



wwPDB EM Model Validation Summary Report ⓘ

Mar 12, 2020 – 02:25 PM EDT

PDB ID : 6QL5
EMDB ID : EMD-4577
Title : Structure of fatty acid synthase complex with bound gamma subunit from *Saccharomyces cerevisiae* at 2.8 angstrom
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.
Deposited on : 2019-01-31
Resolution : 2.80 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

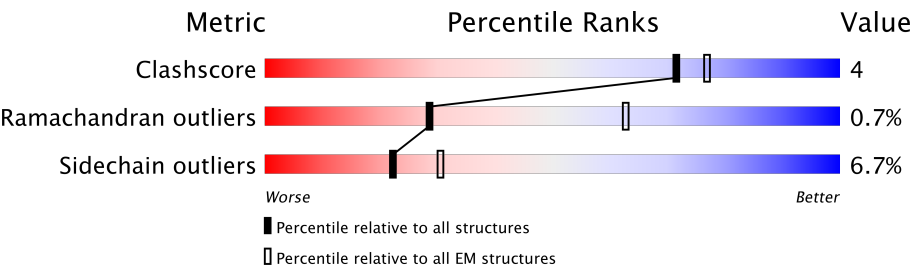
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

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 2.80 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1887	
1	B	1887	
1	C	1887	
1	D	1887	
1	E	1887	
1	F	1887	
2	G	2040	
2	H	2040	
2	I	2040	

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Mol	Chain	Length	Quality of chain
2	J	2040	<div><div></div><div>86%</div><div>12%</div><div></div></div>
2	K	2040	<div><div></div><div>86%</div><div>12%</div><div></div></div>
2	L	2040	<div><div></div><div>86%</div><div>12%</div><div></div></div>
3	M	148	<div><div></div><div>60%</div><div>12%</div><div></div><div>24%</div></div>
3	N	148	<div><div></div><div>60%</div><div>11%</div><div></div><div>24%</div></div>
3	O	148	<div><div></div><div>60%</div><div>12%</div><div></div><div>24%</div></div>
3	P	148	<div><div></div><div>60%</div><div>11%</div><div></div><div>24%</div></div>
3	Q	148	<div><div></div><div>60%</div><div>12%</div><div></div><div>24%</div></div>
3	R	148	<div><div></div><div>60%</div><div>11%</div><div></div><div>24%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 183444 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	B	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	C	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	D	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	E	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	F	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	H	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	I	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	J	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	K	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	L	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		

- Molecule 3 is a protein called Translation machinery-associated protein 17.

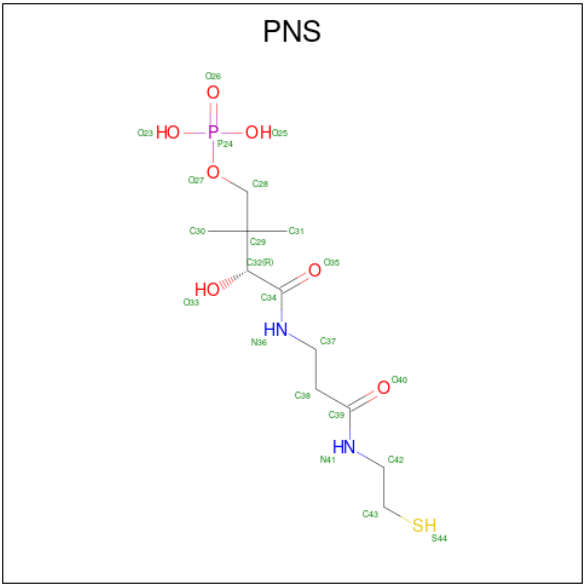
Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	O	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	P	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	Q	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	R	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
4	B	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
4	C	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
4	D	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
4	E	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
4	F	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

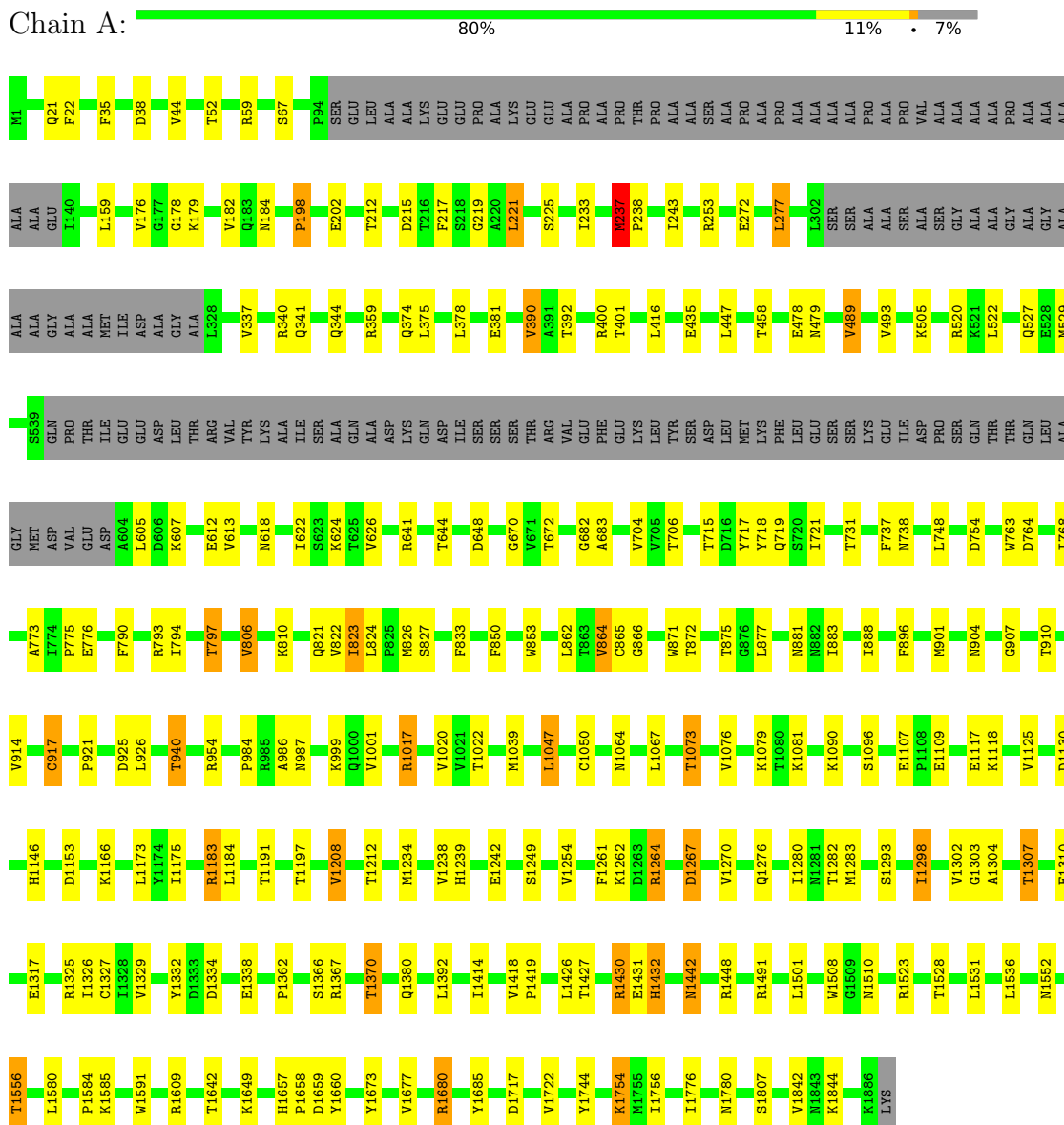
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- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms) attached to a ribityl chain. The ribityl chain is a three-carbon chain with hydroxyl groups at the 2' and 3' positions. The 5' carbon of the ribityl chain is attached to a phosphate group (O1P, O2P, O3P, O4P, O5P). The structure is labeled with atom names: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809,

Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total 31	C 17	N 4	O 9	P 1	0
5	H	1	Total 31	C 17	N 4	O 9	P 1	0
5	I	1	Total 31	C 17	N 4	O 9	P 1	0
5	J	1	Total 31	C 17	N 4	O 9	P 1	0
5	K	1	Total 31	C 17	N 4	O 9	P 1	0
5	L	1	Total 31	C 17	N 4	O 9	P 1	0

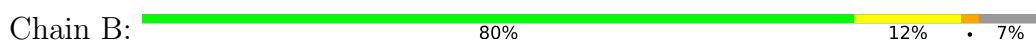
3 Residue-property plots

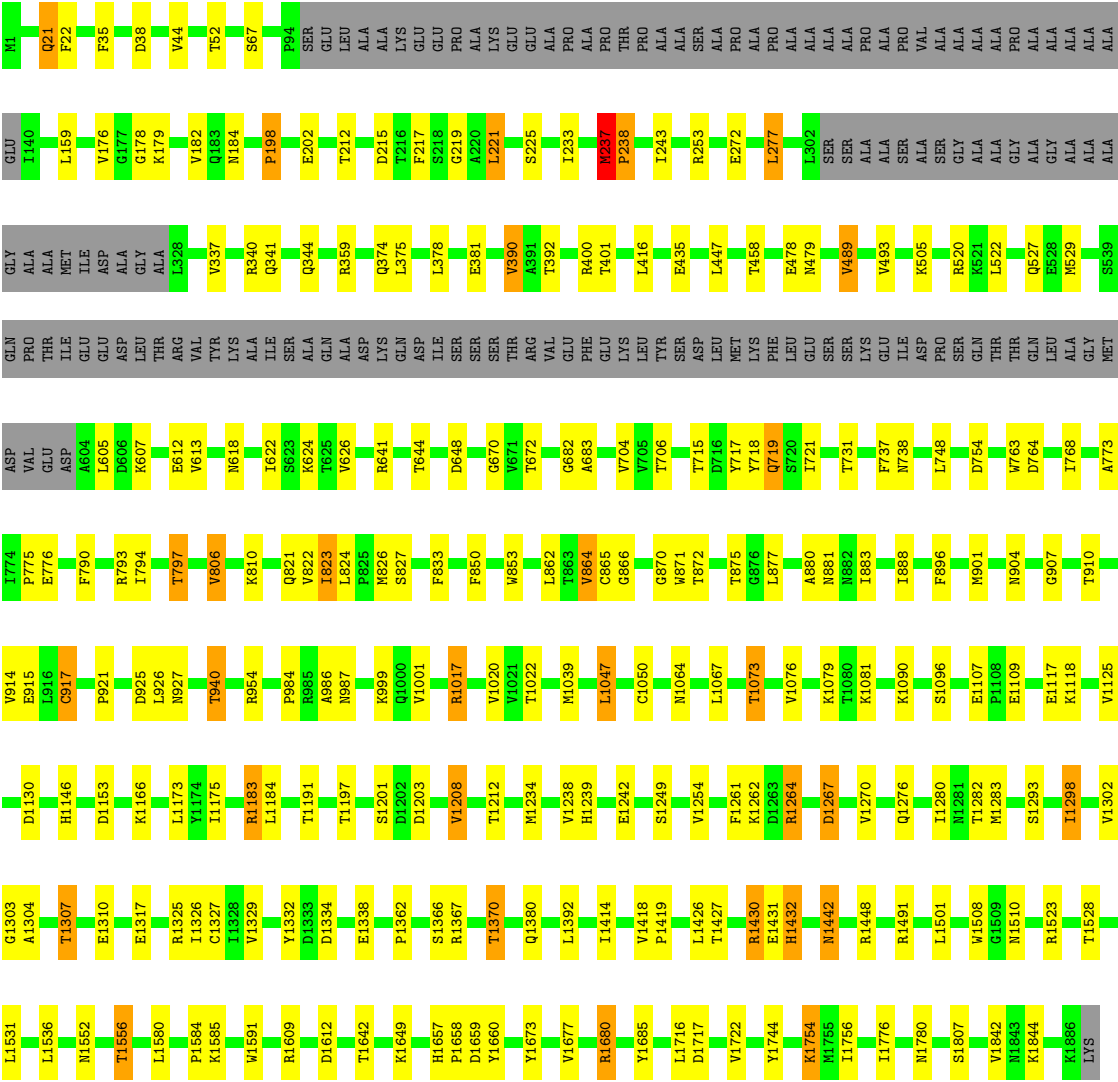
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Fatty acid synthase subunit alpha

