



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 08:38 PM UTC

PDB ID : 7U9Q / pdb_00007u9q
EMDB ID : EMD-26405
Title : Structure of PKA phosphorylated human RyR2 in the closed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 3.11 Å (reported)
Based on initial model : 7U9X

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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:

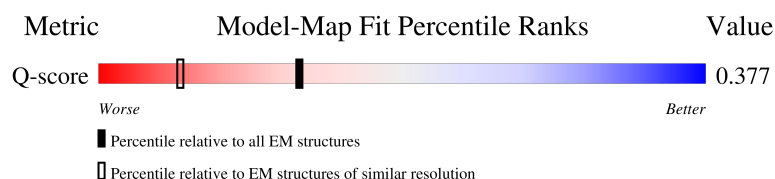
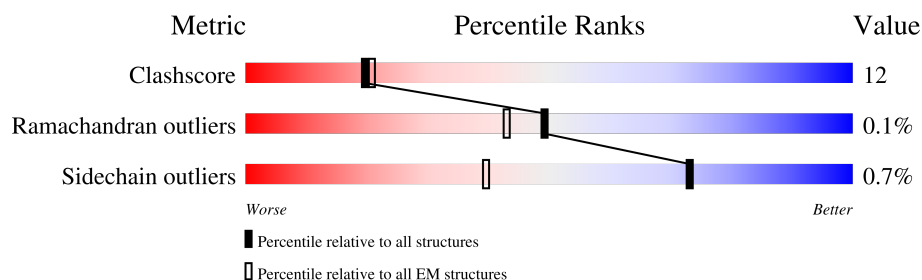
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.61 - 3.61)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	108	80% 17% ...
1	F	108	79% 19% ...
1	G	108	79% 19% ...
1	H	108	77% 20% ...

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Mol	Chain	Length	Quality of chain
2	A	4967	13% 61% 23% 15%
2	B	4967	13% 62% 23% 15%
2	C	4967	13% 62% 23% 15%
2	D	4967	13% 61% 23% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 138608 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

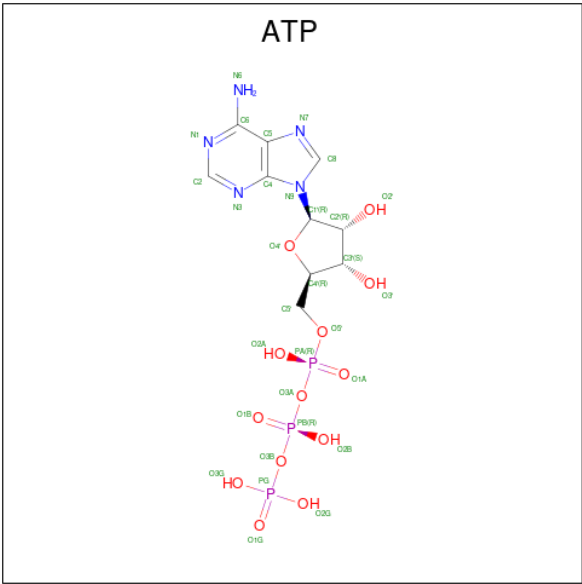
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



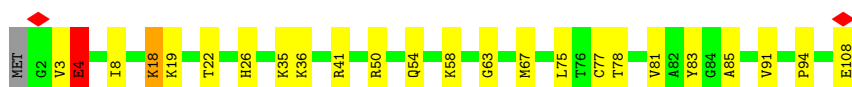
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots

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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



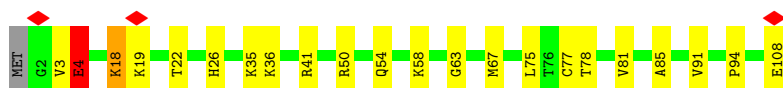
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



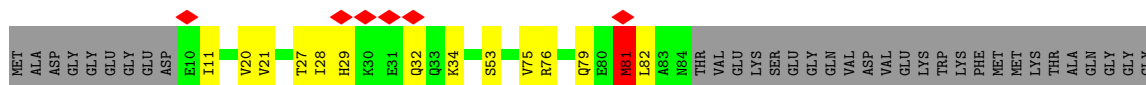
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

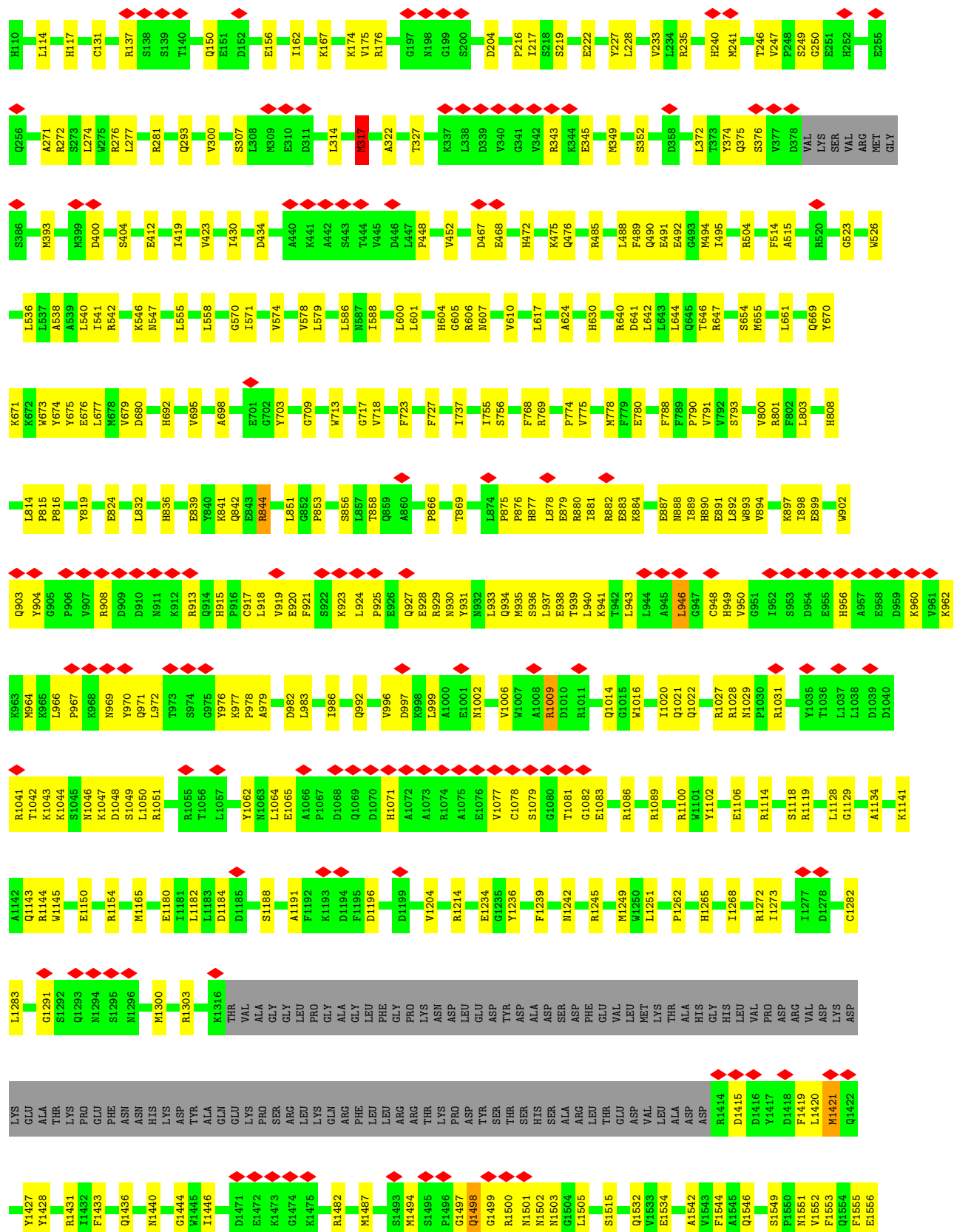
Chain G: 

