Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 03:00 PM JST

PDB ID	:	7YSJ / pdb_00007ysj
EMDB ID	:	EMD-34076
Title	:	GluK1-1a in nanodisc captured in SYM2081 bound desensitized state
Authors	:	Dhingra, S.; Kumar, J.
Deposited on	:	2022-08-12
Resolution	:	5.20 Å(reported)
Based on initial models	:	3C32, 5KUF

This is a Full wwPDB EM Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

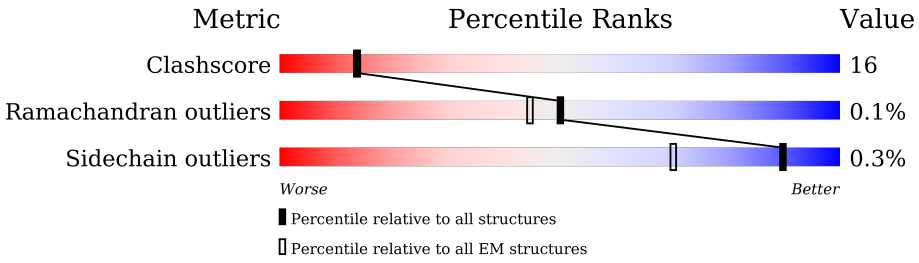
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 5.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1098	39% 22% 39%
1	B	1098	6% 39% 21% 39%
1	C	1098	40% 20% 39%
1	D	1098	42% 19% 39%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21544 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 Glutamate receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	671	Total	C	N	O	S	0	0
			5386	3438	914	1004	30		
1	B	671	Total	C	N	O	S	0	0
			5386	3438	914	1004	30		
1	C	671	Total	C	N	O	S	0	0
			5386	3438	914	1004	30		
1	D	671	Total	C	N	O	S	0	0
			5386	3438	914	1004	30		

