



## wwPDB EM Validation Summary Report ⓘ

Feb 20, 2025 – 06:08 pm GMT

PDB ID : 8S7X  
EMDB ID : EMD-19788  
Title : Methyl-coenzyme M reductase activation complex without the A2 component  
Authors : Ramirez-Amador, F.; Paul, S.; Kumar, A.; Schuller, J.M.  
Deposited on : 2024-03-04  
Resolution : 2.78 Å(reported)  
Based on initial model : .

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

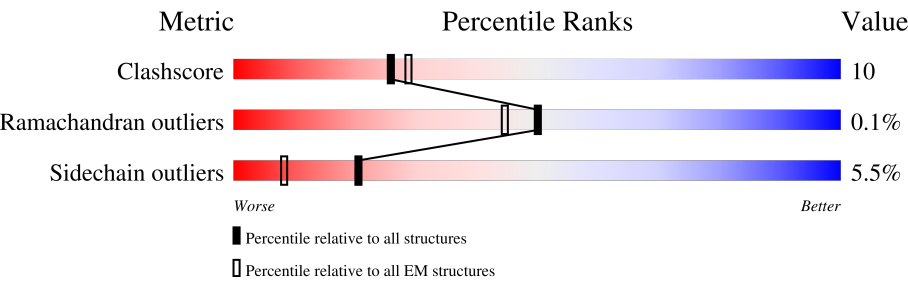
EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.78 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	260	<div><div>80%18%.</div></div>
1	B	260	<div><div>82%17%.</div></div>
2	D	443	<div><div>82%17%</div></div>
2	E	443	<div><div>81%18%.</div></div>
3	C	553	<div><div>77%20%..</div></div>
3	F	553	<div><div>73%15%.10%</div></div>
4	G	183	<div><div>45%16%.38%</div></div>
5	H	304	<div><div>68%27%..</div></div>
6	I	234	<div><div>59%20%.17%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
7	J	501	
8	L	93	

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
10	SHT	E	601	-	-	X	-
9	F43	A	601	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28143 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Methyl-coenzyme M reductase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		
1	B	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		
2	D	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	550	Total	C	N	O	S	0	0
			4284	2707	731	826	20		
3	F	495	Total	C	N	O	S	0	0
			3812	2402	650	740	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	51	SER	ALA	variant	UNP A0A2L1CBB0
F	51	SER	ALA	variant	UNP A0A2L1CBB0

- Molecule 4 is a protein called Methanogenesis marker protein 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	114	Total	C	N	O	S	0	0
			931	600	152	172	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	VAL	ILE	variant	UNP G0H411
G	129	ILE	VAL	variant	UNP G0H411
G	167	GLU	GLN	variant	UNP G0H411
G	168	GLU	ASP	variant	UNP G0H411
G	171	ASN	ASP	variant	UNP G0H411

- Molecule 5 is a protein called Methanogenesis marker protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	296	Total	C	N	O	S	0	0
			2393	1530	411	440	12		

- Molecule 6 is a protein called Methyl-coenzyme M reductase operon protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	194	Total	C	N	O	S	0	0
			1469	929	261	271	8		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-35	MET	-	initiating methionine	UNP G0H3B1
I	-34	SER	-	expression tag	UNP G0H3B1
I	-33	ALA	-	expression tag	UNP G0H3B1
I	-32	TRP	-	expression tag	UNP G0H3B1
I	-31	SER	-	expression tag	UNP G0H3B1
I	-30	HIS	-	expression tag	UNP G0H3B1
I	-29	PRO	-	expression tag	UNP G0H3B1
I	-28	GLN	-	expression tag	UNP G0H3B1
I	-27	PHE	-	expression tag	UNP G0H3B1
I	-26	GLU	-	expression tag	UNP G0H3B1
I	-25	LYS	-	expression tag	UNP G0H3B1
I	-24	GLY	-	expression tag	UNP G0H3B1
I	-23	GLY	-	expression tag	UNP G0H3B1
I	-22	GLY	-	expression tag	UNP G0H3B1
I	-21	SER	-	expression tag	UNP G0H3B1
I	-20	GLY	-	expression tag	UNP G0H3B1
I	-19	GLY	-	expression tag	UNP G0H3B1
I	-18	GLY	-	expression tag	UNP G0H3B1
I	-17	SER	-	expression tag	UNP G0H3B1
I	-16	GLY	-	expression tag	UNP G0H3B1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	-15	GLY	-	expression tag	UNP G0H3B1
I	-14	SER	-	expression tag	UNP G0H3B1
I	-13	ALA	-	expression tag	UNP G0H3B1
I	-12	TRP	-	expression tag	UNP G0H3B1
I	-11	SER	-	expression tag	UNP G0H3B1
I	-10	HIS	-	expression tag	UNP G0H3B1
I	-9	PRO	-	expression tag	UNP G0H3B1
I	-8	GLN	-	expression tag	UNP G0H3B1
I	-7	PHE	-	expression tag	UNP G0H3B1
I	-6	GLU	-	expression tag	UNP G0H3B1
I	-5	LYS	-	expression tag	UNP G0H3B1
I	-4	SER	-	expression tag	UNP G0H3B1
I	-3	ALA	-	expression tag	UNP G0H3B1
I	-2	GLY	-	expression tag	UNP G0H3B1
I	-1	SER	-	expression tag	UNP G0H3B1
I	0	GLY	-	expression tag	UNP G0H3B1

- Molecule 7 is a protein called UPF0288 protein MmarC6\_0796.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	499	Total	C	N	O	S	0	0
			3962	2517	647	790	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	500	SER	LYS	variant	UNP A9A8E0

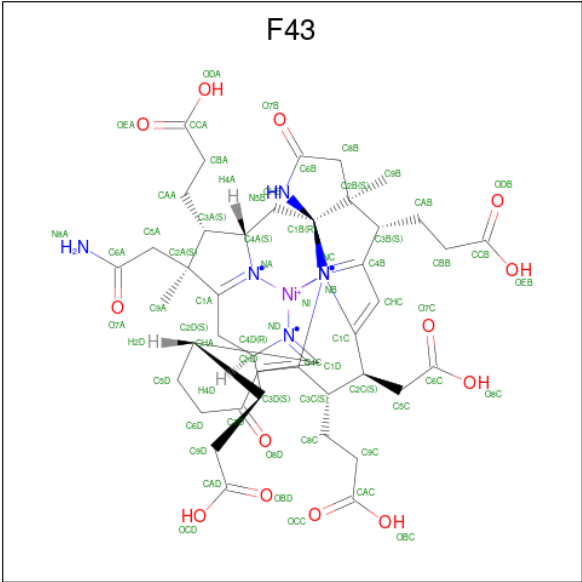
- Molecule 8 is a protein called DUF2098 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	47	Total	C	N	O	0	0
			390	251	61	78		

There is a discrepancy between the modelled and reference sequences:

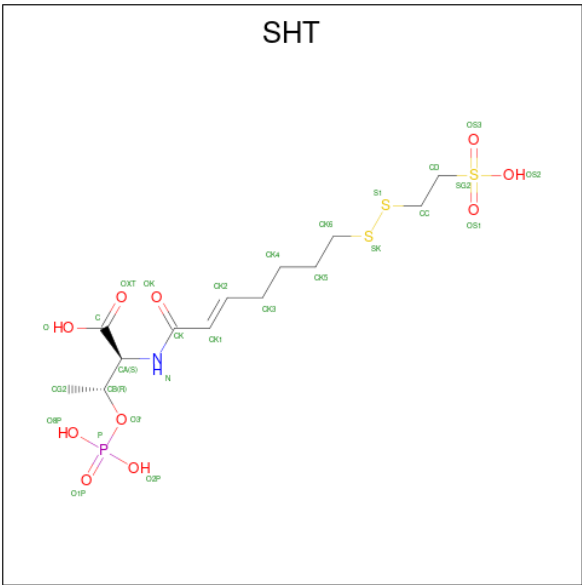
Chain	Residue	Modelled	Actual	Comment	Reference
L	58	LYS	ARG	variant	UNP A0A2L1CAX0

- Molecule 9 is FACTOR 430 (three-letter code: F43) (formula: C<sub>42</sub>H<sub>51</sub>N<sub>6</sub>NiO<sub>13</sub>).



