



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:48 am GMT

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 initial model : 2UV8

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

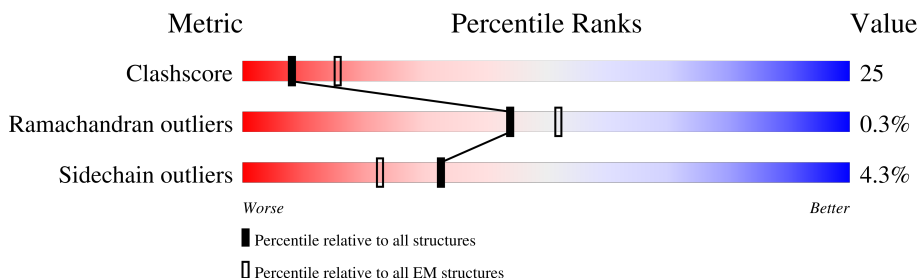
# 1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3089	
1	B	3089	
1	C	3089	
1	D	3089	
1	E	3089	
1	F	3089	

## 2 Entry composition i

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
			Total	C	N	O	S		
1	D	2822	21020	13294	3662	3998	66	0	0
1	E	2822	21020	13294	3662	3998	66	0	0
1	F	2822	21020	13294	3662	3998	66	0	0
1	A	2822	21020	13294	3662	3998	66	0	0
1	B	2822	21020	13294	3662	3998	66	0	0
1	C	2822	21020	13294	3662	3998	66	0	0

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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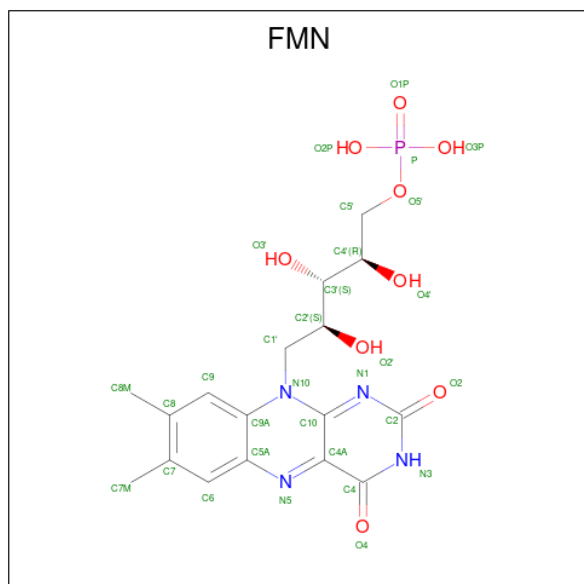
Chain	Residue	Modelled	Actual	Comment	Reference
C	2108	UNK	LEU	conflict	UNP A0R1H7
C	2109	UNK	ALA	conflict	UNP A0R1H7
C	2110	UNK	ALA	conflict	UNP A0R1H7
C	2111	UNK	GLY	conflict	UNP A0R1H7
C	2112	UNK	ARG	conflict	UNP A0R1H7
C	2113	UNK	ASN	conflict	UNP A0R1H7
C	2114	UNK	VAL	conflict	UNP A0R1H7
C	2115	UNK	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: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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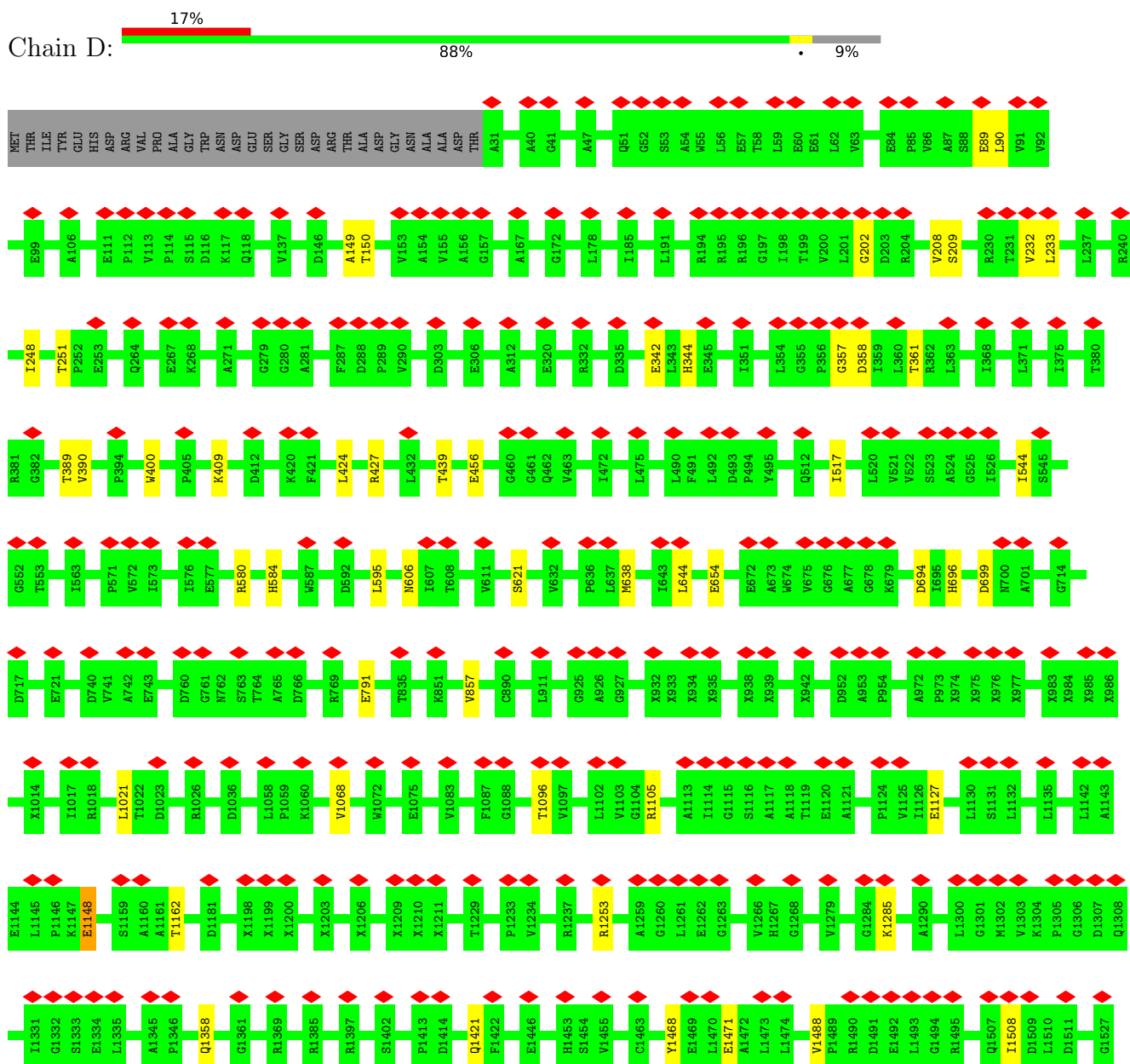
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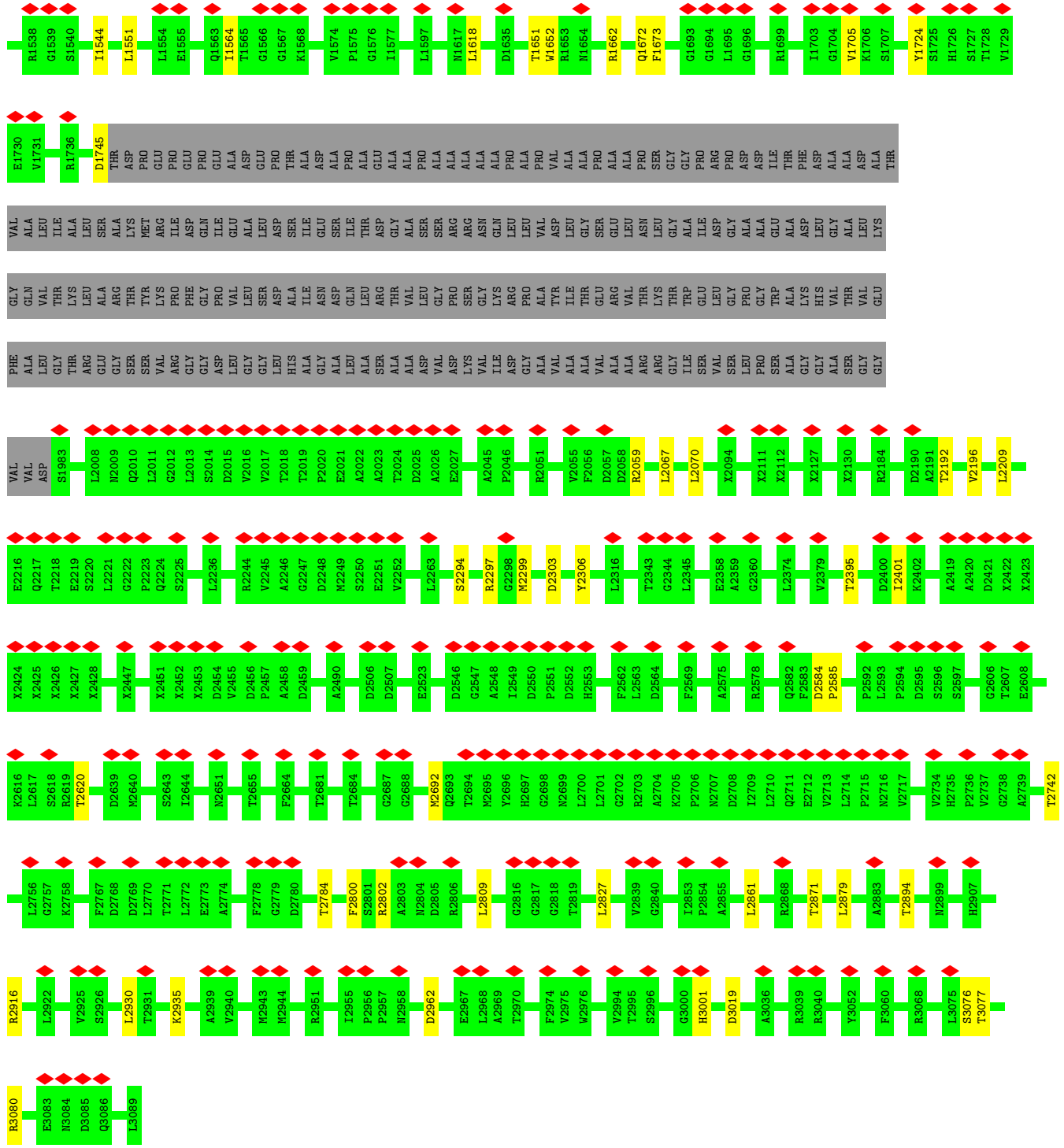
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>AltConf</b>
2	F	1	Total 31	C 17	N 4	O 9	P 1	0
2	A	1	Total 31	C 17	N 4	O 9	P 1	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0