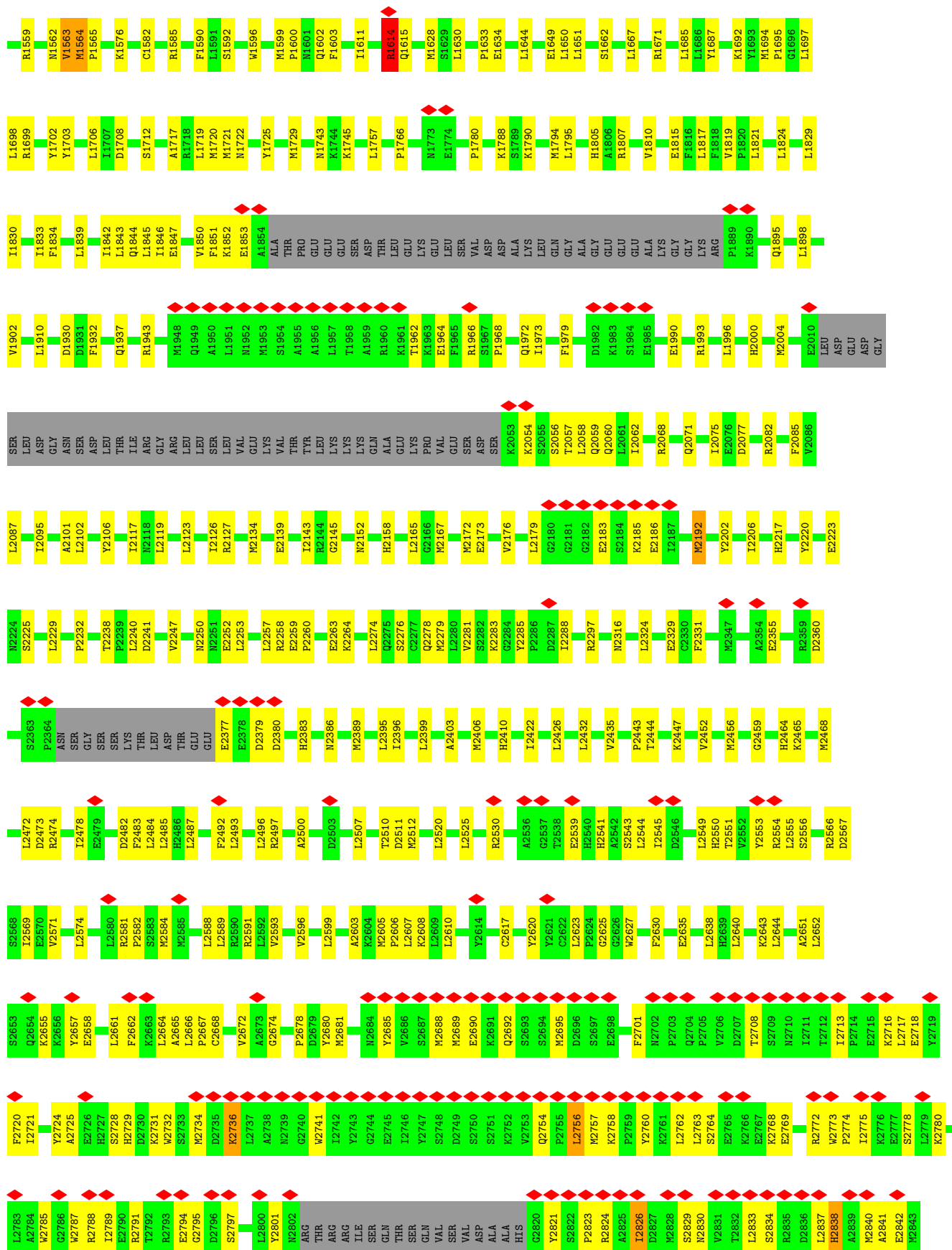


- Molecule 2: Ryanodine receptor 2

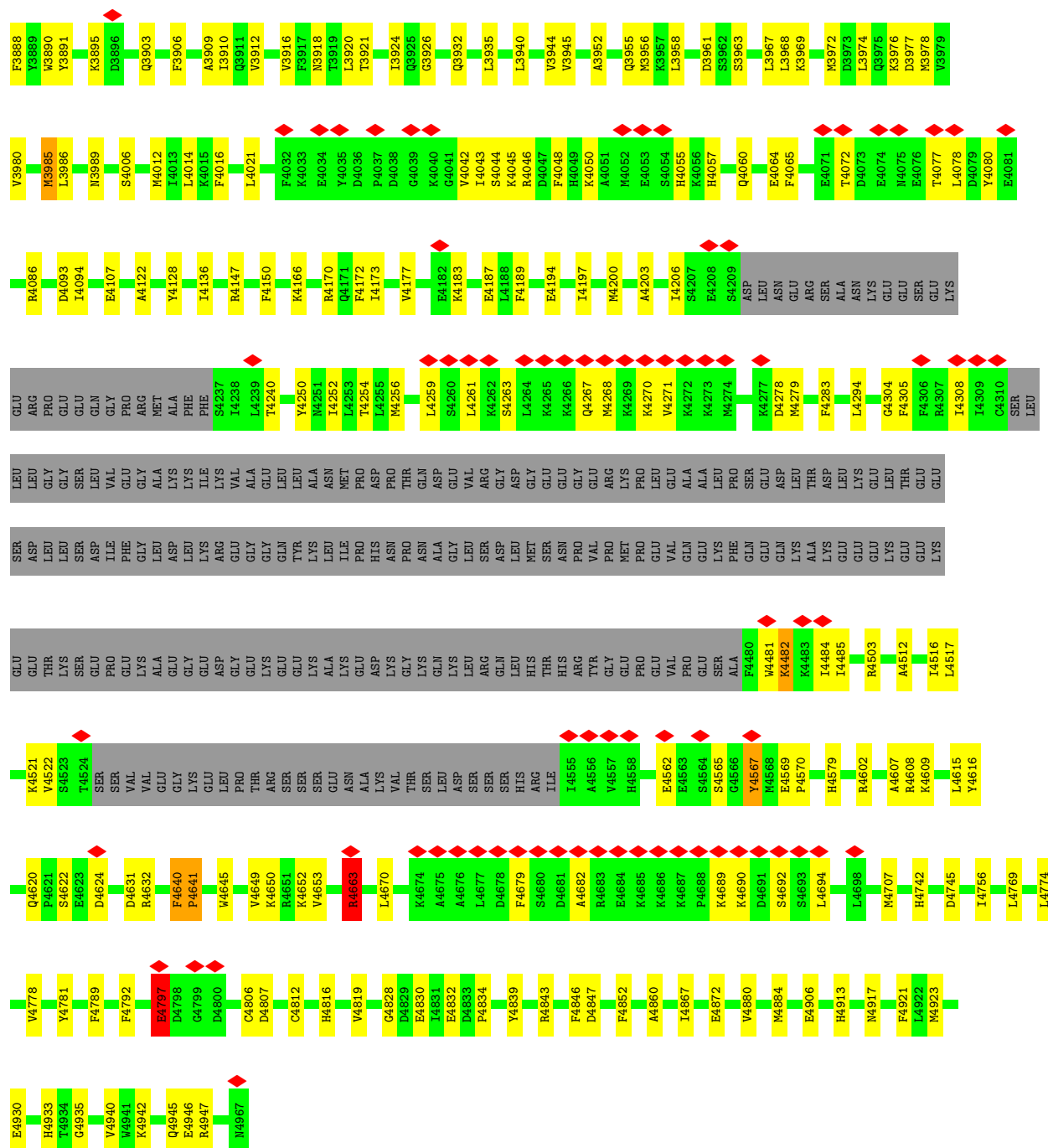
Chain A: 



