



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 04:48 PM EDT

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 : unknown
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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

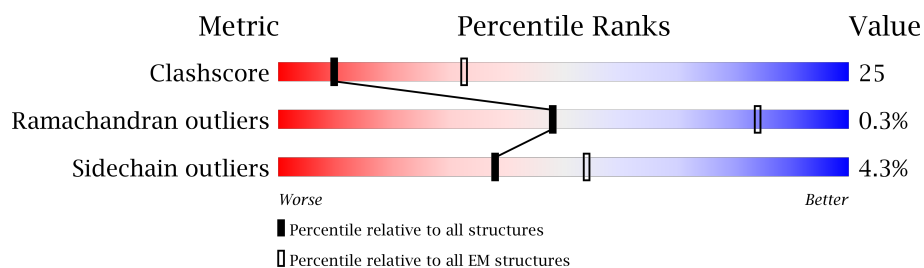
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	
1	B	3089	
1	C	3089	
1	D	3089	
1	E	3089	
1	F	3089	

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 21020	C 13294	N 3662	O 3998	S 66	0	0
1	E	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	F	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	A	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	B	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	C	2822	Total 21020	C 13294	N 3662	O 3998	S 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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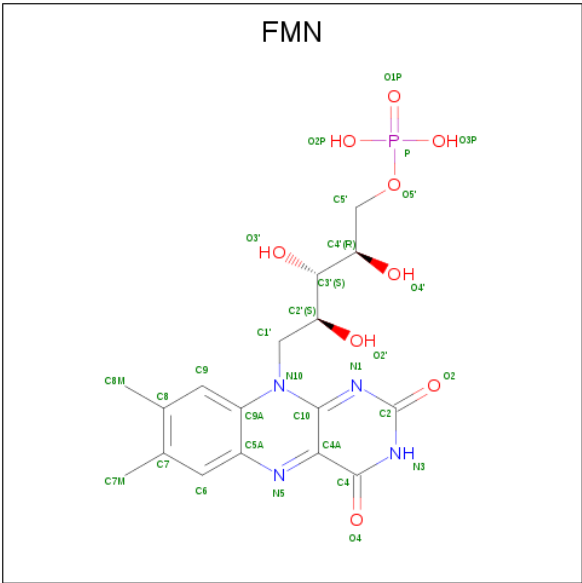
Chain	Residue	Modelled	Actual	Comment	Reference
C	2108	UNK	LEU	CONFLICT	UNP A0R1H7
C	2109	UNK	ALA	CONFLICT	UNP A0R1H7
C	2110	UNK	ALA	CONFLICT	UNP A0R1H7
C	2111	UNK	GLY	CONFLICT	UNP A0R1H7
C	2112	UNK	ARG	CONFLICT	UNP A0R1H7
C	2113	UNK	ASN	CONFLICT	UNP A0R1H7
C	2114	UNK	VAL	CONFLICT	UNP A0R1H7
C	2115	UNK	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: 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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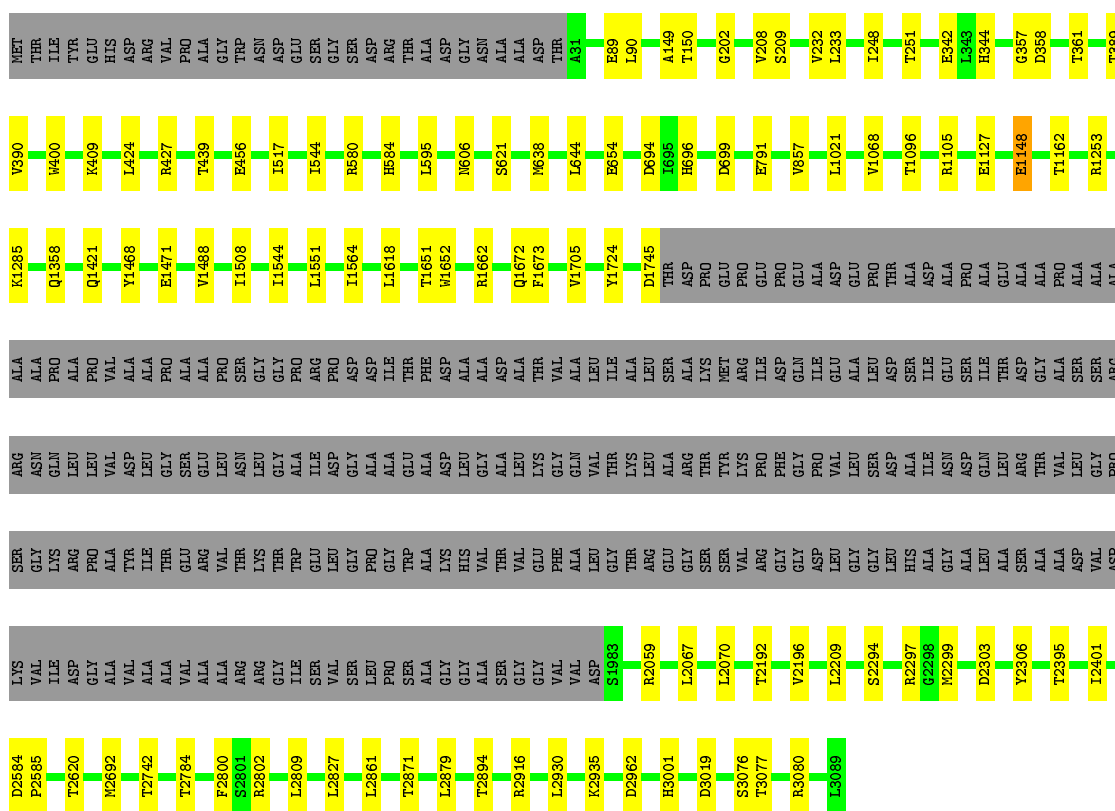
Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