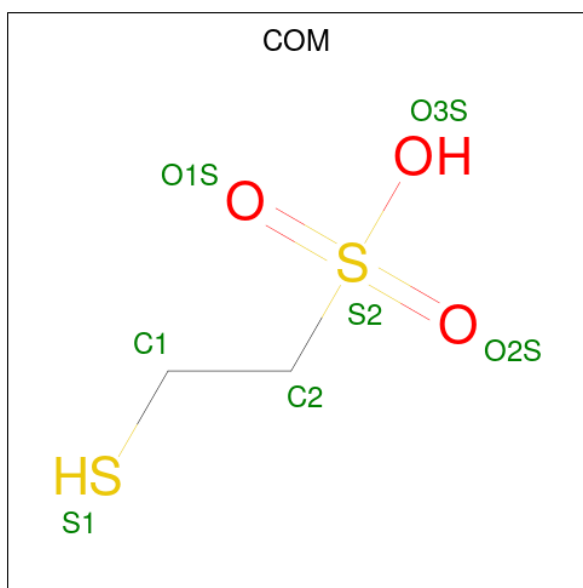
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	Ni	O	0
			62	42	6	1	13	
9	F	1	Total	C	N	Ni	O	0
			62	42	6	1	13	

- Molecule 10 is O-PHOSPHONO-N-[(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL]-L-THREONINE (three-letter code: SHT) (formula: C<sub>13</sub>H<sub>24</sub>NO<sub>10</sub>PS<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



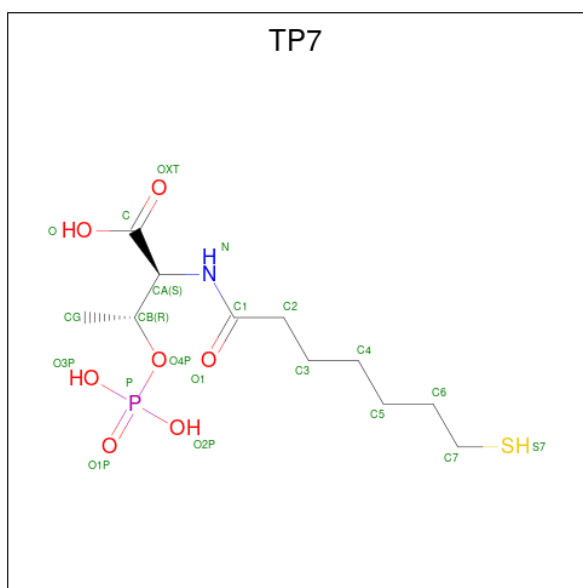
Mol	Chain	Residues	Atoms						AltConf
10	E	1	Total	C	N	O	P	S	0
			28	13	1	10	1	3	

- Molecule 11 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O	S	0
			7	2	3	2	

- Molecule 12 is Coenzyme B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).

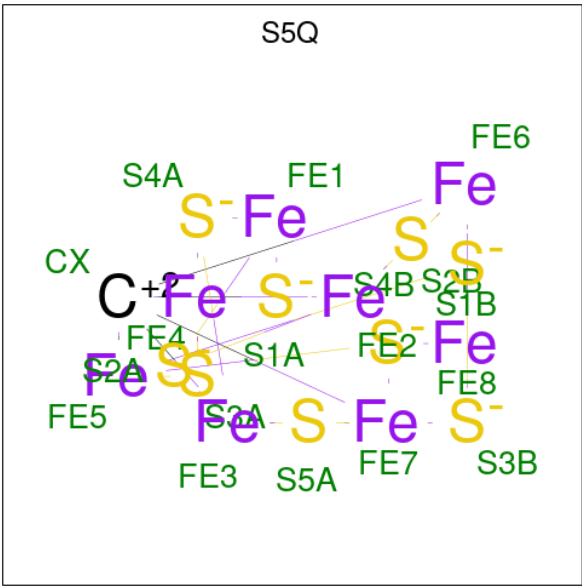


Mol	Chain	Residues	Atoms						AltConf
12	F	1	Total	C	N	O	P	S	0
			21	11	1	7	1	1	

- Molecule 13 is FeFe cofactor (three-letter code: S5Q) (formula:  $CFe_8S_9$ ) (labeled as "Ligand



of Interest" by depositor).

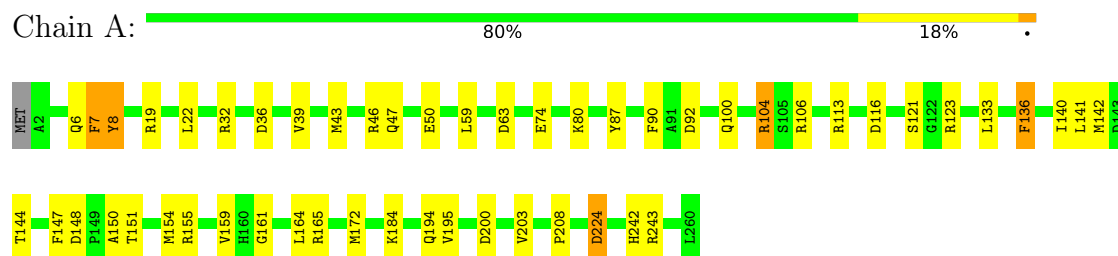


Mol	Chain	Residues	Atoms				AltConf
13	H	1	Total	C	Fe	S	0
			18	1	8	9	
13	I	1	Total	C	Fe	S	0
			18	1	8	9	
13	I	1	Total	C	Fe	S	0
			18	1	8	9	

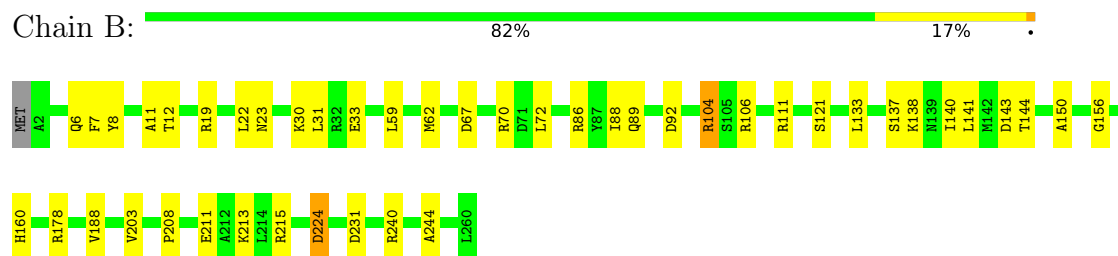
### 3 Residue-property plots [i](#)

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. 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. 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.