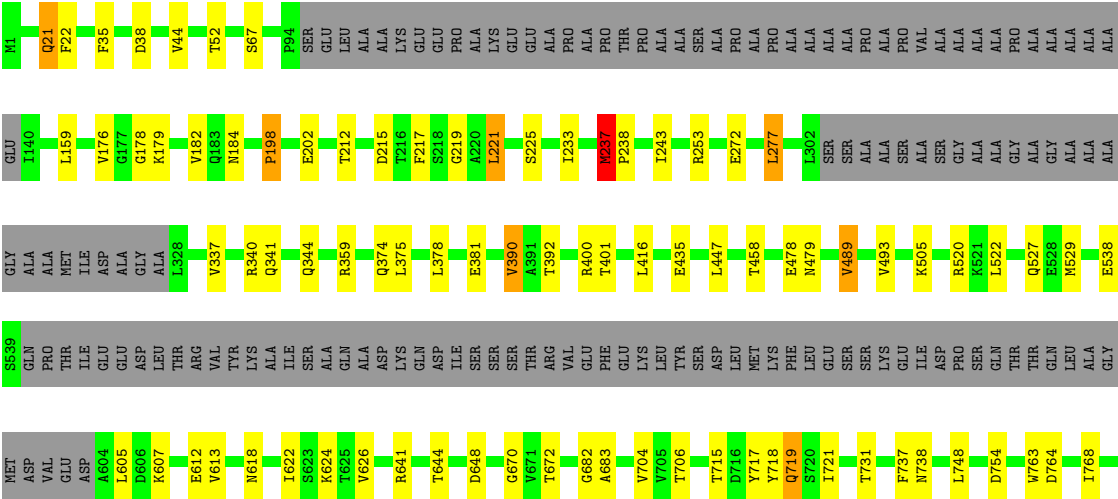
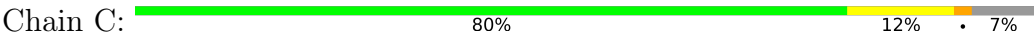


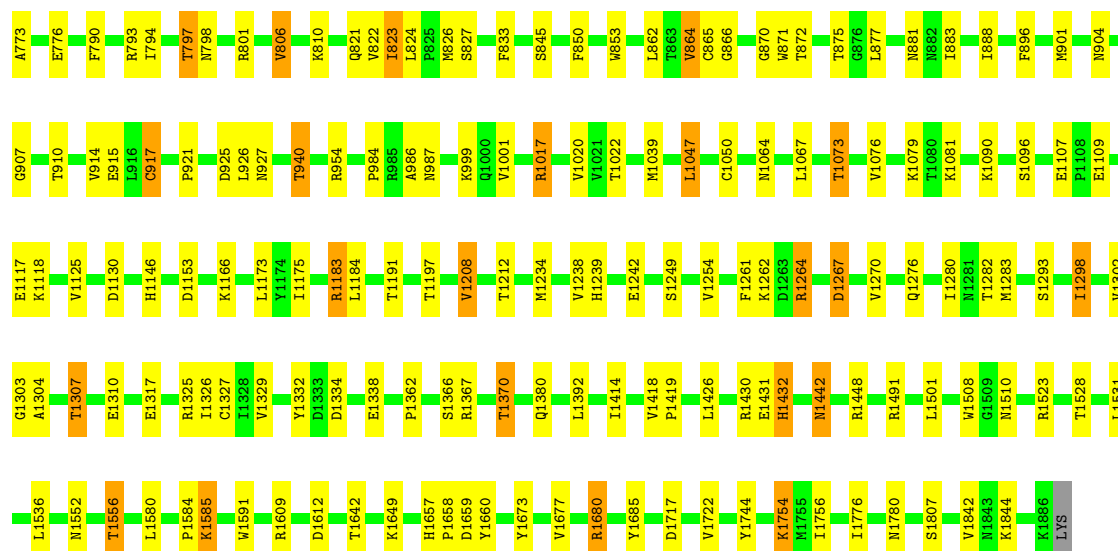
- Molecule 1: Fatty acid synthase subunit alpha





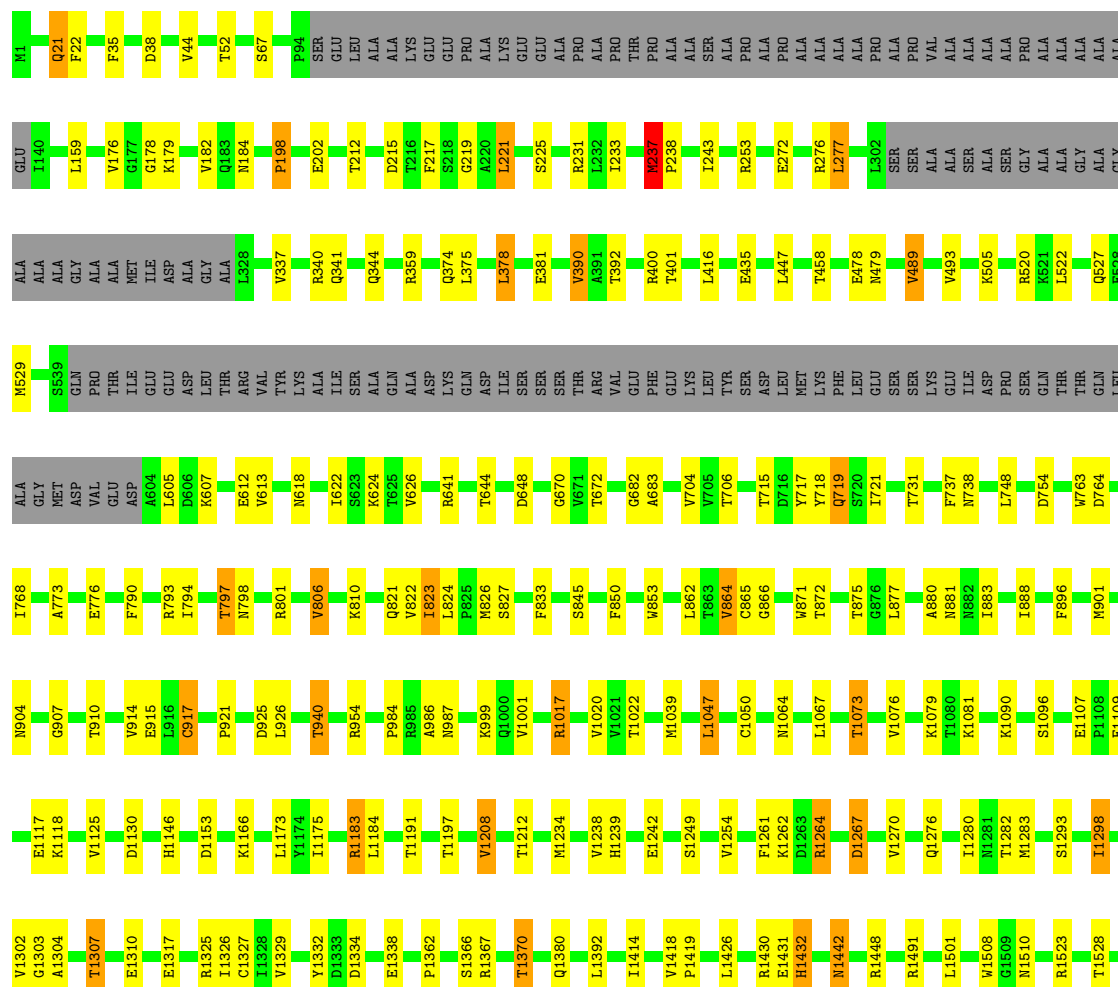
• Molecule 1: Fatty acid synthase subunit alpha





• Molecule 1: Fatty acid synthase subunit alpha

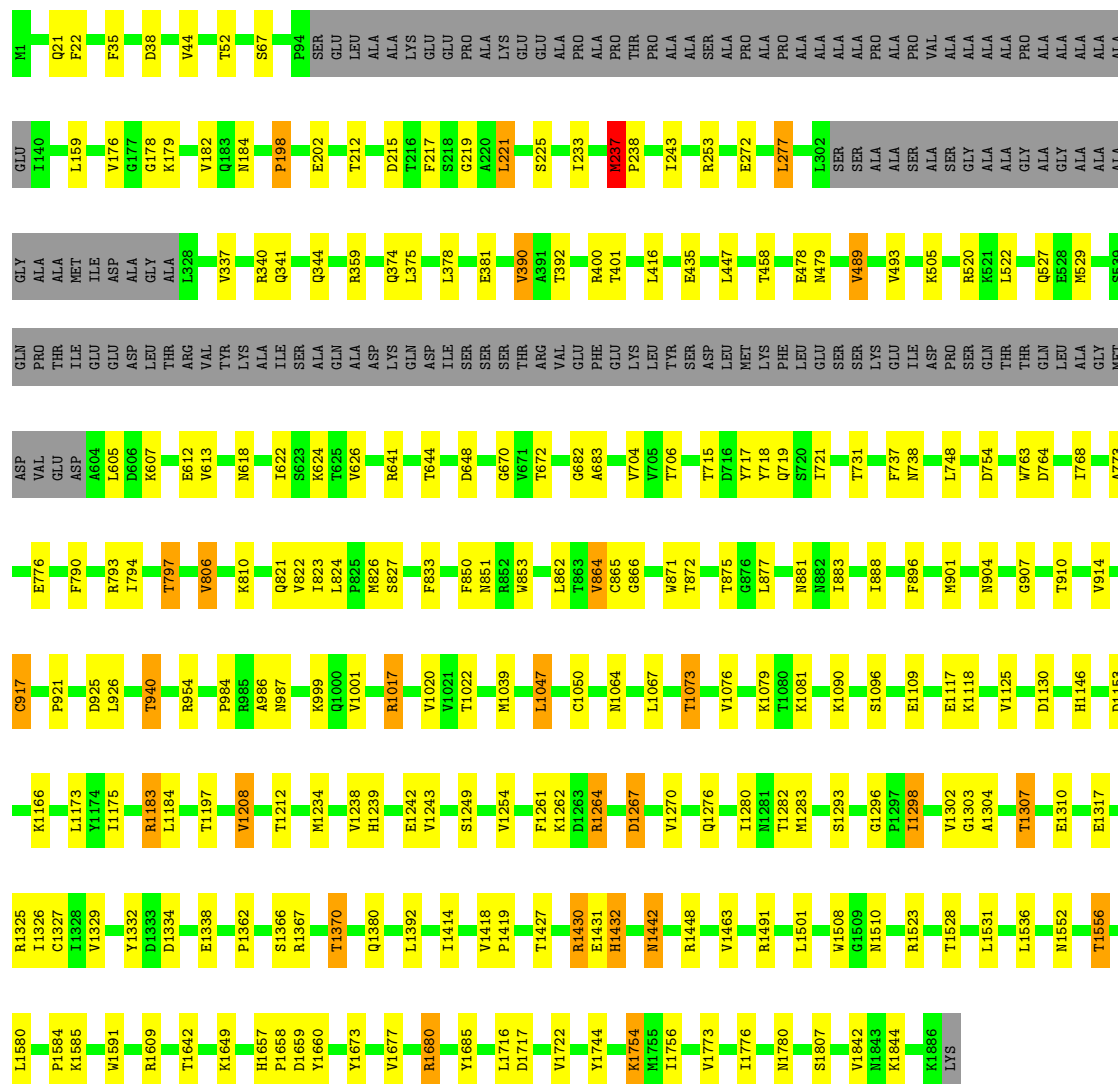
Chain D: 80% 11% 7%





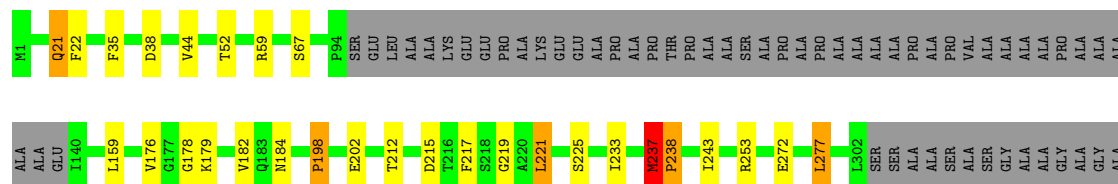
• Molecule 1: Fatty acid synthase subunit alpha