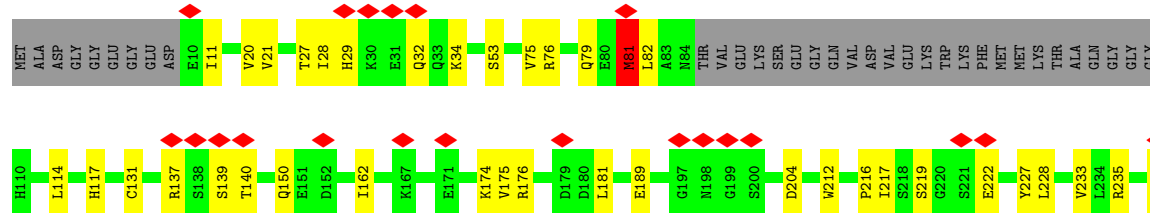




T3743	L3644	LEU	THR	LYS	ARG	L3320	N3256	S3188	E3124	M3046	P2969	R2905	H2844
T3743	A3649	GLU	GLU	ALA	ALA	M3323	N3257	S3189	D3125	K3047	L2970	G2906	A2845
M3754	E3650	GLN	ASP	ALA	TRP	E3324	P3258	R3190	V3126	T3048	F2907	F2907	E2846
T3758	P3651	SER	VAL	VAL	LEU	K3325	E3259	E3191	Q3127	G3049	K2908	K2908	H2847
T3765	P3652	ARG	ASP	ASP	LYS	L3326	R3260	R3192	V3128	D3062	F2975	D2909	Y2848
E3653	E3653	ARG	ILE	GLU	GLU	K3327	A3261	A3193	S3129	R3058	N2977	L2910	K2852
L3766	E3654	GLY	ILE	GLU	PRO	K3328	E3262	A3194	C3130	A3059	N2977	E2911	K2853
D3655	D3655	ARG	ARG	ASN	ASN	K3329	M3263	L3195	L2980	F3060	R2979	L2912	K2854
E3656	E3656	ARG	SER	LYS	PRO	A3330	C3264	S3196	L2981	L3061	L2981	D2913	K2855
L3778	L3778	HIS	SER	LYS	GLU	A3331	C3265	L3197	F2982	D3062	F2982	T2914	K2856
L3796	G3657	TYR	ILE	MET	ALA	A3332	T3266	L3198	L2983	A3065	L2983	T2914	K2857
T3658	T3658	GLU	HIS	ARG	GLU	T3332	T3266	T3199	S2915	E3066	S2987	S2916	K2858
K3659	K3659	LEU	LEU	LYS	LEU	V3333	L3268	N3200	A3139	E3069	S2987	E2916	K2859
R3660	R3660	GLY	GLN	GLY	PHE	V3334	N3269	V3201	L3140	T3071	P2989	L2917	L2860
V3661	V3661	ARG	ARG	ASP	ARG	S3335	E3202	E3202	T3142	K3072	P2989	R2920	L2860
L3664	L3664	HIS	LYS	TYR	VAL	E3336	D3203	V3204	S3143	N3074	L2990	Y2923	E2861
H3665	H3665	GLU	GLU	SER	ALA	E3337	E3271	V3204	K3144	E3072	C2991	S2923	S2862
I3668	I3668	ASP	ASP	MET	GLU	ASP	H3272	C3205	S3145	N3074	S2992	F2925	K2863
E3684	E3684	LEU	ALA	THR	VAL	M3273	M3273	I3208	I3146	L3075	G2994	L2926	G2864
D3685	D3685	LYS	ILE	SER	PHE	L3276	L3276	P3209	Y3147	T3077	E3000	Q2927	G2866
Y3688	Y3688	ALA	ARG	LEU	TRP	L3277	G3276	S3210	V3148	G3078	K3001	Q2928	N2867
H3689	H3689	VAL	TRP	ILE	TRP	L3278	N3279	L3211	E3149	Q3077	E3002	L2929	H2868
Y3691	Y3691	GLN	GLN	VAL	SER	L3279	L3280	E3212	R3150	Q3078	M3003	Y2932	P2869
M3695	M3695	ALA	ALA	ALA	LYS	L3281	L3281	K3213	R3152	Q3079	V3004	E2935	L2870
A3696	A3696	LYS	LYS	LYS	GLY	L3282	K3282	L3214	S3153	F3080	C3009	L2871	L2871
K3697	K3697	ARG	THR	ASN	ASN	L3283	I3283	K3215	A3154	T3081	K3010	H2937	P2873
H3700	H3700	LEU	LEU	LEU	PHE	L3284	I3284	E3216	L3155	THR	K3011	Q2938	D2874
D3701	D3701	GLU	GLU	GLU	GLU	Y3285	Y3285	V3219	G3156	ARG	L3011	H2939	D2875
E3702	E3702	ALA	THR	ASN	ASN	N3286	N3286	A3222	C3158	GLN	L2940	I2940	T2876
ASP	ASP	LEU	ASP	LEU	LEU	N3287	G3288	E3223	L3159	PRO	L2941	E2942	L2877
ASP	ASP	LEU	ASP	LEU	LEU	L3288	G3289	S3224	A3160	K3088	R3016	F2943	T2878
GLY	GLY	GLU	THR	GLY	VAL	L3290	D3291	G3225	A3161	G3089	R3017	D2944	A2879
GLU	GLU	GLN	THR	ASN	GLN	G3291	G3292	T3226	F3162	V3090	R3018	G2945	K2880
GLU	GLU	ASN	ASP	PRO	ASN	G3292	G3293	R3227	A3163	T3091	I3019	G2946	E2881
GLU	GLU	GLY	GLY	GLY	GLY	A3294	G3294	Y3228	G3164	Q3092	I3019	G2946	K2882
GLU	GLU	LEU	GLY	ASP	ILE	M3295	M3295	T3229	A3165	T3093	I3019	G2946	E2887
GLU	GLU	ALA	GLY	ASP	ILE	K3296	K3296	Q3230	F3166	Y3096	I3019	G2946	K2888
GLU	GLU	ARG	ASN	ASP	ALA	K3297	K3297	P3232	M3024	D3025	I3019	G2946	A2889
GLU	GLU	MET	THR	ASP	ASP	F3302	F3302	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	SER	THR	ASP	THR	S3303	S3303	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	PHE	THR	ASP	THR	Q3304	Q3304	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	P3305	P3305	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	L3306	L3306	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	TYR	THR	ASP	THR	I3307	I3307	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	L3308	L3308	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LYS	THR	ASP	THR	K3309	K3309	A3100	D3025	D3025	I3019	G2946	D2890
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GLU	GLU	LYS	THR	ASP	THR	Q3313	Q3313	A3100	D3025	D3025	I3019	G2946	D2890
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GLU	GLU	ASN	THR	ASP	THR	K3315	K3315	A3100	D3025	D3025	I3019	G2946	D2890
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GLU	GLU	ILE	THR	ASP	THR	T3317	T3317	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	SER	THR	ASP	THR	H3318	H3318	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASP	THR	ASP	THR	F3319	F3319	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ALA	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
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GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
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GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
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GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	LEU	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ILE	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	ASN	THR	ASP	THR	E3633	E3633	A3100	D3025	D3025	I3019	G2946	D2890
GLU	GLU	VAL	THR	ASP	THR	E3633	E3633	A3100	D				