There are 1052 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
A	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
A	838	LEU	-	expression tag	UNP A0A0G2K830
A	839	VAL	-	expression tag	UNP A0A0G2K830
A	840	PRO	-	expression tag	UNP A0A0G2K830
A	841	ARG	-	expression tag	UNP A0A0G2K830
A	842	GLY	-	expression tag	UNP A0A0G2K830
A	843	SER	-	expression tag	UNP A0A0G2K830
A	844	ALA	-	expression tag	UNP A0A0G2K830
A	845	ALA	-	expression tag	UNP A0A0G2K830
A	846	ALA	-	expression tag	UNP A0A0G2K830
A	847	ALA	-	expression tag	UNP A0A0G2K830
A	848	VAL	-	expression tag	UNP A0A0G2K830
A	849	SER	-	expression tag	UNP A0A0G2K830
A	850	LYS	-	expression tag	UNP A0A0G2K830
A	851	GLY	-	expression tag	UNP A0A0G2K830
A	852	GLU	-	expression tag	UNP A0A0G2K830
A	853	GLU	-	expression tag	UNP A0A0G2K830
A	854	LEU	-	expression tag	UNP A0A0G2K830
A	855	PHE	-	expression tag	UNP A0A0G2K830
A	856	THR	-	expression tag	UNP A0A0G2K830
A	857	GLY	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	858	VAL	-	expression tag	UNP A0A0G2K830
A	859	VAL	-	expression tag	UNP A0A0G2K830
A	860	PRO	-	expression tag	UNP A0A0G2K830
A	861	ILE	-	expression tag	UNP A0A0G2K830
A	862	LEU	-	expression tag	UNP A0A0G2K830
A	863	VAL	-	expression tag	UNP A0A0G2K830
A	864	GLU	-	expression tag	UNP A0A0G2K830
A	865	LEU	-	expression tag	UNP A0A0G2K830
A	866	ASP	-	expression tag	UNP A0A0G2K830
A	867	GLY	-	expression tag	UNP A0A0G2K830
A	868	ASP	-	expression tag	UNP A0A0G2K830
A	869	VAL	-	expression tag	UNP A0A0G2K830
A	870	ASN	-	expression tag	UNP A0A0G2K830
A	871	GLY	-	expression tag	UNP A0A0G2K830
A	872	HIS	-	expression tag	UNP A0A0G2K830
A	873	LYS	-	expression tag	UNP A0A0G2K830
A	874	PHE	-	expression tag	UNP A0A0G2K830
A	875	SER	-	expression tag	UNP A0A0G2K830
A	876	VAL	-	expression tag	UNP A0A0G2K830
A	877	SER	-	expression tag	UNP A0A0G2K830
A	878	GLY	-	expression tag	UNP A0A0G2K830
A	879	GLU	-	expression tag	UNP A0A0G2K830
A	880	GLY	-	expression tag	UNP A0A0G2K830
A	881	GLU	-	expression tag	UNP A0A0G2K830
A	882	GLY	-	expression tag	UNP A0A0G2K830
A	883	ASP	-	expression tag	UNP A0A0G2K830
A	884	ALA	-	expression tag	UNP A0A0G2K830
A	885	THR	-	expression tag	UNP A0A0G2K830
A	886	TYR	-	expression tag	UNP A0A0G2K830
A	887	GLY	-	expression tag	UNP A0A0G2K830
A	888	LYS	-	expression tag	UNP A0A0G2K830
A	889	LEU	-	expression tag	UNP A0A0G2K830
A	890	THR	-	expression tag	UNP A0A0G2K830
A	891	LEU	-	expression tag	UNP A0A0G2K830
A	892	LYS	-	expression tag	UNP A0A0G2K830
A	893	PHE	-	expression tag	UNP A0A0G2K830
A	894	ILE	-	expression tag	UNP A0A0G2K830
A	895	CYS	-	expression tag	UNP A0A0G2K830
A	896	THR	-	expression tag	UNP A0A0G2K830
A	897	THR	-	expression tag	UNP A0A0G2K830
A	898	GLY	-	expression tag	UNP A0A0G2K830
A	899	LYS	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	900	LEU	-	expression tag	UNP A0A0G2K830
A	901	PRO	-	expression tag	UNP A0A0G2K830
A	902	VAL	-	expression tag	UNP A0A0G2K830
A	903	PRO	-	expression tag	UNP A0A0G2K830
A	904	TRP	-	expression tag	UNP A0A0G2K830
A	905	PRO	-	expression tag	UNP A0A0G2K830
A	906	THR	-	expression tag	UNP A0A0G2K830
A	907	LEU	-	expression tag	UNP A0A0G2K830
A	908	VAL	-	expression tag	UNP A0A0G2K830
A	909	THR	-	expression tag	UNP A0A0G2K830
A	910	THR	-	expression tag	UNP A0A0G2K830
A	911	LEU	-	expression tag	UNP A0A0G2K830
A	912	THR	-	expression tag	UNP A0A0G2K830
A	913	TYR	-	expression tag	UNP A0A0G2K830
A	914	GLY	-	expression tag	UNP A0A0G2K830
A	915	VAL	-	expression tag	UNP A0A0G2K830
A	916	GLN	-	expression tag	UNP A0A0G2K830
A	917	CYS	-	expression tag	UNP A0A0G2K830
A	918	PHE	-	expression tag	UNP A0A0G2K830
A	919	SER	-	expression tag	UNP A0A0G2K830
A	920	ARG	-	expression tag	UNP A0A0G2K830
A	921	TYR	-	expression tag	UNP A0A0G2K830
A	922	PRO	-	expression tag	UNP A0A0G2K830
A	923	ASP	-	expression tag	UNP A0A0G2K830
A	924	HIS	-	expression tag	UNP A0A0G2K830
A	925	MET	-	expression tag	UNP A0A0G2K830
A	926	LYS	-	expression tag	UNP A0A0G2K830
A	927	GLN	-	expression tag	UNP A0A0G2K830
A	928	HIS	-	expression tag	UNP A0A0G2K830
A	929	ASP	-	expression tag	UNP A0A0G2K830
A	930	PHE	-	expression tag	UNP A0A0G2K830
A	931	PHE	-	expression tag	UNP A0A0G2K830
A	932	LYS	-	expression tag	UNP A0A0G2K830
A	933	SER	-	expression tag	UNP A0A0G2K830
A	934	ALA	-	expression tag	UNP A0A0G2K830
A	935	MET	-	expression tag	UNP A0A0G2K830
A	936	PRO	-	expression tag	UNP A0A0G2K830
A	937	GLU	-	expression tag	UNP A0A0G2K830
A	938	GLY	-	expression tag	UNP A0A0G2K830
A	939	TYR	-	expression tag	UNP A0A0G2K830
A	940	VAL	-	expression tag	UNP A0A0G2K830
A	941	GLN	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	942	GLU	-	expression tag	UNP A0A0G2K830
A	943	ARG	-	expression tag	UNP A0A0G2K830
A	944	THR	-	expression tag	UNP A0A0G2K830
A	945	ILE	-	expression tag	UNP A0A0G2K830
A	946	PHE	-	expression tag	UNP A0A0G2K830
A	947	PHE	-	expression tag	UNP A0A0G2K830
A	948	LYS	-	expression tag	UNP A0A0G2K830
A	949	ASP	-	expression tag	UNP A0A0G2K830
A	950	ASP	-	expression tag	UNP A0A0G2K830
A	951	GLY	-	expression tag	UNP A0A0G2K830
A	952	ASN	-	expression tag	UNP A0A0G2K830
A	953	TYR	-	expression tag	UNP A0A0G2K830
A	954	LYS	-	expression tag	UNP A0A0G2K830
A	955	THR	-	expression tag	UNP A0A0G2K830
A	956	ARG	-	expression tag	UNP A0A0G2K830
A	957	ALA	-	expression tag	UNP A0A0G2K830
A	958	GLU	-	expression tag	UNP A0A0G2K830
A	959	VAL	-	expression tag	UNP A0A0G2K830
A	960	LYS	-	expression tag	UNP A0A0G2K830
A	961	PHE	-	expression tag	UNP A0A0G2K830
A	962	GLU	-	expression tag	UNP A0A0G2K830
A	963	GLY	-	expression tag	UNP A0A0G2K830
A	964	ASP	-	expression tag	UNP A0A0G2K830
A	965	THR	-	expression tag	UNP A0A0G2K830
A	966	LEU	-	expression tag	UNP A0A0G2K830
A	967	VAL	-	expression tag	UNP A0A0G2K830
A	968	ASN	-	expression tag	UNP A0A0G2K830
A	969	ARG	-	expression tag	UNP A0A0G2K830
A	970	ILE	-	expression tag	UNP A0A0G2K830
A	971	GLU	-	expression tag	UNP A0A0G2K830
A	972	LEU	-	expression tag	UNP A0A0G2K830
A	973	LYS	-	expression tag	UNP A0A0G2K830
A	974	GLY	-	expression tag	UNP A0A0G2K830
A	975	ILE	-	expression tag	UNP A0A0G2K830
A	976	ASP	-	expression tag	UNP A0A0G2K830
A	977	PHE	-	expression tag	UNP A0A0G2K830
A	978	LYS	-	expression tag	UNP A0A0G2K830
A	979	GLU	-	expression tag	UNP A0A0G2K830
A	980	ASP	-	expression tag	UNP A0A0G2K830
A	981	GLY	-	expression tag	UNP A0A0G2K830
A	982	ASN	-	expression tag	UNP A0A0G2K830
A	983	ILE	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	984	LEU	-	expression tag	UNP A0A0G2K830
A	985	GLY	-	expression tag	UNP A0A0G2K830
A	986	HIS	-	expression tag	UNP A0A0G2K830
A	987	LYS	-	expression tag	UNP A0A0G2K830
A	988	LEU	-	expression tag	UNP A0A0G2K830
A	989	GLU	-	expression tag	UNP A0A0G2K830
A	990	TYR	-	expression tag	UNP A0A0G2K830
A	991	ASN	-	expression tag	UNP A0A0G2K830
A	992	TYR	-	expression tag	UNP A0A0G2K830
A	993	ASN	-	expression tag	UNP A0A0G2K830
A	994	SER	-	expression tag	UNP A0A0G2K830
A	995	HIS	-	expression tag	UNP A0A0G2K830
A	996	ASN	-	expression tag	UNP A0A0G2K830
A	997	VAL	-	expression tag	UNP A0A0G2K830
A	998	TYR	-	expression tag	UNP A0A0G2K830
A	999	ILE	-	expression tag	UNP A0A0G2K830
A	1000	MET	-	expression tag	UNP A0A0G2K830
A	1001	ALA	-	expression tag	UNP A0A0G2K830
A	1002	ASP	-	expression tag	UNP A0A0G2K830
A	1003	LYS	-	expression tag	UNP A0A0G2K830
A	1004	GLN	-	expression tag	UNP A0A0G2K830
A	1005	LYS	-	expression tag	UNP A0A0G2K830
A	1006	ASN	-	expression tag	UNP A0A0G2K830
A	1007	GLY	-	expression tag	UNP A0A0G2K830
A	1008	ILE	-	expression tag	UNP A0A0G2K830
A	1009	LYS	-	expression tag	UNP A0A0G2K830
A	1010	VAL	-	expression tag	UNP A0A0G2K830
A	1011	ASN	-	expression tag	UNP A0A0G2K830
A	1012	PHE	-	expression tag	UNP A0A0G2K830
A	1013	LYS	-	expression tag	UNP A0A0G2K830
A	1014	ILE	-	expression tag	UNP A0A0G2K830
A	1015	ARG	-	expression tag	UNP A0A0G2K830
A	1016	HIS	-	expression tag	UNP A0A0G2K830
A	1017	ASN	-	expression tag	UNP A0A0G2K830
A	1018	ILE	-	expression tag	UNP A0A0G2K830
A	1019	GLU	-	expression tag	UNP A0A0G2K830
A	1020	ASP	-	expression tag	UNP A0A0G2K830
A	1021	GLY	-	expression tag	UNP A0A0G2K830
A	1022	SER	-	expression tag	UNP A0A0G2K830
A	1023	VAL	-	expression tag	UNP A0A0G2K830
A	1024	GLN	-	expression tag	UNP A0A0G2K830
A	1025	LEU	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	-	expression tag	UNP A0A0G2K830
A	1027	ASP	-	expression tag	UNP A0A0G2K830
A	1028	HIS	-	expression tag	UNP A0A0G2K830
A	1029	TYR	-	expression tag	UNP A0A0G2K830
A	1030	GLN	-	expression tag	UNP A0A0G2K830
A	1031	GLN	-	expression tag	UNP A0A0G2K830
A	1032	ASN	-	expression tag	UNP A0A0G2K830
A	1033	THR	-	expression tag	UNP A0A0G2K830
A	1034	PRO	-	expression tag	UNP A0A0G2K830
A	1035	ILE	-	expression tag	UNP A0A0G2K830
A	1036	GLY	-	expression tag	UNP A0A0G2K830
A	1037	ASP	-	expression tag	UNP A0A0G2K830
A	1038	GLY	-	expression tag	UNP A0A0G2K830
A	1039	PRO	-	expression tag	UNP A0A0G2K830
A	1040	VAL	-	expression tag	UNP A0A0G2K830
A	1041	LEU	-	expression tag	UNP A0A0G2K830
A	1042	LEU	-	expression tag	UNP A0A0G2K830
A	1043	PRO	-	expression tag	UNP A0A0G2K830
A	1044	ASP	-	expression tag	UNP A0A0G2K830
A	1045	ASN	-	expression tag	UNP A0A0G2K830
A	1046	HIS	-	expression tag	UNP A0A0G2K830
A	1047	TYR	-	expression tag	UNP A0A0G2K830
A	1048	LEU	-	expression tag	UNP A0A0G2K830
A	1049	SER	-	expression tag	UNP A0A0G2K830
A	1050	THR	-	expression tag	UNP A0A0G2K830
A	1051	GLN	-	expression tag	UNP A0A0G2K830
A	1052	SER	-	expression tag	UNP A0A0G2K830
A	1053	LYS	-	expression tag	UNP A0A0G2K830
A	1054	LEU	-	expression tag	UNP A0A0G2K830
A	1055	SER	-	expression tag	UNP A0A0G2K830
A	1056	LYS	-	expression tag	UNP A0A0G2K830
A	1057	ASP	-	expression tag	UNP A0A0G2K830
A	1058	PRO	-	expression tag	UNP A0A0G2K830
A	1059	ASN	-	expression tag	UNP A0A0G2K830
A	1060	GLU	-	expression tag	UNP A0A0G2K830
A	1061	LYS	-	expression tag	UNP A0A0G2K830
A	1062	ARG	-	expression tag	UNP A0A0G2K830
A	1063	ASP	-	expression tag	UNP A0A0G2K830
A	1064	HIS	-	expression tag	UNP A0A0G2K830
A	1065	MET	-	expression tag	UNP A0A0G2K830
A	1066	VAL	-	expression tag	UNP A0A0G2K830
A	1067	LEU	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1068	LEU	-	expression tag	UNP A0A0G2K830
A	1069	GLU	-	expression tag	UNP A0A0G2K830
A	1070	PHE	-	expression tag	UNP A0A0G2K830
A	1071	VAL	-	expression tag	UNP A0A0G2K830
A	1072	THR	-	expression tag	UNP A0A0G2K830
A	1073	ALA	-	expression tag	UNP A0A0G2K830
A	1074	ALA	-	expression tag	UNP A0A0G2K830
A	1075	GLY	-	expression tag	UNP A0A0G2K830
A	1076	ILE	-	expression tag	UNP A0A0G2K830
A	1077	THR	-	expression tag	UNP A0A0G2K830
A	1078	LEU	-	expression tag	UNP A0A0G2K830
A	1079	GLY	-	expression tag	UNP A0A0G2K830
A	1080	MET	-	expression tag	UNP A0A0G2K830
A	1081	ASP	-	expression tag	UNP A0A0G2K830
A	1082	GLU	-	expression tag	UNP A0A0G2K830
A	1083	LEU	-	expression tag	UNP A0A0G2K830
A	1084	TYR	-	expression tag	UNP A0A0G2K830
A	1085	LYS	-	expression tag	UNP A0A0G2K830
A	1086	SER	-	expression tag	UNP A0A0G2K830
A	1087	GLY	-	expression tag	UNP A0A0G2K830
A	1088	LEU	-	expression tag	UNP A0A0G2K830
A	1089	ARG	-	expression tag	UNP A0A0G2K830
A	1090	SER	-	expression tag	UNP A0A0G2K830
A	1091	HIS	-	expression tag	UNP A0A0G2K830
A	1092	HIS	-	expression tag	UNP A0A0G2K830
A	1093	HIS	-	expression tag	UNP A0A0G2K830
A	1094	HIS	-	expression tag	UNP A0A0G2K830
A	1095	HIS	-	expression tag	UNP A0A0G2K830
A	1096	HIS	-	expression tag	UNP A0A0G2K830
A	1097	HIS	-	expression tag	UNP A0A0G2K830
A	1098	HIS	-	expression tag	UNP A0A0G2K830
B	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
B	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
B	838	LEU	-	expression tag	UNP A0A0G2K830
B	839	VAL	-	expression tag	UNP A0A0G2K830
B	840	PRO	-	expression tag	UNP A0A0G2K830
B	841	ARG	-	expression tag	UNP A0A0G2K830
B	842	GLY	-	expression tag	UNP A0A0G2K830
B	843	SER	-	expression tag	UNP A0A0G2K830
B	844	ALA	-	expression tag	UNP A0A0G2K830
B	845	ALA	-	expression tag	UNP A0A0G2K830
B	846	ALA	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	847	ALA	-	expression tag	UNP A0A0G2K830
B	848	VAL	-	expression tag	UNP A0A0G2K830
B	849	SER	-	expression tag	UNP A0A0G2K830
B	850	LYS	-	expression tag	UNP A0A0G2K830
B	851	GLY	-	expression tag	UNP A0A0G2K830
B	852	GLU	-	expression tag	UNP A0A0G2K830
B	853	GLU	-	expression tag	UNP A0A0G2K830
B	854	LEU	-	expression tag	UNP A0A0G2K830
B	855	PHE	-	expression tag	UNP A0A0G2K830
B	856	THR	-	expression tag	UNP A0A0G2K830
B	857	GLY	-	expression tag	UNP A0A0G2K830
B	858	VAL	-	expression tag	UNP A0A0G2K830
B	859	VAL	-	expression tag	UNP A0A0G2K830
B	860	PRO	-	expression tag	UNP A0A0G2K830
B	861	ILE	-	expression tag	UNP A0A0G2K830
B	862	LEU	-	expression tag	UNP A0A0G2K830
B	863	VAL	-	expression tag	UNP A0A0G2K830
B	864	GLU	-	expression tag	UNP A0A0G2K830
B	865	LEU	-	expression tag	UNP A0A0G2K830
B	866	ASP	-	expression tag	UNP A0A0G2K830
B	867	GLY	-	expression tag	UNP A0A0G2K830
B	868	ASP	-	expression tag	UNP A0A0G2K830
B	869	VAL	-	expression tag	UNP A0A0G2K830
B	870	ASN	-	expression tag	UNP A0A0G2K830
B	871	GLY	-	expression tag	UNP A0A0G2K830
B	872	HIS	-	expression tag	UNP A0A0G2K830
B	873	LYS	-	expression tag	UNP A0A0G2K830
B	874	PHE	-	expression tag	UNP A0A0G2K830
B	875	SER	-	expression tag	UNP A0A0G2K830
B	876	VAL	-	expression tag	UNP A0A0G2K830
B	877	SER	-	expression tag	UNP A0A0G2K830
B	878	GLY	-	expression tag	UNP A0A0G2K830
B	879	GLU	-	expression tag	UNP A0A0G2K830
B	880	GLY	-	expression tag	UNP A0A0G2K830
B	881	GLU	-	expression tag	UNP A0A0G2K830
B	882	GLY	-	expression tag	UNP A0A0G2K830
B	883	ASP	-	expression tag	UNP A0A0G2K830
B	884	ALA	-	expression tag	UNP A0A0G2K830
B	885	THR	-	expression tag	UNP A0A0G2K830
B	886	TYR	-	expression tag	UNP A0A0G2K830
B	887	GLY	-	expression tag	UNP A0A0G2K830
B	888	LYS	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	889	LEU	-	expression tag	UNP A0A0G2K830
B	890	THR	-	expression tag	UNP A0A0G2K830
B	891	LEU	-	expression tag	UNP A0A0G2K830
B	892	LYS	-	expression tag	UNP A0A0G2K830
B	893	PHE	-	expression tag	UNP A0A0G2K830
B	894	ILE	-	expression tag	UNP A0A0G2K830
B	895	CYS	-	expression tag	UNP A0A0G2K830
B	896	THR	-	expression tag	UNP A0A0G2K830
B	897	THR	-	expression tag	UNP A0A0G2K830
B	898	GLY	-	expression tag	UNP A0A0G2K830
B	899	LYS	-	expression tag	UNP A0A0G2K830
B	900	LEU	-	expression tag	UNP A0A0G2K830
B	901	PRO	-	expression tag	UNP A0A0G2K830
B	902	VAL	-	expression tag	UNP A0A0G2K830
B	903	PRO	-	expression tag	UNP A0A0G2K830
B	904	TRP	-	expression tag	UNP A0A0G2K830
B	905	PRO	-	expression tag	UNP A0A0G2K830
B	906	THR	-	expression tag	UNP A0A0G2K830
B	907	LEU	-	expression tag	UNP A0A0G2K830
B	908	VAL	-	expression tag	UNP A0A0G2K830
B	909	THR	-	expression tag	UNP A0A0G2K830
B	910	THR	-	expression tag	UNP A0A0G2K830
B	911	LEU	-	expression tag	UNP A0A0G2K830
B	912	THR	-	expression tag	UNP A0A0G2K830
B	913	TYR	-	expression tag	UNP A0A0G2K830
B	914	GLY	-	expression tag	UNP A0A0G2K830
B	915	VAL	-	expression tag	UNP A0A0G2K830
B	916	GLN	-	expression tag	UNP A0A0G2K830
B	917	CYS	-	expression tag	UNP A0A0G2K830
B	918	PHE	-	expression tag	UNP A0A0G2K830
B	919	SER	-	expression tag	UNP A0A0G2K830
B	920	ARG	-	expression tag	UNP A0A0G2K830
B	921	TYR	-	expression tag	UNP A0A0G2K830
B	922	PRO	-	expression tag	UNP A0A0G2K830
B	923	ASP	-	expression tag	UNP A0A0G2K830
B	924	HIS	-	expression tag	UNP A0A0G2K830
B	925	MET	-	expression tag	UNP A0A0G2K830
B	926	LYS	-	expression tag	UNP A0A0G2K830
B	927	GLN	-	expression tag	UNP A0A0G2K830
B	928	HIS	-	expression tag	UNP A0A0G2K830
B	929	ASP	-	expression tag	UNP A0A0G2K830
B	930	PHE	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	931	PHE	-	expression tag	UNP A0A0G2K830
B	932	LYS	-	expression tag	UNP A0A0G2K830
B	933	SER	-	expression tag	UNP A0A0G2K830
B	934	ALA	-	expression tag	UNP A0A0G2K830
B	935	MET	-	expression tag	UNP A0A0G2K830
B	936	PRO	-	expression tag	UNP A0A0G2K830
B	937	GLU	-	expression tag	UNP A0A0G2K830
B	938	GLY	-	expression tag	UNP A0A0G2K830
B	939	TYR	-	expression tag	UNP A0A0G2K830
B	940	VAL	-	expression tag	UNP A0A0G2K830
B	941	GLN	-	expression tag	UNP A0A0G2K830
B	942	GLU	-	expression tag	UNP A0A0G2K830
B	943	ARG	-	expression tag	UNP A0A0G2K830
B	944	THR	-	expression tag	UNP A0A0G2K830
B	945	ILE	-	expression tag	UNP A0A0G2K830
B	946	PHE	-	expression tag	UNP A0A0G2K830
B	947	PHE	-	expression tag	UNP A0A0G2K830
B	948	LYS	-	expression tag	UNP A0A0G2K830
B	949	ASP	-	expression tag	UNP A0A0G2K830
B	950	ASP	-	expression tag	UNP A0A0G2K830
B	951	GLY	-	expression tag	UNP A0A0G2K830
B	952	ASN	-	expression tag	UNP A0A0G2K830
B	953	TYR	-	expression tag	UNP A0A0G2K830
B	954	LYS	-	expression tag	UNP A0A0G2K830
B	955	THR	-	expression tag	UNP A0A0G2K830
B	956	ARG	-	expression tag	UNP A0A0G2K830
B	957	ALA	-	expression tag	UNP A0A0G2K830
B	958	GLU	-	expression tag	UNP A0A0G2K830
B	959	VAL	-	expression tag	UNP A0A0G2K830
B	960	LYS	-	expression tag	UNP A0A0G2K830
B	961	PHE	-	expression tag	UNP A0A0G2K830
B	962	GLU	-	expression tag	UNP A0A0G2K830
B	963	GLY	-	expression tag	UNP A0A0G2K830
B	964	ASP	-	expression tag	UNP A0A0G2K830
B	965	THR	-	expression tag	UNP A0A0G2K830
B	966	LEU	-	expression tag	UNP A0A0G2K830
B	967	VAL	-	expression tag	UNP A0A0G2K830
B	968	ASN	-	expression tag	UNP A0A0G2K830
B	969	ARG	-	expression tag	UNP A0A0G2K830
B	970	ILE	-	expression tag	UNP A0A0G2K830
B	971	GLU	-	expression tag	UNP A0A0G2K830
B	972	LEU	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	973	LYS	-	expression tag	UNP A0A0G2K830
B	974	GLY	-	expression tag	UNP A0A0G2K830
B	975	ILE	-	expression tag	UNP A0A0G2K830
B	976	ASP	-	expression tag	UNP A0A0G2K830
B	977	PHE	-	expression tag	UNP A0A0G2K830
B	978	LYS	-	expression tag	UNP A0A0G2K830
B	979	GLU	-	expression tag	UNP A0A0G2K830
B	980	ASP	-	expression tag	UNP A0A0G2K830
B	981	GLY	-	expression tag	UNP A0A0G2K830
B	982	ASN	-	expression tag	UNP A0A0G2K830
B	983	ILE	-	expression tag	UNP A0A0G2K830
B	984	LEU	-	expression tag	UNP A0A0G2K830
B	985	GLY	-	expression tag	UNP A0A0G2K830
B	986	HIS	-	expression tag	UNP A0A0G2K830
B	987	LYS	-	expression tag	UNP A0A0G2K830
B	988	LEU	-	expression tag	UNP A0A0G2K830
B	989	GLU	-	expression tag	UNP A0A0G2K830
B	990	TYR	-	expression tag	UNP A0A0G2K830
B	991	ASN	-	expression tag	UNP A0A0G2K830
B	992	TYR	-	expression tag	UNP A0A0G2K830
B	993	ASN	-	expression tag	UNP A0A0G2K830
B	994	SER	-	expression tag	UNP A0A0G2K830
B	995	HIS	-	expression tag	UNP A0A0G2K830
B	996	ASN	-	expression tag	UNP A0A0G2K830
B	997	VAL	-	expression tag	UNP A0A0G2K830
B	998	TYR	-	expression tag	UNP A0A0G2K830
B	999	ILE	-	expression tag	UNP A0A0G2K830
B	1000	MET	-	expression tag	UNP A0A0G2K830
B	1001	ALA	-	expression tag	UNP A0A0G2K830
B	1002	ASP	-	expression tag	UNP A0A0G2K830
B	1003	LYS	-	expression tag	UNP A0A0G2K830
B	1004	GLN	-	expression tag	UNP A0A0G2K830
B	1005	LYS	-	expression tag	UNP A0A0G2K830
B	1006	ASN	-	expression tag	UNP A0A0G2K830
B	1007	GLY	-	expression tag	UNP A0A0G2K830
B	1008	ILE	-	expression tag	UNP A0A0G2K830
B	1009	LYS	-	expression tag	UNP A0A0G2K830
B	1010	VAL	-	expression tag	UNP A0A0G2K830
B	1011	ASN	-	expression tag	UNP A0A0G2K830
B	1012	PHE	-	expression tag	UNP A0A0G2K830
B	1013	LYS	-	expression tag	UNP A0A0G2K830
B	1014	ILE	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1015	ARG	-	expression tag	UNP A0A0G2K830
B	1016	HIS	-	expression tag	UNP A0A0G2K830
B	1017	ASN	-	expression tag	UNP A0A0G2K830
B	1018	ILE	-	expression tag	UNP A0A0G2K830
B	1019	GLU	-	expression tag	UNP A0A0G2K830
B	1020	ASP	-	expression tag	UNP A0A0G2K830
B	1021	GLY	-	expression tag	UNP A0A0G2K830
B	1022	SER	-	expression tag	UNP A0A0G2K830
B	1023	VAL	-	expression tag	UNP A0A0G2K830
B	1024	GLN	-	expression tag	UNP A0A0G2K830
B	1025	LEU	-	expression tag	UNP A0A0G2K830
B	1026	ALA	-	expression tag	UNP A0A0G2K830
B	1027	ASP	-	expression tag	UNP A0A0G2K830
B	1028	HIS	-	expression tag	UNP A0A0G2K830
B	1029	TYR	-	expression tag	UNP A0A0G2K830
B	1030	GLN	-	expression tag	UNP A0A0G2K830
B	1031	GLN	-	expression tag	UNP A0A0G2K830
B	1032	ASN	-	expression tag	UNP A0A0G2K830
B	1033	THR	-	expression tag	UNP A0A0G2K830
B	1034	PRO	-	expression tag	UNP A0A0G2K830
B	1035	ILE	-	expression tag	UNP A0A0G2K830
B	1036	GLY	-	expression tag	UNP A0A0G2K830
B	1037	ASP	-	expression tag	UNP A0A0G2K830
B	1038	GLY	-	expression tag	UNP A0A0G2K830
B	1039	PRO	-	expression tag	UNP A0A0G2K830
B	1040	VAL	-	expression tag	UNP A0A0G2K830
B	1041	LEU	-	expression tag	UNP A0A0G2K830
B	1042	LEU	-	expression tag	UNP A0A0G2K830
B	1043	PRO	-	expression tag	UNP A0A0G2K830
B	1044	ASP	-	expression tag	UNP A0A0G2K830
B	1045	ASN	-	expression tag	UNP A0A0G2K830
B	1046	HIS	-	expression tag	UNP A0A0G2K830
B	1047	TYR	-	expression tag	UNP A0A0G2K830
B	1048	LEU	-	expression tag	UNP A0A0G2K830
B	1049	SER	-	expression tag	UNP A0A0G2K830
B	1050	THR	-	expression tag	UNP A0A0G2K830
B	1051	GLN	-	expression tag	UNP A0A0G2K830
B	1052	SER	-	expression tag	UNP A0A0G2K830
B	1053	LYS	-	expression tag	UNP A0A0G2K830
B	1054	LEU	-	expression tag	UNP A0A0G2K830
B	1055	SER	-	expression tag	UNP A0A0G2K830
B	1056	LYS	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1057	ASP	-	expression tag	UNP A0A0G2K830
B	1058	PRO	-	expression tag	UNP A0A0G2K830
B	1059	ASN	-	expression tag	UNP A0A0G2K830
B	1060	GLU	-	expression tag	UNP A0A0G2K830
B	1061	LYS	-	expression tag	UNP A0A0G2K830
B	1062	ARG	-	expression tag	UNP A0A0G2K830
B	1063	ASP	-	expression tag	UNP A0A0G2K830
B	1064	HIS	-	expression tag	UNP A0A0G2K830
B	1065	MET	-	expression tag	UNP A0A0G2K830
B	1066	VAL	-	expression tag	UNP A0A0G2K830
B	1067	LEU	-	expression tag	UNP A0A0G2K830
B	1068	LEU	-	expression tag	UNP A0A0G2K830
B	1069	GLU	-	expression tag	UNP A0A0G2K830
B	1070	PHE	-	expression tag	UNP A0A0G2K830
B	1071	VAL	-	expression tag	UNP A0A0G2K830
B	1072	THR	-	expression tag	UNP A0A0G2K830
B	1073	ALA	-	expression tag	UNP A0A0G2K830
B	1074	ALA	-	expression tag	UNP A0A0G2K830
B	1075	GLY	-	expression tag	UNP A0A0G2K830
B	1076	ILE	-	expression tag	UNP A0A0G2K830
B	1077	THR	-	expression tag	UNP A0A0G2K830
B	1078	LEU	-	expression tag	UNP A0A0G2K830
B	1079	GLY	-	expression tag	UNP A0A0G2K830
B	1080	MET	-	expression tag	UNP A0A0G2K830
B	1081	ASP	-	expression tag	UNP A0A0G2K830
B	1082	GLU	-	expression tag	UNP A0A0G2K830
B	1083	LEU	-	expression tag	UNP A0A0G2K830
B	1084	TYR	-	expression tag	UNP A0A0G2K830
B	1085	LYS	-	expression tag	UNP A0A0G2K830
B	1086	SER	-	expression tag	UNP A0A0G2K830
