wwPDB EM Validation Summary Report (i)

May 26, 2026 – 10:20 AM EDT

PDB ID	:	11CK / pdb_000011ck
EMDB ID	:	EMD-75617
Title	:	Structure of human TRPV1 in complex with 6-Iodo-CAP (CAY10448)
Authors	:	Lopez, K.E.; Van Horn, W.D.
Deposited on	:	2026-02-17
Resolution	:	2.90 Å(reported)
Based on initial model	:	11CN

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

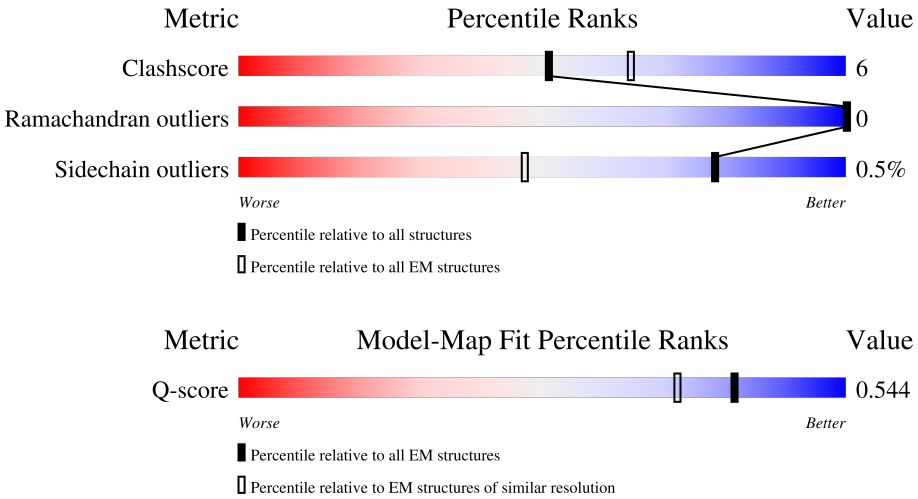
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1100	9% 42% 6% 52%
1	B	1100	9% 41% 7% 52%
1	C	1100	9% 41% 7% 52%
1	D	1100	9% 42% 6% 52%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17340 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	531	Total	C	N	O	S	0	0
			4312	2826	694	763	29		
1	B	531	Total	C	N	O	S	0	0
			4312	2826	694	763	29		
1	C	531	Total	C	N	O	S	0	0
			4312	2826	694	763	29		
1	D	531	Total	C	N	O	S	0	0
			4312	2826	694	763	29		