### 3 Residue-property plots

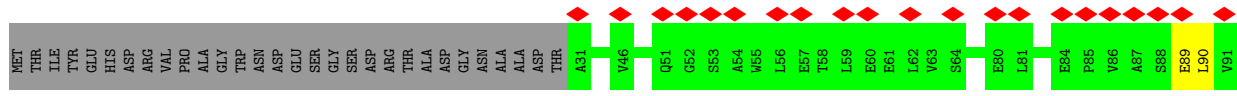
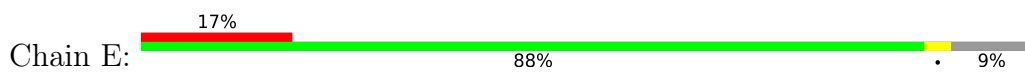
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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





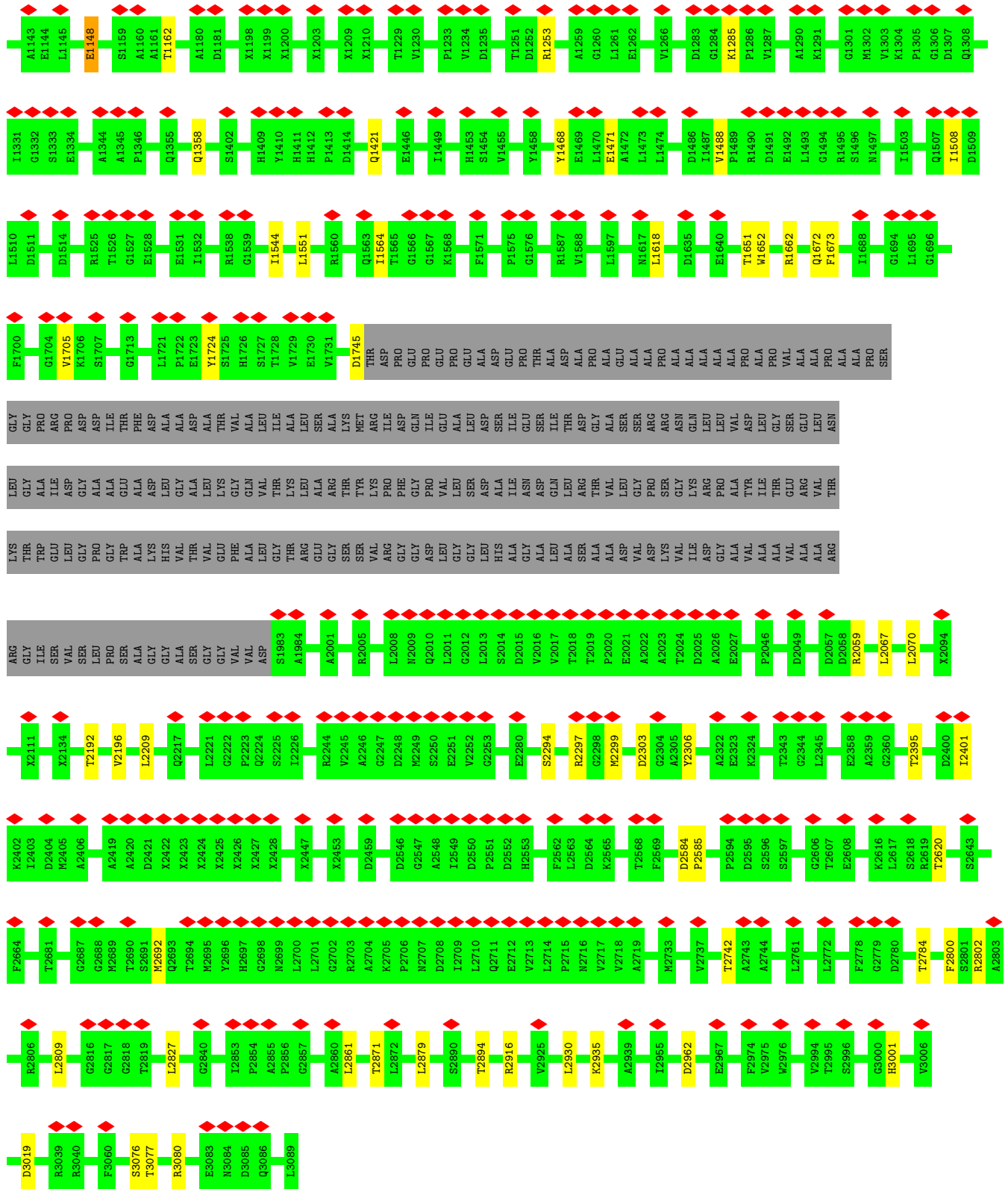
● Molecule 1: FATTY ACID SYNTHASE











• Molecule 1: FATTY ACID SYNTHASE









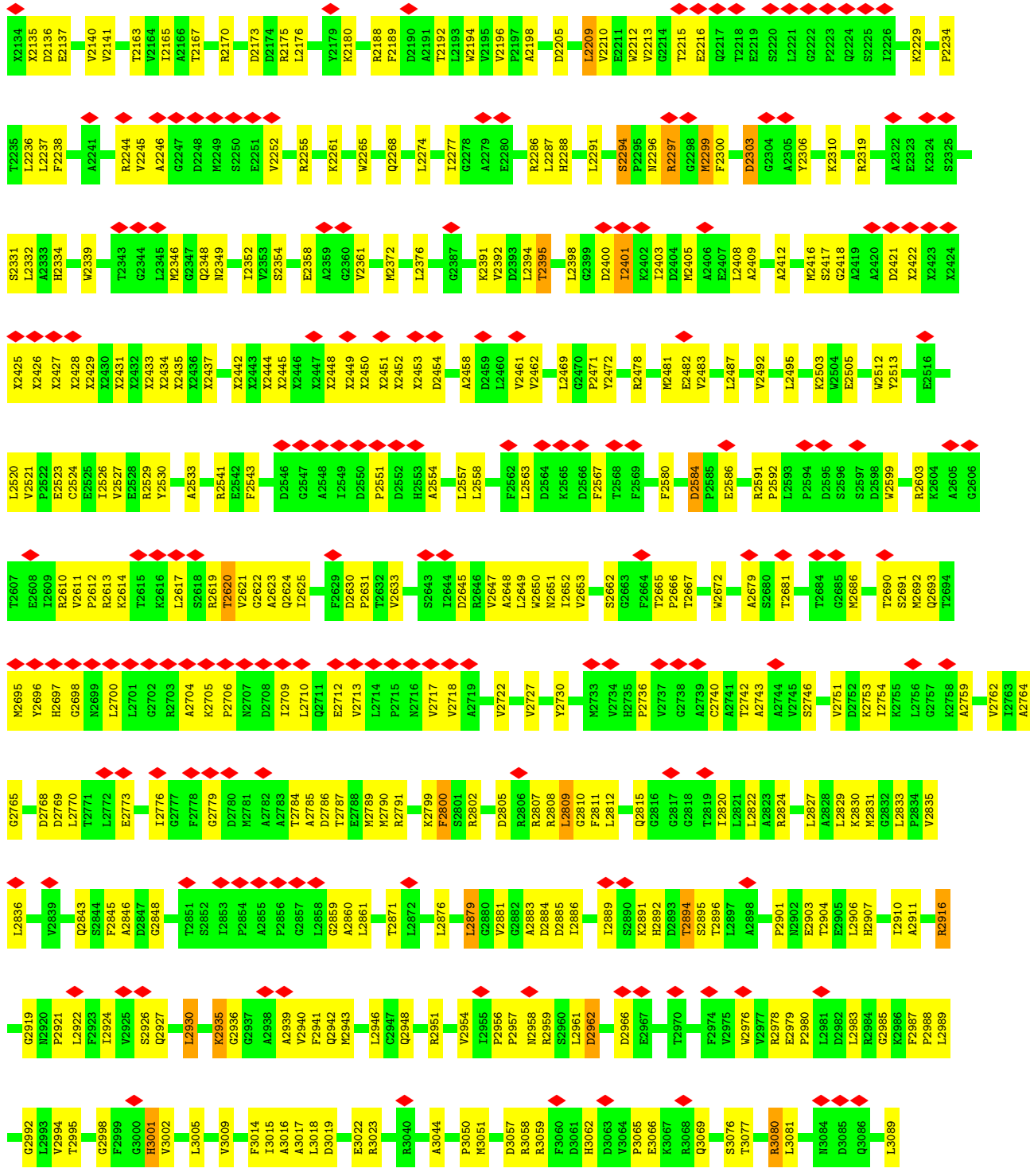
• Molecule 1: FATTY ACID SYNTHASE











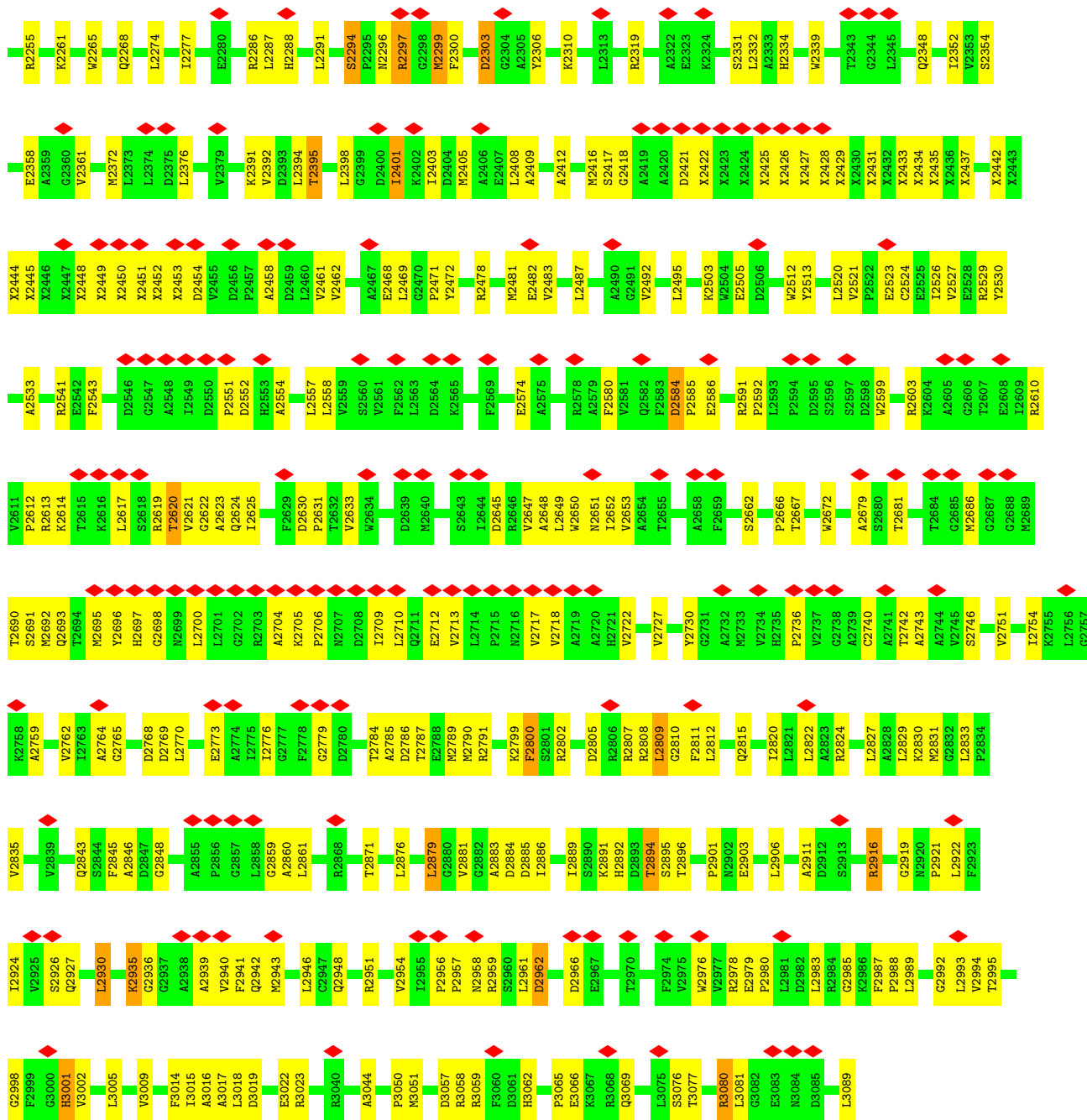
● Molecule 1: FATTY ACID SYNTHASE



MET	G2992	G2919	L2836	G2765	M2695	L2520	X2425	S2331	T2295	G2988	L2930	L3005	L3089
THR	L2993	M2920	V2839	D2768	Y2696	V2521	X2426	L2332	L2236	F2999	K2885	L3009	E60
ILE	V2994	P2921	V2840	D2769	H2697	P2522	X2427	A2333	L2237	G3000	G2937	V3009	E61
GLU	T2995	L2922	Q2843	L2770	G2698	E2523	X2428	F2238	F2237	H3001	A2938	F3014	E62
HIS	G2998	F2923	Q2844	L2771	M2699	E2524	X2429	A2241	A2244	V3002	A2939	I3015	E63
ASP	F2999	L2924	F2845	L2772	G2699	E2525	X2430	R2244	R2244	L3005	V2940	A3016	E64
ARG	G3000	V2925	F2846	L2773	L2700	E2526	X2431	V2244	V2244	L3005	P2941	A3017	E65
VAL	H3001	S2926	D2847	E2773	L2701	V2527	X2432	R2245	R2245	L3005	G2942	A3018	E66
PRO	V3002	S2927	G2848	E2774	G2702	V2528	X2433	A2246	A2246	L3005	M2943	L3019	E67
ALA	L3005	L2930	G2849	L2775	G2703	V2529	X2434	M2466	M2466	L3005	M2944	D3019	E68
GLY	L3005	L2930	G2849	L2776	R2704	A2533	X2435	G2247	D2248	L3005	M2945	E3022	E69
TRP	L3005	L2930	G2849	L2777	A2705	A2533	X2436	G2247	D2248	L3005	M2946	R3023	E70
ASN	L3005	L2930	G2849	L2778	K2705	R2541	X2437	G2247	D2248	L3005	M2947	R3044	E71
ASP	L3005	L2930	G2849	L2779	K2706	R2542	X2438	G2247	D2248	L3005	M2948	A3044	E72
GLU	L3005	L2930	G2849	L2780	P2706	F2543	X2439	G2247	D2248	L3005	M2949	P3050	E73
SER	L3005	L2930	G2849	L2781	M2707	E2542	X2440	G2247	D2248	L3005	M2950	M3051	E74
GLY	L3005	L2930	G2849	L2782	G2708	F2543	X2441	G2247	D2248	L3005	M2951	D3057	E75
SER	L3005	L2930	G2849	L2783	D2708	D2546	X2442	G2247	D2248	L3005	M2952	R3058	E76
ASP	L3005	L2930	G2849	L2784	I2709	G2547	X2443	G2247	D2248	L3005	M2953	R3059	E77
ARG	L3005	L2930	G2849	L2785	I2709	G2547	X2444	G2247	D2248	L3005	M2954	F3060	E78
THR	L3005	L2930	G2849	L2786	G2710	G2547	X2445	G2247	D2248	L3005	M2955	L3061	E79
ALA	L3005	L2930	G2849	L2787	Q2711	G2547	X2446	G2247	D2248	L3005	M2956	H3062	E80
ALA	L3005	L2930	G2849	L2788	E2712	G2547	X2447	G2247	D2248	L3005	M2957	D3063	E81
ASP	L3005	L2930	G2849	L2789	E2713	G2547	X2448	G2247	D2248	L3005	M2958	V3064	E82
THR	L3005	L2930	G2849	L2790	L2714	G2547	X2449	G2247	D2248	L3005	M2959	P3065	E83
GLY	L3005	L2930	G2849	L2791	P2631	D2550	X2450	G2247	D2248	L3005	M2960	E3066	E84
ASN	L3005	L2930	G2849	L2792	V2632	P2551	X2451	G2247	D2248	L3005	M2961	Y44	E85
ALA	L3005	L2930	G2849	L2793	V2633	D2552	X2452	G2247	D2248	L3005	M2962	V46	E86
ASP	L3005	L2930	G2849	L2794	F2629	H2553	X2453	G2247	D2248	L3005	M2963	Q3069	E87
THR	L3005	L2930	G2849	L2795	D2630	A2554	X2454	G2247	D2248	L3005	M2964	S3076	E88
THR	L3005	L2930	G2849	L2796	T2644	L2557	D2454	G2247	D2248	L3005	M2965	T3077	E89
ALA	L3005	L2930	G2849	L2797	D2644	L2558	D2455	G2247	D2248	L3005	M2966	R3080	E90
ASP	L3005	L2930	G2849	L2798	D2645	L2558	D2456	G2247	D2248	L3005	M2967	L3081	E91
THR	L3005	L2930	G2849	L2799	V2647	L2558	D2457	G2247	D2248	L3005	M2968	N3084	E92
ASP	L3005	L2930	G2849	L2800	A2648	F2562	D2458	G2247	D2248	L3005	M2969	D3085	E93