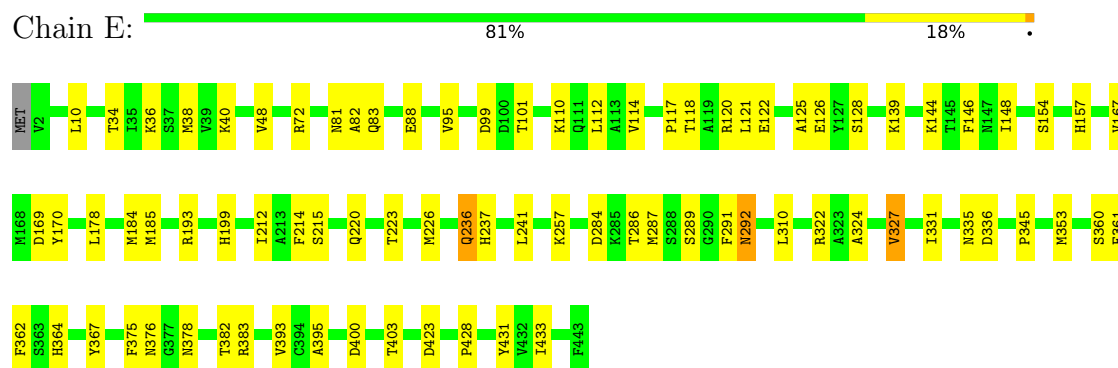
- Molecule 1: Methyl-coenzyme M reductase subunit gamma



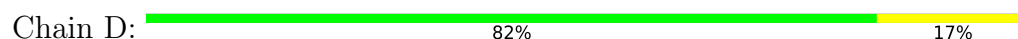
- Molecule 1: Methyl-coenzyme M reductase subunit gamma

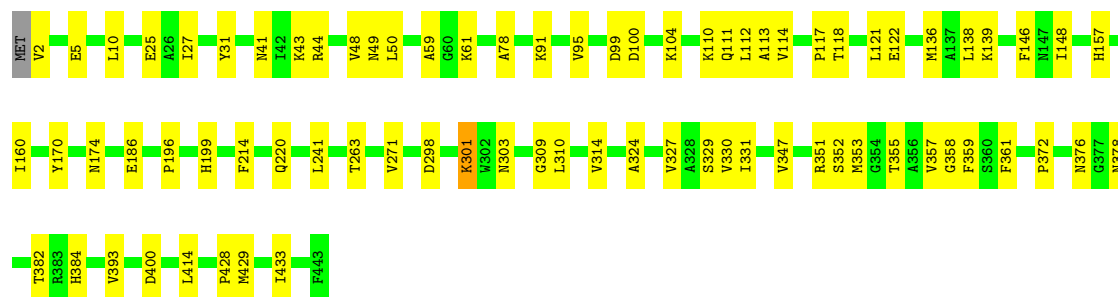


- Molecule 2: Methyl-coenzyme M reductase subunit beta



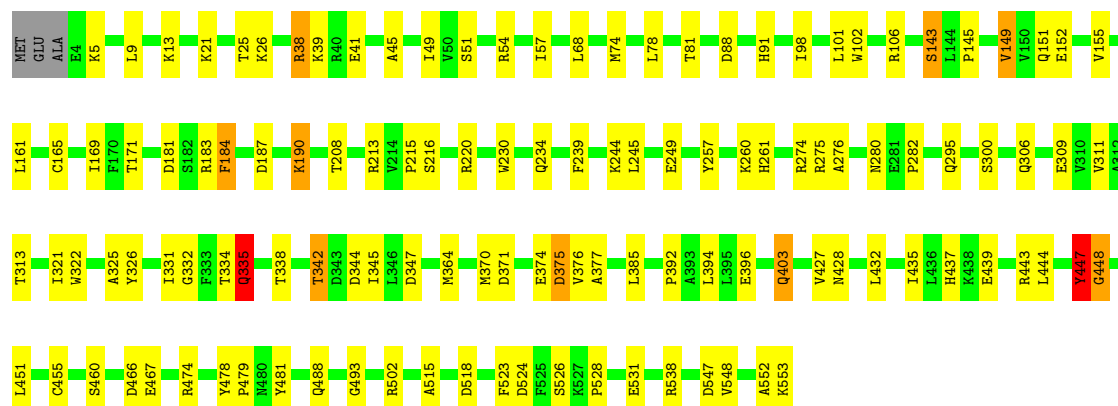
- Molecule 2: Methyl-coenzyme M reductase subunit beta





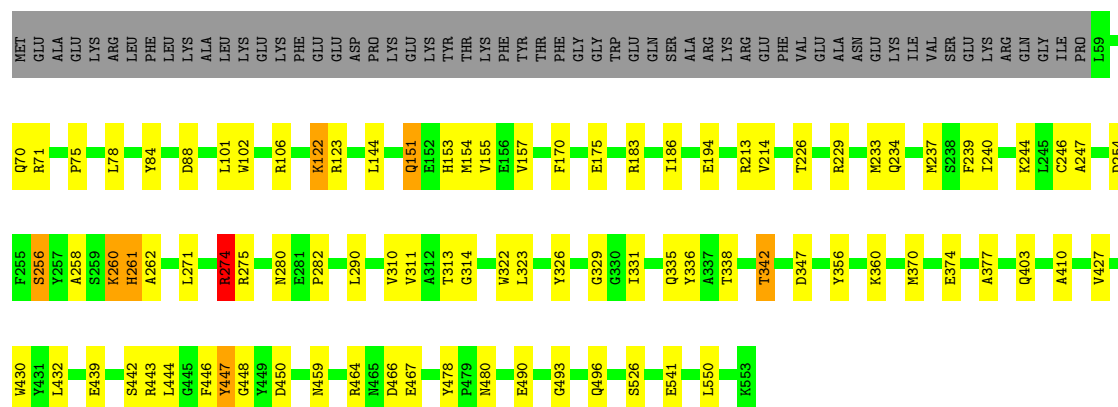
• Molecule 3: Methyl-coenzyme M reductase subunit alpha

Chain C: 77% 20% ..



• Molecule 3: Methyl-coenzyme M reductase subunit alpha

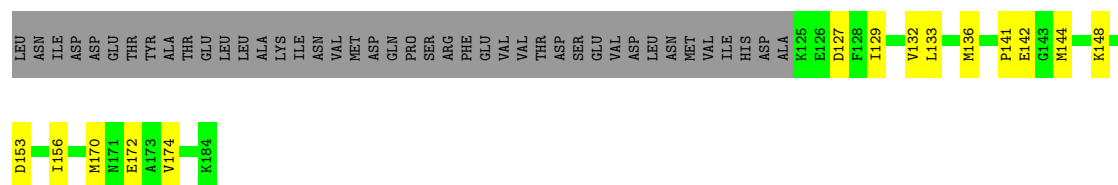
Chain F: 73% 15% 10%



• Molecule 4: Methanogenesis marker protein 17

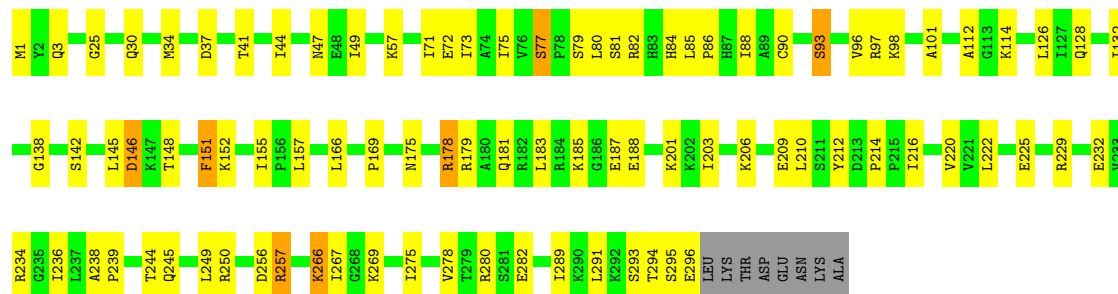
Chain G: 45% 16% 38%





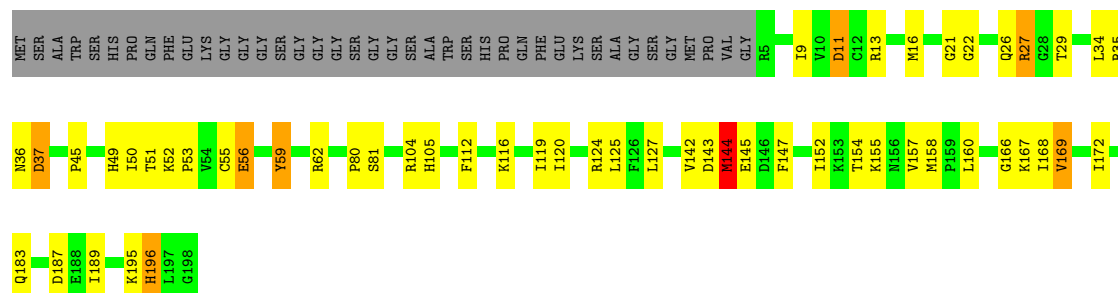
• Molecule 5: Methanogenesis marker protein 7