There are 1048 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	MET	variant	UNP Q8NER1
A	840	GLY	-	expression tag	UNP Q8NER1
A	841	THR	-	expression tag	UNP Q8NER1
A	842	LEU	-	expression tag	UNP Q8NER1
A	843	GLU	-	expression tag	UNP Q8NER1
A	844	VAL	-	expression tag	UNP Q8NER1
A	845	LEU	-	expression tag	UNP Q8NER1
A	846	PHE	-	expression tag	UNP Q8NER1
A	847	GLN	-	expression tag	UNP Q8NER1
A	848	GLY	-	expression tag	UNP Q8NER1
A	849	PRO	-	expression tag	UNP Q8NER1
A	850	GLY	-	expression tag	UNP Q8NER1
A	851	GLY	-	expression tag	UNP Q8NER1
A	852	SER	-	expression tag	UNP Q8NER1
A	853	GLY	-	expression tag	UNP Q8NER1
A	854	GLY	-	expression tag	UNP Q8NER1
A	855	SER	-	expression tag	UNP Q8NER1
A	856	ALA	-	expression tag	UNP Q8NER1
A	857	SER	-	expression tag	UNP Q8NER1
A	858	VAL	-	expression tag	UNP Q8NER1
A	859	ILE	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	860	LYS	-	expression tag	UNP Q8NER1
A	861	PRO	-	expression tag	UNP Q8NER1
A	862	GLU	-	expression tag	UNP Q8NER1
A	863	MET	-	expression tag	UNP Q8NER1
A	864	LYS	-	expression tag	UNP Q8NER1
A	865	ILE	-	expression tag	UNP Q8NER1
A	866	LYS	-	expression tag	UNP Q8NER1
A	867	LEU	-	expression tag	UNP Q8NER1
A	868	ARG	-	expression tag	UNP Q8NER1
A	869	MET	-	expression tag	UNP Q8NER1
A	870	GLU	-	expression tag	UNP Q8NER1
A	871	GLY	-	expression tag	UNP Q8NER1
A	872	ALA	-	expression tag	UNP Q8NER1
A	873	VAL	-	expression tag	UNP Q8NER1
A	874	ASN	-	expression tag	UNP Q8NER1
A	875	GLY	-	expression tag	UNP Q8NER1
A	876	HIS	-	expression tag	UNP Q8NER1
A	877	LYS	-	expression tag	UNP Q8NER1
A	878	PHE	-	expression tag	UNP Q8NER1
A	879	VAL	-	expression tag	UNP Q8NER1
A	880	ILE	-	expression tag	UNP Q8NER1
A	881	GLU	-	expression tag	UNP Q8NER1
A	882	GLY	-	expression tag	UNP Q8NER1
A	883	GLU	-	expression tag	UNP Q8NER1
A	884	GLY	-	expression tag	UNP Q8NER1
A	885	ILE	-	expression tag	UNP Q8NER1
A	886	GLY	-	expression tag	UNP Q8NER1
A	887	LYS	-	expression tag	UNP Q8NER1
A	888	PRO	-	expression tag	UNP Q8NER1
A	889	TYR	-	expression tag	UNP Q8NER1
A	890	GLU	-	expression tag	UNP Q8NER1
A	891	GLY	-	expression tag	UNP Q8NER1
A	892	THR	-	expression tag	UNP Q8NER1
A	893	GLN	-	expression tag	UNP Q8NER1
A	894	THR	-	expression tag	UNP Q8NER1
A	895	LEU	-	expression tag	UNP Q8NER1
A	896	ASP	-	expression tag	UNP Q8NER1
A	897	LEU	-	expression tag	UNP Q8NER1
A	898	THR	-	expression tag	UNP Q8NER1
A	899	VAL	-	expression tag	UNP Q8NER1
A	900	GLU	-	expression tag	UNP Q8NER1
A	901	GLU	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	902	GLY	-	expression tag	UNP Q8NER1
A	903	ALA	-	expression tag	UNP Q8NER1
A	904	PRO	-	expression tag	UNP Q8NER1
A	905	LEU	-	expression tag	UNP Q8NER1
A	906	PRO	-	expression tag	UNP Q8NER1
A	907	PHE	-	expression tag	UNP Q8NER1
A	908	SER	-	expression tag	UNP Q8NER1
A	909	TYR	-	expression tag	UNP Q8NER1
A	910	ASP	-	expression tag	UNP Q8NER1
A	911	ILE	-	expression tag	UNP Q8NER1
A	912	LEU	-	expression tag	UNP Q8NER1
A	913	THR	-	expression tag	UNP Q8NER1
A	914	PRO	-	expression tag	UNP Q8NER1
A	915	ALA	-	expression tag	UNP Q8NER1
A	916	PHE	-	expression tag	UNP Q8NER1
A	917	GLN	-	expression tag	UNP Q8NER1
A	918	TYR	-	expression tag	UNP Q8NER1
A	919	GLY	-	expression tag	UNP Q8NER1
A	920	ASN	-	expression tag	UNP Q8NER1
A	921	ARG	-	expression tag	UNP Q8NER1
A	922	ALA	-	expression tag	UNP Q8NER1
A	923	PHE	-	expression tag	UNP Q8NER1
A	924	THR	-	expression tag	UNP Q8NER1
A	925	LYS	-	expression tag	UNP Q8NER1
A	926	TYR	-	expression tag	UNP Q8NER1
A	927	PRO	-	expression tag	UNP Q8NER1
A	928	GLU	-	expression tag	UNP Q8NER1
A	929	ASP	-	expression tag	UNP Q8NER1
A	930	ILE	-	expression tag	UNP Q8NER1
A	931	PRO	-	expression tag	UNP Q8NER1
A	932	ASP	-	expression tag	UNP Q8NER1
A	933	TYR	-	expression tag	UNP Q8NER1
A	934	PHE	-	expression tag	UNP Q8NER1
A	935	LYS	-	expression tag	UNP Q8NER1
A	936	GLN	-	expression tag	UNP Q8NER1
A	937	ALA	-	expression tag	UNP Q8NER1
A	938	PHE	-	expression tag	UNP Q8NER1
A	939	PRO	-	expression tag	UNP Q8NER1
A	940	GLU	-	expression tag	UNP Q8NER1
A	941	GLY	-	expression tag	UNP Q8NER1
A	942	TYR	-	expression tag	UNP Q8NER1
A	943	SER	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	944	TRP	-	expression tag	UNP Q8NER1
A	945	GLU	-	expression tag	UNP Q8NER1
A	946	ARG	-	expression tag	UNP Q8NER1
A	947	SER	-	expression tag	UNP Q8NER1
A	948	MET	-	expression tag	UNP Q8NER1
A	949	THR	-	expression tag	UNP Q8NER1
A	950	TYR	-	expression tag	UNP Q8NER1
A	951	GLU	-	expression tag	UNP Q8NER1
A	952	ASP	-	expression tag	UNP Q8NER1
A	953	GLN	-	expression tag	UNP Q8NER1
A	954	GLY	-	expression tag	UNP Q8NER1
A	955	ILE	-	expression tag	UNP Q8NER1
A	956	CYS	-	expression tag	UNP Q8NER1
A	957	ILE	-	expression tag	UNP Q8NER1
A	958	ALA	-	expression tag	UNP Q8NER1
A	959	THR	-	expression tag	UNP Q8NER1
A	960	SER	-	expression tag	UNP Q8NER1
A	961	ASP	-	expression tag	UNP Q8NER1
A	962	ILE	-	expression tag	UNP Q8NER1
A	963	THR	-	expression tag	UNP Q8NER1
A	964	MET	-	expression tag	UNP Q8NER1
A	965	GLU	-	expression tag	UNP Q8NER1
A	966	GLY	-	expression tag	UNP Q8NER1
A	967	ASP	-	expression tag	UNP Q8NER1
A	968	CYS	-	expression tag	UNP Q8NER1
A	969	PHE	-	expression tag	UNP Q8NER1
A	970	PHE	-	expression tag	UNP Q8NER1
A	971	TYR	-	expression tag	UNP Q8NER1
A	972	GLU	-	expression tag	UNP Q8NER1
A	973	ILE	-	expression tag	UNP Q8NER1
A	974	ARG	-	expression tag	UNP Q8NER1
A	975	PHE	-	expression tag	UNP Q8NER1
A	976	ASP	-	expression tag	UNP Q8NER1
A	977	GLY	-	expression tag	UNP Q8NER1
A	978	THR	-	expression tag	UNP Q8NER1
A	979	ASN	-	expression tag	UNP Q8NER1
A	980	PHE	-	expression tag	UNP Q8NER1
A	981	PRO	-	expression tag	UNP Q8NER1
A	982	PRO	-	expression tag	UNP Q8NER1
A	983	ASN	-	expression tag	UNP Q8NER1
A	984	GLY	-	expression tag	UNP Q8NER1
A	985	PRO	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	VAL	-	expression tag	UNP Q8NER1
A	987	MET	-	expression tag	UNP Q8NER1
A	988	GLN	-	expression tag	UNP Q8NER1
A	989	LYS	-	expression tag	UNP Q8NER1
A	990	LYS	-	expression tag	UNP Q8NER1
A	991	THR	-	expression tag	UNP Q8NER1
A	992	LEU	-	expression tag	UNP Q8NER1
A	993	LYS	-	expression tag	UNP Q8NER1
A	994	TRP	-	expression tag	UNP Q8NER1
A	995	GLU	-	expression tag	UNP Q8NER1
A	996	PRO	-	expression tag	UNP Q8NER1
A	997	SER	-	expression tag	UNP Q8NER1
A	998	THR	-	expression tag	UNP Q8NER1
A	999	GLU	-	expression tag	UNP Q8NER1
A	1000	LYS	-	expression tag	UNP Q8NER1
A	1001	MET	-	expression tag	UNP Q8NER1
A	1002	TYR	-	expression tag	UNP Q8NER1
A	1003	VAL	-	expression tag	UNP Q8NER1
A	1004	GLU	-	expression tag	UNP Q8NER1
A	1005	ASP	-	expression tag	UNP Q8NER1
A	1006	GLY	-	expression tag	UNP Q8NER1
A	1007	VAL	-	expression tag	UNP Q8NER1
A	1008	LEU	-	expression tag	UNP Q8NER1
A	1009	LYS	-	expression tag	UNP Q8NER1
A	1010	GLY	-	expression tag	UNP Q8NER1
A	1011	ASP	-	expression tag	UNP Q8NER1
A	1012	VAL	-	expression tag	UNP Q8NER1
A	1013	GLU	-	expression tag	UNP Q8NER1
A	1014	MET	-	expression tag	UNP Q8NER1
A	1015	ALA	-	expression tag	UNP Q8NER1
A	1016	LEU	-	expression tag	UNP Q8NER1
A	1017	LEU	-	expression tag	UNP Q8NER1
A	1018	LEU	-	expression tag	UNP Q8NER1
A	1019	GLU	-	expression tag	UNP Q8NER1
A	1020	GLY	-	expression tag	UNP Q8NER1
A	1021	GLY	-	expression tag	UNP Q8NER1
A	1022	GLY	-	expression tag	UNP Q8NER1
A	1023	HIS	-	expression tag	UNP Q8NER1
A	1024	TYR	-	expression tag	UNP Q8NER1
A	1025	ARG	-	expression tag	UNP Q8NER1
A	1026	CYS	-	expression tag	UNP Q8NER1
A	1027	ASP	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1028	PHE	-	expression tag	UNP Q8NER1
A	1029	LYS	-	expression tag	UNP Q8NER1
A	1030	THR	-	expression tag	UNP Q8NER1
A	1031	THR	-	expression tag	UNP Q8NER1
A	1032	TYR	-	expression tag	UNP Q8NER1
A	1033	LYS	-	expression tag	UNP Q8NER1
A	1034	ALA	-	expression tag	UNP Q8NER1
A	1035	LYS	-	expression tag	UNP Q8NER1
A	1036	LYS	-	expression tag	UNP Q8NER1
A	1037	ASP	-	expression tag	UNP Q8NER1
A	1038	VAL	-	expression tag	UNP Q8NER1
A	1039	ARG	-	expression tag	UNP Q8NER1
A	1040	LEU	-	expression tag	UNP Q8NER1
A	1041	PRO	-	expression tag	UNP Q8NER1
A	1042	ASP	-	expression tag	UNP Q8NER1
A	1043	ALA	-	expression tag	UNP Q8NER1
A	1044	HIS	-	expression tag	UNP Q8NER1
A	1045	GLU	-	expression tag	UNP Q8NER1
A	1046	VAL	-	expression tag	UNP Q8NER1
A	1047	ASP	-	expression tag	UNP Q8NER1
A	1048	HIS	-	expression tag	UNP Q8NER1
A	1049	ARG	-	expression tag	UNP Q8NER1
A	1050	ILE	-	expression tag	UNP Q8NER1
A	1051	GLU	-	expression tag	UNP Q8NER1
A	1052	ILE	-	expression tag	UNP Q8NER1
A	1053	LEU	-	expression tag	UNP Q8NER1
A	1054	SER	-	expression tag	UNP Q8NER1
A	1055	HIS	-	expression tag	UNP Q8NER1
A	1056	ASP	-	expression tag	UNP Q8NER1
A	1057	LYS	-	expression tag	UNP Q8NER1
A	1058	ASP	-	expression tag	UNP Q8NER1
A	1059	TYR	-	expression tag	UNP Q8NER1
A	1060	ASN	-	expression tag	UNP Q8NER1
A	1061	LYS	-	expression tag	UNP Q8NER1
A	1062	VAL	-	expression tag	UNP Q8NER1
A	1063	ARG	-	expression tag	UNP Q8NER1
A	1064	LEU	-	expression tag	UNP Q8NER1
A	1065	TYR	-	expression tag	UNP Q8NER1
A	1066	GLU	-	expression tag	UNP Q8NER1
A	1067	HIS	-	expression tag	UNP Q8NER1
A	1068	ALA	-	expression tag	UNP Q8NER1
A	1069	GLU	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1070	ALA	-	expression tag	UNP Q8NER1
A	1071	ARG	-	expression tag	UNP Q8NER1
A	1072	TYR	-	expression tag	UNP Q8NER1
A	1073	SER	-	expression tag	UNP Q8NER1
A	1074	GLY	-	expression tag	UNP Q8NER1
A	1075	GLY	-	expression tag	UNP Q8NER1
A	1076	GLY	-	expression tag	UNP Q8NER1
A	1077	SER	-	expression tag	UNP Q8NER1
A	1078	GLY	-	expression tag	UNP Q8NER1
A	1079	GLY	-	expression tag	UNP Q8NER1
A	1080	GLY	-	expression tag	UNP Q8NER1
A	1081	HIS	-	expression tag	UNP Q8NER1
A	1082	HIS	-	expression tag	UNP Q8NER1
A	1083	HIS	-	expression tag	UNP Q8NER1
A	1084	HIS	-	expression tag	UNP Q8NER1
A	1085	HIS	-	expression tag	UNP Q8NER1
A	1086	HIS	-	expression tag	UNP Q8NER1
A	1087	HIS	-	expression tag	UNP Q8NER1
A	1088	GLY	-	expression tag	UNP Q8NER1
A	1089	GLY	-	expression tag	UNP Q8NER1
A	1090	SER	-	expression tag	UNP Q8NER1
A	1091	GLY	-	expression tag	UNP Q8NER1
A	1092	GLY	-	expression tag	UNP Q8NER1
A	1093	TRP	-	expression tag	UNP Q8NER1
A	1094	SER	-	expression tag	UNP Q8NER1
A	1095	HIS	-	expression tag	UNP Q8NER1
A	1096	PRO	-	expression tag	UNP Q8NER1
A	1097	GLN	-	expression tag	UNP Q8NER1
A	1098	PHE	-	expression tag	UNP Q8NER1
A	1099	GLU	-	expression tag	UNP Q8NER1
A	1100	LYS	-	expression tag	UNP Q8NER1
B	315	ILE	MET	variant	UNP Q8NER1
B	840	GLY	-	expression tag	UNP Q8NER1
B	841	THR	-	expression tag	UNP Q8NER1
B	842	LEU	-	expression tag	UNP Q8NER1
B	843	GLU	-	expression tag	UNP Q8NER1
B	844	VAL	-	expression tag	UNP Q8NER1
B	845	LEU	-	expression tag	UNP Q8NER1
B	846	PHE	-	expression tag	UNP Q8NER1
B	847	GLN	-	expression tag	UNP Q8NER1
B	848	GLY	-	expression tag	UNP Q8NER1
B	849	PRO	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	850	GLY	-	expression tag	UNP Q8NER1
B	851	GLY	-	expression tag	UNP Q8NER1
B	852	SER	-	expression tag	UNP Q8NER1
B	853	GLY	-	expression tag	UNP Q8NER1
B	854	GLY	-	expression tag	UNP Q8NER1
B	855	SER	-	expression tag	UNP Q8NER1
B	856	ALA	-	expression tag	UNP Q8NER1
B	857	SER	-	expression tag	UNP Q8NER1
B	858	VAL	-	expression tag	UNP Q8NER1
B	859	ILE	-	expression tag	UNP Q8NER1
B	860	LYS	-	expression tag	UNP Q8NER1
B	861	PRO	-	expression tag	UNP Q8NER1
B	862	GLU	-	expression tag	UNP Q8NER1
B	863	MET	-	expression tag	UNP Q8NER1
B	864	LYS	-	expression tag	UNP Q8NER1
B	865	ILE	-	expression tag	UNP Q8NER1
B	866	LYS	-	expression tag	UNP Q8NER1
B	867	LEU	-	expression tag	UNP Q8NER1
B	868	ARG	-	expression tag	UNP Q8NER1
B	869	MET	-	expression tag	UNP Q8NER1
B	870	GLU	-	expression tag	UNP Q8NER1
B	871	GLY	-	expression tag	UNP Q8NER1
B	872	ALA	-	expression tag	UNP Q8NER1
B	873	VAL	-	expression tag	UNP Q8NER1
B	874	ASN	-	expression tag	UNP Q8NER1
B	875	GLY	-	expression tag	UNP Q8NER1
B	876	HIS	-	expression tag	UNP Q8NER1
B	877	LYS	-	expression tag	UNP Q8NER1
B	878	PHE	-	expression tag	UNP Q8NER1
B	879	VAL	-	expression tag	UNP Q8NER1
B	880	ILE	-	expression tag	UNP Q8NER1
B	881	GLU	-	expression tag	UNP Q8NER1
B	882	GLY	-	expression tag	UNP Q8NER1
B	883	GLU	-	expression tag	UNP Q8NER1
B	884	GLY	-	expression tag	UNP Q8NER1
B	885	ILE	-	expression tag	UNP Q8NER1
B	886	GLY	-	expression tag	UNP Q8NER1
B	887	LYS	-	expression tag	UNP Q8NER1
B	888	PRO	-	expression tag	UNP Q8NER1
B	889	TYR	-	expression tag	UNP Q8NER1
B	890	GLU	-	expression tag	UNP Q8NER1
B	891	GLY	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	892	THR	-	expression tag	UNP Q8NER1
B	893	GLN	-	expression tag	UNP Q8NER1
B	894	THR	-	expression tag	UNP Q8NER1
B	895	LEU	-	expression tag	UNP Q8NER1
B	896	ASP	-	expression tag	UNP Q8NER1
B	897	LEU	-	expression tag	UNP Q8NER1
B	898	THR	-	expression tag	UNP Q8NER1
B	899	VAL	-	expression tag	UNP Q8NER1
B	900	GLU	-	expression tag	UNP Q8NER1
B	901	GLU	-	expression tag	UNP Q8NER1
B	902	GLY	-	expression tag	UNP Q8NER1
B	903	ALA	-	expression tag	UNP Q8NER1
B	904	PRO	-	expression tag	UNP Q8NER1
B	905	LEU	-	expression tag	UNP Q8NER1
B	906	PRO	-	expression tag	UNP Q8NER1
B	907	PHE	-	expression tag	UNP Q8NER1
B	908	SER	-	expression tag	UNP Q8NER1
B	909	TYR	-	expression tag	UNP Q8NER1
B	910	ASP	-	expression tag	UNP Q8NER1
B	911	ILE	-	expression tag	UNP Q8NER1
B	912	LEU	-	expression tag	UNP Q8NER1
B	913	THR	-	expression tag	UNP Q8NER1
B	914	PRO	-	expression tag	UNP Q8NER1
B	915	ALA	-	expression tag	UNP Q8NER1
B	916	PHE	-	expression tag	UNP Q8NER1
B	917	GLN	-	expression tag	UNP Q8NER1
B	918	TYR	-	expression tag	UNP Q8NER1
B	919	GLY	-	expression tag	UNP Q8NER1
B	920	ASN	-	expression tag	UNP Q8NER1
B	921	ARG	-	expression tag	UNP Q8NER1
B	922	ALA	-	expression tag	UNP Q8NER1
B	923	PHE	-	expression tag	UNP Q8NER1
B	924	THR	-	expression tag	UNP Q8NER1
B	925	LYS	-	expression tag	UNP Q8NER1
B	926	TYR	-	expression tag	UNP Q8NER1
B	927	PRO	-	expression tag	UNP Q8NER1
B	928	GLU	-	expression tag	UNP Q8NER1
B	929	ASP	-	expression tag	UNP Q8NER1
B	930	ILE	-	expression tag	UNP Q8NER1
B	931	PRO	-	expression tag	UNP Q8NER1
B	932	ASP	-	expression tag	UNP Q8NER1
B	933	TYR	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	934	PHE	-	expression tag	UNP Q8NER1
B	935	LYS	-	expression tag	UNP Q8NER1
B	936	GLN	-	expression tag	UNP Q8NER1
B	937	ALA	-	expression tag	UNP Q8NER1
B	938	PHE	-	expression tag	UNP Q8NER1
B	939	PRO	-	expression tag	UNP Q8NER1
B	940	GLU	-	expression tag	UNP Q8NER1
B	941	GLY	-	expression tag	UNP Q8NER1
B	942	TYR	-	expression tag	UNP Q8NER1
B	943	SER	-	expression tag	UNP Q8NER1
B	944	TRP	-	expression tag	UNP Q8NER1
B	945	GLU	-	expression tag	UNP Q8NER1
B	946	ARG	-	expression tag	UNP Q8NER1
B	947	SER	-	expression tag	UNP Q8NER1
B	948	MET	-	expression tag	UNP Q8NER1
B	949	THR	-	expression tag	UNP Q8NER1
B	950	TYR	-	expression tag	UNP Q8NER1
B	951	GLU	-	expression tag	UNP Q8NER1
B	952	ASP	-	expression tag	UNP Q8NER1
B	953	GLN	-	expression tag	UNP Q8NER1
B	954	GLY	-	expression tag	UNP Q8NER1
B	955	ILE	-	expression tag	UNP Q8NER1
B	956	CYS	-	expression tag	UNP Q8NER1
B	957	ILE	-	expression tag	UNP Q8NER1
B	958	ALA	-	expression tag	UNP Q8NER1
B	959	THR	-	expression tag	UNP Q8NER1
B	960	SER	-	expression tag	UNP Q8NER1
B	961	ASP	-	expression tag	UNP Q8NER1
B	962	ILE	-	expression tag	UNP Q8NER1
B	963	THR	-	expression tag	UNP Q8NER1
B	964	MET	-	expression tag	UNP Q8NER1
B	965	GLU	-	expression tag	UNP Q8NER1
B	966	GLY	-	expression tag	UNP Q8NER1
B	967	ASP	-	expression tag	UNP Q8NER1
B	968	CYS	-	expression tag	UNP Q8NER1
B	969	PHE	-	expression tag	UNP Q8NER1
B	970	PHE	-	expression tag	UNP Q8NER1
B	971	TYR	-	expression tag	UNP Q8NER1
B	972	GLU	-	expression tag	UNP Q8NER1
B	973	ILE	-	expression tag	UNP Q8NER1
B	974	ARG	-	expression tag	UNP Q8NER1
B	975	PHE	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	976	ASP	-	expression tag	UNP Q8NER1
B	977	GLY	-	expression tag	UNP Q8NER1
B	978	THR	-	expression tag	UNP Q8NER1
B	979	ASN	-	expression tag	UNP Q8NER1
B	980	PHE	-	expression tag	UNP Q8NER1
B	981	PRO	-	expression tag	UNP Q8NER1
B	982	PRO	-	expression tag	UNP Q8NER1
B	983	ASN	-	expression tag	UNP Q8NER1
B	984	GLY	-	expression tag	UNP Q8NER1
B	985	PRO	-	expression tag	UNP Q8NER1
B	986	VAL	-	expression tag	UNP Q8NER1
B	987	MET	-	expression tag	UNP Q8NER1
B	988	GLN	-	expression tag	UNP Q8NER1
B	989	LYS	-	expression tag	UNP Q8NER1
B	990	LYS	-	expression tag	UNP Q8NER1
B	991	THR	-	expression tag	UNP Q8NER1
B	992	LEU	-	expression tag	UNP Q8NER1
B	993	LYS	-	expression tag	UNP Q8NER1
B	994	TRP	-	expression tag	UNP Q8NER1
B	995	GLU	-	expression tag	UNP Q8NER1
B	996	PRO	-	expression tag	UNP Q8NER1
B	997	SER	-	expression tag	UNP Q8NER1
B	998	THR	-	expression tag	UNP Q8NER1
B	999	GLU	-	expression tag	UNP Q8NER1
B	1000	LYS	-	expression tag	UNP Q8NER1
B	1001	MET	-	expression tag	UNP Q8NER1
B	1002	TYR	-	expression tag	UNP Q8NER1
B	1003	VAL	-	expression tag	UNP Q8NER1
B	1004	GLU	-	expression tag	UNP Q8NER1
B	1005	ASP	-	expression tag	UNP Q8NER1
B	1006	GLY	-	expression tag	UNP Q8NER1
B	1007	VAL	-	expression tag	UNP Q8NER1
B	1008	LEU	-	expression tag	UNP Q8NER1
B	1009	LYS	-	expression tag	UNP Q8NER1
B	1010	GLY	-	expression tag	UNP Q8NER1
B	1011	ASP	-	expression tag	UNP Q8NER1
B	1012	VAL	-	expression tag	UNP Q8NER1
B	1013	GLU	-	expression tag	UNP Q8NER1
B	1014	MET	-	expression tag	UNP Q8NER1
B	1015	ALA	-	expression tag	UNP Q8NER1
B	1016	LEU	-	expression tag	UNP Q8NER1
B	1017	LEU	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1018	LEU	-	expression tag	UNP Q8NER1
B	1019	GLU	-	expression tag	UNP Q8NER1
B	1020	GLY	-	expression tag	UNP Q8NER1
B	1021	GLY	-	expression tag	UNP Q8NER1
B	1022	GLY	-	expression tag	UNP Q8NER1
B	1023	HIS	-	expression tag	UNP Q8NER1
B	1024	TYR	-	expression tag	UNP Q8NER1
B	1025	ARG	-	expression tag	UNP Q8NER1
B	1026	CYS	-	expression tag	UNP Q8NER1
B	1027	ASP	-	expression tag	UNP Q8NER1
B	1028	PHE	-	expression tag	UNP Q8NER1
B	1029	LYS	-	expression tag	UNP Q8NER1
B	1030	THR	-	expression tag	UNP Q8NER1
B	1031	THR	-	expression tag	UNP Q8NER1
B	1032	TYR	-	expression tag	UNP Q8NER1
B	1033	LYS	-	expression tag	UNP Q8NER1
B	1034	ALA	-	expression tag	UNP Q8NER1
B	1035	LYS	-	expression tag	UNP Q8NER1
B	1036	LYS	-	expression tag	UNP Q8NER1
B	1037	ASP	-	expression tag	UNP Q8NER1
B	1038	VAL	-	expression tag	UNP Q8NER1
B	1039	ARG	-	expression tag	UNP Q8NER1
B	1040	LEU	-	expression tag	UNP Q8NER1
B	1041	PRO	-	expression tag	UNP Q8NER1
B	1042	ASP	-	expression tag	UNP Q8NER1
B	1043	ALA	-	expression tag	UNP Q8NER1
B	1044	HIS	-	expression tag	UNP Q8NER1
B	1045	GLU	-	expression tag	UNP Q8NER1
B	1046	VAL	-	expression tag	UNP Q8NER1
B	1047	ASP	-	expression tag	UNP Q8NER1
B	1048	HIS	-	expression tag	UNP Q8NER1
B	1049	ARG	-	expression tag	UNP Q8NER1
B	1050	ILE	-	expression tag	UNP Q8NER1
B	1051	GLU	-	expression tag	UNP Q8NER1
B	1052	ILE	-	expression tag	UNP Q8NER1
B	1053	LEU	-	expression tag	UNP Q8NER1
B	1054	SER	-	expression tag	UNP Q8NER1
B	1055	HIS	-	expression tag	UNP Q8NER1
B	1056	ASP	-	expression tag	UNP Q8NER1
B	1057	LYS	-	expression tag	UNP Q8NER1
B	1058	ASP	-	expression tag	UNP Q8NER1
B	1059	TYR	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1060	ASN	-	expression tag	UNP Q8NER1
B	1061	LYS	-	expression tag	UNP Q8NER1
B	1062	VAL	-	expression tag	UNP Q8NER1
B	1063	ARG	-	expression tag	UNP Q8NER1
B	1064	LEU	-	expression tag	UNP Q8NER1
B	1065	TYR	-	expression tag	UNP Q8NER1
B	1066	GLU	-	expression tag	UNP Q8NER1
B	1067	HIS	-	expression tag	UNP Q8NER1
B	1068	ALA	-	expression tag	UNP Q8NER1
B	1069	GLU	-	expression tag	UNP Q8NER1
B	1070	ALA	-	expression tag	UNP Q8NER1
B	1071	ARG	-	expression tag	UNP Q8NER1
B	1072	TYR	-	expression tag	UNP Q8NER1
B	1073	SER	-	expression tag	UNP Q8NER1
B	1074	GLY	-	expression tag	UNP Q8NER1
B	1075	GLY	-	expression tag	UNP Q8NER1
B	1076	GLY	-	expression tag	UNP Q8NER1
B	1077	SER	-	expression tag	UNP Q8NER1
B	1078	GLY	-	expression tag	UNP Q8NER1
B	1079	GLY	-	expression tag	UNP Q8NER1
B	1080	GLY	-	expression tag	UNP Q8NER1
B	1081	HIS	-	expression tag	UNP Q8NER1
B	1082	HIS	-	expression tag	UNP Q8NER1
B	1083	HIS	-	expression tag	UNP Q8NER1
B	1084	HIS	-	expression tag	UNP Q8NER1
B	1085	HIS	-	expression tag	UNP Q8NER1
B	1086	HIS	-	expression tag	UNP Q8NER1
B	1087	HIS	-	expression tag	UNP Q8NER1
B	1088	GLY	-	expression tag	UNP Q8NER1
B	1089	GLY	-	expression tag	UNP Q8NER1
B	1090	SER	-	expression tag	UNP Q8NER1
B	1091	GLY	-	expression tag	UNP Q8NER1
B	1092	GLY	-	expression tag	UNP Q8NER1
B	1093	TRP	-	expression tag	UNP Q8NER1
B	1094	SER	-	expression tag	UNP Q8NER1
B	1095	HIS	-	expression tag	UNP Q8NER1
B	1096	PRO	-	expression tag	UNP Q8NER1
B	1097	GLN	-	expression tag	UNP Q8NER1
B	1098	PHE	-	expression tag	UNP Q8NER1
B	1099	GLU	-	expression tag	UNP Q8NER1
B	1100	LYS	-	expression tag	UNP Q8NER1
C	315	ILE	MET	variant	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	840	GLY	-	expression tag	UNP Q8NER1
C	841	THR	-	expression tag	UNP Q8NER1
C	842	LEU	-	expression tag	UNP Q8NER1
C	843	GLU	-	expression tag	UNP Q8NER1
C	844	VAL	-	expression tag	UNP Q8NER1
C	845	LEU	-	expression tag	UNP Q8NER1
C	846	PHE	-	expression tag	UNP Q8NER1
C	847	GLN	-	expression tag	UNP Q8NER1
C	848	GLY	-	expression tag	UNP Q8NER1
C	849	PRO	-	expression tag	UNP Q8NER1
C	850	GLY	-	expression tag	UNP Q8NER1
C	851	GLY	-	expression tag	UNP Q8NER1
C	852	SER	-	expression tag	UNP Q8NER1
C	853	GLY	-	expression tag	UNP Q8NER1
C	854	GLY	-	expression tag	UNP Q8NER1
C	855	SER	-	expression tag	UNP Q8NER1
C	856	ALA	-	expression tag	UNP Q8NER1
C	857	SER	-	expression tag	UNP Q8NER1
C	858	VAL	-	expression tag	UNP Q8NER1
C	859	ILE	-	expression tag	UNP Q8NER1
C	860	LYS	-	expression tag	UNP Q8NER1
C	861	PRO	-	expression tag	UNP Q8NER1
C	862	GLU	-	expression tag	UNP Q8NER1
C	863	MET	-	expression tag	UNP Q8NER1
C	864	LYS	-	expression tag	UNP Q8NER1
C	865	ILE	-	expression tag	UNP Q8NER1
C	866	LYS	-	expression tag	UNP Q8NER1
C	867	LEU	-	expression tag	UNP Q8NER1
C	868	ARG	-	expression tag	UNP Q8NER1
C	869	MET	-	expression tag	UNP Q8NER1
C	870	GLU	-	expression tag	UNP Q8NER1
C	871	GLY	-	expression tag	UNP Q8NER1
C	872	ALA	-	expression tag	UNP Q8NER1
C	873	VAL	-	expression tag	UNP Q8NER1
C	874	ASN	-	expression tag	UNP Q8NER1
C	875	GLY	-	expression tag	UNP Q8NER1
C	876	HIS	-	expression tag	UNP Q8NER1
C	877	LYS	-	expression tag	UNP Q8NER1
C	878	PHE	-	expression tag	UNP Q8NER1
C	879	VAL	-	expression tag	UNP Q8NER1
C	880	ILE	-	expression tag	UNP Q8NER1
C	881	GLU	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	882	GLY	-	expression tag	UNP Q8NER1
C	883	GLU	-	expression tag	UNP Q8NER1
C	884	GLY	-	expression tag	UNP Q8NER1
C	885	ILE	-	expression tag	UNP Q8NER1
C	886	GLY	-	expression tag	UNP Q8NER1
C	887	LYS	-	expression tag	UNP Q8NER1
C	888	PRO	-	expression tag	UNP Q8NER1
C	889	TYR	-	expression tag	UNP Q8NER1
C	890	GLU	-	expression tag	UNP Q8NER1
C	891	GLY	-	expression tag	UNP Q8NER1
C	892	THR	-	expression tag	UNP Q8NER1
C	893	GLN	-	expression tag	UNP Q8NER1
C	894	THR	-	expression tag	UNP Q8NER1
C	895	LEU	-	expression tag	UNP Q8NER1
C	896	ASP	-	expression tag	UNP Q8NER1
C	897	LEU	-	expression tag	UNP Q8NER1
C	898	THR	-	expression tag	UNP Q8NER1
C	899	VAL	-	expression tag	UNP Q8NER1
C	900	GLU	-	expression tag	UNP Q8NER1
C	901	GLU	-	expression tag	UNP Q8NER1
C	902	GLY	-	expression tag	UNP Q8NER1
C	903	ALA	-	expression tag	UNP Q8NER1
C	904	PRO	-	expression tag	UNP Q8NER1
C	905	LEU	-	expression tag	UNP Q8NER1
C	906	PRO	-	expression tag	UNP Q8NER1
C	907	PHE	-	expression tag	UNP Q8NER1
C	908	SER	-	expression tag	UNP Q8NER1
C	909	TYR	-	expression tag	UNP Q8NER1
C	910	ASP	-	expression tag	UNP Q8NER1
C	911	ILE	-	expression tag	UNP Q8NER1
C	912	LEU	-	expression tag	UNP Q8NER1
C	913	THR	-	expression tag	UNP Q8NER1
C	914	PRO	-	expression tag	UNP Q8NER1
C	915	ALA	-	expression tag	UNP Q8NER1
C	916	PHE	-	expression tag	UNP Q8NER1
C	917	GLN	-	expression tag	UNP Q8NER1
C	918	TYR	-	expression tag	UNP Q8NER1
C	919	GLY	-	expression tag	UNP Q8NER1
C	920	ASN	-	expression tag	UNP Q8NER1
C	921	ARG	-	expression tag	UNP Q8NER1
C	922	ALA	-	expression tag	UNP Q8NER1
C	923	PHE	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	924	THR	-	expression tag	UNP Q8NER1
C	925	LYS	-	expression tag	UNP Q8NER1
C	926	TYR	-	expression tag	UNP Q8NER1
C	927	PRO	-	expression tag	UNP Q8NER1
C	928	GLU	-	expression tag	UNP Q8NER1
C	929	ASP	-	expression tag	UNP Q8NER1
C	930	ILE	-	expression tag	UNP Q8NER1
C	931	PRO	-	expression tag	UNP Q8NER1
C	932	ASP	-	expression tag	UNP Q8NER1
C	933	TYR	-	expression tag	UNP Q8NER1
C	934	PHE	-	expression tag	UNP Q8NER1
C	935	LYS	-	expression tag	UNP Q8NER1
C	936	GLN	-	expression tag	UNP Q8NER1
C	937	ALA	-	expression tag	UNP Q8NER1
C	938	PHE	-	expression tag	UNP Q8NER1
C	939	PRO	-	expression tag	UNP Q8NER1
C	940	GLU	-	expression tag	UNP Q8NER1
C	941	GLY	-	expression tag	UNP Q8NER1
C	942	TYR	-	expression tag	UNP Q8NER1
C	943	SER	-	expression tag	UNP Q8NER1
C	944	TRP	-	expression tag	UNP Q8NER1
C	945	GLU	-	expression tag	UNP Q8NER1
C	946	ARG	-	expression tag	UNP Q8NER1
C	947	SER	-	expression tag	UNP Q8NER1
C	948	MET	-	expression tag	UNP Q8NER1
C	949	THR	-	expression tag	UNP Q8NER1
C	950	TYR	-	expression tag	UNP Q8NER1
C	951	GLU	-	expression tag	UNP Q8NER1
C	952	ASP	-	expression tag	UNP Q8NER1
C	953	GLN	-	expression tag	UNP Q8NER1
C	954	GLY	-	expression tag	UNP Q8NER1
C	955	ILE	-	expression tag	UNP Q8NER1
C	956	CYS	-	expression tag	UNP Q8NER1
C	957	ILE	-	expression tag	UNP Q8NER1
C	958	ALA	-	expression tag	UNP Q8NER1
C	959	THR	-	expression tag	UNP Q8NER1
C	960	SER	-	expression tag	UNP Q8NER1
C	961	ASP	-	expression tag	UNP Q8NER1
C	962	ILE	-	expression tag	UNP Q8NER1
C	963	THR	-	expression tag	UNP Q8NER1
C	964	MET	-	expression tag	UNP Q8NER1
C	965	GLU	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	966	GLY	-	expression tag	UNP Q8NER1
C	967	ASP	-	expression tag	UNP Q8NER1
C	968	CYS	-	expression tag	UNP Q8NER1
C	969	PHE	-	expression tag	UNP Q8NER1
C	970	PHE	-	expression tag	UNP Q8NER1
C	971	TYR	-	expression tag	UNP Q8NER1
C	972	GLU	-	expression tag	UNP Q8NER1
C	973	ILE	-	expression tag	UNP Q8NER1
C	974	ARG	-	expression tag	UNP Q8NER1
C	975	PHE	-	expression tag	UNP Q8NER1
C	976	ASP	-	expression tag	UNP Q8NER1
C	977	GLY	-	expression tag	UNP Q8NER1
C	978	THR	-	expression tag	UNP Q8NER1
C	979	ASN	-	expression tag	UNP Q8NER1
C	980	PHE	-	expression tag	UNP Q8NER1
C	981	PRO	-	expression tag	UNP Q8NER1
C	982	PRO	-	expression tag	UNP Q8NER1
C	983	ASN	-	expression tag	UNP Q8NER1
C	984	GLY	-	expression tag	UNP Q8NER1
C	985	PRO	-	expression tag	UNP Q8NER1
C	986	VAL	-	expression tag	UNP Q8NER1
C	987	MET	-	expression tag	UNP Q8NER1
C	988	GLN	-	expression tag	UNP Q8NER1
C	989	LYS	-	expression tag	UNP Q8NER1
C	990	LYS	-	expression tag	UNP Q8NER1
C	991	THR	-	expression tag	UNP Q8NER1
C	992	LEU	-	expression tag	UNP Q8NER1
C	993	LYS	-	expression tag	UNP Q8NER1
C	994	TRP	-	expression tag	UNP Q8NER1
C	995	GLU	-	expression tag	UNP Q8NER1
C	996	PRO	-	expression tag	UNP Q8NER1
C	997	SER	-	expression tag	UNP Q8NER1
C	998	THR	-	expression tag	UNP Q8NER1
C	999	GLU	-	expression tag	UNP Q8NER1
C	1000	LYS	-	expression tag	UNP Q8NER1
C	1001	MET	-	expression tag	UNP Q8NER1
C	1002	TYR	-	expression tag	UNP Q8NER1
C	1003	VAL	-	expression tag	UNP Q8NER1
C	1004	GLU	-	expression tag	UNP Q8NER1
C	1005	ASP	-	expression tag	UNP Q8NER1
C	1006	GLY	-	expression tag	UNP Q8NER1
C	1007	VAL	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1008	LEU	-	expression tag	UNP Q8NER1
C	1009	LYS	-	expression tag	UNP Q8NER1
C	1010	GLY	-	expression tag	UNP Q8NER1
C	1011	ASP	-	expression tag	UNP Q8NER1
C	1012	VAL	-	expression tag	UNP Q8NER1
C	1013	GLU	-	expression tag	UNP Q8NER1
C	1014	MET	-	expression tag	UNP Q8NER1
C	1015	ALA	-	expression tag	UNP Q8NER1
C	1016	LEU	-	expression tag	UNP Q8NER1
C	1017	LEU	-	expression tag	UNP Q8NER1
C	1018	LEU	-	expression tag	UNP Q8NER1
C	1019	GLU	-	expression tag	UNP Q8NER1
C	1020	GLY	-	expression tag	UNP Q8NER1
C	1021	GLY	-	expression tag	UNP Q8NER1
C	1022	GLY	-	expression tag	UNP Q8NER1
C	1023	HIS	-	expression tag	UNP Q8NER1
C	1024	TYR	-	expression tag	UNP Q8NER1
C	1025	ARG	-	expression tag	UNP Q8NER1
C	1026	CYS	-	expression tag	UNP Q8NER1
C	1027	ASP	-	expression tag	UNP Q8NER1
C	1028	PHE	-	expression tag	UNP Q8NER1
C	1029	LYS	-	expression tag	UNP Q8NER1
C	1030	THR	-	expression tag	UNP Q8NER1
C	1031	THR	-	expression tag	UNP Q8NER1
C	1032	TYR	-	expression tag	UNP Q8NER1
C	1033	LYS	-	expression tag	UNP Q8NER1
C	1034	ALA	-	expression tag	UNP Q8NER1
C	1035	LYS	-	expression tag	UNP Q8NER1
C	1036	LYS	-	expression tag	UNP Q8NER1
C	1037	ASP	-	expression tag	UNP Q8NER1
C	1038	VAL	-	expression tag	UNP Q8NER1
C	1039	ARG	-	expression tag	UNP Q8NER1
C	1040	LEU	-	expression tag	UNP Q8NER1
C	1041	PRO	-	expression tag	UNP Q8NER1
C	1042	ASP	-	expression tag	UNP Q8NER1
C	1043	ALA	-	expression tag	UNP Q8NER1
C	1044	HIS	-	expression tag	UNP Q8NER1
C	1045	GLU	-	expression tag	UNP Q8NER1
C	1046	VAL	-	expression tag	UNP Q8NER1
C	1047	ASP	-	expression tag	UNP Q8NER1
C	1048	HIS	-	expression tag	UNP Q8NER1
C	1049	ARG	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1050	ILE	-	expression tag	UNP Q8NER1
C	1051	GLU	-	expression tag	UNP Q8NER1
C	1052	ILE	-	expression tag	UNP Q8NER1
C	1053	LEU	-	expression tag	UNP Q8NER1
C	1054	SER	-	expression tag	UNP Q8NER1
C	1055	HIS	-	expression tag	UNP Q8NER1
C	1056	ASP	-	expression tag	UNP Q8NER1
C	1057	LYS	-	expression tag	UNP Q8NER1
C	1058	ASP	-	expression tag	UNP Q8NER1
C	1059	TYR	-	expression tag	UNP Q8NER1
C	1060	ASN	-	expression tag	UNP Q8NER1
C	1061	LYS	-	expression tag	UNP Q8NER1
C	1062	VAL	-	expression tag	UNP Q8NER1
C	1063	ARG	-	expression tag	UNP Q8NER1
C	1064	LEU	-	expression tag	UNP Q8NER1
C	1065	TYR	-	expression tag	UNP Q8NER1
C	1066	GLU	-	expression tag	UNP Q8NER1
C	1067	HIS	-	expression tag	UNP Q8NER1
C	1068	ALA	-	expression tag	UNP Q8NER1
C	1069	GLU	-	expression tag	UNP Q8NER1
C	1070	ALA	-	expression tag	UNP Q8NER1
C	1071	ARG	-	expression tag	UNP Q8NER1
C	1072	TYR	-	expression tag	UNP Q8NER1
C	1073	SER	-	expression tag	UNP Q8NER1
C	1074	GLY	-	expression tag	UNP Q8NER1
C	1075	GLY	-	expression tag	UNP Q8NER1
C	1076	GLY	-	expression tag	UNP Q8NER1
C	1077	SER	-	expression tag	UNP Q8NER1
C	1078	GLY	-	expression tag	UNP Q8NER1
C	1079	GLY	-	expression tag	UNP Q8NER1
C	1080	GLY	-	expression tag	UNP Q8NER1
C	1081	HIS	-	expression tag	UNP Q8NER1
C	1082	HIS	-	expression tag	UNP Q8NER1
C	1083	HIS	-	expression tag	UNP Q8NER1
C	1084	HIS	-	expression tag	UNP Q8NER1
C	1085	HIS	-	expression tag	UNP Q8NER1
C	1086	HIS	-	expression tag	UNP Q8NER1
C	1087	HIS	-	expression tag	UNP Q8NER1
C	1088	GLY	-	expression tag	UNP Q8NER1
C	1089	GLY	-	expression tag	UNP Q8NER1
C	1090	SER	-	expression tag	UNP Q8NER1
C	1091	GLY	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1092	GLY	-	expression tag	UNP Q8NER1
C	1093	TRP	-	expression tag	UNP Q8NER1
C	1094	SER	-	expression tag	UNP Q8NER1
C	1095	HIS	-	expression tag	UNP Q8NER1
C	1096	PRO	-	expression tag	UNP Q8NER1
C	1097	GLN	-	expression tag	UNP Q8NER1
C	1098	PHE	-	expression tag	UNP Q8NER1
C	1099	GLU	-	expression tag	UNP Q8NER1
C	1100	LYS	-	expression tag	UNP Q8NER1
D	315	ILE	MET	variant	UNP Q8NER1
D	840	GLY	-	expression tag	UNP Q8NER1
D	841	THR	-	expression tag	UNP Q8NER1
D	842	LEU	-	expression tag	UNP Q8NER1
D	843	GLU	-	expression tag	UNP Q8NER1
D	844	VAL	-	expression tag	UNP Q8NER1
D	845	LEU	-	expression tag	UNP Q8NER1
D	846	PHE	-	expression tag	UNP Q8NER1
D	847	GLN	-	expression tag	UNP Q8NER1
D	848	GLY	-	expression tag	UNP Q8NER1
D	849	PRO	-	expression tag	UNP Q8NER1
D	850	GLY	-	expression tag	UNP Q8NER1
D	851	GLY	-	expression tag	UNP Q8NER1
D	852	SER	-	expression tag	UNP Q8NER1
D	853	GLY	-	expression tag	UNP Q8NER1
D	854	GLY	-	expression tag	UNP Q8NER1
D	855	SER	-	expression tag	UNP Q8NER1
D	856	ALA	-	expression tag	UNP Q8NER1
D	857	SER	-	expression tag	UNP Q8NER1
D	858	VAL	-	expression tag	UNP Q8NER1
D	859	ILE	-	expression tag	UNP Q8NER1
D	860	LYS	-	expression tag	UNP Q8NER1
D	861	PRO	-	expression tag	UNP Q8NER1
D	862	GLU	-	expression tag	UNP Q8NER1
D	863	MET	-	expression tag	UNP Q8NER1
D	864	LYS	-	expression tag	UNP Q8NER1
D	865	ILE	-	expression tag	UNP Q8NER1
D	866	LYS	-	expression tag	UNP Q8NER1
D	867	LEU	-	expression tag	UNP Q8NER1
D	868	ARG	-	expression tag	UNP Q8NER1
D	869	MET	-	expression tag	UNP Q8NER1
D	870	GLU	-	expression tag	UNP Q8NER1
D	871	GLY	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	872	ALA	-	expression tag	UNP Q8NER1
D	873	VAL	-	expression tag	UNP Q8NER1
D	874	ASN	-	expression tag	UNP Q8NER1
D	875	GLY	-	expression tag	UNP Q8NER1
D	876	HIS	-	expression tag	UNP Q8NER1
D	877	LYS	-	expression tag	UNP Q8NER1
D	878	PHE	-	expression tag	UNP Q8NER1
D	879	VAL	-	expression tag	UNP Q8NER1
D	880	ILE	-	expression tag	UNP Q8NER1
D	881	GLU	-	expression tag	UNP Q8NER1
D	882	GLY	-	expression tag	UNP Q8NER1
D	883	GLU	-	expression tag	UNP Q8NER1
D	884	GLY	-	expression tag	UNP Q8NER1
D	885	ILE	-	expression tag	UNP Q8NER1
D	886	GLY	-	expression tag	UNP Q8NER1
D	887	LYS	-	expression tag	UNP Q8NER1
D	888	PRO	-	expression tag	UNP Q8NER1
D	889	TYR	-	expression tag	UNP Q8NER1
D	890	GLU	-	expression tag	UNP Q8NER1
D	891	GLY	-	expression tag	UNP Q8NER1
D	892	THR	-	expression tag	UNP Q8NER1
D	893	GLN	-	expression tag	UNP Q8NER1
D	894	THR	-	expression tag	UNP Q8NER1
D	895	LEU	-	expression tag	UNP Q8NER1
D	896	ASP	-	expression tag	UNP Q8NER1
D	897	LEU	-	expression tag	UNP Q8NER1
D	898	THR	-	expression tag	UNP Q8NER1
D	899	VAL	-	expression tag	UNP Q8NER1
D	900	GLU	-	expression tag	UNP Q8NER1
D	901	GLU	-	expression tag	UNP Q8NER1
D	902	GLY	-	expression tag	UNP Q8NER1
D	903	ALA	-	expression tag	UNP Q8NER1
D	904	PRO	-	expression tag	UNP Q8NER1
D	905	LEU	-	expression tag	UNP Q8NER1
D	906	PRO	-	expression tag	UNP Q8NER1
D	907	PHE	-	expression tag	UNP Q8NER1
D	908	SER	-	expression tag	UNP Q8NER1
D	909	TYR	-	expression tag	UNP Q8NER1
D	910	ASP	-	expression tag	UNP Q8NER1
D	911	ILE	-	expression tag	UNP Q8NER1
D	912	LEU	-	expression tag	UNP Q8NER1
D	913	THR	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	914	PRO	-	expression tag	UNP Q8NER1
D	915	ALA	-	expression tag	UNP Q8NER1
D	916	PHE	-	expression tag	UNP Q8NER1
D	917	GLN	-	expression tag	UNP Q8NER1
D	918	TYR	-	expression tag	UNP Q8NER1
D	919	GLY	-	expression tag	UNP Q8NER1
D	920	ASN	-	expression tag	UNP Q8NER1
D	921	ARG	-	expression tag	UNP Q8NER1
D	922	ALA	-	expression tag	UNP Q8NER1
D	923	PHE	-	expression tag	UNP Q8NER1
D	924	THR	-	expression tag	UNP Q8NER1
D	925	LYS	-	expression tag	UNP Q8NER1
D	926	TYR	-	expression tag	UNP Q8NER1
D	927	PRO	-	expression tag	UNP Q8NER1
D	928	GLU	-	expression tag	UNP Q8NER1
D	929	ASP	-	expression tag	UNP Q8NER1
D	930	ILE	-	expression tag	UNP Q8NER1
D	931	PRO	-	expression tag	UNP Q8NER1
D	932	ASP	-	expression tag	UNP Q8NER1
D	933	TYR	-	expression tag	UNP Q8NER1
D	934	PHE	-	expression tag	UNP Q8NER1
D	935	LYS	-	expression tag	UNP Q8NER1
D	936	GLN	-	expression tag	UNP Q8NER1
D	937	ALA	-	expression tag	UNP Q8NER1
D	938	PHE	-	expression tag	UNP Q8NER1
D	939	PRO	-	expression tag	UNP Q8NER1
D	940	GLU	-	expression tag	UNP Q8NER1
D	941	GLY	-	expression tag	UNP Q8NER1
D	942	TYR	-	expression tag	UNP Q8NER1
D	943	SER	-	expression tag	UNP Q8NER1
D	944	TRP	-	expression tag	UNP Q8NER1
D	945	GLU	-	expression tag	UNP Q8NER1
D	946	ARG	-	expression tag	UNP Q8NER1
D	947	SER	-	expression tag	UNP Q8NER1
D	948	MET	-	expression tag	UNP Q8NER1
D	949	THR	-	expression tag	UNP Q8NER1
D	950	TYR	-	expression tag	UNP Q8NER1
D	951	GLU	-	expression tag	UNP Q8NER1
D	952	ASP	-	expression tag	UNP Q8NER1
D	953	GLN	-	expression tag	UNP Q8NER1
D	954	GLY	-	expression tag	UNP Q8NER1
D	955	ILE	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	956	CYS	-	expression tag	UNP Q8NER1
D	957	ILE	-	expression tag	UNP Q8NER1
D	958	ALA	-	expression tag	UNP Q8NER1
D	959	THR	-	expression tag	UNP Q8NER1
D	960	SER	-	expression tag	UNP Q8NER1
D	961	ASP	-	expression tag	UNP Q8NER1
D	962	ILE	-	expression tag	UNP Q8NER1
D	963	THR	-	expression tag	UNP Q8NER1
D	964	MET	-	expression tag	UNP Q8NER1
D	965	GLU	-	expression tag	UNP Q8NER1
D	966	GLY	-	expression tag	UNP Q8NER1
D	967	ASP	-	expression tag	UNP Q8NER1
D	968	CYS	-	expression tag	UNP Q8NER1
D	969	PHE	-	expression tag	UNP Q8NER1
D	970	PHE	-	expression tag	UNP Q8NER1
D	971	TYR	-	expression tag	UNP Q8NER1
D	972	GLU	-	expression tag	UNP Q8NER1
D	973	ILE	-	expression tag	UNP Q8NER1
D	974	ARG	-	expression tag	UNP Q8NER1
D	975	PHE	-	expression tag	UNP Q8NER1
D	976	ASP	-	expression tag	UNP Q8NER1
D	977	GLY	-	expression tag	UNP Q8NER1
D	978	THR	-	expression tag	UNP Q8NER1
D	979	ASN	-	expression tag	UNP Q8NER1
D	980	PHE	-	expression tag	UNP Q8NER1
D	981	PRO	-	expression tag	UNP Q8NER1
D	982	PRO	-	expression tag	UNP Q8NER1
D	983	ASN	-	expression tag	UNP Q8NER1
D	984	GLY	-	expression tag	UNP Q8NER1
D	985	PRO	-	expression tag	UNP Q8NER1
D	986	VAL	-	expression tag	UNP Q8NER1
D	987	MET	-	expression tag	UNP Q8NER1
D	988	GLN	-	expression tag	UNP Q8NER1
D	989	LYS	-	expression tag	UNP Q8NER1
D	990	LYS	-	expression tag	UNP Q8NER1
D	991	THR	-	expression tag	UNP Q8NER1
D	992	LEU	-	expression tag	UNP Q8NER1
D	993	LYS	-	expression tag	UNP Q8NER1
D	994	TRP	-	expression tag	UNP Q8NER1
D	995	GLU	-	expression tag	UNP Q8NER1
D	996	PRO	-	expression tag	UNP Q8NER1
D	997	SER	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	998	THR	-	expression tag	UNP Q8NER1
D	999	GLU	-	expression tag	UNP Q8NER1
D	1000	LYS	-	expression tag	UNP Q8NER1
D	1001	MET	-	expression tag	UNP Q8NER1
D	1002	TYR	-	expression tag	UNP Q8NER1
D	1003	VAL	-	expression tag	UNP Q8NER1
D	1004	GLU	-	expression tag	UNP Q8NER1
D	1005	ASP	-	expression tag	UNP Q8NER1
D	1006	GLY	-	expression tag	UNP Q8NER1
D	1007	VAL	-	expression tag	UNP Q8NER1
D	1008	LEU	-	expression tag	UNP Q8NER1
D	1009	LYS	-	expression tag	UNP Q8NER1
D	1010	GLY	-	expression tag	UNP Q8NER1
D	1011	ASP	-	expression tag	UNP Q8NER1
D	1012	VAL	-	expression tag	UNP Q8NER1
D	1013	GLU	-	expression tag	UNP Q8NER1
D	1014	MET	-	expression tag	UNP Q8NER1
D	1015	ALA	-	expression tag	UNP Q8NER1
D	1016	LEU	-	expression tag	UNP Q8NER1
D	1017	LEU	-	expression tag	UNP Q8NER1
D	1018	LEU	-	expression tag	UNP Q8NER1
D	1019	GLU	-	expression tag	UNP Q8NER1
D	1020	GLY	-	expression tag	UNP Q8NER1
D	1021	GLY	-	expression tag	UNP Q8NER1
D	1022	GLY	-	expression tag	UNP Q8NER1
D	1023	HIS	-	expression tag	UNP Q8NER1
D	1024	TYR	-	expression tag	UNP Q8NER1
D	1025	ARG	-	expression tag	UNP Q8NER1
D	1026	CYS	-	expression tag	UNP Q8NER1
D	1027	ASP	-	expression tag	UNP Q8NER1
D	1028	PHE	-	expression tag	UNP Q8NER1
D	1029	LYS	-	expression tag	UNP Q8NER1
D	1030	THR	-	expression tag	UNP Q8NER1
D	1031	THR	-	expression tag	UNP Q8NER1
D	1032	TYR	-	expression tag	UNP Q8NER1
D	1033	LYS	-	expression tag	UNP Q8NER1
D	1034	ALA	-	expression tag	UNP Q8NER1
D	1035	LYS	-	expression tag	UNP Q8NER1
D	1036	LYS	-	expression tag	UNP Q8NER1
D	1037	ASP	-	expression tag	UNP Q8NER1
D	1038	VAL	-	expression tag	UNP Q8NER1
D	1039	ARG	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

