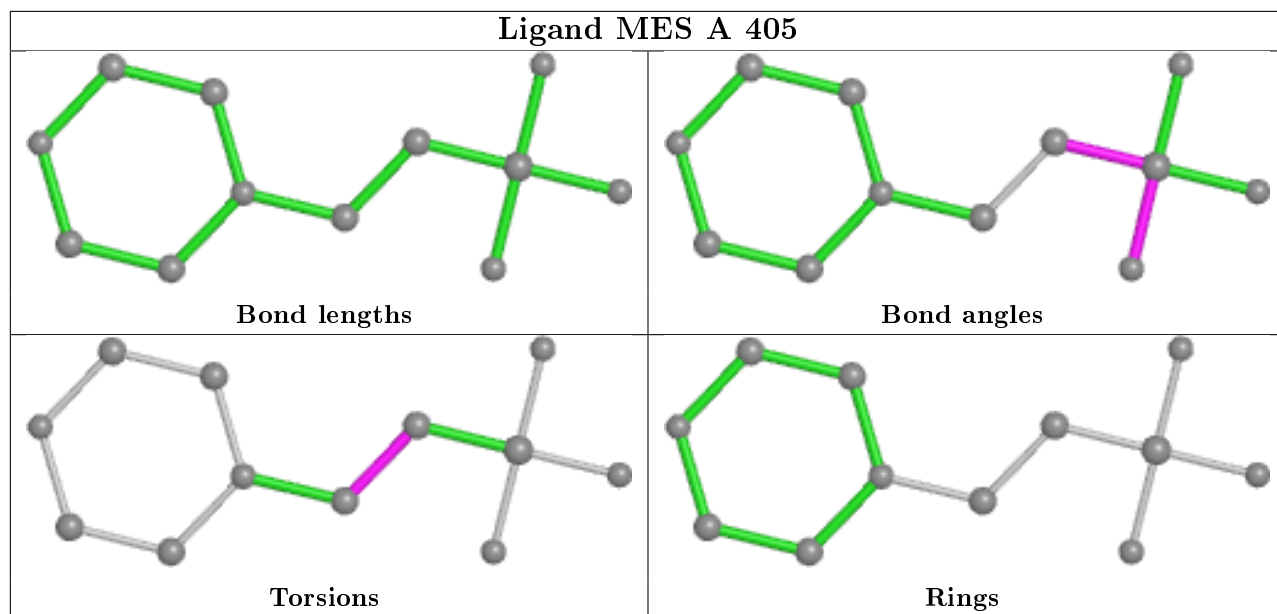
Mol	Chain	Res	Type	Atoms
4	A	405	MES	N4-C7-C8-S
4	B	403	MES	C8-C7-N4-C5
4	A	403	MES	C7-C8-S-O1S
4	A	403	MES	C7-C8-S-O2S
4	A	403	MES	C7-C8-S-O3S
4	B	404	MES	C8-C7-N4-C5
4	A	403	MES	N4-C7-C8-S
4	B	403	MES	C8-C7-N4-C3
4	A	403	MES	C8-C7-N4-C5
3	B	402	FAD	PA-O3P-P-O5'
3	A	402	FAD	PA-O3P-P-O5'
4	A	403	MES	C8-C7-N4-C3
4	B	404	MES	C8-C7-N4-C3
3	B	402	FAD	O4B-C4B-C5B-O5B
3	A	402	FAD	O4B-C4B-C5B-O5B
4	A	404	MES	C8-C7-N4-C5