Chain H: 68% 27%



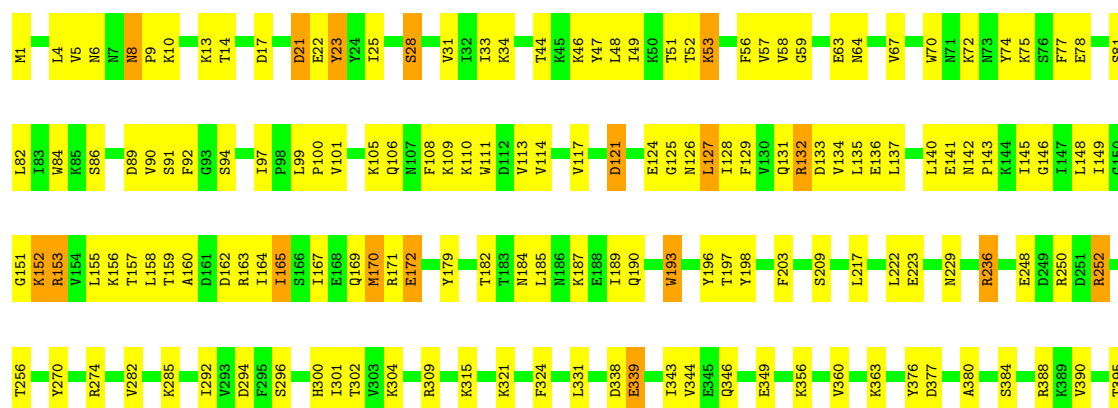
• Molecule 6: Methyl-coenzyme M reductase operon protein C

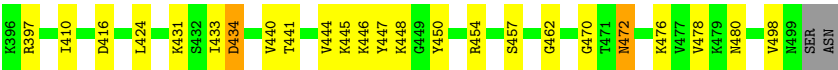
Chain I: 59% 20% 17%



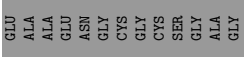
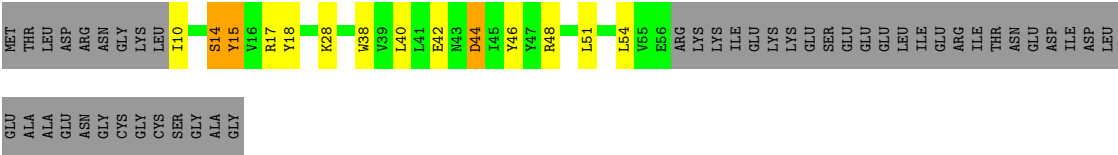
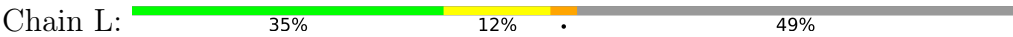
• Molecule 7: UPF0288 protein MmarC6\_0796

Chain J: 64% 32%





- Molecule 8: DUF2098 domain-containing protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	349437	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MHS, SHT, SMC, GL3, COM, MGN, AGM, S5Q, TP7, F43

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	0.31	0/2116	0.57	3/2861 (0.1%)
1	B	0.32	0/2116	0.52	0/2861
2	D	0.33	0/3319	0.47	0/4499
2	E	0.32	0/3319	0.51	1/4499 (0.0%)
3	C	0.33	0/4328	0.51	2/5856 (0.0%)
3	F	0.33	0/3845	0.49	0/5214
4	G	0.28	0/943	0.51	0/1262
5	H	0.32	0/2435	0.53	1/3280 (0.0%)
6	I	0.30	0/1490	0.56	1/2006 (0.0%)
7	J	0.29	0/4027	0.50	0/5444
8	L	0.26	0/398	0.50	0/542
All	All	0.32	0/28336	0.51	8/38324 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	F	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	82	ALA	CB-CA-C	8.72	123.19	110.10
1	A	8	TYR	N-CA-CB	-8.01	96.19	110.60
1	A	7	PHE	N-CA-C	-6.49	93.49	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	447	TYR	CB-CA-C	-6.32	97.77	110.40
5	H	146	ASP	CB-CG-OD1	5.98	123.68	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	274	ARG	Sidechain
3	C	335	GLN	Sidechain
3	F	274	ARG	Sidechain

## 5.2 Too-close contacts

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	2071	0	2012	34	0
1	B	2071	0	2012	35	0
2	D	3263	0	3258	48	0
2	E	3263	0	3258	54	0
3	C	4284	0	4148	99	0
3	F	3812	0	3673	63	0
4	G	931	0	970	21	0
5	H	2393	0	2475	76	0
6	I	1469	0	1534	45	0
7	J	3962	0	4000	165	0
8	L	390	0	378	12	0
9	A	62	0	43	24	0
9	F	62	0	43	7	0
10	E	28	0	21	9	0
11	C	7	0	5	1	0
12	F	21	0	19	1	0
13	H	18	0	0	2	0
13	I	36	0	0	0	0
All	All	28143	0	27849	560	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 10.



The worst 5 of 560 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)
9:A:601:F43:H5D1	3:C:335:GLN:CB	1.53	1.35
9:A:601:F43:OBD	3:C:335:GLN:N	1.83	1.11
9:A:601:F43:H5D1	3:C:335:GLN:HB2	1.10	1.08
5:H:169:PRO:HB3	7:J:135:LEU:HD11	1.38	1.05
2:E:367:TYR:OH	9:F:601:F43:H5A2	1.59	1.02

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 PDB entries followed by that with respect to all EM entries.