THR	L3005	L2930	G2849	L2801	L2649	L2563	D2459	G2247	D2248	L3005	M2970	L3086	E94
ALA	L3005	L2930	G2849	L2802	L2649	L2563	D2460	G2247	D2248	L3005	M2971	L3089	E95
ASP	L3005	L2930	G2849	L2803	L2650	L2563	D2461	G2247	D2248	L3005	M2972	E96	E96
THR	L3005	L2930	G2849	L2804	L2651	L2563	D2462	G2247	D2248	L3005	M2973	E97	E97
THR	L3005	L2930	G2849	L2805	L2652	L2563	D2463	G2247	D2248	L3005	M2974	E98	E98
ASP	L3005	L2930	G2849	L2806	L2653	L2563	D2464	G2247	D2248	L3005	M2975	E99	E99
THR	L3005	L2930	G2849	L2807	S2662	L2563	D2465	G2247	D2248	L3005	M2976	E100	E100
THR	L3005	L2930	G2849	L2808	G2663	L2563	D2466	G2247	D2248	L3005	M2977	E101	E101
THR	L3005	L2930	G2849	L2809	F2664	L2563	D2467	G2247	D2248	L3005	M2978	E102	E102
THR	L3005	L2930	G2849	L2810	G2665	L2563	D2468	G2247	D2248	L3005	M2979	E103	E103
THR	L3005	L2930	G2849	L2811	T2666	L2563	D2469	G2247	D2248	L3005	M2980	E104	E104
THR	L3005	L2930	G2849	L2812	T2667	L2563	D2470	G2247	D2248	L3005	M2981	E105	E105
THR	L3005	L2930	G2849	L2813	G2668	L2563	D2471	G2247	D2248	L3005	M2982	E106	E106
THR	L3005	L2930	G2849	L2814	F2669	L2563	D2472	G2247	D2248	L3005	M2983	E107	E107
THR	L3005	L2930	G2849	L2815	G2670	L2563	D2473	G2247	D2248	L3005	M2984	E108	E108
THR	L3005	L2930	G2849	L2816	F2671	L2563	D2474	G2247	D2248	L3005	M2985	E109	E109
THR	L3005	L2930	G2849	L2817	G2672	L2563	D2475	G2247	D2248	L3005	M2986	E110	E110
THR	L3005	L2930	G2849	L2818	F2673	L2563	D2476	G2247	D2248	L3005	M2987	E111	E111
THR	L3005	L2930	G2849	L2819	G2674	L2563	D2477	G2247	D2248	L3005	M2988	E112	E112
THR	L3005	L2930	G2849	L2820	G2675	L2563	D2478	G2247	D2248	L3005	M2989	E113	E113
THR	L3005	L2930	G2849	L2821	F2676	L2563	D2479	G2247	D2248	L3005	M2990	E114	E114
THR	L3005	L2930	G2849	L2822	G2677	L2563	D2480	G2247	D2248	L3005	M2991	E115	E115
THR	L3005	L2930	G2849	L2823	A2743	L2563	D2481	G2247	D2248	L3005	M2992	E116	E116
THR	L3005	L2930	G2849	L2824	A2744	L2563	D2482	G2247	D2248	L3005	M2993	E117	E117
THR	L3005	L2930	G2849	L2825	G2745	L2563	D2483	G2247	D2248	L3005	M2994	E118	E118
THR	L3005	L2930	G2849	L2826	G2746	L2563	D2484	G2247	D2248	L3005	M2995	E119	E119
THR	L3005	L2930	G2849	L2827	S2746	L2563	D2485	G2247	D2248	L3005	M2996	E120	E120
THR	L3005	L2930	G2849	L2828	V2751	L2563	D2486	G2247	D2248	L3005	M2997	E121	E121
THR	L3005	L2930	G2849	L2829	D2752	L2563	D2487	G2247	D2248	L3005	M2998	E122	E122
THR	L3005	L2930	G2849	L2830	K2753	L2563	D2488	G2247	D2248	L3005	M2999	E123	E123
THR	L3005	L2930	G2849	L2831	L2754	L2563	D2489	G2247	D2248	L3005	M3000	E124	E124
THR	L3005	L2930	G2849	L2832	L2755	L2563	D2490	G2247	D2248	L3005	M3001	E125	E125
THR	L3005	L2930	G2849	L2833	K2756	L2563	D2491	G2247	D2248	L3005	M3002	E126	E126
THR	L3005	L2930	G2849	L2834	L2757	L2563	D2492	G2247	D2248	L3005	M3003	E127	E127
THR	L3005	L2930	G2849	L2835	G2758	L2563	D2493	G2247	D2248	L3005	M3004	E128	E128
THR	L3005	L2930	G2849	L2836	K2759	L2563	D2494	G2247	D2248	L3005	M3005	E129	E129
THR	L3005	L2930	G2849	L2837	L2758	L2563	D2495	G2247	D2248	L3005	M3006	E130	E130
THR	L3005	L2930	G2849	L2838	G2759	L2563	D2496	G2247	D2248	L3005	M3007	E131	E131
THR	L3005	L2930	G2849	L2839	K2603	L2563	D2497	G2247	D2248	L3005	M3008	E132	E132
THR	L3005	L2930	G2849	L2840	A2604	L2563	D2498	G2247	D2248	L3005	M3009	E133	E133
THR	L3005	L2930	G2849	L2841	A2605	L2563	D2499	G2247	D2248	L3005	M3010	E134	E134
THR	L3005	L2930	G2849	L2842	G2606	L2563	D2500	G2247	D2248	L3005	M3011	E135	E135