B	1087	GLY	-	expression tag	UNP A0A0G2K830
B	1088	LEU	-	expression tag	UNP A0A0G2K830
B	1089	ARG	-	expression tag	UNP A0A0G2K830
B	1090	SER	-	expression tag	UNP A0A0G2K830
B	1091	HIS	-	expression tag	UNP A0A0G2K830
B	1092	HIS	-	expression tag	UNP A0A0G2K830
B	1093	HIS	-	expression tag	UNP A0A0G2K830
B	1094	HIS	-	expression tag	UNP A0A0G2K830
B	1095	HIS	-	expression tag	UNP A0A0G2K830
B	1096	HIS	-	expression tag	UNP A0A0G2K830
B	1097	HIS	-	expression tag	UNP A0A0G2K830
B	1098	HIS	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
C	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
C	838	LEU	-	expression tag	UNP A0A0G2K830
C	839	VAL	-	expression tag	UNP A0A0G2K830
C	840	PRO	-	expression tag	UNP A0A0G2K830
C	841	ARG	-	expression tag	UNP A0A0G2K830
C	842	GLY	-	expression tag	UNP A0A0G2K830
C	843	SER	-	expression tag	UNP A0A0G2K830
C	844	ALA	-	expression tag	UNP A0A0G2K830
C	845	ALA	-	expression tag	UNP A0A0G2K830
C	846	ALA	-	expression tag	UNP A0A0G2K830
C	847	ALA	-	expression tag	UNP A0A0G2K830
C	848	VAL	-	expression tag	UNP A0A0G2K830
C	849	SER	-	expression tag	UNP A0A0G2K830
C	850	LYS	-	expression tag	UNP A0A0G2K830
C	851	GLY	-	expression tag	UNP A0A0G2K830
C	852	GLU	-	expression tag	UNP A0A0G2K830
C	853	GLU	-	expression tag	UNP A0A0G2K830
C	854	LEU	-	expression tag	UNP A0A0G2K830
C	855	PHE	-	expression tag	UNP A0A0G2K830
C	856	THR	-	expression tag	UNP A0A0G2K830
C	857	GLY	-	expression tag	UNP A0A0G2K830
C	858	VAL	-	expression tag	UNP A0A0G2K830
C	859	VAL	-	expression tag	UNP A0A0G2K830
C	860	PRO	-	expression tag	UNP A0A0G2K830
C	861	ILE	-	expression tag	UNP A0A0G2K830
C	862	LEU	-	expression tag	UNP A0A0G2K830
C	863	VAL	-	expression tag	UNP A0A0G2K830
C	864	GLU	-	expression tag	UNP A0A0G2K830
C	865	LEU	-	expression tag	UNP A0A0G2K830
C	866	ASP	-	expression tag	UNP A0A0G2K830
C	867	GLY	-	expression tag	UNP A0A0G2K830
C	868	ASP	-	expression tag	UNP A0A0G2K830
C	869	VAL	-	expression tag	UNP A0A0G2K830
C	870	ASN	-	expression tag	UNP A0A0G2K830
C	871	GLY	-	expression tag	UNP A0A0G2K830
C	872	HIS	-	expression tag	UNP A0A0G2K830
C	873	LYS	-	expression tag	UNP A0A0G2K830
C	874	PHE	-	expression tag	UNP A0A0G2K830
C	875	SER	-	expression tag	UNP A0A0G2K830
C	876	VAL	-	expression tag	UNP A0A0G2K830
C	877	SER	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	878	GLY	-	expression tag	UNP A0A0G2K830
C	879	GLU	-	expression tag	UNP A0A0G2K830
C	880	GLY	-	expression tag	UNP A0A0G2K830
C	881	GLU	-	expression tag	UNP A0A0G2K830
C	882	GLY	-	expression tag	UNP A0A0G2K830
C	883	ASP	-	expression tag	UNP A0A0G2K830
C	884	ALA	-	expression tag	UNP A0A0G2K830
C	885	THR	-	expression tag	UNP A0A0G2K830
C	886	TYR	-	expression tag	UNP A0A0G2K830
C	887	GLY	-	expression tag	UNP A0A0G2K830
C	888	LYS	-	expression tag	UNP A0A0G2K830
C	889	LEU	-	expression tag	UNP A0A0G2K830
C	890	THR	-	expression tag	UNP A0A0G2K830
C	891	LEU	-	expression tag	UNP A0A0G2K830
C	892	LYS	-	expression tag	UNP A0A0G2K830
C	893	PHE	-	expression tag	UNP A0A0G2K830
C	894	ILE	-	expression tag	UNP A0A0G2K830
C	895	CYS	-	expression tag	UNP A0A0G2K830
C	896	THR	-	expression tag	UNP A0A0G2K830
C	897	THR	-	expression tag	UNP A0A0G2K830
C	898	GLY	-	expression tag	UNP A0A0G2K830
C	899	LYS	-	expression tag	UNP A0A0G2K830
C	900	LEU	-	expression tag	UNP A0A0G2K830
C	901	PRO	-	expression tag	UNP A0A0G2K830
C	902	VAL	-	expression tag	UNP A0A0G2K830
C	903	PRO	-	expression tag	UNP A0A0G2K830
C	904	TRP	-	expression tag	UNP A0A0G2K830
C	905	PRO	-	expression tag	UNP A0A0G2K830
C	906	THR	-	expression tag	UNP A0A0G2K830
C	907	LEU	-	expression tag	UNP A0A0G2K830
C	908	VAL	-	expression tag	UNP A0A0G2K830
C	909	THR	-	expression tag	UNP A0A0G2K830
C	910	THR	-	expression tag	UNP A0A0G2K830
C	911	LEU	-	expression tag	UNP A0A0G2K830
C	912	THR	-	expression tag	UNP A0A0G2K830
C	913	TYR	-	expression tag	UNP A0A0G2K830
C	914	GLY	-	expression tag	UNP A0A0G2K830
C	915	VAL	-	expression tag	UNP A0A0G2K830
C	916	GLN	-	expression tag	UNP A0A0G2K830
C	917	CYS	-	expression tag	UNP A0A0G2K830
C	918	PHE	-	expression tag	UNP A0A0G2K830
C	919	SER	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	920	ARG	-	expression tag	UNP A0A0G2K830
C	921	TYR	-	expression tag	UNP A0A0G2K830
C	922	PRO	-	expression tag	UNP A0A0G2K830
C	923	ASP	-	expression tag	UNP A0A0G2K830
C	924	HIS	-	expression tag	UNP A0A0G2K830
C	925	MET	-	expression tag	UNP A0A0G2K830
C	926	LYS	-	expression tag	UNP A0A0G2K830
C	927	GLN	-	expression tag	UNP A0A0G2K830
C	928	HIS	-	expression tag	UNP A0A0G2K830
C	929	ASP	-	expression tag	UNP A0A0G2K830
C	930	PHE	-	expression tag	UNP A0A0G2K830
C	931	PHE	-	expression tag	UNP A0A0G2K830
C	932	LYS	-	expression tag	UNP A0A0G2K830
C	933	SER	-	expression tag	UNP A0A0G2K830
C	934	ALA	-	expression tag	UNP A0A0G2K830
C	935	MET	-	expression tag	UNP A0A0G2K830
C	936	PRO	-	expression tag	UNP A0A0G2K830
C	937	GLU	-	expression tag	UNP A0A0G2K830
C	938	GLY	-	expression tag	UNP A0A0G2K830
C	939	TYR	-	expression tag	UNP A0A0G2K830
C	940	VAL	-	expression tag	UNP A0A0G2K830
C	941	GLN	-	expression tag	UNP A0A0G2K830
C	942	GLU	-	expression tag	UNP A0A0G2K830
C	943	ARG	-	expression tag	UNP A0A0G2K830
C	944	THR	-	expression tag	UNP A0A0G2K830
C	945	ILE	-	expression tag	UNP A0A0G2K830
C	946	PHE	-	expression tag	UNP A0A0G2K830
C	947	PHE	-	expression tag	UNP A0A0G2K830
C	948	LYS	-	expression tag	UNP A0A0G2K830
C	949	ASP	-	expression tag	UNP A0A0G2K830
C	950	ASP	-	expression tag	UNP A0A0G2K830
C	951	GLY	-	expression tag	UNP A0A0G2K830
C	952	ASN	-	expression tag	UNP A0A0G2K830
C	953	TYR	-	expression tag	UNP A0A0G2K830
C	954	LYS	-	expression tag	UNP A0A0G2K830
C	955	THR	-	expression tag	UNP A0A0G2K830
C	956	ARG	-	expression tag	UNP A0A0G2K830
C	957	ALA	-	expression tag	UNP A0A0G2K830
C	958	GLU	-	expression tag	UNP A0A0G2K830
C	959	VAL	-	expression tag	UNP A0A0G2K830
C	960	LYS	-	expression tag	UNP A0A0G2K830
C	961	PHE	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	962	GLU	-	expression tag	UNP A0A0G2K830
C	963	GLY	-	expression tag	UNP A0A0G2K830
C	964	ASP	-	expression tag	UNP A0A0G2K830
C	965	THR	-	expression tag	UNP A0A0G2K830
C	966	LEU	-	expression tag	UNP A0A0G2K830
C	967	VAL	-	expression tag	UNP A0A0G2K830
C	968	ASN	-	expression tag	UNP A0A0G2K830
C	969	ARG	-	expression tag	UNP A0A0G2K830
C	970	ILE	-	expression tag	UNP A0A0G2K830
C	971	GLU	-	expression tag	UNP A0A0G2K830
C	972	LEU	-	expression tag	UNP A0A0G2K830
C	973	LYS	-	expression tag	UNP A0A0G2K830
C	974	GLY	-	expression tag	UNP A0A0G2K830
C	975	ILE	-	expression tag	UNP A0A0G2K830
C	976	ASP	-	expression tag	UNP A0A0G2K830
C	977	PHE	-	expression tag	UNP A0A0G2K830
C	978	LYS	-	expression tag	UNP A0A0G2K830
C	979	GLU	-	expression tag	UNP A0A0G2K830
C	980	ASP	-	expression tag	UNP A0A0G2K830
C	981	GLY	-	expression tag	UNP A0A0G2K830
C	982	ASN	-	expression tag	UNP A0A0G2K830
C	983	ILE	-	expression tag	UNP A0A0G2K830
C	984	LEU	-	expression tag	UNP A0A0G2K830
C	985	GLY	-	expression tag	UNP A0A0G2K830
C	986	HIS	-	expression tag	UNP A0A0G2K830
C	987	LYS	-	expression tag	UNP A0A0G2K830
C	988	LEU	-	expression tag	UNP A0A0G2K830
C	989	GLU	-	expression tag	UNP A0A0G2K830
C	990	TYR	-	expression tag	UNP A0A0G2K830
C	991	ASN	-	expression tag	UNP A0A0G2K830
C	992	TYR	-	expression tag	UNP A0A0G2K830
C	993	ASN	-	expression tag	UNP A0A0G2K830
C	994	SER	-	expression tag	UNP A0A0G2K830
C	995	HIS	-	expression tag	UNP A0A0G2K830
C	996	ASN	-	expression tag	UNP A0A0G2K830
C	997	VAL	-	expression tag	UNP A0A0G2K830
C	998	TYR	-	expression tag	UNP A0A0G2K830
C	999	ILE	-	expression tag	UNP A0A0G2K830
C	1000	MET	-	expression tag	UNP A0A0G2K830
C	1001	ALA	-	expression tag	UNP A0A0G2K830
C	1002	ASP	-	expression tag	UNP A0A0G2K830
C	1003	LYS	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1004	GLN	-	expression tag	UNP A0A0G2K830
C	1005	LYS	-	expression tag	UNP A0A0G2K830
C	1006	ASN	-	expression tag	UNP A0A0G2K830
C	1007	GLY	-	expression tag	UNP A0A0G2K830
C	1008	ILE	-	expression tag	UNP A0A0G2K830
C	1009	LYS	-	expression tag	UNP A0A0G2K830
C	1010	VAL	-	expression tag	UNP A0A0G2K830
C	1011	ASN	-	expression tag	UNP A0A0G2K830
C	1012	PHE	-	expression tag	UNP A0A0G2K830
C	1013	LYS	-	expression tag	UNP A0A0G2K830
C	1014	ILE	-	expression tag	UNP A0A0G2K830
C	1015	ARG	-	expression tag	UNP A0A0G2K830
C	1016	HIS	-	expression tag	UNP A0A0G2K830
C	1017	ASN	-	expression tag	UNP A0A0G2K830
C	1018	ILE	-	expression tag	UNP A0A0G2K830
C	1019	GLU	-	expression tag	UNP A0A0G2K830
C	1020	ASP	-	expression tag	UNP A0A0G2K830
C	1021	GLY	-	expression tag	UNP A0A0G2K830
C	1022	SER	-	expression tag	UNP A0A0G2K830
C	1023	VAL	-	expression tag	UNP A0A0G2K830
C	1024	GLN	-	expression tag	UNP A0A0G2K830
C	1025	LEU	-	expression tag	UNP A0A0G2K830
C	1026	ALA	-	expression tag	UNP A0A0G2K830
C	1027	ASP	-	expression tag	UNP A0A0G2K830
C	1028	HIS	-	expression tag	UNP A0A0G2K830
C	1029	TYR	-	expression tag	UNP A0A0G2K830
C	1030	GLN	-	expression tag	UNP A0A0G2K830
C	1031	GLN	-	expression tag	UNP A0A0G2K830
C	1032	ASN	-	expression tag	UNP A0A0G2K830
C	1033	THR	-	expression tag	UNP A0A0G2K830
C	1034	PRO	-	expression tag	UNP A0A0G2K830
C	1035	ILE	-	expression tag	UNP A0A0G2K830
C	1036	GLY	-	expression tag	UNP A0A0G2K830
C	1037	ASP	-	expression tag	UNP A0A0G2K830
C	1038	GLY	-	expression tag	UNP A0A0G2K830
C	1039	PRO	-	expression tag	UNP A0A0G2K830
C	1040	VAL	-	expression tag	UNP A0A0G2K830
C	1041	LEU	-	expression tag	UNP A0A0G2K830
C	1042	LEU	-	expression tag	UNP A0A0G2K830
C	1043	PRO	-	expression tag	UNP A0A0G2K830
C	1044	ASP	-	expression tag	UNP A0A0G2K830
C	1045	ASN	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1046	HIS	-	expression tag	UNP A0A0G2K830
C	1047	TYR	-	expression tag	UNP A0A0G2K830
C	1048	LEU	-	expression tag	UNP A0A0G2K830
C	1049	SER	-	expression tag	UNP A0A0G2K830
C	1050	THR	-	expression tag	UNP A0A0G2K830
C	1051	GLN	-	expression tag	UNP A0A0G2K830
C	1052	SER	-	expression tag	UNP A0A0G2K830
C	1053	LYS	-	expression tag	UNP A0A0G2K830
C	1054	LEU	-	expression tag	UNP A0A0G2K830
C	1055	SER	-	expression tag	UNP A0A0G2K830
C	1056	LYS	-	expression tag	UNP A0A0G2K830
C	1057	ASP	-	expression tag	UNP A0A0G2K830
C	1058	PRO	-	expression tag	UNP A0A0G2K830
C	1059	ASN	-	expression tag	UNP A0A0G2K830
C	1060	GLU	-	expression tag	UNP A0A0G2K830
C	1061	LYS	-	expression tag	UNP A0A0G2K830
C	1062	ARG	-	expression tag	UNP A0A0G2K830
C	1063	ASP	-	expression tag	UNP A0A0G2K830
C	1064	HIS	-	expression tag	UNP A0A0G2K830
C	1065	MET	-	expression tag	UNP A0A0G2K830
C	1066	VAL	-	expression tag	UNP A0A0G2K830
C	1067	LEU	-	expression tag	UNP A0A0G2K830
C	1068	LEU	-	expression tag	UNP A0A0G2K830
C	1069	GLU	-	expression tag	UNP A0A0G2K830
C	1070	PHE	-	expression tag	UNP A0A0G2K830
C	1071	VAL	-	expression tag	UNP A0A0G2K830
C	1072	THR	-	expression tag	UNP A0A0G2K830
C	1073	ALA	-	expression tag	UNP A0A0G2K830
C	1074	ALA	-	expression tag	UNP A0A0G2K830
C	1075	GLY	-	expression tag	UNP A0A0G2K830
C	1076	ILE	-	expression tag	UNP A0A0G2K830
C	1077	THR	-	expression tag	UNP A0A0G2K830
C	1078	LEU	-	expression tag	UNP A0A0G2K830
C	1079	GLY	-	expression tag	UNP A0A0G2K830
C	1080	MET	-	expression tag	UNP A0A0G2K830
C	1081	ASP	-	expression tag	UNP A0A0G2K830
C	1082	GLU	-	expression tag	UNP A0A0G2K830
C	1083	LEU	-	expression tag	UNP A0A0G2K830
C	1084	TYR	-	expression tag	UNP A0A0G2K830
C	1085	LYS	-	expression tag	UNP A0A0G2K830
C	1086	SER	-	expression tag	UNP A0A0G2K830
C	1087	GLY	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1088	LEU	-	expression tag	UNP A0A0G2K830
C	1089	ARG	-	expression tag	UNP A0A0G2K830
C	1090	SER	-	expression tag	UNP A0A0G2K830
C	1091	HIS	-	expression tag	UNP A0A0G2K830
C	1092	HIS	-	expression tag	UNP A0A0G2K830
C	1093	HIS	-	expression tag	UNP A0A0G2K830
C	1094	HIS	-	expression tag	UNP A0A0G2K830
C	1095	HIS	-	expression tag	UNP A0A0G2K830
C	1096	HIS	-	expression tag	UNP A0A0G2K830
C	1097	HIS	-	expression tag	UNP A0A0G2K830
C	1098	HIS	-	expression tag	UNP A0A0G2K830
D	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
D	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
D	838	LEU	-	expression tag	UNP A0A0G2K830
D	839	VAL	-	expression tag	UNP A0A0G2K830
D	840	PRO	-	expression tag	UNP A0A0G2K830
D	841	ARG	-	expression tag	UNP A0A0G2K830
D	842	GLY	-	expression tag	UNP A0A0G2K830
D	843	SER	-	expression tag	UNP A0A0G2K830
D	844	ALA	-	expression tag	UNP A0A0G2K830
D	845	ALA	-	expression tag	UNP A0A0G2K830
D	846	ALA	-	expression tag	UNP A0A0G2K830
D	847	ALA	-	expression tag	UNP A0A0G2K830
D	848	VAL	-	expression tag	UNP A0A0G2K830
D	849	SER	-	expression tag	UNP A0A0G2K830
D	850	LYS	-	expression tag	UNP A0A0G2K830
D	851	GLY	-	expression tag	UNP A0A0G2K830
D	852	GLU	-	expression tag	UNP A0A0G2K830
D	853	GLU	-	expression tag	UNP A0A0G2K830
D	854	LEU	-	expression tag	UNP A0A0G2K830
D	855	PHE	-	expression tag	UNP A0A0G2K830
D	856	THR	-	expression tag	UNP A0A0G2K830
D	857	GLY	-	expression tag	UNP A0A0G2K830
D	858	VAL	-	expression tag	UNP A0A0G2K830
D	859	VAL	-	expression tag	UNP A0A0G2K830
D	860	PRO	-	expression tag	UNP A0A0G2K830
D	861	ILE	-	expression tag	UNP A0A0G2K830
D	862	LEU	-	expression tag	UNP A0A0G2K830
D	863	VAL	-	expression tag	UNP A0A0G2K830
D	864	GLU	-	expression tag	UNP A0A0G2K830
D	865	LEU	-	expression tag	UNP A0A0G2K830
D	866	ASP	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	867	GLY	-	expression tag	UNP A0A0G2K830
D	868	ASP	-	expression tag	UNP A0A0G2K830
D	869	VAL	-	expression tag	UNP A0A0G2K830
D	870	ASN	-	expression tag	UNP A0A0G2K830
D	871	GLY	-	expression tag	UNP A0A0G2K830
D	872	HIS	-	expression tag	UNP A0A0G2K830
D	873	LYS	-	expression tag	UNP A0A0G2K830
D	874	PHE	-	expression tag	UNP A0A0G2K830
D	875	SER	-	expression tag	UNP A0A0G2K830
D	876	VAL	-	expression tag	UNP A0A0G2K830
D	877	SER	-	expression tag	UNP A0A0G2K830
D	878	GLY	-	expression tag	UNP A0A0G2K830
D	879	GLU	-	expression tag	UNP A0A0G2K830
D	880	GLY	-	expression tag	UNP A0A0G2K830
D	881	GLU	-	expression tag	UNP A0A0G2K830
D	882	GLY	-	expression tag	UNP A0A0G2K830
D	883	ASP	-	expression tag	UNP A0A0G2K830
D	884	ALA	-	expression tag	UNP A0A0G2K830
D	885	THR	-	expression tag	UNP A0A0G2K830
D	886	TYR	-	expression tag	UNP A0A0G2K830
D	887	GLY	-	expression tag	UNP A0A0G2K830
D	888	LYS	-	expression tag	UNP A0A0G2K830
D	889	LEU	-	expression tag	UNP A0A0G2K830
D	890	THR	-	expression tag	UNP A0A0G2K830
D	891	LEU	-	expression tag	UNP A0A0G2K830
D	892	LYS	-	expression tag	UNP A0A0G2K830
D	893	PHE	-	expression tag	UNP A0A0G2K830
D	894	ILE	-	expression tag	UNP A0A0G2K830
D	895	CYS	-	expression tag	UNP A0A0G2K830
D	896	THR	-	expression tag	UNP A0A0G2K830
D	897	THR	-	expression tag	UNP A0A0G2K830
D	898	GLY	-	expression tag	UNP A0A0G2K830
D	899	LYS	-	expression tag	UNP A0A0G2K830
D	900	LEU	-	expression tag	UNP A0A0G2K830
D	901	PRO	-	expression tag	UNP A0A0G2K830
D	902	VAL	-	expression tag	UNP A0A0G2K830
D	903	PRO	-	expression tag	UNP A0A0G2K830
D	904	TRP	-	expression tag	UNP A0A0G2K830
D	905	PRO	-	expression tag	UNP A0A0G2K830
D	906	THR	-	expression tag	UNP A0A0G2K830
D	907	LEU	-	expression tag	UNP A0A0G2K830
D	908	VAL	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	909	THR	-	expression tag	UNP A0A0G2K830
D	910	THR	-	expression tag	UNP A0A0G2K830
D	911	LEU	-	expression tag	UNP A0A0G2K830
D	912	THR	-	expression tag	UNP A0A0G2K830
D	913	TYR	-	expression tag	UNP A0A0G2K830
D	914	GLY	-	expression tag	UNP A0A0G2K830
D	915	VAL	-	expression tag	UNP A0A0G2K830
D	916	GLN	-	expression tag	UNP A0A0G2K830
D	917	CYS	-	expression tag	UNP A0A0G2K830
D	918	PHE	-	expression tag	UNP A0A0G2K830
D	919	SER	-	expression tag	UNP A0A0G2K830
D	920	ARG	-	expression tag	UNP A0A0G2K830
D	921	TYR	-	expression tag	UNP A0A0G2K830
D	922	PRO	-	expression tag	UNP A0A0G2K830
D	923	ASP	-	expression tag	UNP A0A0G2K830
D	924	HIS	-	expression tag	UNP A0A0G2K830
D	925	MET	-	expression tag	UNP A0A0G2K830
D	926	LYS	-	expression tag	UNP A0A0G2K830
D	927	GLN	-	expression tag	UNP A0A0G2K830
D	928	HIS	-	expression tag	UNP A0A0G2K830
D	929	ASP	-	expression tag	UNP A0A0G2K830
D	930	PHE	-	expression tag	UNP A0A0G2K830
D	931	PHE	-	expression tag	UNP A0A0G2K830
D	932	LYS	-	expression tag	UNP A0A0G2K830
D	933	SER	-	expression tag	UNP A0A0G2K830
D	934	ALA	-	expression tag	UNP A0A0G2K830
D	935	MET	-	expression tag	UNP A0A0G2K830
D	936	PRO	-	expression tag	UNP A0A0G2K830
D	937	GLU	-	expression tag	UNP A0A0G2K830
D	938	GLY	-	expression tag	UNP A0A0G2K830
D	939	TYR	-	expression tag	UNP A0A0G2K830
D	940	VAL	-	expression tag	UNP A0A0G2K830
D	941	GLN	-	expression tag	UNP A0A0G2K830
D	942	GLU	-	expression tag	UNP A0A0G2K830
D	943	ARG	-	expression tag	UNP A0A0G2K830
D	944	THR	-	expression tag	UNP A0A0G2K830
D	945	ILE	-	expression tag	UNP A0A0G2K830
D	946	PHE	-	expression tag	UNP A0A0G2K830
D	947	PHE	-	expression tag	UNP A0A0G2K830
D	948	LYS	-	expression tag	UNP A0A0G2K830
D	949	ASP	-	expression tag	UNP A0A0G2K830
D	950	ASP	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	951	GLY	-	expression tag	UNP A0A0G2K830
D	952	ASN	-	expression tag	UNP A0A0G2K830
D	953	TYR	-	expression tag	UNP A0A0G2K830
D	954	LYS	-	expression tag	UNP A0A0G2K830
D	955	THR	-	expression tag	UNP A0A0G2K830
D	956	ARG	-	expression tag	UNP A0A0G2K830
D	957	ALA	-	expression tag	UNP A0A0G2K830
D	958	GLU	-	expression tag	UNP A0A0G2K830
D	959	VAL	-	expression tag	UNP A0A0G2K830
D	960	LYS	-	expression tag	UNP A0A0G2K830
D	961	PHE	-	expression tag	UNP A0A0G2K830
D	962	GLU	-	expression tag	UNP A0A0G2K830
D	963	GLY	-	expression tag	UNP A0A0G2K830
D	964	ASP	-	expression tag	UNP A0A0G2K830
D	965	THR	-	expression tag	UNP A0A0G2K830
D	966	LEU	-	expression tag	UNP A0A0G2K830
D	967	VAL	-	expression tag	UNP A0A0G2K830
D	968	ASN	-	expression tag	UNP A0A0G2K830
D	969	ARG	-	expression tag	UNP A0A0G2K830
D	970	ILE	-	expression tag	UNP A0A0G2K830
D	971	GLU	-	expression tag	UNP A0A0G2K830
D	972	LEU	-	expression tag	UNP A0A0G2K830
D	973	LYS	-	expression tag	UNP A0A0G2K830
D	974	GLY	-	expression tag	UNP A0A0G2K830
D	975	ILE	-	expression tag	UNP A0A0G2K830
D	976	ASP	-	expression tag	UNP A0A0G2K830
D	977	PHE	-	expression tag	UNP A0A0G2K830
D	978	LYS	-	expression tag	UNP A0A0G2K830
D	979	GLU	-	expression tag	UNP A0A0G2K830
D	980	ASP	-	expression tag	UNP A0A0G2K830
D	981	GLY	-	expression tag	UNP A0A0G2K830
D	982	ASN	-	expression tag	UNP A0A0G2K830
D	983	ILE	-	expression tag	UNP A0A0G2K830
D	984	LEU	-	expression tag	UNP A0A0G2K830
D	985	GLY	-	expression tag	UNP A0A0G2K830
D	986	HIS	-	expression tag	UNP A0A0G2K830
D	987	LYS	-	expression tag	UNP A0A0G2K830
D	988	LEU	-	expression tag	UNP A0A0G2K830
D	989	GLU	-	expression tag	UNP A0A0G2K830
D	990	TYR	-	expression tag	UNP A0A0G2K830
D	991	ASN	-	expression tag	UNP A0A0G2K830
D	992	TYR	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	993	ASN	-	expression tag	UNP A0A0G2K830
D	994	SER	-	expression tag	UNP A0A0G2K830
D	995	HIS	-	expression tag	UNP A0A0G2K830
D	996	ASN	-	expression tag	UNP A0A0G2K830
D	997	VAL	-	expression tag	UNP A0A0G2K830
D	998	TYR	-	expression tag	UNP A0A0G2K830
D	999	ILE	-	expression tag	UNP A0A0G2K830
D	1000	MET	-	expression tag	UNP A0A0G2K830
D	1001	ALA	-	expression tag	UNP A0A0G2K830
D	1002	ASP	-	expression tag	UNP A0A0G2K830
D	1003	LYS	-	expression tag	UNP A0A0G2K830
D	1004	GLN	-	expression tag	UNP A0A0G2K830
D	1005	LYS	-	expression tag	UNP A0A0G2K830
D	1006	ASN	-	expression tag	UNP A0A0G2K830
D	1007	GLY	-	expression tag	UNP A0A0G2K830
D	1008	ILE	-	expression tag	UNP A0A0G2K830
D	1009	LYS	-	expression tag	UNP A0A0G2K830
D	1010	VAL	-	expression tag	UNP A0A0G2K830
D	1011	ASN	-	expression tag	UNP A0A0G2K830
D	1012	PHE	-	expression tag	UNP A0A0G2K830
D	1013	LYS	-	expression tag	UNP A0A0G2K830
D	1014	ILE	-	expression tag	UNP A0A0G2K830
D	1015	ARG	-	expression tag	UNP A0A0G2K830
D	1016	HIS	-	expression tag	UNP A0A0G2K830
D	1017	ASN	-	expression tag	UNP A0A0G2K830
D	1018	ILE	-	expression tag	UNP A0A0G2K830
D	1019	GLU	-	expression tag	UNP A0A0G2K830
D	1020	ASP	-	expression tag	UNP A0A0G2K830
D	1021	GLY	-	expression tag	UNP A0A0G2K830
D	1022	SER	-	expression tag	UNP A0A0G2K830
D	1023	VAL	-	expression tag	UNP A0A0G2K830
D	1024	GLN	-	expression tag	UNP A0A0G2K830
D	1025	LEU	-	expression tag	UNP A0A0G2K830
D	1026	ALA	-	expression tag	UNP A0A0G2K830
D	1027	ASP	-	expression tag	UNP A0A0G2K830
D	1028	HIS	-	expression tag	UNP A0A0G2K830
D	1029	TYR	-	expression tag	UNP A0A0G2K830
D	1030	GLN	-	expression tag	UNP A0A0G2K830
D	1031	GLN	-	expression tag	UNP A0A0G2K830
D	1032	ASN	-	expression tag	UNP A0A0G2K830
D	1033	THR	-	expression tag	UNP A0A0G2K830
D	1034	PRO	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1035	ILE	-	expression tag	UNP A0A0G2K830
D	1036	GLY	-	expression tag	UNP A0A0G2K830
D	1037	ASP	-	expression tag	UNP A0A0G2K830
D	1038	GLY	-	expression tag	UNP A0A0G2K830
D	1039	PRO	-	expression tag	UNP A0A0G2K830
D	1040	VAL	-	expression tag	UNP A0A0G2K830
D	1041	LEU	-	expression tag	UNP A0A0G2K830
D	1042	LEU	-	expression tag	UNP A0A0G2K830
D	1043	PRO	-	expression tag	UNP A0A0G2K830
D	1044	ASP	-	expression tag	UNP A0A0G2K830
D	1045	ASN	-	expression tag	UNP A0A0G2K830
D	1046	HIS	-	expression tag	UNP A0A0G2K830
D	1047	TYR	-	expression tag	UNP A0A0G2K830
D	1048	LEU	-	expression tag	UNP A0A0G2K830
D	1049	SER	-	expression tag	UNP A0A0G2K830
D	1050	THR	-	expression tag	UNP A0A0G2K830
D	1051	GLN	-	expression tag	UNP A0A0G2K830
D	1052	SER	-	expression tag	UNP A0A0G2K830
D	1053	LYS	-	expression tag	UNP A0A0G2K830
D	1054	LEU	-	expression tag	UNP A0A0G2K830
D	1055	SER	-	expression tag	UNP A0A0G2K830
D	1056	LYS	-	expression tag	UNP A0A0G2K830
D	1057	ASP	-	expression tag	UNP A0A0G2K830
D	1058	PRO	-	expression tag	UNP A0A0G2K830
D	1059	ASN	-	expression tag	UNP A0A0G2K830
D	1060	GLU	-	expression tag	UNP A0A0G2K830
D	1061	LYS	-	expression tag	UNP A0A0G2K830
D	1062	ARG	-	expression tag	UNP A0A0G2K830
D	1063	ASP	-	expression tag	UNP A0A0G2K830
D	1064	HIS	-	expression tag	UNP A0A0G2K830
D	1065	MET	-	expression tag	UNP A0A0G2K830
D	1066	VAL	-	expression tag	UNP A0A0G2K830
D	1067	LEU	-	expression tag	UNP A0A0G2K830
D	1068	LEU	-	expression tag	UNP A0A0G2K830
D	1069	GLU	-	expression tag	UNP A0A0G2K830
D	1070	PHE	-	expression tag	UNP A0A0G2K830
D	1071	VAL	-	expression tag	UNP A0A0G2K830
D	1072	THR	-	expression tag	UNP A0A0G2K830
D	1073	ALA	-	expression tag	UNP A0A0G2K830
D	1074	ALA	-	expression tag	UNP A0A0G2K830
D	1075	GLY	-	expression tag	UNP A0A0G2K830
D	1076	ILE	-	expression tag	UNP A0A0G2K830

