



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 2, 2019 – 10:27 PM EST

PDB ID : 4V8L
EMDB ID: : EMD-2238
Title : Cryo-EM Structure of the Mycobacterial Fatty Acid Synthase
Authors : Boehringer, D.; Ban, N.; Leibundgut, M.
Deposited on : 2012-12-06
Resolution : 7.50 Å(reported)
Based on PDB ID : 2UV8

This is a wwPDB/EMDataBank EM Map/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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
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) : 2.4

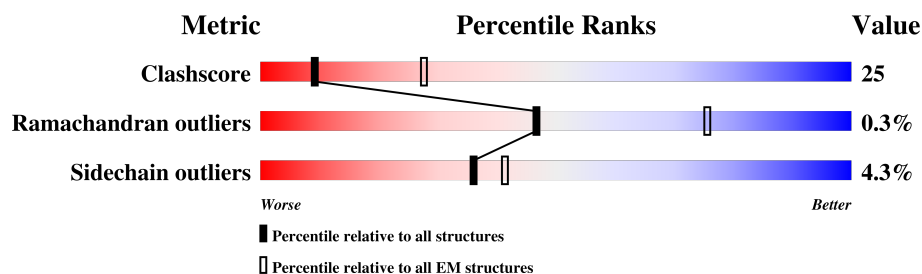
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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. 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. 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	3089	56% 33% • 9%
1	B	3089	56% 33% • 9%
1	C	3089	56% 33% • 9%
1	D	3089	88% • 9%
1	E	3089	88% • 9%
1	F	3089	88% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 126306 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	E	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	F	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	A	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	B	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	C	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		