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	106884	Depositor
Resolution determination method	Not provided	
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
Maximum map value	14.936	Depositor
Minimum map value	-7.793	Depositor
Average map value	-0.133	Depositor
Map value standard deviation	1.076	Depositor
Recommended contour level	2.7	Depositor
Map size ( $\text{\AA}$ )	392.0, 392.0, 392.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.45, 2.45, 2.45	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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  >5	RMSZ	# Z  >5
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

*Continued on next page...*

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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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	41	77
1	B	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	41	77
1	C	2637/3089 (85%)	2489 (94%)	139 (5%)	9 (0%)	41	77
1	D	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	41	77
1	E	2637/3089 (85%)	2488 (94%)	141 (5%)	8 (0%)	41	77
1	F	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	41	77
All	All	15822/18534 (85%)	14931 (94%)	840 (5%)	51 (0%)	44	77

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 [i](#)

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%)	29	53
1	B	2076/2264 (92%)	1986 (96%)	90 (4%)	29	53
1	C	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53

*Continued on next page...*



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
1	E	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
1	F	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
All	All	12456/13584 (92%)	11921 (96%)	535 (4%)	33	53

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

Mol	Chain	Res	Type
1	C	439	THR
1	C	696	HIS
1	C	427	ARG
1	C	2809	LEU
1	F	427	ARG

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

Mol	Chain	Res	Type
1	C	1582	HIS
1	C	1672	GLN
1	C	2699	ASN
1	B	486	GLN
1	B	386	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 monosaccharides 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	E	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	B	4000	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	F	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
2	FMN	D	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	C	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
2	FMN	A	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C4A-N5	4.13	1.38	1.30
2	E	4000	FMN	C4A-N5	4.11	1.38	1.30
2	F	4000	FMN	C4A-N5	4.08	1.38	1.30
2	C	4000	FMN	C4A-N5	4.08	1.38	1.30
2	D	4000	FMN	C4A-N5	4.08	1.38	1.30

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4000	FMN	C4-N3-C2	-3.01	120.08	125.64
2	F	4000	FMN	C4-N3-C2	-3.00	120.09	125.64
2	E	4000	FMN	C4-N3-C2	-2.99	120.11	125.64
2	B	4000	FMN	C4-N3-C2	-2.98	120.13	125.64
2	D	4000	FMN	C4-N3-C2	-2.97	120.15	125.64

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

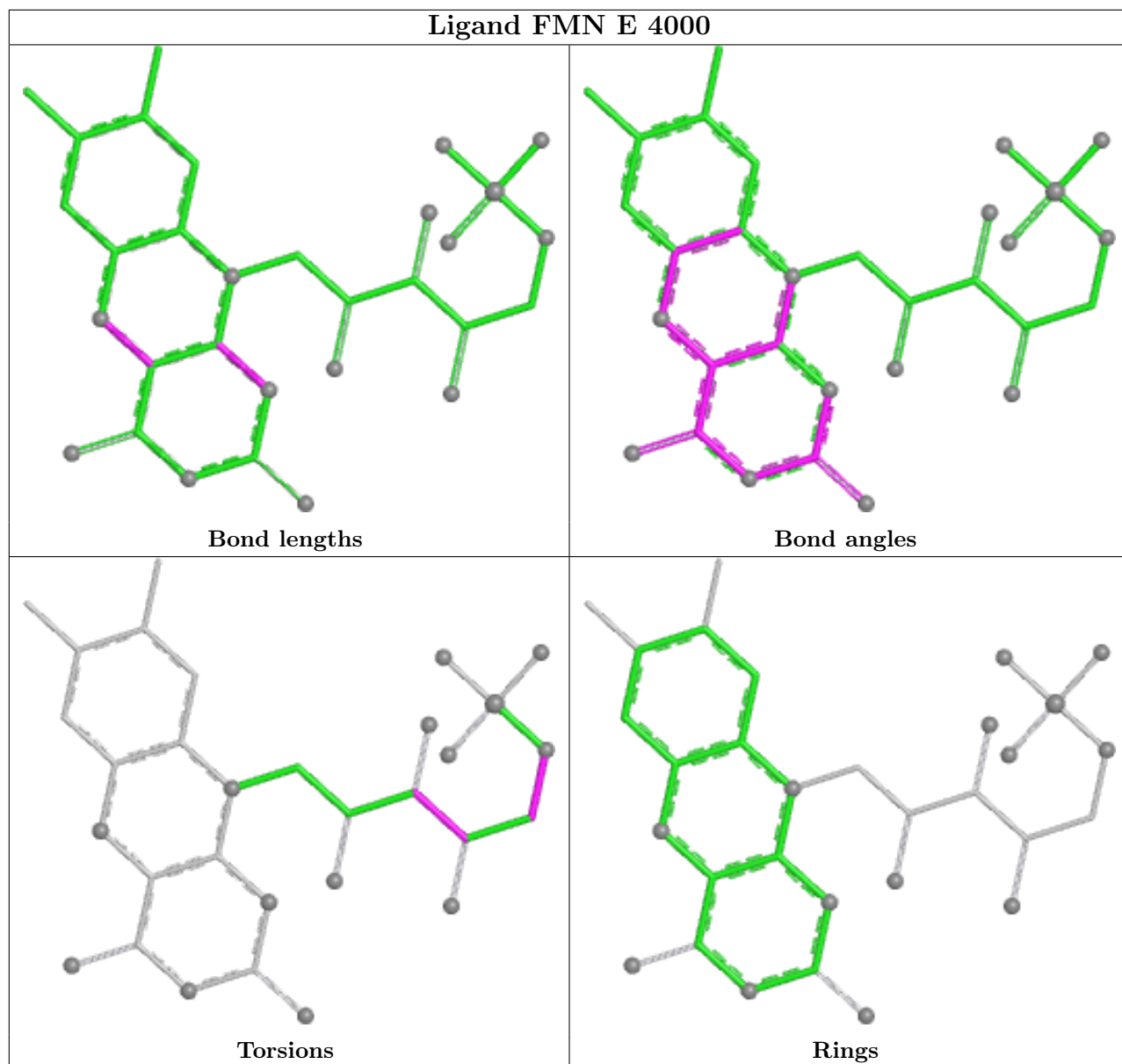
Mol	Chain	Res	Type	Atoms
2	D	4000	FMN	O3'-C3'-C4'-C5'
2	E	4000	FMN	O3'-C3'-C4'-C5'
2	F	4000	FMN	O3'-C3'-C4'-C5'
2	A	4000	FMN	O3'-C3'-C4'-C5'
2	B	4000	FMN	O3'-C3'-C4'-C5'

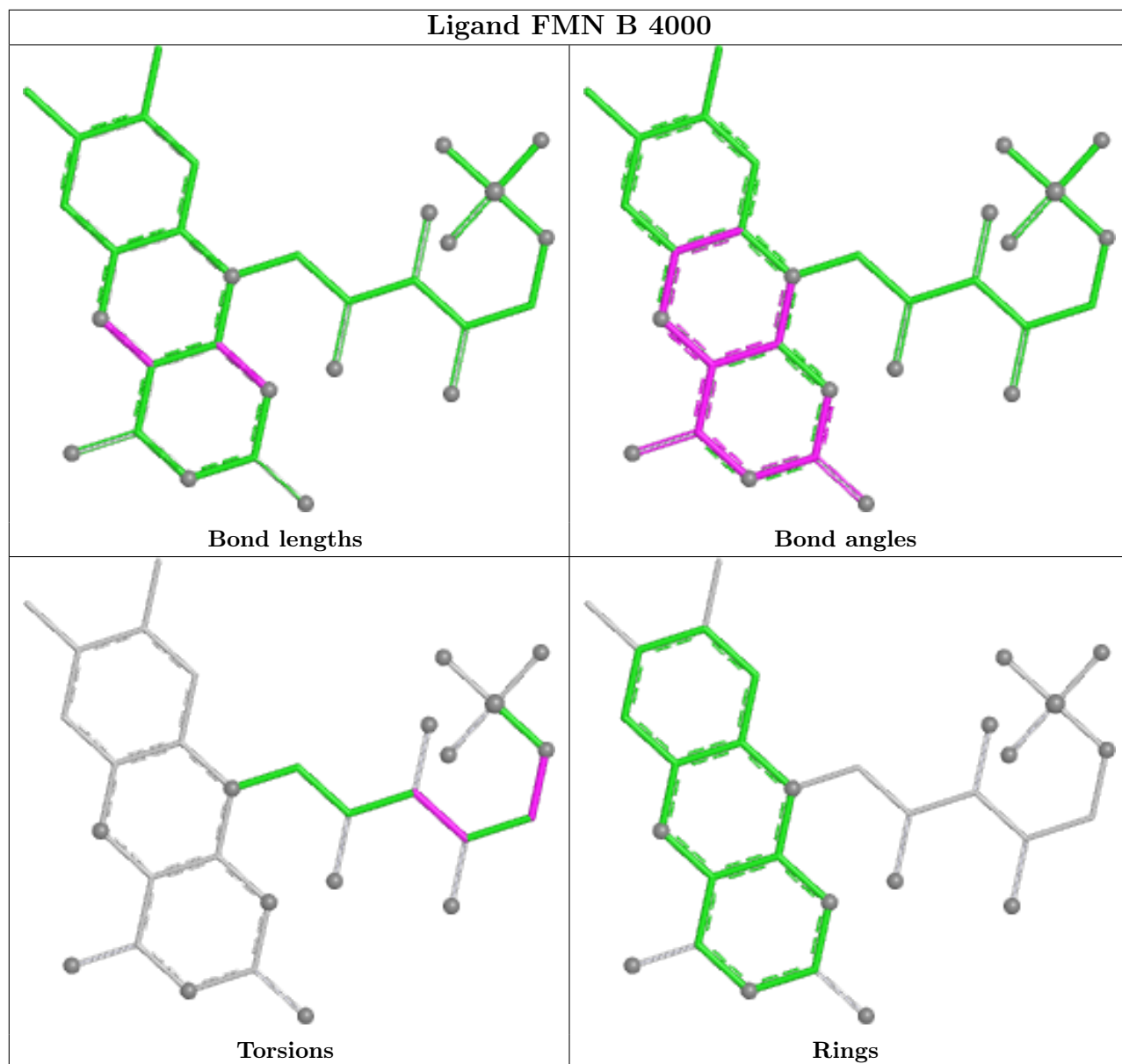
There are no ring outliers.