• Molecule 2: Ryanodine receptor 2

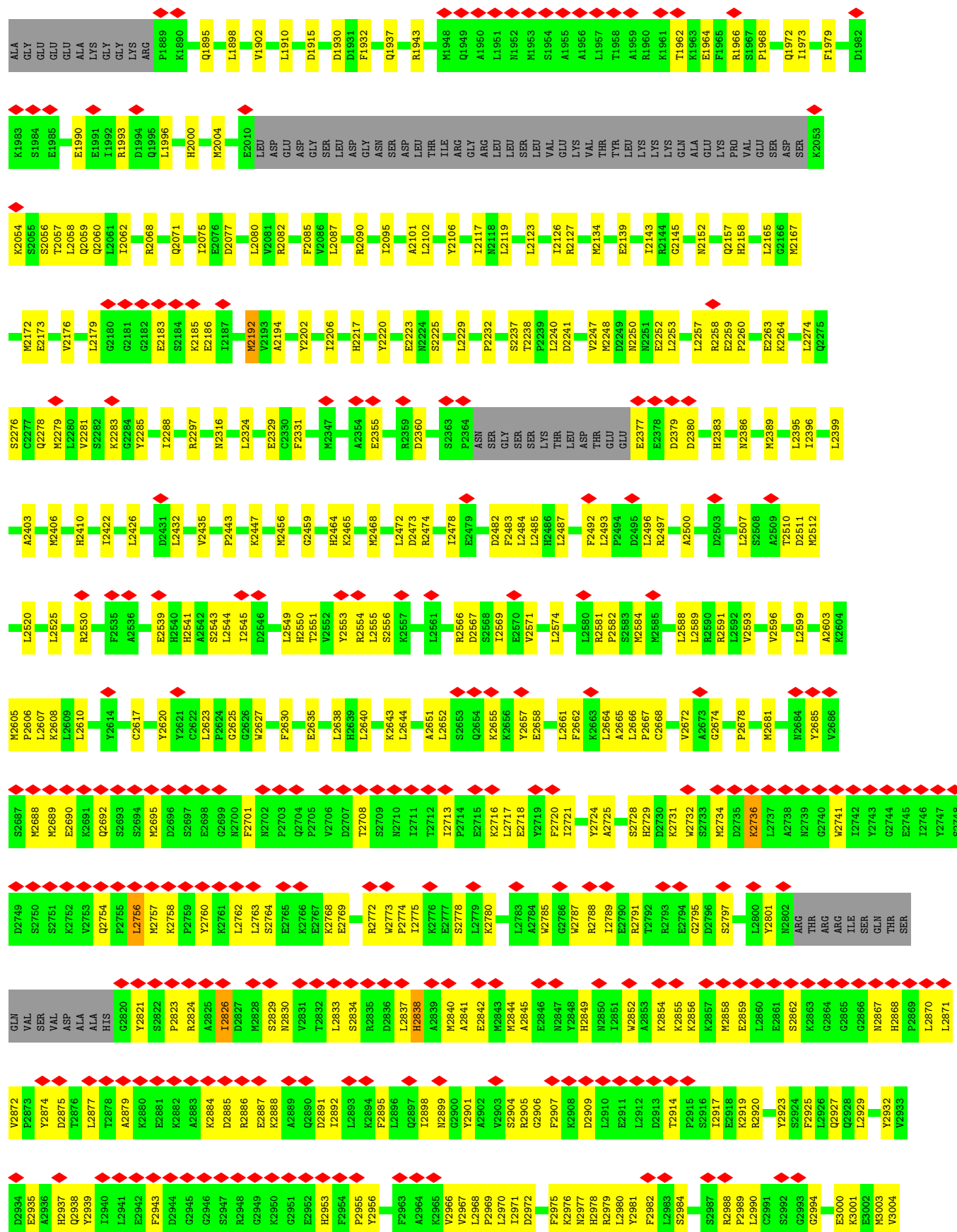




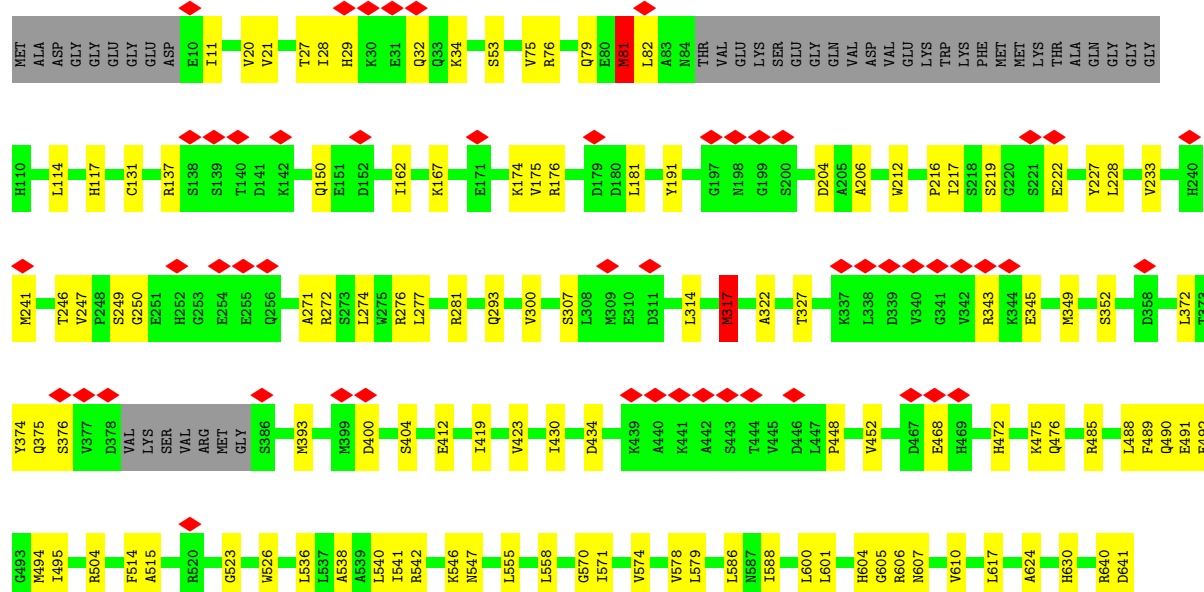












E1990	E1991	I1992	R1993	D1994	Q1995	L1996	H2000	M2004	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	ASN	SER	ASP	LEU	THR	THR	ILE	ARG	GLY	ARG	LEU	LEU	VAL	GLU	LYS	VAL	THR	TYR	LEU	LYS	LYS	GLN	ALA	GLU	LYS	PRO	VAL	SER	ASP	SER	K2053	K2054	S2055	T2057																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	L2312	L2313	L2314	L2315	L2316	L2317	L2318	L2319	L2320	L2321	L2322	L2323	L2324

L2058 Q2059 Q2060 L2061 L2062 R2068 Q2071 L2075 E2076 D2077 L2080 V2081 R2082 F2085 L2087 R2090 L2095 A2101 L2102 Y2106 L2117 E2118 L2119 L2123 L2126 R2127 M2134 V2247 M2248 E2139 L2143 E2252 G2145 N2152 Q2157 H2158 L2165 G2166 M2167 M2172 E2173 M2279	V2176 L2179 G2180 G2181 G2182 S2183 S2184 K2185 E2186 M2192 V2193 A2194 Y2202 L2206 H2217 Y2220 L2221 E2223 H2224 S2225 L2229 P2232 S2237 T2238 L2240 D2241 ASN SER GLY SER SER N2250 L2251 THR LEU ASP THR GLU E2377 E2378 D2379 D2380 H2383 M2386 M2389 L2395	L2396 V2281 S2282 K2283 G2284 Y2285 P2286 L2287 L2288 R2297 M2316 R2322 L2323 L2324 E2329 C2330 F2331 R2336 G2337 E2338 M2347 A2354 E2355 R2359 D2360 S2363 P2364 SER GLY SER SER LYS THR LEU ASP THR GLU E2377 E2378 D2379 D2380 H2383 M2386 M2389 L2395	L2507 S2508 T2510 D2511 M2512 L2520 L2525 R2530 A2535 E2539 H2540 H2541 S2543 L2544 L2545 D2546 L2549 H2550 T2551 V2552 R2566 D2567 S2568 I2569 E2570 V2571 L2574 R2581 P2582 S2583 M2584 M2585 L2588 L2589 R2590 R2591 L2592 V2593 V2596 L2599 A2603	L2604 M2605 P2606 L2607 K2608 L2609 L2610 V2614 C2617 Y2620 Y2621 C2622 L2623 P2624 G2625 G2626 V2627 F2630 E2635 L2638 H2639 L2640 A2651 L2652 S2653 Q2654 L2655 V2656 Y2657 E2658 L2661 L2662 K2663 L2664 A2665 A2666 L2666 C2667 C2668 V2672 G2673 G2674 A2675 P2678 M2681 M2684	Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 L2711 T2712 L2713 P2714 K2715 K2716 L2717 E2718 Y2719 F2720 L2721 Y2724 A2725 S2728 H2729 D2730 K2731 V2732 S2733 M2734 D2735 L2736 A2738 N2739 G2740 V2741 L2742 Y2743 E2744 E2745 L2746	Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 R2772 V2773 P2774 L2775 K2776 E2777 L2779 K2780 L2783 A2784 V2785 G2786 V2787 R2788 L2789 E2790 R2791 L2792 E2794 G2795 D2796 S2797 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN	THR SER GLN VAL SER VAL ASP ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 Y2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 R2844 A2845 E2846 N2847 Y2848 H2849 V2852 A2853 K2854 L2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870	L2871 V2872 P2873 Y2874 D2875 T2876 L2877 L2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 F2895 L2896 Q2897 N2898 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 R2919 K2920 Y2923 S2924 F2925 L2926 Q2927 L2929 Y2932	E2935 A2936 H2937 Q2938 L2939 L2940 L2941 E2942 F2943 D2944 E2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 Y2956 E2957 K2961 A2964 K2965 V2966 V2967 L2968 P2969 L2970 L2971 A2972 F2975 K2976 N2977 H2978 R2979 L2980 Y2981 F2982 S2984 S2987 R2988 P2989 L2990 C2991 S2992 G2993 G2994 E3000 K3001 E3002	M3003 V3004 C3009 K3010 L3011 G3012 V3013 L3014 V3015 R3016 H3017 R3018 R3019 M3024 D3025 A3026 S3028 I3029 V3030 L3033 L3036 L3040 D3041 A3042 R3043 M3046 G3049 A3059 F3060 L3061 D3062 E3066 D3067 L3068 E3069 L3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 Q3078 Q3079 F3080 T3081 HIS THR ARG	ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 L3093 Y3096 T3097 A3100 L3101 L3102 F3103 K3104 F3109 Q3114 H3115 Q3116 F3117 G3118 E3119 D3120 L3121 L3122 L3123 E3124 D3125 V3126 Q3127 V3128 S3129 C3130 V3131 R3132 S3136 L3137 Y3138 A3139 L3140 G3141 T3142 S3143 K3144 S3145 L3146 V3147 V3148 E3149 R3150 Q3151 R3152 S3153 A3154
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.590	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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	E	0.18	0/834	0.53	2/1123 (0.2%)
1	F	0.18	0/834	0.53	2/1123 (0.2%)
1	G	0.17	0/834	0.54	2/1123 (0.2%)
1	H	0.18	0/834	0.53	2/1123 (0.2%)
2	A	0.17	0/34511	0.52	13/46614 (0.0%)
2	B	0.17	0/34511	0.52	12/46614 (0.0%)
2	C	0.17	0/34511	0.52	10/46614 (0.0%)
2	D	0.17	0/34511	0.52	12/46614 (0.0%)
All	All	0.17	0/141380	0.52	55/190948 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1563	VAL	CA-C-N	11.83	136.52	120.67
2	C	1563	VAL	C-N-CA	11.83	136.52	120.67
2	B	1563	VAL	CA-C-N	11.81	136.50	120.67
2	B	1563	VAL	C-N-CA	11.81	136.50	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1563	VAL	CA-C-N	11.80	136.48	120.67