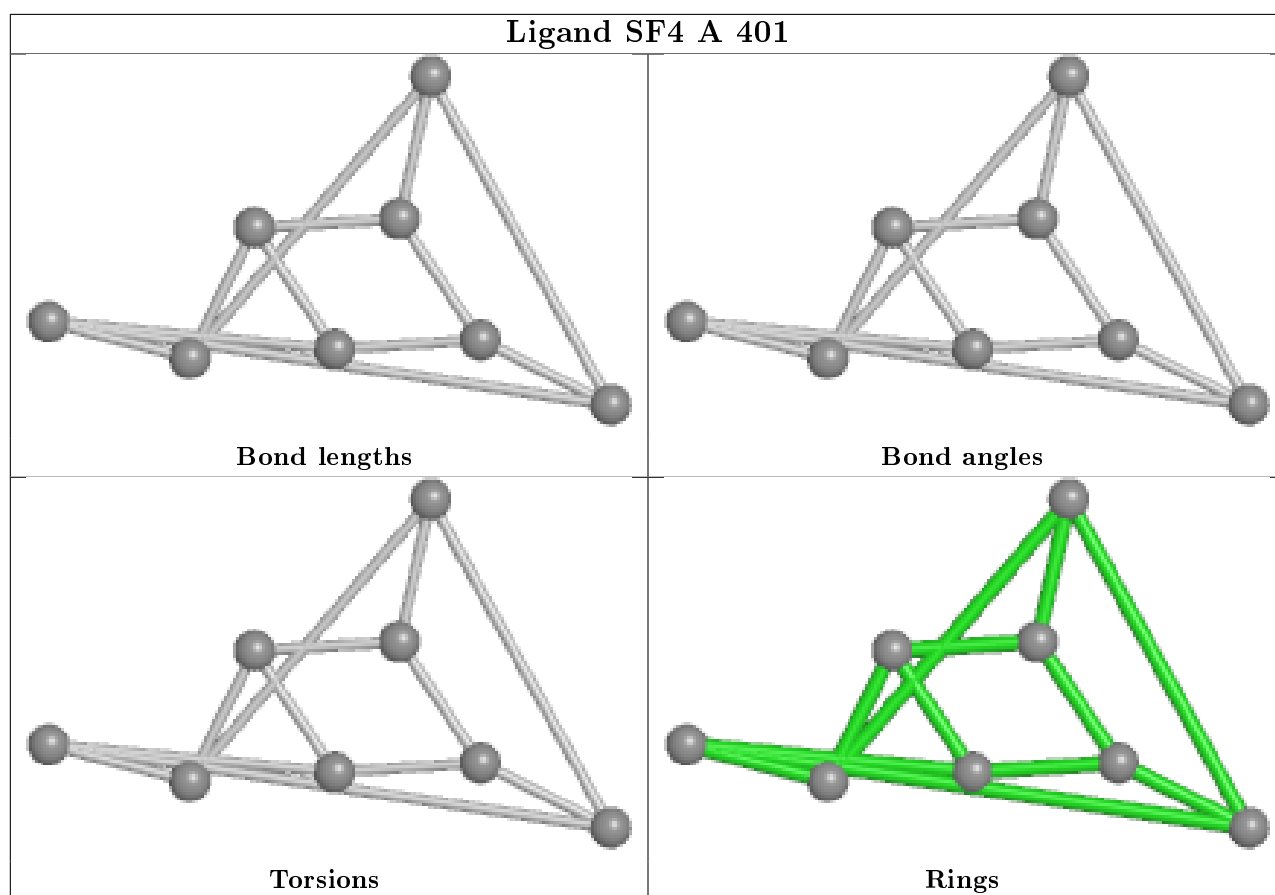
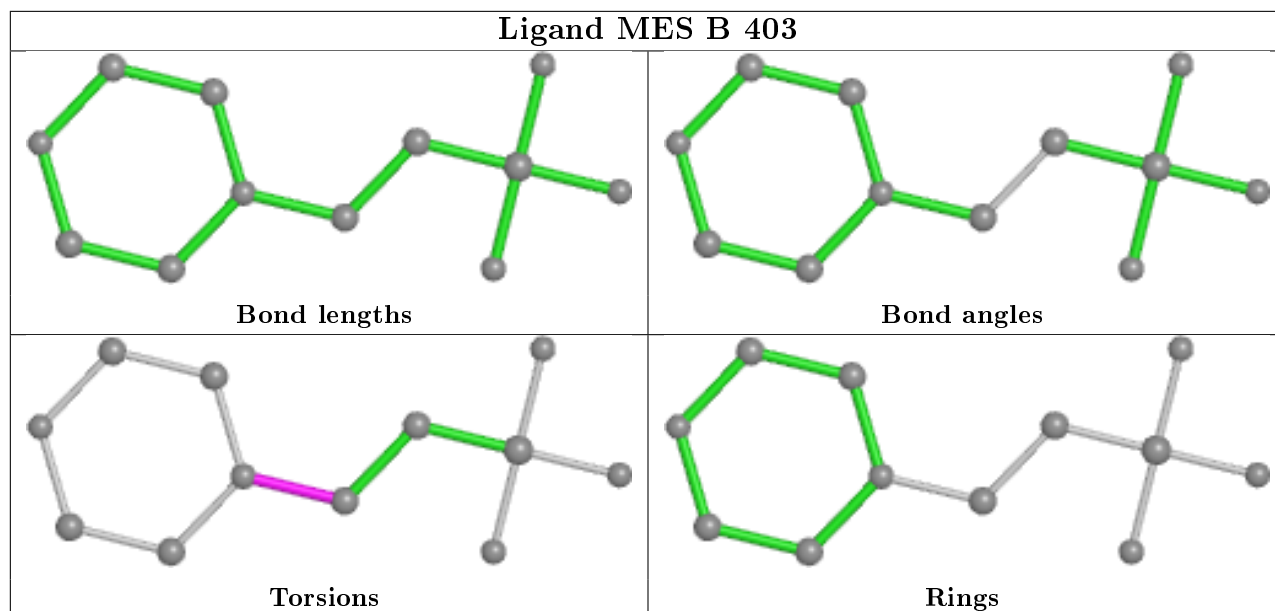
There are no ring outliers.

1 monomer is involved in 2 short contacts:

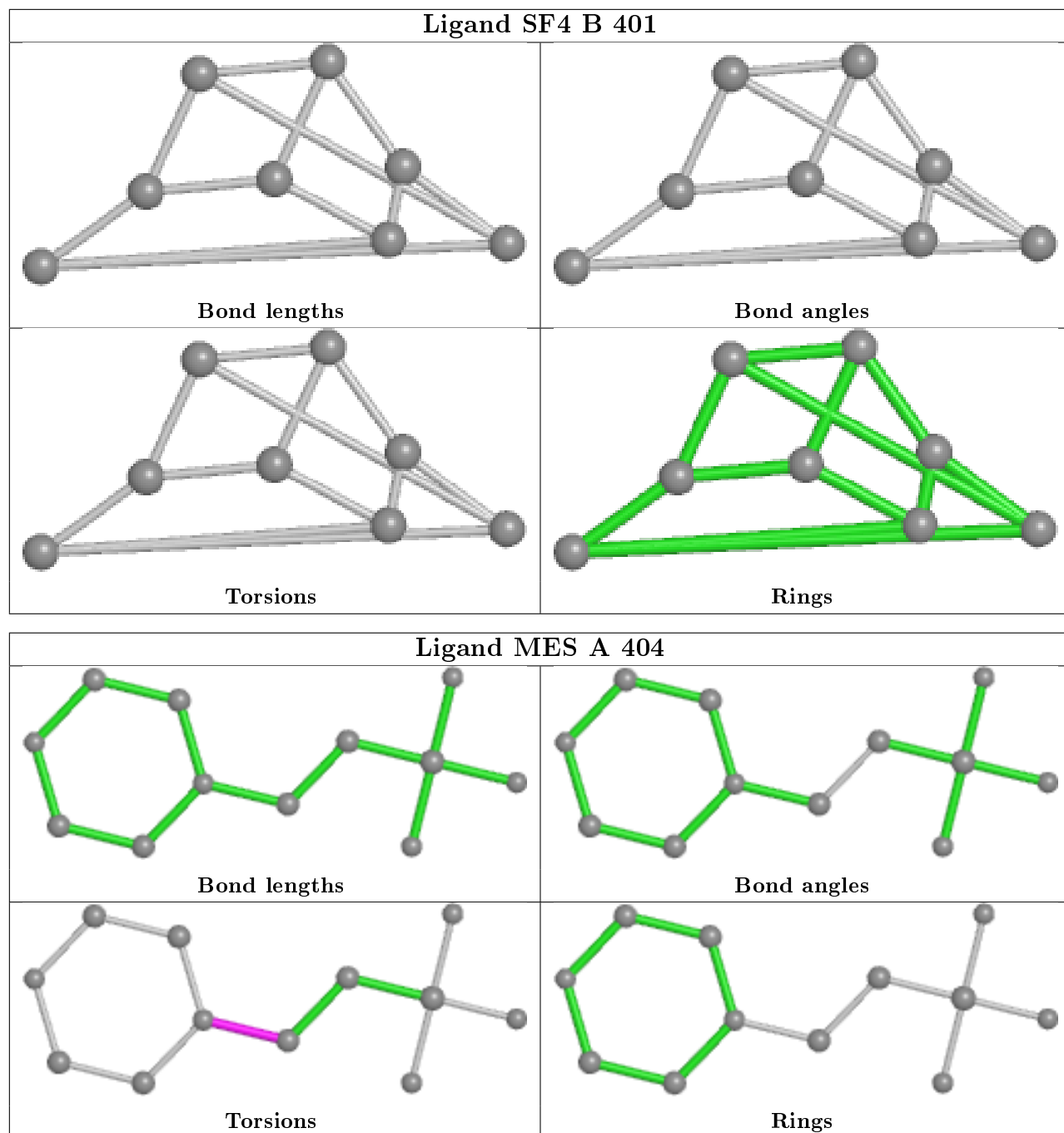
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	MES	2	0

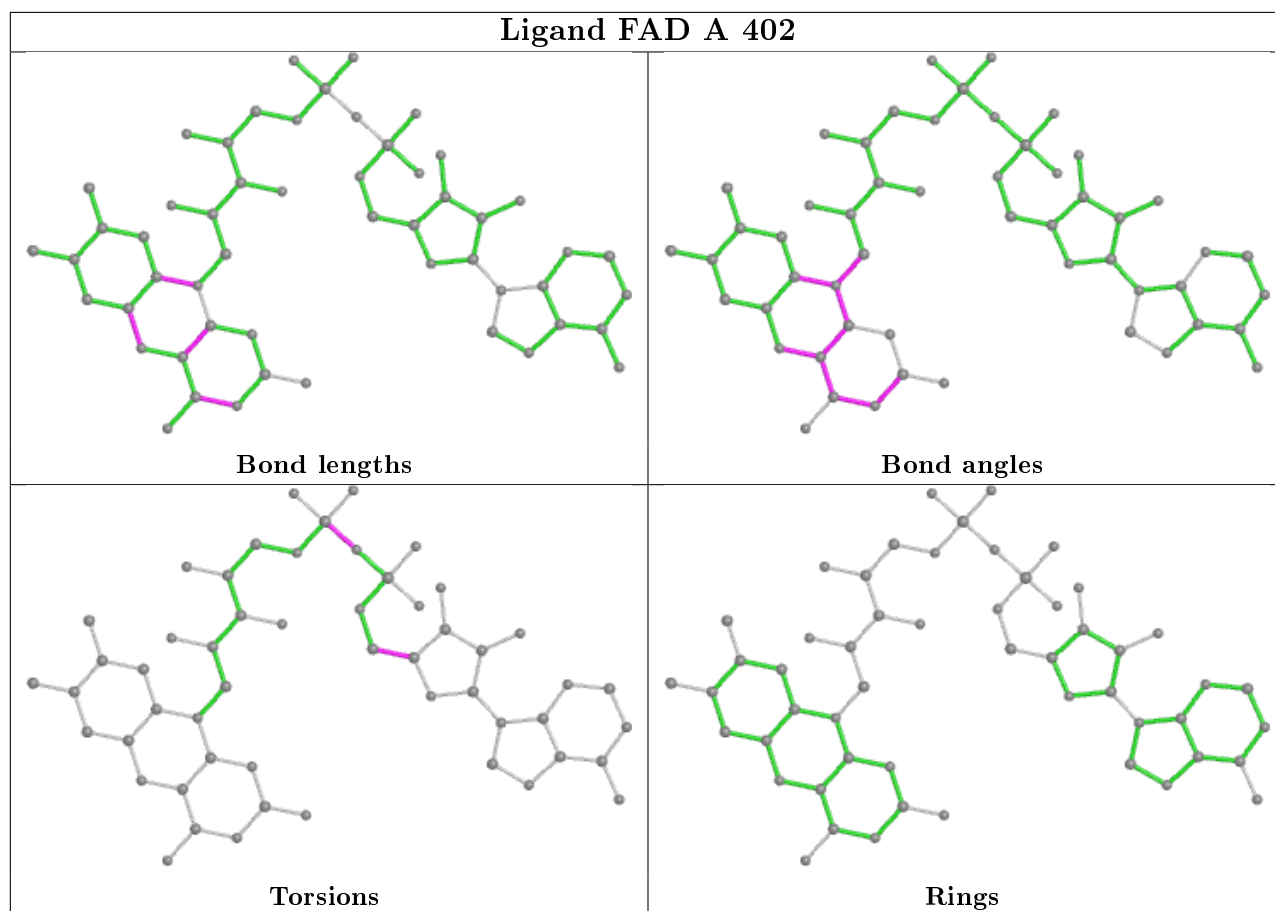
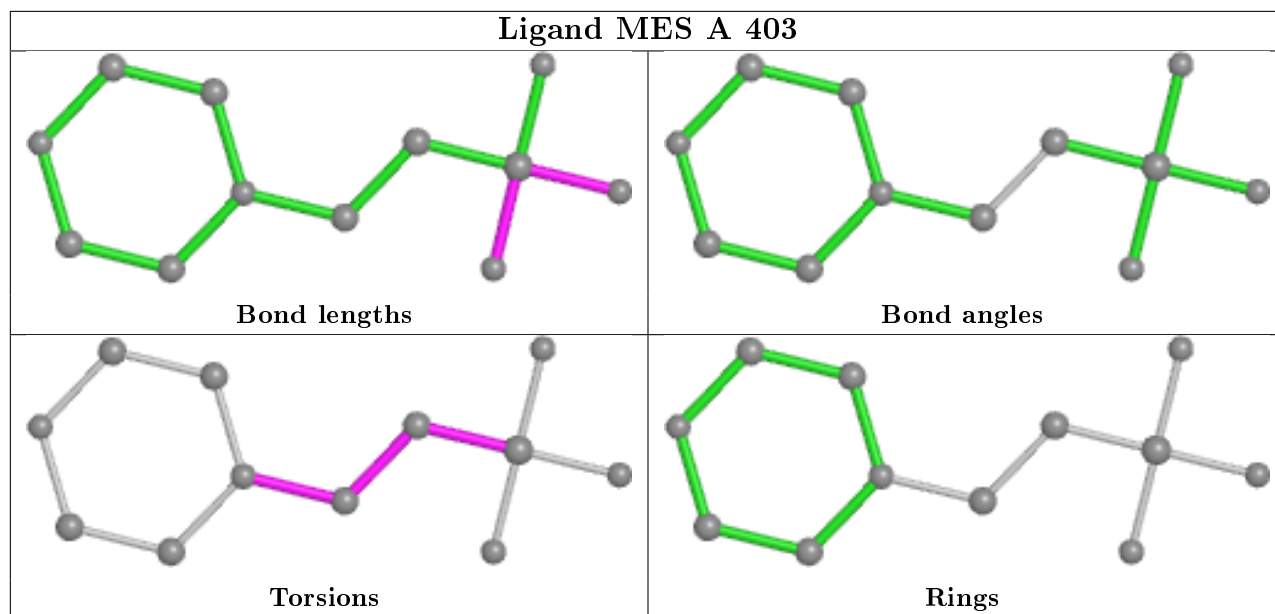
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

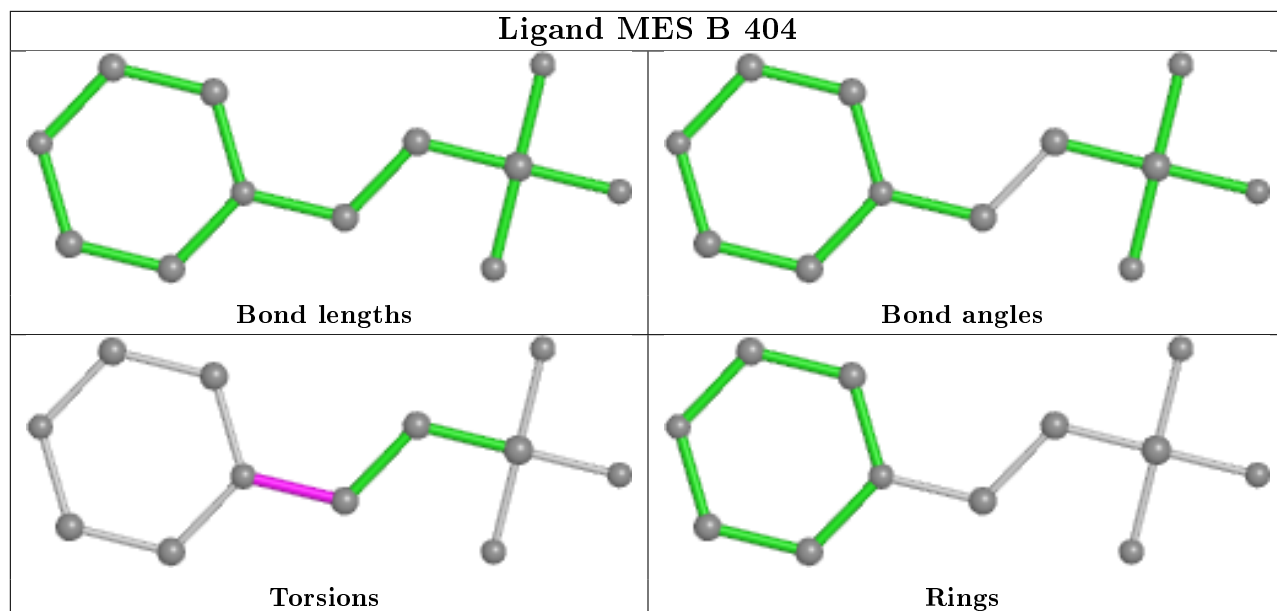