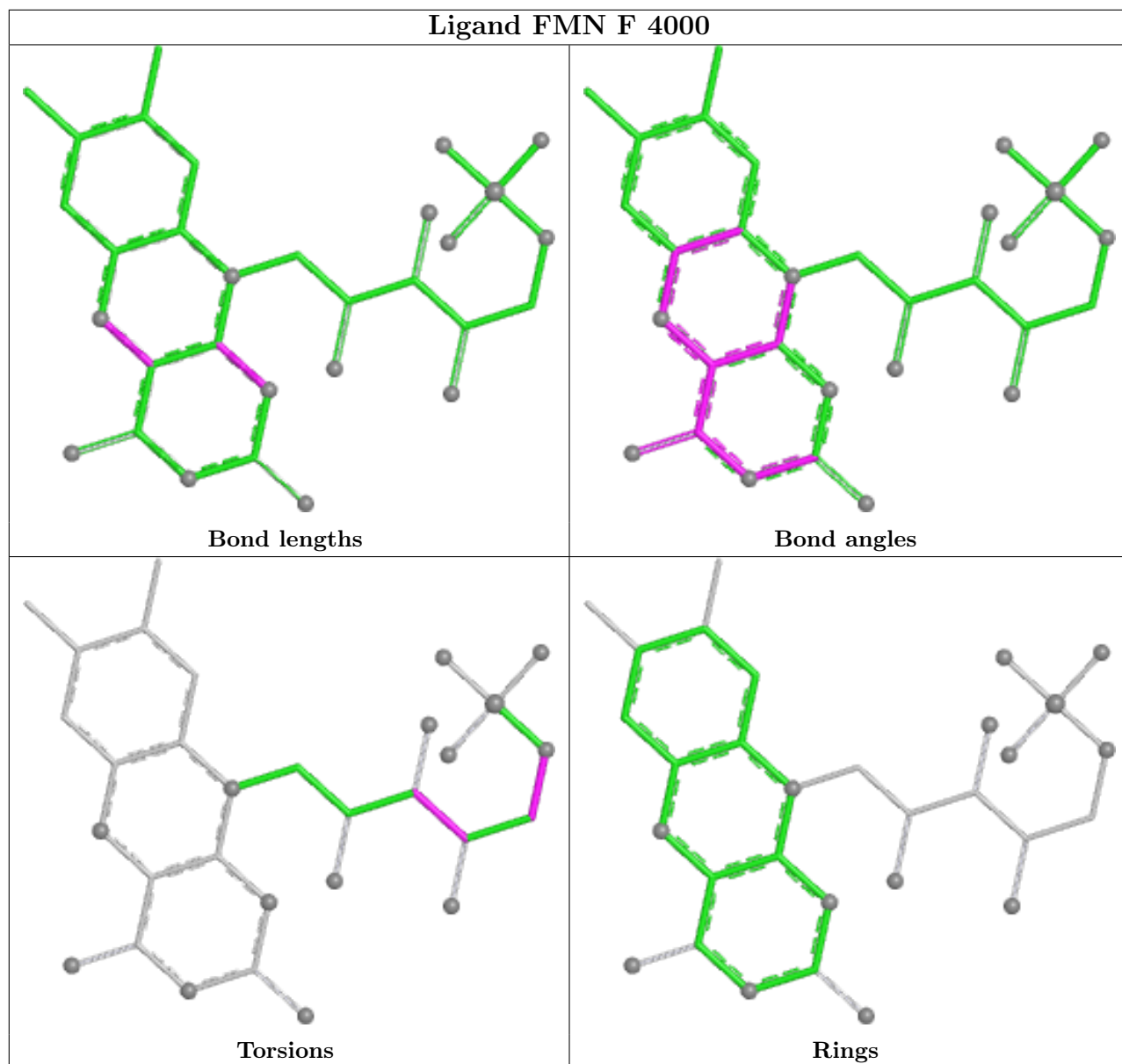
3 monomers are involved in 14 short contacts:

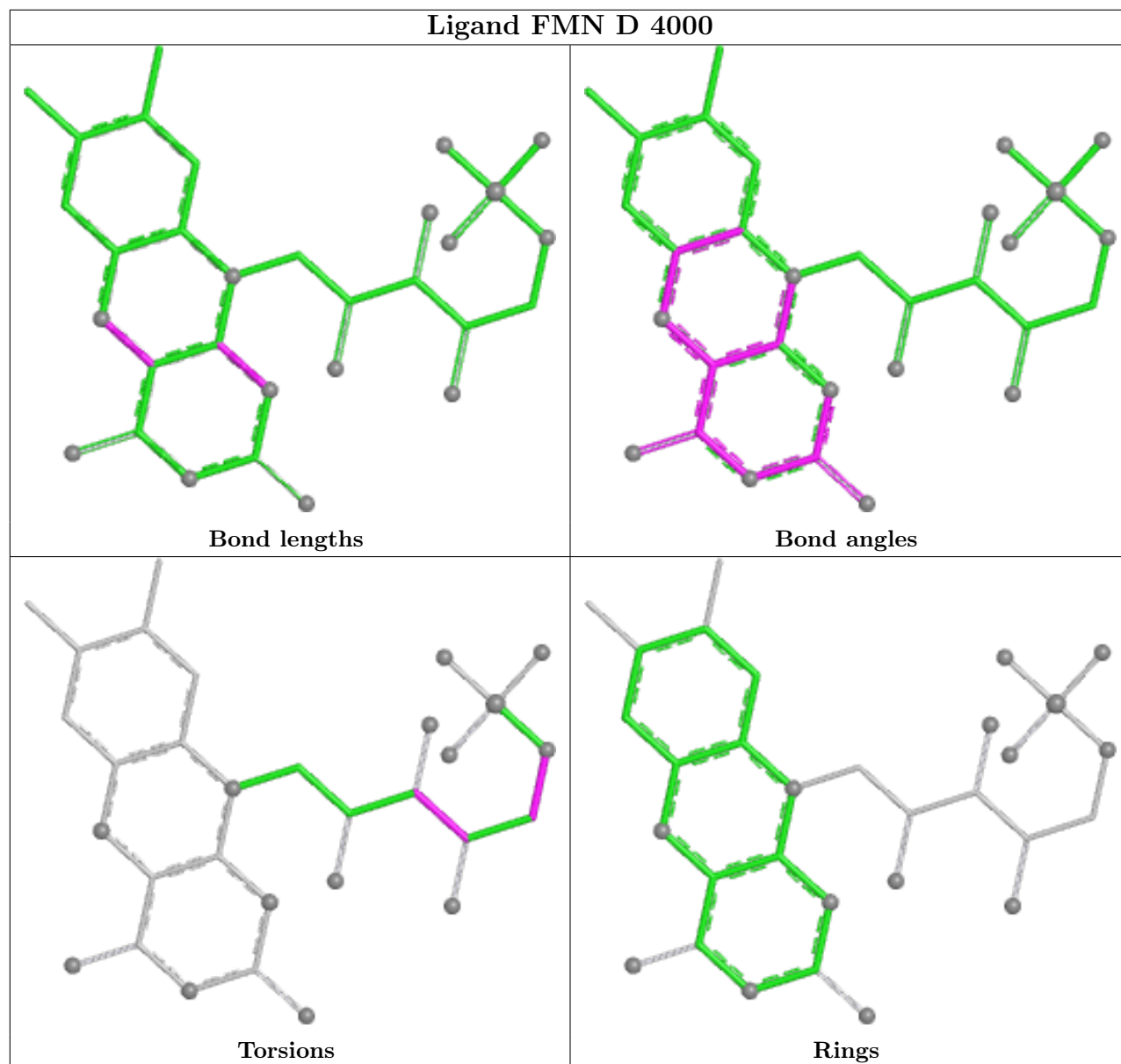
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4000	FMN	5	0
2	C	4000	FMN	4	0
2	A	4000	FMN	5	0

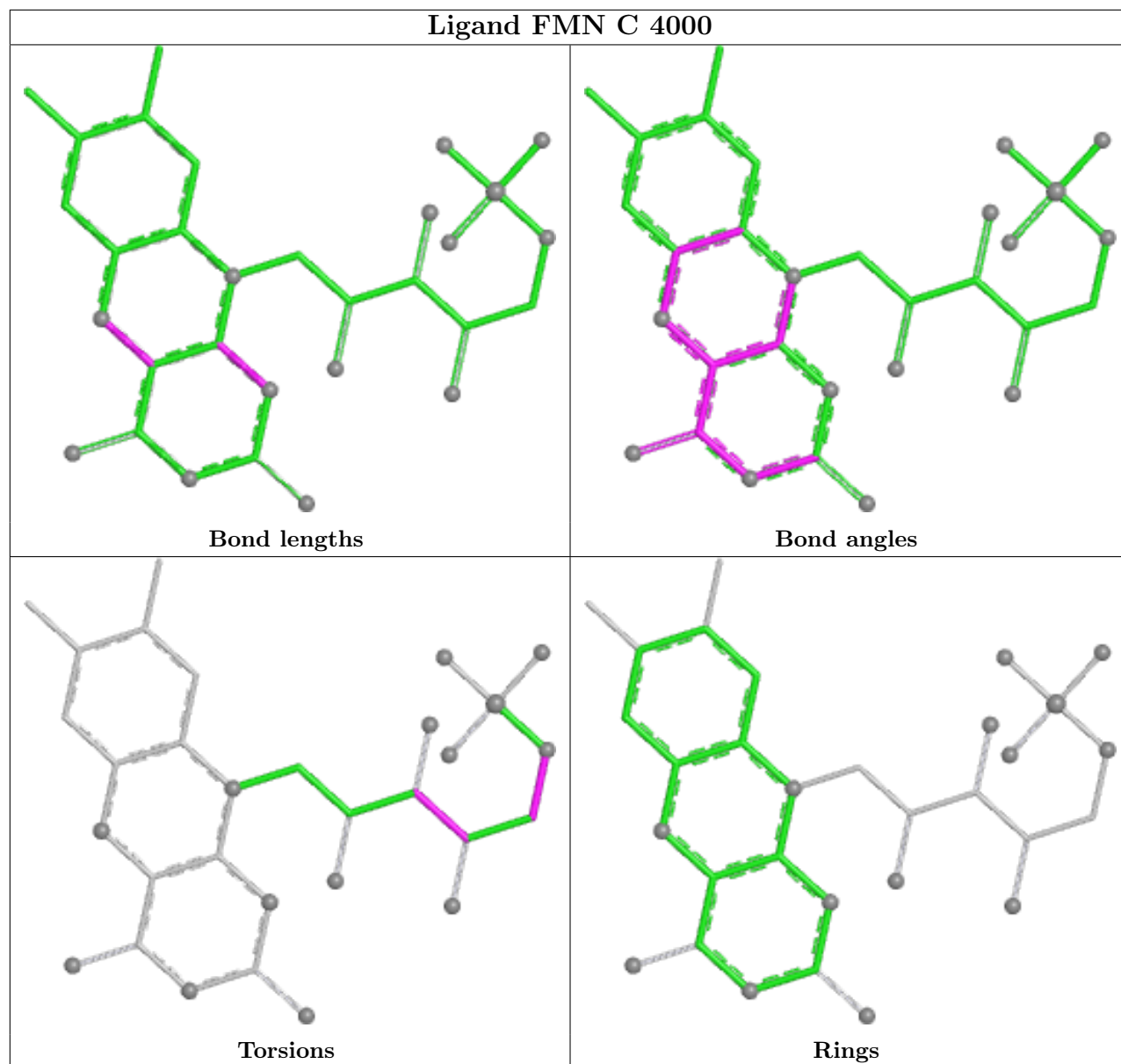
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