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1009	ARG	Sidechain
2	A	4640	PHE	Peptide
2	B	1009	ARG	Sidechain
2	D	1009	ARG	Sidechain
2	D	4640	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	818	0	821	15	0
1	F	818	0	821	16	0
1	G	818	0	821	15	0
1	H	818	0	821	17	0
2	A	33771	0	33455	873	0
2	B	33771	0	33455	862	0
2	C	33771	0	33455	865	0
2	D	33771	0	33455	871	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
All	All	138608	0	137200	3440	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 12.

The worst 5 of 3440 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)
2:A:2732:TRP:CD1	2:A:2736:LYS:HZ1	1.89	0.91
2:C:4663:ARG:HG2	2:C:4663:ARG:HH11	1.37	0.90
2:B:2732:TRP:CD1	2:B:2736:LYS:HZ1	1.90	0.89
2:D:4797:GLU:N	2:D:4797:GLU:OE1	2.07	0.88
2:C:2732:TRP:CD1	2:C:2736:LYS:HZ1	1.90	0.88

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	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	48	77
2	B	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	48	77
2	C	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	48	77
2	D	4198/4967 (84%)	4050 (96%)	144 (3%)	4 (0%)	48	77
All	All	17212/20300 (85%)	16618 (96%)	578 (3%)	16 (0%)	49	77

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2988	ARG
2	A	3292	GLU
2	A	4641	PRO
2	D	2988	ARG

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Mol	Chain	Res	Type
2	D	3292	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/89 (99%)	85 (97%)	3 (3%)	32	60
1	F	88/89 (99%)	85 (97%)	3 (3%)	32	60
1	G	88/89 (99%)	85 (97%)	3 (3%)	32	60
1	H	88/89 (99%)	85 (97%)	3 (3%)	32	60
2	A	3708/4358 (85%)	3685 (99%)	23 (1%)	78	81
2	B	3708/4358 (85%)	3685 (99%)	23 (1%)	78	81
2	C	3708/4358 (85%)	3685 (99%)	23 (1%)	78	81
2	D	3708/4358 (85%)	3685 (99%)	23 (1%)	78	81
All	All	15184/17788 (85%)	15080 (99%)	104 (1%)	73	80

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	4797	GLU
2	B	2838[A]	HIS
2	C	4256	MET
2	B	317	MET
2	B	1614	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2464	HIS
2	C	2830	ASN
2	C	4579	HIS
2	D	2410	HIS

Continued on next page...

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Mol	Chain	Res	Type
2	D	1844	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	A	5003	-	32,33,33	0.26	0	48,52,52	0.29	0
4	ATP	C	5003	-	32,33,33	0.25	0	48,52,52	0.29	0
4	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.34	0
4	ATP	B	5003	-	32,33,33	0.25	0	48,52,52	0.29	0
4	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.34	0
4	ATP	D	5003	-	32,33,33	0.25	0	48,52,52	0.29	0
4	ATP	C	5002	-	32,33,33	0.27	0	48,52,52	0.34	0
4	ATP	B	5002	-	32,33,33	0.27	0	48,52,52	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	5003	-	-	11/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	11/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	11/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	11/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	C5'-O5'-PA-O1A

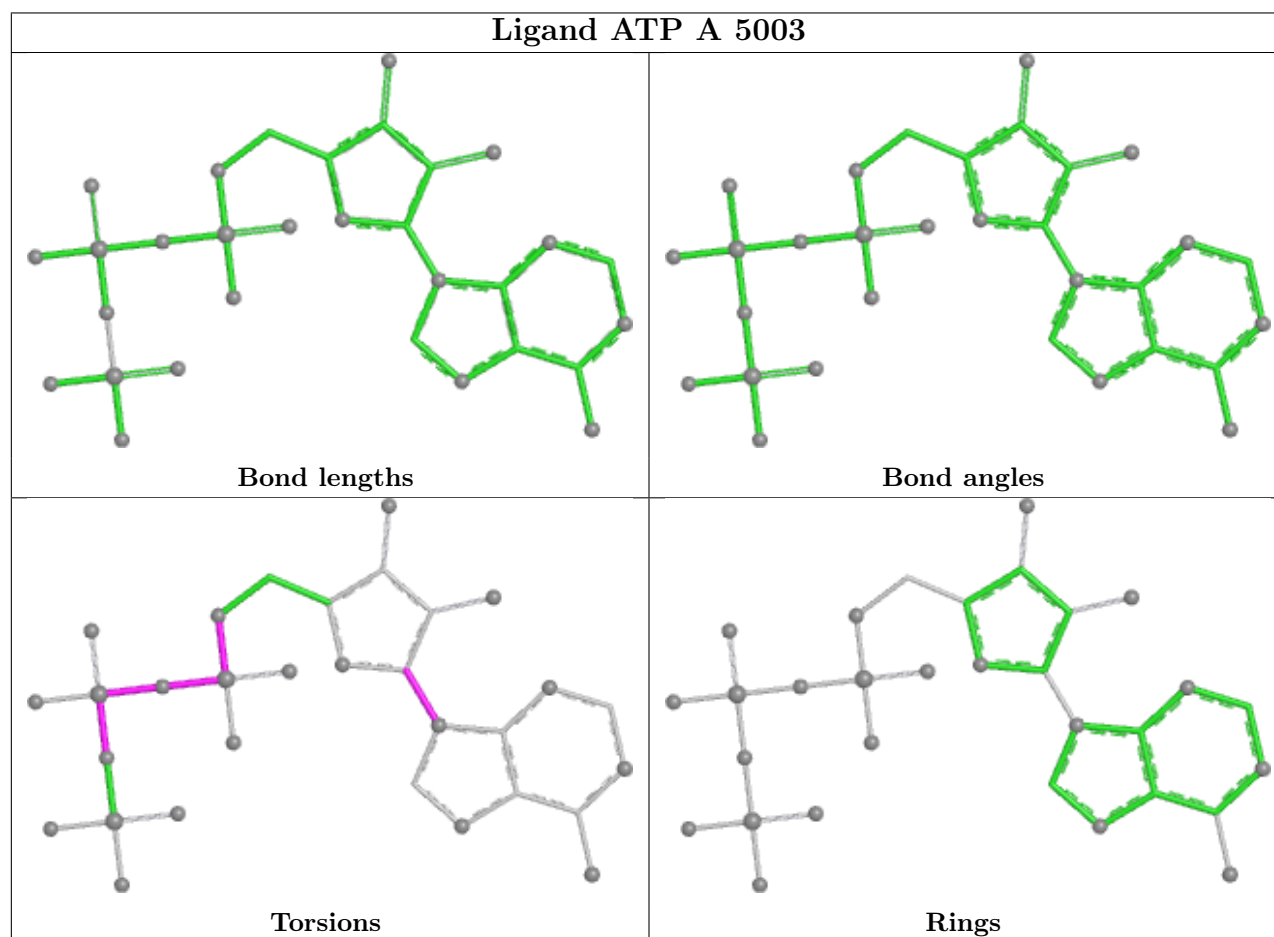
There are no ring outliers.