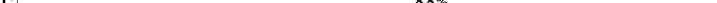
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

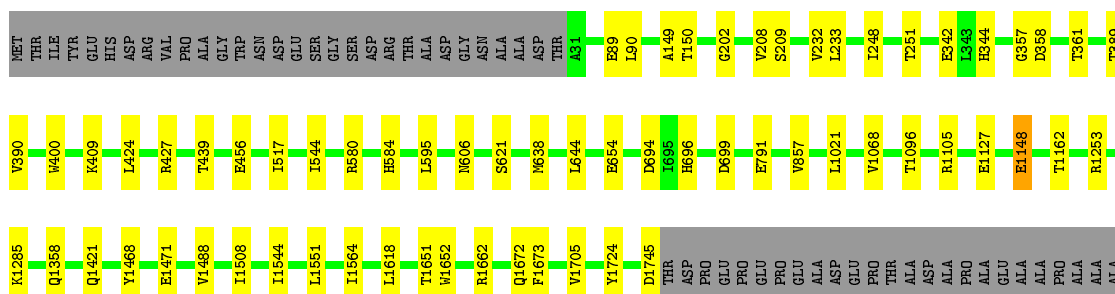
- Molecule 1: FATTY ACID SYNTHASE

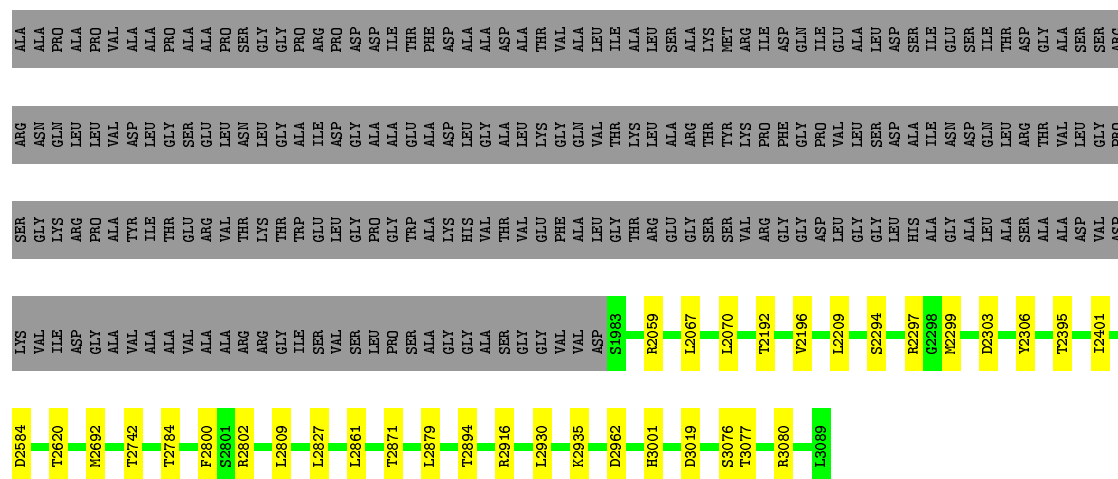
Chain D:  88% 9%



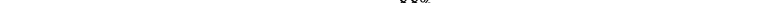
- Molecule 1: FATTY ACID SYNTHASE

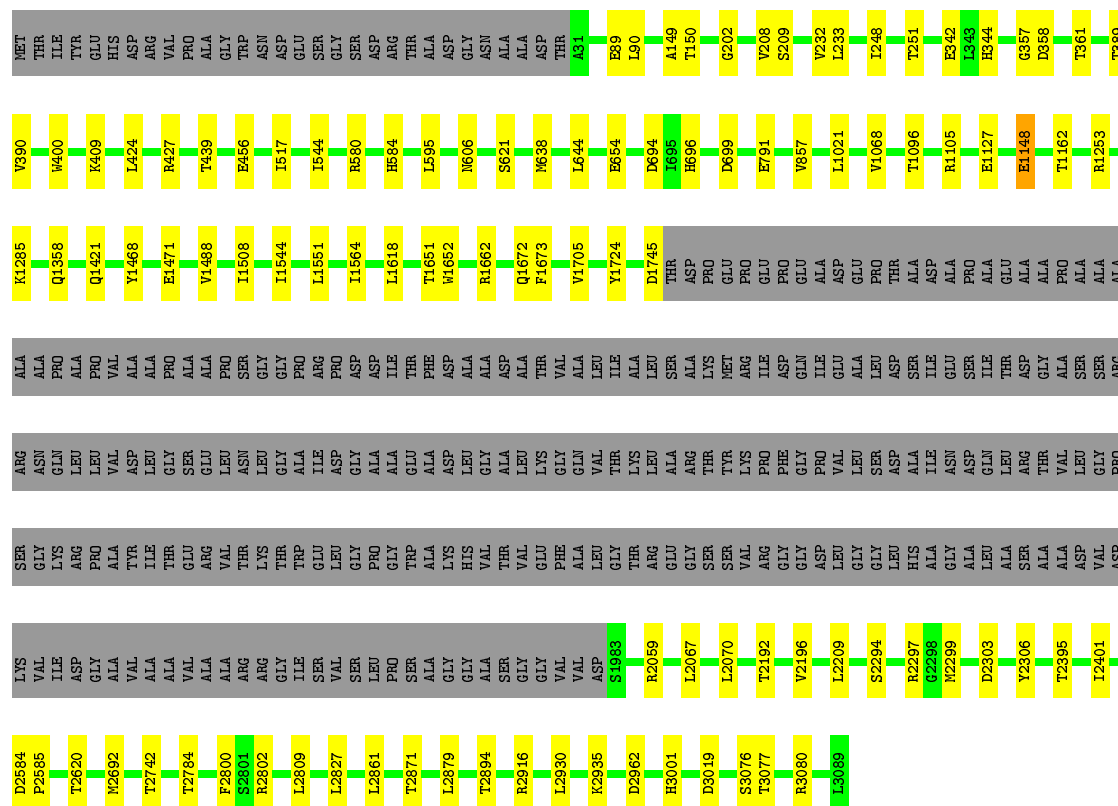
Chain E:  88% . 9%





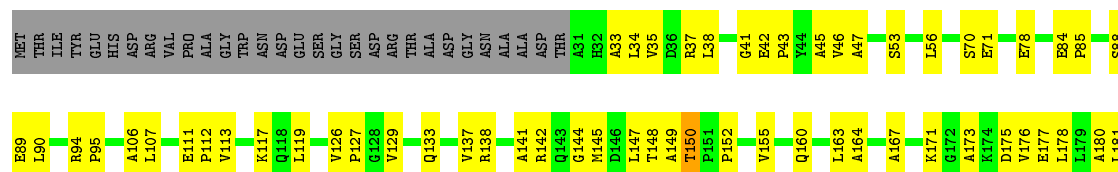
- Molecule 1: FATTY ACID SYNTHASE

Chain F:  88% 9%



- Molecule 1: FATTY ACID SYNTHASE

Chain A:  56% 33% • 9%



WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

- Molecule 1: FATTY ACID SYNTHASE

Response	Percentage
Yes	56%
No	33%
Don't know	9%

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

ALA	I1703	I1611	R1495	V1408	K1304	A1193	T1096	X989	L787	G676	H584	L479	V376	D288	A180	L179
ALA	G1704	G1612	S1496	H1412	D1307	I1194	V1097	X990	L787	G676	H585	R483	P377	P289	L181	
ALA	V1705	R1613	S1496	H1412	D1307	R1195	P1098	X991	A790	A680	S586	R483	R381	V292	L182	
ALA	S1707	R1614	R1503	P1413	Q1308	X1196	D1100	X992	A791	A681	E588	I485	Q384	E293	Q183	
SER	T1710	H1615	R1504	D1414	X1309	X1198	V1103	X993	E792	N682	D589	Q486	Q384	V294	L184	
GLY	V1711	H1617	Q1507	C1415	D1310	X1199	G1104	X994	R793	G683	L590	F487	I488	L301	R195	
GLY	V1712	L1618	T1508	V1416	F1311	X1204	C1105	X995	L794	M684	L593	I489	V390	I305	I198	
PRO	G1713	V1619	T1508	L1417	R1312	X1205	C1106	X996	H795	S686	L594	L490	V393	E306	I198	
ARG	L1714	P1620	D1511	T1420	V1314	X1206	F1110	X997	Q797	G687	L595	Q500	V393	I307	D203	
PRO	P1722	R1621	D1514	Q1421	R1315	X1207	F1111	X1000	D798	R688	V598	V501	E395	I307	D203	
ASP	E1723	F1623	D1514	T1423	G1317	X1212	A1117	X1002	E803	D684	R602	R504	W400	W311	R204	
ASP	T1725	L1625	V1519	Q1424	I1318	X1213	A1118	X1003	A928	H696	R606	R505	P405	T314	P206	