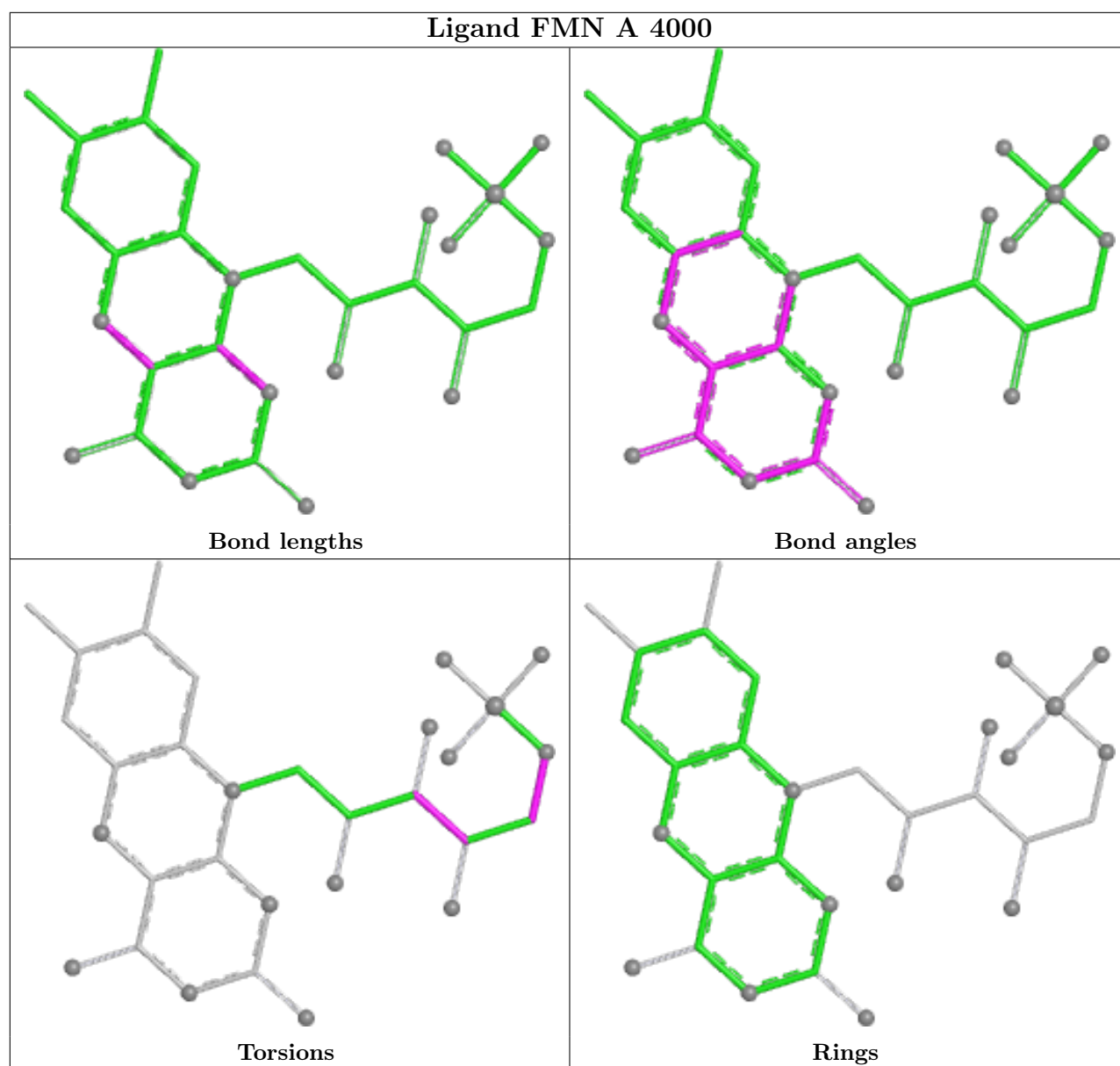












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

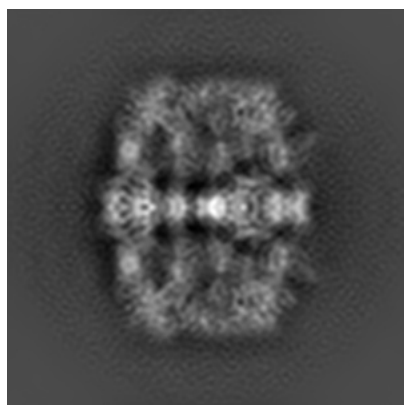
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2238. These allow visual inspection of the internal detail of the map and identification of artifacts.

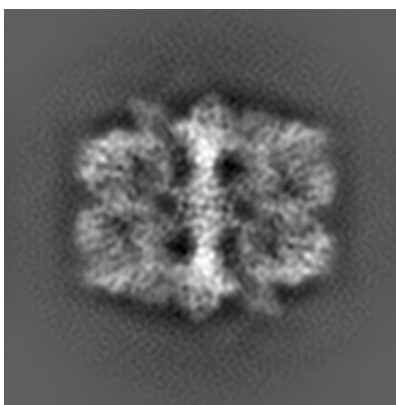
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

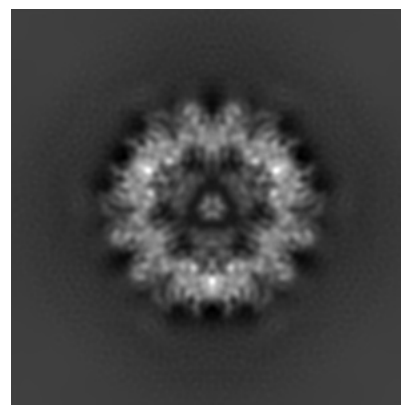
#### 6.1.1 Primary map



X



Y

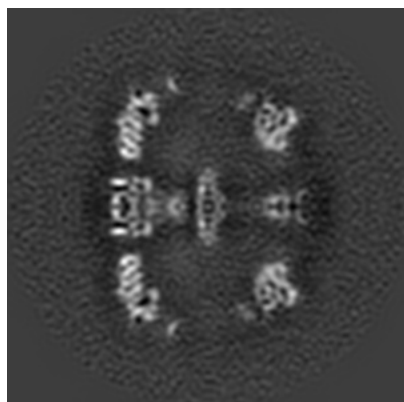


Z

The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

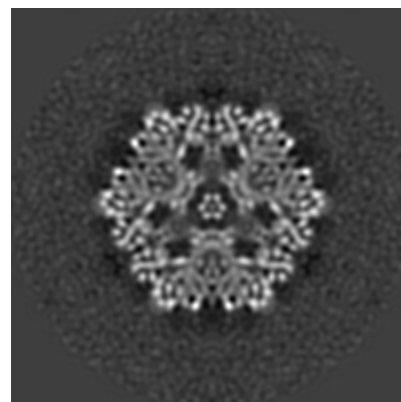
#### 6.2.1 Primary map



X Index: 80



Y Index: 80

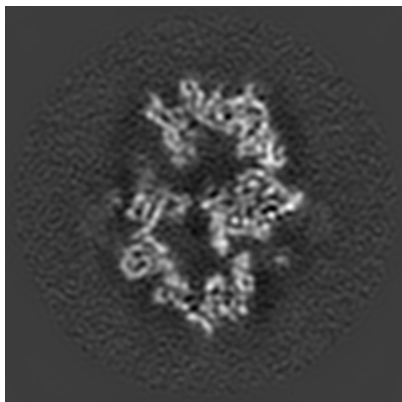


Z Index: 80

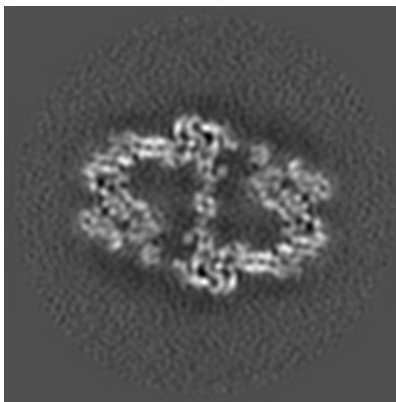
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

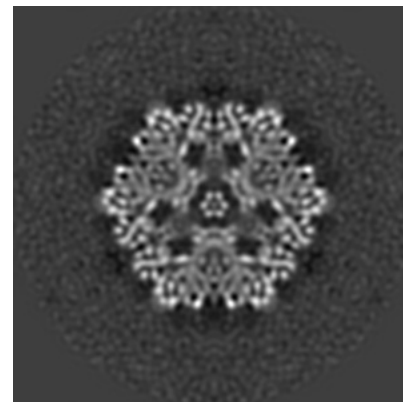
### 6.3.1 Primary map



X Index: 55



Y Index: 105

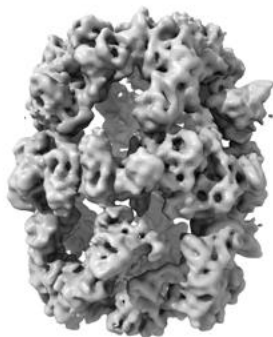


Z Index: 80

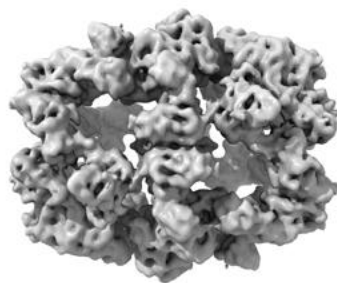
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