There are 1086 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	929	UNK	GLU	conflict	UNP A0R1H7
D	930	UNK	PRO	conflict	UNP A0R1H7
D	931	UNK	VAL	conflict	UNP A0R1H7
D	932	UNK	GLU	conflict	UNP A0R1H7
D	933	UNK	VAL	conflict	UNP A0R1H7
D	934	UNK	LEU	conflict	UNP A0R1H7
D	935	UNK	SER	conflict	UNP A0R1H7
D	936	UNK	ARG	conflict	UNP A0R1H7
D	937	UNK	ARG	conflict	UNP A0R1H7
D	938	UNK	GLN	conflict	UNP A0R1H7
D	939	UNK	ALA	conflict	UNP A0R1H7
D	940	UNK	ARG	conflict	UNP A0R1H7
D	941	UNK	ARG	conflict	UNP A0R1H7
D	942	UNK	ASP	conflict	UNP A0R1H7
D	943	UNK	ALA	conflict	UNP A0R1H7
D	944	UNK	SER	conflict	UNP A0R1H7
D	974	UNK	THR	conflict	UNP A0R1H7
D	975	UNK	GLU	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	976	UNK	TRP	conflict	UNP A0R1H7
D	977	UNK	GLN	conflict	UNP A0R1H7
D	978	UNK	VAL	conflict	UNP A0R1H7
D	979	UNK	ARG	conflict	UNP A0R1H7
D	980	UNK	GLU	conflict	UNP A0R1H7
D	981	UNK	GLY	conflict	UNP A0R1H7
D	982	UNK	SER	conflict	UNP A0R1H7
D	983	UNK	ASP	conflict	UNP A0R1H7
D	984	UNK	ASN	conflict	UNP A0R1H7
D	985	UNK	ARG	conflict	UNP A0R1H7
D	986	UNK	SER	conflict	UNP A0R1H7
D	987	UNK	ALA	conflict	UNP A0R1H7
D	988	UNK	SER	conflict	UNP A0R1H7
D	989	UNK	HIS	conflict	UNP A0R1H7
D	990	UNK	PRO	conflict	UNP A0R1H7
D	991	UNK	SER	conflict	UNP A0R1H7
D	992	UNK	THR	conflict	UNP A0R1H7
D	993	UNK	GLY	conflict	UNP A0R1H7
D	994	UNK	ALA	conflict	UNP A0R1H7
D	995	UNK	ARG	conflict	UNP A0R1H7
D	996	UNK	LEU	conflict	UNP A0R1H7
D	997	UNK	GLU	conflict	UNP A0R1H7
D	998	UNK	VAL	conflict	UNP A0R1H7
D	999	UNK	ALA	conflict	UNP A0R1H7
D	1000	UNK	ASP	conflict	UNP A0R1H7
D	1001	UNK	ASP	conflict	UNP A0R1H7
D	1002	UNK	GLN	conflict	UNP A0R1H7
D	1003	UNK	HIS	conflict	UNP A0R1H7
D	1004	UNK	VAL	conflict	UNP A0R1H7
D	1005	UNK	VAL	conflict	UNP A0R1H7
D	1006	UNK	LEU	conflict	UNP A0R1H7
D	1007	UNK	SER	conflict	UNP A0R1H7
D	1008	UNK	VAL	conflict	UNP A0R1H7
D	1009	UNK	PRO	conflict	UNP A0R1H7
D	1010	UNK	LEU	conflict	UNP A0R1H7
D	1011	UNK	SER	conflict	UNP A0R1H7
D	1012	UNK	GLY	conflict	UNP A0R1H7
D	1013	UNK	THR	conflict	UNP A0R1H7
D	1014	UNK	TRP	conflict	UNP A0R1H7
D	1196	UNK	GLY	conflict	UNP A0R1H7
D	1197	UNK	ARG	conflict	UNP A0R1H7
D	1198	UNK	THR	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1199	UNK	GLY	conflict	UNP A0R1H7
D	1200	UNK	ALA	conflict	UNP A0R1H7
D	1201	UNK	ALA	conflict	UNP A0R1H7
D	1202	UNK	GLU	conflict	UNP A0R1H7
D	1203	UNK	LEU	conflict	UNP A0R1H7
D	1204	UNK	THR	conflict	UNP A0R1H7
D	1205	UNK	ASP	conflict	UNP A0R1H7
D	1206	UNK	PRO	conflict	UNP A0R1H7
D	1207	UNK	VAL	conflict	UNP A0R1H7
D	1208	UNK	ARG	conflict	UNP A0R1H7
D	1209	UNK	ALA	conflict	UNP A0R1H7
D	1210	UNK	GLY	conflict	UNP A0R1H7
D	1211	UNK	GLY	conflict	UNP A0R1H7
D	1212	UNK	ALA	conflict	UNP A0R1H7
D	1213	UNK	ILE	conflict	UNP A0R1H7
D	1214	UNK	SER	conflict	UNP A0R1H7
D	1215	UNK	ASP	conflict	UNP A0R1H7
D	1216	UNK	ASN	conflict	UNP A0R1H7
D	1217	UNK	ALA	conflict	UNP A0R1H7
D	1218	UNK	THR	conflict	UNP A0R1H7
D	1219	UNK	ASP	conflict	UNP A0R1H7
D	1220	UNK	THR	conflict	UNP A0R1H7
D	1221	UNK	PRO	conflict	UNP A0R1H7
D	1222	UNK	ARG	conflict	UNP A0R1H7
D	1223	UNK	ARG	conflict	UNP A0R1H7
D	1224	UNK	ARG	conflict	UNP A0R1H7
D	1225	UNK	ARG	conflict	UNP A0R1H7
D	1226	UNK	ARG	conflict	UNP A0R1H7
D	1227	UNK	ASP	conflict	UNP A0R1H7
D	2076	UNK	GLY	conflict	UNP A0R1H7
D	2077	UNK	ASP	conflict	UNP A0R1H7
D	2078	UNK	ILE	conflict	UNP A0R1H7
D	2079	UNK	ASP	conflict	UNP A0R1H7
D	2080	UNK	ALA	conflict	UNP A0R1H7
D	2081	UNK	GLN	conflict	UNP A0R1H7
D	2082	UNK	TRP	conflict	UNP A0R1H7
D	2083	UNK	GLU	conflict	UNP A0R1H7
D	2084	UNK	GLN	conflict	UNP A0R1H7
D	2085	UNK	LEU	conflict	UNP A0R1H7
D	2086	UNK	SER	conflict	UNP A0R1H7
D	2087	UNK	GLN	conflict	UNP A0R1H7
D	2088	UNK	ARG	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2089	UNK	PHE	conflict	UNP A0R1H7
D	2090	UNK	GLU	conflict	UNP A0R1H7
D	2091	UNK	GLY	conflict	UNP A0R1H7
D	2092	UNK	THR	conflict	UNP A0R1H7
D	2093	UNK	GLY	conflict	UNP A0R1H7
D	2094	UNK	HIS	conflict	UNP A0R1H7
D	2095	UNK	VAL	conflict	UNP A0R1H7
D	2096	UNK	VAL	conflict	UNP A0R1H7
D	2097	UNK	ALA	conflict	UNP A0R1H7
D	2098	UNK	THR	conflict	UNP A0R1H7
D	2099	UNK	GLN	conflict	UNP A0R1H7
D	2100	UNK	ALA	conflict	UNP A0R1H7
D	2101	UNK	ASN	conflict	UNP A0R1H7
D	2102	UNK	TRP	conflict	UNP A0R1H7
D	2103	UNK	TRP	conflict	UNP A0R1H7
D	2104	UNK	GLN	conflict	UNP A0R1H7
D	2105	UNK	GLY	conflict	UNP A0R1H7
D	2106	UNK	LYS	conflict	UNP A0R1H7
D	2107	UNK	ALA	conflict	UNP A0R1H7
D	2108	UNK	LEU	conflict	UNP A0R1H7
D	2109	UNK	ALA	conflict	UNP A0R1H7
D	2110	UNK	ALA	conflict	UNP A0R1H7
D	2111	UNK	GLY	conflict	UNP A0R1H7
D	2112	UNK	ARG	conflict	UNP A0R1H7
D	2113	UNK	ASN	conflict	UNP A0R1H7
D	2114	UNK	VAL	conflict	UNP A0R1H7
D	2115	UNK	HIS	conflict	UNP A0R1H7
D	2116	UNK	ALA	conflict	UNP A0R1H7
D	2117	UNK	SER	conflict	UNP A0R1H7
D	2118	UNK	LEU	conflict	UNP A0R1H7
D	2119	UNK	PHE	conflict	UNP A0R1H7
D	2120	UNK	GLY	conflict	UNP A0R1H7
D	2121	UNK	ARG	conflict	UNP A0R1H7
D	2122	UNK	ILE	conflict	UNP A0R1H7
D	2123	UNK	ALA	conflict	UNP A0R1H7
D	2124	UNK	ALA	conflict	UNP A0R1H7
D	2125	UNK	GLY	conflict	UNP A0R1H7
D	2126	UNK	ALA	conflict	UNP A0R1H7
D	2127	UNK	GLU	conflict	UNP A0R1H7
D	2128	UNK	ASN	conflict	UNP A0R1H7
D	2129	UNK	PRO	conflict	UNP A0R1H7
D	2130	UNK	GLY	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2131	UNK	LYS	conflict	UNP A0R1H7
D	2132	UNK	GLY	conflict	UNP A0R1H7
D	2133	UNK	ARG	conflict	UNP A0R1H7
D	2134	UNK	TYR	conflict	UNP A0R1H7
D	2135	UNK	SER	conflict	UNP A0R1H7
D	2422	UNK	GLU	conflict	UNP A0R1H7
D	2423	UNK	SER	conflict	UNP A0R1H7
D	2424	UNK	ASP	conflict	UNP A0R1H7
D	2425	UNK	ASP	conflict	UNP A0R1H7
D	2426	UNK	GLU	conflict	UNP A0R1H7
D	2427	UNK	ALA	conflict	UNP A0R1H7
D	2428	UNK	PRO	conflict	UNP A0R1H7
D	2429	UNK	ALA	conflict	UNP A0R1H7
D	2430	UNK	GLY	conflict	UNP A0R1H7
D	2431	UNK	THR	conflict	UNP A0R1H7
D	2432	UNK	ILE	conflict	UNP A0R1H7
D	2433	UNK	ARG	conflict	UNP A0R1H7
D	2434	UNK	ALA	conflict	UNP A0R1H7
D	2435	UNK	LEU	conflict	UNP A0R1H7
D	2436	UNK	PRO	conflict	UNP A0R1H7
D	2437	UNK	SER	conflict	UNP A0R1H7
D	2438	UNK	PRO	conflict	UNP A0R1H7
D	2439	UNK	PRO	conflict	UNP A0R1H7
D	2440	UNK	ARG	conflict	UNP A0R1H7
D	2441	UNK	GLY	conflict	UNP A0R1H7
D	2442	UNK	TYR	conflict	UNP A0R1H7
D	2443	UNK	ASN	conflict	UNP A0R1H7
D	2444	UNK	PRO	conflict	UNP A0R1H7
D	2445	UNK	ALA	conflict	UNP A0R1H7
D	2446	UNK	PRO	conflict	UNP A0R1H7
D	2447	UNK	ALA	conflict	UNP A0R1H7
D	2448	UNK	PRO	conflict	UNP A0R1H7
D	2449	UNK	GLU	conflict	UNP A0R1H7
D	2450	UNK	TRP	conflict	UNP A0R1H7
D	2451	UNK	ASP	conflict	UNP A0R1H7
D	2452	UNK	ASP	conflict	UNP A0R1H7
D	2453	UNK	LEU	conflict	UNP A0R1H7
E	929	UNK	GLU	conflict	UNP A0R1H7
E	930	UNK	PRO	conflict	UNP A0R1H7
E	931	UNK	VAL	conflict	UNP A0R1H7
E	932	UNK	GLU	conflict	UNP A0R1H7
E	933	UNK	VAL	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	934	UNK	LEU	conflict	UNP A0R1H7
E	935	UNK	SER	conflict	UNP A0R1H7
E	936	UNK	ARG	conflict	UNP A0R1H7
E	937	UNK	ARG	conflict	UNP A0R1H7
E	938	UNK	GLN	conflict	UNP A0R1H7
E	939	UNK	ALA	conflict	UNP A0R1H7
E	940	UNK	ARG	conflict	UNP A0R1H7
E	941	UNK	ARG	conflict	UNP A0R1H7
E	942	UNK	ASP	conflict	UNP A0R1H7
E	943	UNK	ALA	conflict	UNP A0R1H7
E	944	UNK	SER	conflict	UNP A0R1H7
E	974	UNK	THR	conflict	UNP A0R1H7
E	975	UNK	GLU	conflict	UNP A0R1H7
E	976	UNK	TRP	conflict	UNP A0R1H7
E	977	UNK	GLN	conflict	UNP A0R1H7
E	978	UNK	VAL	conflict	UNP A0R1H7
E	979	UNK	ARG	conflict	UNP A0R1H7
E	980	UNK	GLU	conflict	UNP A0R1H7
E	981	UNK	GLY	conflict	UNP A0R1H7
E	982	UNK	SER	conflict	UNP A0R1H7
E	983	UNK	ASP	conflict	UNP A0R1H7
E	984	UNK	ASN	conflict	UNP A0R1H7
E	985	UNK	ARG	conflict	UNP A0R1H7
E	986	UNK	SER	conflict	UNP A0R1H7
E	987	UNK	ALA	conflict	UNP A0R1H7
E	988	UNK	SER	conflict	UNP A0R1H7
E	989	UNK	HIS	conflict	UNP A0R1H7
E	990	UNK	PRO	conflict	UNP A0R1H7
E	991	UNK	SER	conflict	UNP A0R1H7
E	992	UNK	THR	conflict	UNP A0R1H7
E	993	UNK	GLY	conflict	UNP A0R1H7
E	994	UNK	ALA	conflict	UNP A0R1H7
E	995	UNK	ARG	conflict	UNP A0R1H7
E	996	UNK	LEU	conflict	UNP A0R1H7
E	997	UNK	GLU	conflict	UNP A0R1H7
E	998	UNK	VAL	conflict	UNP A0R1H7
E	999	UNK	ALA	conflict	UNP A0R1H7
E	1000	UNK	ASP	conflict	UNP A0R1H7
E	1001	UNK	ASP	conflict	UNP A0R1H7
E	1002	UNK	GLN	conflict	UNP A0R1H7
E	1003	UNK	HIS	conflict	UNP A0R1H7
E	1004	UNK	VAL	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1005	UNK	VAL	conflict	UNP A0R1H7
E	1006	UNK	LEU	conflict	UNP A0R1H7
E	1007	UNK	SER	conflict	UNP A0R1H7
E	1008	UNK	VAL	conflict	UNP A0R1H7
E	1009	UNK	PRO	conflict	UNP A0R1H7
E	1010	UNK	LEU	conflict	UNP A0R1H7
E	1011	UNK	SER	conflict	UNP A0R1H7
E	1012	UNK	GLY	conflict	UNP A0R1H7
E	1013	UNK	THR	conflict	UNP A0R1H7
E	1014	UNK	TRP	conflict	UNP A0R1H7
E	1196	UNK	GLY	conflict	UNP A0R1H7
E	1197	UNK	ARG	conflict	UNP A0R1H7
E	1198	UNK	THR	conflict	UNP A0R1H7
E	1199	UNK	GLY	conflict	UNP A0R1H7
E	1200	UNK	ALA	conflict	UNP A0R1H7
E	1201	UNK	ALA	conflict	UNP A0R1H7
E	1202	UNK	GLU	conflict	UNP A0R1H7
E	1203	UNK	LEU	conflict	UNP A0R1H7
E	1204	UNK	THR	conflict	UNP A0R1H7
E	1205	UNK	ASP	conflict	UNP A0R1H7
E	1206	UNK	PRO	conflict	UNP A0R1H7
E	1207	UNK	VAL	conflict	UNP A0R1H7
E	1208	UNK	ARG	conflict	UNP A0R1H7
E	1209	UNK	ALA	conflict	UNP A0R1H7
E	1210	UNK	GLY	conflict	UNP A0R1H7
E	1211	UNK	GLY	conflict	UNP A0R1H7
E	1212	UNK	ALA	conflict	UNP A0R1H7
E	1213	UNK	ILE	conflict	UNP A0R1H7
E	1214	UNK	SER	conflict	UNP A0R1H7
E	1215	UNK	ASP	conflict	UNP A0R1H7
E	1216	UNK	ASN	conflict	UNP A0R1H7
E	1217	UNK	ALA	conflict	UNP A0R1H7
E	1218	UNK	THR	conflict	UNP A0R1H7
E	1219	UNK	ASP	conflict	UNP A0R1H7
E	1220	UNK	THR	conflict	UNP A0R1H7
E	1221	UNK	PRO	conflict	UNP A0R1H7
E	1222	UNK	ARG	conflict	UNP A0R1H7
E	1223	UNK	ARG	conflict	UNP A0R1H7
E	1224	UNK	ARG	conflict	UNP A0R1H7
E	1225	UNK	ARG	conflict	UNP A0R1H7
E	1226	UNK	ARG	conflict	UNP A0R1H7
E	1227	UNK	ASP	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2076	UNK	GLY	conflict	UNP A0R1H7
E	2077	UNK	ASP	conflict	UNP A0R1H7
E	2078	UNK	ILE	conflict	UNP A0R1H7
E	2079	UNK	ASP	conflict	UNP A0R1H7
E	2080	UNK	ALA	conflict	UNP A0R1H7
E	2081	UNK	GLN	conflict	UNP A0R1H7
E	2082	UNK	TRP	conflict	UNP A0R1H7
E	2083	UNK	GLU	conflict	UNP A0R1H7
E	2084	UNK	GLN	conflict	UNP A0R1H7
E	2085	UNK	LEU	conflict	UNP A0R1H7
E	2086	UNK	SER	conflict	UNP A0R1H7
E	2087	UNK	GLN	conflict	UNP A0R1H7
E	2088	UNK	ARG	conflict	UNP A0R1H7
E	2089	UNK	PHE	conflict	UNP A0R1H7
E	2090	UNK	GLU	conflict	UNP A0R1H7
E	2091	UNK	GLY	conflict	UNP A0R1H7
E	2092	UNK	THR	conflict	UNP A0R1H7
E	2093	UNK	GLY	conflict	UNP A0R1H7
E	2094	UNK	HIS	conflict	UNP A0R1H7
E	2095	UNK	VAL	conflict	UNP A0R1H7
E	2096	UNK	VAL	conflict	UNP A0R1H7
E	2097	UNK	ALA	conflict	UNP A0R1H7
E	2098	UNK	THR	conflict	UNP A0R1H7
E	2099	UNK	GLN	conflict	UNP A0R1H7
E	2100	UNK	ALA	conflict	UNP A0R1H7
E	2101	UNK	ASN	conflict	UNP A0R1H7
E	2102	UNK	TRP	conflict	UNP A0R1H7
E	2103	UNK	TRP	conflict	UNP A0R1H7
E	2104	UNK	GLN	conflict	UNP A0R1H7
E	2105	UNK	GLY	conflict	UNP A0R1H7
E	2106	UNK	LYS	conflict	UNP A0R1H7
E	2107	UNK	ALA	conflict	UNP A0R1H7
E	2108	UNK	LEU	conflict	UNP A0R1H7
E	2109	UNK	ALA	conflict	UNP A0R1H7
E	2110	UNK	ALA	conflict	UNP A0R1H7
E	2111	UNK	GLY	conflict	UNP A0R1H7
E	2112	UNK	ARG	conflict	UNP A0R1H7
E	2113	UNK	ASN	conflict	UNP A0R1H7
E	2114	UNK	VAL	conflict	UNP A0R1H7
E	2115	UNK	HIS	conflict	UNP A0R1H7
E	2116	UNK	ALA	conflict	UNP A0R1H7
E	2117	UNK	SER	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2118	UNK	LEU	conflict	UNP A0R1H7
E	2119	UNK	PHE	conflict	UNP A0R1H7
E	2120	UNK	GLY	conflict	UNP A0R1H7
E	2121	UNK	ARG	conflict	UNP A0R1H7
E	2122	UNK	ILE	conflict	UNP A0R1H7
E	2123	UNK	ALA	conflict	UNP A0R1H7
E	2124	UNK	ALA	conflict	UNP A0R1H7
E	2125	UNK	GLY	conflict	UNP A0R1H7
E	2126	UNK	ALA	conflict	UNP A0R1H7
E	2127	UNK	GLU	conflict	UNP A0R1H7
E	2128	UNK	ASN	conflict	UNP A0R1H7
E	2129	UNK	PRO	conflict	UNP A0R1H7
E	2130	UNK	GLY	conflict	UNP A0R1H7
E	2131	UNK	LYS	conflict	UNP A0R1H7
E	2132	UNK	GLY	conflict	UNP A0R1H7
E	2133	UNK	ARG	conflict	UNP A0R1H7
E	2134	UNK	TYR	conflict	UNP A0R1H7
E	2135	UNK	SER	conflict	UNP A0R1H7
E	2422	UNK	GLU	conflict	UNP A0R1H7
E	2423	UNK	SER	conflict	UNP A0R1H7
E	2424	UNK	ASP	conflict	UNP A0R1H7
E	2425	UNK	ASP	conflict	UNP A0R1H7
E	2426	UNK	GLU	conflict	UNP A0R1H7
E	2427	UNK	ALA	conflict	UNP A0R1H7
E	2428	UNK	PRO	conflict	UNP A0R1H7
E	2429	UNK	ALA	conflict	UNP A0R1H7
E	2430	UNK	GLY	conflict	UNP A0R1H7
E	2431	UNK	THR	conflict	UNP A0R1H7
E	2432	UNK	ILE	conflict	UNP A0R1H7
E	2433	UNK	ARG	conflict	UNP A0R1H7
E	2434	UNK	ALA	conflict	UNP A0R1H7
E	2435	UNK	LEU	conflict	UNP A0R1H7
E	2436	UNK	PRO	conflict	UNP A0R1H7
E	2437	UNK	SER	conflict	UNP A0R1H7
E	2438	UNK	PRO	conflict	UNP A0R1H7
E	2439	UNK	PRO	conflict	UNP A0R1H7
E	2440	UNK	ARG	conflict	UNP A0R1H7
E	2441	UNK	GLY	conflict	UNP A0R1H7
E	2442	UNK	TYR	conflict	UNP A0R1H7
E	2443	UNK	ASN	conflict	UNP A0R1H7
E	2444	UNK	PRO	conflict	UNP A0R1H7
E	2445	UNK	ALA	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2446	UNK	PRO	conflict	UNP A0R1H7
E	2447	UNK	ALA	conflict	UNP A0R1H7
E	2448	UNK	PRO	conflict	UNP A0R1H7
E	2449	UNK	GLU	conflict	UNP A0R1H7
E	2450	UNK	TRP	conflict	UNP A0R1H7
E	2451	UNK	ASP	conflict	UNP A0R1H7
E	2452	UNK	ASP	conflict	UNP A0R1H7
E	2453	UNK	LEU	conflict	UNP A0R1H7
F	929	UNK	GLU	conflict	UNP A0R1H7
F	930	UNK	PRO	conflict	UNP A0R1H7
F	931	UNK	VAL	conflict	UNP A0R1H7
F	932	UNK	GLU	conflict	UNP A0R1H7
F	933	UNK	VAL	conflict	UNP A0R1H7
F	934	UNK	LEU	conflict	UNP A0R1H7
F	935	UNK	SER	conflict	UNP A0R1H7
F	936	UNK	ARG	conflict	UNP A0R1H7
F	937	UNK	ARG	conflict	UNP A0R1H7
F	938	UNK	GLN	conflict	UNP A0R1H7
F	939	UNK	ALA	conflict	UNP A0R1H7
F	940	UNK	ARG	conflict	UNP A0R1H7
F	941	UNK	ARG	conflict	UNP A0R1H7
F	942	UNK	ASP	conflict	UNP A0R1H7
F	943	UNK	ALA	conflict	UNP A0R1H7
F	944	UNK	SER	conflict	UNP A0R1H7
F	974	UNK	THR	conflict	UNP A0R1H7
F	975	UNK	GLU	conflict	UNP A0R1H7
F	976	UNK	TRP	conflict	UNP A0R1H7
F	977	UNK	GLN	conflict	UNP A0R1H7
F	978	UNK	VAL	conflict	UNP A0R1H7
F	979	UNK	ARG	conflict	UNP A0R1H7
F	980	UNK	GLU	conflict	UNP A0R1H7
F	981	UNK	GLY	conflict	UNP A0R1H7
F	982	UNK	SER	conflict	UNP A0R1H7
F	983	UNK	ASP	conflict	UNP A0R1H7
F	984	UNK	ASN	conflict	UNP A0R1H7
F	985	UNK	ARG	conflict	UNP A0R1H7
F	986	UNK	SER	conflict	UNP A0R1H7
F	987	UNK	ALA	conflict	UNP A0R1H7
F	988	UNK	SER	conflict	UNP A0R1H7
F	989	UNK	HIS	conflict	UNP A0R1H7
F	990	UNK	PRO	conflict	UNP A0R1H7
F	991	UNK	SER	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	992	UNK	THR	conflict	UNP A0R1H7
F	993	UNK	GLY	conflict	UNP A0R1H7
F	994	UNK	ALA	conflict	UNP A0R1H7
F	995	UNK	ARG	conflict	UNP A0R1H7
F	996	UNK	LEU	conflict	UNP A0R1H7
F	997	UNK	GLU	conflict	UNP A0R1H7
F	998	UNK	VAL	conflict	UNP A0R1H7
F	999	UNK	ALA	conflict	UNP A0R1H7
F	1000	UNK	ASP	conflict	UNP A0R1H7
F	1001	UNK	ASP	conflict	UNP A0R1H7
F	1002	UNK	GLN	conflict	UNP A0R1H7
F	1003	UNK	HIS	conflict	UNP A0R1H7
F	1004	UNK	VAL	conflict	UNP A0R1H7
F	1005	UNK	VAL	conflict	UNP A0R1H7
F	1006	UNK	LEU	conflict	UNP A0R1H7
F	1007	UNK	SER	conflict	UNP A0R1H7
F	1008	UNK	VAL	conflict	UNP A0R1H7
F	1009	UNK	PRO	conflict	UNP A0R1H7
F	1010	UNK	LEU	conflict	UNP A0R1H7
F	1011	UNK	SER	conflict	UNP A0R1H7
F	1012	UNK	GLY	conflict	UNP A0R1H7
F	1013	UNK	THR	conflict	UNP A0R1H7
F	1014	UNK	TRP	conflict	UNP A0R1H7
F	1196	UNK	GLY	conflict	UNP A0R1H7
F	1197	UNK	ARG	conflict	UNP A0R1H7
F	1198	UNK	THR	conflict	UNP A0R1H7
F	1199	UNK	GLY	conflict	UNP A0R1H7
F	1200	UNK	ALA	conflict	UNP A0R1H7
F	1201	UNK	ALA	conflict	UNP A0R1H7
F	1202	UNK	GLU	conflict	UNP A0R1H7
F	1203	UNK	LEU	conflict	UNP A0R1H7
F	1204	UNK	THR	conflict	UNP A0R1H7
F	1205	UNK	ASP	conflict	UNP A0R1H7
F	1206	UNK	PRO	conflict	UNP A0R1H7
F	1207	UNK	VAL	conflict	UNP A0R1H7
F	1208	UNK	ARG	conflict	UNP A0R1H7
F	1209	UNK	ALA	conflict	UNP A0R1H7
F	1210	UNK	GLY	conflict	UNP A0R1H7
F	1211	UNK	GLY	conflict	UNP A0R1H7
F	1212	UNK	ALA	conflict	UNP A0R1H7
F	1213	UNK	ILE	conflict	UNP A0R1H7
F	1214	UNK	SER	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1215	UNK	ASP	conflict	UNP A0R1H7
F	1216	UNK	ASN	conflict	UNP A0R1H7
F	1217	UNK	ALA	conflict	UNP A0R1H7
F	1218	UNK	THR	conflict	UNP A0R1H7
F	1219	UNK	ASP	conflict	UNP A0R1H7
F	1220	UNK	THR	conflict	UNP A0R1H7
F	1221	UNK	PRO	conflict	UNP A0R1H7
F	1222	UNK	ARG	conflict	UNP A0R1H7
F	1223	UNK	ARG	conflict	UNP A0R1H7
F	1224	UNK	ARG	conflict	UNP A0R1H7
F	1225	UNK	ARG	conflict	UNP A0R1H7
F	1226	UNK	ARG	conflict	UNP A0R1H7
F	1227	UNK	ASP	conflict	UNP A0R1H7
F	2076	UNK	GLY	conflict	UNP A0R1H7
F	2077	UNK	ASP	conflict	UNP A0R1H7
F	2078	UNK	ILE	conflict	UNP A0R1H7
F	2079	UNK	ASP	conflict	UNP A0R1H7
F	2080	UNK	ALA	conflict	UNP A0R1H7
F	2081	UNK	GLN	conflict	UNP A0R1H7
F	2082	UNK	TRP	conflict	UNP A0R1H7
F	2083	UNK	GLU	conflict	UNP A0R1H7
F	2084	UNK	GLN	conflict	UNP A0R1H7
F	2085	UNK	LEU	conflict	UNP A0R1H7
F	2086	UNK	SER	conflict	UNP A0R1H7
F	2087	UNK	GLN	conflict	UNP A0R1H7
F	2088	UNK	ARG	conflict	UNP A0R1H7
F	2089	UNK	PHE	conflict	UNP A0R1H7
F	2090	UNK	GLU	conflict	UNP A0R1H7
F	2091	UNK	GLY	conflict	UNP A0R1H7
F	2092	UNK	THR	conflict	UNP A0R1H7
F	2093	UNK	GLY	conflict	UNP A0R1H7
F	2094	UNK	HIS	conflict	UNP A0R1H7
F	2095	UNK	VAL	conflict	UNP A0R1H7
F	2096	UNK	VAL	conflict	UNP A0R1H7
F	2097	UNK	ALA	conflict	UNP A0R1H7
F	2098	UNK	THR	conflict	UNP A0R1H7
F	2099	UNK	GLN	conflict	UNP A0R1H7
F	2100	UNK	ALA	conflict	UNP A0R1H7
F	2101	UNK	ASN	conflict	UNP A0R1H7
F	2102	UNK	TRP	conflict	UNP A0R1H7
F	2103	UNK	TRP	conflict	UNP A0R1H7
F	2104	UNK	GLN	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2105	UNK	GLY	conflict	UNP A0R1H7
F	2106	UNK	LYS	conflict	UNP A0R1H7
F	2107	UNK	ALA	conflict	UNP A0R1H7
F	2108	UNK	LEU	conflict	UNP A0R1H7
F	2109	UNK	ALA	conflict	UNP A0R1H7
F	2110	UNK	ALA	conflict	UNP A0R1H7
F	2111	UNK	GLY	conflict	UNP A0R1H7
F	2112	UNK	ARG	conflict	UNP A0R1H7
F	2113	UNK	ASN	conflict	UNP A0R1H7
F	2114	UNK	VAL	conflict	UNP A0R1H7
F	2115	UNK	HIS	conflict	UNP A0R1H7
F	2116	UNK	ALA	conflict	UNP A0R1H7
F	2117	UNK	SER	conflict	UNP A0R1H7
F	2118	UNK	LEU	conflict	UNP A0R1H7
F	2119	UNK	PHE	conflict	UNP A0R1H7
F	2120	UNK	GLY	conflict	UNP A0R1H7
F	2121	UNK	ARG	conflict	UNP A0R1H7
F	2122	UNK	ILE	conflict	UNP A0R1H7
F	2123	UNK	ALA	conflict	UNP A0R1H7
F	2124	UNK	ALA	conflict	UNP A0R1H7
F	2125	UNK	GLY	conflict	UNP A0R1H7
F	2126	UNK	ALA	conflict	UNP A0R1H7
F	2127	UNK	GLU	conflict	UNP A0R1H7
F	2128	UNK	ASN	conflict	UNP A0R1H7
F	2129	UNK	PRO	conflict	UNP A0R1H7
F	2130	UNK	GLY	conflict	UNP A0R1H7
F	2131	UNK	LYS	conflict	UNP A0R1H7
F	2132	UNK	GLY	conflict	UNP A0R1H7
F	2133	UNK	ARG	conflict	UNP A0R1H7
F	2134	UNK	TYR	conflict	UNP A0R1H7
F	2135	UNK	SER	conflict	UNP A0R1H7
F	2422	UNK	GLU	conflict	UNP A0R1H7