Continued on next page...

Continued from previous page...

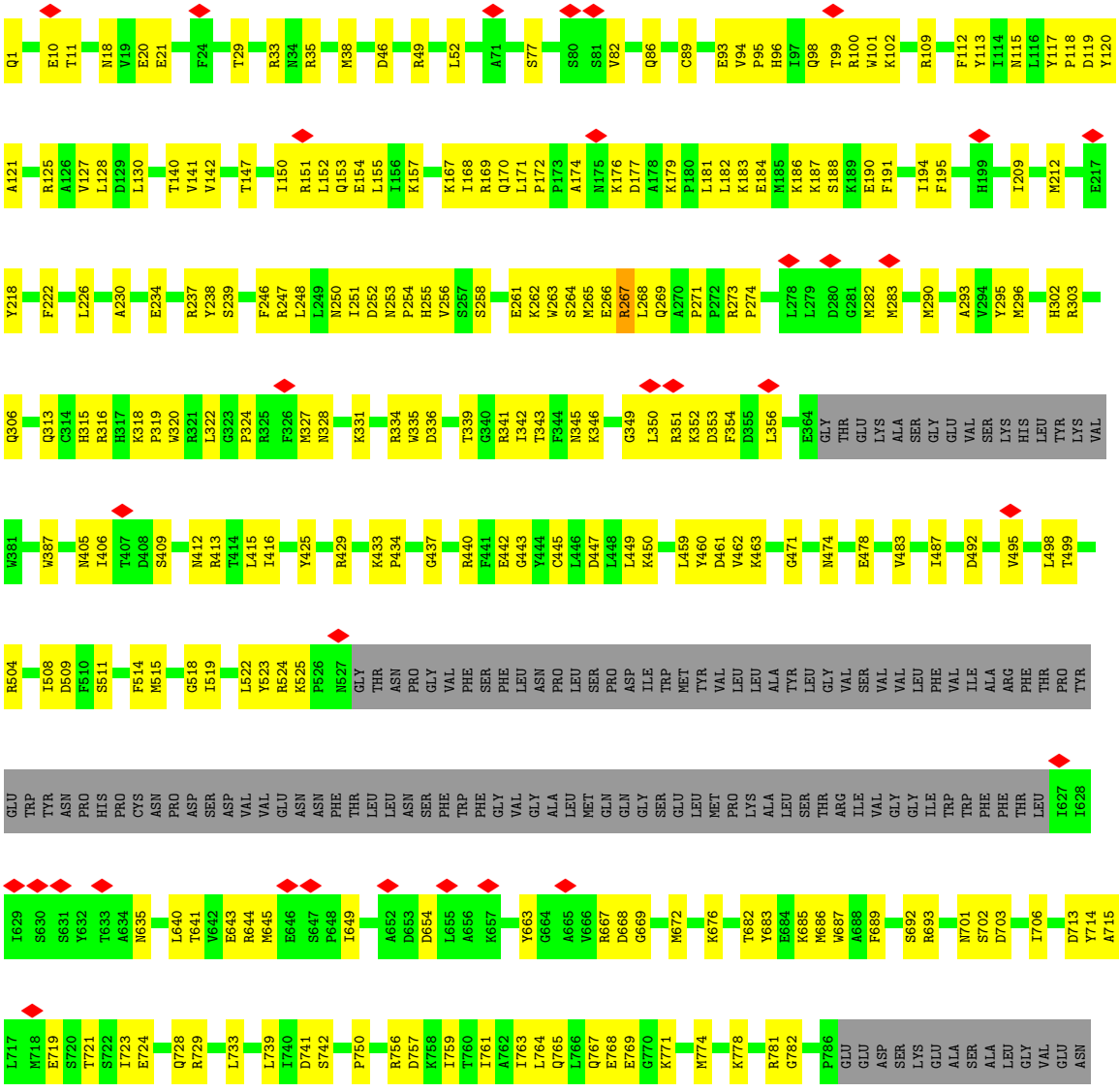
Chain	Residue	Modelled	Actual	Comment	Reference
D	1077	THR	-	expression tag	UNP A0A0G2K830
D	1078	LEU	-	expression tag	UNP A0A0G2K830
D	1079	GLY	-	expression tag	UNP A0A0G2K830
D	1080	MET	-	expression tag	UNP A0A0G2K830
D	1081	ASP	-	expression tag	UNP A0A0G2K830
D	1082	GLU	-	expression tag	UNP A0A0G2K830
D	1083	LEU	-	expression tag	UNP A0A0G2K830
D	1084	TYR	-	expression tag	UNP A0A0G2K830
D	1085	LYS	-	expression tag	UNP A0A0G2K830
D	1086	SER	-	expression tag	UNP A0A0G2K830
D	1087	GLY	-	expression tag	UNP A0A0G2K830
D	1088	LEU	-	expression tag	UNP A0A0G2K830
D	1089	ARG	-	expression tag	UNP A0A0G2K830
D	1090	SER	-	expression tag	UNP A0A0G2K830
D	1091	HIS	-	expression tag	UNP A0A0G2K830
D	1092	HIS	-	expression tag	UNP A0A0G2K830
D	1093	HIS	-	expression tag	UNP A0A0G2K830
D	1094	HIS	-	expression tag	UNP A0A0G2K830
D	1095	HIS	-	expression tag	UNP A0A0G2K830
D	1096	HIS	-	expression tag	UNP A0A0G2K830
D	1097	HIS	-	expression tag	UNP A0A0G2K830
D	1098	HIS	-	expression tag	UNP A0A0G2K830

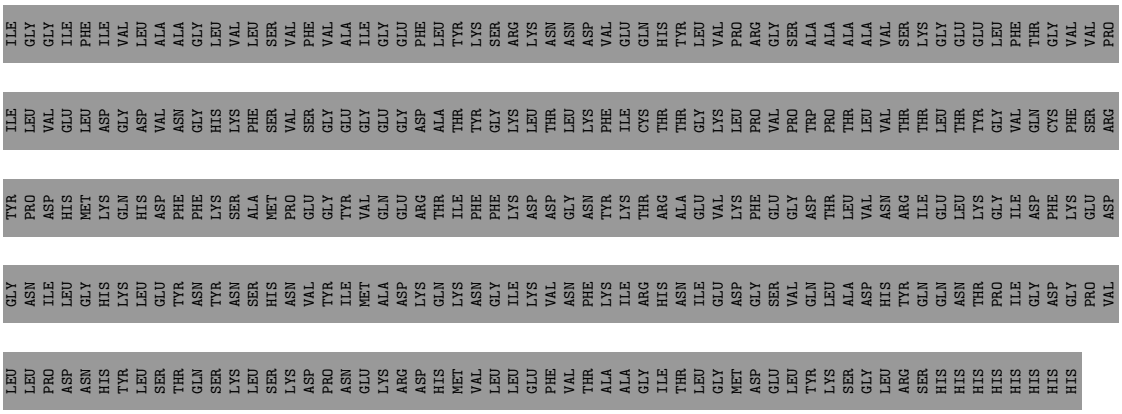
3 Residue-property plots (i)

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: Glutamate receptor

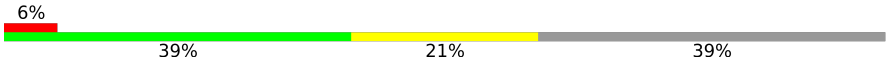
Chain A:

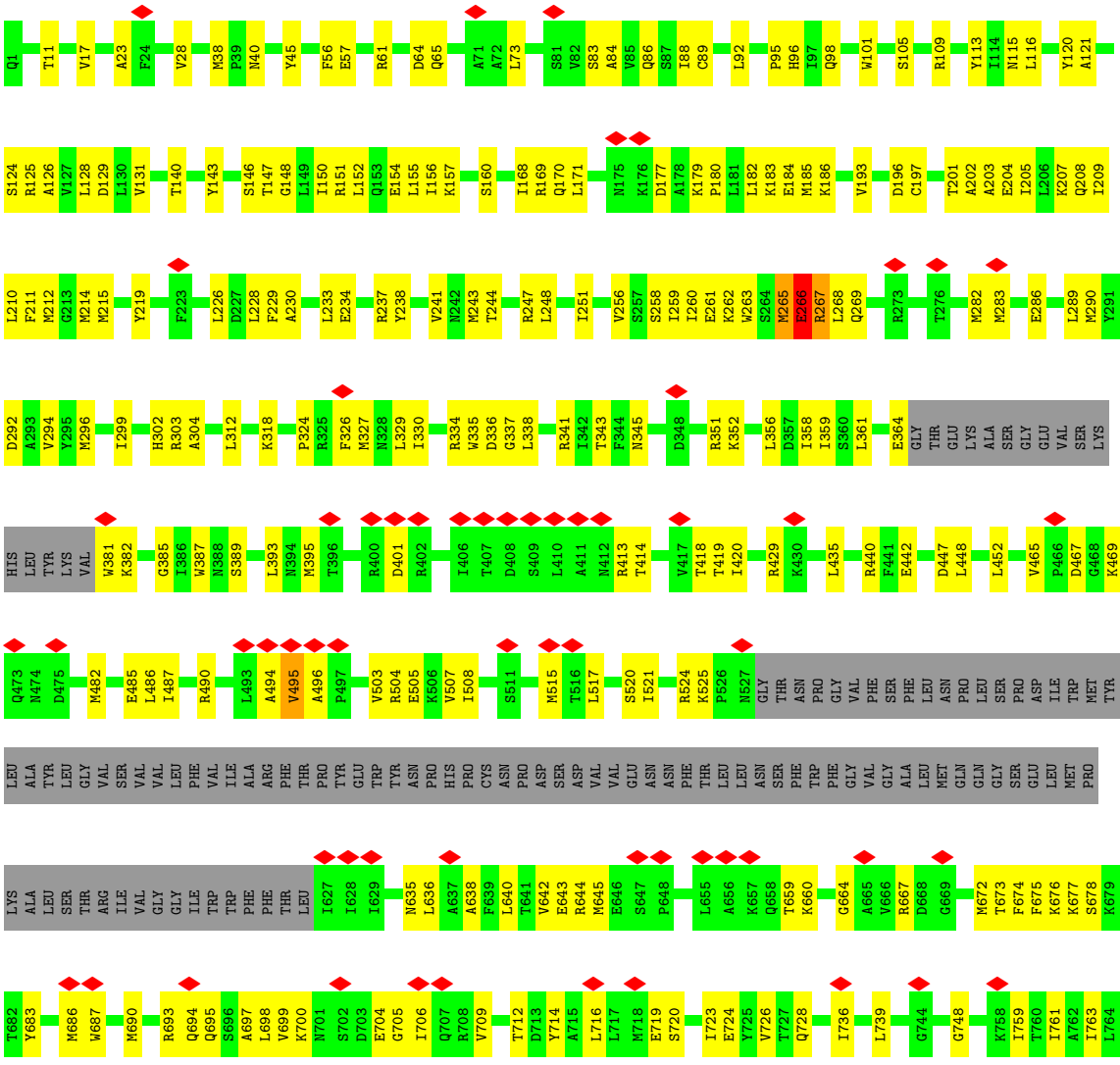


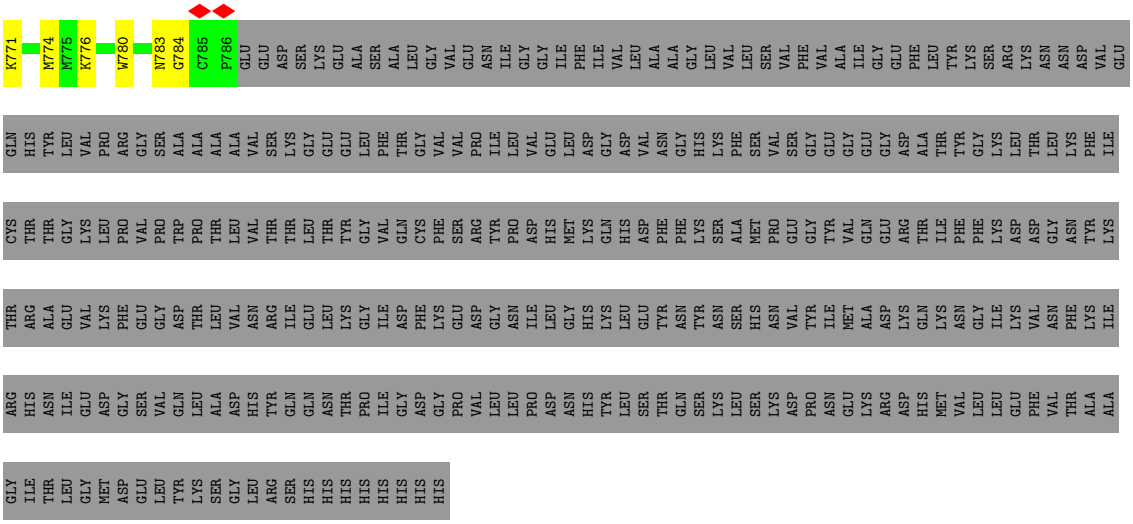


• Molecule 1: Glutamate receptor

Chain B:

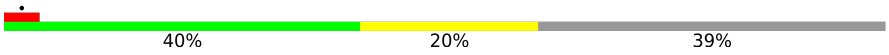


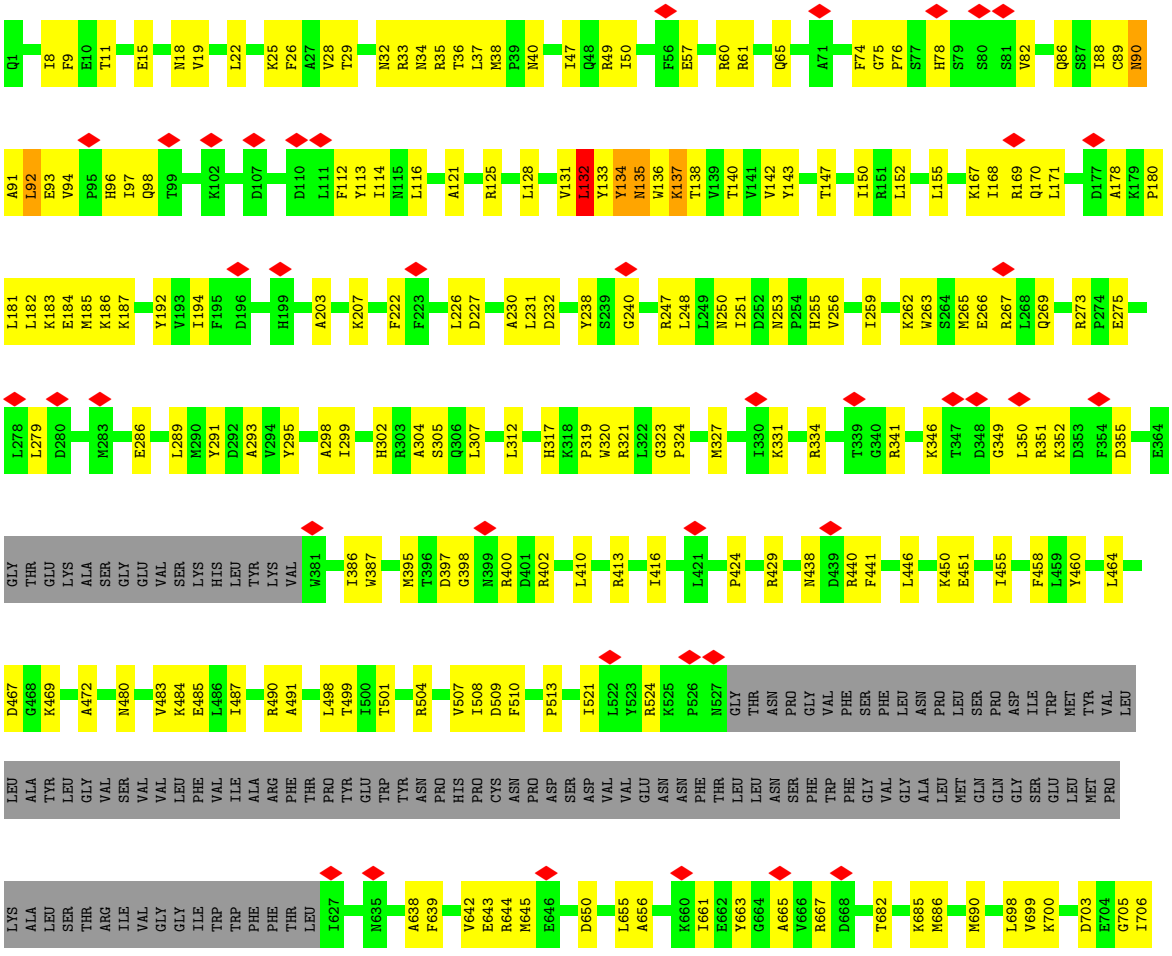


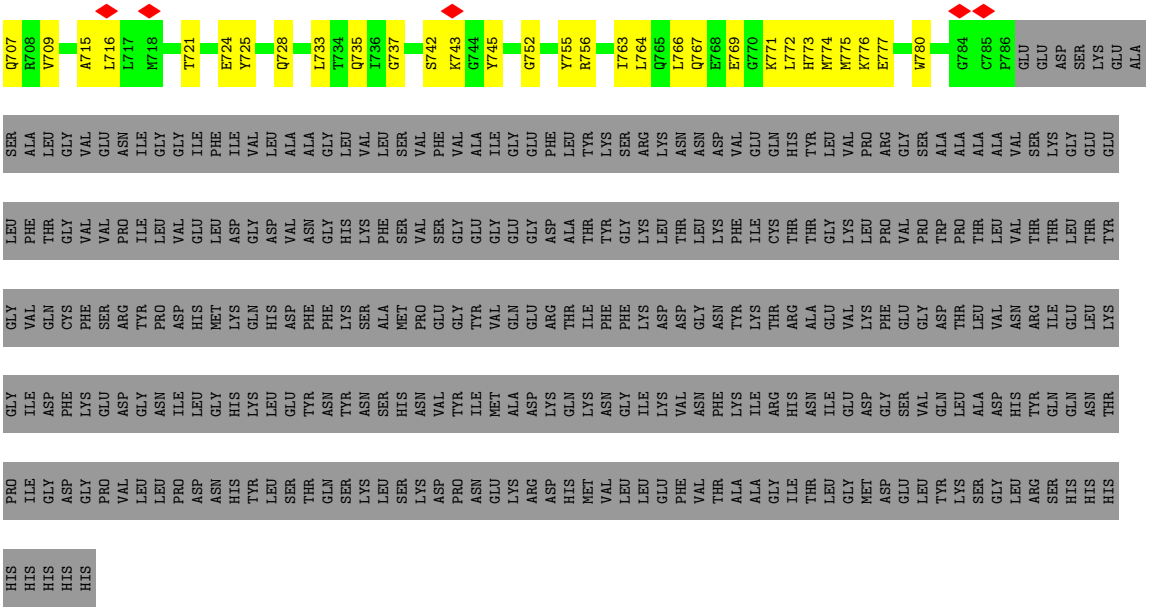


• Molecule 1: Glutamate receptor

Chain C:

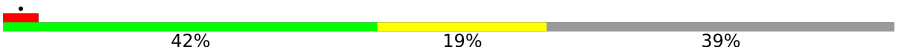


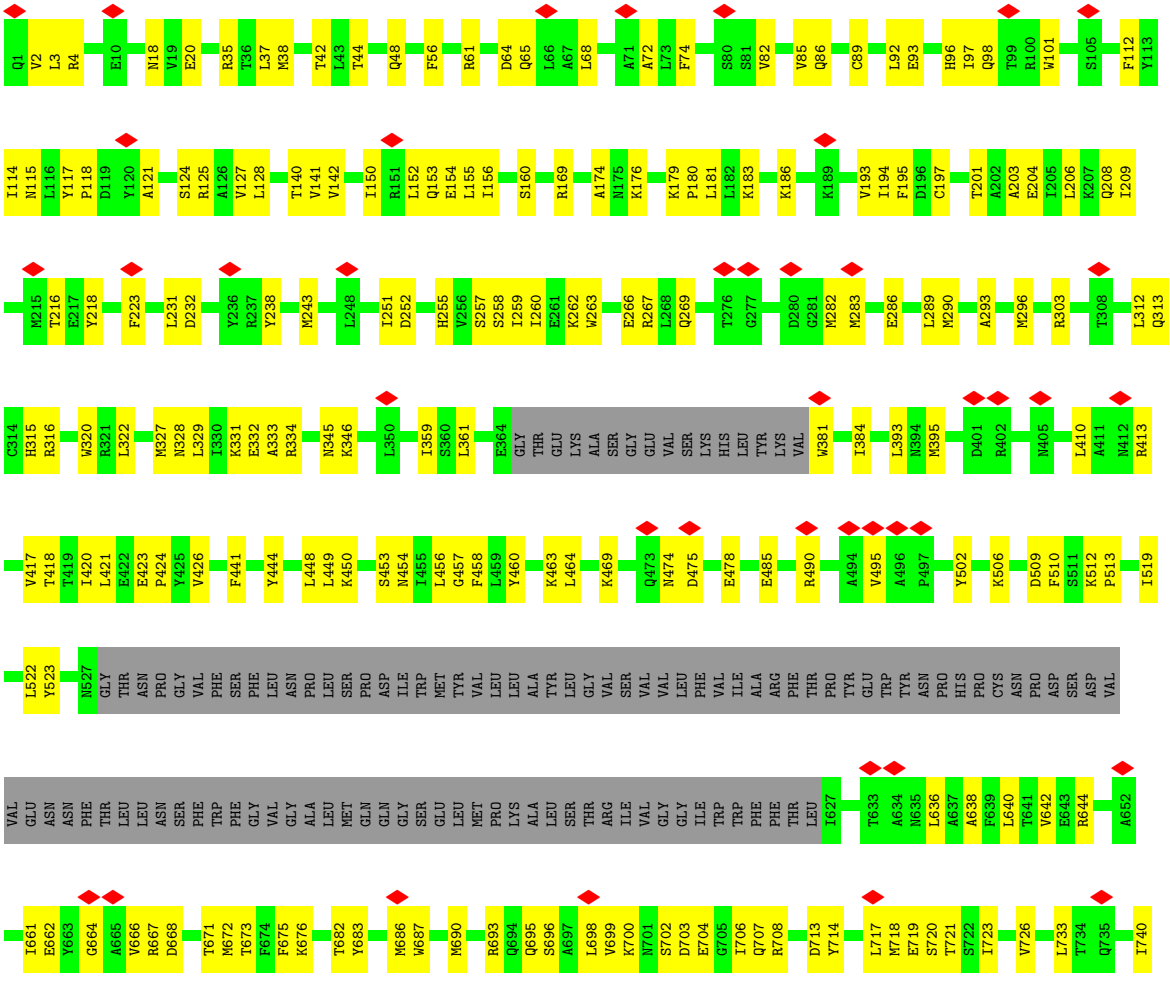


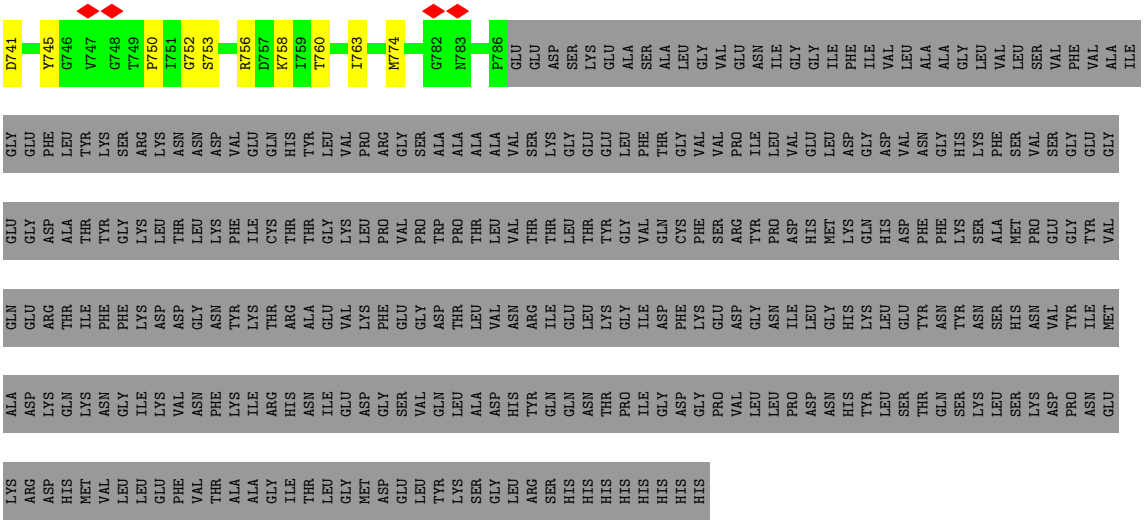


• Molecule 1: Glutamate receptor

Chain D:






D741 Y745 G746 V747 G748 T749 P750 I751 G752 S753 R756 D757 K758 I759 T760 I763 M774 G782 N783 P786
GLU GLU ASP SER LYS GLU ALA SER ALA LEU GLY VAL GLU ASN ILE GLY GLY ILE PHE ILE VAL LEU ALA ALA GLY LEU VAL LEU SER VAL PHE VAL ALA ILE
GLY GLU PHE LEU TYR LYS SER ARG LYS ASN ASN ASP VAL GLU GLN HIS TYR LEU VAL PRO ARG GLY SER ALA ALA ALA VAL SER LYS GLY GLU THR GLY VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL SER GLY GLU GLY
GLU GLY ASP ALA THR TYR GLY LYS LEU THR LEU LYS PHE ILE CYS THR THR GLY LYS LEU PRO VAL PRO TRP PRO THR LEU VAL THR THR LEU THR GLY GLY VAL GLN CYS PHE SER ARG TYR PRO ASP HIS MET LYS GLN HIS ASP PHE PHE LYS SER ALA MET PRO GLU GLY TYR VAL
GLN GLU ARG THR ILE PHE PHE LYS ASP ASP GLY ASN TYR LYS THR ARG ALA GLU VAL LYS PHE GLU GLY ASP THR LEU VAL ASN ARG ILE GLU LEU LYS GLY ILE ASP PHE LYS GLU ASP GLY ASN ILE LEU GLY HIS LYS LEU GLU TYR ASN TYR ASN SER HIS ASN VAL TYR ILE MET
ALA ASP LYS GLN LYS ASN GLY ILE LYS VAL ASN PHE LYS ILE ARG HIS ASN ILE GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL LEU LEU PRO ASP ASN HIS TYR LEU SER THR GLN SER LYS LEU SER LYS ASP PRO ASN GLU
LYS ARG ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR LEU GLY MET ASP GLU LEU TYR LYS SER GLY LEU ARG SER HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.017	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	360.96, 360.96, 360.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.41, 1.41, 1.41	Depositor

5 Model quality

5.1 Standard geometry

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	0.18	0/5498	0.47	2/7437 (0.0%)
1	B	0.22	1/5498 (0.0%)	0.51	2/7437 (0.0%)
1	C	0.28	0/5498	0.54	4/7437 (0.1%)
1	D	0.15	0/5498	0.46	0/7437
All	All	0.22	1/21992 (0.0%)	0.50	8/29748 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	MET	CA-C	-5.37	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	132	LEU	N-CA-C	-6.60	104.08	111.28
1	B	266	GLU	N-CA-C	-6.45	104.25	111.28
1	C	90	ASN	N-CA-C	-6.30	104.46	111.71
1	B	495	VAL	N-CA-C	-6.07	105.45	111.88
1	C	134	TYR	N-CA-C	-6.00	105.81	113.01
1	A	267	ARG	CB-CG-CD	5.23	123.34	111.30
1	A	271	PRO	N-CA-C	5.21	117.06	110.70
1	C	40	ASN	N-CA-C	-5.17	108.23	114.75

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	5386	0	5408	188	0
1	B	5386	0	5408	176	0
1	C	5386	0	5408	180	0
1	D	5386	0	5408	144	0
All	All	21544	0	21632	672	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 16.