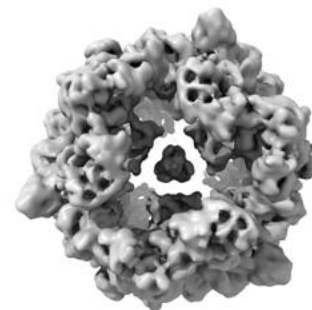
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

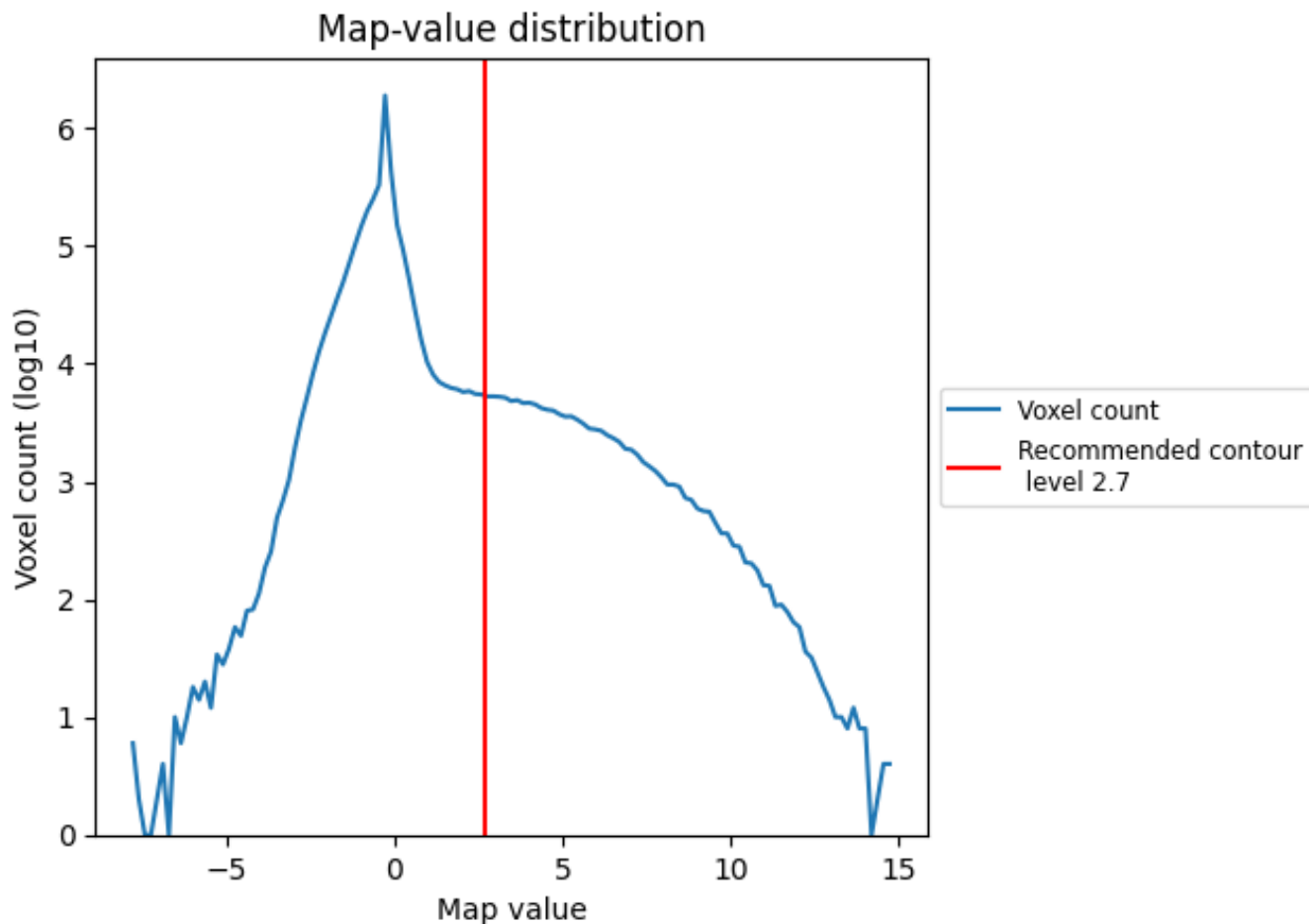
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

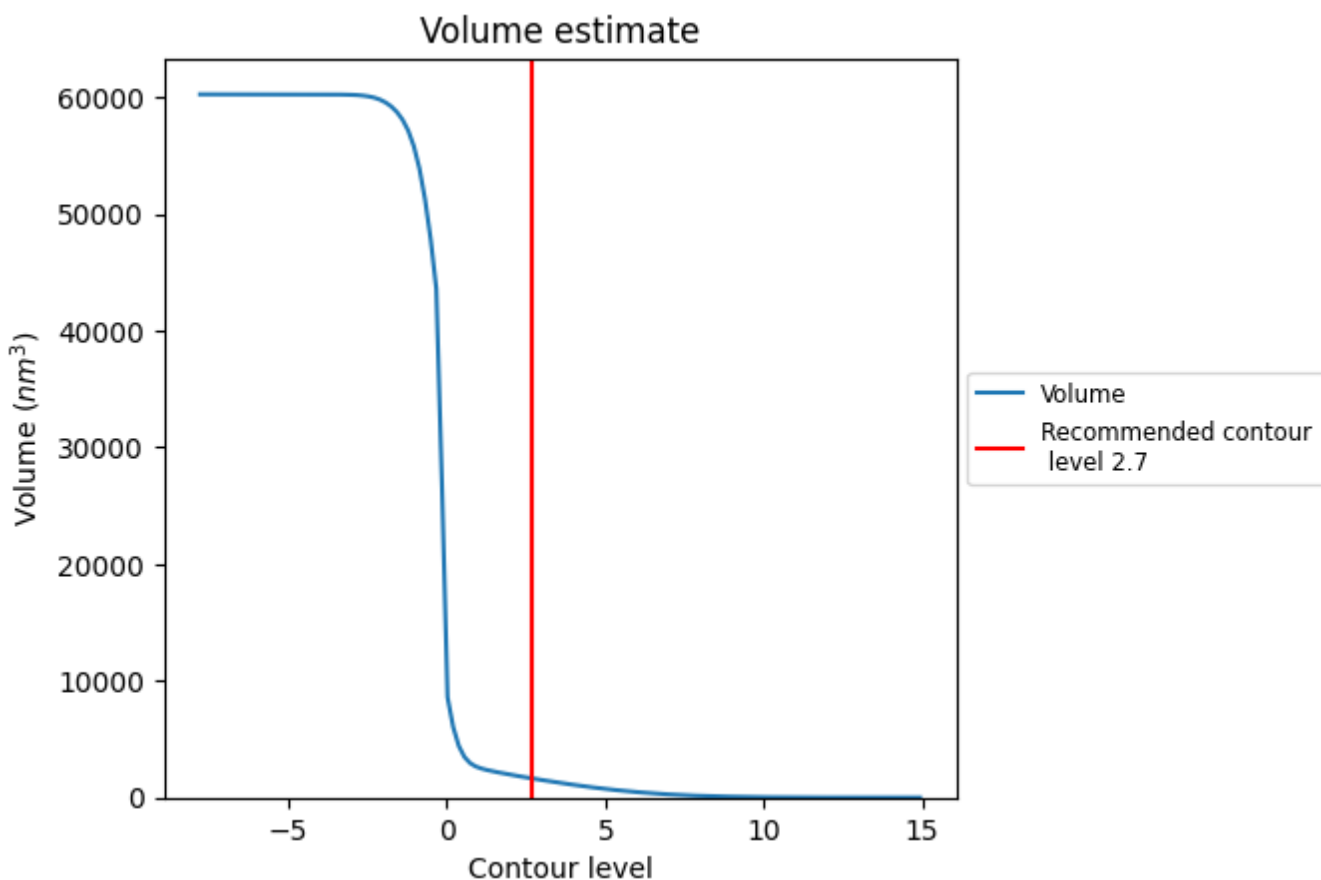
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

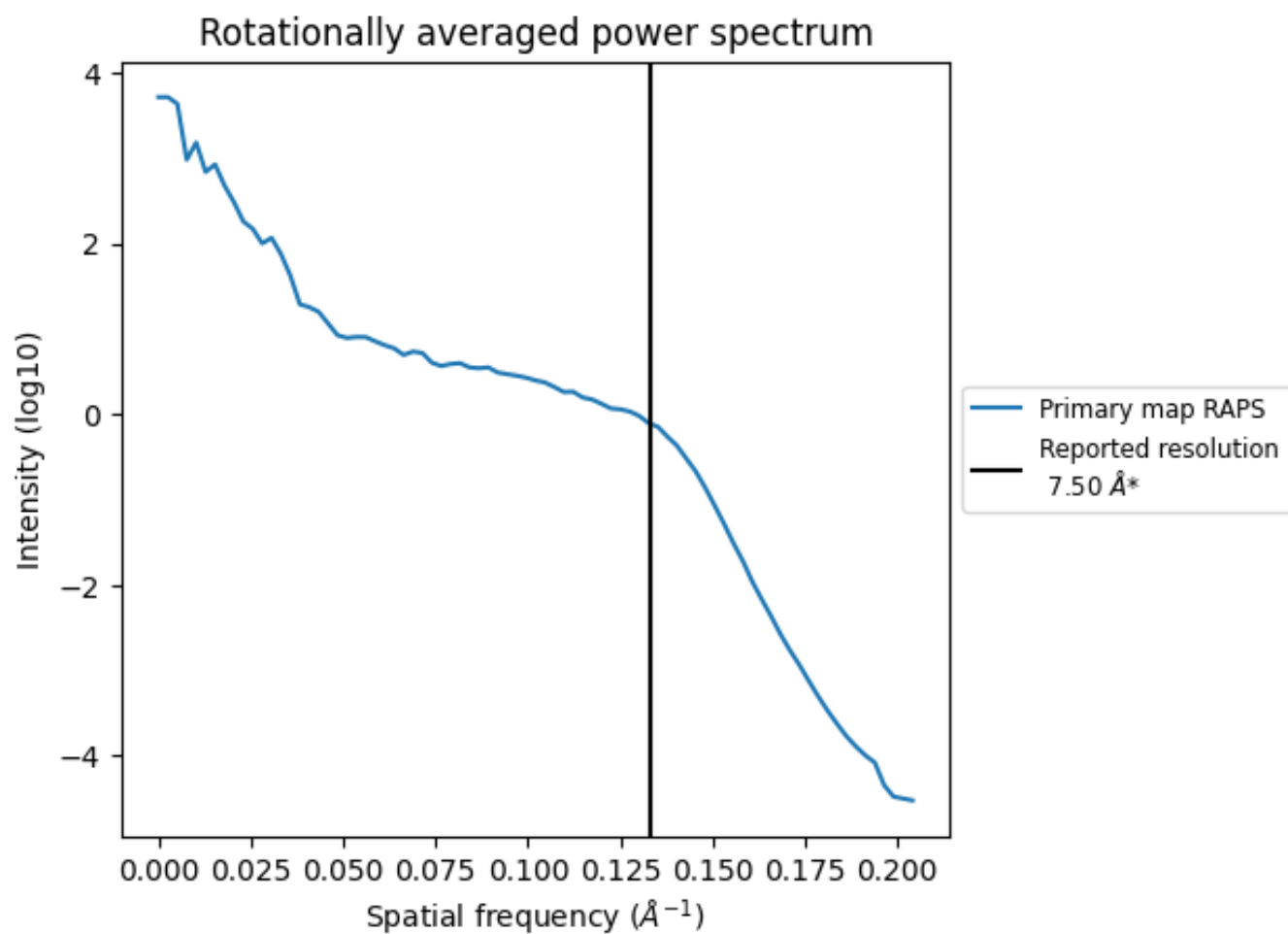
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1634 nm<sup>3</sup>; this corresponds to an approximate mass of 1476 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.133 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