F	2423	UNK	SER	conflict	UNP A0R1H7
F	2424	UNK	ASP	conflict	UNP A0R1H7
F	2425	UNK	ASP	conflict	UNP A0R1H7
F	2426	UNK	GLU	conflict	UNP A0R1H7
F	2427	UNK	ALA	conflict	UNP A0R1H7
F	2428	UNK	PRO	conflict	UNP A0R1H7
F	2429	UNK	ALA	conflict	UNP A0R1H7
F	2430	UNK	GLY	conflict	UNP A0R1H7
F	2431	UNK	THR	conflict	UNP A0R1H7
F	2432	UNK	ILE	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2433	UNK	ARG	conflict	UNP A0R1H7
F	2434	UNK	ALA	conflict	UNP A0R1H7
F	2435	UNK	LEU	conflict	UNP A0R1H7
F	2436	UNK	PRO	conflict	UNP A0R1H7
F	2437	UNK	SER	conflict	UNP A0R1H7
F	2438	UNK	PRO	conflict	UNP A0R1H7
F	2439	UNK	PRO	conflict	UNP A0R1H7
F	2440	UNK	ARG	conflict	UNP A0R1H7
F	2441	UNK	GLY	conflict	UNP A0R1H7
F	2442	UNK	TYR	conflict	UNP A0R1H7
F	2443	UNK	ASN	conflict	UNP A0R1H7
F	2444	UNK	PRO	conflict	UNP A0R1H7
F	2445	UNK	ALA	conflict	UNP A0R1H7
F	2446	UNK	PRO	conflict	UNP A0R1H7
F	2447	UNK	ALA	conflict	UNP A0R1H7
F	2448	UNK	PRO	conflict	UNP A0R1H7
F	2449	UNK	GLU	conflict	UNP A0R1H7
F	2450	UNK	TRP	conflict	UNP A0R1H7
F	2451	UNK	ASP	conflict	UNP A0R1H7
F	2452	UNK	ASP	conflict	UNP A0R1H7
F	2453	UNK	LEU	conflict	UNP A0R1H7
A	929	UNK	GLU	conflict	UNP A0R1H7
A	930	UNK	PRO	conflict	UNP A0R1H7
A	931	UNK	VAL	conflict	UNP A0R1H7
A	932	UNK	GLU	conflict	UNP A0R1H7
A	933	UNK	VAL	conflict	UNP A0R1H7
A	934	UNK	LEU	conflict	UNP A0R1H7
A	935	UNK	SER	conflict	UNP A0R1H7
A	936	UNK	ARG	conflict	UNP A0R1H7
A	937	UNK	ARG	conflict	UNP A0R1H7
A	938	UNK	GLN	conflict	UNP A0R1H7
A	939	UNK	ALA	conflict	UNP A0R1H7
A	940	UNK	ARG	conflict	UNP A0R1H7
A	941	UNK	ARG	conflict	UNP A0R1H7
A	942	UNK	ASP	conflict	UNP A0R1H7
A	943	UNK	ALA	conflict	UNP A0R1H7
A	944	UNK	SER	conflict	UNP A0R1H7
A	974	UNK	THR	conflict	UNP A0R1H7
A	975	UNK	GLU	conflict	UNP A0R1H7
A	976	UNK	TRP	conflict	UNP A0R1H7
A	977	UNK	GLN	conflict	UNP A0R1H7
A	978	UNK	VAL	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	979	UNK	ARG	conflict	UNP A0R1H7
A	980	UNK	GLU	conflict	UNP A0R1H7
A	981	UNK	GLY	conflict	UNP A0R1H7
A	982	UNK	SER	conflict	UNP A0R1H7
A	983	UNK	ASP	conflict	UNP A0R1H7
A	984	UNK	ASN	conflict	UNP A0R1H7
A	985	UNK	ARG	conflict	UNP A0R1H7
A	986	UNK	SER	conflict	UNP A0R1H7
A	987	UNK	ALA	conflict	UNP A0R1H7
A	988	UNK	SER	conflict	UNP A0R1H7
A	989	UNK	HIS	conflict	UNP A0R1H7
A	990	UNK	PRO	conflict	UNP A0R1H7
A	991	UNK	SER	conflict	UNP A0R1H7
A	992	UNK	THR	conflict	UNP A0R1H7
A	993	UNK	GLY	conflict	UNP A0R1H7
A	994	UNK	ALA	conflict	UNP A0R1H7
A	995	UNK	ARG	conflict	UNP A0R1H7
A	996	UNK	LEU	conflict	UNP A0R1H7
A	997	UNK	GLU	conflict	UNP A0R1H7
A	998	UNK	VAL	conflict	UNP A0R1H7
A	999	UNK	ALA	conflict	UNP A0R1H7
A	1000	UNK	ASP	conflict	UNP A0R1H7
A	1001	UNK	ASP	conflict	UNP A0R1H7
A	1002	UNK	GLN	conflict	UNP A0R1H7
A	1003	UNK	HIS	conflict	UNP A0R1H7
A	1004	UNK	VAL	conflict	UNP A0R1H7
A	1005	UNK	VAL	conflict	UNP A0R1H7
A	1006	UNK	LEU	conflict	UNP A0R1H7
A	1007	UNK	SER	conflict	UNP A0R1H7
A	1008	UNK	VAL	conflict	UNP A0R1H7
A	1009	UNK	PRO	conflict	UNP A0R1H7
A	1010	UNK	LEU	conflict	UNP A0R1H7
A	1011	UNK	SER	conflict	UNP A0R1H7
A	1012	UNK	GLY	conflict	UNP A0R1H7
A	1013	UNK	THR	conflict	UNP A0R1H7
A	1014	UNK	TRP	conflict	UNP A0R1H7
A	1196	UNK	GLY	conflict	UNP A0R1H7
A	1197	UNK	ARG	conflict	UNP A0R1H7
A	1198	UNK	THR	conflict	UNP A0R1H7
A	1199	UNK	GLY	conflict	UNP A0R1H7
A	1200	UNK	ALA	conflict	UNP A0R1H7
A	1201	UNK	ALA	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1202	UNK	GLU	conflict	UNP A0R1H7
A	1203	UNK	LEU	conflict	UNP A0R1H7
A	1204	UNK	THR	conflict	UNP A0R1H7
A	1205	UNK	ASP	conflict	UNP A0R1H7
A	1206	UNK	PRO	conflict	UNP A0R1H7
A	1207	UNK	VAL	conflict	UNP A0R1H7
A	1208	UNK	ARG	conflict	UNP A0R1H7
A	1209	UNK	ALA	conflict	UNP A0R1H7
A	1210	UNK	GLY	conflict	UNP A0R1H7
A	1211	UNK	GLY	conflict	UNP A0R1H7
A	1212	UNK	ALA	conflict	UNP A0R1H7
A	1213	UNK	ILE	conflict	UNP A0R1H7
A	1214	UNK	SER	conflict	UNP A0R1H7
A	1215	UNK	ASP	conflict	UNP A0R1H7
A	1216	UNK	ASN	conflict	UNP A0R1H7
A	1217	UNK	ALA	conflict	UNP A0R1H7
A	1218	UNK	THR	conflict	UNP A0R1H7
A	1219	UNK	ASP	conflict	UNP A0R1H7
A	1220	UNK	THR	conflict	UNP A0R1H7
A	1221	UNK	PRO	conflict	UNP A0R1H7
A	1222	UNK	ARG	conflict	UNP A0R1H7
A	1223	UNK	ARG	conflict	UNP A0R1H7
A	1224	UNK	ARG	conflict	UNP A0R1H7
A	1225	UNK	ARG	conflict	UNP A0R1H7
A	1226	UNK	ARG	conflict	UNP A0R1H7
A	1227	UNK	ASP	conflict	UNP A0R1H7
A	2076	UNK	GLY	conflict	UNP A0R1H7
A	2077	UNK	ASP	conflict	UNP A0R1H7
A	2078	UNK	ILE	conflict	UNP A0R1H7
A	2079	UNK	ASP	conflict	UNP A0R1H7
A	2080	UNK	ALA	conflict	UNP A0R1H7
A	2081	UNK	GLN	conflict	UNP A0R1H7
A	2082	UNK	TRP	conflict	UNP A0R1H7
A	2083	UNK	GLU	conflict	UNP A0R1H7
A	2084	UNK	GLN	conflict	UNP A0R1H7
A	2085	UNK	LEU	conflict	UNP A0R1H7
A	2086	UNK	SER	conflict	UNP A0R1H7
A	2087	UNK	GLN	conflict	UNP A0R1H7
A	2088	UNK	ARG	conflict	UNP A0R1H7
A	2089	UNK	PHE	conflict	UNP A0R1H7
A	2090	UNK	GLU	conflict	UNP A0R1H7
A	2091	UNK	GLY	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2092	UNK	THR	conflict	UNP A0R1H7
A	2093	UNK	GLY	conflict	UNP A0R1H7
A	2094	UNK	HIS	conflict	UNP A0R1H7
A	2095	UNK	VAL	conflict	UNP A0R1H7
A	2096	UNK	VAL	conflict	UNP A0R1H7
A	2097	UNK	ALA	conflict	UNP A0R1H7
A	2098	UNK	THR	conflict	UNP A0R1H7
A	2099	UNK	GLN	conflict	UNP A0R1H7
A	2100	UNK	ALA	conflict	UNP A0R1H7
A	2101	UNK	ASN	conflict	UNP A0R1H7
A	2102	UNK	TRP	conflict	UNP A0R1H7
A	2103	UNK	TRP	conflict	UNP A0R1H7
A	2104	UNK	GLN	conflict	UNP A0R1H7
A	2105	UNK	GLY	conflict	UNP A0R1H7
A	2106	UNK	LYS	conflict	UNP A0R1H7
A	2107	UNK	ALA	conflict	UNP A0R1H7
A	2108	UNK	LEU	conflict	UNP A0R1H7
A	2109	UNK	ALA	conflict	UNP A0R1H7
A	2110	UNK	ALA	conflict	UNP A0R1H7
A	2111	UNK	GLY	conflict	UNP A0R1H7
A	2112	UNK	ARG	conflict	UNP A0R1H7
A	2113	UNK	ASN	conflict	UNP A0R1H7
A	2114	UNK	VAL	conflict	UNP A0R1H7
A	2115	UNK	HIS	conflict	UNP A0R1H7
A	2116	UNK	ALA	conflict	UNP A0R1H7
A	2117	UNK	SER	conflict	UNP A0R1H7
A	2118	UNK	LEU	conflict	UNP A0R1H7
A	2119	UNK	PHE	conflict	UNP A0R1H7
A	2120	UNK	GLY	conflict	UNP A0R1H7
A	2121	UNK	ARG	conflict	UNP A0R1H7
A	2122	UNK	ILE	conflict	UNP A0R1H7
A	2123	UNK	ALA	conflict	UNP A0R1H7
A	2124	UNK	ALA	conflict	UNP A0R1H7
A	2125	UNK	GLY	conflict	UNP A0R1H7
A	2126	UNK	ALA	conflict	UNP A0R1H7
A	2127	UNK	GLU	conflict	UNP A0R1H7
A	2128	UNK	ASN	conflict	UNP A0R1H7
A	2129	UNK	PRO	conflict	UNP A0R1H7
A	2130	UNK	GLY	conflict	UNP A0R1H7
A	2131	UNK	LYS	conflict	UNP A0R1H7
A	2132	UNK	GLY	conflict	UNP A0R1H7
A	2133	UNK	ARG	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2134	UNK	TYR	conflict	UNP A0R1H7
A	2135	UNK	SER	conflict	UNP A0R1H7
A	2422	UNK	GLU	conflict	UNP A0R1H7
A	2423	UNK	SER	conflict	UNP A0R1H7
A	2424	UNK	ASP	conflict	UNP A0R1H7
A	2425	UNK	ASP	conflict	UNP A0R1H7
A	2426	UNK	GLU	conflict	UNP A0R1H7
A	2427	UNK	ALA	conflict	UNP A0R1H7
A	2428	UNK	PRO	conflict	UNP A0R1H7
A	2429	UNK	ALA	conflict	UNP A0R1H7
A	2430	UNK	GLY	conflict	UNP A0R1H7
A	2431	UNK	THR	conflict	UNP A0R1H7
A	2432	UNK	ILE	conflict	UNP A0R1H7
A	2433	UNK	ARG	conflict	UNP A0R1H7
A	2434	UNK	ALA	conflict	UNP A0R1H7
A	2435	UNK	LEU	conflict	UNP A0R1H7
A	2436	UNK	PRO	conflict	UNP A0R1H7
A	2437	UNK	SER	conflict	UNP A0R1H7
A	2438	UNK	PRO	conflict	UNP A0R1H7
A	2439	UNK	PRO	conflict	UNP A0R1H7
A	2440	UNK	ARG	conflict	UNP A0R1H7
A	2441	UNK	GLY	conflict	UNP A0R1H7
A	2442	UNK	TYR	conflict	UNP A0R1H7
A	2443	UNK	ASN	conflict	UNP A0R1H7
A	2444	UNK	PRO	conflict	UNP A0R1H7
A	2445	UNK	ALA	conflict	UNP A0R1H7
A	2446	UNK	PRO	conflict	UNP A0R1H7
A	2447	UNK	ALA	conflict	UNP A0R1H7
A	2448	UNK	PRO	conflict	UNP A0R1H7
A	2449	UNK	GLU	conflict	UNP A0R1H7
A	2450	UNK	TRP	conflict	UNP A0R1H7
A	2451	UNK	ASP	conflict	UNP A0R1H7
A	2452	UNK	ASP	conflict	UNP A0R1H7
A	2453	UNK	LEU	conflict	UNP A0R1H7
B	929	UNK	GLU	conflict	UNP A0R1H7
B	930	UNK	PRO	conflict	UNP A0R1H7
B	931	UNK	VAL	conflict	UNP A0R1H7
B	932	UNK	GLU	conflict	UNP A0R1H7
B	933	UNK	VAL	conflict	UNP A0R1H7
B	934	UNK	LEU	conflict	UNP A0R1H7
B	935	UNK	SER	conflict	UNP A0R1H7
B	936	UNK	ARG	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	937	UNK	ARG	conflict	UNP A0R1H7
B	938	UNK	GLN	conflict	UNP A0R1H7
B	939	UNK	ALA	conflict	UNP A0R1H7
B	940	UNK	ARG	conflict	UNP A0R1H7
B	941	UNK	ARG	conflict	UNP A0R1H7
B	942	UNK	ASP	conflict	UNP A0R1H7
B	943	UNK	ALA	conflict	UNP A0R1H7
B	944	UNK	SER	conflict	UNP A0R1H7
B	974	UNK	THR	conflict	UNP A0R1H7
B	975	UNK	GLU	conflict	UNP A0R1H7
B	976	UNK	TRP	conflict	UNP A0R1H7
B	977	UNK	GLN	conflict	UNP A0R1H7
B	978	UNK	VAL	conflict	UNP A0R1H7
B	979	UNK	ARG	conflict	UNP A0R1H7
B	980	UNK	GLU	conflict	UNP A0R1H7
B	981	UNK	GLY	conflict	UNP A0R1H7
B	982	UNK	SER	conflict	UNP A0R1H7
B	983	UNK	ASP	conflict	UNP A0R1H7
B	984	UNK	ASN	conflict	UNP A0R1H7
B	985	UNK	ARG	conflict	UNP A0R1H7
B	986	UNK	SER	conflict	UNP A0R1H7
B	987	UNK	ALA	conflict	UNP A0R1H7
B	988	UNK	SER	conflict	UNP A0R1H7
B	989	UNK	HIS	conflict	UNP A0R1H7
B	990	UNK	PRO	conflict	UNP A0R1H7
B	991	UNK	SER	conflict	UNP A0R1H7
B	992	UNK	THR	conflict	UNP A0R1H7
B	993	UNK	GLY	conflict	UNP A0R1H7
B	994	UNK	ALA	conflict	UNP A0R1H7
B	995	UNK	ARG	conflict	UNP A0R1H7
B	996	UNK	LEU	conflict	UNP A0R1H7
B	997	UNK	GLU	conflict	UNP A0R1H7
B	998	UNK	VAL	conflict	UNP A0R1H7
B	999	UNK	ALA	conflict	UNP A0R1H7
B	1000	UNK	ASP	conflict	UNP A0R1H7
B	1001	UNK	ASP	conflict	UNP A0R1H7
B	1002	UNK	GLN	conflict	UNP A0R1H7
B	1003	UNK	HIS	conflict	UNP A0R1H7
B	1004	UNK	VAL	conflict	UNP A0R1H7
B	1005	UNK	VAL	conflict	UNP A0R1H7
B	1006	UNK	LEU	conflict	UNP A0R1H7
B	1007	UNK	SER	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1008	UNK	VAL	conflict	UNP A0R1H7
B	1009	UNK	PRO	conflict	UNP A0R1H7
B	1010	UNK	LEU	conflict	UNP A0R1H7
B	1011	UNK	SER	conflict	UNP A0R1H7
B	1012	UNK	GLY	conflict	UNP A0R1H7
B	1013	UNK	THR	conflict	UNP A0R1H7
B	1014	UNK	TRP	conflict	UNP A0R1H7
B	1196	UNK	GLY	conflict	UNP A0R1H7
B	1197	UNK	ARG	conflict	UNP A0R1H7
B	1198	UNK	THR	conflict	UNP A0R1H7
B	1199	UNK	GLY	conflict	UNP A0R1H7
B	1200	UNK	ALA	conflict	UNP A0R1H7
B	1201	UNK	ALA	conflict	UNP A0R1H7
B	1202	UNK	GLU	conflict	UNP A0R1H7
B	1203	UNK	LEU	conflict	UNP A0R1H7
B	1204	UNK	THR	conflict	UNP A0R1H7
B	1205	UNK	ASP	conflict	UNP A0R1H7
B	1206	UNK	PRO	conflict	UNP A0R1H7
B	1207	UNK	VAL	conflict	UNP A0R1H7
B	1208	UNK	ARG	conflict	UNP A0R1H7
B	1209	UNK	ALA	conflict	UNP A0R1H7
B	1210	UNK	GLY	conflict	UNP A0R1H7
B	1211	UNK	GLY	conflict	UNP A0R1H7
B	1212	UNK	ALA	conflict	UNP A0R1H7
B	1213	UNK	ILE	conflict	UNP A0R1H7
B	1214	UNK	SER	conflict	UNP A0R1H7
B	1215	UNK	ASP	conflict	UNP A0R1H7
B	1216	UNK	ASN	conflict	UNP A0R1H7
B	1217	UNK	ALA	conflict	UNP A0R1H7
B	1218	UNK	THR	conflict	UNP A0R1H7
B	1219	UNK	ASP	conflict	UNP A0R1H7
B	1220	UNK	THR	conflict	UNP A0R1H7
B	1221	UNK	PRO	conflict	UNP A0R1H7
B	1222	UNK	ARG	conflict	UNP A0R1H7
B	1223	UNK	ARG	conflict	UNP A0R1H7
B	1224	UNK	ARG	conflict	UNP A0R1H7
B	1225	UNK	ARG	conflict	UNP A0R1H7
B	1226	UNK	ARG	conflict	UNP A0R1H7
B	1227	UNK	ASP	conflict	UNP A0R1H7
B	2076	UNK	GLY	conflict	UNP A0R1H7
B	2077	UNK	ASP	conflict	UNP A0R1H7
B	2078	UNK	ILE	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2079	UNK	ASP	conflict	UNP A0R1H7
B	2080	UNK	ALA	conflict	UNP A0R1H7
B	2081	UNK	GLN	conflict	UNP A0R1H7
B	2082	UNK	TRP	conflict	UNP A0R1H7
B	2083	UNK	GLU	conflict	UNP A0R1H7
B	2084	UNK	GLN	conflict	UNP A0R1H7
B	2085	UNK	LEU	conflict	UNP A0R1H7
B	2086	UNK	SER	conflict	UNP A0R1H7
B	2087	UNK	GLN	conflict	UNP A0R1H7
B	2088	UNK	ARG	conflict	UNP A0R1H7
B	2089	UNK	PHE	conflict	UNP A0R1H7
B	2090	UNK	GLU	conflict	UNP A0R1H7
B	2091	UNK	GLY	conflict	UNP A0R1H7
B	2092	UNK	THR	conflict	UNP A0R1H7
B	2093	UNK	GLY	conflict	UNP A0R1H7
B	2094	UNK	HIS	conflict	UNP A0R1H7
B	2095	UNK	VAL	conflict	UNP A0R1H7
B	2096	UNK	VAL	conflict	UNP A0R1H7
B	2097	UNK	ALA	conflict	UNP A0R1H7
B	2098	UNK	THR	conflict	UNP A0R1H7
B	2099	UNK	GLN	conflict	UNP A0R1H7
B	2100	UNK	ALA	conflict	UNP A0R1H7
B	2101	UNK	ASN	conflict	UNP A0R1H7
B	2102	UNK	TRP	conflict	UNP A0R1H7
B	2103	UNK	TRP	conflict	UNP A0R1H7
B	2104	UNK	GLN	conflict	UNP A0R1H7
B	2105	UNK	GLY	conflict	UNP A0R1H7
B	2106	UNK	LYS	conflict	UNP A0R1H7
B	2107	UNK	ALA	conflict	UNP A0R1H7
B	2108	UNK	LEU	conflict	UNP A0R1H7
B	2109	UNK	ALA	conflict	UNP A0R1H7
B	2110	UNK	ALA	conflict	UNP A0R1H7
B	2111	UNK	GLY	conflict	UNP A0R1H7
B	2112	UNK	ARG	conflict	UNP A0R1H7
B	2113	UNK	ASN	conflict	UNP A0R1H7
B	2114	UNK	VAL	conflict	UNP A0R1H7
B	2115	UNK	HIS	conflict	UNP A0R1H7
B	2116	UNK	ALA	conflict	UNP A0R1H7
B	2117	UNK	SER	conflict	UNP A0R1H7
B	2118	UNK	LEU	conflict	UNP A0R1H7
B	2119	UNK	PHE	conflict	UNP A0R1H7
B	2120	UNK	GLY	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2121	UNK	ARG	conflict	UNP A0R1H7
B	2122	UNK	ILE	conflict	UNP A0R1H7
B	2123	UNK	ALA	conflict	UNP A0R1H7
B	2124	UNK	ALA	conflict	UNP A0R1H7
B	2125	UNK	GLY	conflict	UNP A0R1H7
B	2126	UNK	ALA	conflict	UNP A0R1H7
B	2127	UNK	GLU	conflict	UNP A0R1H7
B	2128	UNK	ASN	conflict	UNP A0R1H7
B	2129	UNK	PRO	conflict	UNP A0R1H7
B	2130	UNK	GLY	conflict	UNP A0R1H7
B	2131	UNK	LYS	conflict	UNP A0R1H7
B	2132	UNK	GLY	conflict	UNP A0R1H7
B	2133	UNK	ARG	conflict	UNP A0R1H7
B	2134	UNK	TYR	conflict	UNP A0R1H7
B	2135	UNK	SER	conflict	UNP A0R1H7
B	2422	UNK	GLU	conflict	UNP A0R1H7
B	2423	UNK	SER	conflict	UNP A0R1H7
B	2424	UNK	ASP	conflict	UNP A0R1H7
B	2425	UNK	ASP	conflict	UNP A0R1H7
B	2426	UNK	GLU	conflict	UNP A0R1H7
B	2427	UNK	ALA	conflict	UNP A0R1H7
B	2428	UNK	PRO	conflict	UNP A0R1H7
B	2429	UNK	ALA	conflict	UNP A0R1H7
B	2430	UNK	GLY	conflict	UNP A0R1H7
B	2431	UNK	THR	conflict	UNP A0R1H7
B	2432	UNK	ILE	conflict	UNP A0R1H7
B	2433	UNK	ARG	conflict	UNP A0R1H7
B	2434	UNK	ALA	conflict	UNP A0R1H7
B	2435	UNK	LEU	conflict	UNP A0R1H7
B	2436	UNK	PRO	conflict	UNP A0R1H7
B	2437	UNK	SER	conflict	UNP A0R1H7
B	2438	UNK	PRO	conflict	UNP A0R1H7
B	2439	UNK	PRO	conflict	UNP A0R1H7
B	2440	UNK	ARG	conflict	UNP A0R1H7
B	2441	UNK	GLY	conflict	UNP A0R1H7
B	2442	UNK	TYR	conflict	UNP A0R1H7
B	2443	UNK	ASN	conflict	UNP A0R1H7
B	2444	UNK	PRO	conflict	UNP A0R1H7
B	2445	UNK	ALA	conflict	UNP A0R1H7
B	2446	UNK	PRO	conflict	UNP A0R1H7
B	2447	UNK	ALA	conflict	UNP A0R1H7
B	2448	UNK	PRO	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2449	UNK	GLU	conflict	UNP A0R1H7
B	2450	UNK	TRP	conflict	UNP A0R1H7
B	2451	UNK	ASP	conflict	UNP A0R1H7
B	2452	UNK	ASP	conflict	UNP A0R1H7
B	2453	UNK	LEU	conflict	UNP A0R1H7
C	929	UNK	GLU	conflict	UNP A0R1H7
C	930	UNK	PRO	conflict	UNP A0R1H7
C	931	UNK	VAL	conflict	UNP A0R1H7
C	932	UNK	GLU	conflict	UNP A0R1H7
C	933	UNK	VAL	conflict	UNP A0R1H7
C	934	UNK	LEU	conflict	UNP A0R1H7
C	935	UNK	SER	conflict	UNP A0R1H7
C	936	UNK	ARG	conflict	UNP A0R1H7
C	937	UNK	ARG	conflict	UNP A0R1H7
C	938	UNK	GLN	conflict	UNP A0R1H7
C	939	UNK	ALA	conflict	UNP A0R1H7
C	940	UNK	ARG	conflict	UNP A0R1H7
C	941	UNK	ARG	conflict	UNP A0R1H7
C	942	UNK	ASP	conflict	UNP A0R1H7
C	943	UNK	ALA	conflict	UNP A0R1H7
C	944	UNK	SER	conflict	UNP A0R1H7
C	974	UNK	THR	conflict	UNP A0R1H7
C	975	UNK	GLU	conflict	UNP A0R1H7
C	976	UNK	TRP	conflict	UNP A0R1H7
C	977	UNK	GLN	conflict	UNP A0R1H7
C	978	UNK	VAL	conflict	UNP A0R1H7
C	979	UNK	ARG	conflict	UNP A0R1H7
C	980	UNK	GLU	conflict	UNP A0R1H7
C	981	UNK	GLY	conflict	UNP A0R1H7
C	982	UNK	SER	conflict	UNP A0R1H7
C	983	UNK	ASP	conflict	UNP A0R1H7
C	984	UNK	ASN	conflict	UNP A0R1H7
C	985	UNK	ARG	conflict	UNP A0R1H7
C	986	UNK	SER	conflict	UNP A0R1H7
C	987	UNK	ALA	conflict	UNP A0R1H7
C	988	UNK	SER	conflict	UNP A0R1H7
C	989	UNK	HIS	conflict	UNP A0R1H7
C	990	UNK	PRO	conflict	UNP A0R1H7
C	991	UNK	SER	conflict	UNP A0R1H7
C	992	UNK	THR	conflict	UNP A0R1H7
C	993	UNK	GLY	conflict	UNP A0R1H7
C	994	UNK	ALA	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	995	UNK	ARG	conflict	UNP A0R1H7
C	996	UNK	LEU	conflict	UNP A0R1H7
C	997	UNK	GLU	conflict	UNP A0R1H7
C	998	UNK	VAL	conflict	UNP A0R1H7
C	999	UNK	ALA	conflict	UNP A0R1H7
C	1000	UNK	ASP	conflict	UNP A0R1H7
C	1001	UNK	ASP	conflict	UNP A0R1H7
C	1002	UNK	GLN	conflict	UNP A0R1H7
C	1003	UNK	HIS	conflict	UNP A0R1H7
C	1004	UNK	VAL	conflict	UNP A0R1H7
C	1005	UNK	VAL	conflict	UNP A0R1H7
C	1006	UNK	LEU	conflict	UNP A0R1H7
C	1007	UNK	SER	conflict	UNP A0R1H7
C	1008	UNK	VAL	conflict	UNP A0R1H7
C	1009	UNK	PRO	conflict	UNP A0R1H7
C	1010	UNK	LEU	conflict	UNP A0R1H7
C	1011	UNK	SER	conflict	UNP A0R1H7
C	1012	UNK	GLY	conflict	UNP A0R1H7
C	1013	UNK	THR	conflict	UNP A0R1H7
C	1014	UNK	TRP	conflict	UNP A0R1H7
C	1196	UNK	GLY	conflict	UNP A0R1H7
C	1197	UNK	ARG	conflict	UNP A0R1H7
C	1198	UNK	THR	conflict	UNP A0R1H7
C	1199	UNK	GLY	conflict	UNP A0R1H7
C	1200	UNK	ALA	conflict	UNP A0R1H7
C	1201	UNK	ALA	conflict	UNP A0R1H7
C	1202	UNK	GLU	conflict	UNP A0R1H7
C	1203	UNK	LEU	conflict	UNP A0R1H7
C	1204	UNK	THR	conflict	UNP A0R1H7
C	1205	UNK	ASP	conflict	UNP A0R1H7
C	1206	UNK	PRO	conflict	UNP A0R1H7
C	1207	UNK	VAL	conflict	UNP A0R1H7
C	1208	UNK	ARG	conflict	UNP A0R1H7
C	1209	UNK	ALA	conflict	UNP A0R1H7
C	1210	UNK	GLY	conflict	UNP A0R1H7
C	1211	UNK	GLY	conflict	UNP A0R1H7
C	1212	UNK	ALA	conflict	UNP A0R1H7
C	1213	UNK	ILE	conflict	UNP A0R1H7
C	1214	UNK	SER	conflict	UNP A0R1H7
C	1215	UNK	ASP	conflict	UNP A0R1H7
C	1216	UNK	ASN	conflict	UNP A0R1H7
C	1217	UNK	ALA	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	UNK	THR	conflict	UNP A0R1H7
C	1219	UNK	ASP	conflict	UNP A0R1H7
C	1220	UNK	THR	conflict	UNP A0R1H7
C	1221	UNK	PRO	conflict	UNP A0R1H7
C	1222	UNK	ARG	conflict	UNP A0R1H7
C	1223	UNK	ARG	conflict	UNP A0R1H7
C	1224	UNK	ARG	conflict	UNP A0R1H7
C	1225	UNK	ARG	conflict	UNP A0R1H7
C	1226	UNK	ARG	conflict	UNP A0R1H7
C	1227	UNK	ASP	conflict	UNP A0R1H7
C	2076	UNK	GLY	conflict	UNP A0R1H7
C	2077	UNK	ASP	conflict	UNP A0R1H7
C	2078	UNK	ILE	conflict	UNP A0R1H7
C	2079	UNK	ASP	conflict	UNP A0R1H7
C	2080	UNK	ALA	conflict	UNP A0R1H7
C	2081	UNK	GLN	conflict	UNP A0R1H7
C	2082	UNK	TRP	conflict	UNP A0R1H7
C	2083	UNK	GLU	conflict	UNP A0R1H7
C	2084	UNK	GLN	conflict	UNP A0R1H7
C	2085	UNK	LEU	conflict	UNP A0R1H7
C	2086	UNK	SER	conflict	UNP A0R1H7
C	2087	UNK	GLN	conflict	UNP A0R1H7
C	2088	UNK	ARG	conflict	UNP A0R1H7
C	2089	UNK	PHE	conflict	UNP A0R1H7
C	2090	UNK	GLU	conflict	UNP A0R1H7
C	2091	UNK	GLY	conflict	UNP A0R1H7
C	2092	UNK	THR	conflict	UNP A0R1H7
C	2093	UNK	GLY	conflict	UNP A0R1H7
C	2094	UNK	HIS	conflict	UNP A0R1H7
C	2095	UNK	VAL	conflict	UNP A0R1H7
C	2096	UNK	VAL	conflict	UNP A0R1H7
C	2097	UNK	ALA	conflict	UNP A0R1H7
C	2098	UNK	THR	conflict	UNP A0R1H7
C	2099	UNK	GLN	conflict	UNP A0R1H7
C	2100	UNK	ALA	conflict	UNP A0R1H7
C	2101	UNK	ASN	conflict	UNP A0R1H7
C	2102	UNK	TRP	conflict	UNP A0R1H7
C	2103	UNK	TRP	conflict	UNP A0R1H7
C	2104	UNK	GLN	conflict	UNP A0R1H7
C	2105	UNK	GLY	conflict	UNP A0R1H7
C	2106	UNK	LYS	conflict	UNP A0R1H7
C	2107	UNK	ALA	conflict	UNP A0R1H7