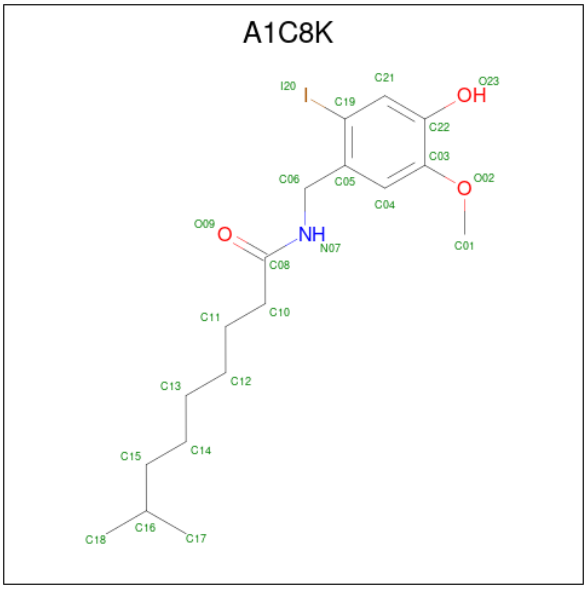
Chain	Residue	Modelled	Actual	Comment	Reference
D	1040	LEU	-	expression tag	UNP Q8NER1
D	1041	PRO	-	expression tag	UNP Q8NER1
D	1042	ASP	-	expression tag	UNP Q8NER1
D	1043	ALA	-	expression tag	UNP Q8NER1
D	1044	HIS	-	expression tag	UNP Q8NER1
D	1045	GLU	-	expression tag	UNP Q8NER1
D	1046	VAL	-	expression tag	UNP Q8NER1
D	1047	ASP	-	expression tag	UNP Q8NER1
D	1048	HIS	-	expression tag	UNP Q8NER1
D	1049	ARG	-	expression tag	UNP Q8NER1
D	1050	ILE	-	expression tag	UNP Q8NER1
D	1051	GLU	-	expression tag	UNP Q8NER1
D	1052	ILE	-	expression tag	UNP Q8NER1
D	1053	LEU	-	expression tag	UNP Q8NER1
D	1054	SER	-	expression tag	UNP Q8NER1
D	1055	HIS	-	expression tag	UNP Q8NER1
D	1056	ASP	-	expression tag	UNP Q8NER1
D	1057	LYS	-	expression tag	UNP Q8NER1
D	1058	ASP	-	expression tag	UNP Q8NER1
D	1059	TYR	-	expression tag	UNP Q8NER1
D	1060	ASN	-	expression tag	UNP Q8NER1
D	1061	LYS	-	expression tag	UNP Q8NER1
D	1062	VAL	-	expression tag	UNP Q8NER1
D	1063	ARG	-	expression tag	UNP Q8NER1
D	1064	LEU	-	expression tag	UNP Q8NER1
D	1065	TYR	-	expression tag	UNP Q8NER1
D	1066	GLU	-	expression tag	UNP Q8NER1
D	1067	HIS	-	expression tag	UNP Q8NER1
D	1068	ALA	-	expression tag	UNP Q8NER1
D	1069	GLU	-	expression tag	UNP Q8NER1
D	1070	ALA	-	expression tag	UNP Q8NER1
D	1071	ARG	-	expression tag	UNP Q8NER1
D	1072	TYR	-	expression tag	UNP Q8NER1
D	1073	SER	-	expression tag	UNP Q8NER1
D	1074	GLY	-	expression tag	UNP Q8NER1
D	1075	GLY	-	expression tag	UNP Q8NER1
D	1076	GLY	-	expression tag	UNP Q8NER1
D	1077	SER	-	expression tag	UNP Q8NER1
D	1078	GLY	-	expression tag	UNP Q8NER1
D	1079	GLY	-	expression tag	UNP Q8NER1
D	1080	GLY	-	expression tag	UNP Q8NER1
D	1081	HIS	-	expression tag	UNP Q8NER1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1082	HIS	-	expression tag	UNP Q8NER1
D	1083	HIS	-	expression tag	UNP Q8NER1
D	1084	HIS	-	expression tag	UNP Q8NER1
D	1085	HIS	-	expression tag	UNP Q8NER1
D	1086	HIS	-	expression tag	UNP Q8NER1
D	1087	HIS	-	expression tag	UNP Q8NER1
D	1088	GLY	-	expression tag	UNP Q8NER1
D	1089	GLY	-	expression tag	UNP Q8NER1
D	1090	SER	-	expression tag	UNP Q8NER1
D	1091	GLY	-	expression tag	UNP Q8NER1
D	1092	GLY	-	expression tag	UNP Q8NER1
D	1093	TRP	-	expression tag	UNP Q8NER1
D	1094	SER	-	expression tag	UNP Q8NER1
D	1095	HIS	-	expression tag	UNP Q8NER1
D	1096	PRO	-	expression tag	UNP Q8NER1
D	1097	GLN	-	expression tag	UNP Q8NER1
D	1098	PHE	-	expression tag	UNP Q8NER1
D	1099	GLU	-	expression tag	UNP Q8NER1
D	1100	LYS	-	expression tag	UNP Q8NER1