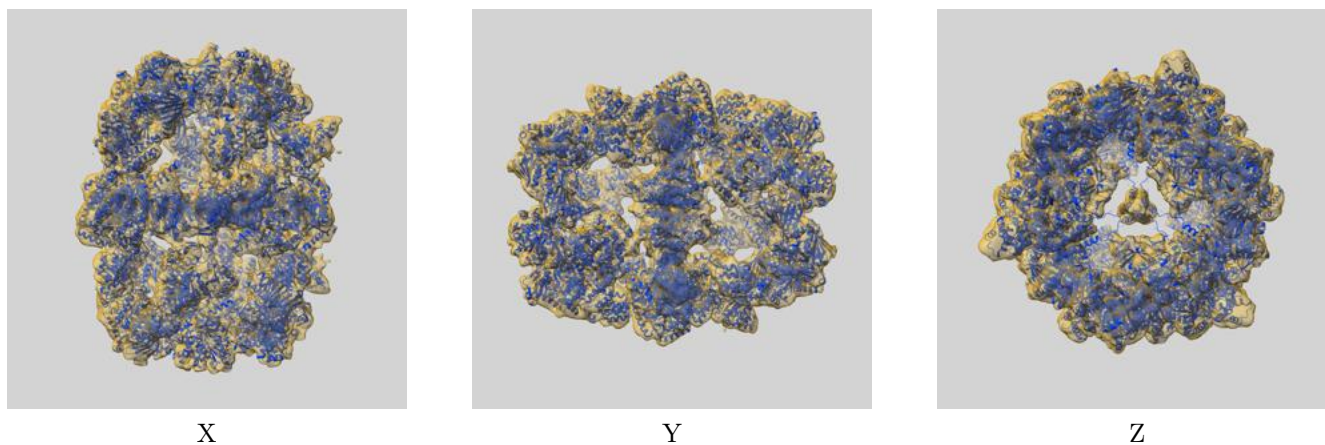
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

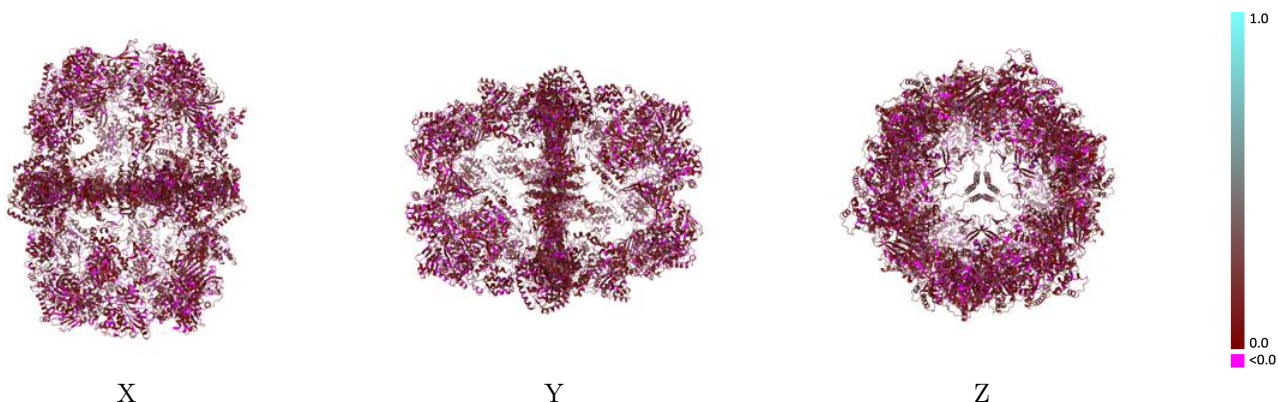
This section contains information regarding the fit between EMDB map EMD-2238 and PDB model 4V8L. Per-residue inclusion information can be found in section 3 on page 31.

### 9.1 Map-model overlay [i](#)



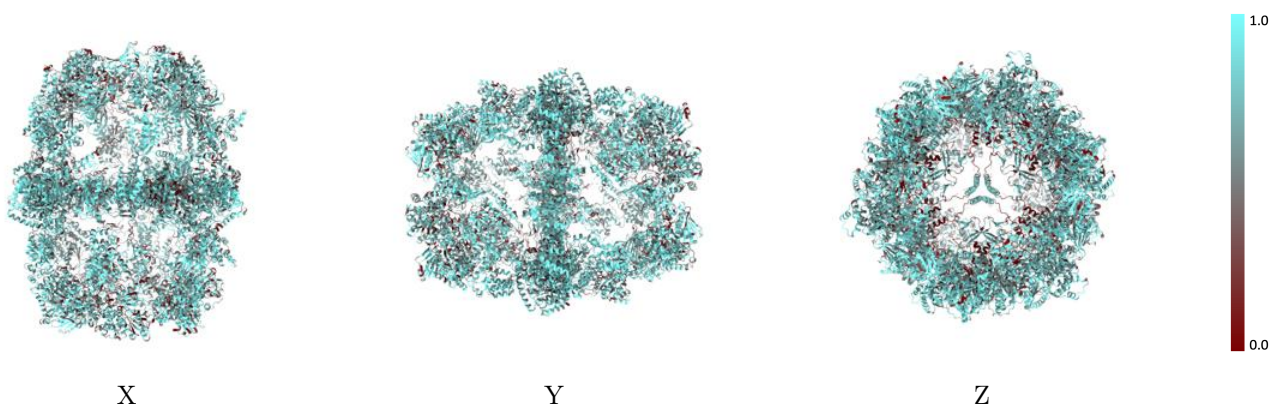
The images above show the 3D surface view of the map at the recommended contour level 2.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



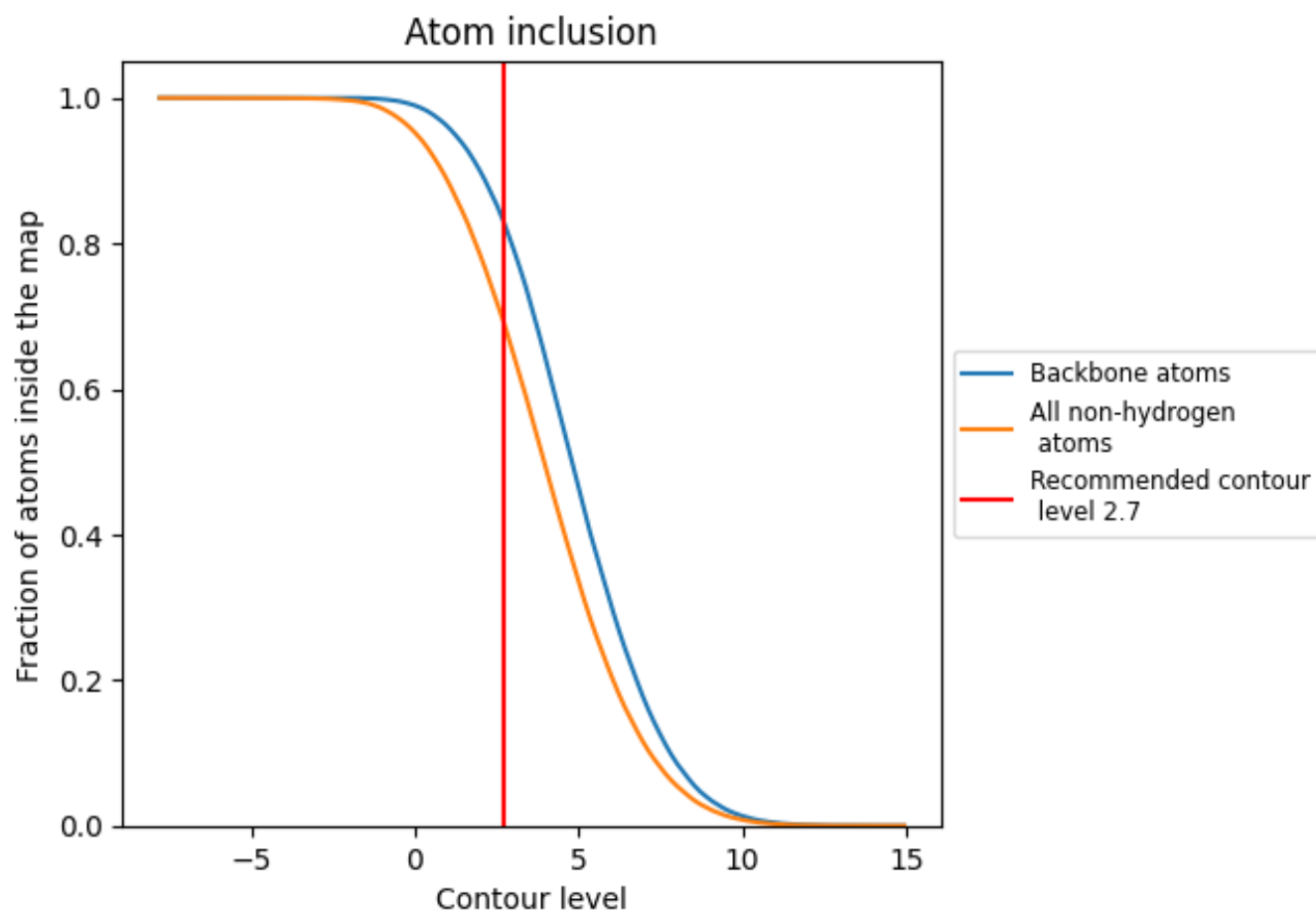
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.7).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6932	 0.1100
A	 0.6749	 0.1000
B	 0.6945	 0.1130
C	 0.6892	 0.1090
D	 0.6976	 0.1120
E	 0.6908	 0.1080
F	 0.7121	 0.1200