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	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
1	B	257/260 (99%)	251 (98%)	6 (2%)	0	100	100
2	D	440/443 (99%)	418 (95%)	22 (5%)	0	100	100
2	E	440/443 (99%)	416 (94%)	24 (6%)	0	100	100
3	C	543/553 (98%)	511 (94%)	31 (6%)	1 (0%)	44	71
3	F	488/553 (88%)	460 (94%)	28 (6%)	0	100	100
4	G	110/183 (60%)	106 (96%)	4 (4%)	0	100	100
5	H	294/304 (97%)	284 (97%)	10 (3%)	0	100	100
6	I	192/234 (82%)	183 (95%)	9 (5%)	0	100	100
7	J	495/501 (99%)	456 (92%)	37 (8%)	2 (0%)	30	58
8	L	45/93 (48%)	45 (100%)	0	0	100	100
All	All	3561/3827 (93%)	3380 (95%)	178 (5%)	3 (0%)	50	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	J	165	ILE
7	J	6	ASN
3	C	145	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	223/224 (100%)	212 (95%)	11 (5%)	21	49
1	B	223/224 (100%)	218 (98%)	5 (2%)	47	76
2	D	341/343 (99%)	333 (98%)	8 (2%)	45	75
2	E	341/343 (99%)	331 (97%)	10 (3%)	37	68
3	C	437/439 (100%)	413 (94%)	24 (6%)	18	44
3	F	388/439 (88%)	368 (95%)	20 (5%)	19	47
4	G	104/168 (62%)	95 (91%)	9 (9%)	8	24
5	H	264/271 (97%)	241 (91%)	23 (9%)	8	24
6	I	160/186 (86%)	147 (92%)	13 (8%)	9	27
7	J	452/454 (100%)	416 (92%)	36 (8%)	10	27
8	L	43/81 (53%)	39 (91%)	4 (9%)	7	21
All	All	2976/3172 (94%)	2813 (94%)	163 (6%)	20	44

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	59	TYR
7	J	187	LYS
6	I	167	LYS
7	J	72	LYS
7	J	344	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
5	H	181	GLN
7	J	64	ASN
7	J	126	ASN
3	C	509	ASN
3	C	335	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	MHS	C	261	3	7,11,12	0.77	0	6,14,16	0.89	0
3	MGN	C	403	3	6,9,10	0.78	0	5,12,14	1.34	1 (20%)
3	SMC	C	455	3	5,6,7	0.71	0	2,6,8	1.06	0
3	GL3	F	448	3	2,3,4	1.84	1 (50%)	1,2,4	0.11	0
3	MHS	F	261	3	7,11,12	0.81	0	6,14,16	1.86	1 (16%)
3	MGN	F	403	3	6,9,10	0.78	0	5,12,14	1.02	0
3	SMC	F	455	3	5,6,7	0.69	0	2,6,8	0.80	0
3	AGM	F	275	3	10,11,12	0.48	0	6,13,15	0.21	0
3	AGM	C	275	3	10,11,12	0.46	0	6,13,15	0.22	0
3	GL3	C	448	3	2,3,4	1.85	1 (50%)	1,2,4	0.47	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
3	MHS	C	261	3	-	1/5/6/8	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGN	C	403	3	-	4/7/9/12	-
3	SMC	C	455	3	-	3/3/5/7	-
3	GL3	F	448	3	-	1/1/1/2	-
3	MHS	F	261	3	-	4/5/6/8	0/1/1/1
3	MGN	F	403	3	-	0/7/9/12	-
3	SMC	F	455	3	-	2/3/5/7	-
3	AGM	F	275	3	-	5/10/11/13	-
3	AGM	C	275	3	-	3/10/11/13	-
3	GL3	C	448	3	-	0/1/1/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	448	GL3	C-S	-2.59	1.71	1.80
3	F	448	GL3	C-S	-2.58	1.71	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	261	MHS	CB-CA-C	-4.19	103.62	111.47
3	C	403	MGN	CB2-CA-CB1	-2.74	106.17	111.00

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	261	MHS	O-C-CA-CB
3	C	275	AGM	O-C-CA-CB
3	C	403	MGN	N-CA-CB1-CG
3	C	403	MGN	CB2-CA-CB1-CG
3	C	403	MGN	C-CA-CB1-CG

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	261	MHS	1	0
3	C	403	MGN	2	0
3	C	455	SMC	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	261	MHS	1	0
3	F	403	MGN	1	0
3	F	275	AGM	1	0
3	C	275	AGM	1	0
3	C	448	GL3	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
13	S5Q	I	201	6	18,30,30	2.68	12 (66%)	-		
9	F43	F	601	-	61,71,71	1.97	4 (6%)	64,118,118	1.02	5 (7%)
9	F43	A	601	11,3	61,71,71	2.04	4 (6%)	64,118,118	1.11	4 (6%)
13	S5Q	I	202	6	18,30,30	2.62	11 (61%)	-		
13	S5Q	H	401	5	18,30,30	2.62	12 (66%)	-		
12	TP7	F	602	-	19,20,20	1.58	3 (15%)	24,26,26	1.16	2 (8%)
11	COM	C	601	9	6,6,6	0.42	0	7,8,8	0.62	0
10	SHT	E	601	-	26,27,27	1.29	1 (3%)	30,36,36	0.77	1 (3%)

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
9	F43	F	601	-	-	10/28/185/185	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	F43	A	601	11,3	-	14/28/185/185	-
12	TP7	F	602	-	-	3/24/24/24	-
11	COM	C	601	9	-	4/4/4/4	-
10	SHT	E	601	-	-	14/31/31/31	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	F43	NI-NA	9.70	2.10	1.89
9	F	601	F43	NI-NA	9.40	2.09	1.89
9	A	601	F43	NI-NB	9.16	2.09	1.89
9	F	601	F43	NI-NB	9.09	2.09	1.89
9	A	601	F43	NI-ND	7.20	2.05	1.89

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	601	F43	C2B-C1B-NB	3.45	107.00	101.84
9	A	601	F43	C3D-C4D-ND	3.24	107.39	102.34
9	F	601	F43	C2A-C3A-C4A	-3.24	97.42	102.36
9	F	601	F43	C3D-C4D-ND	3.15	107.24	102.34
9	F	601	F43	C2B-C3B-C4B	-2.71	98.57	101.63

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	F43	C2A-C3A-CAA-CBA
9	A	601	F43	C4A-C3A-CAA-CBA
9	F	601	F43	C1A-C2A-C5A-C6A
9	F	601	F43	C9A-C2A-C5A-C6A
9	F	601	F43	C2A-C3A-CAA-CBA

There are no ring outliers.

6 monomers are involved in 44 short contacts:

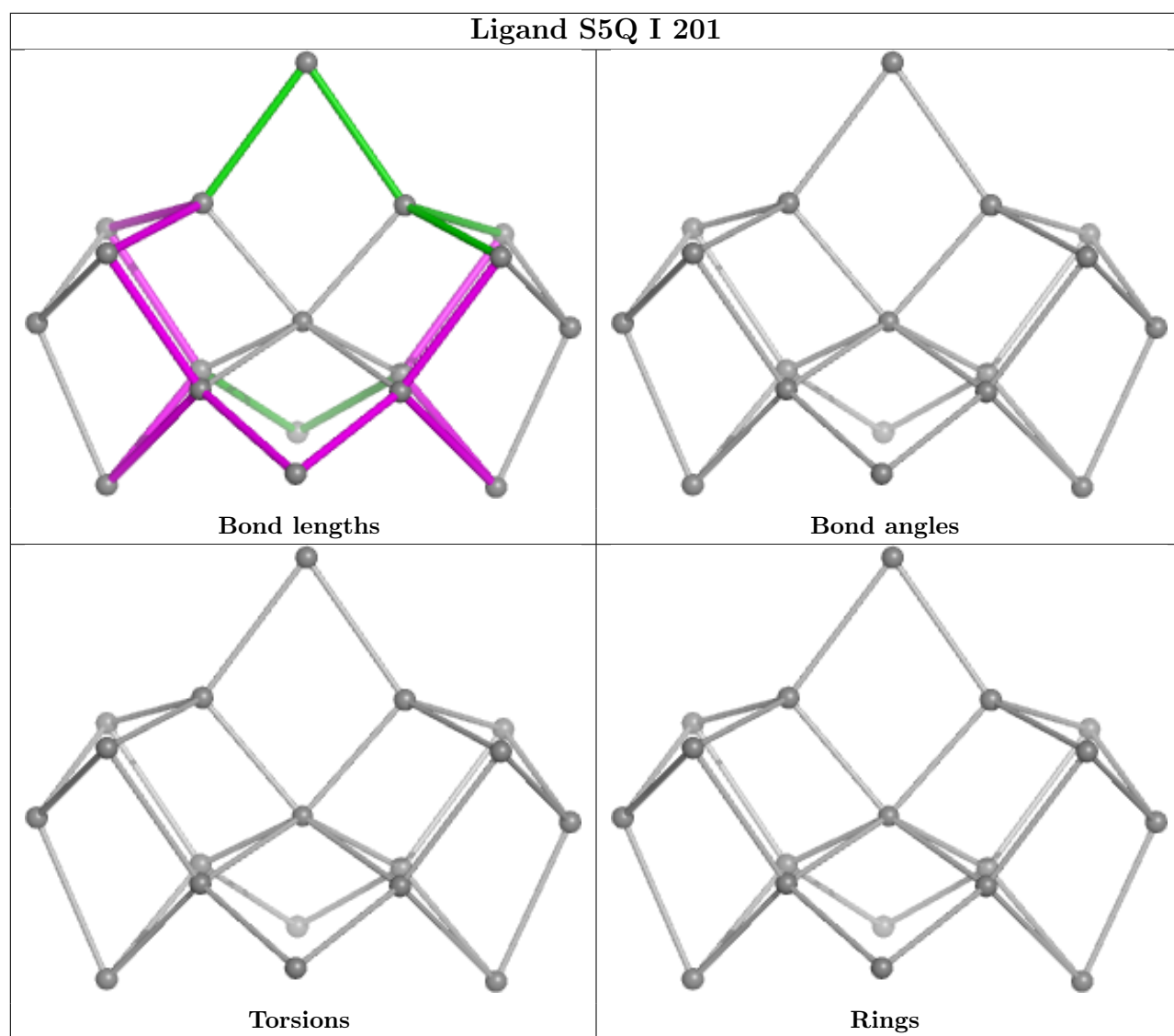
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	601	F43	7	0
9	A	601	F43	24	0
13	H	401	S5Q	2	0