PHE	E1730	R1634	L1530	V1430	V1320	X1215	T1119	X1005	A808	E697	N606	T405	P405	V315	N207	
ALA	V1731	V1532	L1532	A1431	E1323	X1216	E1120	X1006	X931	E698	G613	Q508	T406	G316	V208	
ALA	L1732	V1637	V1533	A1431	V1324	X1218	F1123	X1007	X932	D611	G614	R511	V407	L317	S209	
ASP	L1733	P1638	V1533	V1435	V1324	X1218	P1124	X1008	X933	L616	G614	R511	V408	E327	T211	
ALA	E1734	A1639	F1535	V1326	E1326	X1219	T1125	X1009	X934	E817	P618	A515	L410	S328	L222	
THR	E1735	N1536	N1536	Q1441	V1327	X1220	I1126	X1010	X935	E817	P618	A515	L410	S328	L222	
VAL	R1736	L1651	L1537	Q1441	V1327	X1221	E1127	X1011	X936	L709	S621	I517	D412	L330	L222	
ALA	D1737	V1652	L1538	V1445	X1328	X1224	G1128	X1012	X937	A713	W624	D518	V415	V232	V232	
LEU			G1539	V1445	X1329	X1225	L1129	X1013	X938	L616	W624	D518	V415	L233	L233	
ILE	L1741	K1656	S1540	A1448	I1331	X1226	L1132	X1014	X939	A716	W625	V521	R416	V236	V236	
ALA	D1745	P1657	P1541	I1449	L1327	X1227	L1133	T1017	X940	W745	L625	V521	R416	V236	V236	
LEU		K1658	Y1542	A1450	M1336	X1228	F1133	R1018	X941	Y746	N629	S523	L417	L237	L237	
SER	THR	E1659	A1543	M1337	V1337	V1228	X943	F1019	X942	L747	N629	S523	L417	L237	L237	
ALA	ASP	L1660	I1544	V1455	A1338	R1237	P1146	X1020	X944	Q748	W636	I526	K420	E342	E342	
LYS	PRO	G1661		V1456	A1339	R1237	L1147	L1021	X957	W736	W636	I526	K420	L343	L248	
NET	GLU	R1662	L1551	E1457	R1253	R1253	E1147	L1021	X957	W737	W636	I526	K420	H344	L249	
ARG	PRO	K1663	E1552	E1458	R1342	G1268	P1149	V1025	R961	T745	D641	E538	R427	A348	T251	
ILE	GLU	A1553	L1554	T1459	L1343	G1268	A1150	E1034	M962	Y746	G642	L539	R427	R349	T251	
ASP	PRO	L1554	A1460	A1460	M1269	M1269	E1151	V1035	S963	L747	G642	L539	R427	R349	T251	
GLN	GLU	E1555	L1461	A1345	W1270	W1270	T1162	D1036	S963	Q748	G642	L539	R427	R349	T251	
ILE	ALA	E1556	A1462	P1346	L1271	L1271	D1163	D1037	S963	Q748	G642	L539	R427	R349	T251	