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	340/349 (97%)	0.64	16 (4%) 31 32	13, 19, 39, 95	0
1	B	340/349 (97%)	0.95	47 (13%) 2 2	14, 23, 54, 97	0
All	All	680/698 (97%)	0.80	63 (9%) 8 9	13, 21, 51, 97	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	28.3
1	A	253	VAL	21.4
1	B	252	LEU	17.6
1	B	253	VAL	16.1
1	A	255	ARG	13.6
1	B	251	THR	9.9
1	B	254	LYS	9.8
1	B	259	ILE	9.3
1	B	257	ILE	9.0
1	A	254	LYS	8.7
1	B	255	ARG	8.3
1	A	256	PRO	8.0
1	B	256	PRO	7.3
1	A	251	THR	7.1
1	B	117	VAL	6.6
1	B	258	THR	6.4
1	B	219	TRP	5.2
1	B	242	LYS	4.8
1	A	257	ILE	4.6
1	A	250	ASP	4.6
1	B	250	ASP	4.3
1	A	249	GLU	4.1
1	B	170	GLN	3.9
1	B	122	TRP	3.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	260	PRO	3.9
1	A	259	ILE	3.8
1	A	258	THR	3.6
1	B	249	GLU	3.6
1	B	246	VAL	3.6
1	B	127	PHE	3.4
1	B	197	ASP	3.3
1	B	118	ASN	3.2
1	B	247	LYS	3.2
1	B	248	GLY	3.1
1	B	234	ILE	3.1
1	A	340	GLY	3.1
1	B	171	ILE	3.1
1	A	219[A]	TRP	3.0
1	B	126	MET	3.0
1	B	199	HIS	2.9
1	A	42[A]	PHE	2.8
1	B	42[A]	PHE	2.8