All (672) 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:640:LEU:HG	1:B:644:ARG:HH12	1.28	0.96
1:C:92:LEU:HA	1:C:319:PRO:HA	1.48	0.95
1:A:264:SER:O	1:A:267:ARG:NH1	2.07	0.86
1:B:170:GLN:NE2	1:B:171:LEU:O	2.11	0.84
1:C:91:ALA:O	1:C:94:VAL:HG23	1.77	0.83
1:B:504:ARG:HH12	1:B:673:THR:HG21	1.45	0.81
1:C:89:CYS:HA	1:C:94:VAL:HB	1.61	0.81
1:A:341:ARG:NH1	1:A:353:ASP:O	2.14	0.78
1:D:666:VAL:H	1:D:718:MET:HE3	1.50	0.77
1:D:150:ILE:O	1:D:153:GLN:NE2	2.18	0.77
1:A:239:SER:HA	1:A:413:ARG:HD2	1.67	0.76
1:A:682:THR:HG22	1:A:686:MET:HE1	1.66	0.75
1:C:682:THR:HG22	1:C:685:LYS:HZ3	1.52	0.75
1:B:385:GLY:HA3	1:B:395:MET:HG2	1.68	0.74
1:D:703:ASP:O	1:D:707:GLN:NE2	2.21	0.73
1:A:729:ARG:HH22	1:A:782:GLY:HA2	1.52	0.72
1:C:355:ASP:HB3	1:C:386:ILE:HD11	1.71	0.72
1:C:703:ASP:O	1:C:707:GLN:NE2	2.23	0.71
1:C:86:GLN:HA	1:C:89:CYS:HB2	1.72	0.71
1:B:129:ASP:HB3	1:B:393:LEU:HD23	1.73	0.71
1:C:61:ARG:O	1:C:65:GLN:NE2	2.24	0.71
1:C:121:ALA:HB1	1:C:125:ARG:HH12	1.54	0.71
1:C:298:ALA:O	1:C:302:HIS:ND1	2.24	0.71
1:D:293:ALA:HA	1:D:296:MET:HE2	1.73	0.70
1:D:152:LEU:HD22	1:D:155:LEU:HD12	1.72	0.70
1:B:247:ARG:HH12	1:B:251:ILE:HG12	1.57	0.70
1:C:509:ASP:HB3	1:C:756:ARG:HE	1.56	0.70
1:B:147:THR:O	1:B:151:ARG:NH1	2.25	0.69
1:C:499:THR:C	1:C:504:ARG:HH21	2.01	0.69
1:A:335:TRP:CD1	1:A:336:ASP:H	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:LYS:HG3	1:B:677:LYS:HD2	1.75	0.69
1:C:643:GLU:HG2	1:C:644:ARG:HD3	1.74	0.68
1:A:461:ASP:OD1	1:A:463:LYS:NZ	2.26	0.68
1:B:520:SER:HB3	1:B:739:LEU:HD13	1.75	0.68
1:A:499:THR:O	1:A:504:ARG:NH1	2.27	0.68
1:B:312:LEU:HD21	1:B:318:LYS:H	1.58	0.68
1:C:89:CYS:CA	1:C:94:VAL:HB	2.24	0.68
1:D:522:LEU:HB2	1:D:723:ILE:HG23	1.75	0.67
1:C:484:LYS:HA	1:C:487:ILE:HG12	1.76	0.67
1:A:644:ARG:NH2	1:D:638:ALA:HB1	2.10	0.67
1:C:22:LEU:HA	1:C:25:LYS:HZ2	1.60	0.66
1:A:635:ASN:OD1	1:B:644:ARG:NH2	2.28	0.66
1:C:183:LYS:HA	1:C:186:LYS:HG2	1.77	0.66
1:B:263:TRP:CD1	1:B:267:ARG:HH22	2.14	0.66
1:A:474:ASN:ND2	1:A:478:GLU:OE2	2.29	0.66
1:A:117:TYR:CD1	1:A:118:PRO:HD2	2.31	0.66
1:A:683:TYR:HA	1:A:686:MET:HE2	1.77	0.66
1:D:140:THR:HB	1:D:193:VAL:HG22	1.78	0.66
1:D:251:ILE:HG13	1:D:252:ASP:H	1.59	0.66
1:B:635:ASN:HA	1:C:644:ARG:HH22	1.61	0.65
1:D:121:ALA:HB1	1:D:125:ARG:HH12	1.61	0.65
1:A:416:ILE:HA	1:A:463:LYS:HZ1	1.60	0.65
1:B:435:LEU:HB3	1:B:440:ARG:HG2	1.79	0.65
1:A:77:SER:OG	1:A:100:ARG:NH1	2.28	0.65
1:B:101:TRP:HA	1:B:115:ASN:HD21	1.61	0.65
1:B:304:ALA:HB2	1:B:329:LEU:HD11	1.77	0.65
1:D:86:GLN:OE1	1:D:96:HIS:ND1	2.29	0.65
1:A:182:LEU:HD13	1:A:186:LYS:HZ3	1.60	0.65
1:D:522:LEU:HD11	1:D:733:LEU:HB2	1.78	0.65
1:B:667:ARG:NH1	1:B:699:VAL:O	2.29	0.65
1:B:664:GLY:HA2	1:B:698:LEU:HG	1.78	0.64
1:A:522:LEU:HD13	1:A:723:ILE:HG23	1.80	0.64
1:A:334:ARG:HG3	1:A:343:THR:HB	1.80	0.64
1:B:202:ALA:HA	1:B:205:ILE:HG12	1.80	0.64
1:A:524:ARG:HA	1:A:733:LEU:HG	1.80	0.64
1:A:409:SER:OG	1:A:413:ARG:NH1	2.30	0.64
1:A:522:LEU:HD22	1:A:723:ILE:HG12	1.79	0.63
1:B:186:LYS:HG2	1:B:214:MET:HE3	1.80	0.63
1:A:765:GLN:NE2	1:A:768:GLU:OE2	2.30	0.63
1:C:121:ALA:HB1	1:C:125:ARG:NH1	2.14	0.63
1:D:303:ARG:NH2	1:D:329:LEU:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:ASN:ND2	1:D:478:GLU:OE1	2.29	0.62
1:A:761:ILE:HA	1:A:764:LEU:HD12	1.79	0.62
1:C:266:GLU:HA	1:C:269:GLN:HG2	1.80	0.62
1:A:11:THR:HB	1:A:49:ARG:HH22	1.65	0.62
1:A:449:LEU:HD21	1:A:495:VAL:HG11	1.82	0.62
1:A:518:GLY:HA2	1:A:742:SER:HA	1.81	0.62
1:C:25:LYS:HA	1:C:28:VAL:HG12	1.81	0.62
1:A:771:LYS:HA	1:A:774:MET:HE2	1.81	0.62
1:D:673:THR:HA	1:D:676:LYS:HE3	1.81	0.62
1:C:395:MET:HE1	1:C:397:ASP:HB2	1.82	0.62
1:A:141:VAL:HG12	1:A:194:ILE:HB	1.81	0.61
1:D:328:ASN:HA	1:D:331:LYS:HZ3	1.65	0.61
1:A:295:TYR:HD2	1:A:335:TRP:CH2	2.19	0.61
1:C:75:GLY:O	1:C:96:HIS:NE2	2.29	0.61
1:D:195:PHE:HD2	1:D:223:PHE:HE1	1.46	0.61
1:C:90:ASN:HA	1:C:112:PHE:CD2	2.35	0.61
1:A:405:ASN:OD1	1:A:406:ILE:N	2.34	0.61
1:C:116:LEU:C	1:C:351:ARG:HE	2.08	0.60
1:D:257:SER:O	1:D:260:ILE:HG22	2.01	0.60
1:D:313:GLN:OE1	1:D:316:ARG:N	2.33	0.60
1:A:640:LEU:HG	1:A:644:ARG:HE	1.67	0.60
1:B:148:GLY:HA2	1:B:151:ARG:NH2	2.16	0.60
1:B:387:TRP:CZ3	1:B:389:SER:HA	2.37	0.60
1:A:184:GLU:HA	1:A:187:LYS:HG2	1.83	0.60
1:D:98:GLN:HE21	1:D:115:ASN:HB2	1.66	0.59
1:C:231:LEU:HD12	1:C:232:ASP:H	1.66	0.59
1:B:267:ARG:HE	1:B:283:MET:CE	2.15	0.59
1:B:180:PRO:HA	1:B:183:LYS:HG2	1.84	0.59
1:D:449:LEU:HD21	1:D:495:VAL:HG11	1.85	0.59
1:A:152:LEU:HD22	1:A:155:LEU:HD12	1.84	0.58
1:A:247:ARG:HH21	1:A:251:ILE:HG12	1.68	0.58
1:B:209:ILE:HA	1:B:212:MET:HE1	1.84	0.58
1:C:639:PHE:HA	1:C:642:VAL:HG22	1.85	0.58
1:D:509:ASP:OD2	1:D:752:GLY:N	2.32	0.58
1:A:769:GLU:HG3	1:A:771:LYS:HG2	1.86	0.58
1:B:180:PRO:O	1:B:183:LYS:HG2	2.03	0.58
1:C:37:LEU:O	1:C:38:MET:HE2	2.03	0.58
1:C:699:VAL:HG11	1:C:705:GLY:HA2	1.86	0.58
1:D:128:LEU:HD11	1:D:154:GLU:HB3	1.84	0.58
1:A:296:MET:HE1	1:A:335:TRP:HB3	1.86	0.57
1:B:517:LEU:HD12	1:B:719:GLU:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASN:ND2	1:D:20:GLU:OE2	2.36	0.57
1:B:709:VAL:HG21	1:B:716:LEU:HD23	1.86	0.57
1:A:29:THR:O	1:A:33:ARG:HG2	2.05	0.57
1:C:524:ARG:HA	1:C:733:LEU:HD13	1.86	0.57
1:D:260:ILE:HD11	1:D:282:MET:HA	1.85	0.57
1:D:519:ILE:HG13	1:D:740:ILE:HB	1.86	0.57
1:D:522:LEU:HD12	1:D:523:TYR:H	1.69	0.57
1:B:229:PHE:HD2	1:B:282:MET:HB3	1.70	0.57
1:B:243:MET:HB3	1:B:361:LEU:HB2	1.86	0.56
1:A:10:GLU:HB3	1:A:52:LEU:HA	1.87	0.56
1:D:328:ASN:HD22	1:D:331:LYS:NZ	2.03	0.56
1:A:498:LEU:HD23	1:A:504:ARG:HH22	1.70	0.56
1:B:635:ASN:OD1	1:B:636:LEU:N	2.38	0.56
1:A:437:GLY:O	1:A:440:ARG:NH1	2.38	0.56
1:B:121:ALA:HB1	1:B:125:ARG:NH1	2.21	0.56
1:B:267:ARG:HE	1:B:283:MET:HE1	1.71	0.56
1:A:471:GLY:N	1:A:668:ASP:OD2	2.24	0.56
1:B:11:THR:HG21	1:B:17:VAL:HG13	1.87	0.56
1:C:735:GLN:NE2	1:C:737:GLY:O	2.36	0.56
1:A:77:SER:HG	1:A:100:ARG:HH11	1.51	0.56
1:C:90:ASN:HA	1:C:112:PHE:CE2	2.40	0.56
1:A:142:VAL:HB	1:A:169:ARG:HB2	1.88	0.55
1:A:263:TRP:O	1:A:266:GLU:HG3	2.05	0.55
1:A:127:VAL:HA	1:A:130:LEU:HG	1.86	0.55
1:A:186:LYS:NZ	1:A:212:MET:HG2	2.21	0.55
1:D:328:ASN:HD22	1:D:331:LYS:HZ3	1.53	0.55
1:A:118:PRO:HA	1:A:354:PHE:CE2	2.41	0.55
1:B:147:THR:O	1:B:150:ILE:HG12	2.06	0.55
1:B:143:TYR:HA	1:B:196:ASP:HB3	1.89	0.55
1:B:667:ARG:HH22	1:B:698:LEU:HD22	1.72	0.55
1:C:147:THR:HA	1:C:150:ILE:HD13	1.88	0.55
1:C:227:ASP:HB3	1:C:230:ALA:HB3	1.89	0.55
1:A:433:LYS:HD2	1:A:434:PRO:HD2	1.87	0.55
1:C:143:TYR:HE1	1:C:168:ILE:HB	1.71	0.55
1:C:182:LEU:HA	1:C:185:MET:HE2	1.87	0.55
1:C:35:ARG:HH21	1:C:38:MET:HE1	1.72	0.55
1:D:216:THR:HG23	1:D:218:TYR:H	1.72	0.55
1:A:525:LYS:H	1:A:733:LEU:HA	1.71	0.54
1:A:644:ARG:NH1	1:A:644:ARG:HB2	2.23	0.54
1:A:128:LEU:HD11	1:A:154:GLU:HB3	1.89	0.54
1:B:487:ILE:HG12	1:B:507:VAL:HG11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:ARG:HH22	1:D:333:ALA:HB2	1.72	0.54
1:B:86:GLN:HA	1:B:89:CYS:SG	2.47	0.54
1:C:140:THR:OG1	1:C:192:TYR:O	2.24	0.54
1:C:238:TYR:HD1	1:C:240:GLY:H	1.56	0.54
1:A:95:PRO:HA	1:A:112:PHE:HB3	1.90	0.54
1:A:266:GLU:O	1:A:269:GLN:HG2	2.07	0.54
1:A:701:ASN:OD1	1:A:702:SER:N	2.40	0.54
1:A:109:ARG:NH2	1:A:113:TYR:O	2.41	0.54
1:B:169:ARG:NH2	1:B:184:GLU:OE2	2.32	0.54
1:D:89:CYS:O	1:D:93:GLU:N	2.40	0.54
1:D:92:LEU:HD12	1:D:312:LEU:HD13	1.90	0.54
1:B:258:SER:HA	1:B:261:GLU:CD	2.32	0.54
1:C:9:PHE:HB2	1:C:49:ARG:HH21	1.72	0.54
1:C:32:ASN:O	1:C:35:ARG:NH1	2.38	0.54
1:C:769:GLU:HB2	1:C:771:LYS:NZ	2.23	0.54
1:D:141:VAL:HG12	1:D:194:ILE:HB	1.90	0.53
1:D:502:TYR:O	1:D:506:LYS:NZ	2.38	0.53
1:A:447:ASP:HA	1:A:450:LYS:HG2	1.91	0.53
1:B:418:THR:OG1	1:B:485:GLU:OE1	2.16	0.53
1:A:264:SER:OG	1:A:267:ARG:NH1	2.42	0.53
1:B:101:TRP:CG	1:B:120:TYR:HH	2.26	0.53
1:C:183:LYS:O	1:C:187:LYS:HG2	2.09	0.53
1:D:719:GLU:OE2	1:D:721:THR:HG23	2.08	0.53
1:C:665:ALA:HA	1:C:716:LEU:HD12	1.91	0.53
1:D:361:LEU:HA	1:D:381:TRP:HA	1.90	0.53
1:D:112:PHE:CD1	1:D:327:MET:HE1	2.43	0.53
1:A:194:ILE:HD12	1:A:222:PHE:HD2	1.73	0.53
1:B:286:GLU:HA	1:B:289:LEU:HG	1.91	0.53
1:D:686:MET:O	1:D:690:MET:HG2	2.08	0.53
1:A:264:SER:HA	1:A:267:ARG:HD2	1.91	0.53
1:C:291:TYR:CE2	1:C:295:TYR:HE2	2.27	0.53
1:B:674:PHE:O	1:B:678:SER:OG	2.26	0.53
1:C:262:LYS:O	1:C:265:MET:HG3	2.09	0.53
1:D:101:TRP:HB2	1:D:117:TYR:CD2	2.45	0.52
1:A:669:GLY:H	1:A:672:MET:HE2	1.72	0.52
1:A:262:LYS:O	1:A:265:MET:HG3	2.10	0.52
1:A:757:ASP:OD1	1:A:757:ASP:N	2.42	0.52
1:B:771:LYS:HA	1:B:774:MET:HE2	1.92	0.52
1:C:142:VAL:HG22	1:C:169:ARG:HB2	1.91	0.52
1:D:726:VAL:HG12	1:D:733:LEU:HD11	1.91	0.52
1:B:364:GLU:OE2	1:B:381:TRP:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:VAL:O	1:A:487:ILE:HG12	2.10	0.52
1:B:256:VAL:HG22	1:B:338:LEU:HD23	1.91	0.52
1:B:143:TYR:HE1	1:B:168:ILE:HG23	1.75	0.52
1:B:324:PRO:HA	1:B:327:MET:HG2	1.91	0.52
1:C:501:THR:HG22	1:C:504:ARG:NH1	2.24	0.52
1:D:74:PHE:CD2	1:D:290:MET:HE1	2.43	0.52
1:D:117:TYR:CD1	1:D:118:PRO:HD2	2.45	0.52
1:A:331:LYS:HZ2	1:A:346:LYS:HA	1.73	0.52
1:B:105:SER:O	1:B:109:ARG:NH2	2.37	0.52
1:C:724:GLU:HG3	1:C:780:TRP:HZ2	1.73	0.52
1:A:140:THR:HG22	1:A:167:LYS:HB2	1.90	0.52
1:A:741:ASP:OD1	1:D:693:ARG:NH2	2.41	0.52
1:C:682:THR:HB	1:C:686:MET:HE1	1.92	0.52
1:C:89:CYS:HA	1:C:94:VAL:CB	2.37	0.52
1:C:467:ASP:HB2	1:C:469:LYS:NZ	2.25	0.52
1:D:332:GLU:O	1:D:334:ARG:NH1	2.43	0.52
1:A:101:TRP:HB2	1:A:117:TYR:CE2	2.45	0.52
1:D:774:MET:O	1:D:774:MET:HE3	2.09	0.51
1:A:250:ASN:ND2	1:A:252:ASP:OD1	2.27	0.51
1:B:706:ILE:HG12	1:B:726:VAL:HG21	1.92	0.51
1:C:521:ILE:HD11	1:C:715:ALA:HB1	1.93	0.51
1:D:522:LEU:HD11	1:D:733:LEU:HD13	1.92	0.51
1:B:84:ALA:O	1:B:88:ILE:HD12	2.10	0.51
1:D:696:SER:O	1:D:708:ARG:NH2	2.44	0.51
1:A:518:GLY:HA3	1:A:739:LEU:HD22	1.92	0.51
1:D:124:SER:HB2	1:D:154:GLU:HB2	1.90	0.51
1:A:238:TYR:O	1:A:409:SER:OG	2.27	0.51
1:A:335:TRP:CG	1:A:336:ASP:N	2.78	0.51
1:D:97:ILE:HG13	1:D:114:ILE:HB	1.91	0.51
1:A:498:LEU:HD23	1:A:504:ARG:NH2	2.24	0.51
1:B:121:ALA:HB1	1:B:125:ARG:HH12	1.75	0.51
1:A:663:TYR:HB3	1:A:715:ALA:HB3	1.92	0.51
1:B:208:GLN:HA	1:B:211:PHE:HD1	1.75	0.51
1:D:417:VAL:HG21	1:D:460:TYR:HB2	1.93	0.51
1:A:248:LEU:HD13	1:A:339:THR:HG22	1.93	0.51
1:A:415:LEU:N	1:A:459:LEU:O	2.26	0.51
1:C:184:GLU:HA	1:C:187:LYS:HG2	1.93	0.51
1:D:667:ARG:HH22	1:D:695:GLN:HB3	1.76	0.51
1:A:447:ASP:O	1:A:450:LYS:HG2	2.11	0.51
1:C:416:ILE:HB	1:C:491:ALA:HA	1.93	0.51
1:B:783:ASN:OD1	1:B:784:GLY:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:PHE:O	1:B:330:ILE:HG12	2.11	0.50
1:D:384:ILE:HG22	1:D:395:MET:HE1	1.93	0.50
1:A:168:ILE:HG13	1:B:157:LYS:HZ3	1.77	0.50
1:A:429:ARG:HG2	1:A:442:GLU:HG3	1.92	0.50
1:B:116:LEU:HD23	1:B:289:LEU:HB2	1.92	0.50
1:C:181:LEU:HA	1:C:184:GLU:CD	2.37	0.50
1:C:22:LEU:HD23	1:C:25:LYS:HZ2	1.77	0.50
1:C:472:ALA:N	1:C:480:ASN:OD1	2.41	0.50
1:A:77:SER:HG	1:A:100:ARG:NH1	2.09	0.50
1:A:327:MET:SD	1:A:328:ASN:ND2	2.85	0.50
1:B:209:ILE:HG13	1:B:215:MET:SD	2.52	0.50
1:B:234:GLU:HG3	1:B:237:ARG:HH21	1.77	0.50
1:D:395:MET:HE2	1:D:395:MET:HA	1.94	0.50
1:A:188:SER:OG	1:A:190:GLU:OE2	2.21	0.50
1:A:234:GLU:O	1:A:237:ARG:NH2	2.37	0.50
1:A:415:LEU:HB3	1:A:460:TYR:HB3	1.94	0.50
1:A:645:MET:HE1	1:D:642:VAL:HG22	1.93	0.50
1:C:152:LEU:HD13	1:C:155:LEU:HD21	1.94	0.50
1:C:397:ASP:HA	1:C:400:ARG:HH12	1.77	0.50
1:C:181:LEU:HA	1:C:184:GLU:OE2	2.12	0.50
1:A:195:PHE:HE2	1:A:209:ILE:HD11	1.77	0.49
1:A:273:ARG:HD2	1:A:274:PRO:HD2	1.94	0.49
1:B:267:ARG:O	1:B:268:LEU:C	2.55	0.49
1:C:256:VAL:HA	1:C:259:ILE:HG12	1.94	0.49
1:D:266:GLU:OE2	1:D:267:ARG:NH1	2.40	0.49
1:B:243:MET:HE3	1:B:244:THR:N	2.28	0.49
1:A:119:ASP:OD1	1:A:120:TYR:N	2.46	0.49
1:A:331:LYS:NZ	1:A:346:LYS:HA	2.27	0.49
1:B:292:ASP:O	1:B:296:MET:HG2	2.11	0.49
1:A:101:TRP:HB2	1:A:117:TYR:CD2	2.47	0.49
1:C:226:LEU:HD12	1:C:248:LEU:H	1.77	0.49
1:D:313:GLN:HE22	1:D:315:HIS:HB2	1.77	0.49
1:D:750:PRO:HB2	1:D:753:SER:HB2	1.93	0.49
1:C:47:ILE:HB	1:C:49:ARG:HH12	1.78	0.49
1:A:331:LYS:NZ	1:A:345:ASN:O	2.30	0.49
1:C:667:ARG:HH21	1:C:700:LYS:HD3	1.76	0.49
1:D:456:LEU:HD22	1:D:758:LYS:HG3	1.95	0.49
1:B:92:LEU:HD22	1:B:312:LEU:HD23	1.95	0.49
1:A:342:ILE:HG13	1:A:351:ARG:HH21	1.78	0.49
1:B:120:TYR:CG	1:B:151:ARG:HG3	2.48	0.49
1:C:22:LEU:HD23	1:C:25:LYS:NZ	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:GLU:HA	1:D:490:ARG:HE	1.78	0.49
1:B:95:PRO:HD3	1:B:327:MET:HE2	1.95	0.49
1:B:259:ILE:HA	1:B:262:LYS:HD2	1.95	0.49
1:A:253:ASN:O	1:A:255:HIS:N	2.46	0.48
1:A:461:ASP:O	1:A:463:LYS:NZ	2.43	0.48
1:B:230:ALA:HB2	1:B:283:MET:HA	1.94	0.48
1:C:263:TRP:HA	1:C:266:GLU:CD	2.38	0.48
1:B:61:ARG:NH2	1:B:64:ASP:OD2	2.46	0.48
1:D:82:VAL:HA	1:D:85:VAL:HG12	1.96	0.48
1:D:258:SER:O	1:D:262:LYS:HG2	2.13	0.48
1:D:699:VAL:HB	1:D:704:GLU:HB2	1.95	0.48
1:C:642:VAL:HG21	1:D:644:ARG:HH21	1.78	0.48
1:D:636:LEU:O	1:D:640:LEU:HG	2.13	0.48
1:A:120:TYR:HB3	1:A:151:ARG:HA	1.95	0.48
1:A:356:LEU:HD12	1:A:387:TRP:HE3	1.77	0.48
1:A:667:ARG:HA	1:A:672:MET:HE1	1.95	0.48
1:B:177:ASP:HA	1:B:179:LYS:NZ	2.29	0.48
1:B:485:GLU:HG2	1:B:490:ARG:CZ	2.43	0.48
1:D:206:LEU:HA	1:D:209:ILE:HG12	1.95	0.48
1:B:334:ARG:HD3	1:B:343:THR:HG22	1.96	0.48
1:B:693:ARG:HH12	1:C:742:SER:N	2.11	0.48
1:C:133:TYR:C	1:C:135:ASN:N	2.68	0.48
1:C:480:ASN:HA	1:C:484:LYS:NZ	2.28	0.48
1:D:263:TRP:HB2	1:D:283:MET:HE2	1.95	0.48
1:C:398:GLY:H	1:C:400:ARG:HH11	1.62	0.48
1:C:499:THR:HG22	1:C:743:LYS:HB3	1.96	0.48
1:A:508:ILE:HD11	1:A:750:PRO:HA	1.95	0.48
1:A:640:LEU:HG	1:A:644:ARG:HH21	1.78	0.48
1:C:140:THR:HG22	1:C:167:LYS:HB3	1.96	0.48
1:B:124:SER:OG	1:B:154:GLU:OE2	2.31	0.48
1:C:429:ARG:HH22	1:C:438:ASN:HB2	1.79	0.48
1:D:197:CYS:HB2	1:D:201:THR:OG1	2.14	0.48
1:A:511:SER:HB3	1:A:756:ARG:NH2	2.29	0.47
1:B:705:GLY:O	1:B:709:VAL:HG23	2.14	0.47
1:B:214:MET:HB3	1:B:219:TYR:CE2	2.48	0.47
1:B:265:MET:O	1:B:268:LEU:HB2	2.15	0.47
1:D:3:LEU:O	1:D:44:THR:N	2.42	0.47
1:B:228:LEU:HD21	1:B:359:ILE:HG13	1.97	0.47
1:D:142:VAL:HA	1:D:169:ARG:O	2.14	0.47
1:D:169:ARG:HD3	1:D:181:LEU:HD22	1.96	0.47
1:B:680:ILE:O	1:B:683:TYR:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LEU:O	1:C:352:LYS:NZ	2.29	0.47
1:D:418:THR:HB	1:D:463:LYS:HE3	1.95	0.47
1:D:522:LEU:HD12	1:D:523:TYR:N	2.28	0.47
1:D:720:SER:O	1:D:723:ILE:N	2.48	0.47
1:A:120:TYR:CG	1:A:151:ARG:HG2	2.48	0.47
1:A:649:ILE:HG23	1:A:654:ASP:HB2	1.97	0.47
1:B:515:MET:HE3	1:B:517:LEU:HD13	1.97	0.47
1:C:773:HIS:NE2	1:C:777:GLU:OE2	2.46	0.47
1:D:4:ARG:HA	1:D:44:THR:HB	1.97	0.47
1:A:253:ASN:O	1:A:256:VAL:N	2.47	0.47
1:B:467:ASP:CG	1:B:469:LYS:HD2	2.40	0.47
1:C:143:TYR:CE1	1:C:168:ILE:HB	2.50	0.47
1:A:170:GLN:HB2	1:B:157:LYS:HZ1	1.80	0.47
1:B:266:GLU:HG2	1:B:267:ARG:N	2.29	0.47
1:B:507:VAL:HG23	1:B:508:ILE:HG23	1.96	0.47
1:B:640:LEU:HD12	1:B:643:GLU:OE2	2.15	0.47
1:B:694:GLN:O	1:B:695:GLN:HG3	2.15	0.47