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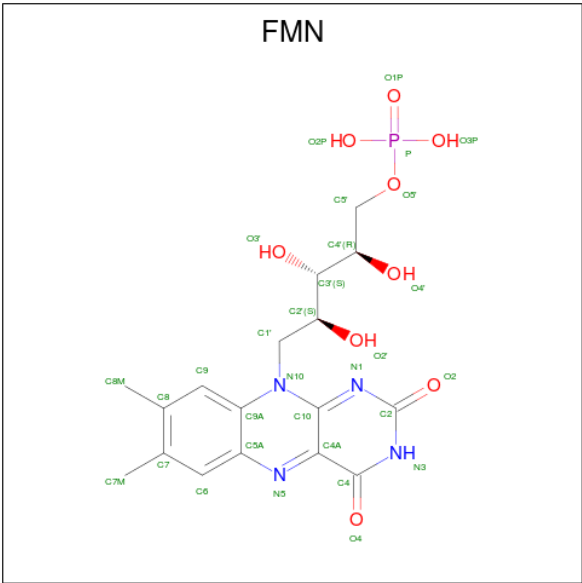
Chain	Residue	Modelled	Actual	Comment	Reference
C	2108	UNK	LEU	conflict	UNP A0R1H7
C	2109	UNK	ALA	conflict	UNP A0R1H7
C	2110	UNK	ALA	conflict	UNP A0R1H7
C	2111	UNK	GLY	conflict	UNP A0R1H7
C	2112	UNK	ARG	conflict	UNP A0R1H7
C	2113	UNK	ASN	conflict	UNP A0R1H7
C	2114	UNK	VAL	conflict	UNP A0R1H7
C	2115	UNK	HIS	conflict	UNP A0R1H7
C	2116	UNK	ALA	conflict	UNP A0R1H7
C	2117	UNK	SER	conflict	UNP A0R1H7
C	2118	UNK	LEU	conflict	UNP A0R1H7
C	2119	UNK	PHE	conflict	UNP A0R1H7
C	2120	UNK	GLY	conflict	UNP A0R1H7
C	2121	UNK	ARG	conflict	UNP A0R1H7
C	2122	UNK	ILE	conflict	UNP A0R1H7
C	2123	UNK	ALA	conflict	UNP A0R1H7
C	2124	UNK	ALA	conflict	UNP A0R1H7
C	2125	UNK	GLY	conflict	UNP A0R1H7
C	2126	UNK	ALA	conflict	UNP A0R1H7
C	2127	UNK	GLU	conflict	UNP A0R1H7
C	2128	UNK	ASN	conflict	UNP A0R1H7
C	2129	UNK	PRO	conflict	UNP A0R1H7
C	2130	UNK	GLY	conflict	UNP A0R1H7
C	2131	UNK	LYS	conflict	UNP A0R1H7
C	2132	UNK	GLY	conflict	UNP A0R1H7
C	2133	UNK	ARG	conflict	UNP A0R1H7
C	2134	UNK	TYR	conflict	UNP A0R1H7
C	2135	UNK	SER	conflict	UNP A0R1H7
C	2422	UNK	GLU	conflict	UNP A0R1H7
C	2423	UNK	SER	conflict	UNP A0R1H7
C	2424	UNK	ASP	conflict	UNP A0R1H7
C	2425	UNK	ASP	conflict	UNP A0R1H7
C	2426	UNK	GLU	conflict	UNP A0R1H7
C	2427	UNK	ALA	conflict	UNP A0R1H7
C	2428	UNK	PRO	conflict	UNP A0R1H7
C	2429	UNK	ALA	conflict	UNP A0R1H7
C	2430	UNK	GLY	conflict	UNP A0R1H7
C	2431	UNK	THR	conflict	UNP A0R1H7
C	2432	UNK	ILE	conflict	UNP A0R1H7
C	2433	UNK	ARG	conflict	UNP A0R1H7
C	2434	UNK	ALA	conflict	UNP A0R1H7
C	2435	UNK	LEU	conflict	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2436	UNK	PRO	conflict	UNP A0R1H7
C	2437	UNK	SER	conflict	UNP A0R1H7
C	2438	UNK	PRO	conflict	UNP A0R1H7
C	2439	UNK	PRO	conflict	UNP A0R1H7
C	2440	UNK	ARG	conflict	UNP A0R1H7
C	2441	UNK	GLY	conflict	UNP A0R1H7
C	2442	UNK	TYR	conflict	UNP A0R1H7
C	2443	UNK	ASN	conflict	UNP A0R1H7
C	2444	UNK	PRO	conflict	UNP A0R1H7
C	2445	UNK	ALA	conflict	UNP A0R1H7
C	2446	UNK	PRO	conflict	UNP A0R1H7
C	2447	UNK	ALA	conflict	UNP A0R1H7
C	2448	UNK	PRO	conflict	UNP A0R1H7
C	2449	UNK	GLU	conflict	UNP A0R1H7
C	2450	UNK	TRP	conflict	UNP A0R1H7
C	2451	UNK	ASP	conflict	UNP A0R1H7
C	2452	UNK	ASP	conflict	UNP A0R1H7
C	2453	UNK	LEU	conflict	UNP A0R1H7