1	B	239	SER	2.8
1	B	128	PRO	2.7
1	B	226	LYS	2.7
1	B	245	ILE	2.7
1	B	341	ARG	2.7
1	B	322	ILE	2.6
1	B	233	ARG	2.6
1	A	341	ARG	2.5
1	B	241	GLY	2.5
1	B	340	GLY	2.4
1	B	201	TYR	2.4
1	B	91	THR	2.3
1	B	2	LYS	2.3
1	B	179	ILE	2.2
1	B	48	LEU	2.2
1	B	243	GLN	2.2
1	B	84	ASP	2.1
1	A	169	ARG	2.1
1	B	205	MET	2.0
1	B	240	ASP	2.0
1	B	183	VAL	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](#)

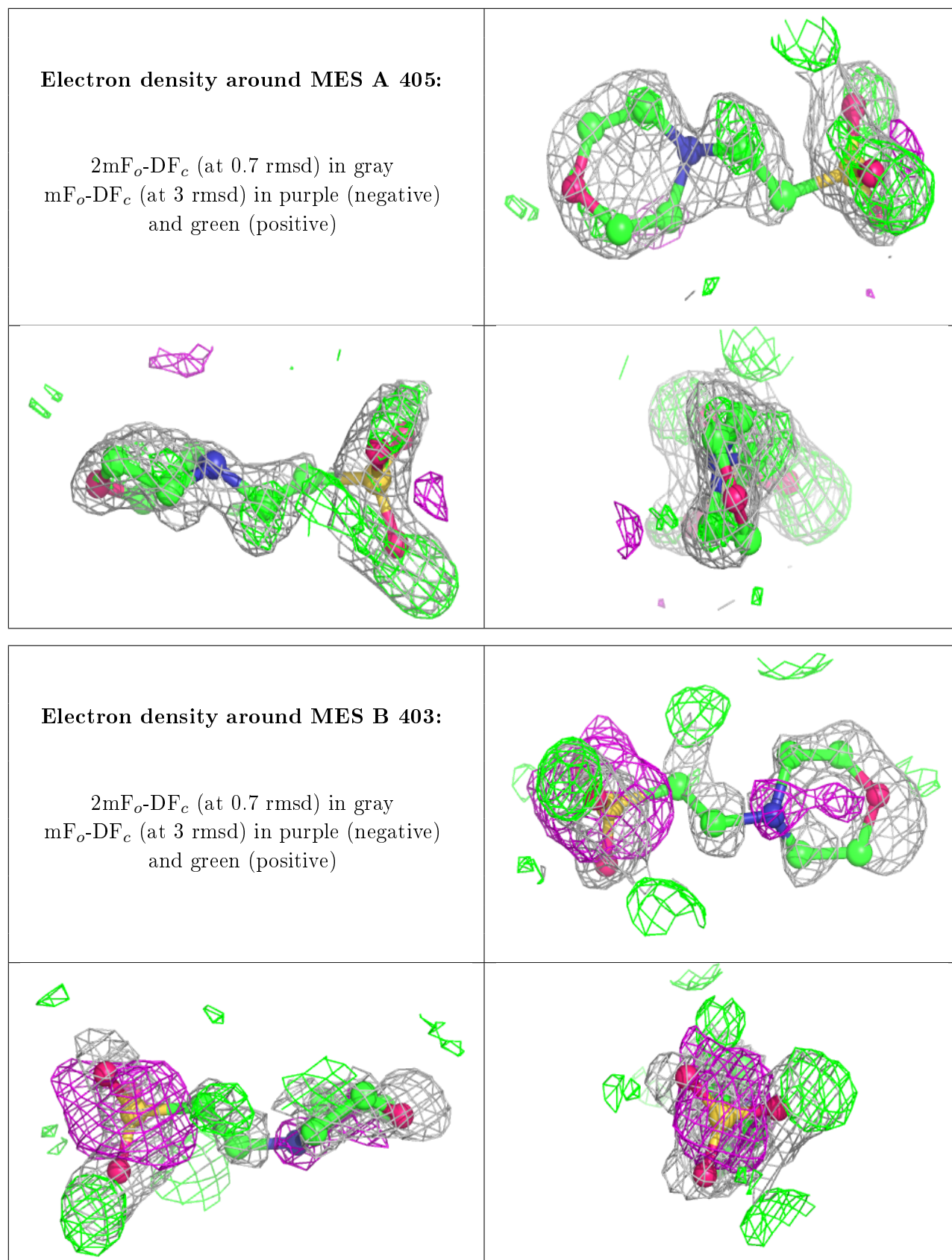
There are no monosaccharides in this entry.