Chain E: 80% 11% 7%

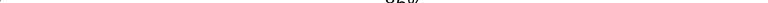


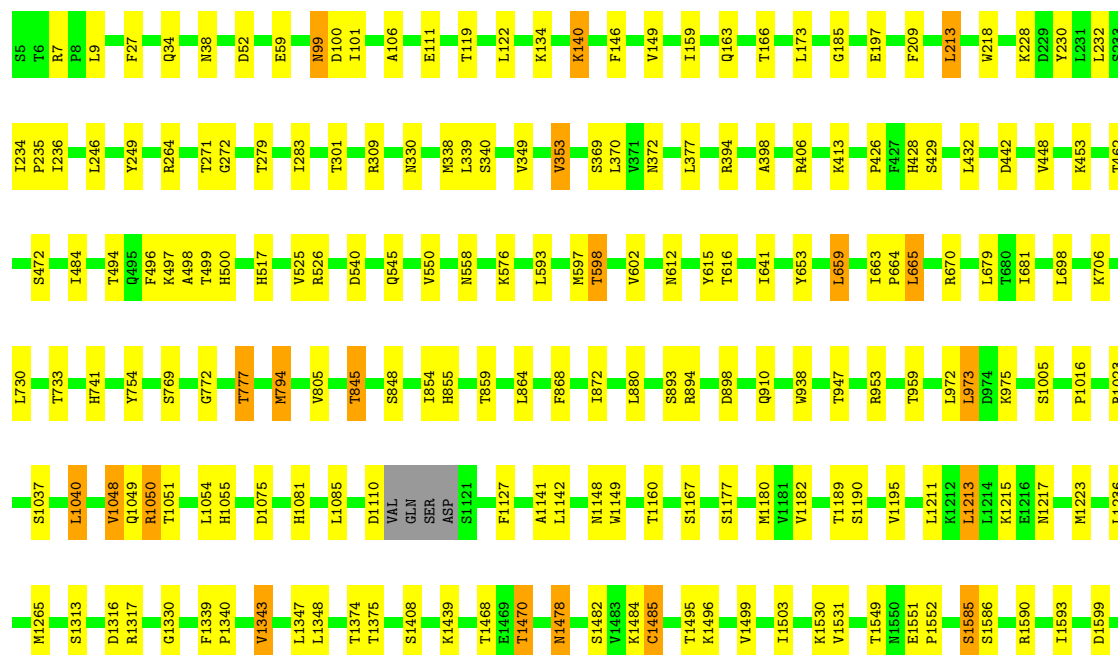
• Molecule 1: Fatty acid synthase subunit alpha

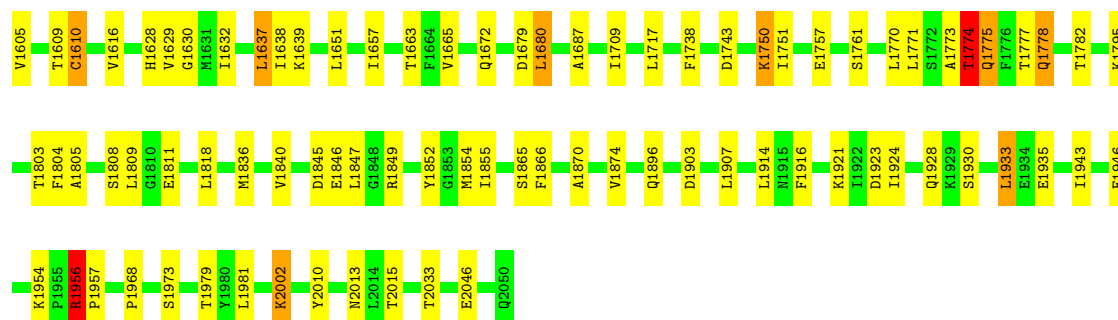
Chain F: 80% 11% 7%





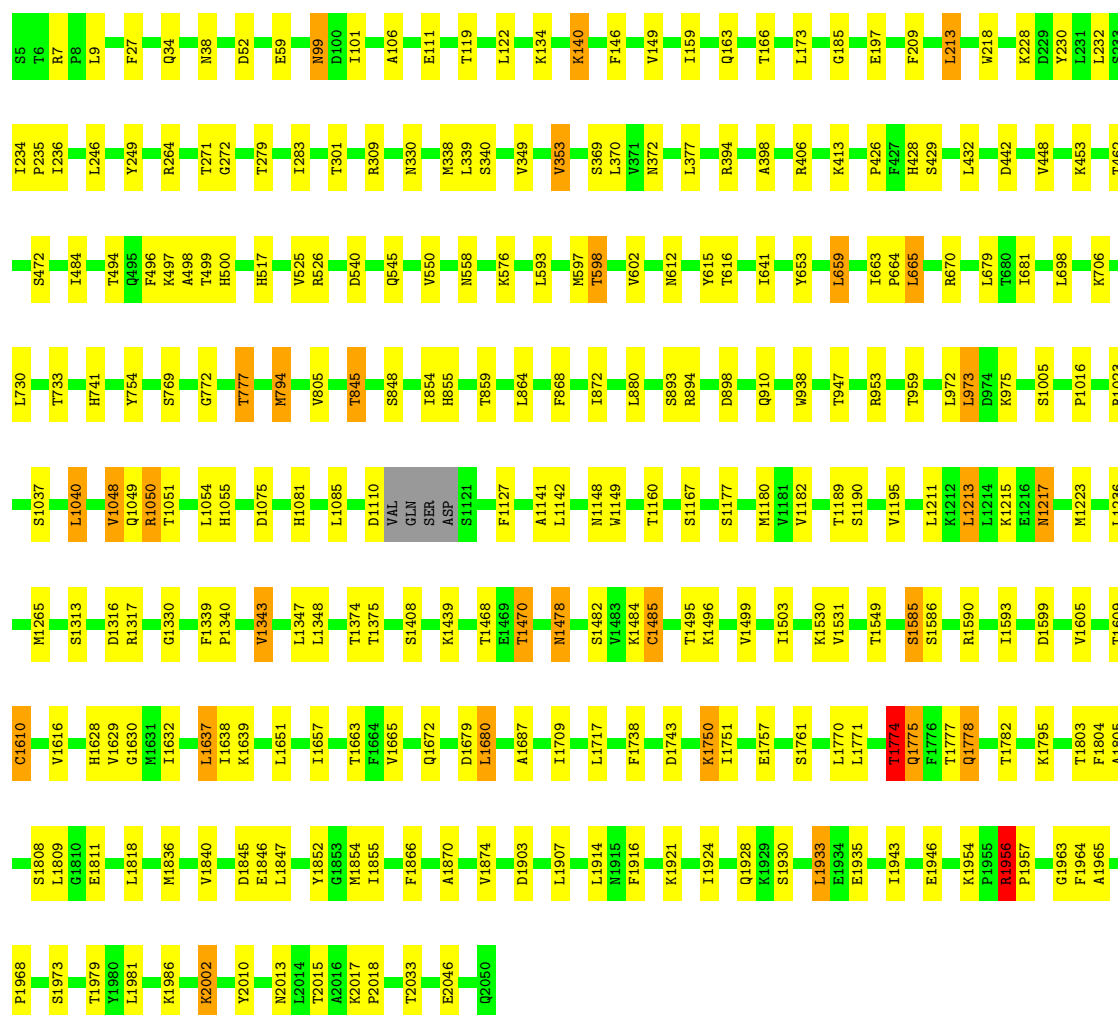
Chain G:  86% 12%





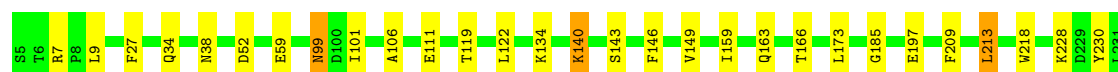
• Molecule 2: Fatty acid synthase subunit beta

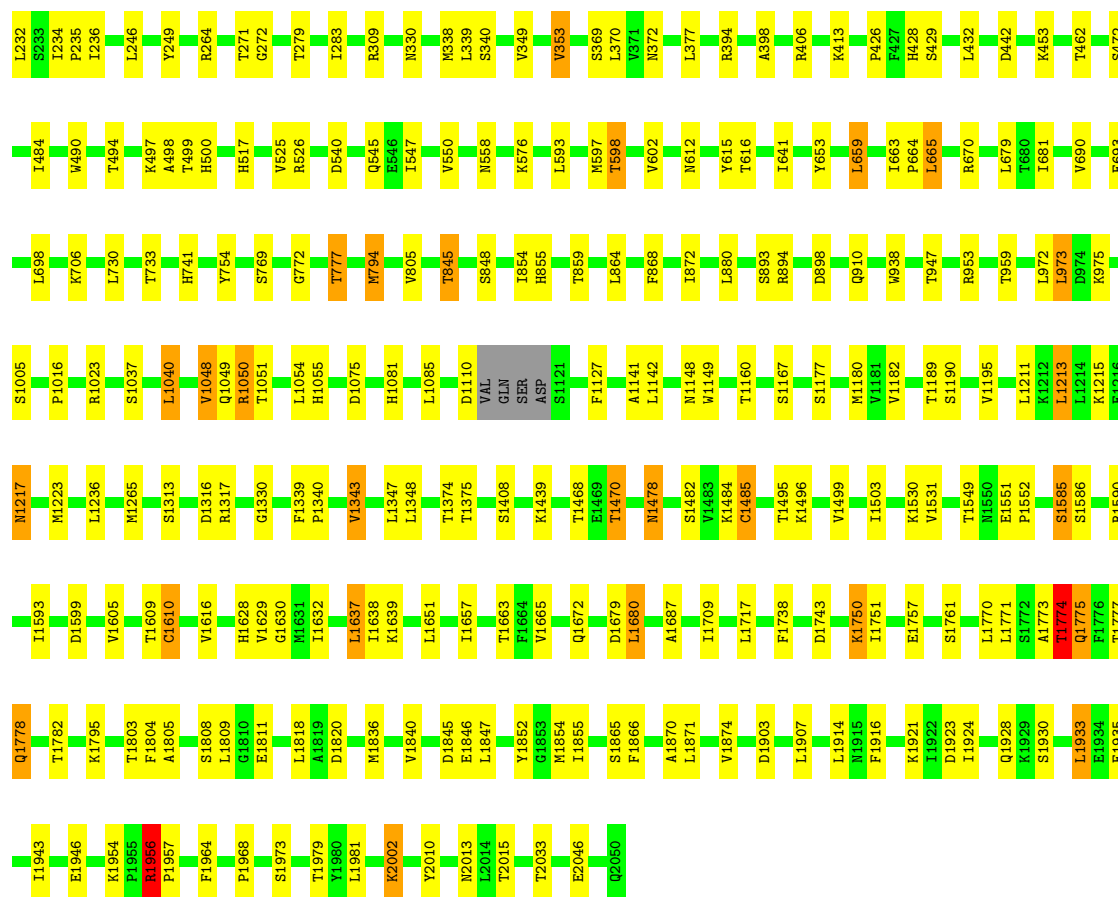
Chain H: 86% 12% .