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	

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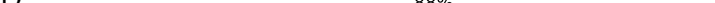
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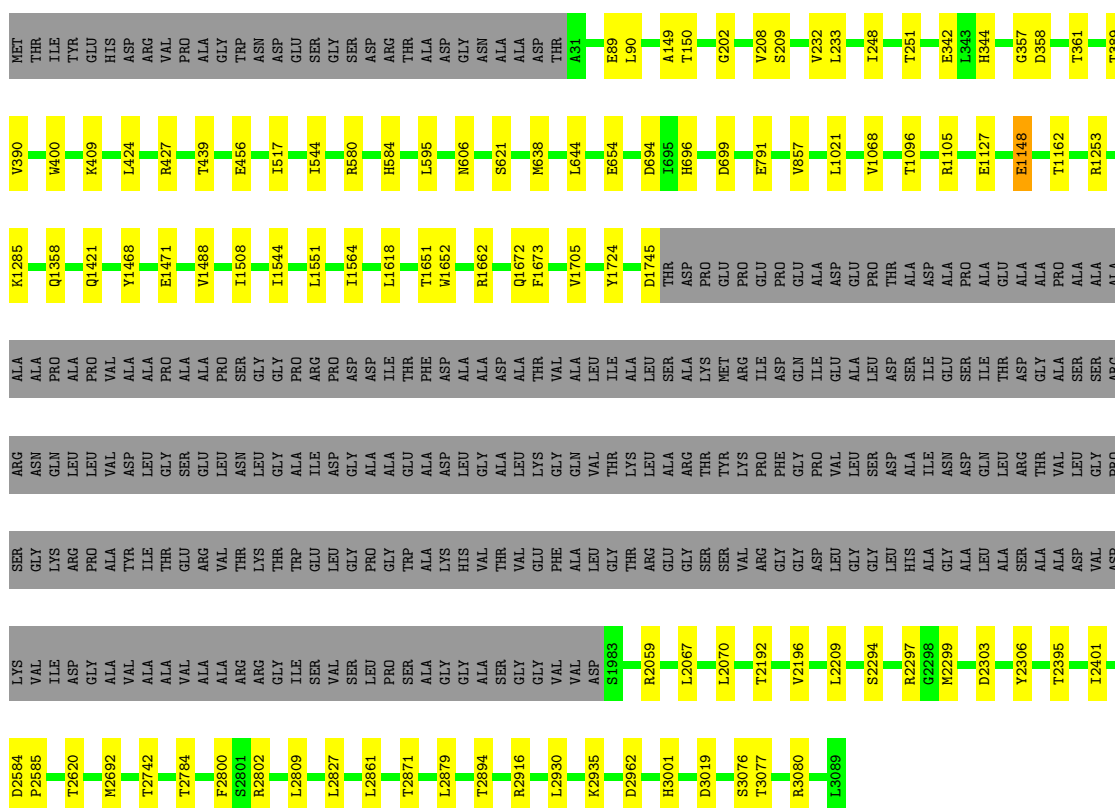
Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

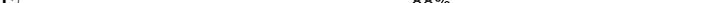
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

