



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

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

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

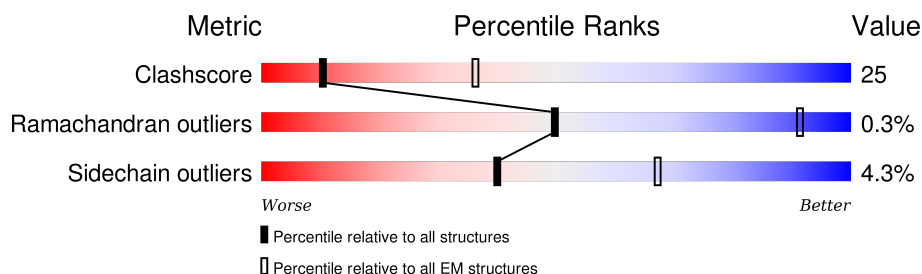
# 1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	3089	 56% 33% • 9%
1	B	3089	 56% 33% • 9%
1	C	3089	 56% 33% • 9%
1	D	3089	 88% • 9%
1	E	3089	 88% • 9%
1	F	3089	 88% • 9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 126306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FATTY ACID SYNTHASE.

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

There are 1086 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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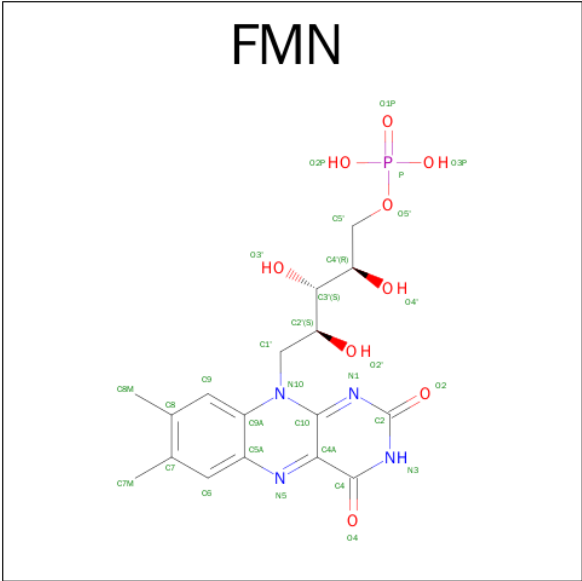
Chain	Residue	Modelled	Actual	Comment	Reference
C	2108	UNK	LEU	CONFLICT	UNP A0R1H7
C	2109	UNK	ALA	CONFLICT	UNP A0R1H7
C	2110	UNK	ALA	CONFLICT	UNP A0R1H7
C	2111	UNK	GLY	CONFLICT	UNP A0R1H7
C	2112	UNK	ARG	CONFLICT	UNP A0R1H7
C	2113	UNK	ASN	CONFLICT	UNP A0R1H7
C	2114	UNK	VAL	CONFLICT	UNP A0R1H7
C	2115	UNK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