*Continued on next page...*

*Continued from previous page...*

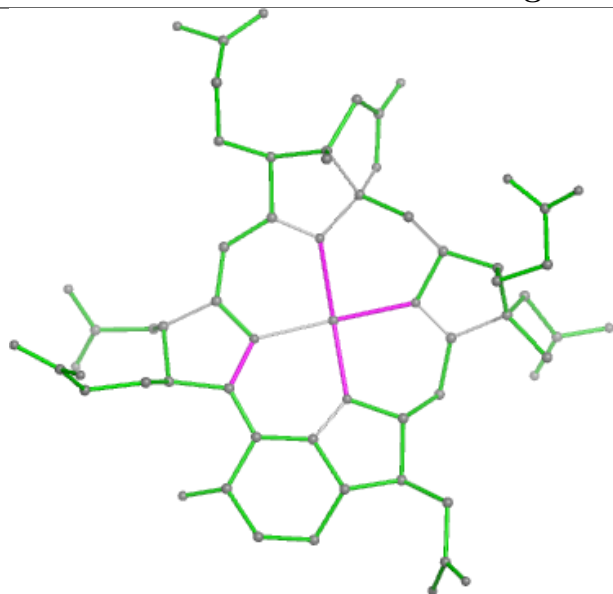
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	602	TP7	1	0
11	C	601	COM	1	0
10	E	601	SHT	9	0