• Molecule 2: Fatty acid synthase subunit beta

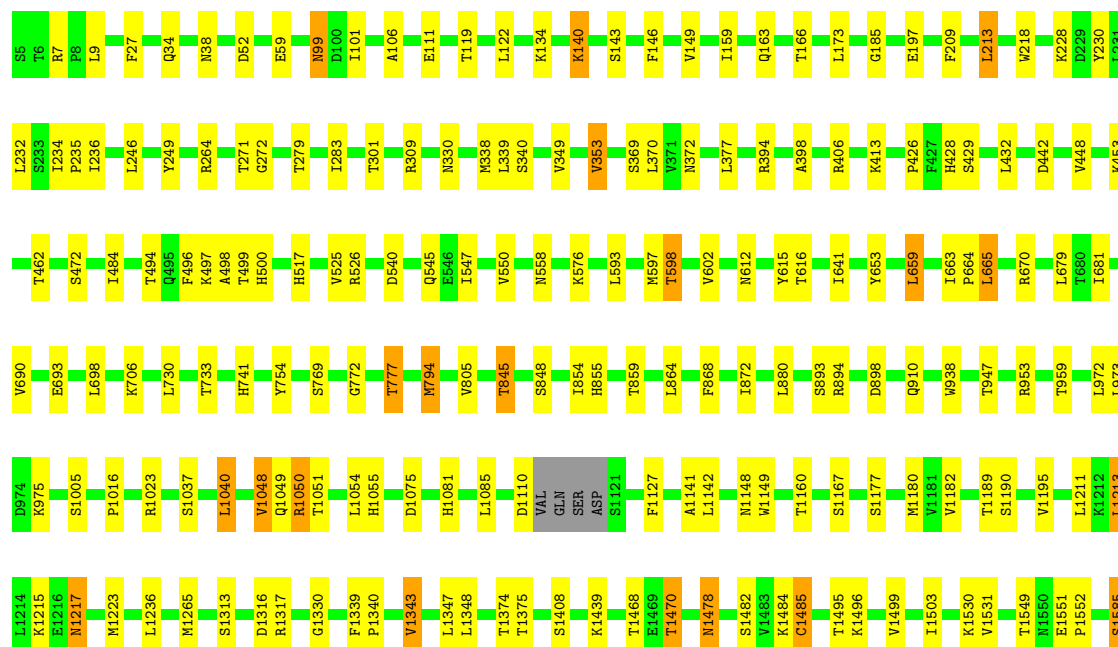
Chain I: 86% 12% .

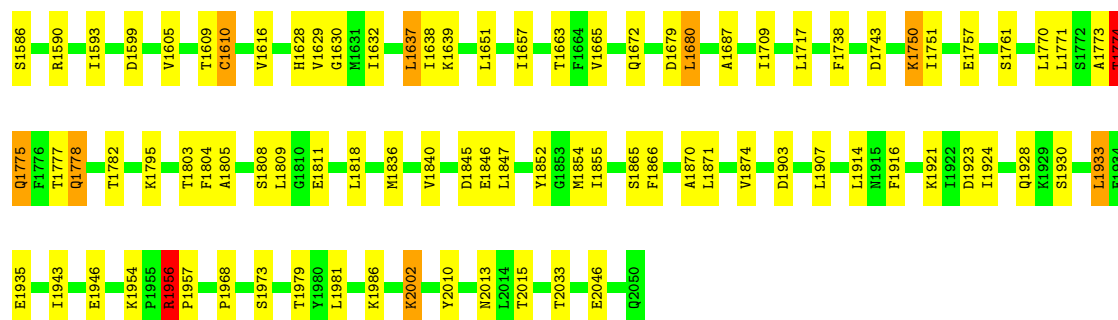




• Molecule 2: Fatty acid synthase subunit beta

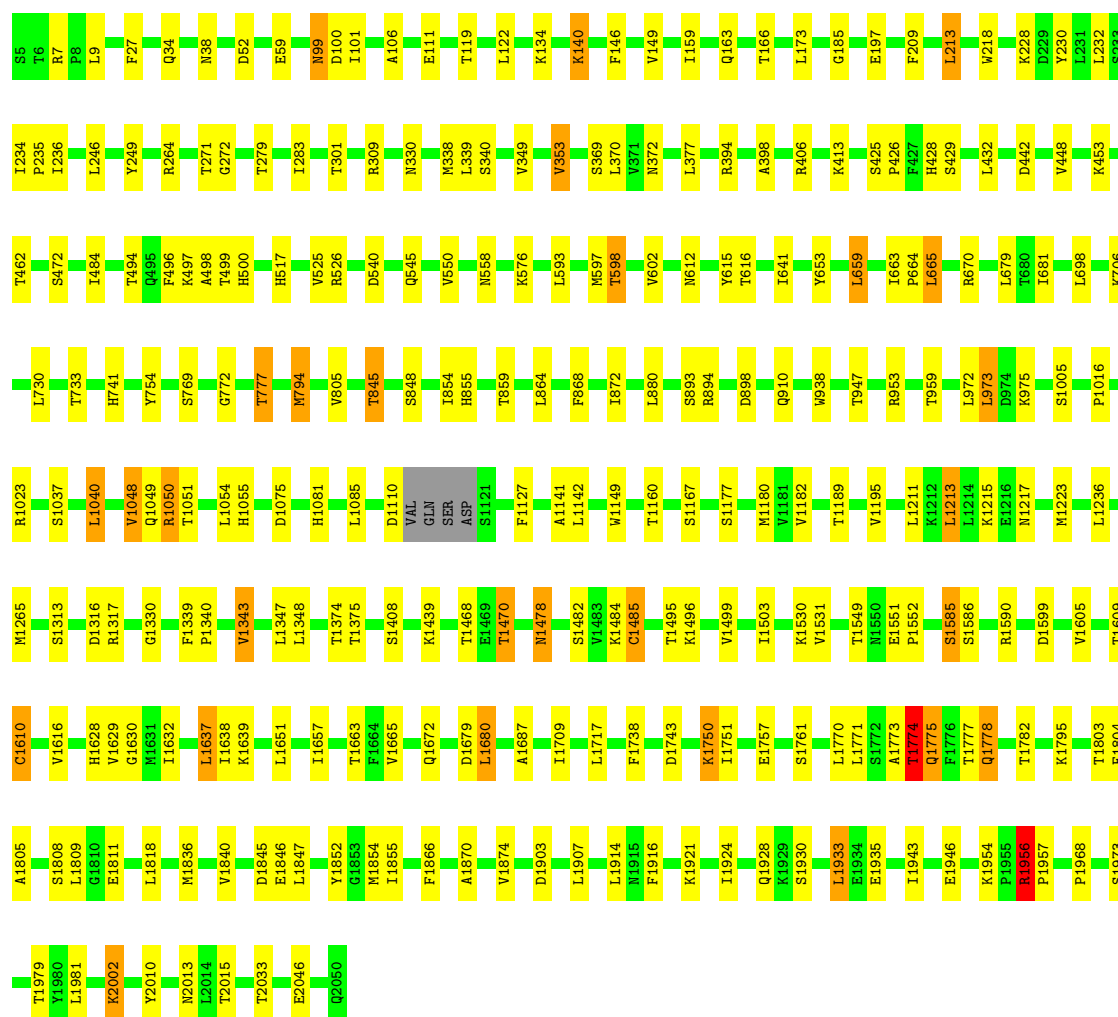
Chain J: 86% 12% .





• Molecule 2: Fatty acid synthase subunit beta

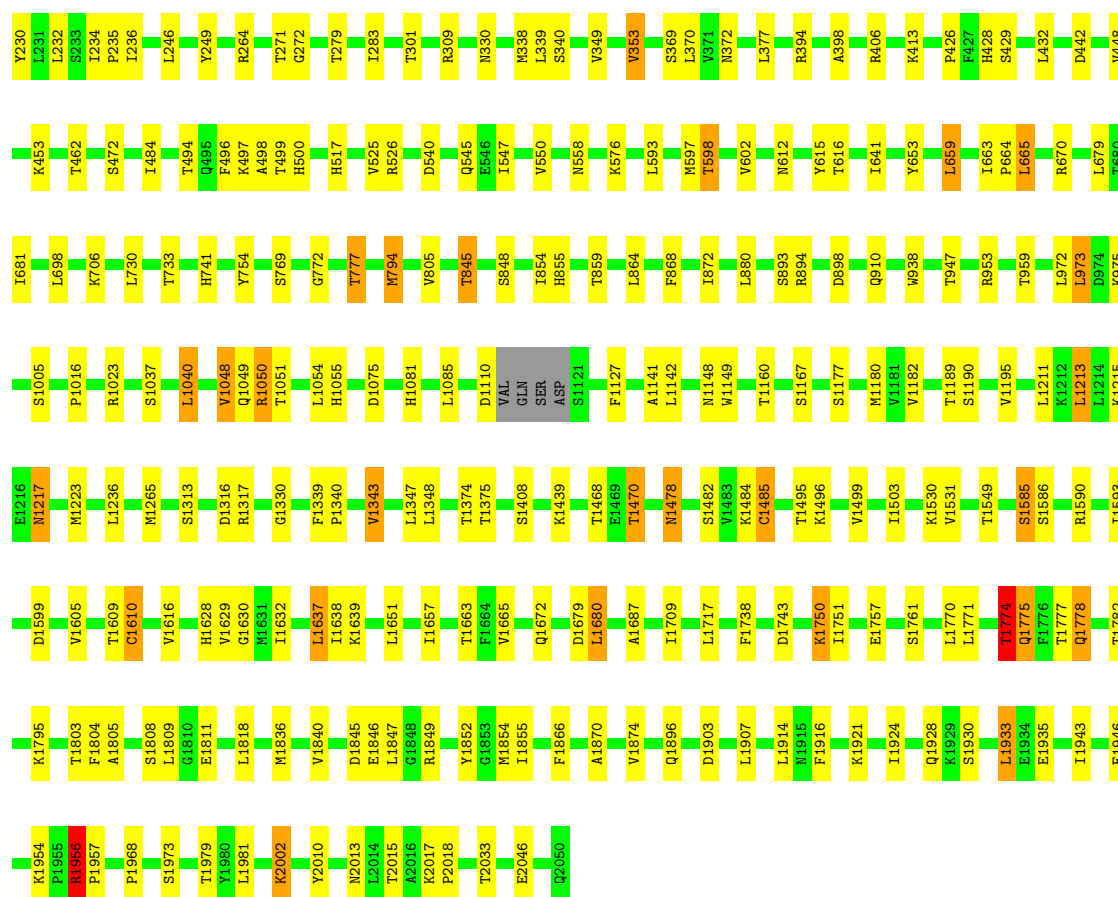
Chain K: 86% 12% .



• Molecule 2: Fatty acid synthase subunit beta

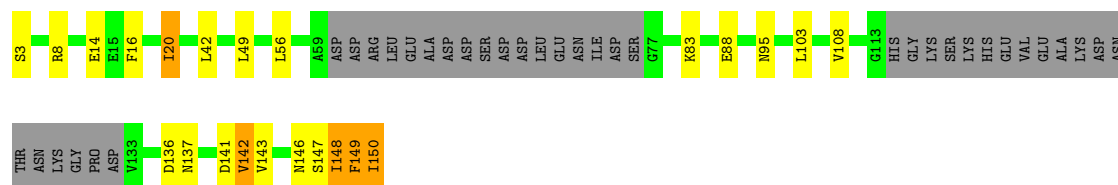
Chain L: 86% 12% .





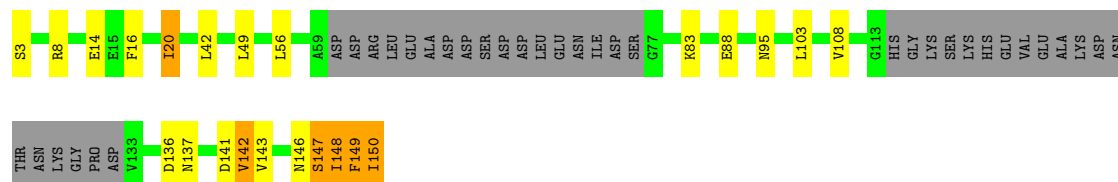
• Molecule 3: Translation machinery-associated protein 17

Chain M: 60% 12% 24%



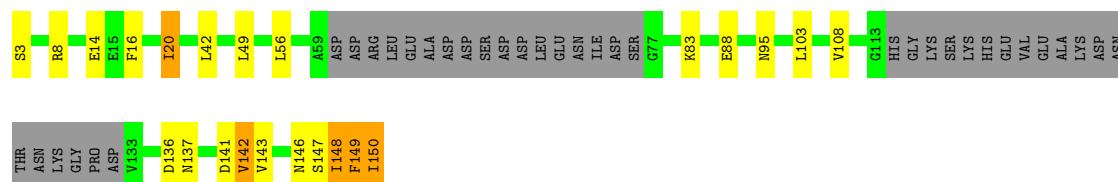
• Molecule 3: Translation machinery-associated protein 17