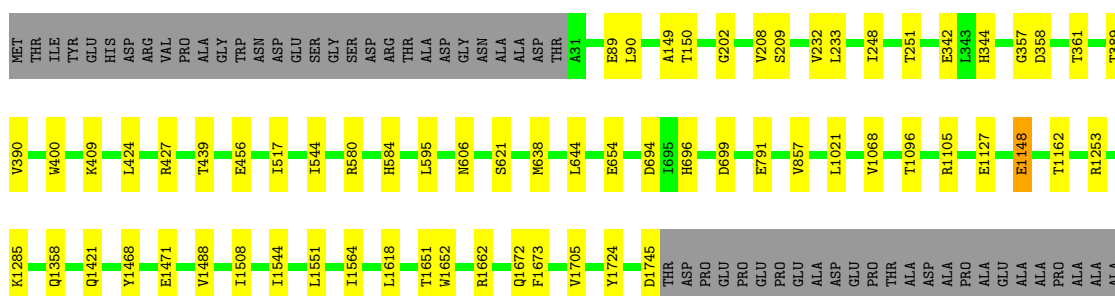
- Molecule 1: FATTY ACID SYNTHASE

Chain D:  88% . 9%



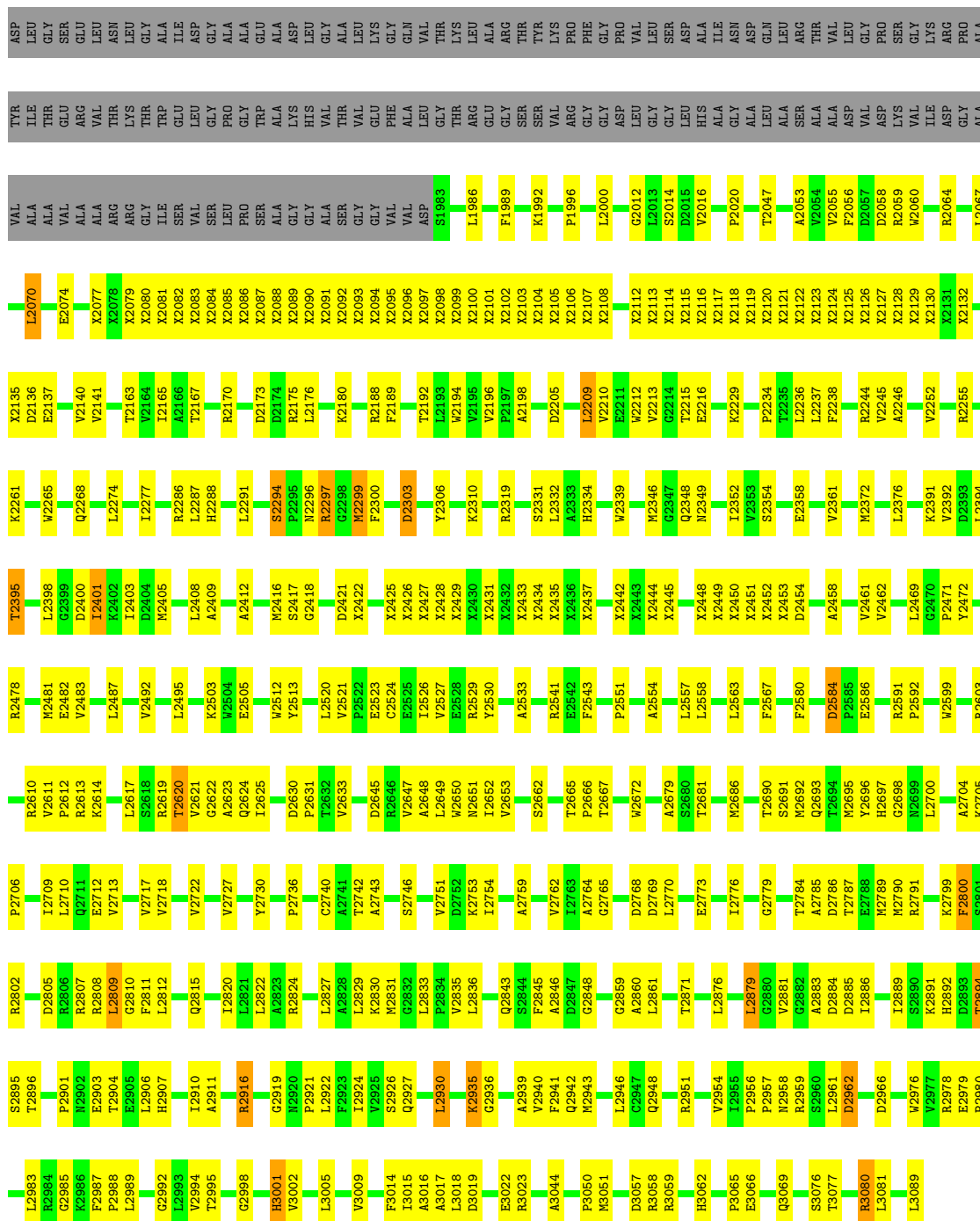
- Molecule 1: FATTY ACID SYNTHASE

Chain E:  88% . 9%



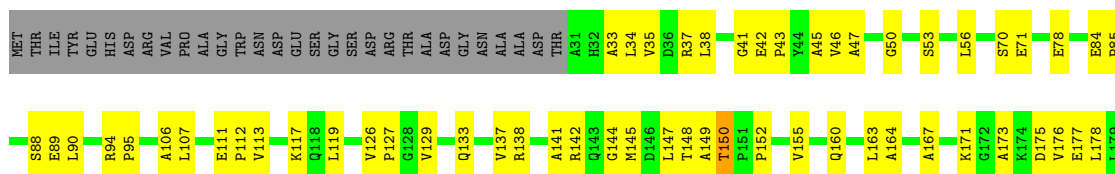
ALA	K1706	T1503	H1412	R1195	P1099	X994	G990	A792	N682	T485	R381	V292	A182
PRO	P1616	R1504	Q1307	X1196	D1100	X996	L901	R793	G683	Q486	R381	V292	Q183
SER	M1617	Q1507	D1308	X1197	X1198	X997	V904	L794	M684	R487	R381	V292	Q184
GLY	V1711	Q1508	V1309	X1198	G1103	X998	V904	H795	A685	T488	Q384	V294	R195
PRO	V1712	Q1508	D1310	X1199	G1104	X999	F915	P796	S686	T489	T389	L301	R195
GLY	V1713	Q1508	F1311	V1416	R1105	X999	F915	Q797	G687	L490	T389	L301	R195
PRO	G1713	Q1508	F1311	V1416	R1105	X999	F915	Q797	G687	L490	T389	L301	R195
ALA	L1714	D1511	R1312	X1204	C1106	X1000	L924	P798	R688	Q500	V390	L305	I198
PRO	P1622	D1511	R1313	X1205	X1206	X1001	L924	P799	R688	Q500	V390	L305	I198
ASP	T1623	D1514	T1420	X1206	F1110	X1002	A928	E803	O694	V501	P393	E306	G202
ASP	T1624	D1514	R1314	X1207	F1111	X1003	A928	E803	O694	V501	P393	E306	G202
ASP	L1625	V1519	D1315	X1207	F1111	X1003	A928	E803	O694	V501	P393	E306	G202
ILE	V1724	V1519	F1422	X1210	E1120	X1008	A928	E803	O694	V501	P393	E306	G202
THR	S1725	F1629	G1317	X1212	A1117	X1005	X930	A808	E697	R505	E395	R311	R204
PHE	F1629	F1629	G1317	X1212	A1117	X1005	X930	A808	E697	R505	E395	R311	R204
ASP	I1633	L1580	I1318	X1213	A1118	X1006	X931	A808	E697	R505	E395	R311	R204
ALA	R1634	E1532	D1319	X1215	E1120	X1007	A928	E803	O694	V501	P393	E306	G202
ALA	V1731	V1533	D1319	X1215	E1120	X1007	A928	E803	O694	V501	P393	E306	G202
ASP	N1733	N1534	V1430	A1431	F1123	X1010	X935	E817	A701	R511	P405	V315	R205
ASP	P1637	N1534	V1430	A1431	F1123	X1010	X935	E817	A701	R511	P405	V315	R205
ALA	P1638	F1535	V1324	X1218	P1124	X1011	X936	E817	A701	R511	P405	V315	R205
ALA	S1734	F1638	V1324	X1218	P1124	X1011	X936	E817	A701	R511	P405	V315	R205
THR	E1735	N1536	L1325	X1219	V1125	X1012	X937	L826	L709	P516	V407	G316	V210
VAL	R1736	L1537	E1326	X1220	I1126	X1013	X938	L827	A713	D518	L410	G328	T211
ALA	T1651	G1538	V1327	X1221	E1127	X1014	X939	L827	A713	D518	L410	G328	T211
LEU	V1652	G1539	S1328	X1224	G1128	X1017	X940	D832	A716	V521	D412	L330	V232
ALA	S1429	G1539	S1328	X1224	G1128	X1017	X940	D832	A716	V521	D412	L330	V232
ILE	S1540	Q1541	A1329	X1225	L1129	R1018	X941	A833	V719	S523	V415	K336	L233
ALA	Q1541	Q1541	A1329	X1225	L1129	R1018	X941	A833	V719	S523	V415	K336	L233
LEU	P1657	Y1542	R1330	X1226	L1132	F1019	X943	T635	K735	I526	L416	E339	V236
SER	K1658	A1543	I1449	X1227	V1133	F1019	X943	T635	K735	I526	L416	E339	V236
ALA	E1659	I1544	I1449	X1227	V1133	F1019	X943	T635	K735	I526	L416	E339	V236
LYS	L1660	I1544	V1336	V1228	P1146	T1021	L957	V837	P736	D534	T419	T341	V237
MET	C1661	L1551	M1337	V1228	P1146	T1021	L957	V837	P736	D534	T419	T341	V237

ALA	I1703	V1408	K1304	A1193	T1096	X989	L787	V676	H584	L479	V376	D288	L179
ALA	G1704			I1194	V1097	X990		G676	H585	R483	P377	P289	A180
PRO	V1705	H1412	D1307	R1196	P1098	X991	T895	A680	S586	R483		P289	A181
ALA	K1706	P1413	Q1308	X1197	D1100	X992	A899	A681	N587	R381		V292	L181
ALA	S1707	R1503	R1309	X1198	V1103	X993	A899	N682	E588			E293	Q183
PRO	T1710	R1504	D1310	X1199	V1104	X994	G900	G683	D589	Q384		V294	L184
SER	P1616	G1415	F1311		G1104	X995	L901	M684	L590			L301	R195
GLY	H1617	V1416	F1312	X1204	G1105	X996	V904	A685	L593	T389		L301	R195
PRO	L1618	L1417	R1312	X1205	C1106	X997	H795	G686	L594	V390		I305	I198
PRO	V1619	T1420	D1314	X1206	F1110	X998	F915	G687	L595	V393		I307	G202
ARG	P1620	Q1421	R1315	X1207	V1110	X1000	L924	R688		P394		I307	D203
PRO	D1511	F1422	V1316		F1111	X1001			V598	V501		W311	R204
ASP	D1514	T1423	G1317	X1212		X1002	A928	D684	R602		W400		P205
ASP	V1519	Q1424	I1318	A1213	A1117	X1003	X929	L695	R504	R505		T314	P206
THR	L1625	V1425	D1319	X1214	A1118	X1004	X930	H696	N606			V315	N207
PHE	L1530		V1320	X1215	T1119	X1005	X931	E697				G316	V208
ALA	E1531	V1430	E1323	X1216	E1120	X1006	X932	L698	Q508	T406		L317	S209
ALA	L1532	A1431	E1324	X1217	F1123	X1007	X933	D699	R511	V407		E327	V210
ALA	V1533	V1324	V1324	X1218	F1124	X1008	X934	A701		V403			T211
ASP	N1534	V1435	L1325	A1219	P1124	X1009	X935		A515			S328	
ALA	A1639	F1535	E1326	X1220	V1125	X1010	X936	L709	P516	L410		I329	L222
THR	E1735	Q1441	V1327	X1221	I1126	X1011	X937		I517	D412		L330	
VAL	R1736	L1537	S1328		E1127	X1012	X938	A713	D518				V232
ALA	W1652	V1445	A1329	X1224	G1128	X1013	X938					W336	L233
LEU			R1330	X1225	L1129	X1014	X939	A716	V624	V415			V236
ILE	L1741	A1448	I1331	X1226			X940	L416	L625	L416			V236
ALA	D1745	I1449	V1336	X1227	L1132	I1017	X941	V521	V521	V521		E339	
LEU		A1450	V1337	V1228	V1133	R1018	X942	S523	S523			I340	L237
SER			M1337			F1019	X943	V719	N629			T341	S238
LYS	ASP	V1455	A1338	R1237	P1146	T1020	X944	K735	P636	I526		E342	
LYS	PRO	G1456	A1339		L1147	L1021		F736	L437			L343	T248
MET	GLU	E1457		R1253	E1147		L957	Y737	M638	D534		H344	T249
ARG	GLU	E1458	R1342	G1268	P1149	V1025	R961	T745	D641	E538		A348	T251
ILE	GLU	T1459	L1343	M1269	E1151	E1034	M962	Y746	G642			R349	
ASN	PRO	A1460	A1344	W1270	E1151	V1035	S963	L747	I643	N540		W350	L255
GLN	GLU	L1461	A1345	L1271	T1162	D1036	V964	Q748	L644	E541		I351	S256
ILE	ALA	A1462	P1346		D1163	D1037	S965	W749		V542		L352	R257
GLU	ASP	C1463			T1164		S965	W750	T647	G543		D353	
ALA	GLU	V1464	Y1350	A1274	G1167	V1045	V967	L751		I544		L354	L260
LEU	PRO	V1467	A1351	A1275		L1046		L756	E654	S545		G355	A266
ASP	THR	Y1468	P1352	Q1276	R1168				A655	H546		P356	A266
SER	ALA	E1469	P1353	H1277		V1068	A971		T657			G357	E267
ILE	ALA	L1470	I1357	V1279	P1171			S763		F549		D358	A266
GLU	PRO	E1471	Q1358	T1280	V1172	W1072	X974	D766	S658	R550		L360	E269
ILE	ALA		M1362	A1281	V1174	V1077	X975			P551		L360	E270
THR	GLU	L1474		T1282			X976	S873	V661		N450	T361	A271
ASP	ALA		D1283	D1283			X977	K768	K662	S559		R362	E272
GLY	ALA	R1480	V1376	G1284	R1177	T1084	X978	S875	G663	V560		L363	R273
ALA	PRO			K1285	N1178		X979	L775	L664		E456	T364	
SER	ALA	K1483	A1380	P1286	N1179	F1087	X980	D776		I563		A365	K276
SER	ALA	D1381	V1287	V1287	A1179	G1088	X981	T777	V666		G461	P366	L277
ARG	ALA	H1485	P1288	L1184	L1184	A1089	X982	T778	E667	H575	Q462	V367	
ARG	ALA	S1391	P1289	L1185	L1185	P1090	X983	W779	T668			I368	G280
ASN	ALA	I1487	A1290	L1188		L1091	X984	R780	K669	E577	F468	R369	G281
GLN	PRO	V1488	K1291	L1188	L1188	A1092	X985	D781	G670			I373	V282
LEU	ALA	F1489	L1292	P1093		P1093	X986	R782	T671	R580		G374	V286
LEU	PRO	R1490	T1401	X987	R1191	T1094	X987	F783		E476		I375	F287
VAL	VAL	D1491	A1405	W1295	F1192	L1095	X988	E784	N674				



- Molecule 1: FATTY ACID SYNTHASE

Chain C:






G2992	L2906	A2911	R2916	G2919	R2920	P2921	L2922	F2923	L2924	V2925	S2926	Q2927	L2930	K2935	G2936	A2939	V2940	F2941	Q2942	M2943	M3051	L2946	G2947	Q2948	R2951	V2954	I2955	P2956	P2957	R2958	R2959	S2960	L2961	D2962	D2966	V2976	R2977	R2978	E2979	P2980	L2983	R2984	G2985	K2986	F2987	P2988	L2989								
R2808	L2809	G2810	F2811	L2812	Q2815	L2820	L2821	L2822	A2823	R2824	L2827	A2828	L2829	K2830	M2831	G2832	L2833	P2834	V2835	Q2843	S2844	F2845	A2846	L2847	G2848	G2859	A2860	L2861	T2871	L2876	L2879	G2880	V2881	G2882	A2883	D2884	D2885	I2886	L2889	S2890	K2891	H2892	L2893	T2894	S2895	T2896	P2901	N2902	E2903						
Q2711	E2712	V2713	V2717	V2718	V2722	V2727	Y2730	P2736	C2740	A2741	T2742	A2743	S2746	V2751	L2754	L2759	L2762	L2763	A2764	G2765	D2768	D2769	L2770	E2773	L2776	G2779	T2784	A2785	D2786	T2787	E2788	M2789	M2790	R2791	K2799	D2800	S2801	R2802	D2805	R2806	R2807														
P2612	R2613	K2614	L2617	S2618	R2619	T2620	V2621	G2622	A2623	Q2624	L2625	D2630	P2631	T2632	V2633	D2645	R2646	V2647	A2648	L2649	L2650	V2651	N2651	S2662	P2666	T2667	W2672	A2679	S2680	T2681	M2686	T2690	S2691	M2692	Q2693	T2694	M2695	Y2696	H2697	G2698	R2699	L2700	A2704	K2705	P2706	I2709	L2710								
M2481	E2482	V2483	L2487	V2492	L2495	K2503	W2504	E2505	W2512	Y2513	L2520	V2521	F2522	E2523	C2524	E2526	L2526	V2527	E2528	X2431	Y2530	R2541	E2542	F2543	P2551	D2552	H2553	A2554	L2557	L2558	E2574	F2580	D2584	P2585	E2586	R2591	P2592	W2599	G2470	P2471	Y2472	R2603	V2610	V2611											
L2398	T2401	K2402	I2403	D2404	M2405	L2408	A2409	A2412	M2416	S2417	G2418	D2421	X2422	X2425	X2426	X2427	X2428	X2429	X2430	X2431	X2432	X2433	X2434	X2435	X2436	X2437	X2442	X2443	X2444	X2445	X2448	X2449	X2450	X2451	X2452	X2453	D2454	A2458	V2461	V2462	E2468	L2469	G2470	P2471	Y2472	R2478									
D2136	E2137	V2140	V2141	T2163	V2164	I2165	T2167	R2170	D2173	D2174	R2175	L2176	K2180	R2188	F2189	T2192	L2193	V2194	T2196	P2197	A2198	R2199	M2200	D2205	L2209	V2210	E2211	W2212	V2213	G2214	T2215	E2216	K2229	P2234	T2235	L2236	L2237	F2238	R2244	V2245	A2246	V2252	R2255												
K2261	W2265	I2265	Q2268	L2274	I2277	R2286	L2287	H2288	L2291	S2294	P2295	R2296	G2298	M2299	F2300	D2303	Y2306	K2310	R2319	S2331	L2332	H2334	W2339	Q2348	L2352	V2353	S2354	E2358	V2361	W2372	L2376	K2391	V2392	D2393	L2394	T2395	R2399	R2478																	
L2070	E2074	X2077	X2078	X2079	X2080	X2081	X2082	X2083	X2084	X2085	X2086	X2087	X2088	X2089	X2090	X2091	X2092	X2093	X2094	X2095	X2096	X2097	X2098	X2099	X2100	X2101	X2102	X2103	X2104	X2105	X2106	X2107	X2108	X2112	X2113	X2114	X2115	X2116	X2117	X2118	X2119	X2120	X2121	X2122	X2123	X2124	X2125	X2126	X2127	X2128	X2129	X2130	X2131	X2132	X2135
VAL	ALA	ARG	ARG	GLY	ILE	SER	VAL	PRO	ALA	PRO	SER	ALA	ALA	LYS	HIS	THR	THR	GLY	VAL	ASP	S1983	L1986	F1989	K1992	P1996	L2000	Q2010	L2011	G2012	L2013	S2014	D2015	V2016	P2020	T2047	A2053	V2054	V2055	F2056	D2057	R2058	W2059	W2060	R2064	L2067										
GLU	ARG	VAL	THR	LYS	THR	TRP	GLU	LEU	GLY	PRO	GLY	ALA	ALA	LYS	HIS	VAL	THR	VAL	PHE	VAL	ASP	THR	LYS	LEU	ALA	ARG	GLY	ASP	LEU	GLY	SER	GLY	ALA	THR	ALA	VAL	ASP	VAL	ASP	LYS	VAL	ILE	LYS	ARG	PRO	ALA	TYR	ILE	ALA						
SER	GLU	LEU	ASN	LEU	GLY	ALA	ILE	ASP	GLY	ALA	ALA	ALA	ASP	LEU	GLY	ALA	LYS	GLY	GLN	VAL	THR	LYS	LEU	ALA	ARG	PHE	GLY	PRO	VAL	LEU	GLY	SER	THR	ALA	THR	ALA	VAL	ASP	VAL	ASP	LYS	VAL	ILE	LYS	ARG	PRO	ALA	TYR	ILE	ALA					

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	106884	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON I (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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.24	0/20319	0.48	0/27667
1	B	0.24	0/20319	0.48	0/27667
1	C	0.24	0/20319	0.48	0/27667
1	D	0.24	0/20319	0.48	0/27667
1	E	0.24	0/20319	0.48	0/27667
1	F	0.24	0/20319	0.48	0/27667
All	All	0.24	0/121914	0.48	0/166002

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	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
All	All	0	30

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1148	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	D	150	THR	Peptide
1	D	202	GLY	Peptide
1	D	2584	ASP	Peptide
1	D	357	GLY	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	21020	0	20990	1056	0
1	B	21020	0	20990	1067	0
1	C	21020	0	20990	1051	0
1	D	21020	0	20990	0	0
1	E	21020	0	20990	0	0
1	F	21020	0	20990	0	0
2	A	31	0	19	5	0
2	B	31	0	19	5	0
2	C	31	0	19	4	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
All	All	126306	0	126054	3117	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 25.

The worst 5 of 3117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:O	1:A:2435:UNK:HG2	1.31	1.30
1:B:793:ARG:O	1:B:2435:UNK:HG2	1.31	1.28
1:B:2100:UNK:O	1:B:2103:UNK:HG3	1.36	1.26
1:A:2105:UNK:O	1:A:2108:UNK:HG3	1.34	1.25
1:B:2105:UNK:O	1:B:2108:UNK:HG3	1.34	1.25

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	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	43	81
1	B	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	43	81
1	C	2637/3089 (85%)	2489 (94%)	139 (5%)	9 (0%)	43	81
1	D	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	43	81
1	E	2637/3089 (85%)	2488 (94%)	141 (5%)	8 (0%)	43	81
1	F	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	43	81
All	All	15822/18534 (85%)	14931 (94%)	840 (5%)	51 (0%)	47	81

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1148	GLU
1	E	1148	GLU
1	F	1148	GLU
1	A	1148	GLU
1	B	1148	GLU

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	2076/2264 (92%)	1987 (96%)	89 (4%)	32	61
1	B	2076/2264 (92%)	1986 (96%)	90 (4%)	32	61
1	C	2076/2264 (92%)	1987 (96%)	89 (4%)	32	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	2076/2264 (92%)	1987 (96%)	89 (4%)	32	61
1	E	2076/2264 (92%)	1987 (96%)	89 (4%)	32	61
1	F	2076/2264 (92%)	1987 (96%)	89 (4%)	32	61
All	All	12456/13584 (92%)	11921 (96%)	535 (4%)	36	61

5 of 535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	2303	ASP
1	A	791	GLU
1	C	1564	ILE
1	F	2784	THR
1	A	233	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1355	GLN
1	B	2349	ASN
1	C	2699	ASN
1	B	1582	HIS
1	B	2288	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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
2	FMN	A	4000	-	31,33,33	1.35	4 (12%)	40,50,50	1.58	7 (17%)
2	FMN	B	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.57	7 (17%)
2	FMN	C	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.56	7 (17%)
2	FMN	D	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.57	7 (17%)
2	FMN	E	4000	-	31,33,33	1.36	4 (12%)	40,50,50	1.57	7 (17%)
2	FMN	F	4000	-	31,33,33	1.35	4 (12%)	40,50,50	1.56	7 (17%)

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
2	FMN	A	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	B	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	C	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	D	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	E	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	F	4000	-	-	5/18/18/18	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C4A-N5	3.76	1.38	1.33
2	E	4000	FMN	C4A-N5	3.73	1.38	1.33
2	C	4000	FMN	C4A-N5	3.69	1.38	1.33
2	F	4000	FMN	C4A-N5	3.69	1.38	1.33
2	A	4000	FMN	C4A-N5	3.69	1.38	1.33

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	FMN	C4-N3-C2	5.93	120.15	115.14
2	D	4000	FMN	C4-N3-C2	5.93	120.15	115.14
2	B	4000	FMN	C4-N3-C2	5.91	120.13	115.14
2	E	4000	FMN	C4-N3-C2	5.88	120.11	115.14
2	F	4000	FMN	C4-N3-C2	5.86	120.09	115.14

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4000	FMN	O3'-C3'-C4'-C5'
2	C	4000	FMN	O3'-C3'-C4'-C5'
2	A	4000	FMN	O3'-C3'-C4'-C5'
2	F	4000	FMN	O3'-C3'-C4'-C5'
2	D	4000	FMN	O3'-C3'-C4'-C5'

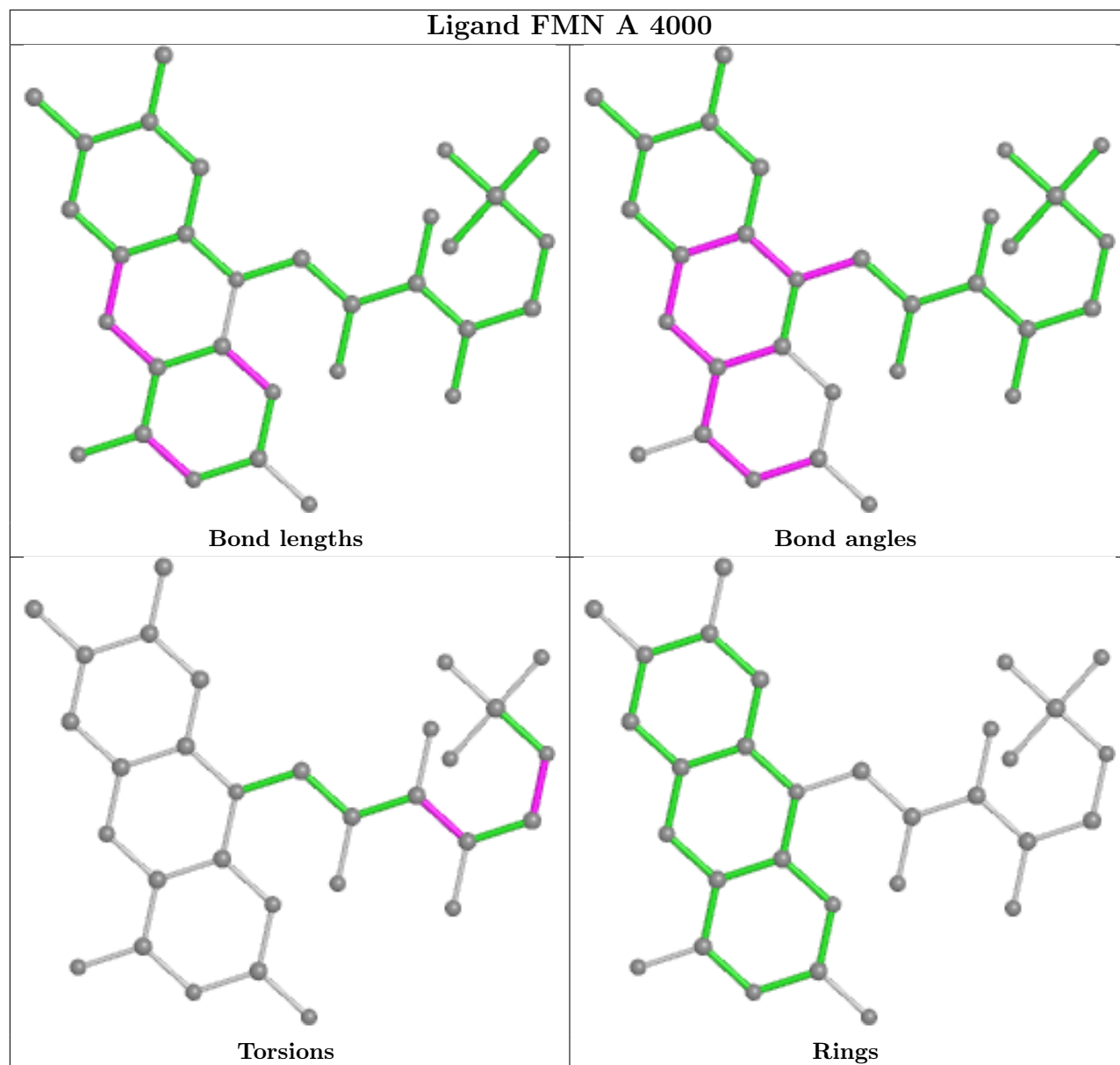
There are no ring outliers.

3 monomers are involved in 14 short contacts:

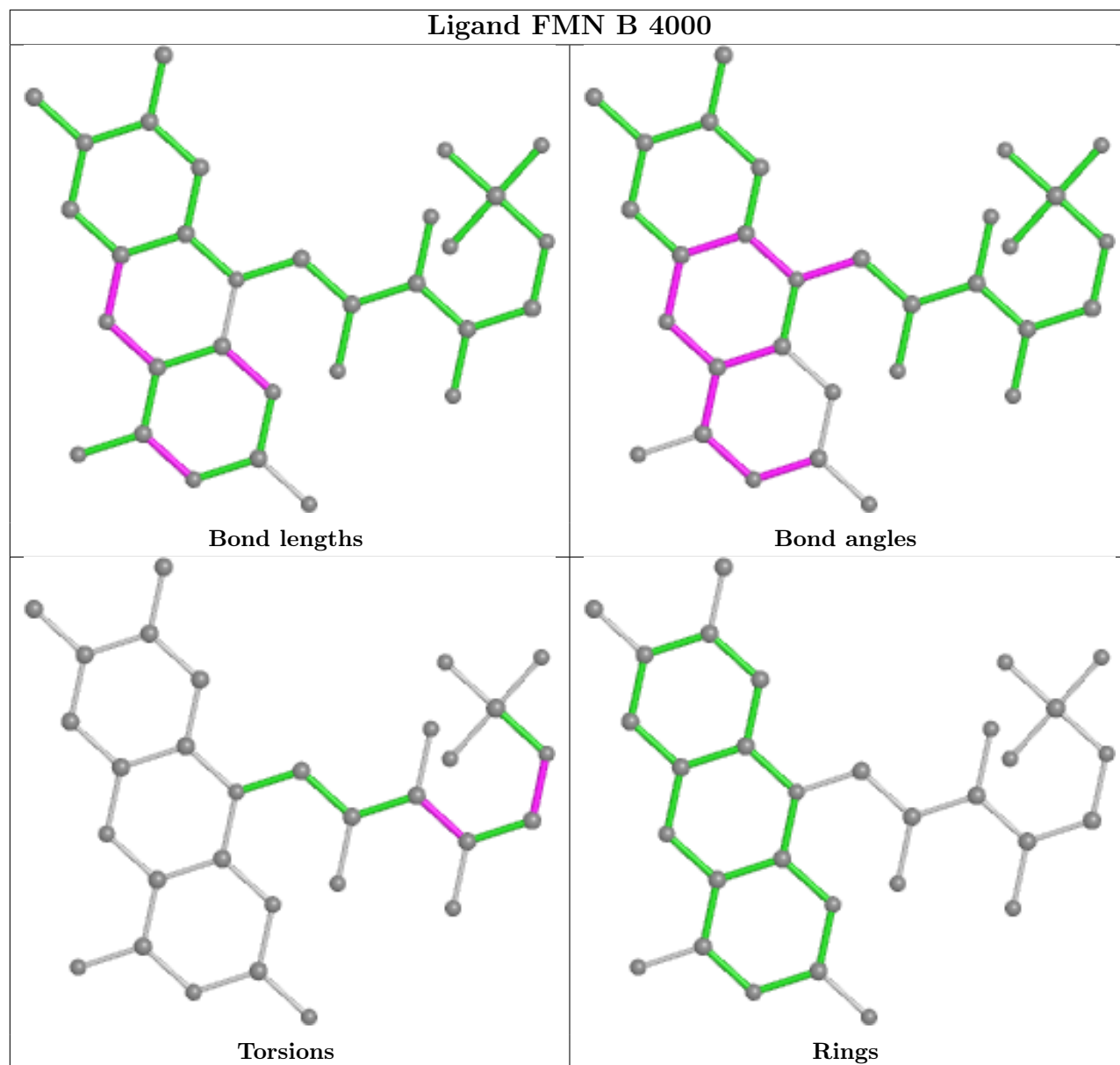
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	FMN	5	0
2	B	4000	FMN	5	0
2	C	4000	FMN	4	0

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.