1:C:91:ALA:O	1:C:93:GLU:N	2.48	0.47
1:C:398:GLY:H	1:C:400:ARG:NH1	2.13	0.47
1:C:446:LEU:HG	1:C:450:LYS:NZ	2.30	0.47
1:C:764:LEU:O	1:C:767:GLN:HG3	2.14	0.47
1:C:771:LYS:HA	1:C:774:MET:HE2	1.97	0.47
1:A:128:LEU:HD23	1:A:155:LEU:HD23	1.96	0.47
1:B:700:LYS:N	1:B:704:GLU:OE2	2.46	0.47
1:C:15:GLU:HG2	1:C:18:ASN:H	1.79	0.47
1:C:771:LYS:HB3	1:C:775:MET:HE1	1.97	0.47
1:B:263:TRP:CG	1:B:267:ARG:HH12	2.32	0.47
1:C:319:PRO:HG2	1:C:321:ARG:HH22	1.79	0.47
1:D:203:ALA:O	1:D:206:LEU:HG	2.15	0.47
1:A:282:MET:HE2	1:A:282:MET:HB3	1.87	0.47
1:A:692:SER:O	1:A:693:ARG:HD3	2.15	0.47
1:C:11:THR:N	1:C:50:ILE:O	2.36	0.47
1:B:723:ILE:HA	1:B:726:VAL:HG12	1.98	0.46
1:C:295:TYR:O	1:C:299:ILE:HD12	2.15	0.46
1:A:230:ALA:HA	1:A:282:MET:HG3	1.97	0.46
1:B:659:THR:HG23	1:B:660:LYS:HD3	1.97	0.46
1:C:34:ASN:OD1	1:C:36:THR:HG22	2.14	0.46
1:C:170:GLN:NE2	1:C:171:LEU:O	2.48	0.46
1:A:509:ASP:HB3	1:A:756:ARG:NH1	2.31	0.46
1:C:88:ILE:HD12	1:C:88:ILE:H	1.81	0.46
1:B:98:GLN:HE22	1:B:113:TYR:HA	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ARG:NH2	1:D:68:LEU:O	2.29	0.46
1:D:98:GLN:NE2	1:D:115:ASN:HB2	2.31	0.46
1:B:420:ILE:HG22	1:B:496:ALA:HB1	1.98	0.46
1:C:458:PHE:HE2	1:C:460:TYR:HB3	1.80	0.46
1:C:725:TYR:HA	1:C:728:GLN:HE21	1.80	0.46
1:D:61:ARG:HH11	1:D:64:ASP:HB2	1.79	0.46
1:D:359:ILE:HG13	1:D:381:TRP:CE3	2.50	0.46
1:A:320:TRP:CZ2	1:A:322:LEU:HB2	2.51	0.46
1:B:56:PHE:CG	1:B:57:GLU:N	2.84	0.46
1:C:19:VAL:HA	1:C:22:LEU:HD12	1.98	0.46
1:C:76:PRO:HD3	1:C:96:HIS:CE1	2.51	0.46
1:D:695:GLN:HG3	1:D:698:LEU:HD12	1.98	0.46
1:B:180:PRO:O	1:B:184:GLU:OE1	2.33	0.46
1:D:666:VAL:N	1:D:718:MET:HE3	2.25	0.46
1:B:180:PRO:HA	1:B:183:LYS:HE3	1.98	0.46
1:C:93:GLU:OE2	1:C:319:PRO:HB2	2.15	0.46
1:C:263:TRP:NE1	1:C:267:ARG:HH11	2.14	0.46
1:D:174:ALA:O	1:D:176:LYS:HE2	2.16	0.46
1:A:522:LEU:HD11	1:A:733:LEU:HD21	1.98	0.46
1:B:150:ILE:HG13	1:B:151:ARG:HD3	1.97	0.46
1:B:312:LEU:HD11	1:B:318:LYS:HD3	1.98	0.46
1:B:759:ILE:O	1:B:763:ILE:HG12	2.16	0.46
1:C:721:THR:HA	1:C:724:GLU:OE2	2.16	0.46
1:C:116:LEU:HG	1:C:293:ALA:HB2	1.97	0.45
1:D:4:ARG:H	1:D:4:ARG:HD3	1.81	0.45
1:D:231:LEU:HD23	1:D:232:ASP:N	2.31	0.45
1:D:664:GLY:HA2	1:D:690:MET:HE1	1.98	0.45
1:A:350:LEU:O	1:A:352:LYS:NZ	2.49	0.45
1:B:98:GLN:N	1:B:98:GLN:OE1	2.50	0.45
1:B:505:GLU:HA	1:B:508:ILE:O	2.16	0.45
1:C:136:TRP:C	1:C:138:THR:H	2.23	0.45
1:A:183:LYS:HA	1:A:186:LYS:HD3	1.99	0.45
1:B:680:ILE:HG12	1:B:683:TYR:CD2	2.51	0.45
1:C:312:LEU:HD21	1:C:320:TRP:CD1	2.51	0.45
1:D:420:ILE:HG13	1:D:421:LEU:H	1.80	0.45
1:A:176:LYS:HA	1:A:179:LYS:HZ3	1.81	0.45
1:A:258:SER:O	1:A:262:LYS:HG2	2.17	0.45
1:A:263:TRP:CZ3	1:A:283:MET:HA	2.52	0.45
1:C:451:GLU:O	1:C:455:ILE:HG12	2.16	0.45
1:A:261:GLU:OE1	1:A:262:LYS:HE3	2.16	0.45
1:B:525:LYS:HG2	1:B:736:ILE:HD11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ALA:C	1:C:93:GLU:H	2.24	0.45
1:D:519:ILE:HG12	1:D:741:ASP:OD1	2.16	0.45
1:D:671:THR:HB	1:D:675:PHE:CZ	2.52	0.45
1:D:682:THR:O	1:D:686:MET:HG2	2.16	0.45
1:B:61:ARG:O	1:B:65:GLN:HG2	2.16	0.45
1:C:263:TRP:HA	1:C:266:GLU:OE2	2.16	0.45
1:C:317:HIS:CE1	1:D:56:PHE:HZ	2.33	0.45
1:C:655:LEU:HD22	1:C:661:ILE:HG21	1.98	0.45
1:A:692:SER:C	1:A:693:ARG:HD3	2.41	0.45
1:B:447:ASP:OD1	1:B:448:LEU:N	2.50	0.45
1:B:448:LEU:O	1:B:452:LEU:HD23	2.17	0.45
1:C:250:ASN:OD1	1:C:251:ILE:N	2.49	0.45
1:B:203:ALA:O	1:B:207:LYS:NZ	2.42	0.45
1:C:98:GLN:N	1:C:114:ILE:O	2.36	0.45
1:C:125:ARG:HA	1:C:128:LEU:HG	1.99	0.45
1:C:298:ALA:C	1:C:302:HIS:HD1	2.21	0.45
1:A:154:GLU:HA	1:A:157:LYS:HG2	1.99	0.45
1:A:415:LEU:HD12	1:A:492:ASP:HB2	1.99	0.45
1:B:248:LEU:HD21	1:B:351:ARG:HH22	1.81	0.45
1:B:335:TRP:CZ3	1:B:337:GLY:HA3	2.51	0.45
1:B:420:ILE:HB	1:B:482:MET:SD	2.57	0.45
1:D:700:LYS:N	1:D:704:GLU:OE1	2.50	0.45
1:A:86:GLN:HE22	1:A:96:HIS:HB3	1.81	0.45
1:A:171:LEU:HD23	1:A:181:LEU:HD12	1.98	0.45
1:A:186:LYS:HZ1	1:A:212:MET:HG2	1.81	0.45
1:B:83:SER:O	1:B:86:GLN:HG3	2.17	0.45
1:B:140:THR:HG23	1:B:193:VAL:HG23	1.99	0.45
1:C:180:PRO:HA	1:C:183:LYS:HG2	1.99	0.45
1:C:650:ASP:OD1	1:C:650:ASP:N	2.48	0.44
1:A:121:ALA:HB1	1:A:125:ARG:NH1	2.32	0.44
1:A:169:ARG:NH2	1:B:160:SER:HB3	2.32	0.44
1:B:508:ILE:HD12	1:B:748:GLY:HA3	2.00	0.44
1:C:8:ILE:HG23	1:C:50:ILE:HD13	1.99	0.44
1:C:91:ALA:C	1:C:93:GLU:N	2.76	0.44
1:C:232:ASP:HB2	1:C:279:LEU:HD11	1.98	0.44
1:C:253:ASN:O	1:C:255:HIS:N	2.50	0.44
1:C:410:LEU:HA	1:C:413:ARG:HH21	1.81	0.44
1:A:168:ILE:HG13	1:B:157:LYS:NZ	2.31	0.44
1:B:126:ALA:HA	1:B:387:TRP:NE1	2.32	0.44
1:B:761:ILE:HG22	1:B:765:GLN:OE1	2.18	0.44
1:C:331:LYS:HE3	1:C:346:LYS:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:LEU:HA	1:C:775:MET:HE2	2.00	0.44
1:D:510:PHE:O	1:D:756:ARG:NH2	2.41	0.44
1:D:760:THR:HA	1:D:763:ILE:HG22	1.98	0.44
1:A:186:LYS:HE2	1:A:212:MET:HE2	1.97	0.44
1:A:335:TRP:CG	1:A:336:ASP:H	2.36	0.44
1:A:445:CYS:O	1:A:449:LEU:HD23	2.17	0.44
1:B:381:TRP:C	1:B:382:LYS:HD3	2.42	0.44
1:B:486:LEU:HD11	1:B:494:ALA:HB2	2.00	0.44
1:B:699:VAL:HB	1:B:704:GLU:OE2	2.18	0.44
1:C:90:ASN:HA	1:C:112:PHE:HD2	1.82	0.44
1:C:194:ILE:HG23	1:C:222:PHE:HD2	1.81	0.44
1:C:763:ILE:O	1:C:766:LEU:HB2	2.17	0.44
1:D:667:ARG:HG2	1:D:700:LYS:HD2	1.98	0.44
1:A:415:LEU:HD12	1:A:416:ILE:N	2.33	0.44
1:A:416:ILE:HG23	1:A:463:LYS:HE3	1.99	0.44
1:C:424:PRO:HB3	1:C:725:TYR:CZ	2.52	0.44
1:C:769:GLU:HB2	1:C:771:LYS:HZ3	1.82	0.44
1:A:93:GLU:HG2	1:A:319:PRO:HB3	1.98	0.44
1:A:226:LEU:HB3	1:A:248:LEU:HD23	1.99	0.44
1:A:324:PRO:HA	1:A:327:MET:HG3	1.98	0.44
1:B:38:MET:HB2	1:B:302:HIS:ND1	2.32	0.44
1:B:73:LEU:HB2	1:B:96:HIS:HD2	1.82	0.44
1:B:429:ARG:HD3	1:B:442:GLU:HB3	2.00	0.44
1:C:776:LYS:O	1:C:780:TRP:CB	2.66	0.44
1:C:485:GLU:HA	1:C:490:ARG:HH21	1.83	0.44
1:C:498:LEU:HD11	1:C:510:PHE:HE1	1.83	0.44
1:A:302:HIS:HD2	1:A:303:ARG:NH1	2.15	0.44
1:B:23:ALA:HB2	1:B:263:TRP:HH2	1.82	0.44
1:B:667:ARG:HG2	1:B:667:ARG:HH11	1.83	0.44
1:D:255:HIS:O	1:D:259:ILE:HG12	2.18	0.44
1:D:269:GLN:OE1	1:D:269:GLN:N	2.48	0.44
1:D:662:GLU:HG3	1:D:714:TYR:HD1	1.83	0.44
1:B:345:ASN:HD21	1:B:352:LYS:HG3	1.82	0.43
1:D:512:LYS:HD2	1:D:513:PRO:O	2.18	0.43
1:D:672:MET:HA	1:D:675:PHE:CD2	2.52	0.43
1:A:267:ARG:NH1	1:A:268:LEU:HD23	2.33	0.43
1:A:682:THR:HG23	1:A:685:LYS:NZ	2.33	0.43
1:B:208:GLN:HA	1:B:211:PHE:CD1	2.53	0.43
1:A:689:PHE:O	1:A:693:ARG:NH1	2.51	0.43
1:C:690:MET:HB3	1:C:698:LEU:HD11	2.00	0.43
1:A:523:TYR:CE1	1:A:713:ASP:HA	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:HD11	1:B:237:ARG:HD2	2.00	0.43
1:C:286:GLU:O	1:C:289:LEU:HG	2.18	0.43
1:D:421:LEU:HA	1:D:426:VAL:HB	2.00	0.43
1:A:82:VAL:O	1:A:86:GLN:HG2	2.19	0.43
1:A:641:THR:O	1:A:645:MET:HG2	2.17	0.43
1:B:125:ARG:O	1:B:128:LEU:HG	2.18	0.43
1:B:214:MET:HB3	1:B:219:TYR:HE2	1.83	0.43
1:B:267:ARG:C	1:B:269:GLN:N	2.75	0.43
1:C:253:ASN:O	1:C:256:VAL:N	2.39	0.43
1:C:483:VAL:O	1:C:487:ILE:HG23	2.19	0.43
1:A:462:VAL:C	1:A:463:LYS:HD3	2.43	0.43
1:A:759:ILE:O	1:A:763:ILE:HG12	2.19	0.43
1:B:152:LEU:HA	1:B:155:LEU:HD23	2.01	0.43
1:B:265:MET:HE3	1:B:265:MET:HB3	1.91	0.43
1:A:176:LYS:HA	1:A:179:LYS:NZ	2.33	0.43
1:C:89:CYS:O	1:C:90:ASN:C	2.58	0.43
1:C:724:GLU:O	1:C:728:GLN:HG3	2.19	0.43
1:A:676:LYS:HB2	1:A:687:TRP:CD1	2.54	0.43
1:B:28:VAL:HG11	1:B:45:TYR:CD1	2.54	0.43
1:C:26:PHE:CZ	1:C:266:GLU:HG3	2.54	0.43
1:C:397:ASP:OD2	1:C:402:ARG:NH2	2.52	0.43
1:D:393:LEU:HD23	1:D:393:LEU:H	1.84	0.43
1:A:153:GLN:NE2	1:B:146:SER:HB3	2.34	0.43
1:B:364:GLU:N	1:B:364:GLU:OE1	2.52	0.43
1:B:676:LYS:HB3	1:B:687:TRP:CZ3	2.54	0.43
1:C:355:ASP:HA	1:C:387:TRP:O	2.19	0.43
1:D:48:GLN:NE2	1:D:61:ARG:HH21	2.16	0.43
1:C:29:THR:O	1:C:33:ARG:HG2	2.19	0.42
1:C:78:HIS:O	1:C:82:VAL:HG23	2.19	0.42
1:D:257:SER:O	1:D:260:ILE:N	2.51	0.42
1:B:672:MET:O	1:B:676:LYS:HG2	2.19	0.42
1:C:178:ALA:O	1:C:181:LEU:HG	2.19	0.42
1:D:450:LYS:HE2	1:D:454:ASN:HD21	1.84	0.42
1:A:168:ILE:HG21	1:B:156:ILE:HD12	2.01	0.42
1:A:183:LYS:O	1:A:186:LYS:HB2	2.19	0.42
1:B:197:CYS:HB2	1:B:201:THR:OG1	2.19	0.42
1:D:37:LEU:O	1:D:38:MET:HE2	2.18	0.42
1:D:713:ASP:OD1	1:D:713:ASP:N	2.52	0.42
1:A:425:TYR:O	1:A:443:GLY:HA3	2.19	0.42
1:B:38:MET:HE3	1:B:40:ASN:H	1.83	0.42
1:B:697:ALA:C	1:B:698:LEU:HD12	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLN:HE21	1:C:86:GLN:HB2	1.69	0.42
1:C:304:ALA:HB1	1:C:307:LEU:HD12	2.02	0.42
1:D:2:VAL:HA	1:D:42:THR:HB	2.02	0.42
1:B:201:THR:HA	1:B:204:GLU:OE2	2.19	0.42
1:B:495:VAL:HG12	1:B:495:VAL:O	2.20	0.42
1:C:92:LEU:HD22	1:C:312:LEU:HB3	2.02	0.42
1:D:72:ALA:HB1	1:D:97:ILE:HD13	2.01	0.42
1:A:89:CYS:HB3	1:A:94:VAL:O	2.19	0.42
1:B:299:ILE:O	1:B:303:ARG:NH1	2.51	0.42
1:B:638:ALA:O	1:B:642:VAL:HG23	2.20	0.42
1:C:32:ASN:HB3	1:C:33:ARG:HH21	1.83	0.42
1:C:37:LEU:HB3	1:C:302:HIS:CD2	2.55	0.42
1:C:136:TRP:C	1:C:138:THR:N	2.76	0.42
1:C:334:ARG:HA	1:C:341:ARG:HH12	1.85	0.42
1:A:316:ARG:HH21	1:A:318:LYS:HG2	1.85	0.42
1:A:719:GLU:OE2	1:A:721:THR:N	2.53	0.42
1:B:521:ILE:HD12	1:B:716:LEU:O	2.19	0.42
1:C:513:PRO:HA	1:C:745:TYR:O	2.20	0.42
1:D:453:SER:OG	1:D:458:PHE:O	2.25	0.42
1:A:351:ARG:NH1	1:A:354:PHE:HD2	2.18	0.42
1:B:238:TYR:HB2	1:B:241:VAL:HG22	2.02	0.42
1:B:672:MET:HA	1:B:675:PHE:CD1	2.55	0.42
1:C:89:CYS:O	1:C:94:VAL:HB	2.19	0.42
1:D:179:LYS:HG3	1:D:180:PRO:HD3	2.02	0.42
1:D:243:MET:HB3	1:D:361:LEU:HD23	2.01	0.42
1:B:183:LYS:O	1:B:186:LYS:HG3	2.20	0.42
1:B:419:THR:O	1:B:465:VAL:N	2.53	0.42
1:C:247:ARG:HH12	1:C:251:ILE:HG23	1.84	0.42
1:C:638:ALA:O	1:C:642:VAL:HG13	2.20	0.42
1:D:201:THR:HA	1:D:204:GLU:HG3	2.02	0.42
1:D:413:ARG:HG2	1:D:458:PHE:CE1	2.55	0.42
1:D:475:ASP:OD1	1:D:475:ASP:N	2.52	0.42
1:D:513:PRO:HG3	1:D:745:TYR:H	1.84	0.42
1:A:100:ARG:HG3	1:A:102:LYS:HE2	2.02	0.42
1:A:264:SER:O	1:A:267:ARG:HD3	2.20	0.42
1:A:447:ASP:O	1:A:450:LYS:N	2.53	0.42
1:A:640:LEU:O	1:A:643:GLU:HG2	2.20	0.42
1:A:714:TYR:HE2	1:A:716:LEU:HD13	1.85	0.42
1:A:778:LYS:HA	1:A:781:ARG:NH1	2.35	0.42
1:C:169:ARG:NH2	1:D:160:SER:OG	2.53	0.42
1:D:259:ILE:HG22	1:D:283:MET:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:GLN:O	1:A:768:GLU:HG3	2.19	0.41
1:C:74:PHE:HD1	1:C:97:ILE:HD11	1.85	0.41
1:C:93:GLU:HB3	1:C:323:GLY:HA3	2.02	0.41
1:D:176:LYS:HA	1:D:176:LYS:HD3	1.83	0.41
1:A:172:PRO:HB2	1:A:177:ASP:OD2	2.20	0.41
1:A:191:PHE:CE2	1:A:218:TYR:HB3	2.55	0.41
1:B:233:LEU:HD13	1:B:361:LEU:HD11	2.01	0.41
1:B:680:ILE:O	1:B:681:SER:C	2.64	0.41
1:C:262:LYS:HA	1:C:265:MET:HG3	2.02	0.41
1:C:324:PRO:HA	1:C:327:MET:HG3	2.02	0.41
1:A:109:ARG:HH21	1:A:349:GLY:H	1.68	0.41
1:A:351:ARG:HH11	1:A:354:PHE:HD2	1.68	0.41
1:B:675:PHE:CD1	1:B:686:MET:HE1	2.55	0.41
1:D:204:GLU:O	1:D:208:GLN:HG2	2.20	0.41
1:D:243:MET:H	1:D:361:LEU:HD21	1.85	0.41
1:B:256:VAL:O	1:B:260:ILE:HG13	2.20	0.41
1:B:413:ARG:HE	1:B:414:THR:N	2.18	0.41
1:B:645:MET:HE3	1:C:645:MET:HE1	2.01	0.41
1:C:133:TYR:C	1:C:135:ASN:H	2.29	0.41
1:C:424:PRO:HB3	1:C:725:TYR:CE2	2.55	0.41
1:C:499:THR:HB	1:C:743:LYS:HD2	2.02	0.41
1:A:222:PHE:HZ	1:A:246:PHE:CE2	2.38	0.41
1:A:514:PHE:HD2	1:A:515:MET:HG2	1.85	0.41
1:B:690:MET:HG2	1:B:698:LEU:HD13	2.02	0.41
1:B:709:VAL:HG22	1:B:714:TYR:HD2	1.86	0.41
1:C:509:ASP:OD2	1:C:752:GLY:N	2.54	0.41
1:D:35:ARG:H	1:D:35:ARG:HD3	1.85	0.41
1:D:238:TYR:CD2	1:D:361:LEU:HD22	2.55	0.41
1:D:661:ILE:HD12	1:D:713:ASP:OD2	2.20	0.41
1:D:675:PHE:CD1	1:D:683:TYR:HD1	2.38	0.41
1:A:11:THR:HB	1:A:49:ARG:NH2	2.32	0.41
1:A:18:ASN:HD21	1:A:21:GLU:HG3	1.85	0.41
1:A:35:ARG:NH1	1:A:38:MET:O	2.53	0.41
1:A:682:THR:HG23	1:A:685:LYS:HZ3	1.84	0.41
1:B:720:SER:HB3	1:B:739:LEU:HD11	2.02	0.41
1:C:137:LYS:HD2	1:C:137:LYS:HA	1.67	0.41
1:C:323:GLY:N	1:C:324:PRO:HD2	2.36	0.41
1:C:776:LYS:O	1:C:780:TRP:HB3	2.21	0.41
1:A:99:THR:HG21	1:A:290:MET:SD	2.60	0.41
1:A:147:THR:HA	1:A:150:ILE:HD13	2.02	0.41
1:A:293:ALA:O	1:A:296:MET:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:LYS:HG3	1:A:781:ARG:HH22	1.86	0.41
1:B:336:ASP:OD1	1:B:341:ARG:NE	2.54	0.41
1:C:706:ILE:HA	1:C:709:VAL:HG22	2.03	0.41
1:D:469:LYS:HD2	1:D:668:ASP:HB2	2.01	0.41
1:A:1:GLN:HG2	1:A:306:GLN:HB2	2.03	0.41
1:A:18:ASN:HD22	1:A:20:GLU:CD	2.28	0.41
1:A:98:GLN:NE2	1:A:115:ASN:HB2	2.35	0.41
1:B:503:VAL:HG23	1:B:504:ARG:HD3	2.03	0.41
1:C:113:TYR:O	1:C:349:GLY:HA3	2.21	0.41
1:C:203:ALA:C	1:C:207:LYS:HZ2	2.29	0.41
1:A:118:PRO:HA	1:A:354:PHE:CD2	2.55	0.41
1:A:669:GLY:H	1:A:672:MET:CE	2.34	0.41
1:A:724:GLU:O	1:A:728:GLN:HG2	2.20	0.41
1:B:243:MET:HE3	1:B:244:THR:H	1.85	0.41
1:B:358:ILE:HG13	1:B:395:MET:SD	2.61	0.41
1:C:273:ARG:HD3	1:C:275:GLU:O	2.21	0.41
1:C:305:SER:O	1:C:307:LEU:HG	2.21	0.41
1:C:429:ARG:HH21	1:C:440:ARG:HA	1.85	0.41
1:D:286:GLU:HA	1:D:289:LEU:HG	2.03	0.41
1:D:413:ARG:NH2	1:D:457:GLY:O	2.46	0.41
1:D:441:PHE:HZ	1:D:464:LEU:HD11	1.86	0.41
1:D:717:LEU:O	1:D:718:MET:HE2	2.21	0.41
1:A:313:GLN:HG3	1:A:315:HIS:H	1.86	0.41
1:B:128:LEU:HA	1:B:131:VAL:HG12	2.03	0.41
1:B:524:ARG:HH21	1:B:712:THR:C	2.28	0.41
1:C:441:PHE:HE1	1:C:464:LEU:HD11	1.85	0.41
1:C:507:VAL:HG23	1:C:508:ILE:HG23	2.03	0.41
1:D:410:LEU:HB3	1:D:413:ARG:HD2	2.03	0.41
1:D:675:PHE:HB2	1:D:687:TRP:HB2	2.03	0.41
1:A:46:ASP:OD1	1:A:46:ASP:N	2.53	0.40
1:B:485:GLU:HG2	1:B:490:ARG:NH1	2.36	0.40
1:C:131:VAL:O	1:C:132:LEU:C	2.65	0.40
1:D:61:ARG:NH1	1:D:65:GLN:OE1	2.54	0.40
1:D:127:VAL:HG21	1:D:155:LEU:HD11	2.04	0.40
1:D:263:TRP:HA	1:D:266:GLU:HG2	2.03	0.40
1:D:320:TRP:CZ2	1:D:322:LEU:HB2	2.55	0.40
1:A:342:ILE:HG13	1:A:351:ARG:NH2	2.37	0.40
1:B:116:LEU:HD12	1:B:351:ARG:HD3	2.03	0.40
1:B:776:LYS:HA	1:B:780:TRP:CE3	2.56	0.40
1:C:656:ALA:HA	1:C:663:TYR:CE1	2.55	0.40
1:C:728:GLN:NE2	1:C:780:TRP:O	2.32	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:TYR:O	1:C:756:ARG:C	2.64	0.40
1:A:519:ILE:N	1:A:741:ASP:O	2.54	0.40
1:A:764:LEU:O	1:A:767:GLN:HG3	2.21	0.40
1:B:182:LEU:HA	1:B:185:MET:HE3	2.03	0.40
1:B:256:VAL:HG13	1:B:338:LEU:HD22	2.04	0.40
1:C:167:LYS:HD3	1:C:168:ILE:H	1.87	0.40
1:D:140:THR:O	1:D:193:VAL:HA	2.21	0.40
1:D:152:LEU:O	1:D:156:ILE:HG13	2.21	0.40
1:D:183:LYS:HA	1:D:186:LYS:HE3	2.04	0.40
1:D:423:GLU:HA	1:D:424:PRO:HA	1.88	0.40
1:D:702:SER:O	1:D:706:ILE:HG13	2.21	0.40
1:A:641:THR:HA	1:A:644:ARG:NH2	2.37	0.40
1:A:703:ASP:HA	1:A:706:ILE:HG12	2.04	0.40
1:A:728:GLN:OE1	1:A:782:GLY:HA3	2.21	0.40
1:B:120:TYR:CZ	1:B:151:ARG:HD2	2.56	0.40
1:B:401:ASP:N	1:B:401:ASP:OD1	2.53	0.40
1:C:135:ASN:HD22	1:C:135:ASN:HA	1.45	0.40
1:C:183:LYS:HA	1:C:186:LYS:CG	2.49	0.40
1:D:444:TYR:CE2	1:D:448:LEU:HD11	2.56	0.40
1:A:412:ASN:C	1:A:413:ARG:HD3	2.46	0.40
1:B:226:LEU:HD11	1:B:356:LEU:HD22	2.04	0.40
1:B:290:MET:O	1:B:294:VAL:HG23	2.21	0.40
1:B:724:GLU:O	1:B:728:GLN:HG2	2.21	0.40
1:C:36:THR:HG23	1:C:37:LEU:CD2	2.51	0.40
1:C:57:GLU:HA	1:C:60:ARG:HG2	2.04	0.40
1:D:313:GLN:CD	1:D:315:HIS:H	2.30	0.40
1:D:345:ASN:OD1	1:D:346:LYS:N	2.51	0.40