- Molecule 2 is N-[(4-hydroxy-2-iodo-5-methoxyphenyl)methyl]-8-methylnonanamide (CCD ID: A1C8K) (formula: $C_{18}H_{28}INO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	I	N	O	0
			23	18	1	1	3	

Continued on next page...

Continued from previous page...

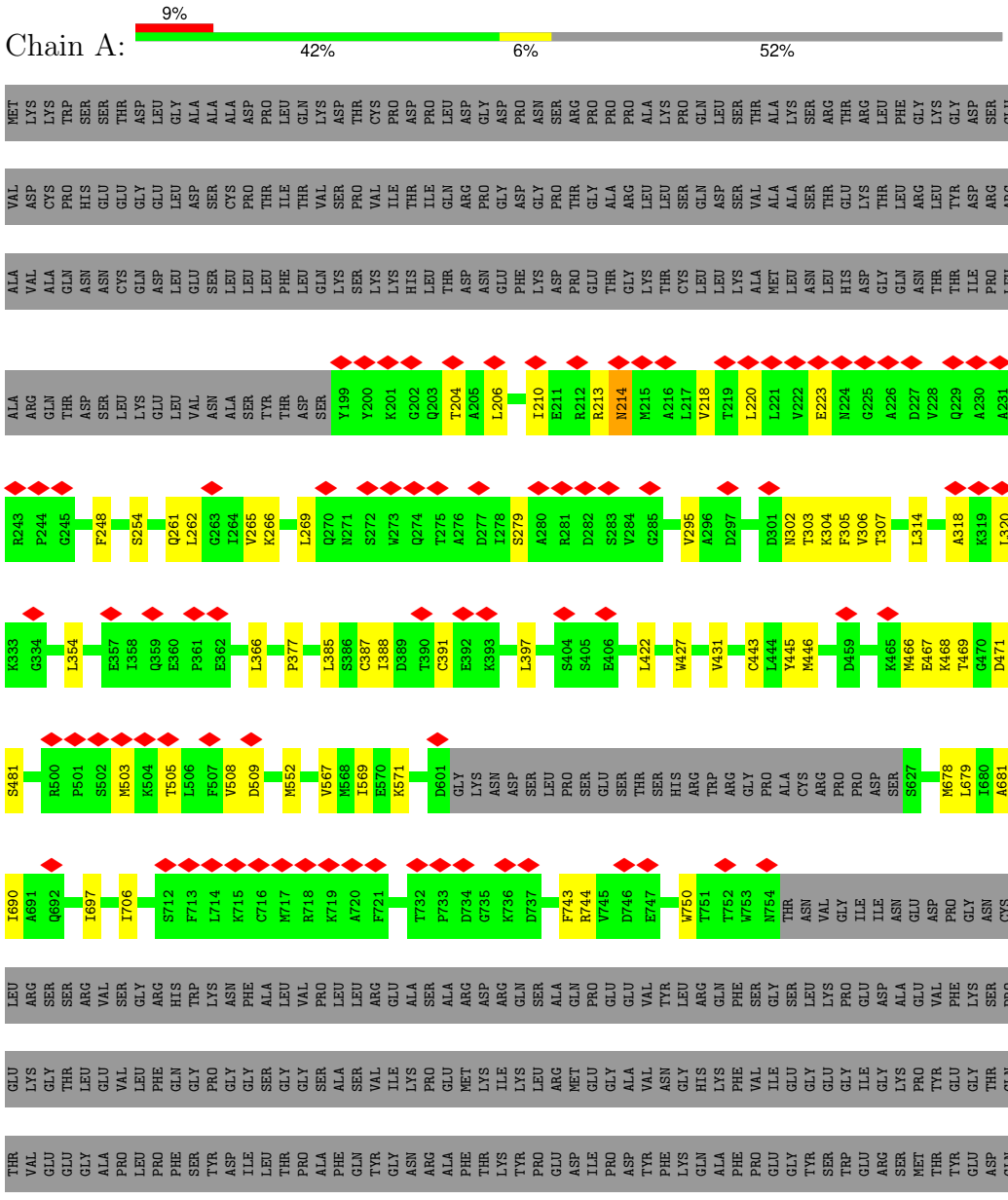
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	I	N	O	0
			23	18	1	1	3	
2	C	1	Total	C	I	N	O	0
			23	18	1	1	3	
2	D	1	Total	C	I	N	O	0
			23	18	1	1	3	