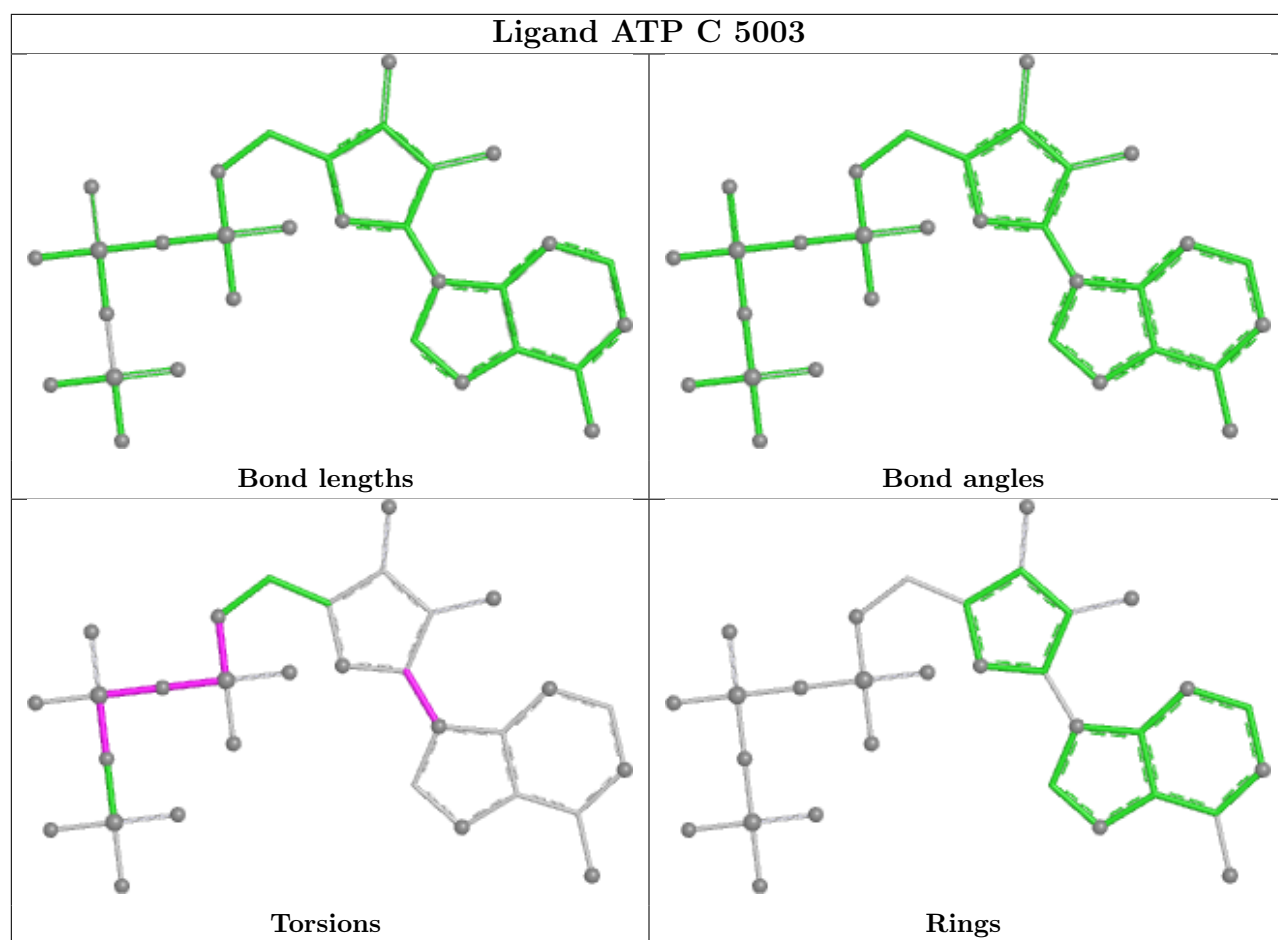
8 monomers are involved in 8 short contacts:

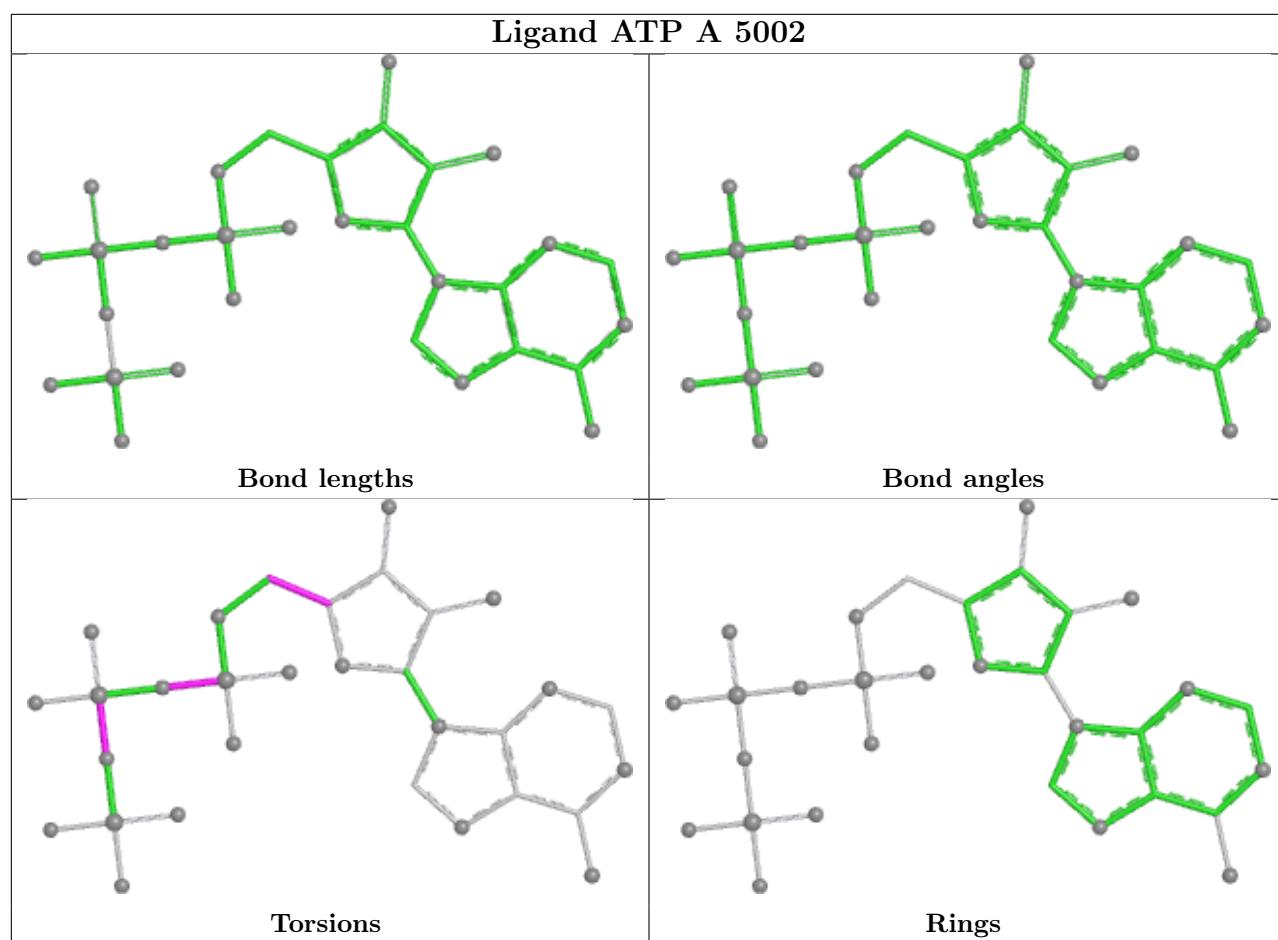
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5003	ATP	1	0
4	C	5003	ATP	1	0
4	A	5002	ATP	1	0
4	B	5003	ATP	1	0
4	D	5002	ATP	1	0
4	D	5003	ATP	1	0
4	C	5002	ATP	1	0
4	B	5002	ATP	1	0