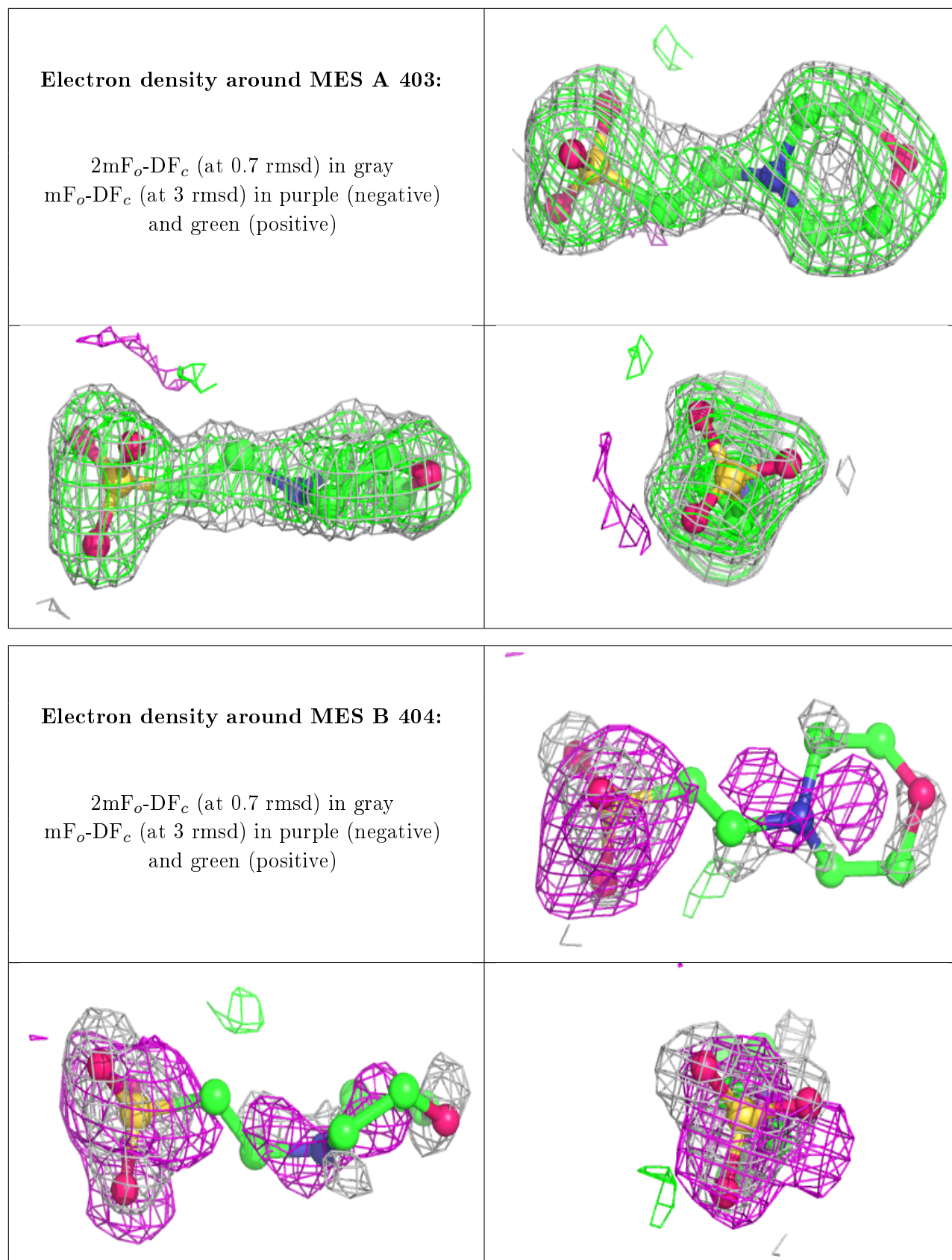
## 6.4 Ligands [i](#)

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.

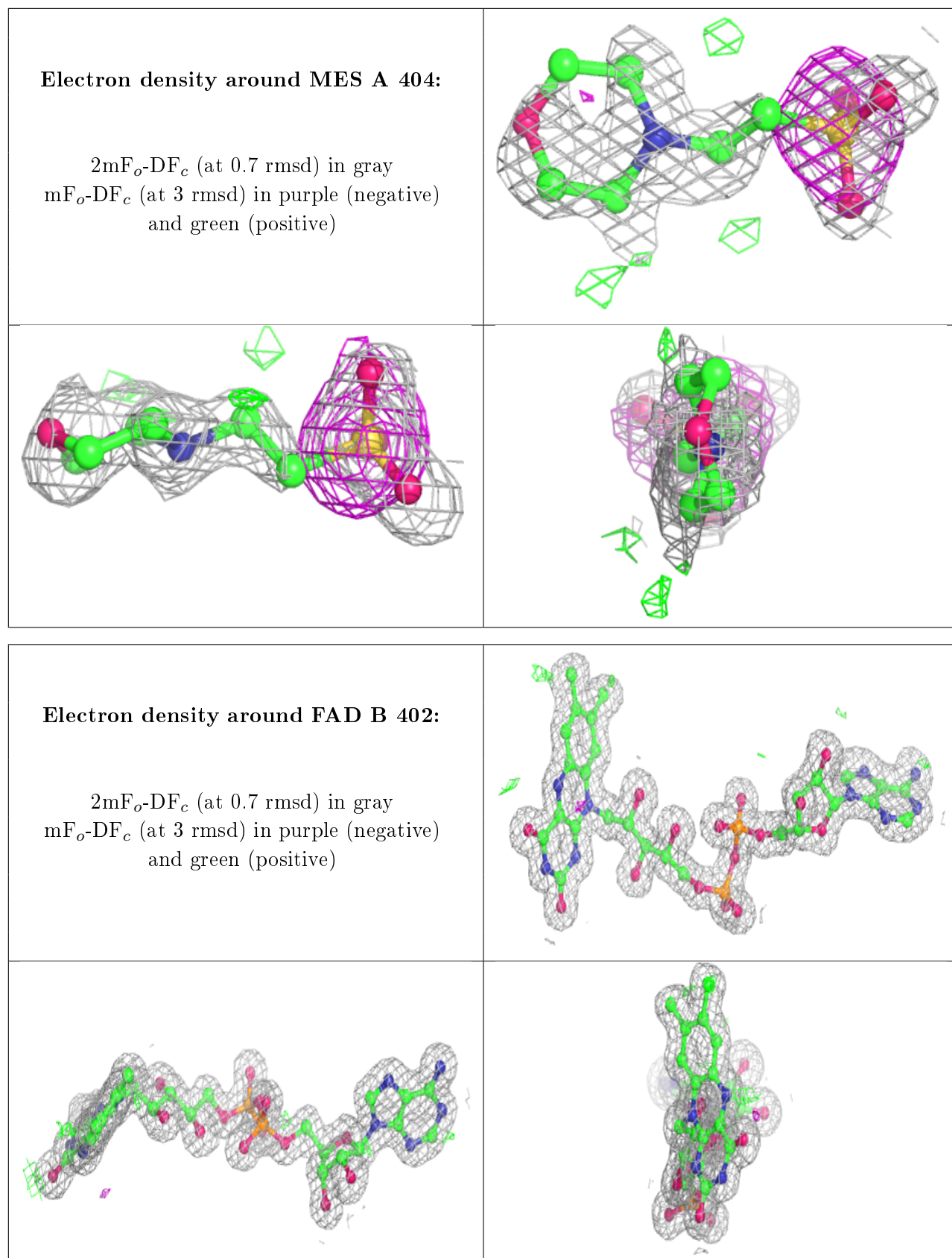
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MES	A	405	12/12	0.48	0.55	127,130,131,131	0
4	MES	B	403	12/12	0.63	0.32	46,54,59,60	0