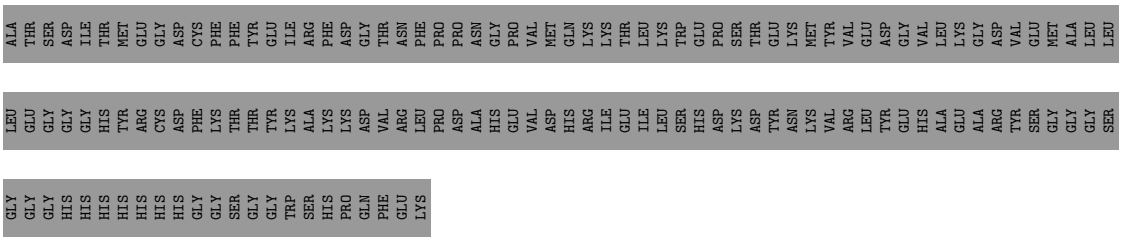
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transient receptor potential cation channel subfamily V member 1

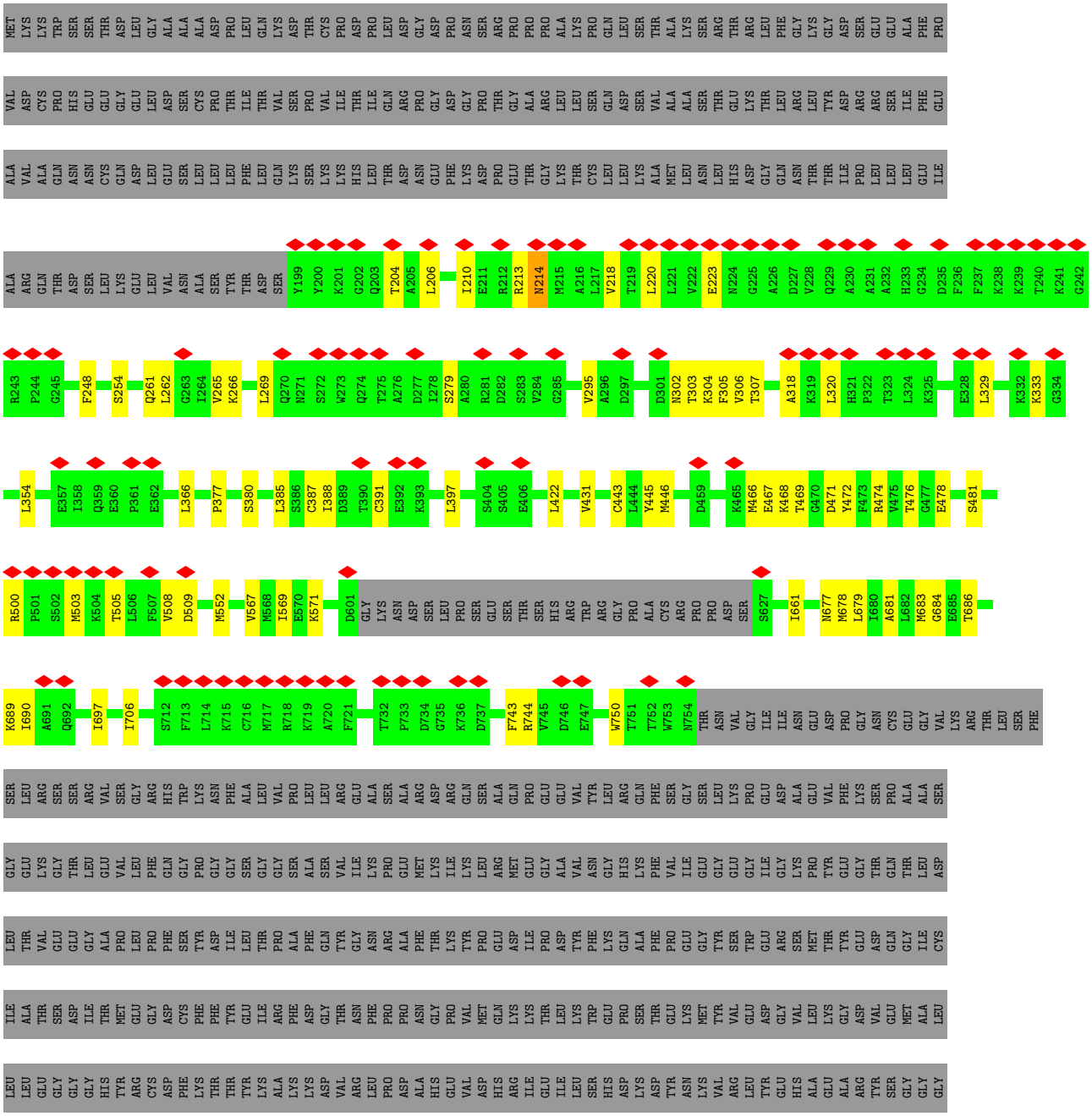
Chain A:





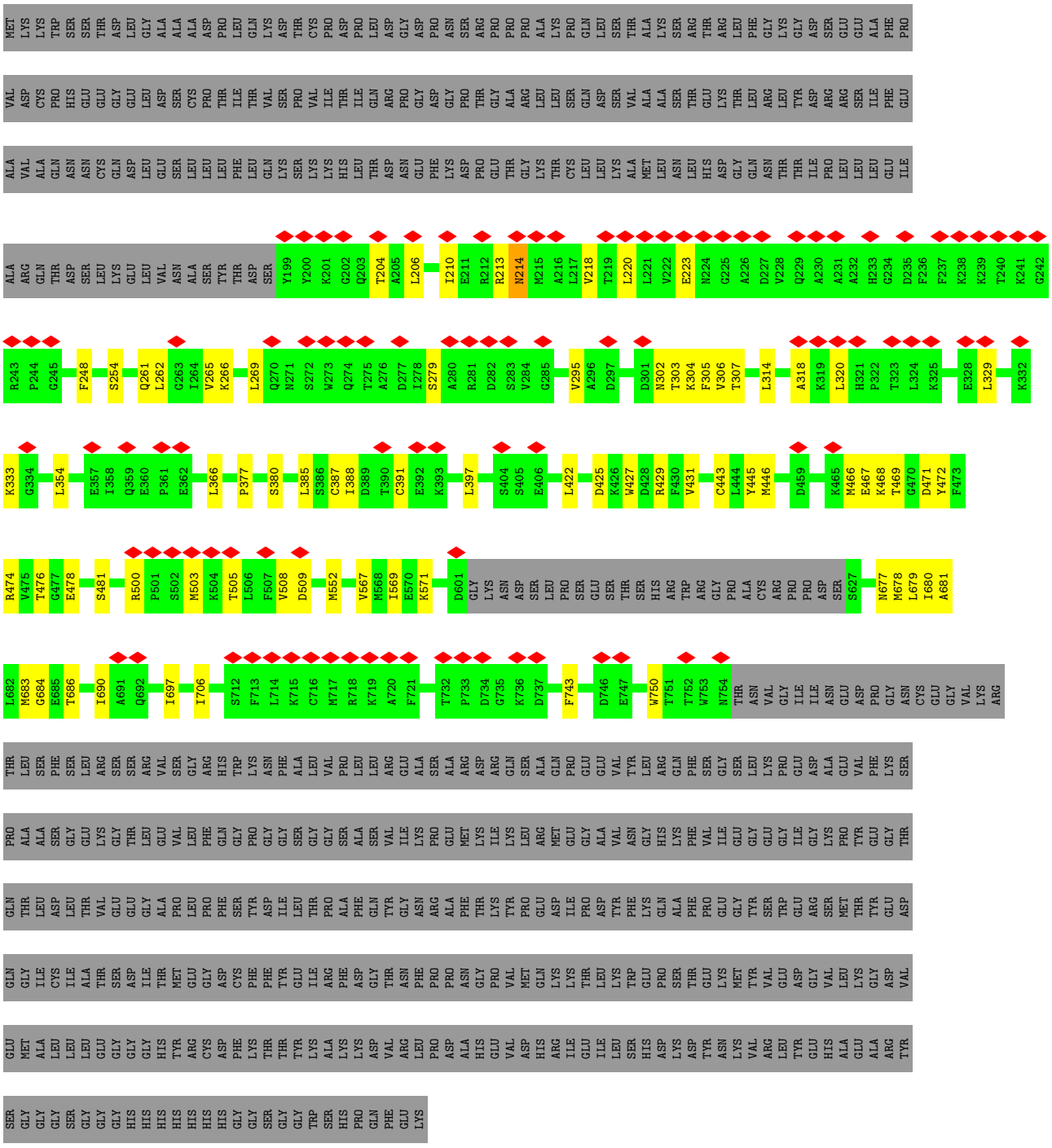
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain B:



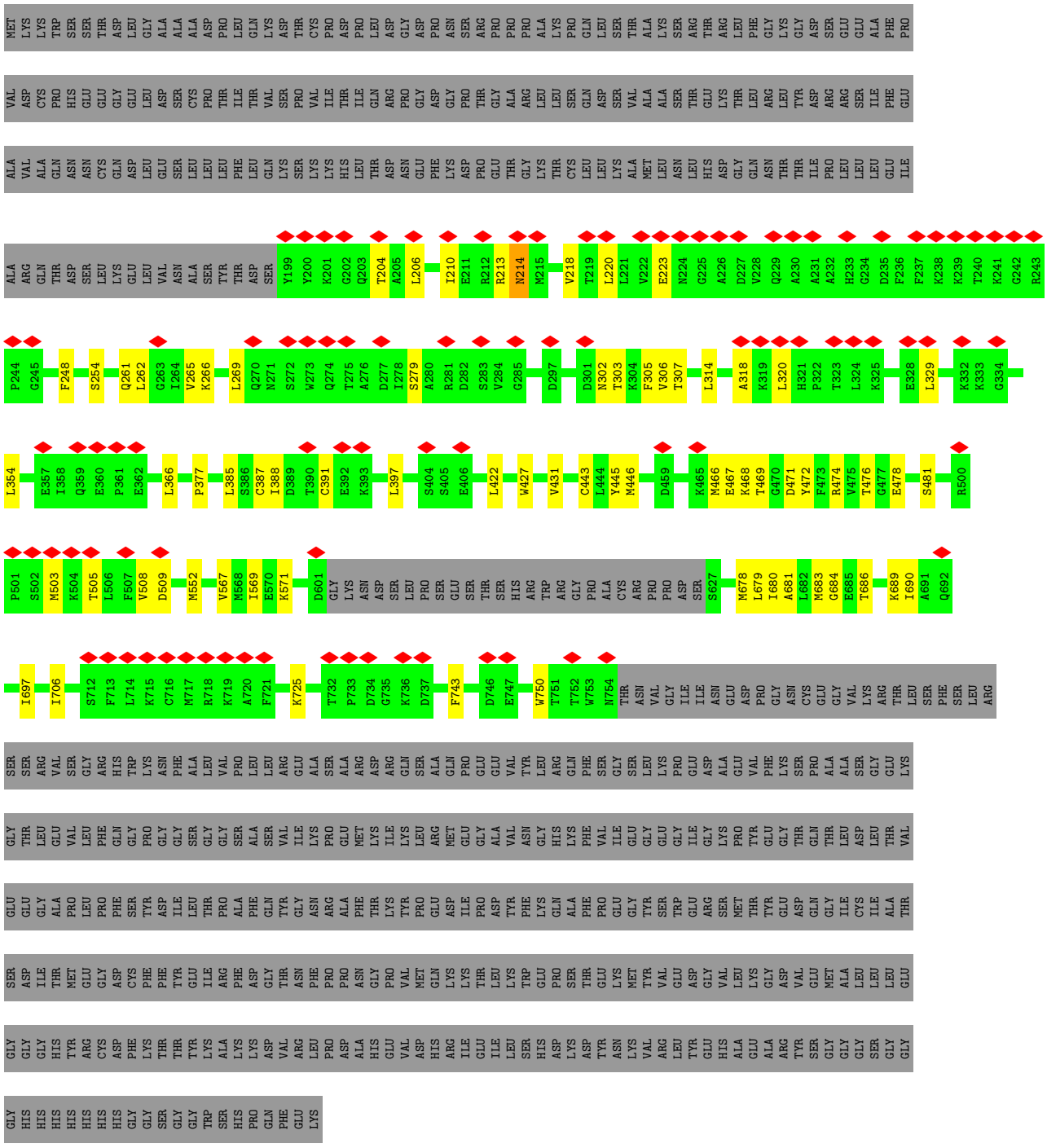
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain D:


MET LYS LYS TRP SER SER THR ASP LEU GLY ALA ALA ASP PRO LEU GLN LYS ASP THR CYS PRO ASP PRO LEU ASP GLY ASP PRO ASN SER ARG PRO PRO PRO ALA LYS PRO GLN LEU SER THR ALA LYS SER ARG THR ARG LEU PHE GLY LYS GLY ASP SER GLU GLU ALA PHE PRO
VAL ASP CYS PRO HIS GLU GLU GLY GLU LEU ASP SER CYS PRO THR ILE THR VAL SER PRO VAL ILE THR ILE GLN GLN ARG PRO GLY ASP GLY PRO THR GLY ALA ARG LEU LEU SER GLN ASP SER VAL ALA ALA SER THR GLU LYS THR LEU ARG LEU TYR ASP ARG ARG SER ILE PHE GLU
ALA VAL ALA GLN ASN ASN CYS GLN ASP LEU GLU SER LEU LEU LEU PHE LEU GLN LYS SER LYS LYS HIS LEU THR ASP ASN GLU PHE LYS ASP PRO GLU THR GLY LYS THR CYS LEU LEU LYS ALA MET LEU ASN LEU HIS ASP GLY GLN ASN THR THR ILE PRO LEU LEU LEU GLU GLU ILE
ALA ARG GLN THR ASP SER LEU LYS GLU LEU VAL ASN ALA SER TYR THR ASP SER Y199 Y200 K201 G202 Q203 T204 A205 L206 I210 E211 R212 R213 N214 M215 V218 T219 L220 L221 V222 E223 N224 G225 A226 D227 V228 Q229 A230 A231 A232 H233 G234 D235 F236 F237 K238 K239 T240 K241 G242 R243
P244 G245 F248 S254 Q261 L262 G263 I264 V265 K266 L269 Q270 N271 S272 W273 Q274 T275 A276 D277 I278 S279 A280 R281 D282 S283 V284 G285 D297 D301 N302 T303 K304 F305 V306 T307 L314 A318 K319 L320 H321 P322 T323 L324 K325 E328 L329 K332 K333 G334
L354 E357 I358 Q359 E360 P361 E362 L366 P377 L385 S386 C387 I388 D389 T390 C391 E392 K393 L397 S404 S405 E406 L422 W427 V431 C443 L444 Y445 M446 D459 K465 M466 E467 K468 T469 G470 D471 Y472 F473 R474 V475 T476 G477 E478 S481 R500
P501 S502 M503 K504 T505 L506 F507 V508 D509 M552 V567 M568 I569 E570 K571 D601 GLY LYS ASN ASP SER LEU PRO SER GLU SER THR SER HIS ARG TRP ARG GLY PRO ALA CYS ARG PRO PRO ASP SER S627 M678 L679 I680 A681 L682 H683 G684 E685 T686 K689 I690 A691 Q692
I697 I706 S712 F713 L714 K715 C716 M717 R718 K719 A720 F721 K725 T732 P733 D734 G735 K736 D737 F743 D746 E747 W750 T751 T752 W753 N754 THR ASN VAL GLY ILE ILE ASN GLU ASP PRO GLY ASN CYS GLU GLY VAL LYS ARG THR LEU SER PHE SER LEU ARG
SER SER ARG VAL SER GLY ARG HIS TRP LYS ASN PHE ALA LEU VAL PRO LEU LEU LEU ARG GLU GLU ALA SER ALA ARG ASP ARG GLN SER ALA GLN PRO GLU GLU VAL TYR LEU ARG GLN PHE SER GLY SER LEU LYS PRO GLU ASP ALA GLU VAL PHE LYS SER PRO ALA ALA SER GLY GLU LYS
GLY THR LEU GLU VAL LEU PHE GLN GLY PRO GLY GLY SER GLY GLY GLY SER ALA ALA SER VAL ILE LYS PRO GLU MET LYS ILE LYS LEU ARG MET GLU GLY ALA VAL ASN GLY HIS LYS PHE VAL ILE GLU GLY GLU GLY ILE GLY LYS PRO TYR GLU GLY THR GLN THR LEU ASP LEU THR VAL
GLU GLU GLY ALA PRO LEU PRO PHE SER TYR ASP ILE LEU THR PRO ALA PHE GLN TYR GLY ASN ARG ALA PHE THR LYS TYR PRO GLU ASP ILE PRO ASP TYR PHE LYS GLN ALA PHE PRO GLU GLY TYR SER TRP GLU ARG SER MET THR TYR GLU ASP GLN THR LEU ASP LEU THR ALA THR
SER ASP ILE THR MET GLU GLY ASP CYS PHE PHE TYR GLU ILE ARG PHE ASP GLY THR ASN PHE PRO PRO ASN GLY PRO VAL MET GLN LYS LYS THR LEU LYS TRP GLU PRO SER THR GLU LYS MET TYR VAL GLU ASP GLY VAL LEU LYS GLY ASP VAL GLU MET ALA LEU LEU LEU GLU
GLY GLY GLY HIS TYR ARG CYS ASP PHE LYS THR THR TYR LYS ALA LYS LYS ASP VAL ARG LEU PRO ASP ALA HIS GLU VAL ASP HIS ARG ILE GLU ILE LEU SER HIS ASP LYS ASP TYR ASN LYS VAL ARG LEU TYR GLU HIS ALA GLU ALA ARG TYR SER GLY GLY GLY SER GLY GLY
GLY HIS HIS HIS HIS HIS HIS GLY GLY SER GLY GLY TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	75798	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.989	Depositor
Minimum map value	-1.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.222	Depositor
Map size (Å)	343.19998, 343.19998, 343.19998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8249999, 0.8249999, 0.8249999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1C8K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.15	0/4415	0.31	0/5974
1	B	0.15	0/4415	0.31	0/5974
1	C	0.15	0/4415	0.31	0/5974
1	D	0.14	0/4415	0.31	0/5974
All	All	0.15	0/17660	0.31	0/23896

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4312	0	4347	49	0
1	B	4312	0	4347	53	0
1	C	4312	0	4347	53	0
1	D	4312	0	4347	49	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
All	All	17340	0	17388	191	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 6.