GLU	ASP	E1557	C1463	P1346	L1271	L1271	D1164	D1037	S963	Q748	G642	L539	R427	R349	T251	
ALA	GLU	W1671	V1464	V1350	A1274	A1274	T1164	V1045	P966	W749	W647	S545	V440	L354	L260	
LEU	PRO	F1672	V1467	A1351	A1275	A1275	G1167	L1046	P967	W749	W647	S545	V440	L354	L260	
ASP	THR	A1674	Y1468	F1352	Q1276	Q1276	R1168	V1046	P967	W749	W647	S545	V440	L354	L260	
SER	ALA		E1469	P1353	H1277	H1277	R1168	V1046	P967	W749	W647	S545	V440	L354	L260	
ILE	ASP	W1679	L1470	V1357	V1278	V1278	P1171	V1068	A971	L756	W656	H546	K443	P356	A266	
GLU	ALA		E1471	Q1358	V1279	V1279	P1172	V1072	X974	S763	W657	H546	K443	P356	A266	
SER	PRO			Q1358	T1280	T1280	V1173	W1072	X974	S763	W657	H546	K443	P356	A266	
ILE	ALA			Q1358	A1281	A1281	V1174	V1077	X975	D766	S658	P551	V445	I359	K266	
THR	GLU			M1362	T1282	T1282	W1174	V1077	X976	D766	S658	P551	V445	I359	K266	
ASP	ALA			D1283	D1283	D1283	D674	K768	X977	K768	W661	S559	N450	T361	E270	
GLY	ALA			G1284	G1284	G1284	S875	X978	X978	K768	W661	S559	N450	T361	E270	
ALA	PRO			V1376	K1285	K1285	R1177	T1084	X979	L775	W661	S559	N450	T361	E270	
SER	ALA			A1380	P1286	P1286	N1178	V1084	X979	L775	W661	S559	N450	T361	E270	
SER	ALA			D1381	V1287	V1287	N1179	F1087	X980	D776	W661	S559	N450	T361	E270	
ARG	ALA			H1485	P1288	P1288	L1184	G1088	X981	T777	W666	H575	Q462	V367	L277	
ALA	ALA			S1391	P1289	P1289	L1185	A1089	X982	T777	W666	H575	Q462	V367	L277	
ASN	ALA			V1590	P1289	P1289	L1185	P1090	X983	W779	W666	H575	Q462	V367	L277	
ASN	ALA			I1487	A1290	A1290	L1185	L1091	X984	W779	W666	H575	Q462	V367	L277	
GLN	PRO			V1488	K1291	K1291	L1188	A1092	X985	D761	W666	H575	Q462	V367	L277	
LEU	ALA			P1489	L1292	L1292	L1188	P1093	X986	D761	W666	H575	Q462	V367	L277	
LEU	PRO			R1490	L1292	L1292	R1191	T1094	X987	F782	W666	H575	Q462	V367	L277	
VAL	VAL			D1491	W1295	W1295	F1192	L1095	X988	E784	W666	H575	Q462	V367	L277	