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

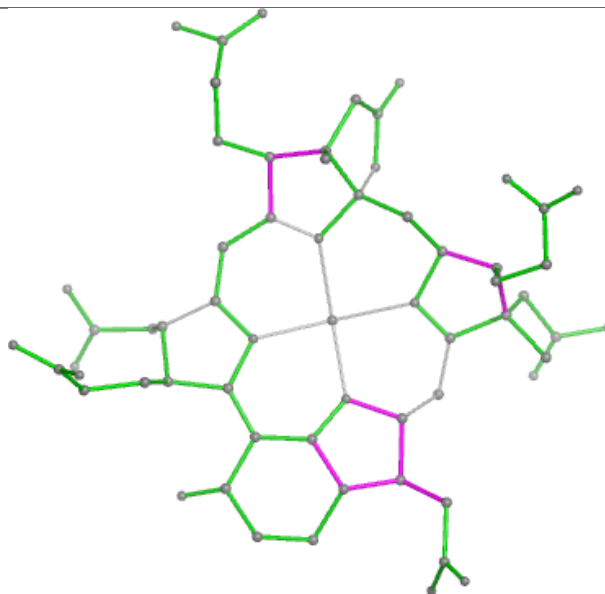




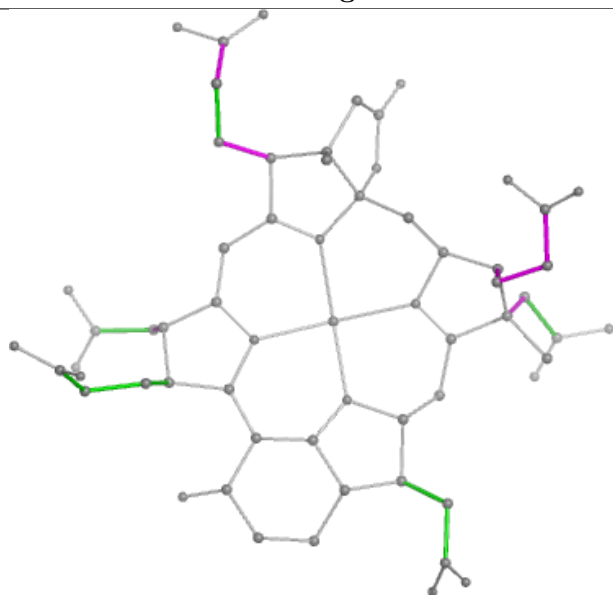
## Ligand F43 F 601



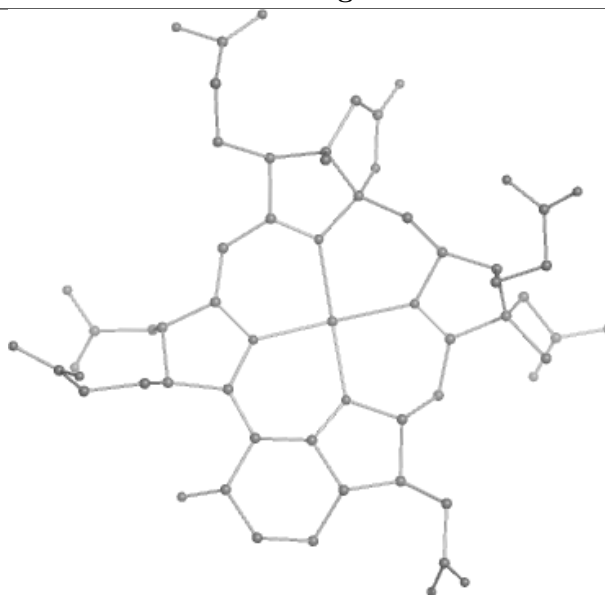
Bond lengths



Bond angles

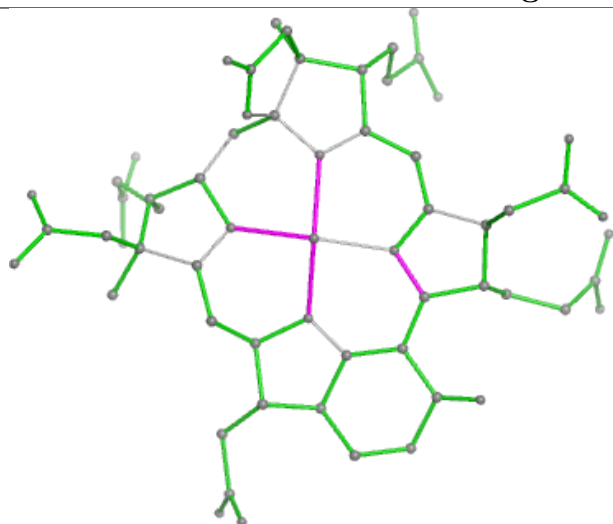


Torsions

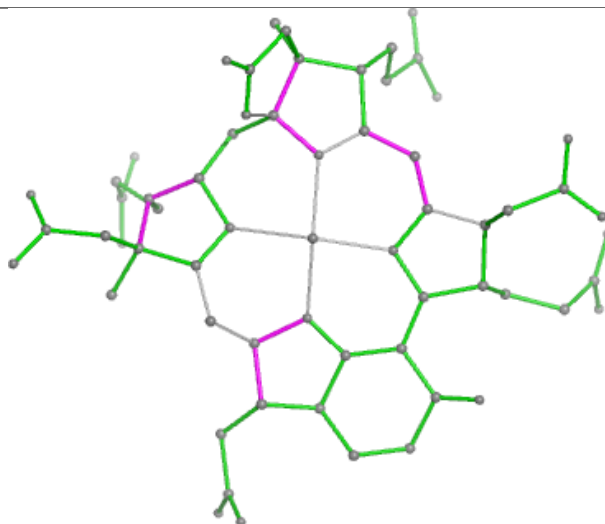


Rings