Chain N: 60% 11% 24%

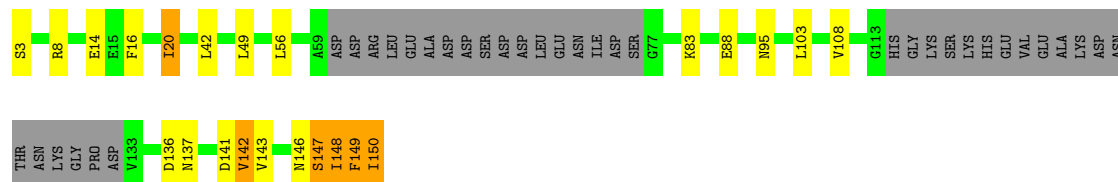


• Molecule 3: Translation machinery-associated protein 17

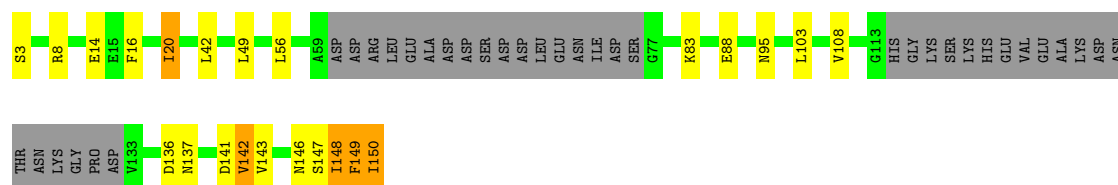
Chain O: 60% 12% 24%



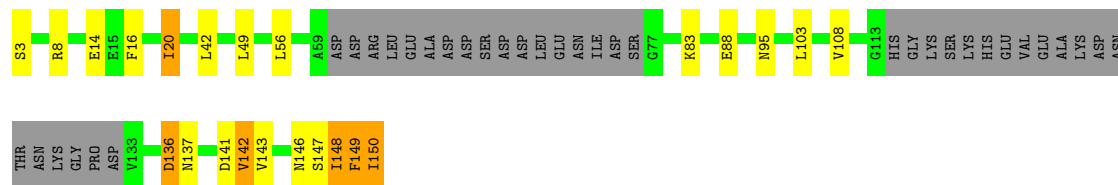
• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	110597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (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: FMN, PNS

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	0.75	0/13878	0.93	4/18755 (0.0%)
1	B	0.75	0/13878	0.93	4/18755 (0.0%)
1	C	0.75	0/13878	0.93	4/18755 (0.0%)
1	D	0.75	0/13878	0.93	4/18755 (0.0%)
1	E	0.75	0/13878	0.93	4/18755 (0.0%)
1	F	0.75	0/13878	0.93	4/18755 (0.0%)
2	G	0.67	0/16383	0.86	1/22229 (0.0%)
2	H	0.67	0/16383	0.86	1/22229 (0.0%)
2	I	0.67	0/16383	0.87	1/22229 (0.0%)
2	J	0.67	0/16383	0.86	1/22229 (0.0%)
2	K	0.67	0/16383	0.86	1/22229 (0.0%)
2	L	0.67	0/16383	0.86	1/22229 (0.0%)
3	M	0.76	0/885	0.91	0/1189
3	N	0.76	0/885	0.91	0/1189
3	O	0.76	0/885	0.91	0/1189
3	P	0.76	0/885	0.91	0/1189
3	Q	0.76	0/885	0.91	0/1189
3	R	0.76	0/885	0.91	0/1189
All	All	0.71	0/186876	0.90	30/253038 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	G	0	6
2	H	0	6
2	I	0	6
2	J	0	6
2	K	0	6
2	L	0	6
All	All	0	42

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1264	ARG	CG-CD-NE	-6.20	98.78	111.80
1	E	1264	ARG	CG-CD-NE	-6.20	98.79	111.80
1	D	1264	ARG	CG-CD-NE	-6.20	98.79	111.80
1	F	1264	ARG	CG-CD-NE	-6.19	98.79	111.80
1	C	1264	ARG	CG-CD-NE	-6.18	98.81	111.80

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	MET	Peptide
1	B	237	MET	Peptide
1	C	237	MET	Peptide
1	D	237	MET	Peptide
1	E	237	MET	Peptide

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	13625	0	13615	117	0
1	B	13625	0	13615	123	0
1	C	13625	0	13615	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	13625	0	13615	124	0
1	E	13625	0	13615	117	0
1	F	13625	0	13615	120	0
2	G	16018	0	15993	117	0
2	H	16018	0	15993	113	0
2	I	16018	0	15993	114	0
2	J	16018	0	15993	114	0
2	K	16018	0	15993	112	0
2	L	16018	0	15993	114	0
3	M	879	0	871	19	0
3	N	879	0	871	20	0
3	O	879	0	871	19	0
3	P	879	0	871	19	0
3	Q	879	0	871	18	0
3	R	879	0	871	20	0
4	A	21	0	21	3	0
4	B	21	0	21	4	0
4	C	21	0	21	3	0
4	D	21	0	21	3	0
4	E	21	0	21	3	0
4	F	21	0	21	3	0
5	G	31	0	19	3	0
5	H	31	0	19	3	0
5	I	31	0	19	3	0
5	J	31	0	19	3	0
5	K	31	0	19	3	0
5	L	31	0	19	3	0
All	All	183444	0	183114	1374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1374 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)
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	1.80	1.00
2:H:1811:GLU:OE2	2:H:2010:TYR:OH	1.80	1.00
2:K:1811:GLU:OE2	2:K:2010:TYR:OH	1.80	0.99
2:G:1811:GLU:OE2	2:G:2010:TYR:OH	1.80	0.99
2:I:1811:GLU:OE2	2:I:2010:TYR:OH	1.80	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	B	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	C	1744/1887 (92%)	1612 (92%)	119 (7%)	13 (1%)	24	57
1	D	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	E	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	24	57
1	F	1744/1887 (92%)	1613 (92%)	119 (7%)	12 (1%)	24	57
2	G	2032/2040 (100%)	1843 (91%)	177 (9%)	12 (1%)	27	60
2	H	2032/2040 (100%)	1843 (91%)	176 (9%)	13 (1%)	27	60
2	I	2032/2040 (100%)	1844 (91%)	174 (9%)	14 (1%)	24	57
2	J	2032/2040 (100%)	1842 (91%)	178 (9%)	12 (1%)	27	60
2	K	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	27	60
2	L	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	27	60
3	M	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	N	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	O	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	P	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	Q	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
3	R	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	9	28
All	All	23292/24450 (95%)	21327 (92%)	1805 (8%)	160 (1%)	28	57

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	ASP

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Mol	Chain	Res	Type
1	B	1130	ASP
1	C	1130	ASP
1	D	1130	ASP
1	E	1130	ASP

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	1476/1566 (94%)	1381 (94%)	95 (6%)	19	48
1	B	1476/1566 (94%)	1380 (94%)	96 (6%)	19	48
1	C	1476/1566 (94%)	1380 (94%)	96 (6%)	19	48
1	D	1476/1566 (94%)	1379 (93%)	97 (7%)	18	47
1	E	1476/1566 (94%)	1381 (94%)	95 (6%)	19	48
1	F	1476/1566 (94%)	1378 (93%)	98 (7%)	18	47
2	G	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
2	H	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
2	I	1775/1779 (100%)	1661 (94%)	114 (6%)	19	48
2	J	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
2	K	1775/1779 (100%)	1661 (94%)	114 (6%)	19	48
2	L	1775/1779 (100%)	1660 (94%)	115 (6%)	19	48
3	M	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	N	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	O	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	P	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	Q	97/129 (75%)	83 (86%)	14 (14%)	3	11
3	R	97/129 (75%)	82 (84%)	15 (16%)	3	9
All	All	20088/20844 (96%)	18738 (93%)	1350 (7%)	22	46

5 of 1350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	777	THR
2	H	1348	LEU
2	L	1795	LYS
2	G	1167	SER
2	G	1956	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 420 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1476	ASN
2	H	1712	ASN
2	L	1595	ASN
2	G	1669	GLN
2	H	572	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	PNS	A	1901	1	13,20,21	0.76	0	18,26,29	1.53	5 (27%)
4	PNS	B	1901	1	13,20,21	0.75	0	18,26,29	1.50	4 (22%)
4	PNS	C	1901	1	13,20,21	0.75	0	18,26,29	1.52	5 (27%)
4	PNS	D	1901	1	13,20,21	0.76	0	18,26,29	1.51	4 (22%)
4	PNS	E	1901	1	13,20,21	0.76	0	18,26,29	1.51	4 (22%)
4	PNS	F	1901	1	13,20,21	0.75	0	18,26,29	1.52	5 (27%)
5	FMN	G	2101	-	31,33,33	2.09	8 (25%)	40,50,50	2.59	12 (30%)
5	FMN	H	2101	-	31,33,33	2.10	7 (22%)	40,50,50	2.61	13 (32%)
5	FMN	I	2101	-	31,33,33	2.11	8 (25%)	40,50,50	2.60	13 (32%)
5	FMN	J	2101	-	31,33,33	2.10	8 (25%)	40,50,50	2.59	12 (30%)
5	FMN	K	2101	-	31,33,33	2.10	8 (25%)	40,50,50	2.60	13 (32%)
5	FMN	L	2101	-	31,33,33	2.08	8 (25%)	40,50,50	2.58	13 (32%)

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	PNS	A	1901	1	-	6/24/26/27	-
4	PNS	B	1901	1	-	7/24/26/27	-
4	PNS	C	1901	1	-	6/24/26/27	-
4	PNS	D	1901	1	-	7/24/26/27	-
4	PNS	E	1901	1	-	6/24/26/27	-
4	PNS	F	1901	1	-	6/24/26/27	-
5	FMN	G	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	H	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	J	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	K	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	L	2101	-	-	6/18/18/18	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	2101	FMN	C4A-C10	8.44	1.47	1.38
5	I	2101	FMN	C4A-C10	8.40	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2101	FMN	C4A-C10	8.39	1.47	1.38
5	J	2101	FMN	C4A-C10	8.34	1.47	1.38
5	G	2101	FMN	C4A-C10	8.34	1.47	1.38

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2101	FMN	C4-N3-C2	9.32	123.01	115.14
5	H	2101	FMN	C4-N3-C2	9.31	123.00	115.14
5	J	2101	FMN	C4-N3-C2	9.27	122.97	115.14
5	L	2101	FMN	C4-N3-C2	9.24	122.94	115.14
5	G	2101	FMN	C4-N3-C2	9.22	122.93	115.14

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1901	PNS	O27-C28-C29-C32
4	A	1901	PNS	N36-C37-C38-C39
4	A	1901	PNS	N41-C42-C43-S44
4	D	1901	PNS	O27-C28-C29-C32
4	D	1901	PNS	N36-C37-C38-C39

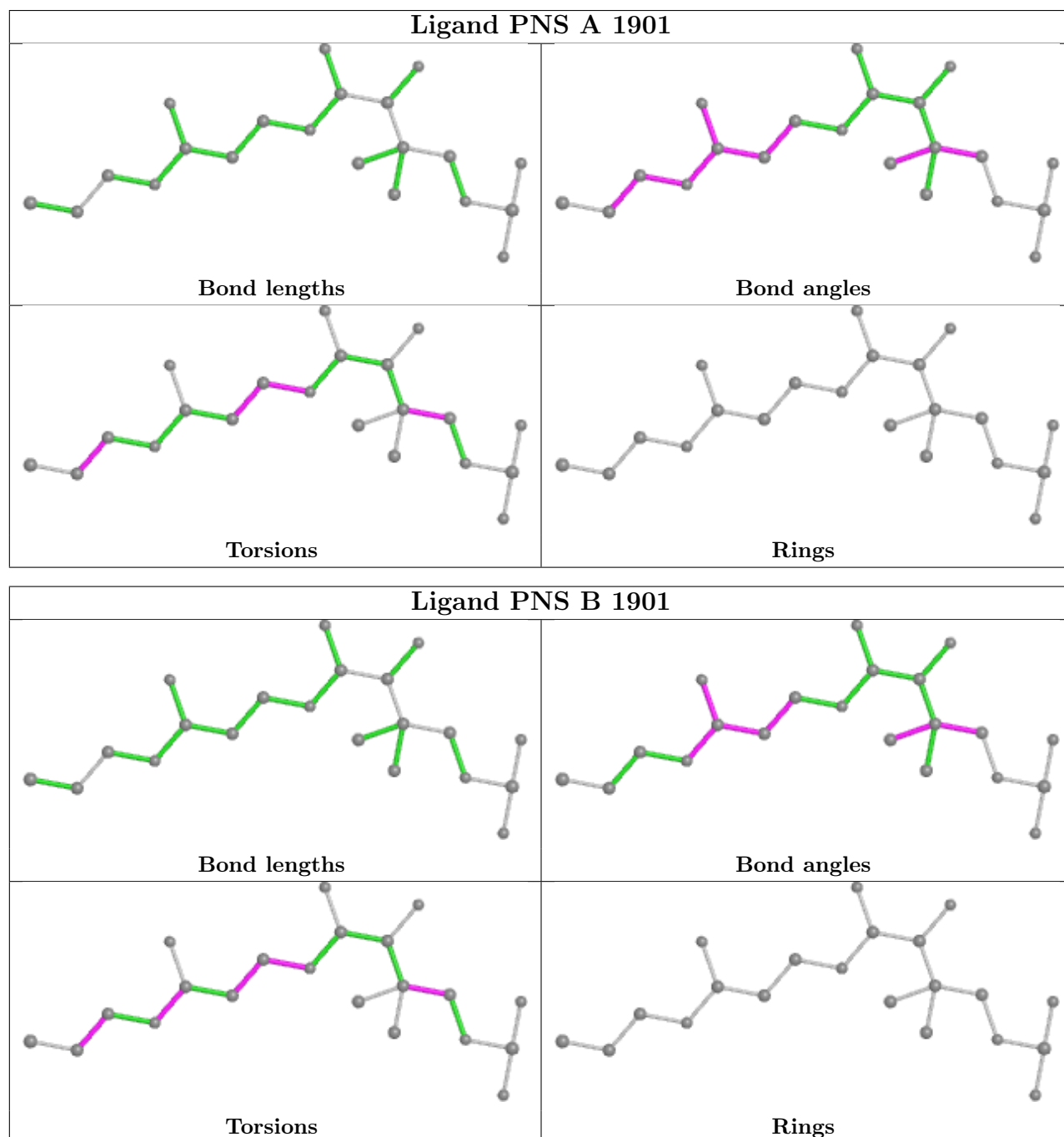
There are no ring outliers.