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	665/1098 (61%)	636 (96%)	27 (4%)	2 (0%)	37 72
1	B	665/1098 (61%)	635 (96%)	30 (4%)	0	100 100
1	C	665/1098 (61%)	643 (97%)	22 (3%)	0	100 100
1	D	665/1098 (61%)	650 (98%)	15 (2%)	0	100 100
All	All	2660/4392 (61%)	2564 (96%)	94 (4%)	2 (0%)	50 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ALA
1	A	254	PRO

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	593/960 (62%)	593 (100%)	0	100 100
1	B	593/960 (62%)	591 (100%)	2 (0%)	91 92
1	C	593/960 (62%)	588 (99%)	5 (1%)	79 85
1	D	593/960 (62%)	593 (100%)	0	100 100
All	All	2372/3840 (62%)	2365 (100%)	7 (0%)	90 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	266	GLU
1	B	267	ARG
1	C	92	LEU
1	C	132	LEU
1	C	134	TYR
1	C	135	ASN
1	C	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	135	ASN
1	A	255	HIS
1	A	315	HIS
1	A	328	ASN
1	A	694	GLN
1	A	765	GLN
1	B	115	ASN
1	B	255	HIS
1	B	345	ASN
1	C	65	GLN
1	C	135	ASN
1	C	170	GLN
1	C	313	GLN
1	C	315	HIS
1	C	732	ASN
1	C	765	GLN
1	D	98	GLN
1	D	250	ASN
1	D	315	HIS
1	D	328	ASN
1	D	635	ASN
1	D	707	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

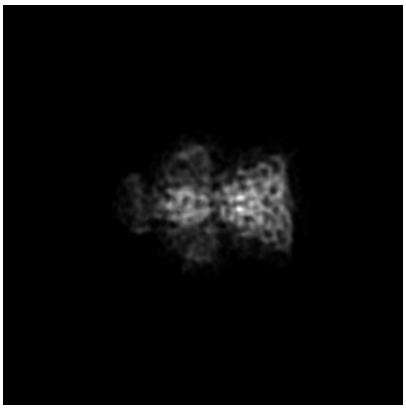
This section contains visualisations of the EMDB entry EMD-34076. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

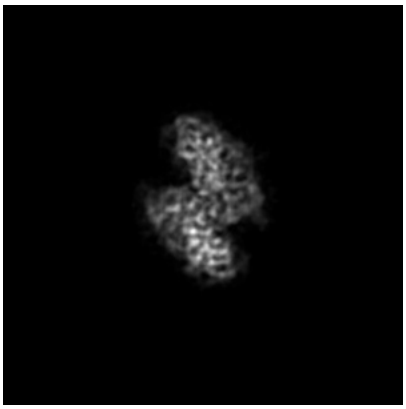
6.1 Orthogonal projections

6.1.1 Primary map

X

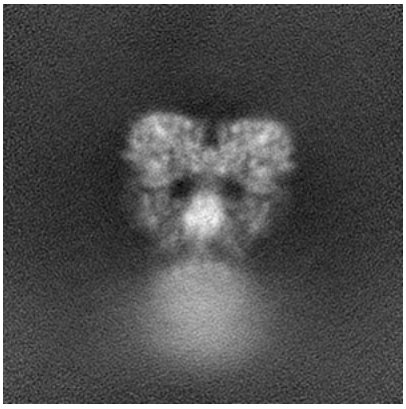


Y

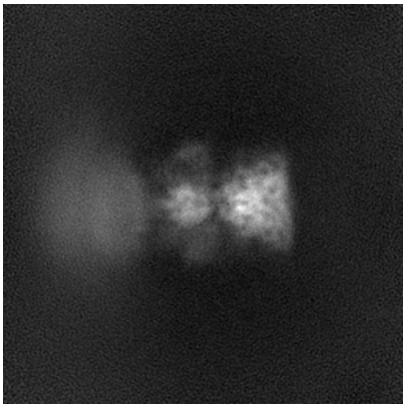


Z

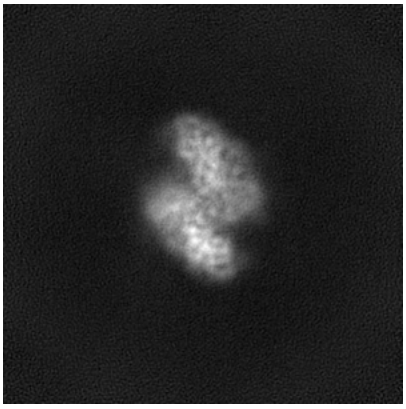
6.1.2 Raw map



X



Y



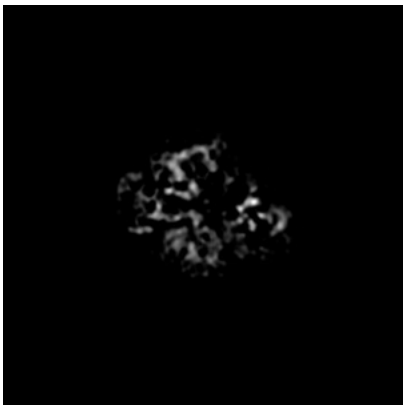
Z

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

6.2 Central slices (i)

6.2.1 Primary map

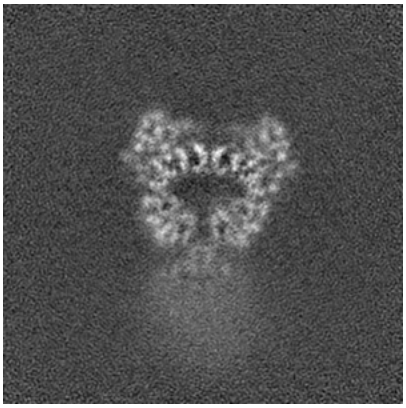
X Index: 128



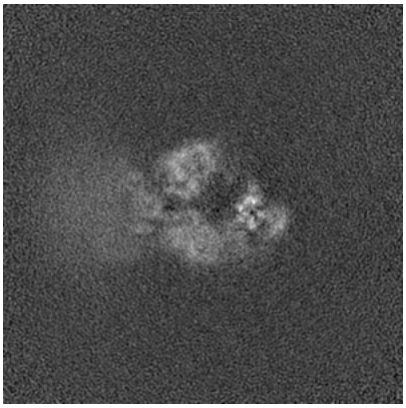
Y Index: 128

Z Index: 128

6.2.2 Raw map



X Index: 128



Y Index: 128

Z Index: 128

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

6.3 Largest variance slices (i)

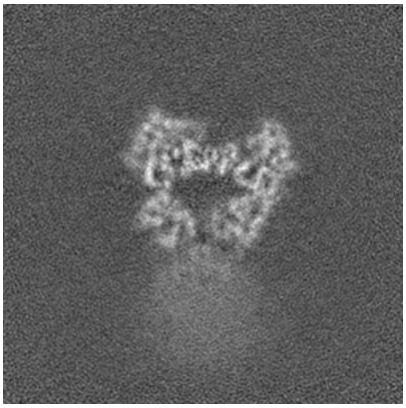
6.3.1 Primary map

X Index: 125

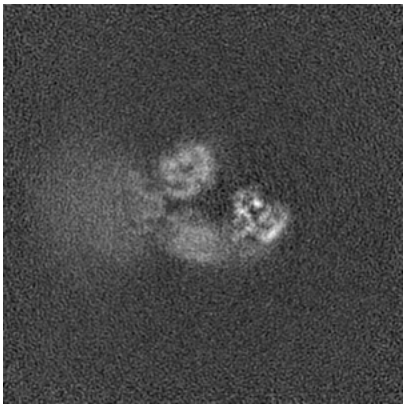
Y Index: 104

Z Index: 159

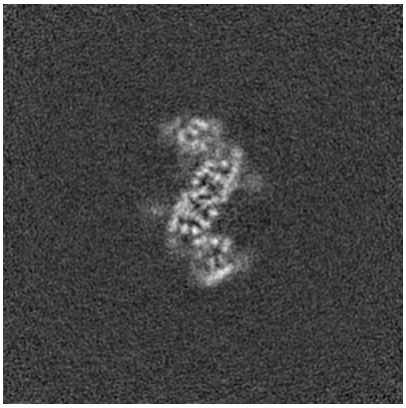
6.3.2 Raw map



X Index: 125



Y Index: 125



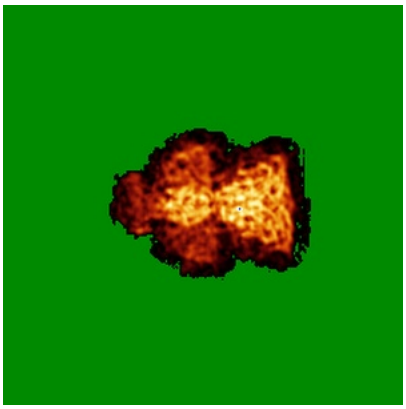
Z Index: 158

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

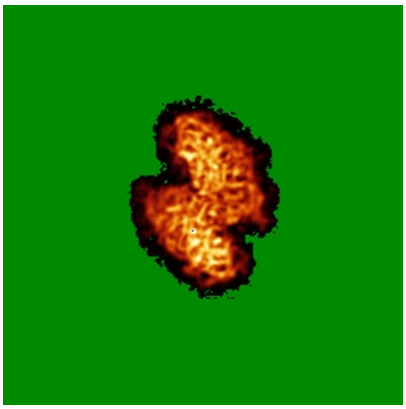
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

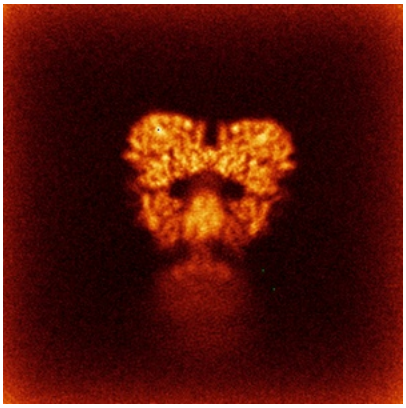


Y

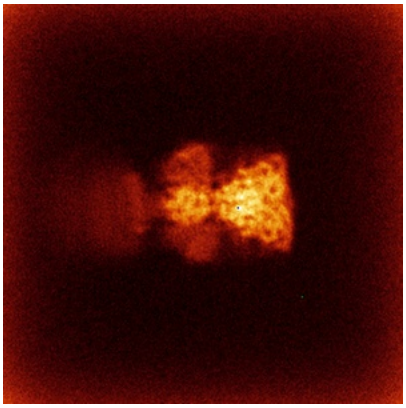


Z

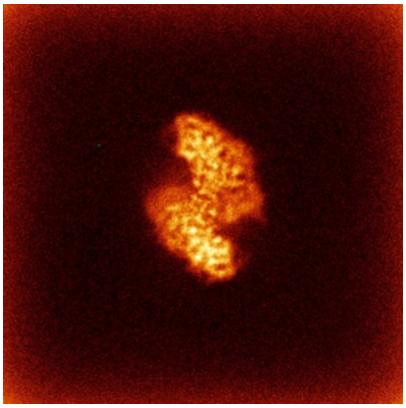
6.4.2 Raw map



X



Y

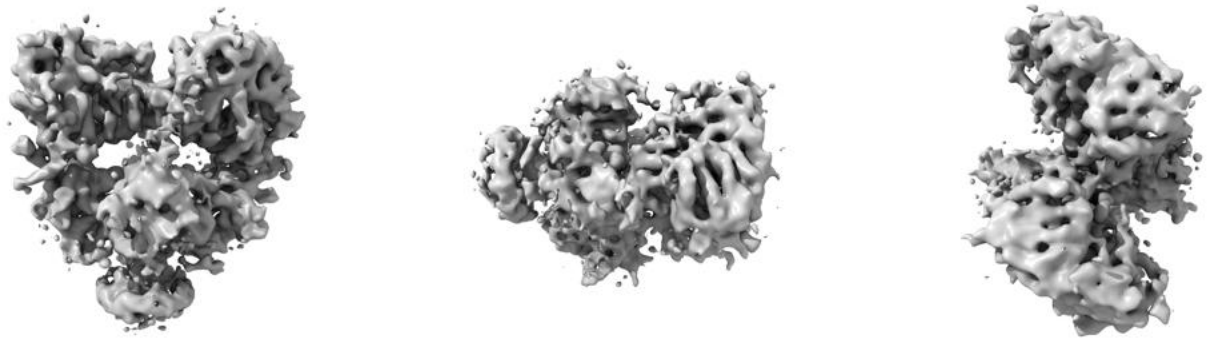


Z

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 0.25. 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.