- Molecule 1: FATTY ACID SYNTHASE

ALA	V1705	I1611	R1495	A1405	W1295	R1191	T1094	X987	L787	G676	H584	L479	V376	D288	A180
ALA	K1706	G1612	S1496	V1408	K1304	F1192	L1095	X988	L787	G676	H585	R483	P377	P289	L181
PRO		R1613				A1193	T1097	X989	A790	A680	S586	R483	P377	P289	L182
GLY	T1710	P1616	R1503	V1408	K1304	A1194	V1096	X990	A790	A680	S587	R483	P377	P289	L183
GLY	A1712	H1617	R1504	H1412	D1307	R1195	P1098	X991	E791	A681	E588	I485	R381	V292	L184
PRO	G1713	L1618	I1503	P1413	Q1308	X1196	P1099	X992	A792	N682	D589	Q486	Q384	E293	
ARG	L1714	V1619	Q1507	D1414	V1309	X1197	D1100	X993	R793	G683	L590	P487	Q384	V294	
PRO		P1620	T1508	G1415	D1310	X1199	V1103	X994	L794	M684	L590	M488	T389	L301	R195
ASP	P1722	R1621	D1511	V1416	F1311	X1204	G1104	X995	H795	G685	L593	T489	T389	L301	
ASP	E1723	F1622	D1511	V1416	F1311	X1205	G1104	X996	T796	G686	L594	T489	T389	L301	
ILE	Y1724	F1623	D1514	L1417	F1312	X1206	G1106	X997	T797	G687	L595	T489	T389	L301	
THR	S1725	L1625	D1514	L1417	F1312	X1206	G1106	X998	D798	R688	L598	T489	T389	L301	
PHE						X1207		X999	F799						
ASP	E1730	R1634	V1519	F1422	V1316	X1207	V1110	X1000	E803	D684	R602	R504	R400	W311	I198
ALA	V1731			T1423	G1317	X1212	F1111	X1001	E803	D684	R602	R504	R400	W311	
ALA	L1732					X1213	A1117	X1002	A808	H696	N606	R505	P405	T314	
ASP	N1733	V1637	E1531	Q1424	I1318	X1214	A1117	X1003	A808	H696	N606	R505	P405	T314	
ALA	S1734	P1638	V1532	V1425	D1319	X1215	T1119	X1004	X929	I698	T406	Q508	T406	G315	V208
ALA	E1735	A1639	V1533	V1430	V1320	X1216	E1120	X1005	X930	I699	G613	R511	V407	G316	S209
THR						X1217	E1121	X1006	X931	I700	G614	R511	V407	G316	V210
VAL						X1218	E1122	X1007	X932	A701	G614	R511	V407	G316	T211
ALA						X1219	E1123	X1008	X933	L709	P618	A515	L410	S328	
ALA						X1220	V1125	X1009	X934	L709	P618	A515	L410	S328	
ALA						X1221	V1126	X1010	X935	A713	S621	I517	D412	V232	
ALA						X1222	E1127	X1011	X936	A713	S621	I517	D412	V232	
ALA						X1223	E1128	X1012	X937	A713	S621	I517	D412	V232	
ALA						X1224	E1129	X1013	X938	A716	L625	V521	L416	W336	L233
ALA						X1225	E1130	X1014	X939	A716	L625	V521	L416	W336	
ALA						X1226	E1131	X1015	X940	A716	L625	V521	L416	W336	
ALA						X1227	E1132	X1016	X941	A716	L625	V521	L416	W336	
ALA						X1228	E1133	X1017	X942	A716	L625	V521	L416	W336	
ALA						X1229	E1134	X1018	X943	A716	L625	V521	L416	W336	
ALA						X1230	E1135	X1019	X944	A716	L625	V521	L416	W336	
ALA						X1231	E1136	X1020	X945	A716	L625	V521	L416	W336	
ALA						X1232	E1137	X1021	X946	A716	L625	V521	L416	W336	
ALA						X1233	E1138	X1022	X947	A716	L625	V521	L416	W336	
ALA						X1234	E1139	X1023	X948	A716	L625	V521	L416	W336	
ALA						X1235	E1140	X1024	X949	A716	L625	V521	L416	W336	
ALA						X1236	E1141	X1025	X950	A716	L625	V521	L416	W336	
ALA						X1237	E1142	X1026	X951	A716	L625	V521	L416	W336	
ALA						X1238	E1143	X1027	X952	A716	L625	V521	L416	W336	
ALA						X1239	E1144	X1028	X953	A716	L625	V521	L416	W336	
ALA						X1240	E1145	X1029	X954	A716	L625	V521	L416	W336	
ALA						X1241	E1146	X1030	X955	A716	L625	V521	L416	W336	
ALA						X1242	E1147	X1031	X956	A716	L625	V521	L416	W336	
ALA						X1243	E1148	X1032	X957	A716	L625	V521	L416	W336	
ALA						X1244	E1149	X1033	X958	A716	L625	V521	L416	W336	
ALA						X1245	E1150	X1034	X959	A716	L625	V521	L416	W336	
ALA						X1246	E1151	X1035	X960	A716	L625	V521	L416	W336	
ALA						X1247	E1152	X1036	X961	A716	L625	V521	L416	W336	