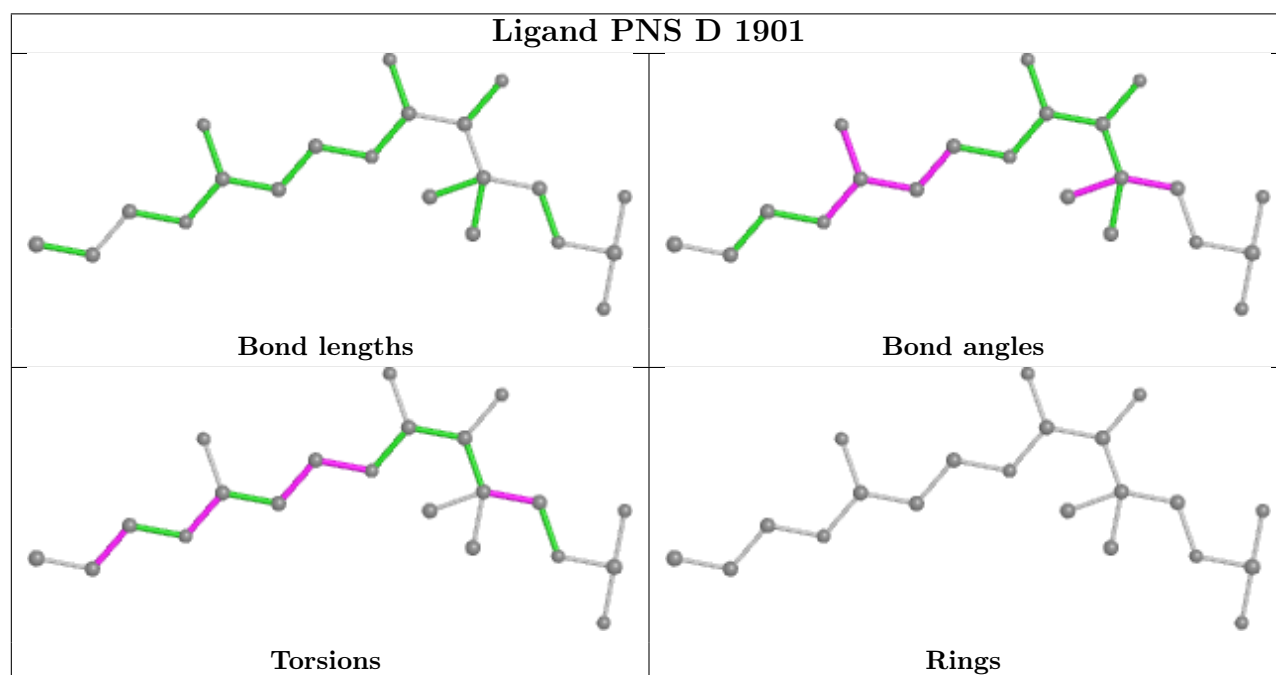
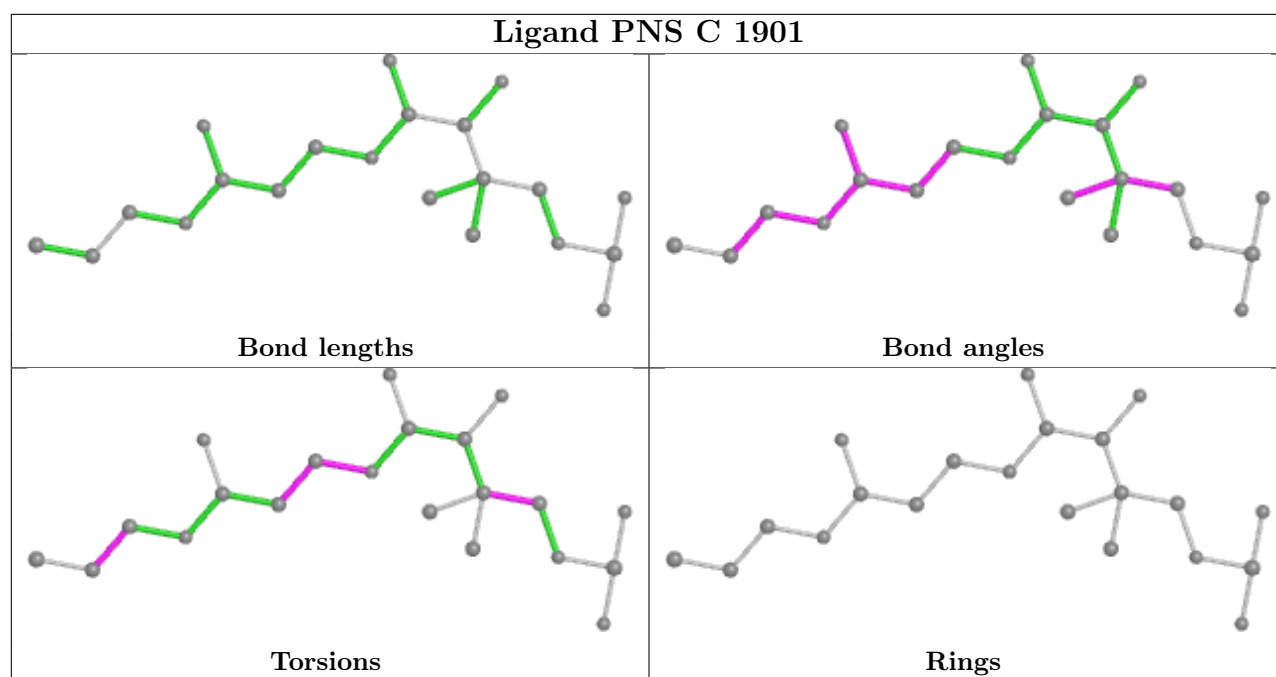
12 monomers are involved in 37 short contacts:

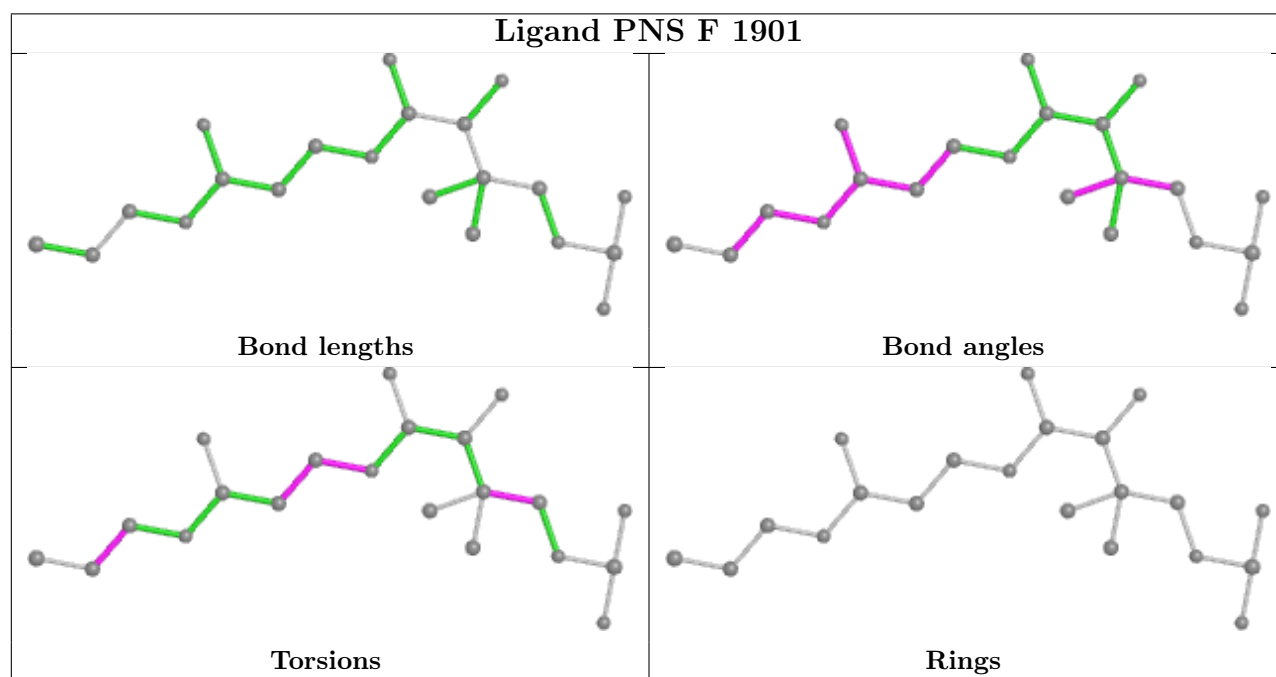
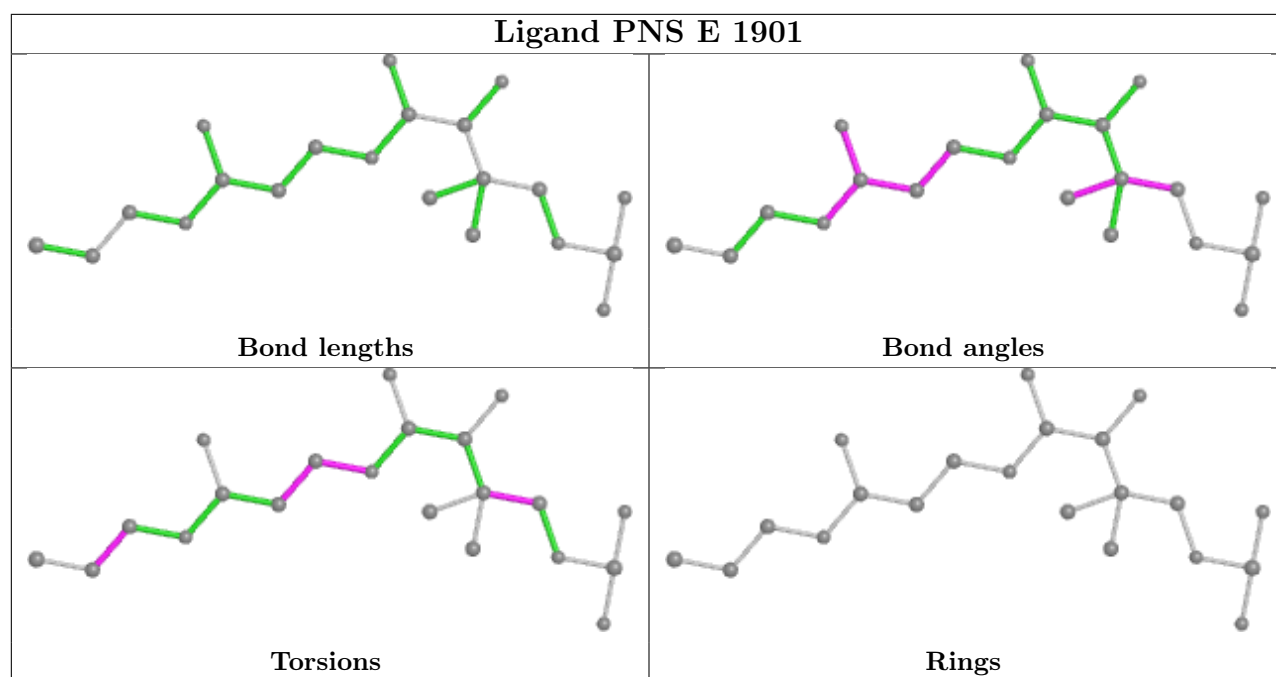
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1901	PNS	3	0
4	B	1901	PNS	4	0
4	C	1901	PNS	3	0
4	D	1901	PNS	3	0
4	E	1901	PNS	3	0
4	F	1901	PNS	3	0
5	G	2101	FMN	3	0
5	H	2101	FMN	3	0
5	I	2101	FMN	3	0
5	J	2101	FMN	3	0
5	K	2101	FMN	3	0
5	L	2101	FMN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