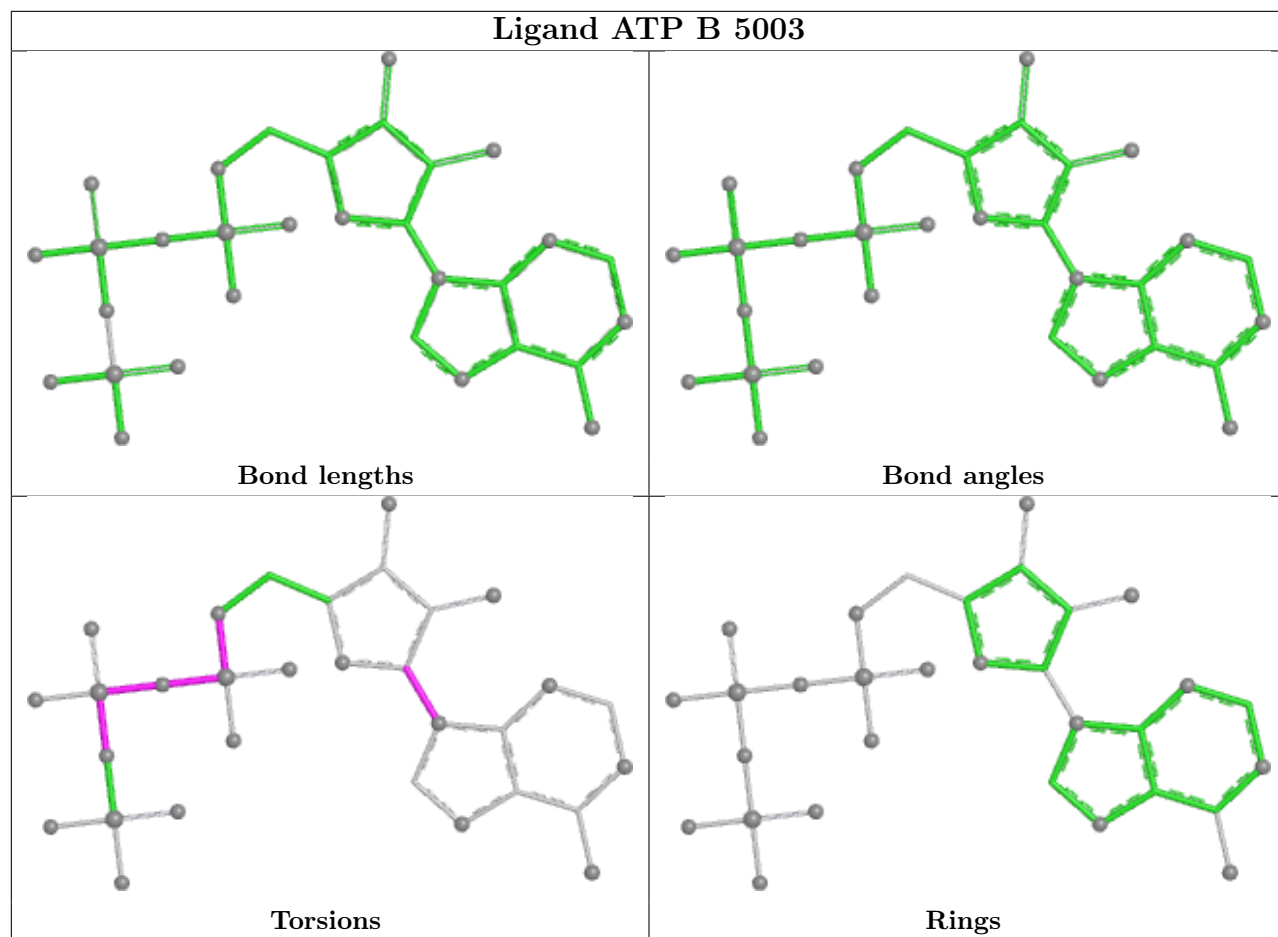
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

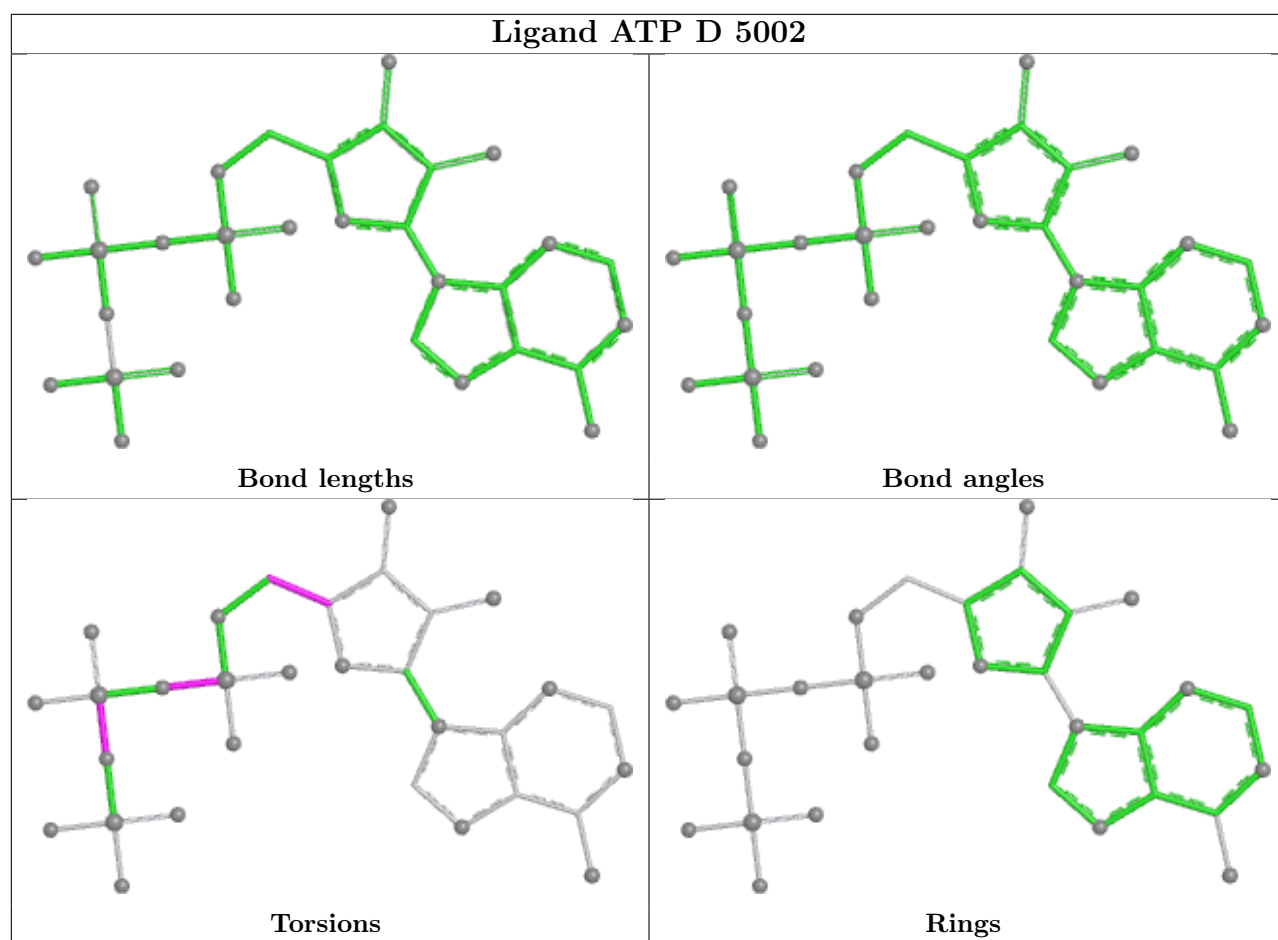
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