4	MES	A	403	12/12	0.75	1.04	189,189,191,191	0
4	MES	B	404	12/12	0.88	0.41	41,55,64,65	0
4	MES	A	404	12/12	0.89	0.29	33,48,59,59	0
3	FAD	B	402	53/53	0.96	0.10	14,16,20,24	0
3	FAD	A	402	53/53	0.97	0.09	12,14,18,21	0
2	SF4	A	401	8/8	0.99	0.08	13,14,15,15	0
2	SF4	B	401	8/8	0.99	0.08	14,16,16,16	0

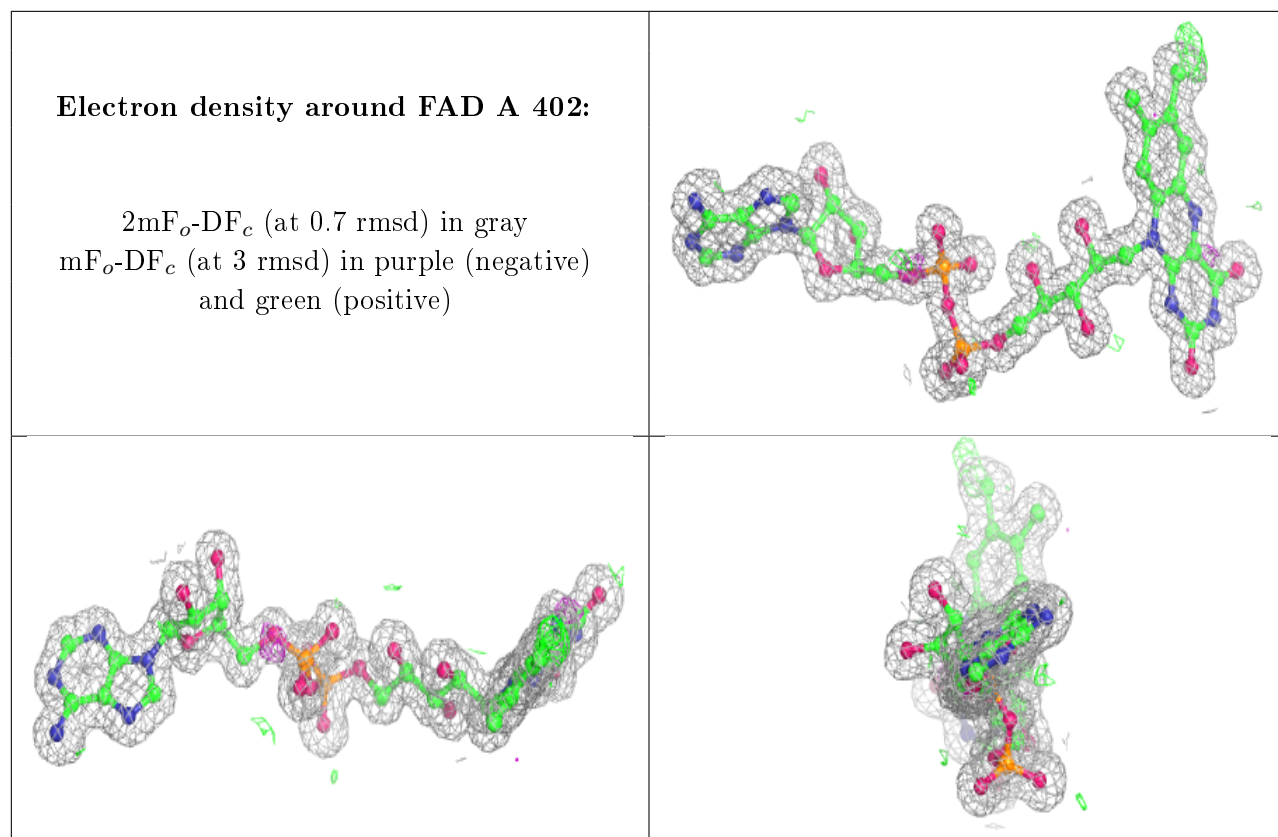