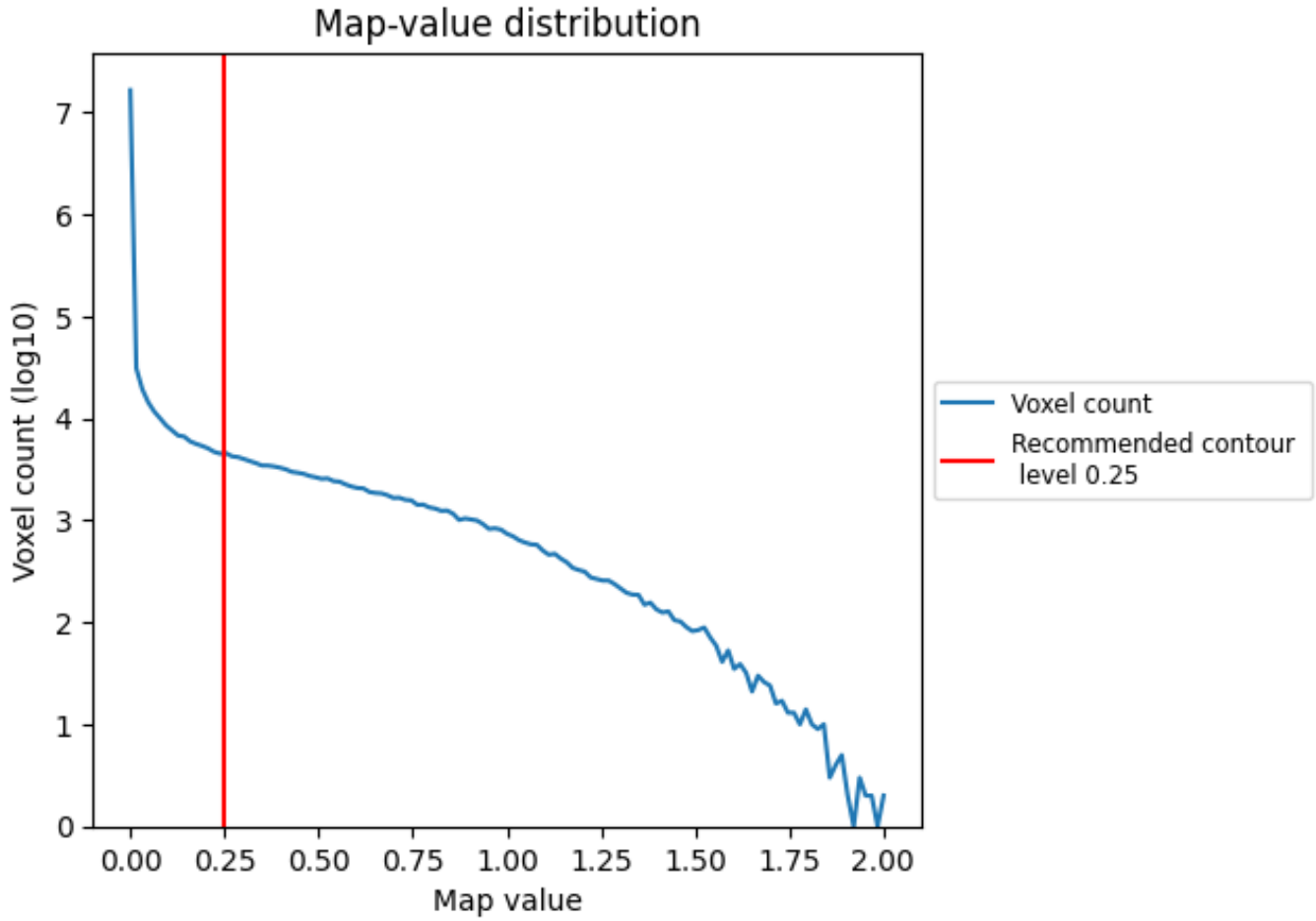
6.6 Mask visualisation (i)

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

7 Map analysis

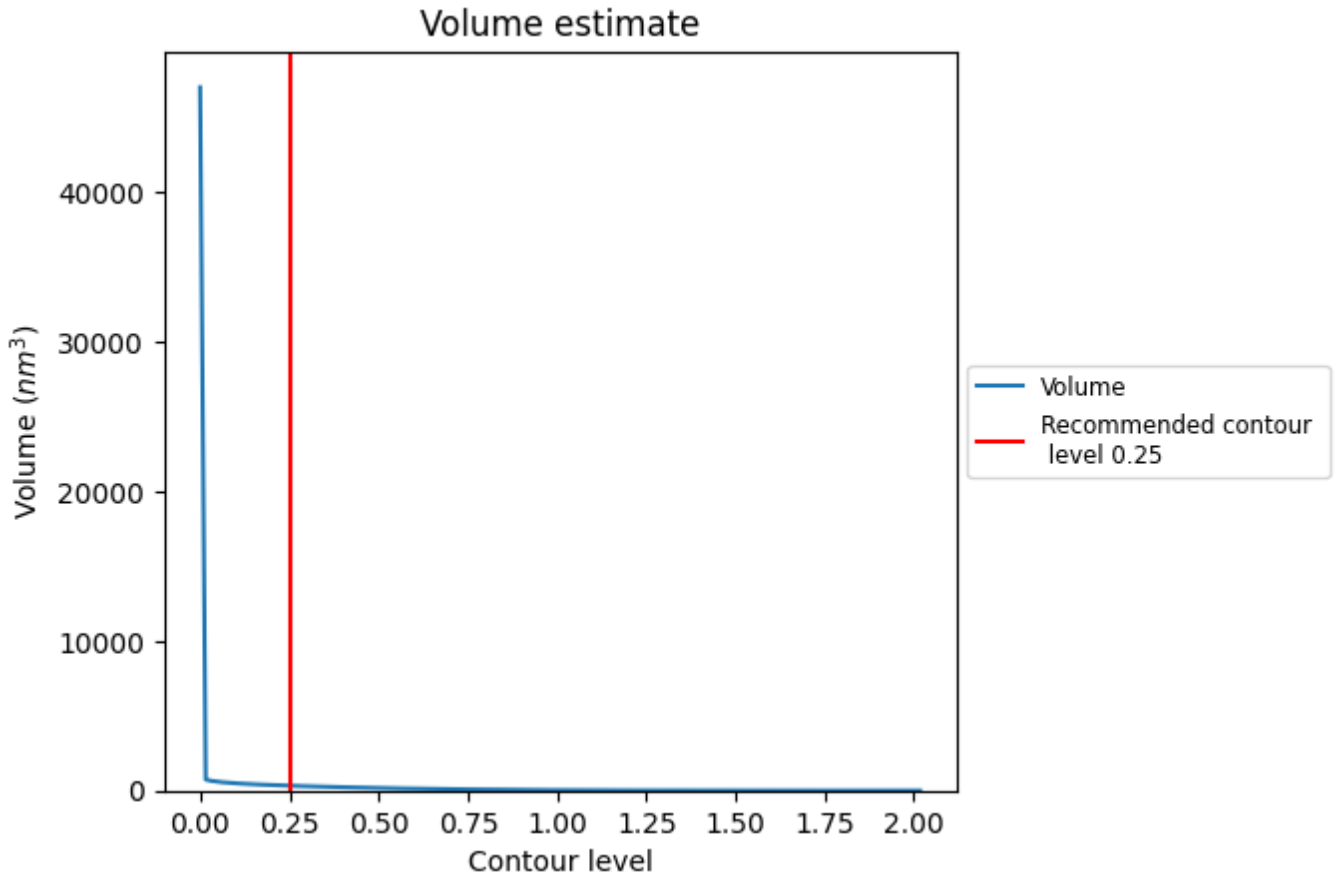
This section contains the results of statistical analysis of the map.

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.

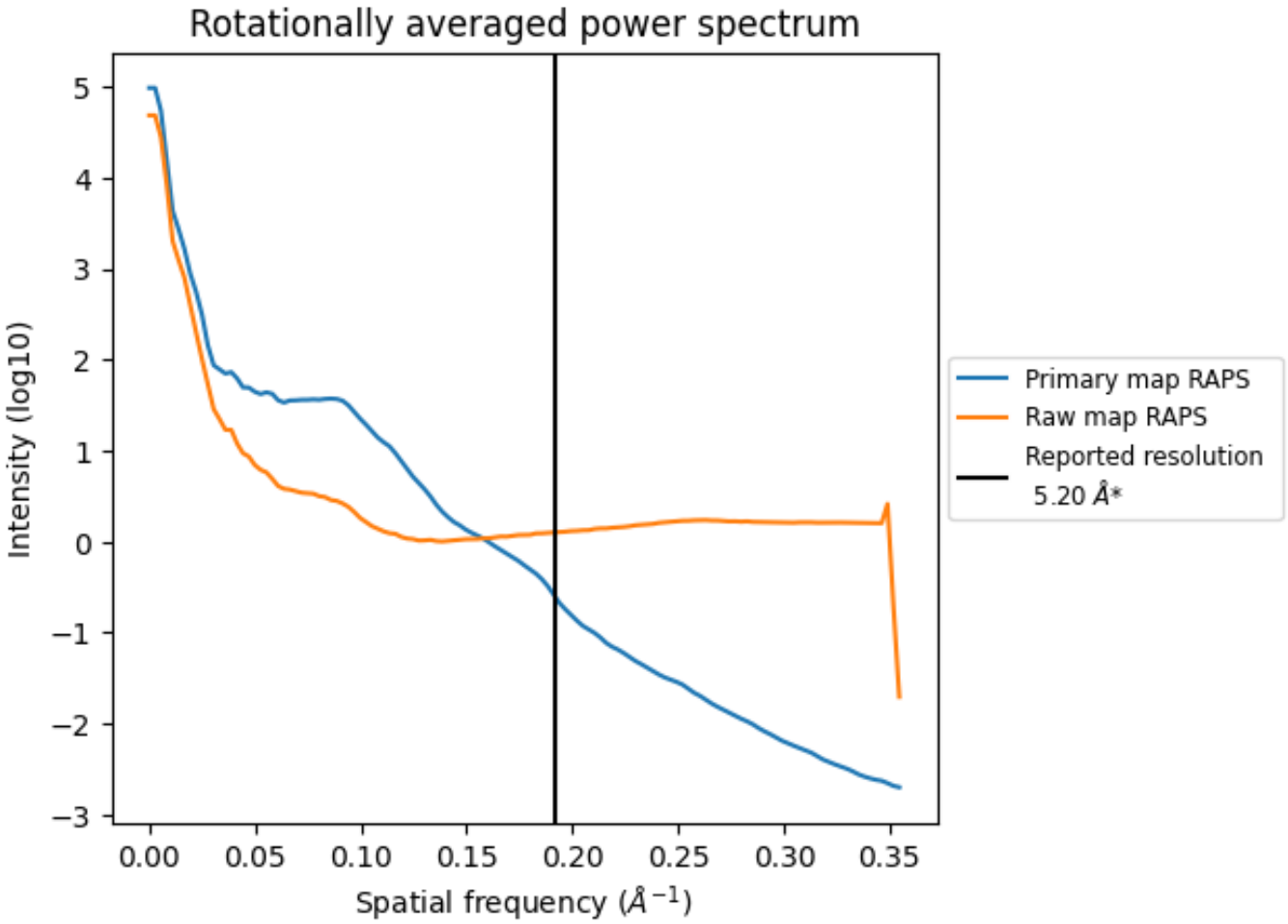
7.2 Volume estimate



The volume at the recommended contour level is 326 nm^3; this corresponds to an approximate mass of 294 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)

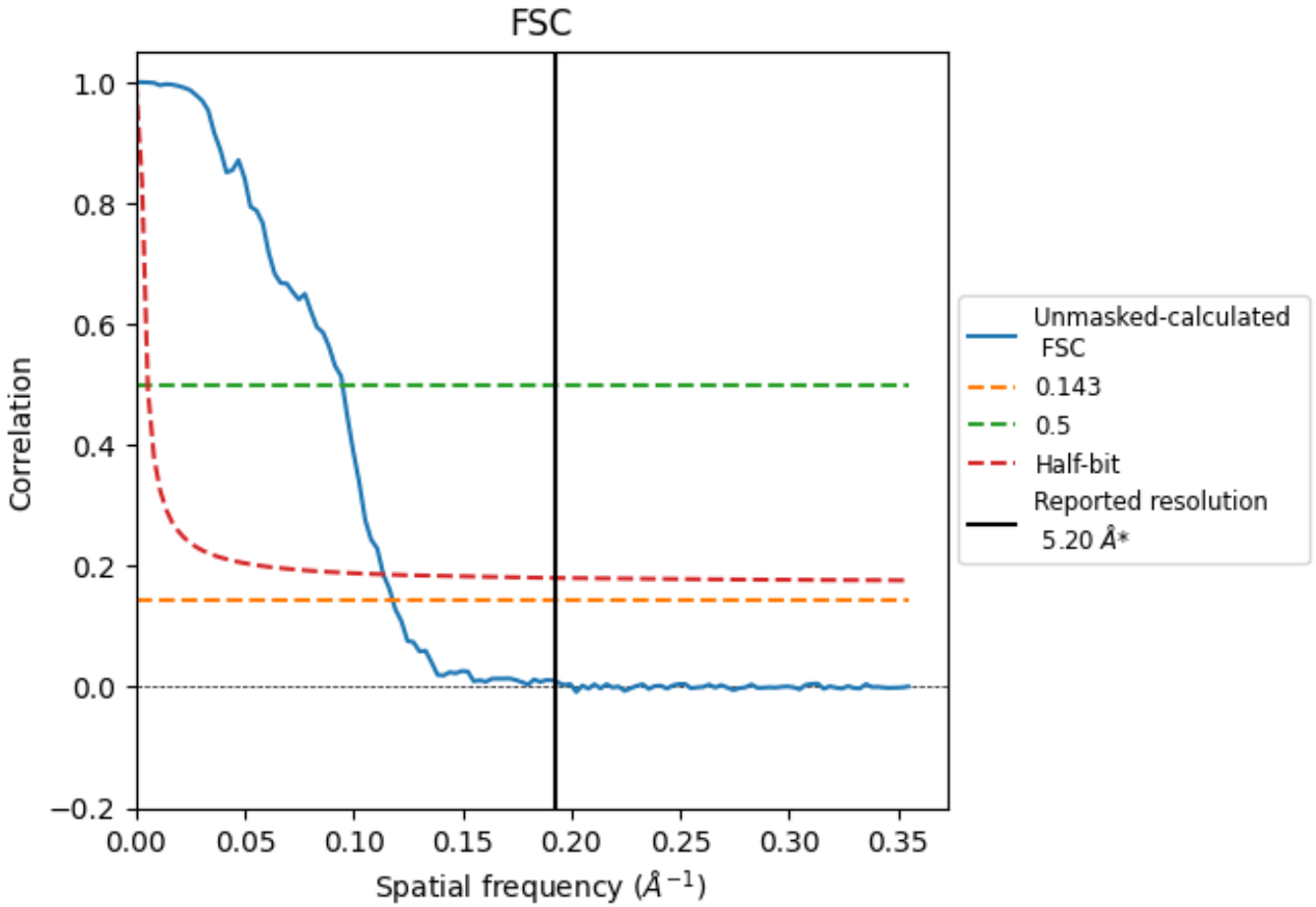


*Reported resolution corresponds to spatial frequency of 0.192 Å^{-1}

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 0.192 Å^{-1}

8.2 Resolution estimates (i)

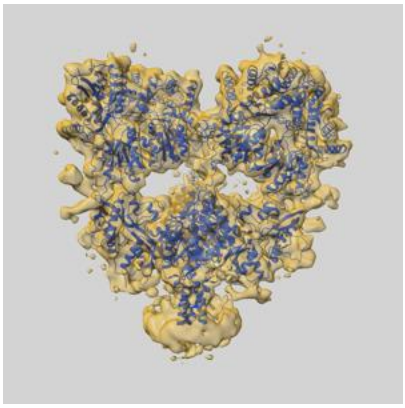
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.48	10.55	8.80

*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 8.48 differs from the reported value 5.2 by more than 10 %

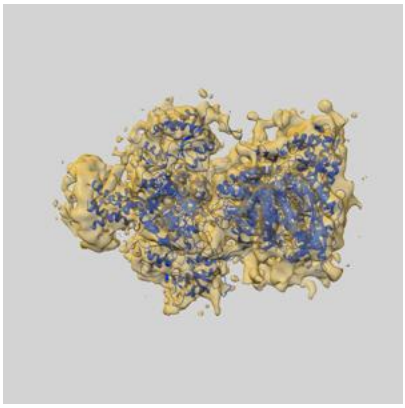
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34076 and PDB model 7YSJ. Per-residue inclusion information can be found in section 3 on page 29.

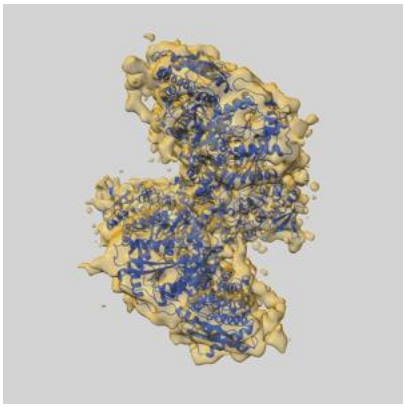
9.1 Map-model overlay



X



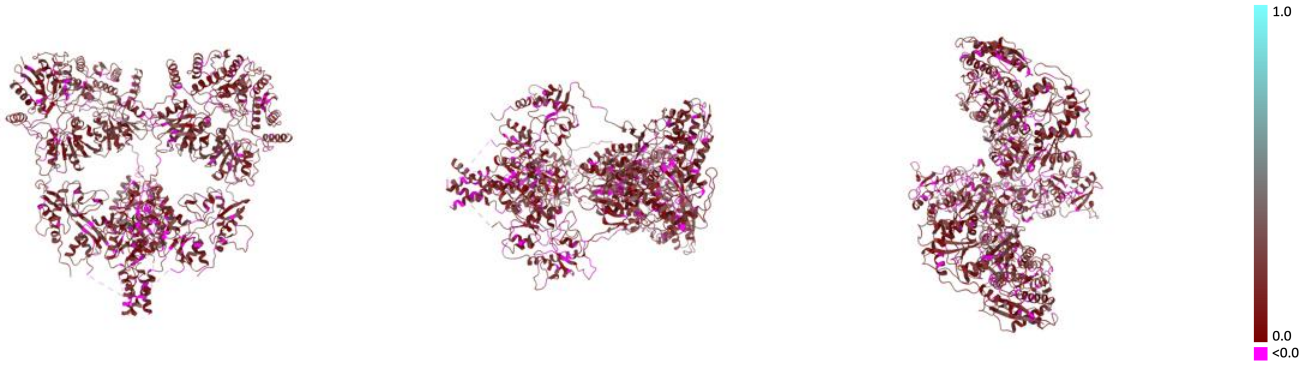
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

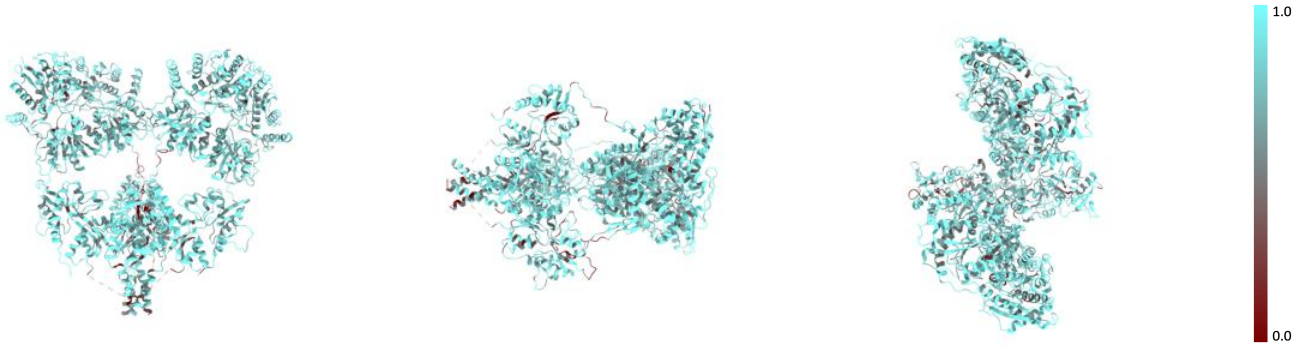
9.2 Q-score mapped to coordinate model



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.

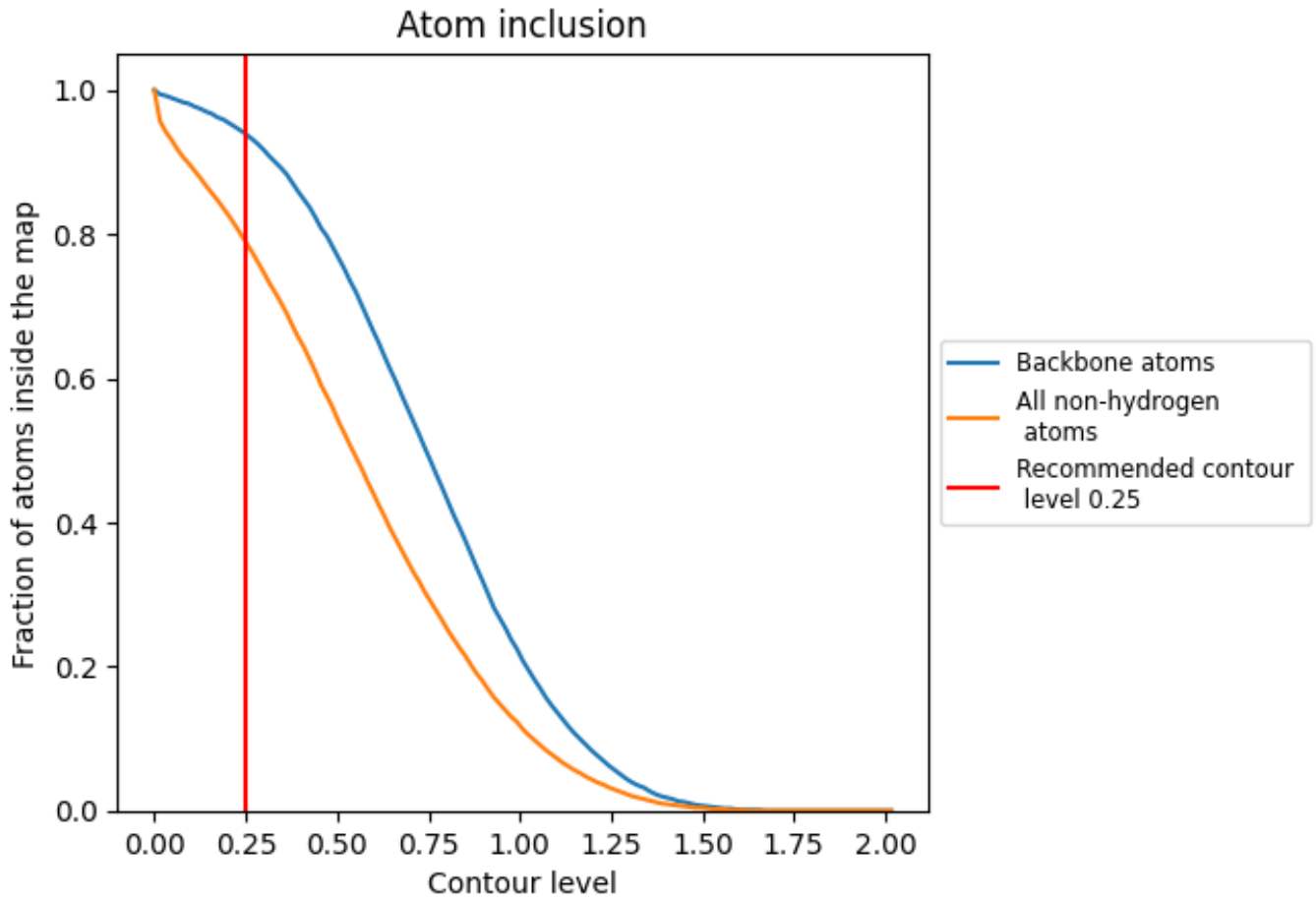
9.3 Atom inclusion mapped to coordinate model



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 79% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.1620
A	0.8070	0.1700
B	0.7640	0.1520
C	0.7900	0.1610
D	0.7960	0.1640