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

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

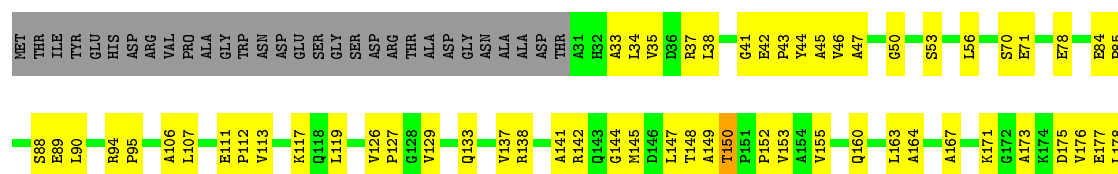






WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM



ALA	I1703	I1611	R1495	V1408	K1304	A1193	T1096	X989		L787	G676	H584	L479	V376	D288	L179
ALA	G1704	G1612	S1496	H1412	D1307	I1194	V1097	X990		T895	A680	H585	R483	P377	P289	A180
PRO	V1705	R1613	S1496	H1412	D1307	R1195	P1098	X991		A896	A680	S586	R483	P377	P289	L181
ALA	S1707	R1614	R1503	P1413	Q1308	R1196	D1100	X992		A899	A681	E588	I485	R381	V292	L182
PRO	T1710	H1615	R1504	D1414	X1309	X1198	V1103	X993		G900	N682	D589	Q384	Q384	E293	Q183
SER	P1711	P1616	Q1507	C1415	D1310	X1199	G1104	X994		I901	N683	L590	F487		V294	L184
GLY	V1712	H1617	T1508	V1416	F1311		C1106	X995		P904	N684	L593	I488	T389	L301	R195
PRO	G1713	L1618	T1508	L1417	R1312	X1204		X996		H795	G685	L593	T389			
ARG	L1714	P1620	D1511	T1420	V1314	X1205	F1110	X997		F915	S686	L595	L490	V390	E306	I198
PRO	P1722	R1621	D1514	Q1421	R1315	X1206	V1110	X998		L824	R688	L598	Q500	P394	I307	D203
ASP	E1723	F1623		F1422	R1316	X1207	F1111	X999					V501	E395		R204
ASP	T1725	L1625		T1423	G1317		A1117	X1000		A928	D684	R602	R504	W400	W311	P205
THR	P1726	L1625		Q1424	I1318	X1213	A1118	X1003		X929	H696	R606	R505		T314	P206
PHE	E1730	R1634	L1530	V1430	V1320	X1215	T1119	X1005		X930	E697	N606	P405	P405	V315	N207
ALA	E1731		L1532	A1431		X1216	E1120	X1006		X931	E698	G613	Q508	T406	G316	V208
ALA	L1732	V1637	V1533	A1431	E1323	X1217	F1123	X1007		X932	D611	G614	R511	V407	L317	S209
ASP	L1733	P1638	V1533	V1435	V1324	X1218	P1124	X1008		X933	L616	G614		V408	E327	V210
ALA	A1639	A1639	F1535	V1326	L1325	X1219	T1125	X1009		X934	E317	P618	A515	L410	S328	T211
THR	E1735	N1536	N1536	Q1441	V1327	X1220	I1126	X1010		X935			P516	L410	I329	L222
VAL	R1736	T1651	L1537	Q1441	V1327	X1221	E1127	X1011		X936	L709	S621	I517	D412	L330	
ALA	D1737	W1652	R1538	V1445	X1328	X1224	G1128	X1012		X937	A713	W624	D518		V232	
LEU			G1539	V1445	A1329	X1225	L1129	X1013		X938		W624		V415	L233	
ILE	L1741	K1656	S1540	A1448	I1331	X1226	L1132	X1014		X939	A716	L625	V521	L416	W336	
ALA	D1745	P1657	Q1541	I1449	L1332	X1227	L1133			X940	T745	L625	V521	L416		V236
LEU		K1658	Y1542	A1450	V1228	X1227	R1018	X1017		X941	Y746	N629	S523	R417	E339	L237
SER	ASP	E1659	A1543	M1337	V1228		F1019	X1018		X942	L747	N629		T419	I340	
ALA	ASP	L1660	I1544	V1455	R1237		T1162	X1019		X943	Q748	L644	V542	T419	T341	S238
LYS	PRO	G1661		V1456	R1237		D1163	X1020		X944	W749	L644		K420	E342	
NET	GLU	R1662	L1551	E1457	R1253		T1164	L1021			Y737	L637	D534	K420	I343	L248
ARG	PRO	K1663	E1552	E1458			P1149			L957		W639		L424	H344	T249
ILE	GLU	A1553	L1554	T1459	R1342	G1268	E1150	V1025		R961	T745	D641	E538	R427	A348	T251
ASP	PRO	L1554	A1460	A1344	L1343	M1269	E1151	E1034		N962	G842	N642	N540	T436	R349	L255
GLN	GLU	E1555	L1461	A1345	M1270	M1269	T1035	X1035		S963	L747	G643	E541	T436	H350	L255
ILE	ALA	E1556	A1462	P1346	L1271		D1036	D1036		N964	Q748	L644	P437	P437	I351	S256
GLU	ASP	E1557	C1463				D1037	D1037		N965	W749	W647	V542	T438	L352	R257
ALA	GLU	W1671	V1464			A1274	T1164	V1045		P966	L750		G543	T439	D353	
LEU	PRO	F1672	V1467		A1275	A1275	G1167	L1046		P967	R751	E654	S545	V440	L354	L260
ASP	ALA	A1674	Y1468		Q1276	Q1276	R1168				R751	E655	H546	A442	G355	A266
ILE	ASP	W1679	E1469		H1277	H1277		V1068		1970	L756	W656	H546	A442	P356	A266
SER	PRO		L1470		V1278	V1278	P1171	V1068		A971	S763	W657	F549	K443	G357	E267
ILE	ALA		E1471		V1279	V1279	V1172	W1072		X974	D766	S658	R500	V445	D358	K266
THR	GLU	D1578			A1281	A1281	V1174	V1077		X975	D766		P551		L360	E270
ASP	GLU	L1585	P1580	L1474	T1282	T1282	W1174	V1077		X976	S873	W661		N450	T361	A271
GLY	ALA	F1581	F1581		D1283	D1283	R1177	T1084		X977	K768	K662	S559		R362	E272
ALA	PRO	H1582		R1480	G1284	G1284	R1177	T1084		X978	S875	G663	V560	E456	L363	R273
SER	ALA		K1483		K1285	K1285	N1178			X979	L775	L664			T364	
SER	ALA	L1586	D1381	A1380	P1286	P1286	N1178	F1087		X980	D776	L665	I563	G460	K276	K276
ARG	ALA		D1381	D1381	V1287	V1287	G1088	G1088		X981	T777	W666		G461	L277	L277
ALA	ALA	V1590	H1485	H1485	P1288	P1288	L1184	A1089		X982	T778	E367	H575	Q462	V367	
ASN	ALA	L1695	D1486	S1391	P1289	P1289	L1185	P1090		X983	W779	W669	I576	Q462	I368	G280
GLN	ALA		I1487		A1290	A1290	L1185	L1091		X984	R780	K669	E577	F468	R369	G281
PRO	PRO	E1598	V1488	P1400	K1291	K1291	L1188	A1092		X985	D781	G670	R500	L475	I373	V282
LEU	ALA	F1700	P1489	T1401	L1292	L1292	L1188	P1093		X986	R782	W671	R500	E476	G374	V286
LEU	PRO		R1490				R1191	T1094		X987	E784				I375	F287
VAL	VAL	E1702	K1605	D1491	A1405	W1295	F1192	L1095		X988		W674	G583			