ALA						X1248	E1153	X1037	X962	A716	L625	V521	L416	W336	
ALA						X1249	E1154	X1038	X963	A716	L625	V521	L416	W336	
ALA						X1250	E1155	X1039	X964	A716	L625	V521	L416	W336	
ALA						X1251	E1156	X1040	X965	A716	L625	V521	L416	W336	
ALA						X1252	E1157	X1041	X966	A716	L625	V521	L416	W336	
ALA						X1253	E1158	X1042	X967	A716	L625	V521	L416	W336	
ALA						X1254	E1159	X1043	X968	A716	L625	V521	L416	W336	
ALA						X1255	E1160	X1044	X969	A716	L625	V521	L416	W336	
ALA						X1256	E1161	X1045	X970	A716	L625	V521	L416	W336	
ALA						X1257	E1162	X1046	X971	A716	L625	V521	L416	W336	
ALA						X1258	E1163	X1047	X972	A716	L625	V521	L416	W336	
ALA						X1259	E1164	X1048	X973	A716	L625	V521	L416	W336	
ALA						X1260	E1165	X1049	X974	A716	L625	V521	L416	W336	
ALA						X1261	E1166	X1050	X975	A716	L625	V521	L416	W336	
ALA						X1262	E1167	X1051	X976	A716	L625	V521	L416	W336	
ALA						X1263	E1168	X1052	X977	A716	L625	V521	L416	W336	
ALA						X1264	E1169	X1053	X978	A716	L625	V521	L416	W336	
ALA						X1265	E1170	X1054	X979	A716	L625	V521	L416	W336	
ALA						X1266	E1171	X1055	X980	A716	L625	V521	L416	W336	
ALA						X1267	E1172	X1056	X981	A716	L625	V521	L416	W336	
ALA						X1268	E1173	X1057	X982	A716	L625	V521	L416	W336	
ALA						X1269	E1174	X1058	X983	A716	L625	V521	L416	W336	
ALA						X1270	E1175	X1059	X984	A716	L625	V521	L416	W336	
ALA						X1271	E1176	X1060	X985	A716	L625	V521	L416	W336	
ALA						X1272	E1177	X1061	X986	A716	L625	V521	L416	W336	
ALA						X1273	E1178	X1062	X987	A716	L625	V521	L416	W336	
ALA						X1274	E1179	X1063	X988	A716	L625	V521	L416	W336	
ALA						X1275	E1180	X1064	X989	A716	L625	V521	L416	W336	
ALA						X1276	E1181	X1065	X990	A716	L625	V521	L416	W336	
ALA						X1277	E1182	X1066	X991	A716	L625	V521	L416	W336	
ALA						X1278	E1183	X1067	X992	A716	L625	V521	L416	W336	
ALA						X1279	E1184	X1068	X993	A716	L625	V521	L416	W336	
ALA						X1280	E1185	X1069	X994	A716	L625	V521	L416	W336	
ALA						X1281	E1186	X1070	X995	A716	L625	V521	L416	W336	
ALA						X1282	E1187	X1071	X996	A716	L625	V521	L416	W336	
ALA						X1283	E1188	X1072	X997	A716	L625	V521	L416	W336	
ALA						X1284	E1189	X1073	X998	A716	L625	V521	L416	W336	
ALA						X1285	E1190	X1074	X999	A716	L625	V521	L416	W336	
ALA						X1286	E1191	X1075	X1000	A716	L625	V521	L416	W336	
ALA						X1287	E1192	X1076	X1001	A716	L625	V521	L416	W336	
ALA						X1288	E1193	X1077	X1002	A716	L625	V521	L416	W336	
ALA						X1289	E1194	X1078	X1003	A716	L625	V521	L416	W336	
ALA						X1290	E1195	X1079	X1004	A716	L625	V521	L416	W336	
ALA						X1291	E1196	X1080	X1005	A716	L625	V521	L416	W336	
ALA						X1292	E1197	X1081	X1006	A716	L625	V521	L416	W336	
ALA						X1293	E1198	X1082	X1007	A716	L625	V521	L416	W336	
ALA						X1294	E1199	X1083	X1008	A716	L625	V521	L416	W336	
ALA						X1295	E1200	X1084	X1009	A716	L625	V521	L416	W336	
ALA						X1296	E1201	X1085	X1010	A716	L625	V521	L416	W336	
ALA						X1297	E1202	X1086	X1011	A716	L625	V521	L416	W336	
ALA						X1298	E1203	X1087	X1012	A716	L625	V521	L416	W336	
ALA						X1299	E1204	X1088	X1013	A716	L625	V521	L416	W336	
ALA						X1300	E1205	X1089	X1014	A716	L625	V521	L416	W336	
ALA						X1301	E1206	X1090	X1015	A716	L625	V521	L416	W336	
ALA						X1302	E1207	X1091	X1016	A716	L625	V521	L416	W336	
ALA						X1303	E1208	X1092	X1017	A716	L625	V521	L416	W336	
ALA						X1304	E1209	X1093	X1018	A716	L625	V521	L416	W336	
ALA						X1305	E1210	X1094	X1019	A716					