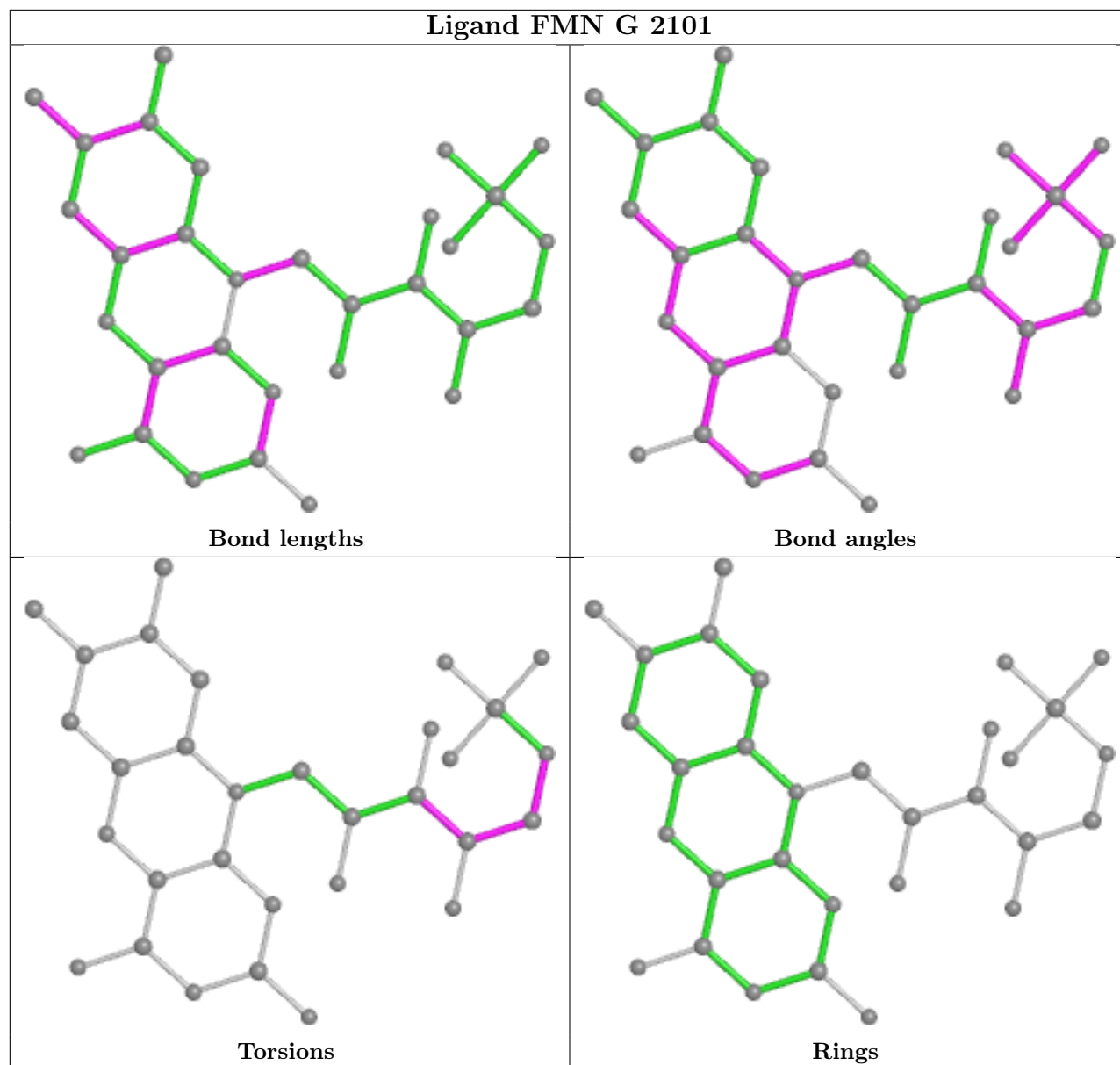
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