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	T1710	R1613				A1193	T1097	X989	A790	A680	S586	R483	P377	P289	L182
GLY	V1711	H1617	R1503	H1412	D1307	R1194	V1096	X990	A791	A681	H587	R381	R381	V292	Q183
GLY	A1712	L1618	I1504	P1413	Q1308	R1195	P1099	X991	A792	N682	E588	I485	Q384	E293	L184
PRO	G1713	L1618	R1503	P1413	Q1308	R1196	P1099	X992	A793	N683	D589	Q486	Q384	E294	
ARG	L1714	V1619	Q1507	D1414	V1309	R1197	D1100	X993	R793	G683	L590	R487	T389	L301	R195
PRO		P1620	T1508	G1415	D1310	X1199	V1103	X994	H795	A684	L593	I488	T389	L301	
ASP	P1722	R1621	D1511	V1416	F1311	X1204	G1104	X995	T796	S686	L594	R489	V390	I305	I198
ASP	E1723	F1622		L1417	F1311	X1205	R1105	X996	Q797	S687	L595	L490	V393	I307	G202
ILE	Y1724	T1624	D1514	L1417	F1311	X1206	G1106	X997	D798	R688	L598	V501	E395	I307	D203
THR	S1725	L1625				X1207		X998	F799						R204
PHE								X999							P205
ASP	E1730		V1519	Q1421	R1315	X1207	V1110	X1000	E803	D684	R602	R504	R400	W311	P206
ALA	V1731	R1634		F1422	G1317	X1212	F1111	X1001	E803	I695	R602	R505		T314	P207
ALA	L1732		L1530	T1423	G1317	X1212		X1002	A808	H696					
ASP	N1733	V1637	E1531	Q1424	I1318	X1213	A1117	X1003	A808	E697	N606	Q508	P405	V315	V208
ASP	N1734	P1638	I1532	V1425	D1319	X1214	A1118	X1004	X929	I698			T406	G316	S209
ALA	E1735	A1639	V1533	V1430	V1320	X1215	T1119	X1005	X930	D611	G613	R511	V407	I317	V210
THR						X1216	E1120	X1006	X931		G614		V403		T211
VAL						X1217		X1007	L216	A701			R409	E327	
ALA						X1218	F1123	X1008	E817	L709	P618	A515	L410	S328	L222
ALA						X1219	L1128	X1009	X934	A713		I517	D412	L330	V232
ILE	W1652					X1220	V1125	X1010	X935		S621				L233
ALA						X1221	I1126	X1011	X936						
ALA						X1222	E1127	X1012	X937						
LEU						X1223	G1128	X1013	X938	A716				W336	
LEU						X1224	L1129	X1014	X939	L416					
SER						X1225	L1129	X1014	X940	V521	L625			E339	V236
ALA						X1226		X1015	X941	V522				L417	L237
LYS						X1227		X1016	X942	S523				I340	S238
NET						X1228		X1017	X943	T419				T341	
ARG						X1229		X1018	X944	K420				E342	T248
ILE						X1230		X1019	X945	I526				I343	T249
ASP						X1231		X1020	X946	D634				H344	G250
GLN						X1232		X1021	X947						T251
GLU						X1233		X1022	X948						
GLU						X1234		X1023	X949						
GLU						X1235		X1024	X950						
GLU						X1236		X1025	X951						
GLU						X1237		X1026	X952						
GLU						X1238		X1027	X953						
GLU						X1239		X1028	X954						
GLU						X1240		X1029	X955						
GLU						X1241		X1030	X956						
GLU						X1242		X1031	X957						
GLU						X1243		X1032	X958						
GLU						X1244		X1033	X959						
GLU						X1245		X1034	X960						
GLU						X1246		X1035	X961						
GLU						X1247		X1036	X962						
GLU						X1248		X1037	X963						
GLU						X1249		X1038	X964						
GLU						X1250		X1039	X965						
GLU						X1251		X1040	X966						
GLU						X1252		X1041	X967						
GLU						X1253		X1042	X968						
GLU						X1254		X1043	X969						
GLU						X1255		X1044	X970						
GLU						X1256		X1045	X971						
GLU						X1257		X1046	X972						
GLU						X1258		X1047	X973						
GLU						X1259		X1048	X974						
GLU						X1260		X1049	X975						
GLU						X1261		X1050	X976						
GLU						X1262		X1051	X977						
GLU						X1263		X1052	X978						
GLU						X1264		X1053	X979						
GLU						X1265		X1054	X980						
GLU						X1266		X1055	X981						
GLU						X1267		X1056	X982						
GLU						X1268		X1057	X983						
GLU						X1269		X1058	X984						
GLU						X1270		X1059	X985						
GLU						X1271		X1060	X986						
GLU						X1272		X1061	X987						
GLU						X1273		X1062	X988						
GLU						X1274		X1063	X989						
GLU						X1275		X1064	X990						
GLU						X1276		X1065	X991						
GLU						X1277		X1066	X992						
GLU						X1278		X1067	X993						
GLU						X1279		X1068	X994						
GLU						X1280		X1069	X995						
GLU						X1281		X1070	X996						
GLU						X1282		X1071	X997						
GLU						X1283		X1072	X998						
GLU						X1284		X1073	X999						
GLU						X1285		X1074	X1000						
GLU						X1286		X1075	X1001						
GLU						X1287		X1076	X1002						
GLU						X1288		X1077	X1003						
GLU						X1289		X1078	X1004						
GLU						X1290		X1079	X1005						
GLU						X1291		X1080	X1006						
GLU						X1292		X1081	X1007						
GLU						X1293		X1082	X1008						
GLU						X1294		X1083	X1009						
GLU						X1295		X1084	X1010						
GLU						X1296		X1085	X1011						
GLU						X1297		X1086	X1012						
GLU						X1298		X1087	X1013						
GLU						X1299		X1088	X1014						
GLU						X1300		X1089	X1015						
GLU						X1301		X1090	X1016						
GLU						X1302		X1091	X1017						
GLU						X1303		X1092	X1018						
GLU						X1304		X1093	X1019						
GLU						X1305		X1094	X1020						
GLU						X1306		X1095	X1021						
GLU						X1307		X1096	X1022						
GLU						X1308		X1097	X1023						
GLU						X1309		X1098	X1024						
GLU						X1310		X1099	X1025						
GLU						X1311		X1100	X1026						
GLU						X1312		X1101	X1027						
GLU						X1313		X1102	X1028						
GLU						X1314		X1103	X1029						
GLU						X1315		X1104	X1030						
GLU						X1316		X1105	X1031						
GLU						X1317		X1106	X1032						
GLU						X1318		X1107	X1033						
GLU						X1319		X1108	X1034						
GLU						X1320		X1109	X1035						
GLU						X1321		X1110	X1036						
GLU						X1322		X1111	X1037						
GLU						X1323		X1112	X1038						
GLU						X1324		X1113	X1039						
GLU						X13									