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





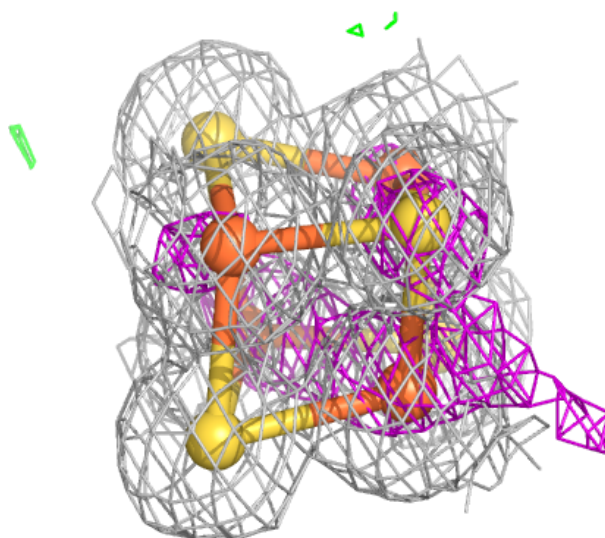
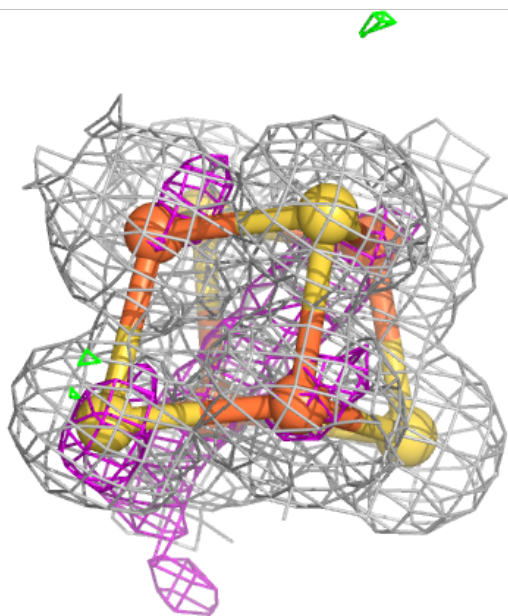
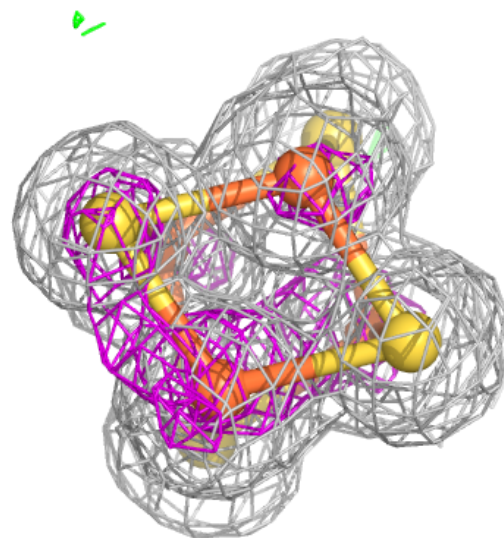


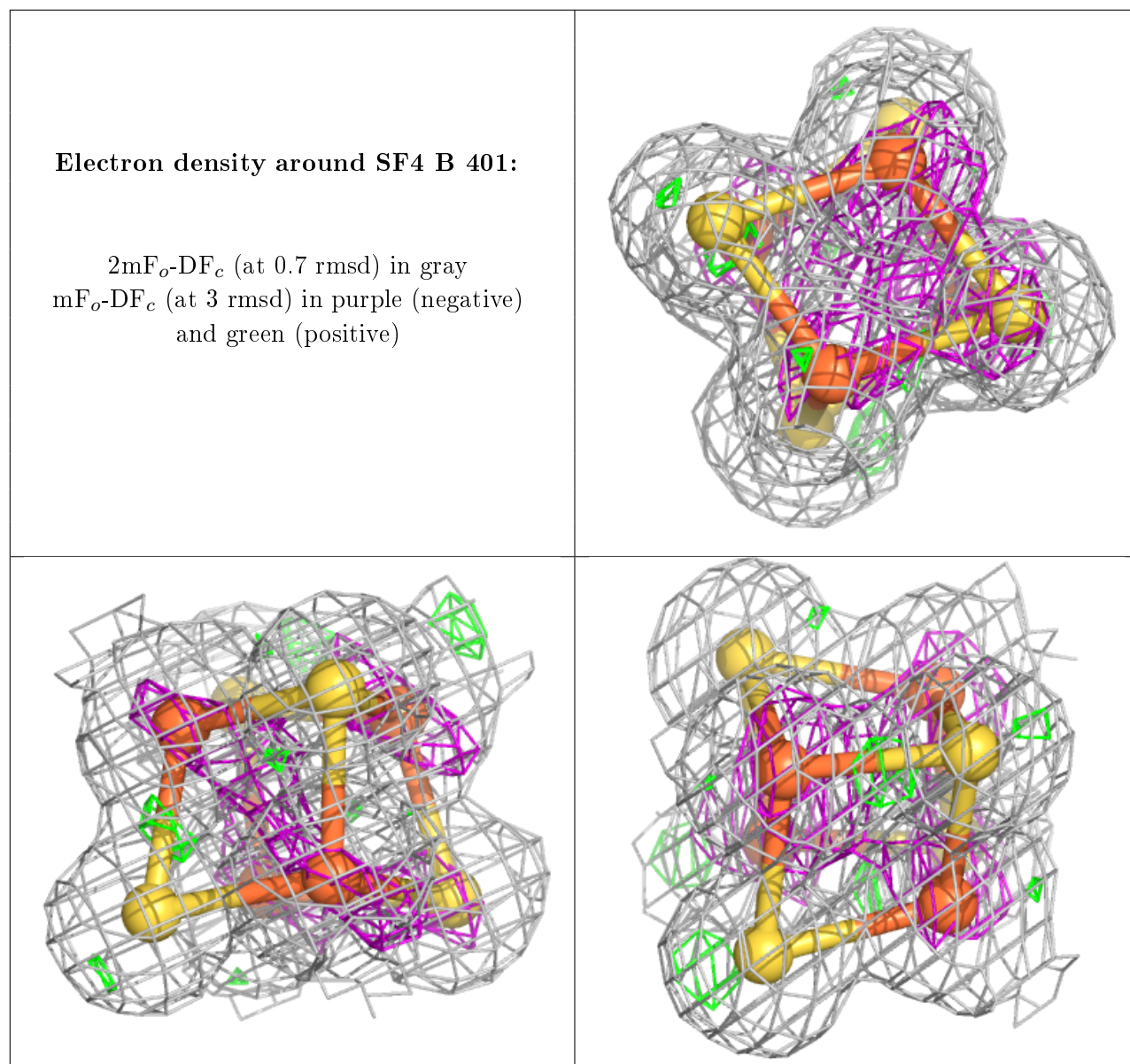




**Electron density around SF4 A 401:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.