G2992	L2906	A2911	R2916	G2919	N2920	P2921	L2922	F2923	L2924	V2925	S2926	Q2927	L2930	K2935	G2936	A2939	V2940	F2941	Q2942	M2943	L2946	G2947	Q2948	R2951	V2954	P2955	P2957	N2958	R2959	L2961	D2962	D2966	W2976	V2977	R2978	E2979	P2980	L2983	R2984	G2985	K2986	F2987	P2988	L2989										
R2808	L2809	E2810	F2811	L2812	Q2815	L2820	L2821	L2822	A2823	R2824	L2827	A2828	L2829	K2830	M2831	G2832	L2833	P2834	V2835	Q2843	S2844	F2845	A2846	D2847	G2848	G2859	A2860	L2861	T2871	L2876	L2879	G2880	V2881	G2882	A2883	D2884	D2885	L2886	L2889	S2890	K2891	H2892	D2893	T2894	S2895	T2896	P2901	N2902	E2903					
Q2711	E2712	V2713	V2717	V2718	V2722	V2727	V2727	Y2730	P2736	C2740	A2741	T2742	A2743	S2746	V2751	L2754	A2759	L2763	A2764	G2765	D2768	D2769	L2770	E2773	L2776	G2779	T2784	A2785	D2786	Q2693	T2787	E2788	M2789	M2790	R2791	K2799	L2700	A2704	S2801	K2705	P2706	D2805	R2806	R2807										
P2612	R2613	K2614	L2617	S2618	R2619	T2620	G2622	A2623	Q2624	L2625	D2630	P2631	T2632	V2633	D2645	R2646	V2647	A2648	L2649	W2650	N2651	S2662	P2666	T2667	W2672	A2679	S2680	T2681	M2686	T2690	S2691	M2692	Q2693	T2694	M2695	Y2696	H2697	G2698	N2699	L2700	A2704	S2801	K2705	P2706	D2805	R2806	R2807							
M2481	E2482	V2483	L2487	V2492	L2495	K2503	W2504	E2505	W2512	Y2513	L2520	P2521	F2522	E2523	C2524	E2525	A2526	L2526	W2527	E2528	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						
K2261	E2137	V2140	V2141	T2163	W2164	L2165	A2166	T2167	R2170	D2173	D2174	R2175	L2176	K2180	R2188	F2189	T2192	L2193	W2194	T2195	V2196	P2197	A2198	E2199	M2200	D2205	L2209	W2210	E2211	W2212	V2213	G2214	T2215	E2216	R2229	P2234	T2235	L2236	L2237	F2238	R2244	V2245	A2246	V2252	R2255									
L2070	E2074	X2077	X2078	X2079	X2080	X2081	X2082	A2083	X2084	X2085	X2086	X2087	X2088	X2089	X2090	X2091	X2092	X2093	X2094	X2095	X2096	X2097	X2098	X2099	X2100	X2101	X2102	X2103	X2104	X2105	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	ALA	ARG	ARG	THR	THR	THR	TRP	GLY	LEU	LEU	LEU	ASP	PRO	GLY	TRP	ALA	ALA	LYS	GLY	GLY	GLY	VAL	VAL	ASP	S1983	L1986	F1989	K1992	P1996	L2000	Q2010	L2011	G2012	L2013	S2014	D2015	V2016	P2020	T2047	A2053	W2054	V2055	F2056	D2057	D2058	R2059	W2060	R2064	L2067	ALA			
SER	GLU	LEU	ASN	LEU	GLY	ALA	ILE	ASP	GLY	ALA	ALA	GLU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	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%)	44	81
1	B	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	44	81
1	C	2637/3089 (85%)	2489 (94%)	139 (5%)	9 (0%)	44	81
1	D	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	44	81
1	E	2637/3089 (85%)	2488 (94%)	141 (5%)	8 (0%)	44	81
1	F	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	44	81
All	All	15822/18534 (85%)	14931 (94%)	840 (5%)	51 (0%)	48	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%)	33	64
1	B	2076/2264 (92%)	1986 (96%)	90 (4%)	33	64
1	C	2076/2264 (92%)	1987 (96%)	89 (4%)	33	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	2076 / 2264 (92%)	1987 (96%)	89 (4%)	33	64
1	E	2076 / 2264 (92%)	1987 (96%)	89 (4%)	33	64
1	F	2076 / 2264 (92%)	1987 (96%)	89 (4%)	33	64
All	All	12456 / 13584 (92%)	11921 (96%)	535 (4%)	38	64