G2992	L2906	A2911	R2916	G2919	N2920	P2921	L2922	P2923	L2924	V2925	S2926	Q2927	L2930	K2935	G2936	A2939	V2940	F2941	Q2942	M2943	L2946	G2947	Q2948	R2951	V2954	P2955	P2957	N2958	S2960	L2961	D2962	D2966	W2976	V2977	R2978	E2979	P2980	L2983	R2984	G2985	K2986	F2987	P2988	L2989								
R2808	L2809	G2810	F2811	L2812	Q2815	L2820	L2821	L2822	A2823	R2824	L2827	A2828	L2829	K2830	M2831	G2832	L2833	P2834	V2835	Q2843	S2844	F2845	A2846	G2847	G2848	G2859	A2860	L2861	T2871	L2876	L2879	G2880	V2881	G2882	A2883	D2884	D2885	I2886	L2889	S2890	K2891	H2892	D2893	T2894	S2895	T2896	P2901	N2902	E2903			
Q2711	E2712	V2713	V2717	S2618	R2619	T2620	G2622	A2623	Q2624	L2625	D2630	P2631	T2632	V2633	D2645	R2646	V2647	A2648	L2649	W2650	N2651	L2754	A2755	V2751	V2762	L2763	A2764	G2765	D2768	D2769	L2770	E2773	L2776	G2779	T2784	A2785	D2786	T2787	E2788	M2789	M2790	R2791	K2799	L2700	A2704	W2599	G2470	P2471	Y2472	R2603	R2610	V2611
P2612	R2613	K2614	L2487	L2489	V2492	L2495	K2503	W2504	E2505	W2512	Y2513	L2520	P2521	F2522	E2523	C2524	E2525	L2526	X2428	Y2527	E2528	R2541	E2542	F2543	P2551	D2552	H2553	A2554	L2557	L2558	E2574	F2580	D2584	P2585	E2586	R2591	P2592	L2469	G2470	P2471	Y2472	R2603	R2610	V2611								
L2398	K2261	W2265	Q2268	L2274	L2277	R2286	L2287	H2288	M2416	S2417	G2418	D2421	X2422	X2425	X2426	X2427	X2428	X2429	X2430	X2431	X2432	X2433	X2434	X2435	X2436	X2437	X2442	X2443	X2444	X2445	X2448	X2449	X2450	X2451	X2452	X2453	D2454	A2458	V2361	L2236	M2372	F2238	L2376	K2391	V2392	D2393	L2394	T2395	R2478			
D2136	E2137	V2140	V2141	T2163	V2164	I2165	A2166	T2167	R2170	D2173	R2175	L2176	K2180	R2188	F2189	T2192	W2194	V2195	V2196	F2197	K2310	R2319	W2200	D2205	L2209	V2210	E2211	W2212	W2213	G2214	T2215	E2216	K2229	P2234	T2235	X2123	X2124	X2125	X2126	X2127	X2128	W2245	A2246	X2129	X2130	X2131	X2132	P2245	Y2135			
GLU	ARG	ALA	VAL	THR	LYS	THR	TRP	GLU	LEU	ALA	ILE	ASP	GLY	PRO	ALA	GLY	TRP	ALA	LYS	ASP	GLY	HIS	VAL	THR	GLY	LEU	ALA	GLY	LEU	VAL	THR	LYS	THR	ARG	GLY	LEU	ASP	VAL	HIS	ALA	ILE	ASP	GLY	ASN	ASP	GLN	VAL	THR	LYS	LEU	THR	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	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	59000	Depositor
Image detector	FEI FALCON I	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%)	46	83
1	B	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	46	83
1	C	2637/3089 (85%)	2489 (94%)	139 (5%)	9 (0%)	46	83
1	D	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	46	83
1	E	2637/3089 (85%)	2488 (94%)	141 (5%)	8 (0%)	46	83
1	F	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	46	83
All	All	15822/18534 (85%)	14931 (94%)	840 (5%)	51 (0%)	50	83