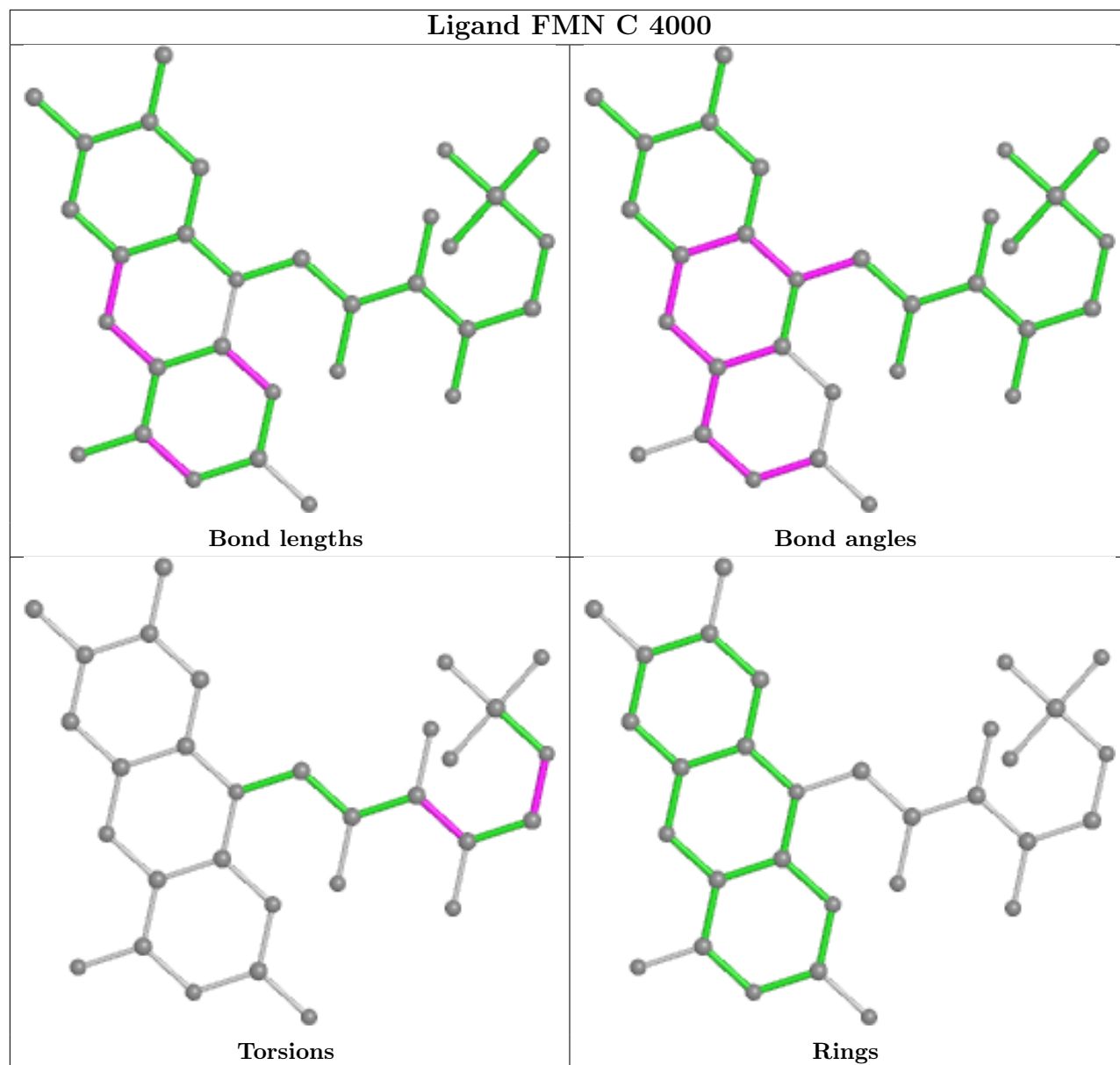
Ligand FMN A 4000



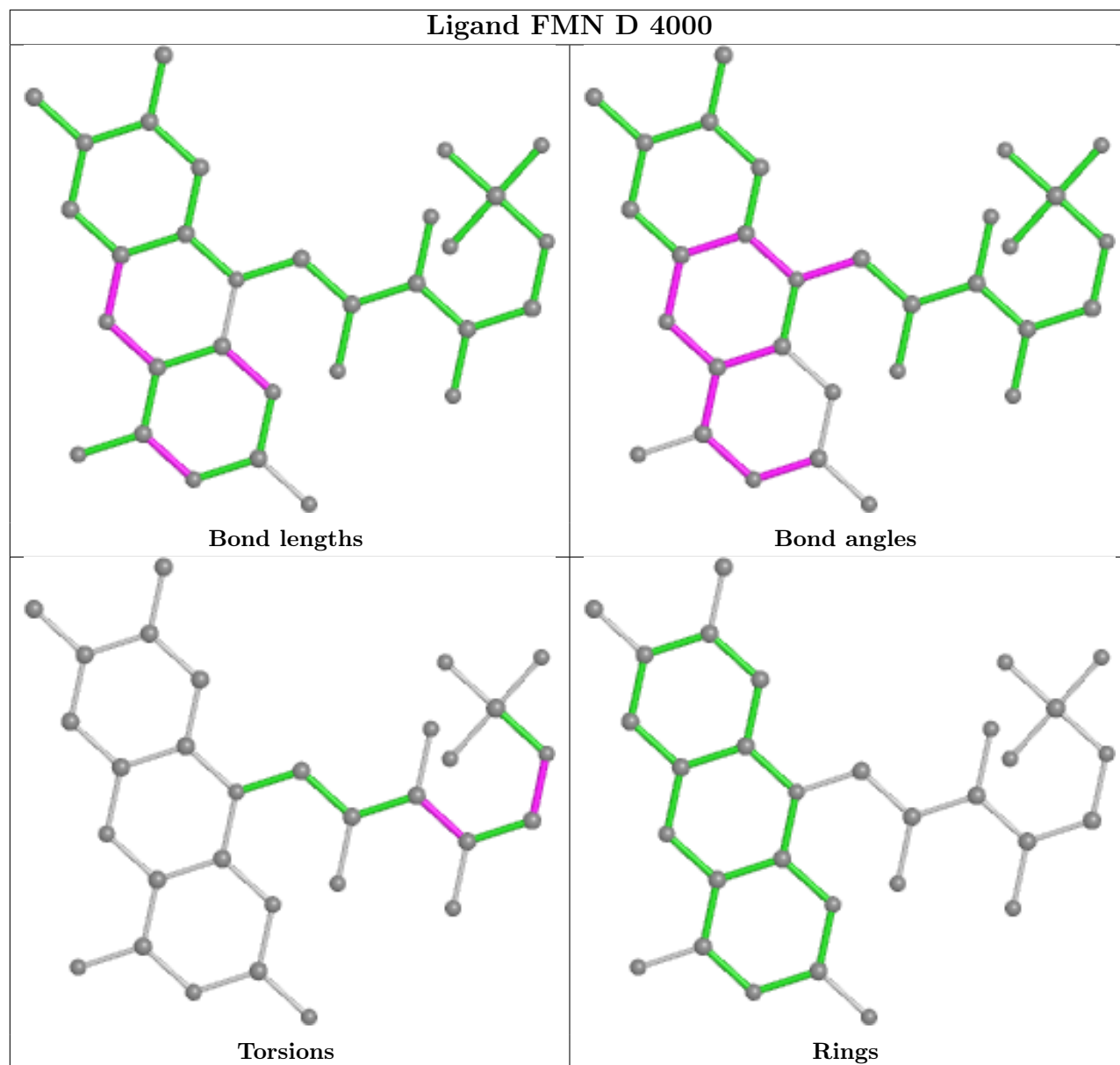
Ligand FMN B 4000



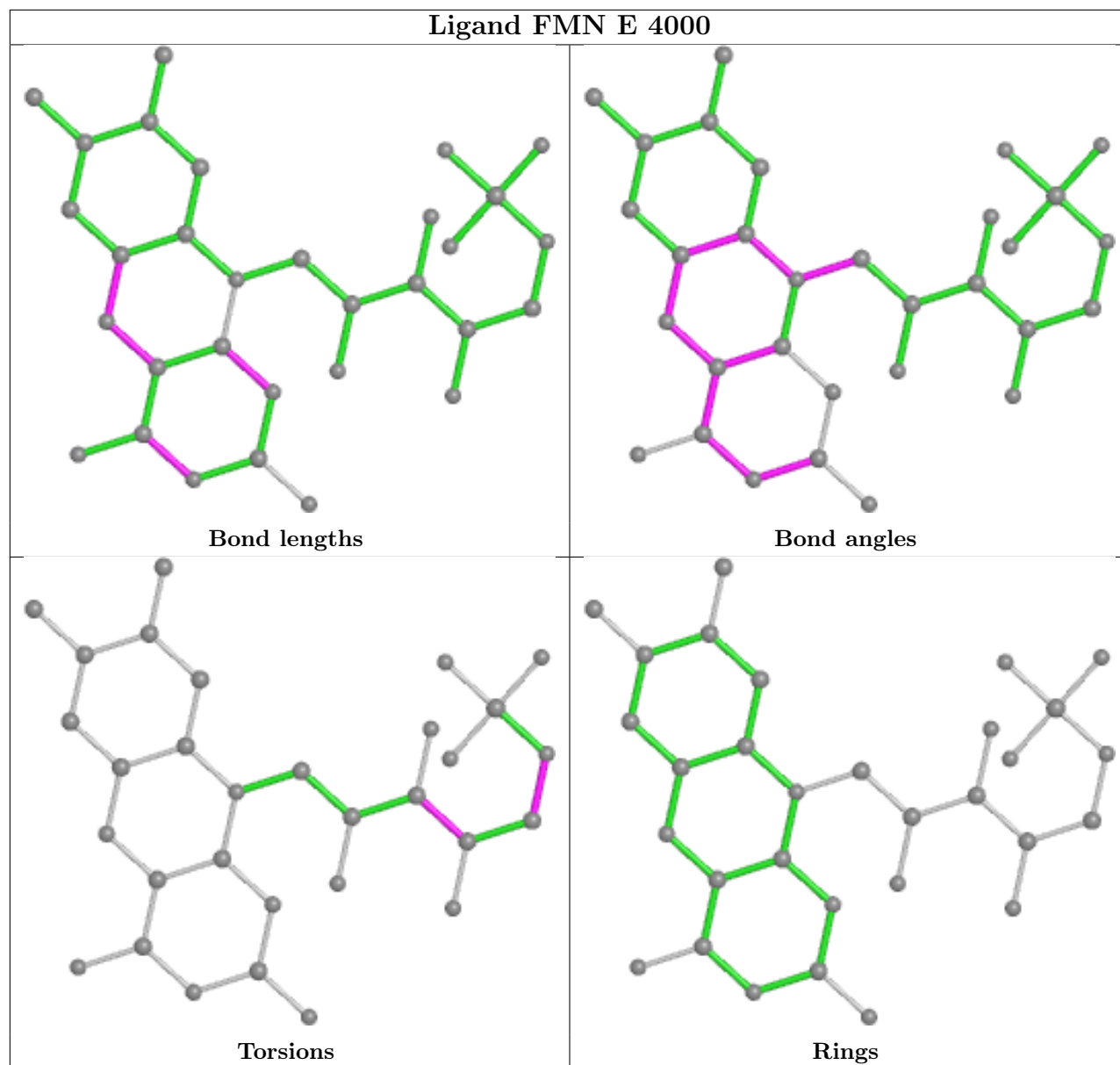
Ligand FMN C 4000

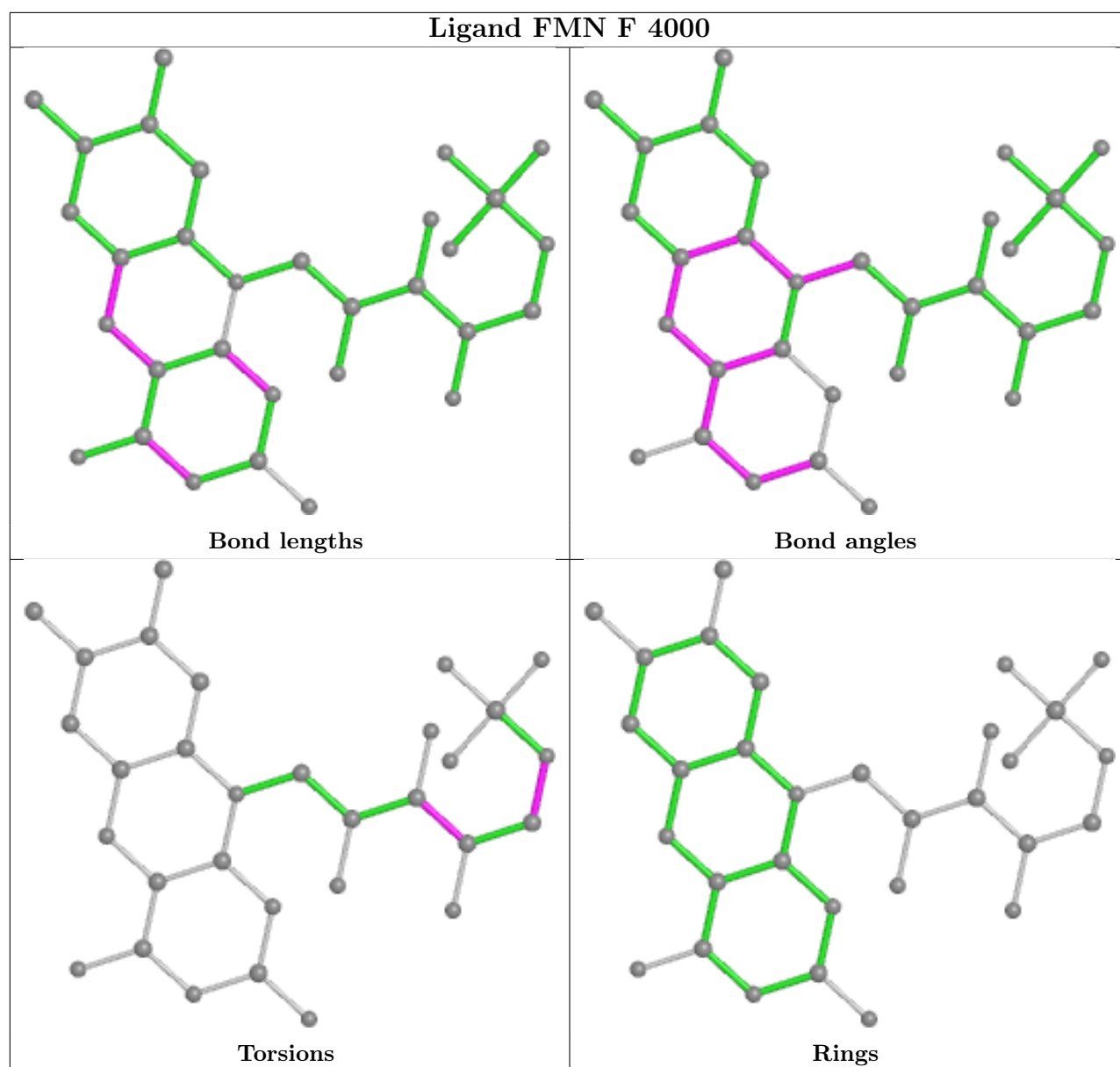


Ligand FMN D 4000



Ligand FMN E 4000





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.