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	1.34	4 (12%)	38,50,50	1.51	6 (15%)
2	FMN	B	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	C	4000	-	31,33,33	1.36	4 (12%)	38,50,50	1.49	6 (15%)
2	FMN	D	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.51	6 (15%)
2	FMN	E	4000	-	31,33,33	1.36	4 (12%)	38,50,50	1.50	6 (15%)
2	FMN	F	4000	-	31,33,33	1.35	4 (12%)	38,50,50	1.49	6 (15%)

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	-	-	0/16/18/18	0/3/3/3
2	FMN	B	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	C	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	D	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	E	4000	-	-	0/16/18/18	0/3/3/3
2	FMN	F	4000	-	-	0/16/18/18	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	E	4000	FMN	C5A-N5	2.29	1.38	1.35
2	A	4000	FMN	C5A-N5	2.30	1.38	1.35
2	B	4000	FMN	C5A-N5	2.30	1.38	1.35
2	D	4000	FMN	C5A-N5	2.36	1.38	1.35
2	C	4000	FMN	C5A-N5	2.37	1.38	1.35

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	FMN	C4A-C4-N3	-2.59	119.80	123.48
2	D	4000	FMN	C4A-C4-N3	-2.59	119.80	123.48
2	F	4000	FMN	C4A-C4-N3	-2.58	119.81	123.48
2	C	4000	FMN	C4A-C4-N3	-2.58	119.81	123.48
2	E	4000	FMN	C4A-C4-N3	-2.58	119.82	123.48

There are no chirality outliers.

There are no torsion outliers.

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

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.