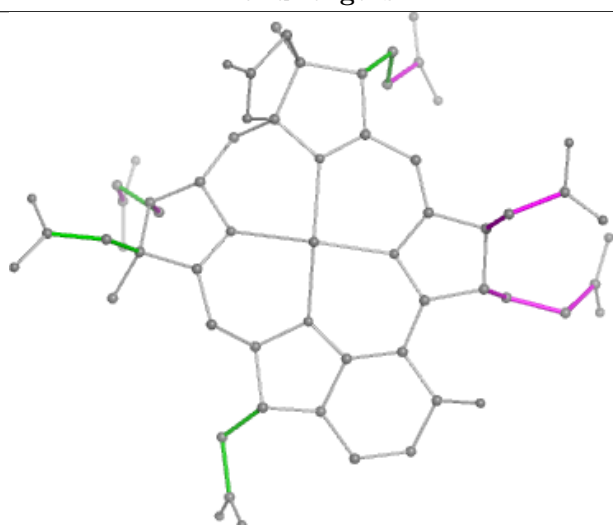
## Ligand F43 A 601



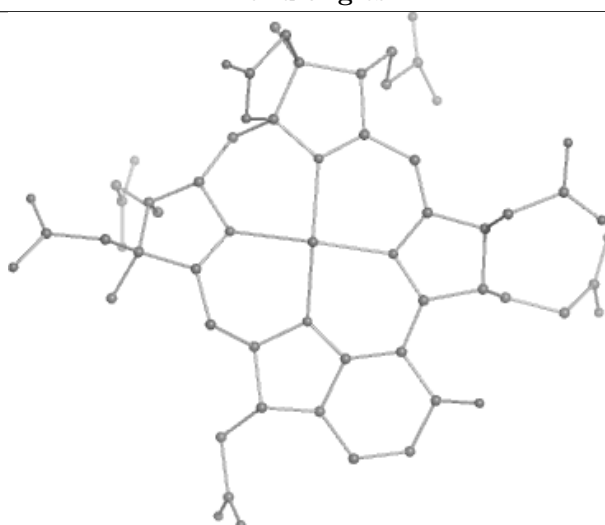
Bond lengths



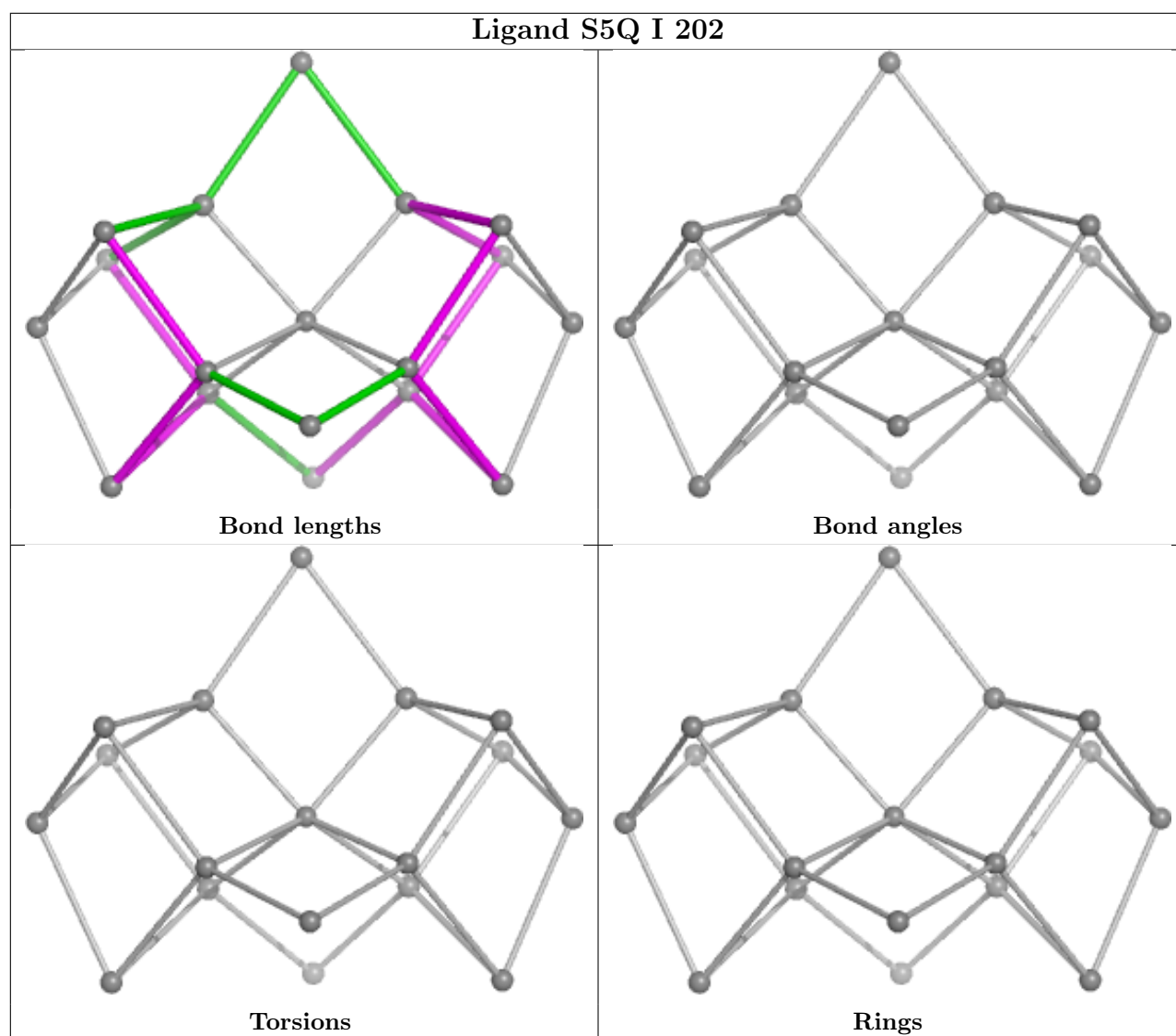
Bond angles

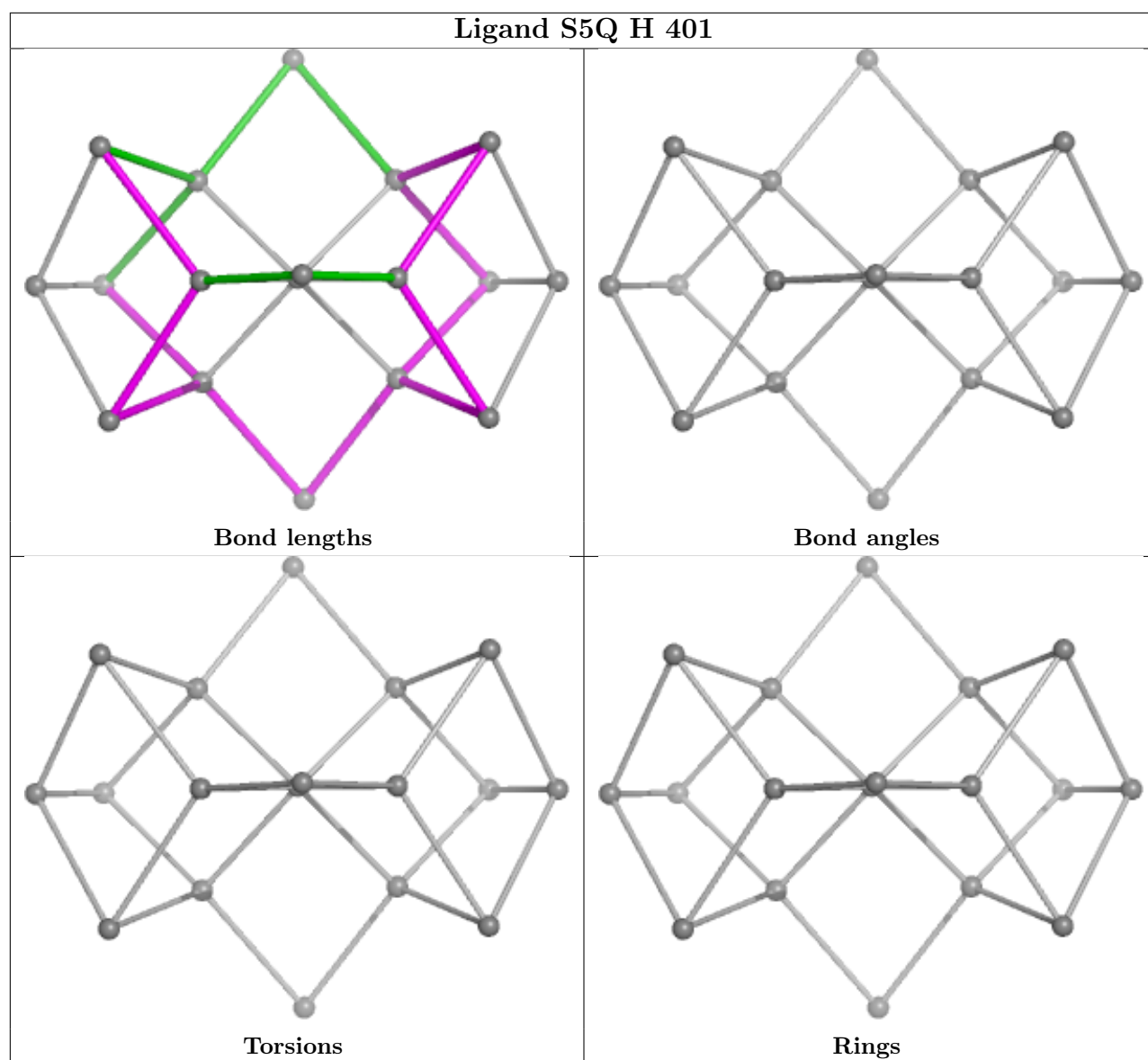


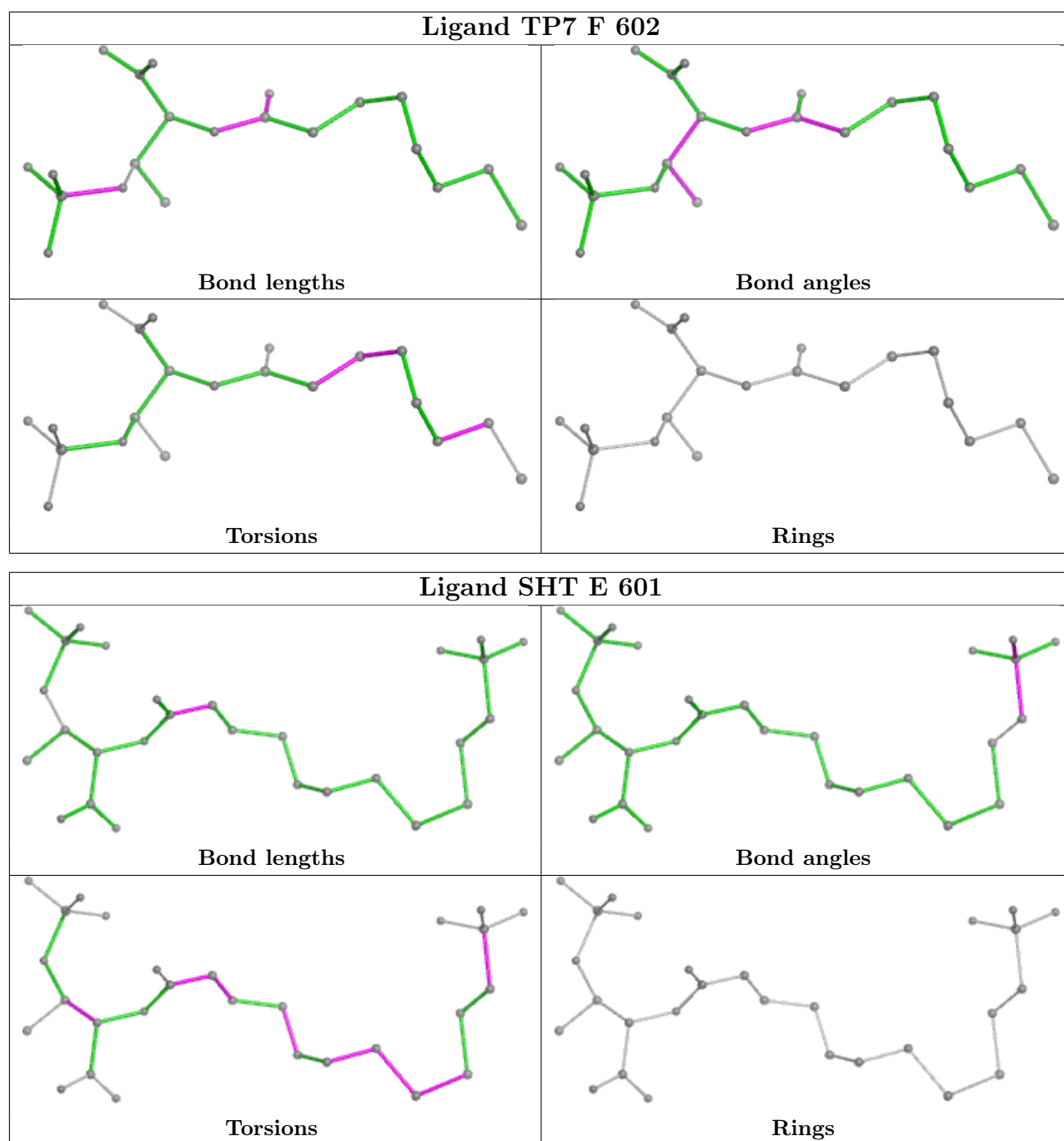
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	183:THR	C	184:ASN	N	3.25