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%)	35	70
1	B	2076/2264 (92%)	1986 (96%)	90 (4%)	35	70
1	C	2076/2264 (92%)	1987 (96%)	89 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	2076 / 2264 (92%)	1987 (96%)	89 (4%)	35	70
1	E	2076 / 2264 (92%)	1987 (96%)	89 (4%)	35	70
1	F	2076 / 2264 (92%)	1987 (96%)	89 (4%)	35	70
All	All	12456 / 13584 (92%)	11921 (96%)	535 (4%)	40	70

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	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	B	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	C	4000	-	32,33,33	1.22	3 (9%)	34,50,50	1.70	7 (20%)
2	FMN	D	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	E	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	F	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.70	7 (20%)

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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4000	FMN	C5A-N5	2.23	1.38	1.35
2	A	4000	FMN	C5A-N5	2.24	1.38	1.35
2	B	4000	FMN	C5A-N5	2.25	1.38	1.35
2	D	4000	FMN	C5A-N5	2.30	1.38	1.35
2	C	4000	FMN	C5A-N5	2.31	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	4000	FMN	N3-C2-N1	-4.47	120.16	127.69
2	B	4000	FMN	N3-C2-N1	-4.46	120.19	127.69
2	D	4000	FMN	N3-C2-N1	-4.45	120.19	127.69
2	E	4000	FMN	N3-C2-N1	-4.45	120.20	127.69
2	C	4000	FMN	N3-C2-N1	-4.44	120.22	127.69

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.