The worst 5 of 191 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:B:279:SER:HB2	1:B:329:LEU:HD11	1.68	0.76
1:A:279:SER:HB2	1:A:329:LEU:HD11	1.68	0.74
1:D:279:SER:HB2	1:D:329:LEU:HD11	1.68	0.73
1:C:279:SER:HB2	1:C:329:LEU:HD11	1.68	0.73
1:A:204:THR:HG22	1:A:206:LEU:H	1.54	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/1100 (48%)	512 (97%)	15 (3%)	0	100	100
1	B	527/1100 (48%)	511 (97%)	16 (3%)	0	100	100
1	C	527/1100 (48%)	511 (97%)	16 (3%)	0	100	100
1	D	527/1100 (48%)	511 (97%)	16 (3%)	0	100	100
All	All	2108/4400 (48%)	2045 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	467/950 (49%)	465 (100%)	2 (0%)	84	94
1	B	467/950 (49%)	464 (99%)	3 (1%)	78	93
1	C	467/950 (49%)	464 (99%)	3 (1%)	78	93
1	D	467/950 (49%)	465 (100%)	2 (0%)	84	94
All	All	1868/3800 (49%)	1858 (100%)	10 (0%)	78	93

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	380	SER
1	D	214	ASN
1	D	305	PHE
1	B	305	PHE
1	B	380	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	409	ASN
1	C	561	GLN
1	C	533	HIS
1	D	214	ASN
1	B	214	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	A1C8K	A	1201	-	23,23,23	2.30	6 (26%)	28,29,29	1.16	3 (10%)
2	A1C8K	B	1201	-	23,23,23	2.30	6 (26%)	28,29,29	1.16	3 (10%)
2	A1C8K	D	1201	-	23,23,23	2.30	6 (26%)	28,29,29	1.16	3 (10%)
2	A1C8K	C	1201	-	23,23,23	2.30	6 (26%)	28,29,29	1.16	3 (10%)

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	A1C8K	A	1201	-	-	9/16/16/16	0/1/1/1
2	A1C8K	B	1201	-	-	9/16/16/16	0/1/1/1
2	A1C8K	D	1201	-	-	9/16/16/16	0/1/1/1
2	A1C8K	C	1201	-	-	9/16/16/16	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	A1C8K	C08-N07	6.96	1.49	1.33
2	A	1201	A1C8K	C08-N07	6.95	1.49	1.33
2	C	1201	A1C8K	C08-N07	6.95	1.49	1.33
2	D	1201	A1C8K	C08-N07	6.93	1.49	1.33
2	B	1201	A1C8K	C10-C08	4.04	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	A1C8K	O02-C03-C22	3.34	119.56	114.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1201	A1C8K	O02-C03-C22	3.34	119.55	114.55
2	A	1201	A1C8K	O02-C03-C22	3.33	119.54	114.55
2	C	1201	A1C8K	O02-C03-C22	3.33	119.54	114.55
2	D	1201	A1C8K	C10-C08-N07	2.22	120.39	116.34

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

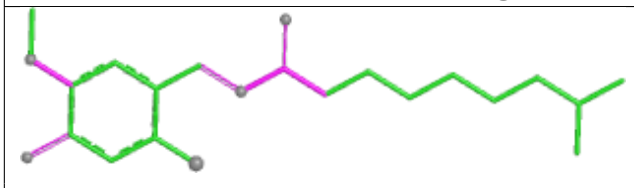
Mol	Chain	Res	Type	Atoms
2	A	1201	A1C8K	C19-C05-C06-N07
2	B	1201	A1C8K	C19-C05-C06-N07
2	C	1201	A1C8K	C19-C05-C06-N07
2	D	1201	A1C8K	C19-C05-C06-N07
2	A	1201	A1C8K	C14-C15-C16-C18

There are no ring outliers.

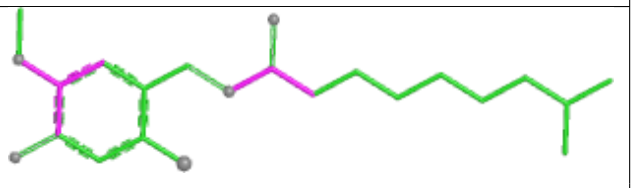
No monomer is involved in short contacts.

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

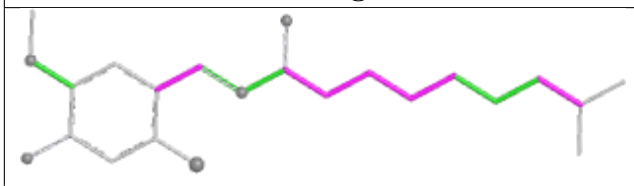
Ligand A1C8K A 1201



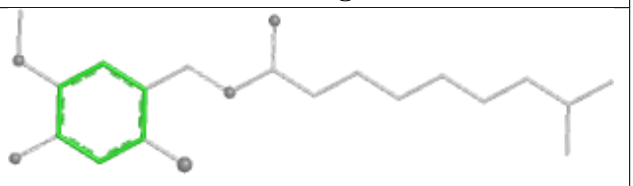
Bond lengths



Bond angles

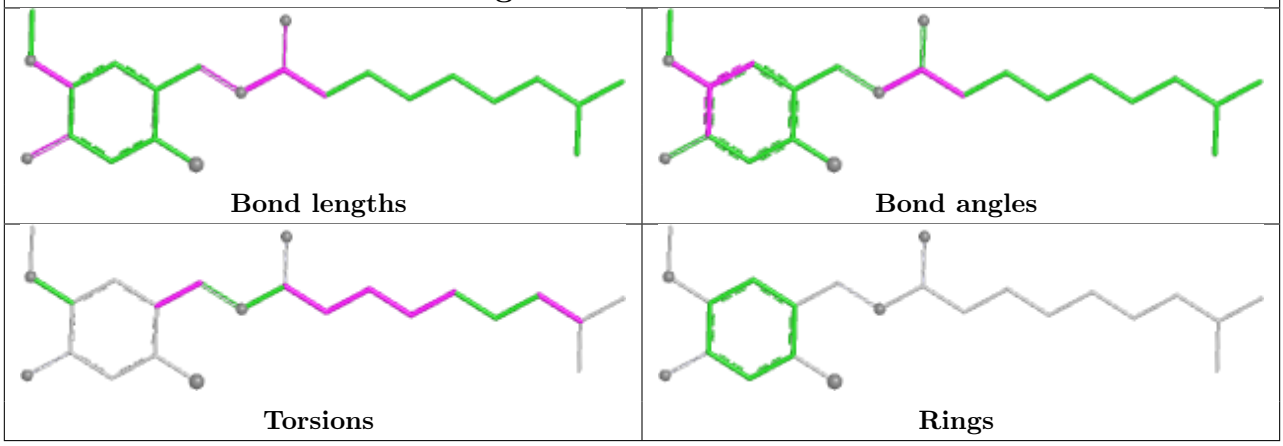


Torsions

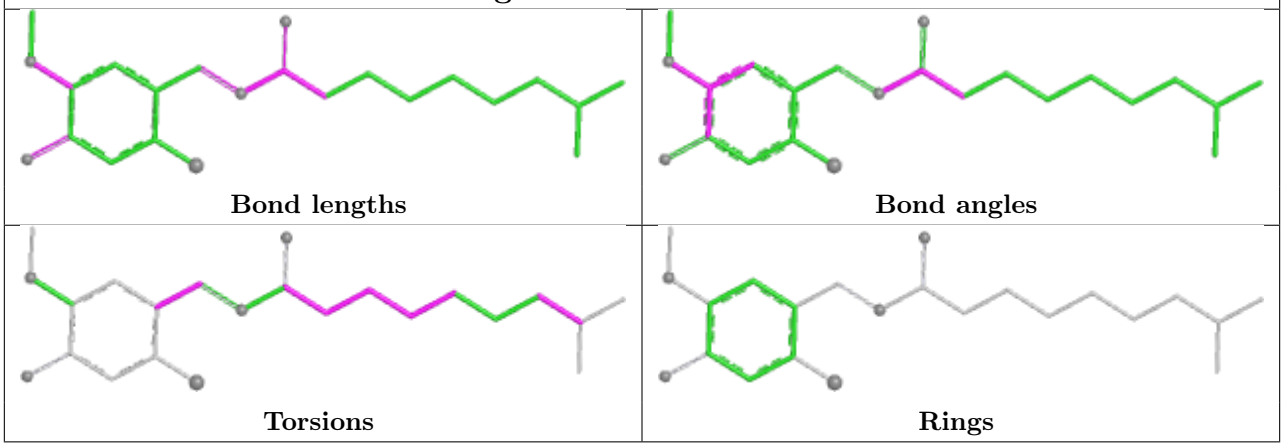


Rings

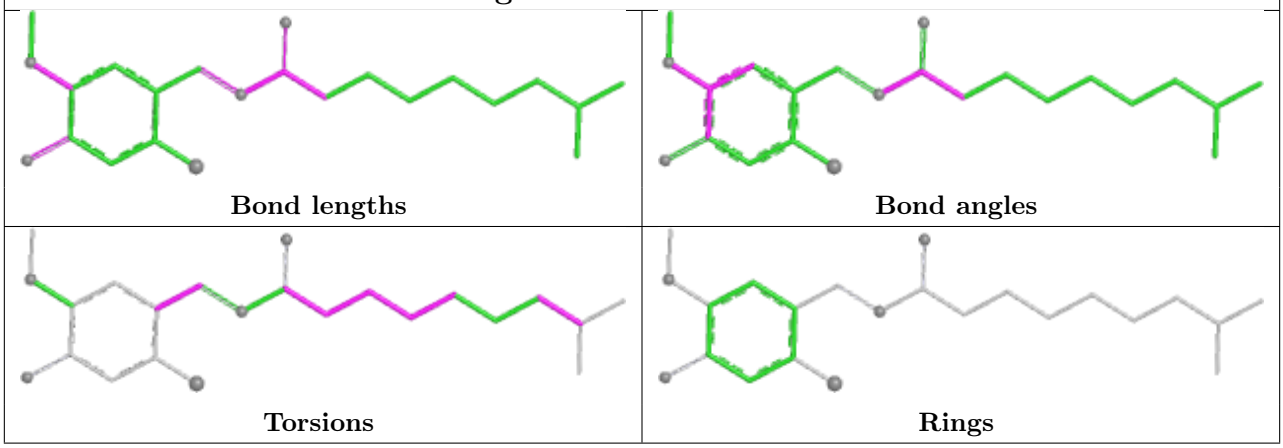
Ligand A1C8K B 1201



Ligand A1C8K D 1201



Ligand A1C8K C 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

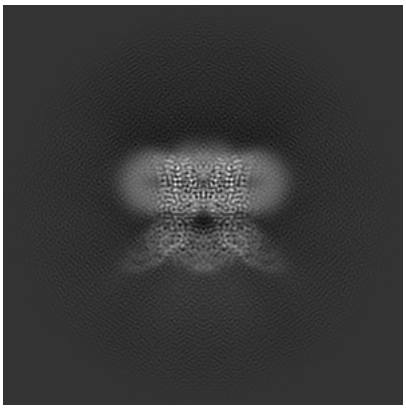
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-75617. These allow visual inspection of the internal detail of the map and identification of artifacts.

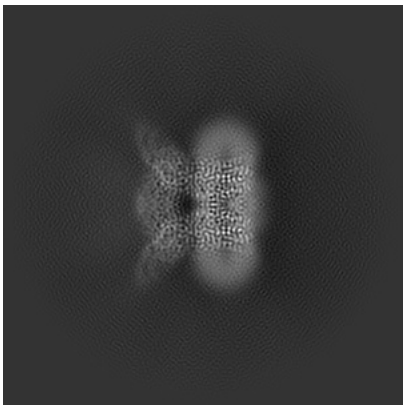
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

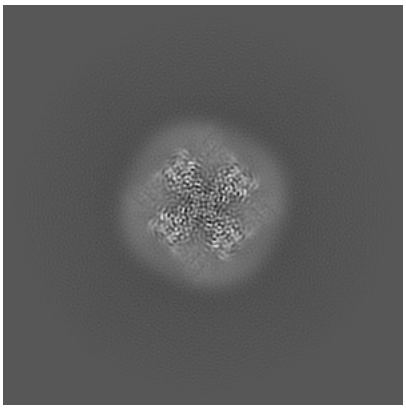
6.1.1 Primary map



X

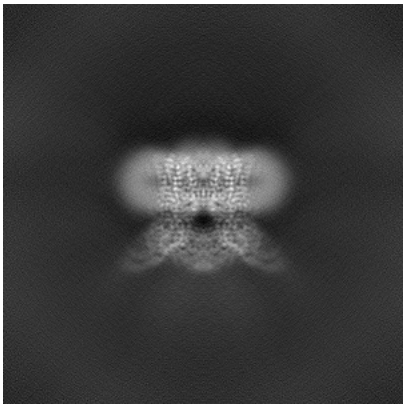


Y

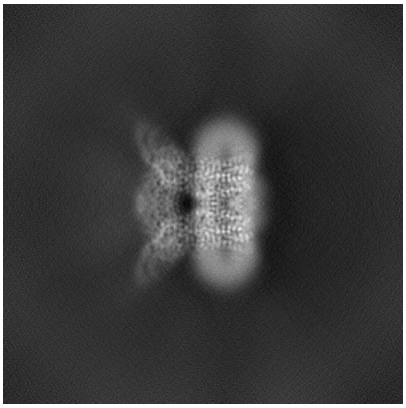


Z

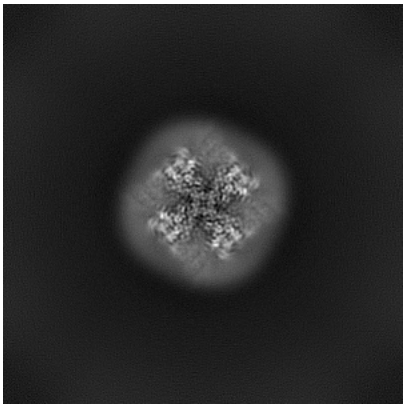
6.1.2 Raw map



X



Y



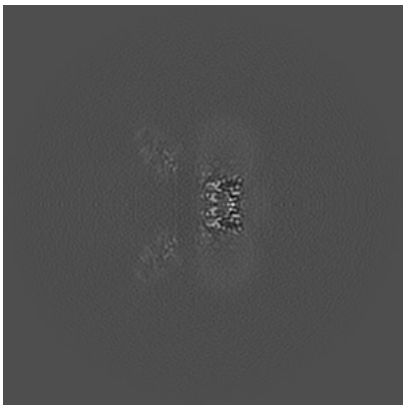
Z

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

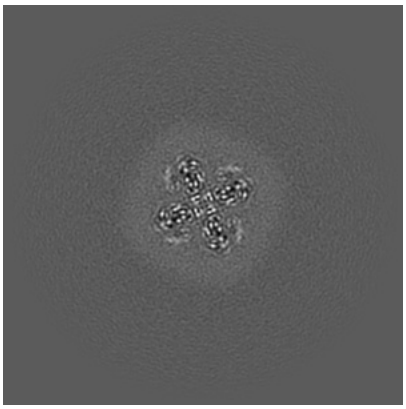
6.2 Central slices (i)