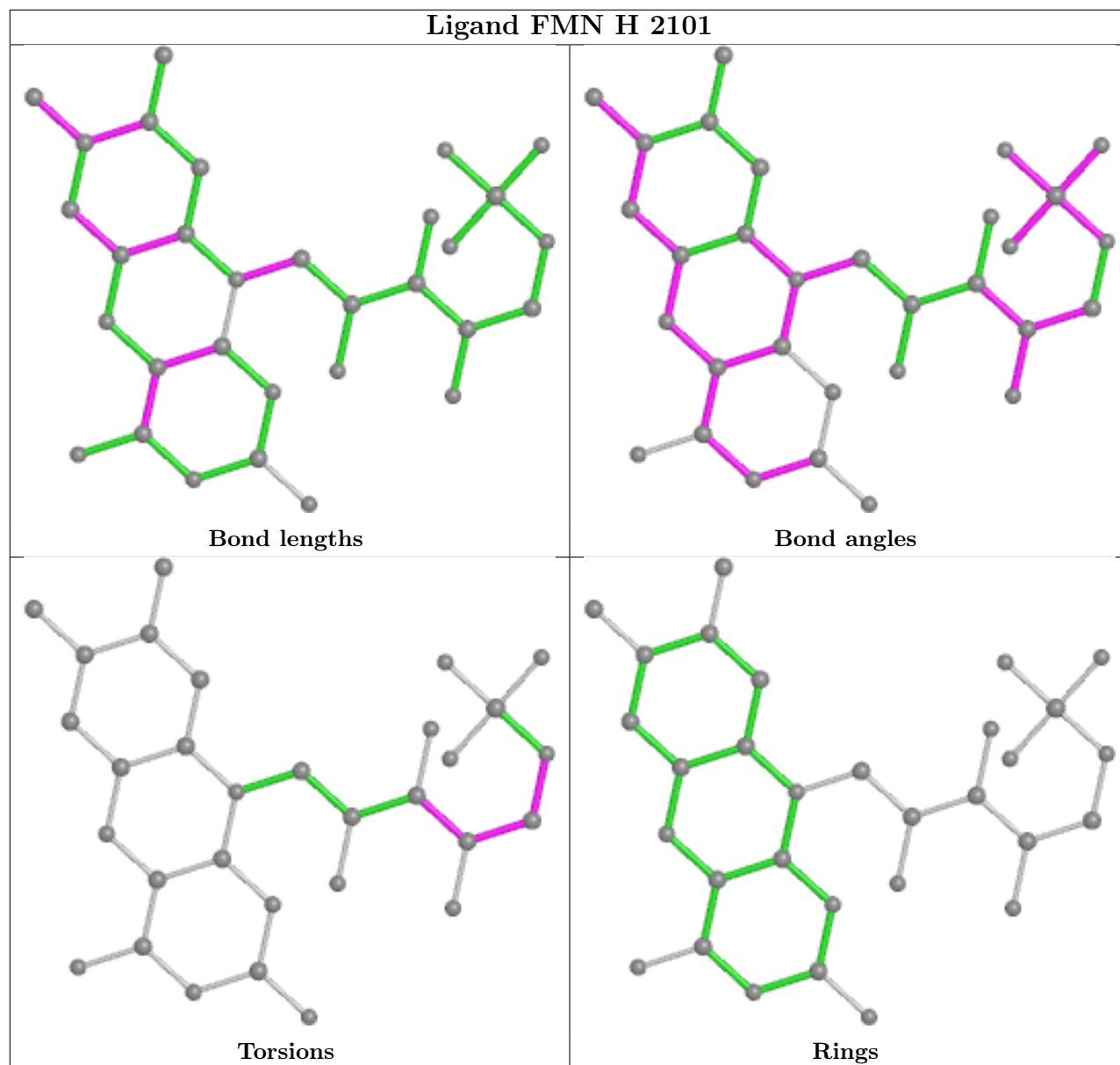


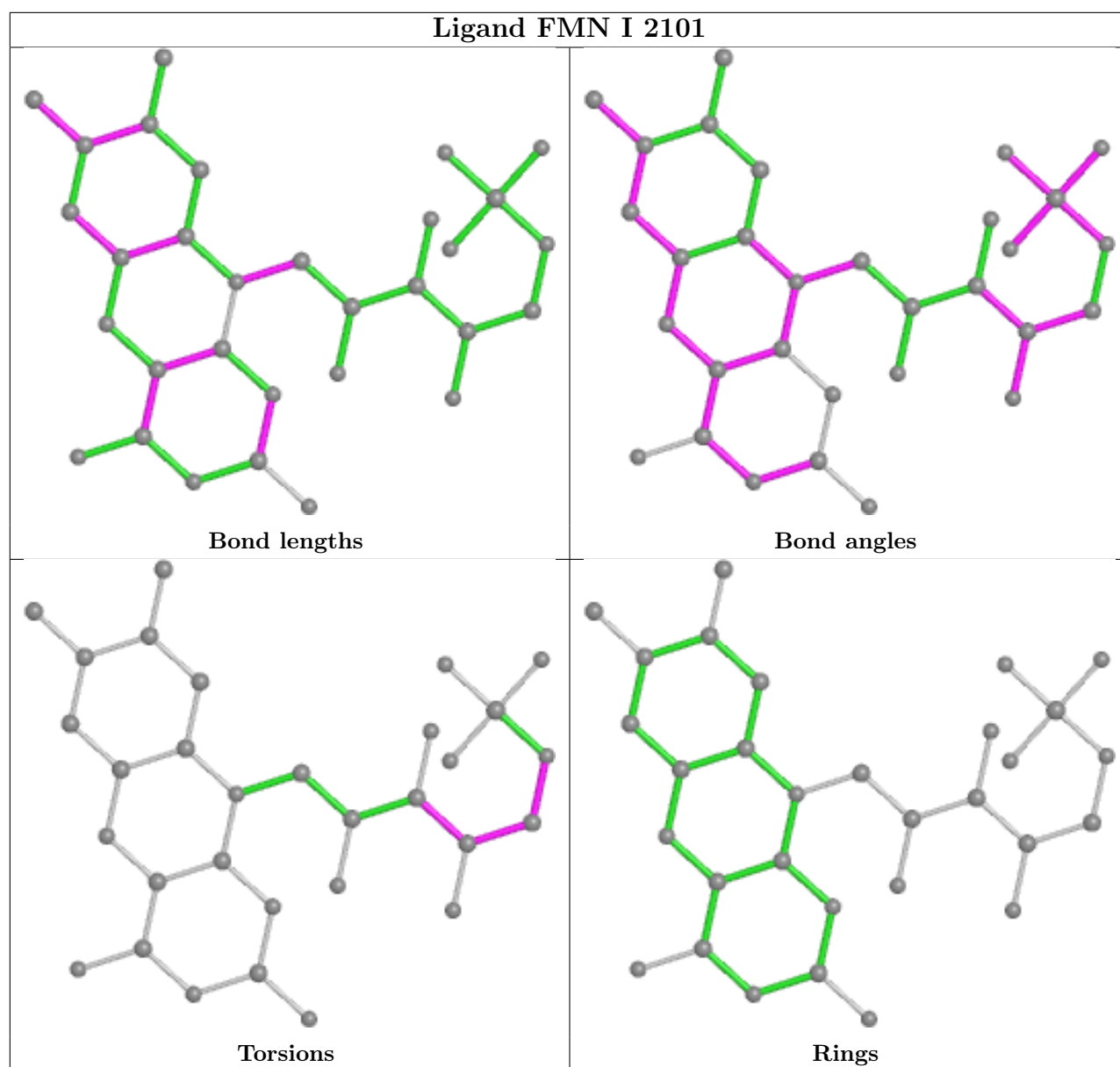


Ligand FMN G 2101

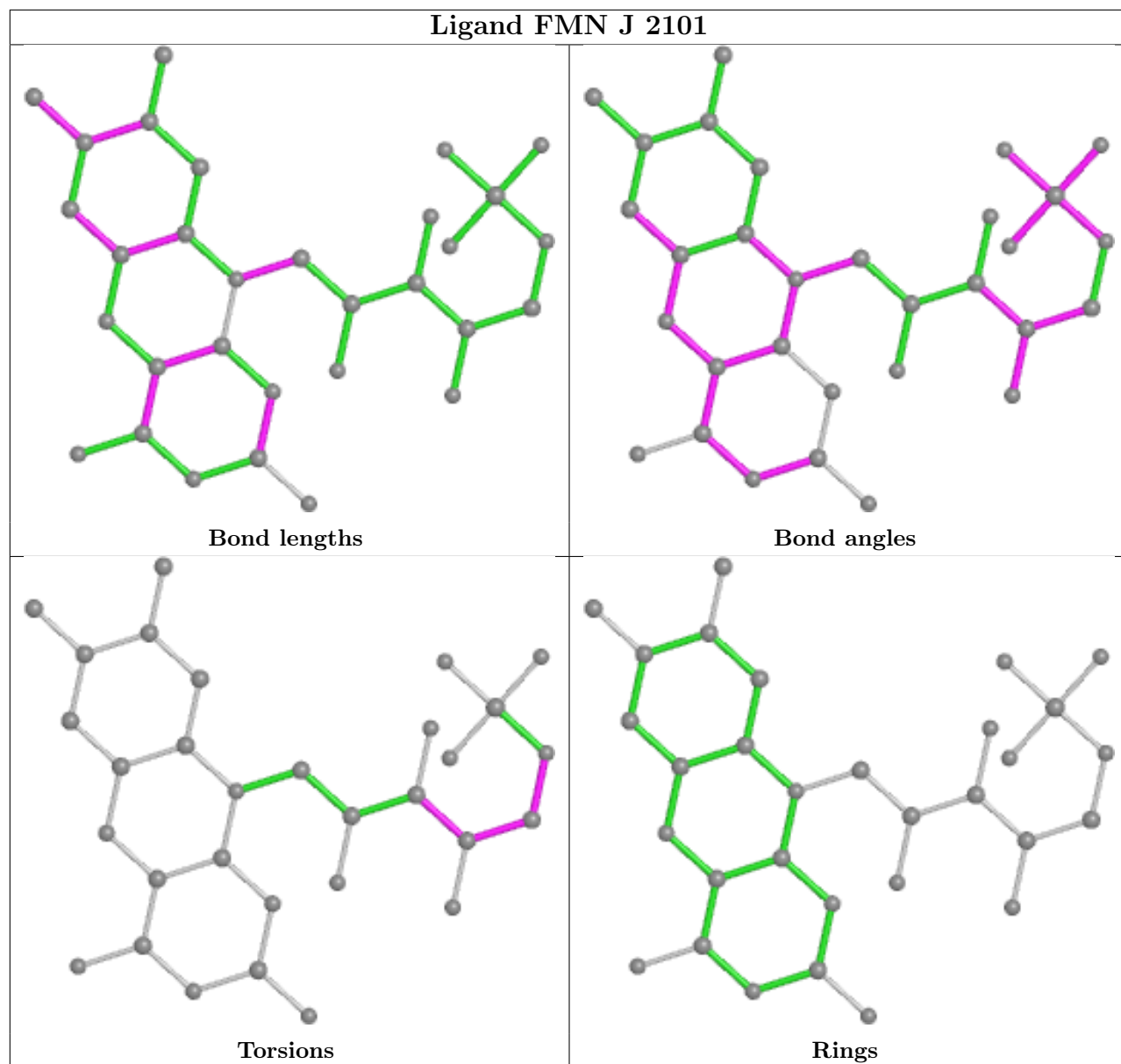


Ligand FMN H 2101

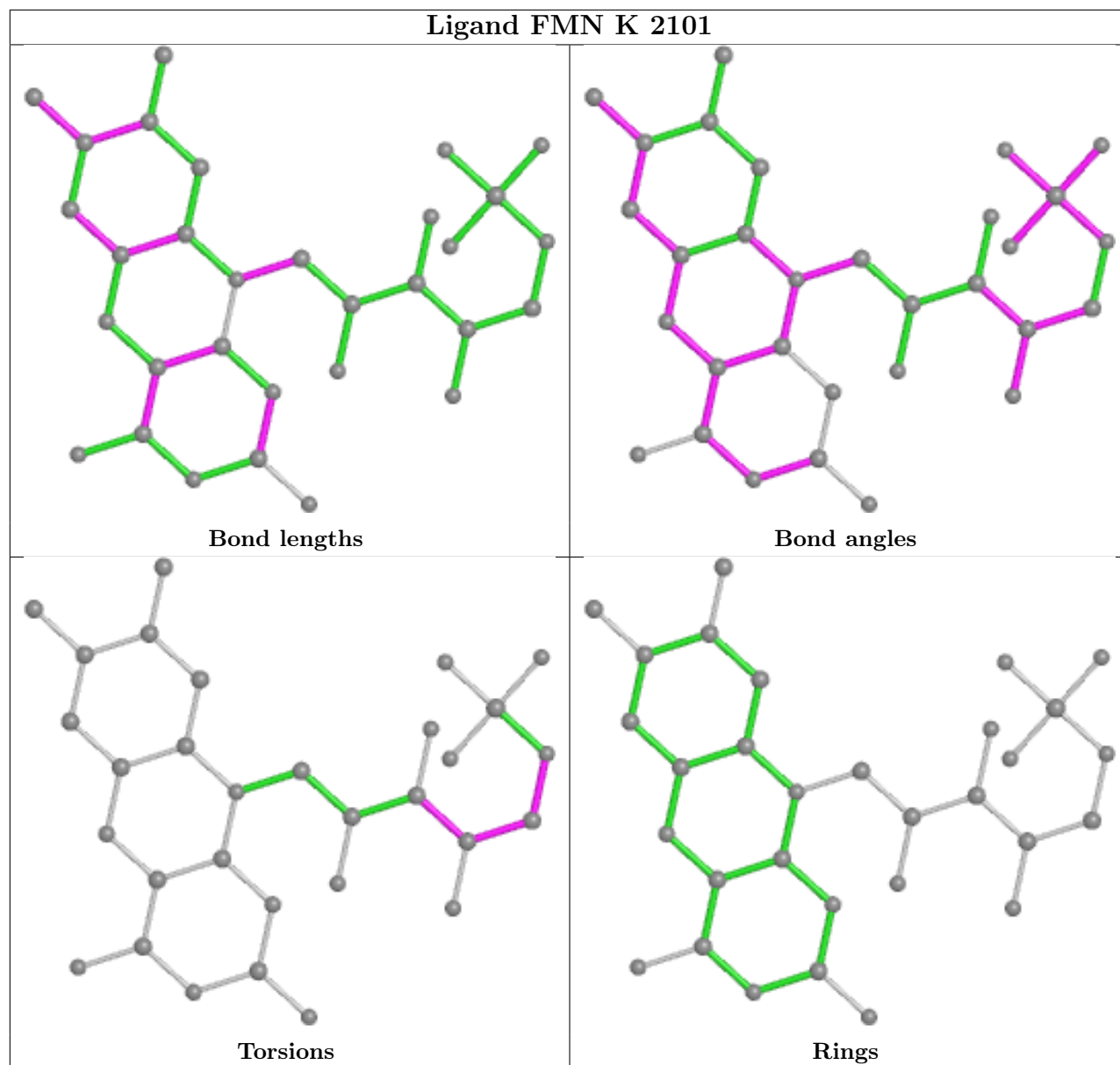


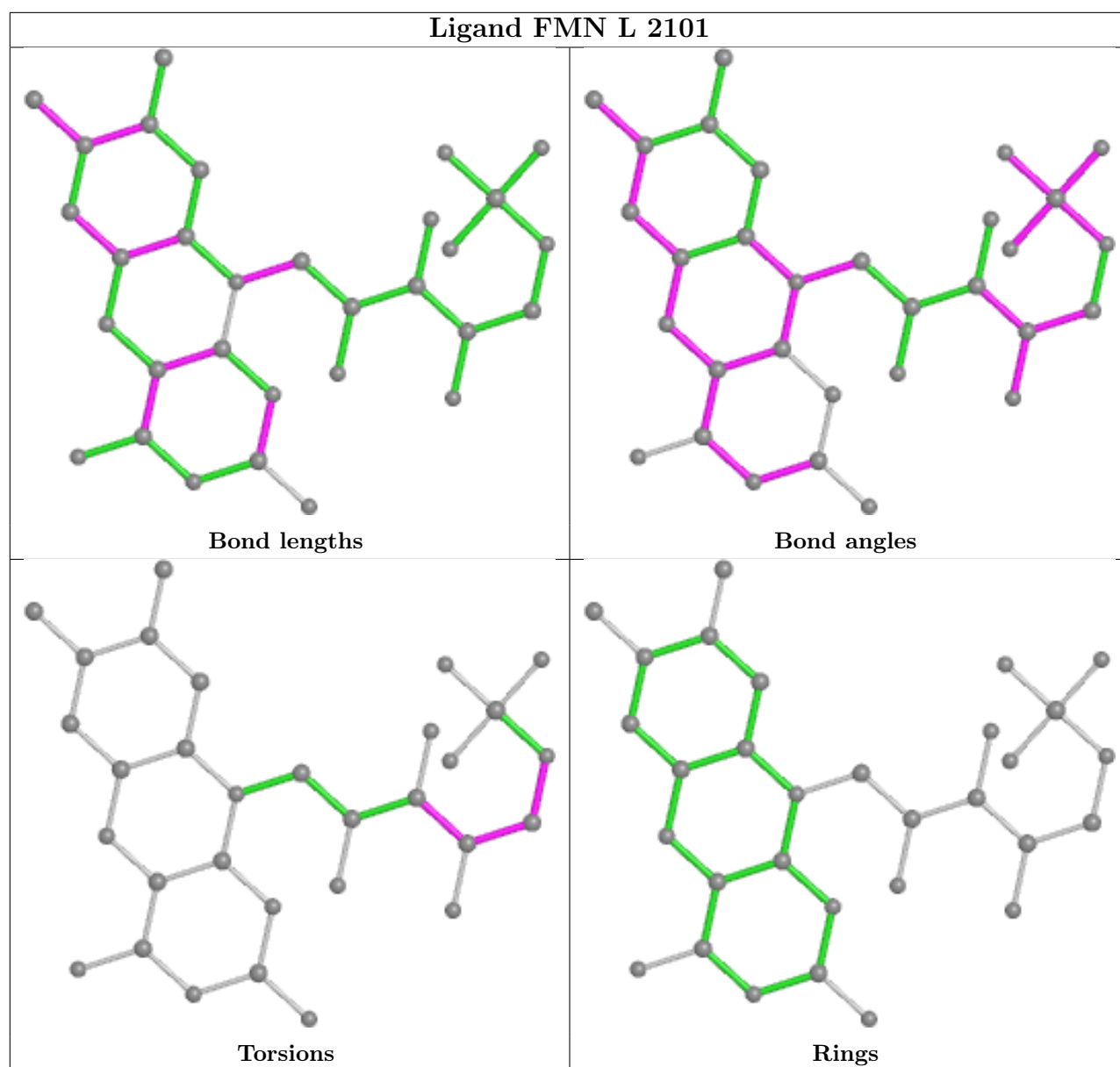


Ligand FMN J 2101



Ligand FMN K 2101





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.