6.2.1 Primary map

X Index: 208

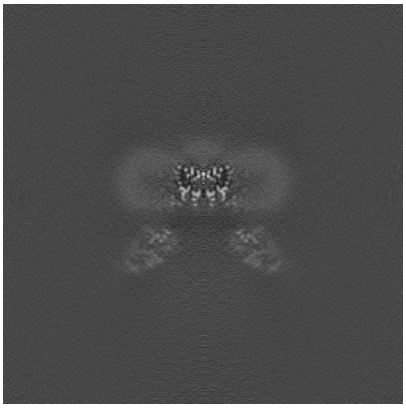


Y Index: 208

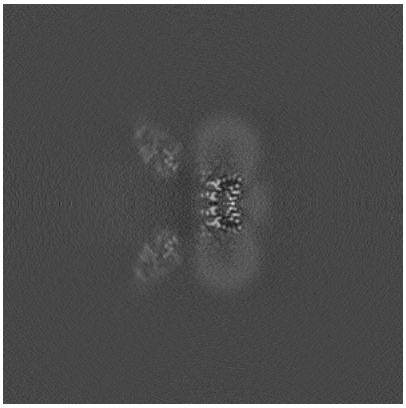


Z Index: 208

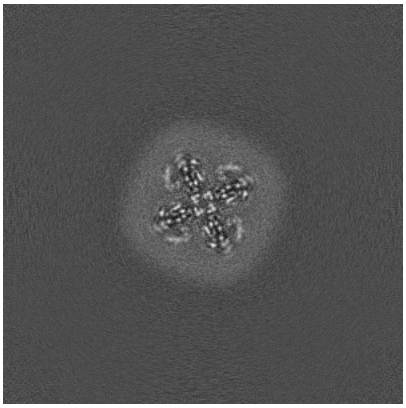
6.2.2 Raw map



X Index: 208



Y Index: 208

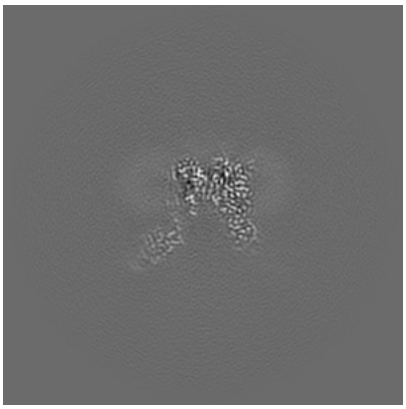


Z Index: 208

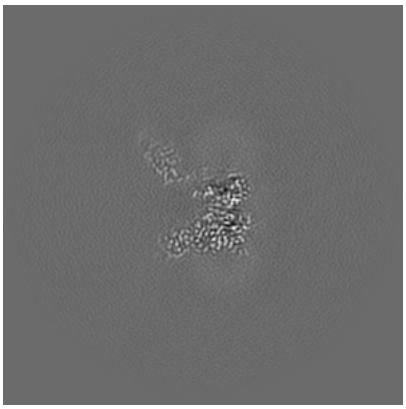
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

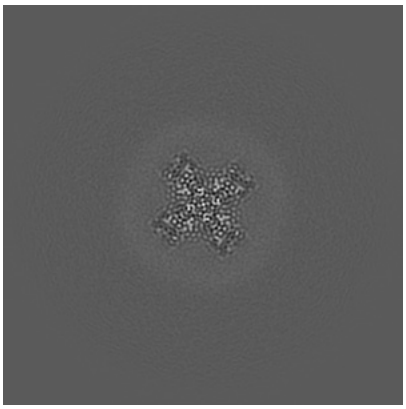
6.3.1 Primary map



X Index: 192

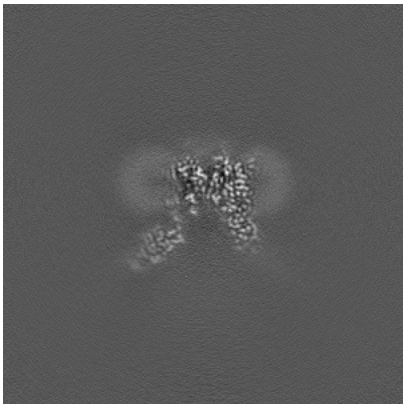


Y Index: 192

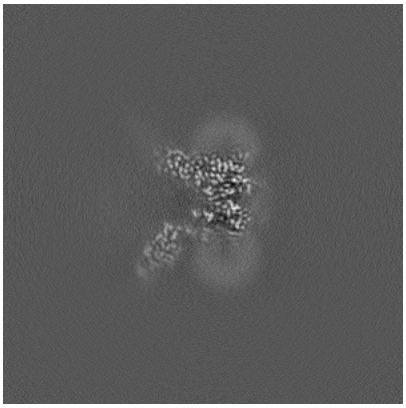


Z Index: 238

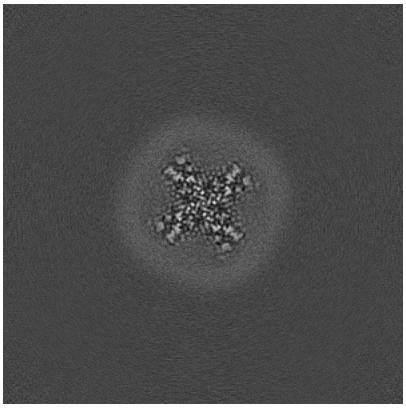
6.3.2 Raw map



X Index: 192



Y Index: 224

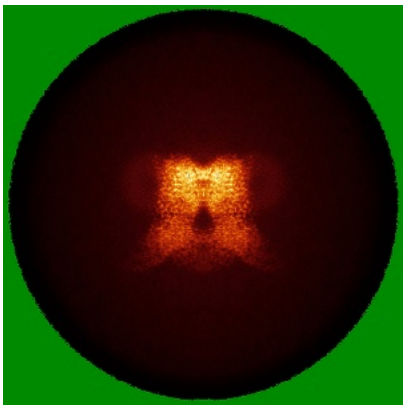


Z Index: 240

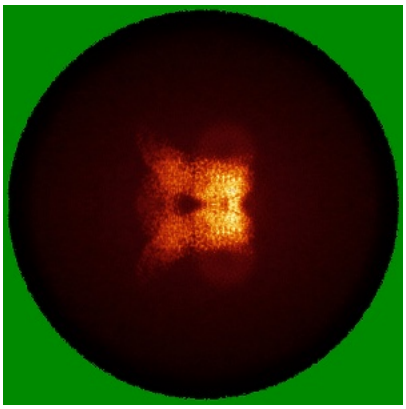
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

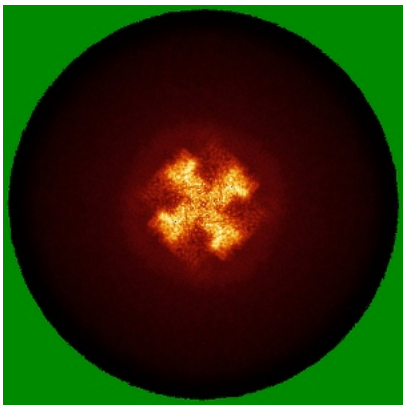
6.4.1 Primary map



X

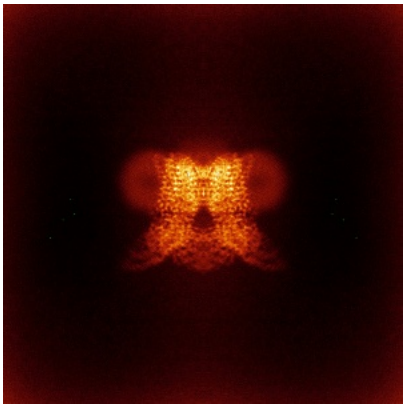


Y

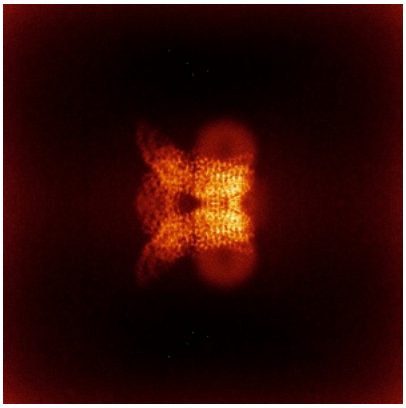


Z

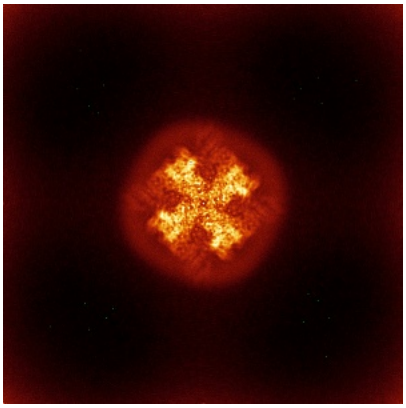
6.4.2 Raw map



X



Y

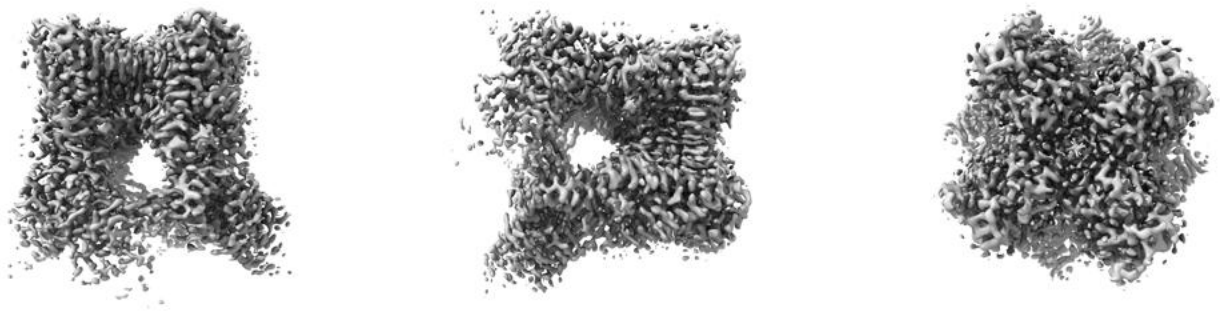


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

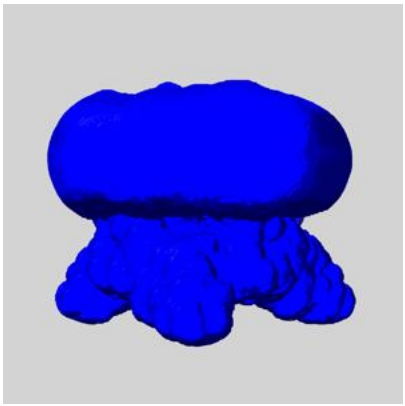
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

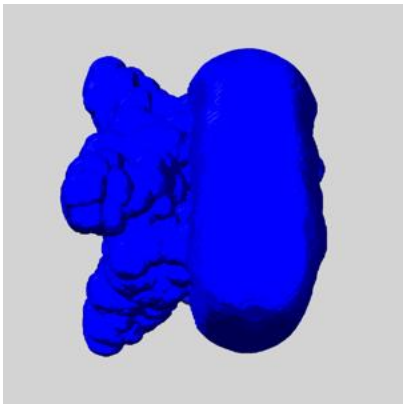
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

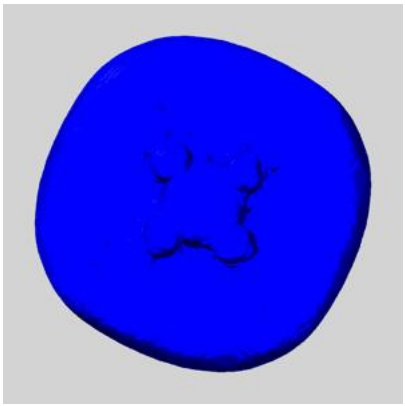
6.6.1 emd_75617_msk_1.map (i)



X



Y

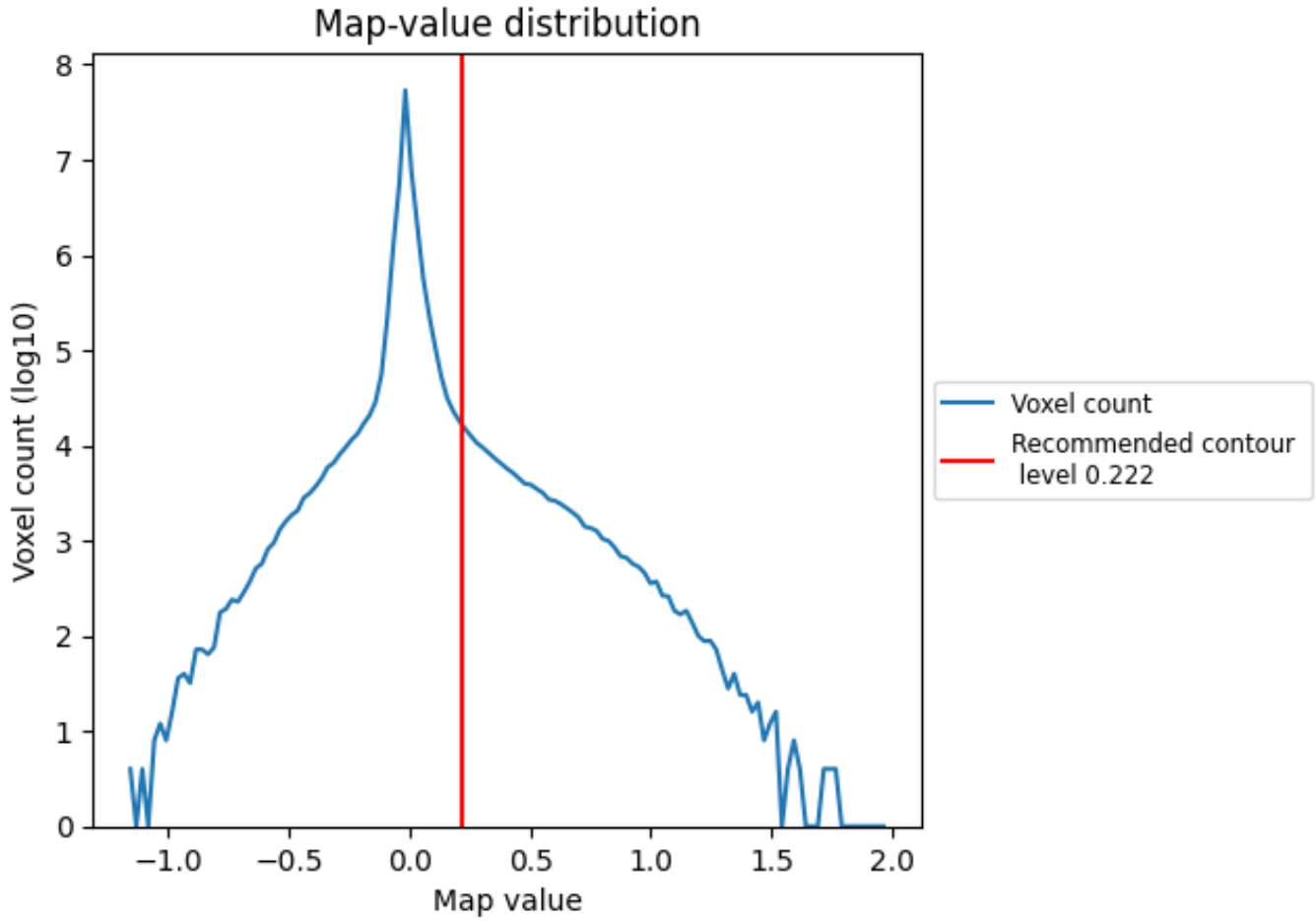


Z

7 Map analysis

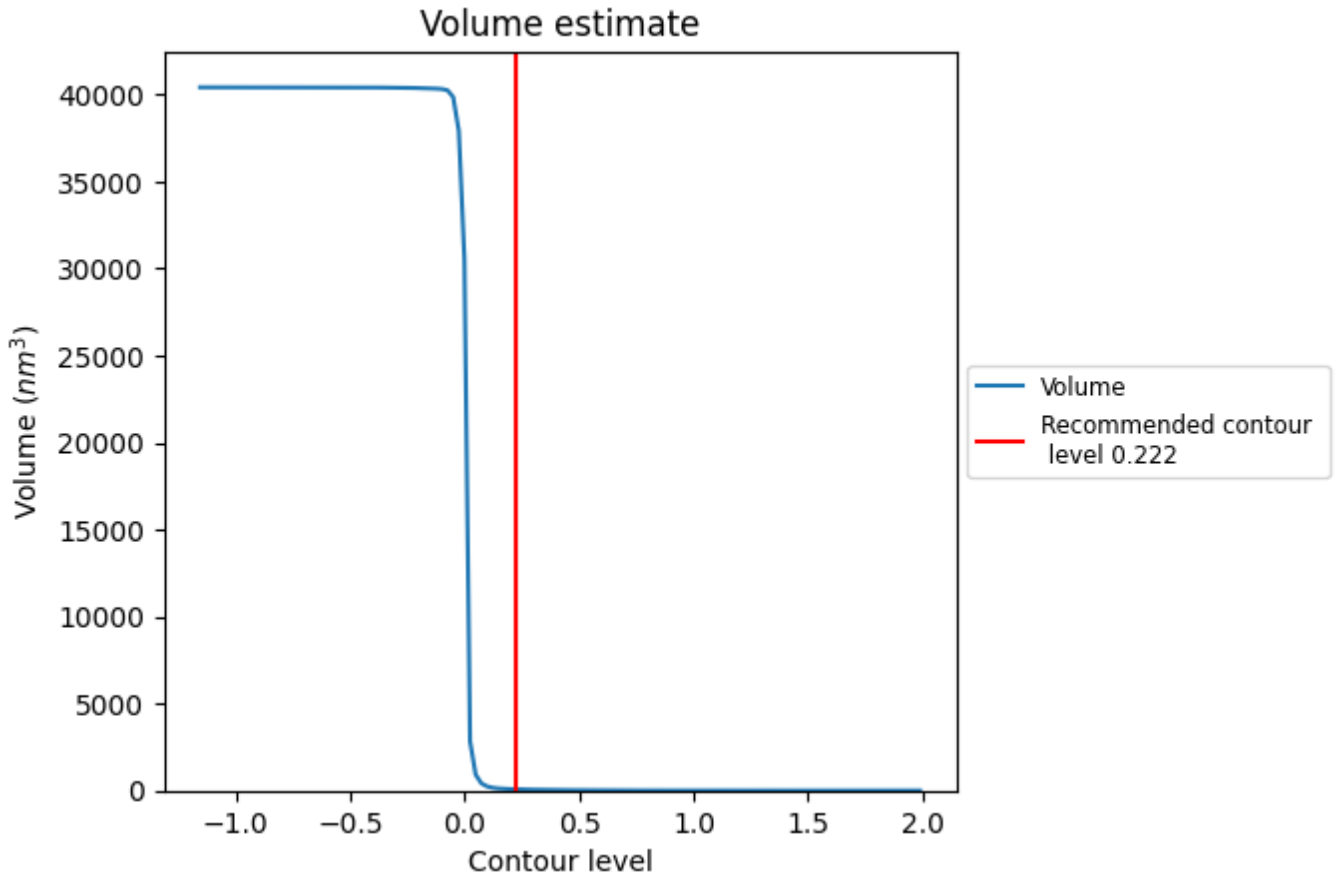
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

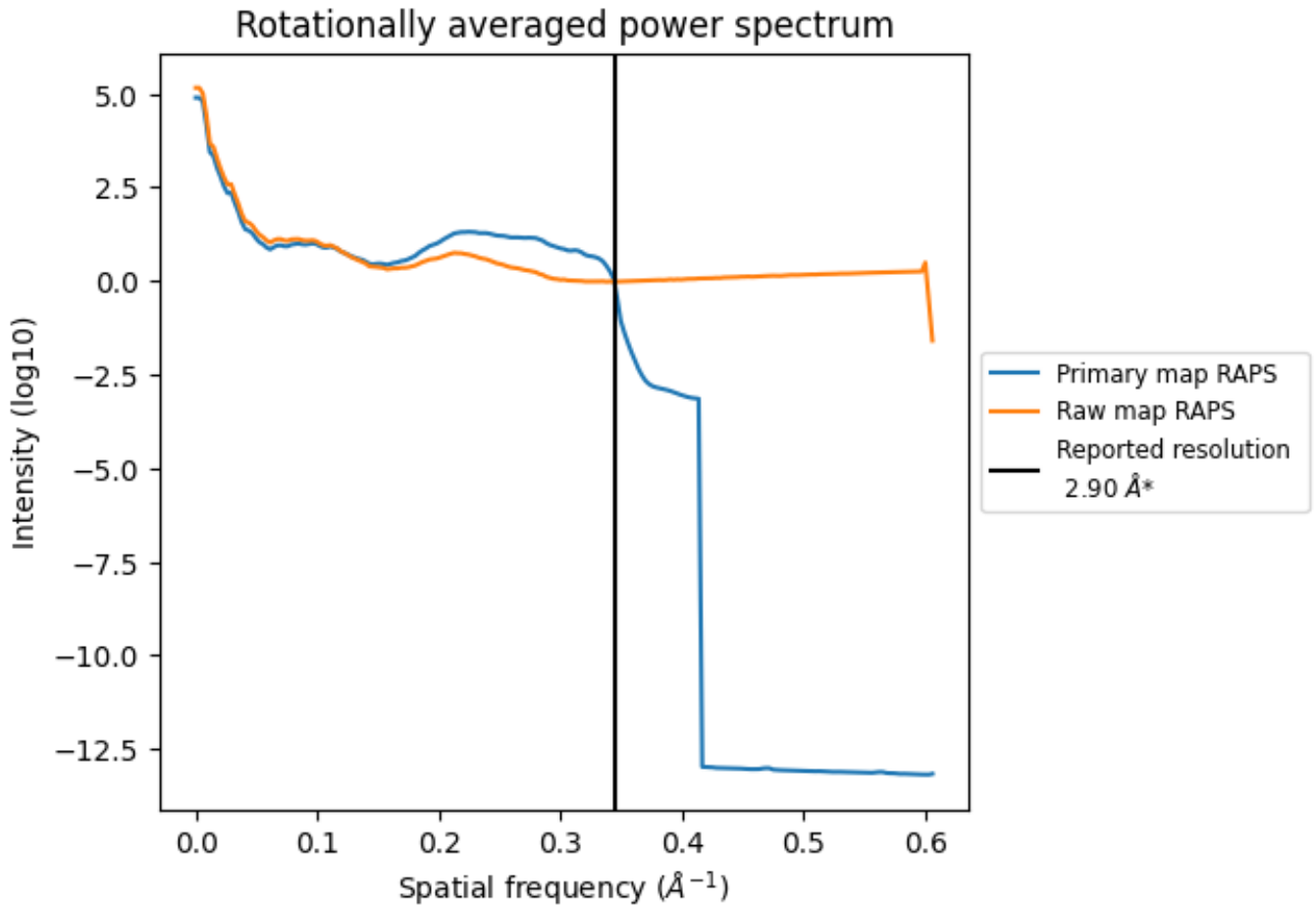
7.2 Volume estimate (i)



The volume at the recommended contour level is 74 nm^3; this corresponds to an approximate mass of 67 kDa.

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

7.3 Rotationally averaged power spectrum (i)

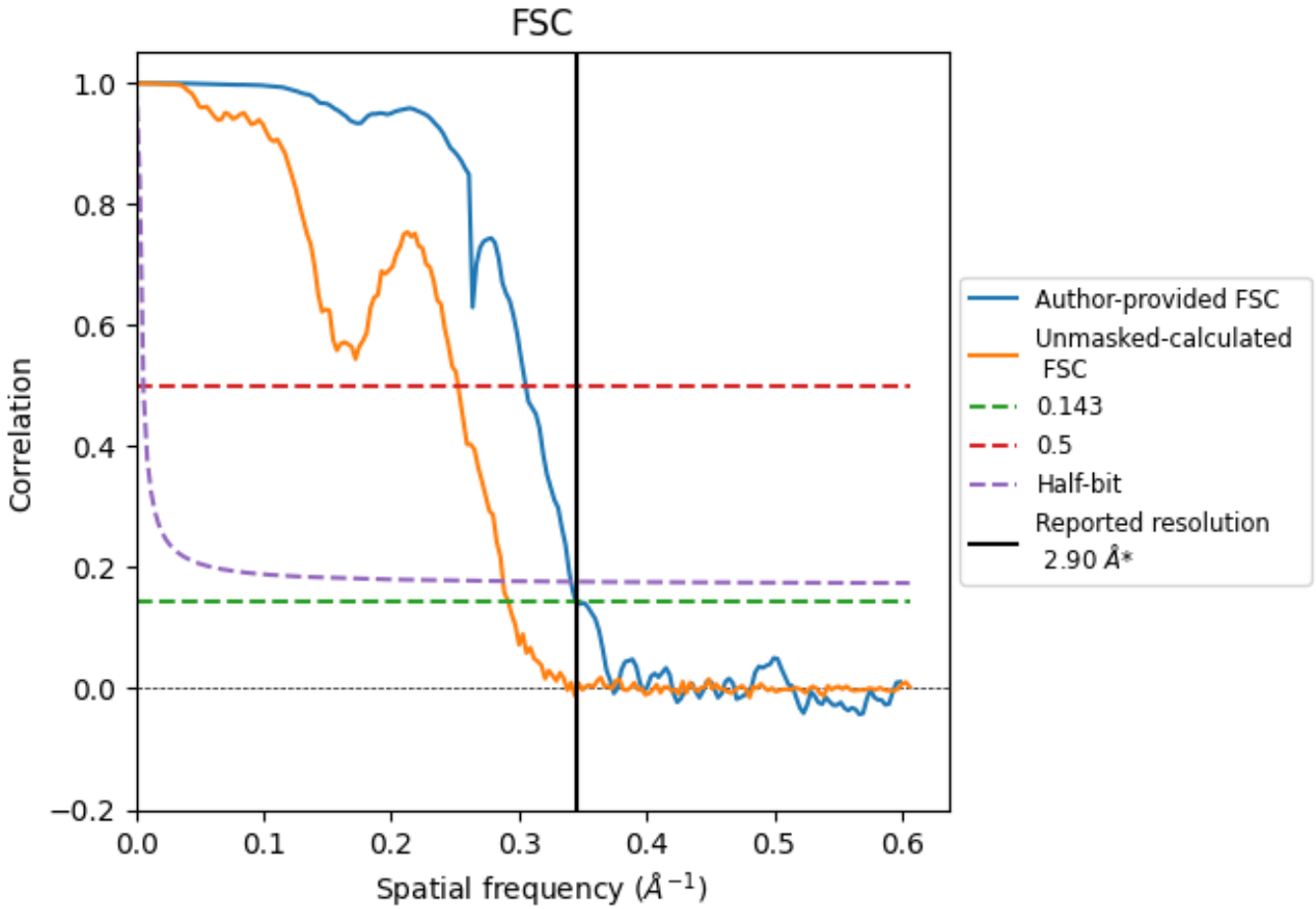


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

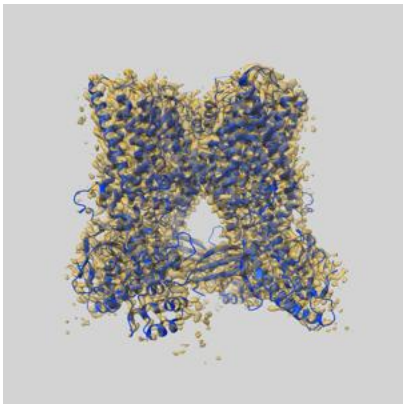
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.27	2.93
Unmasked-calculated*	3.43	3.96	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.9 by more than 10 %

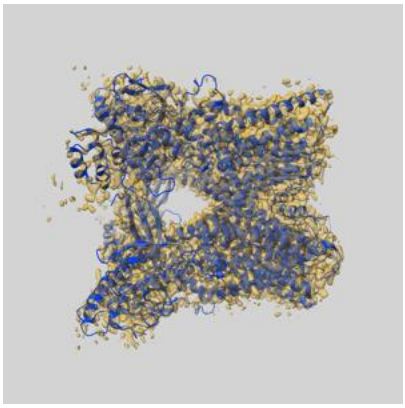
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-75617 and PDB model 11CK. Per-residue inclusion information can be found in section 3 on page 30.

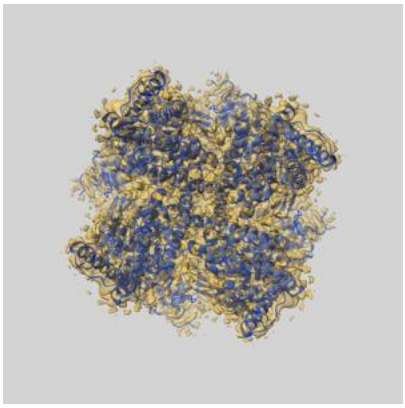
9.1 Map-model overlay



X



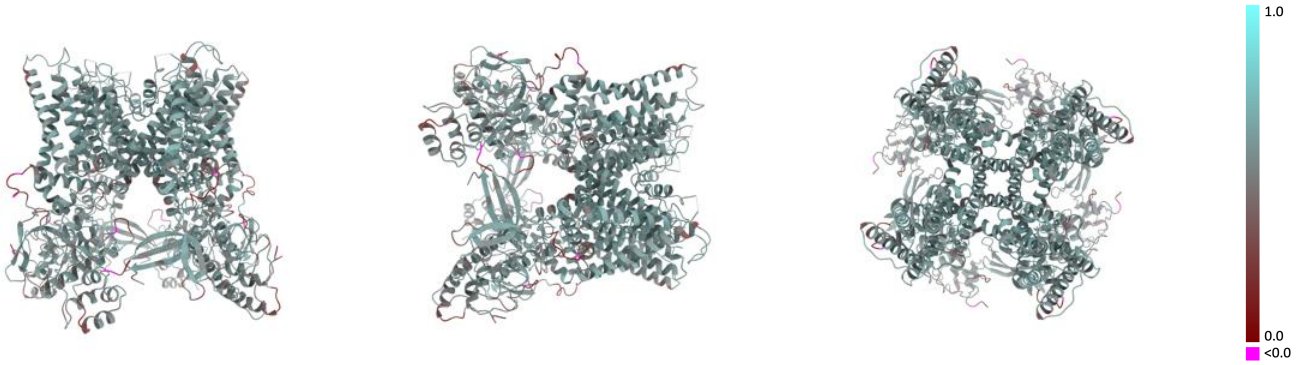
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

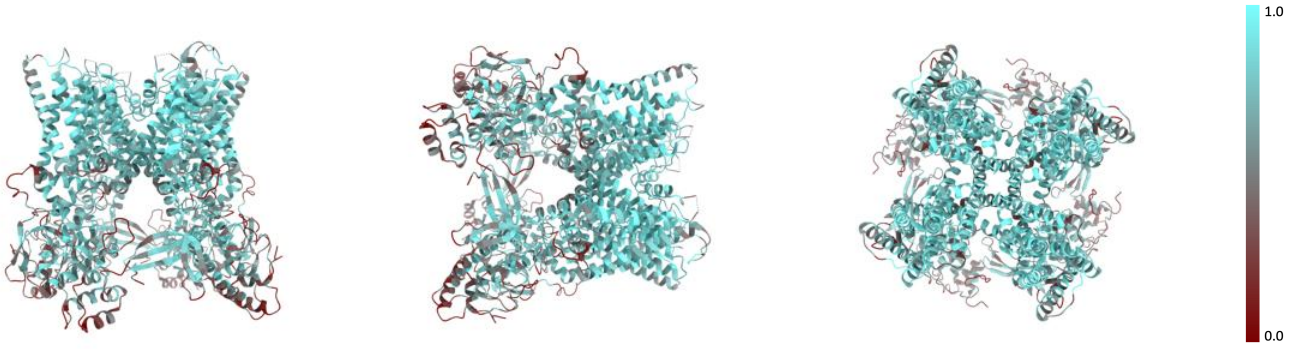
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

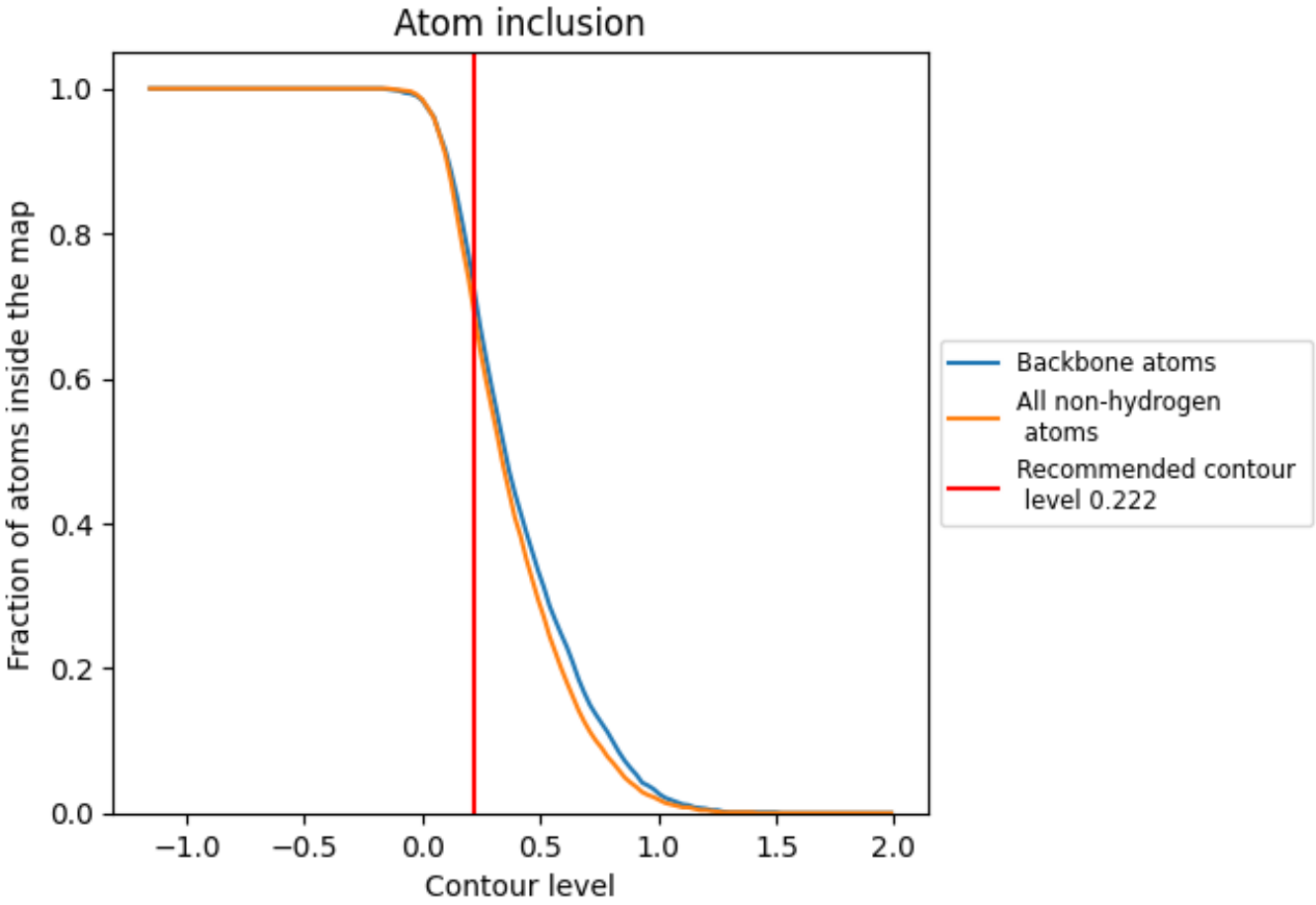
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.222).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6850	0.5440
A	0.6850	0.5430
B	0.6850	0.5440
C	0.6840	0.5440
D	0.6850	0.5440