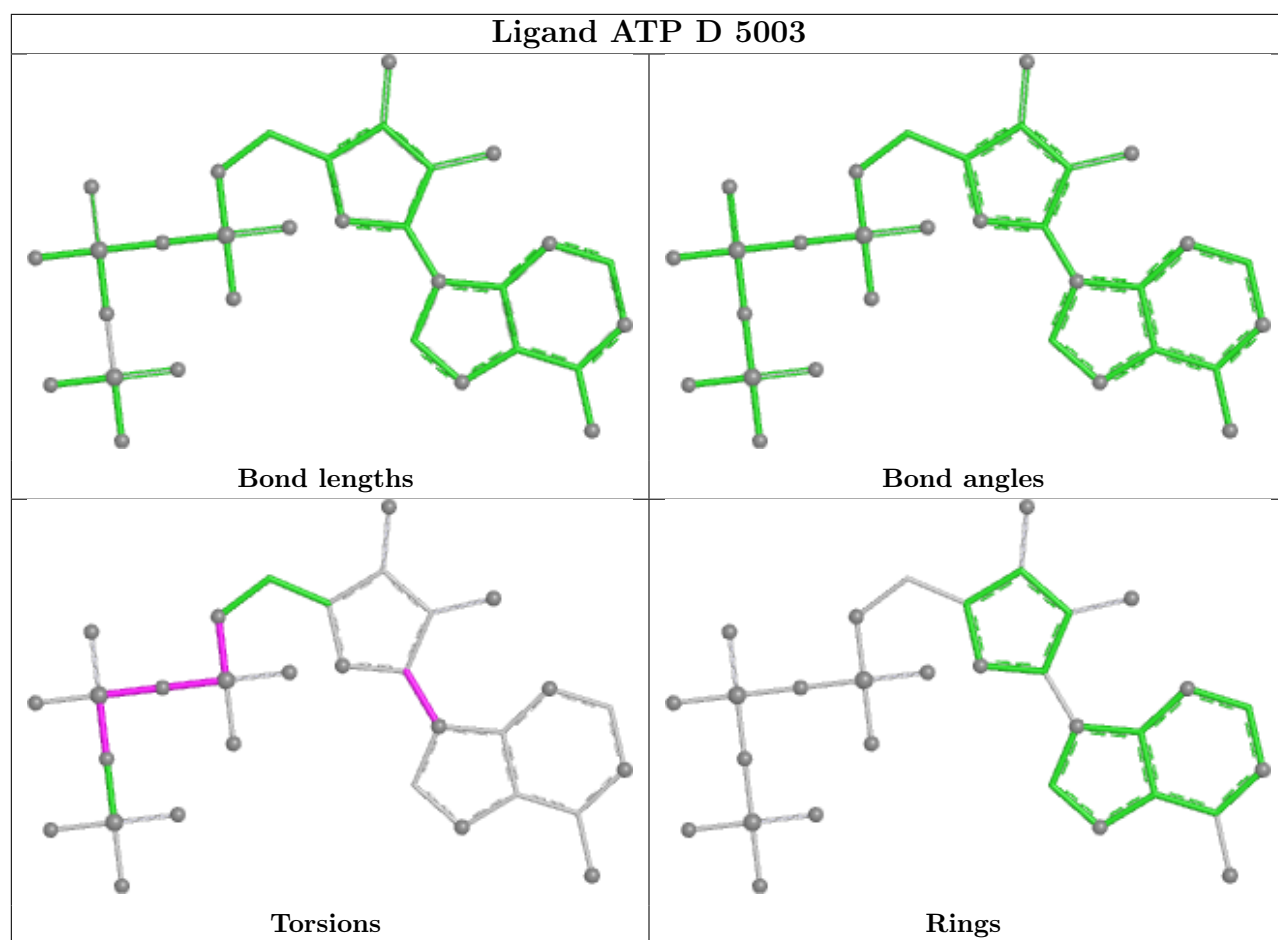


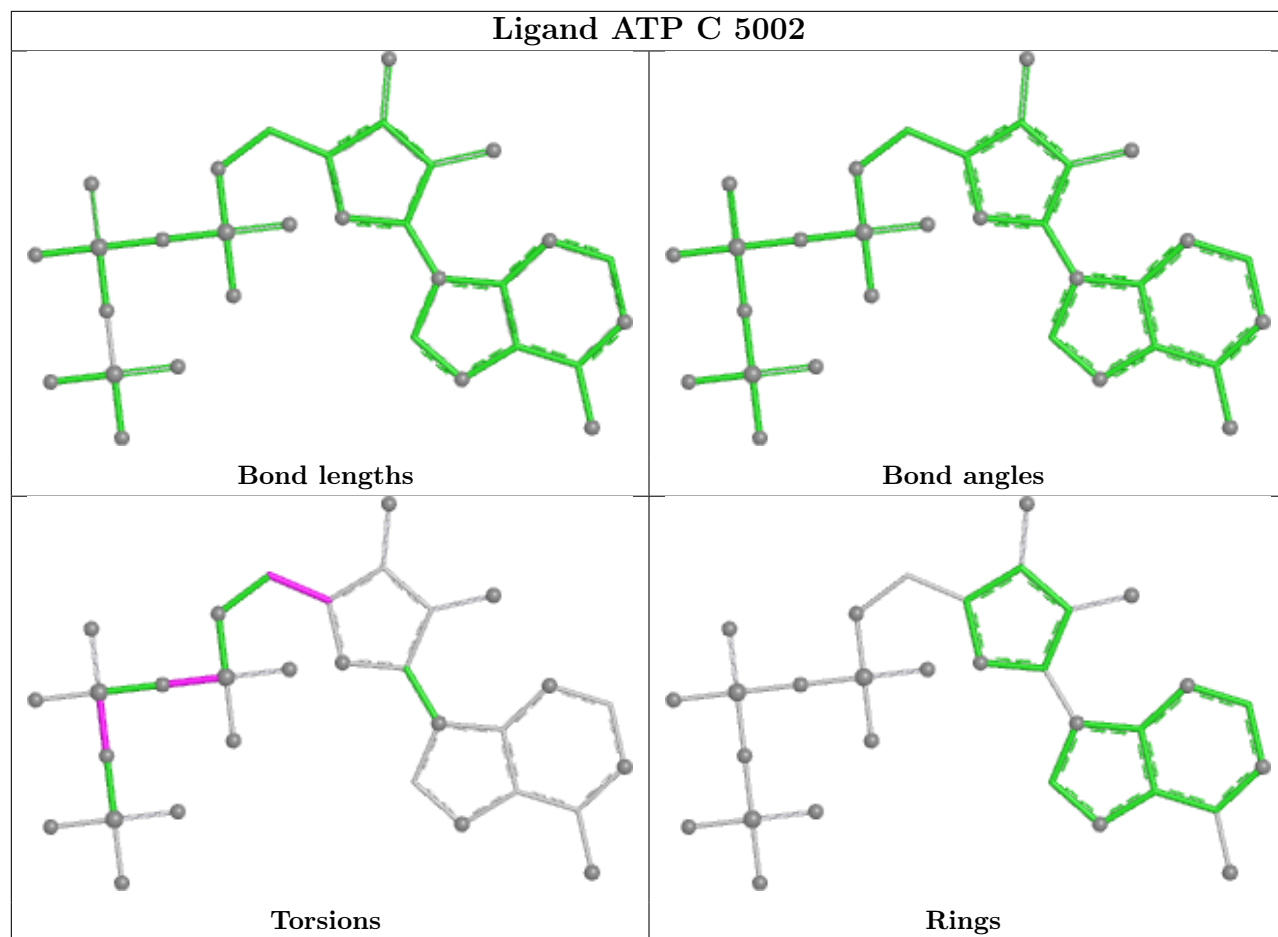


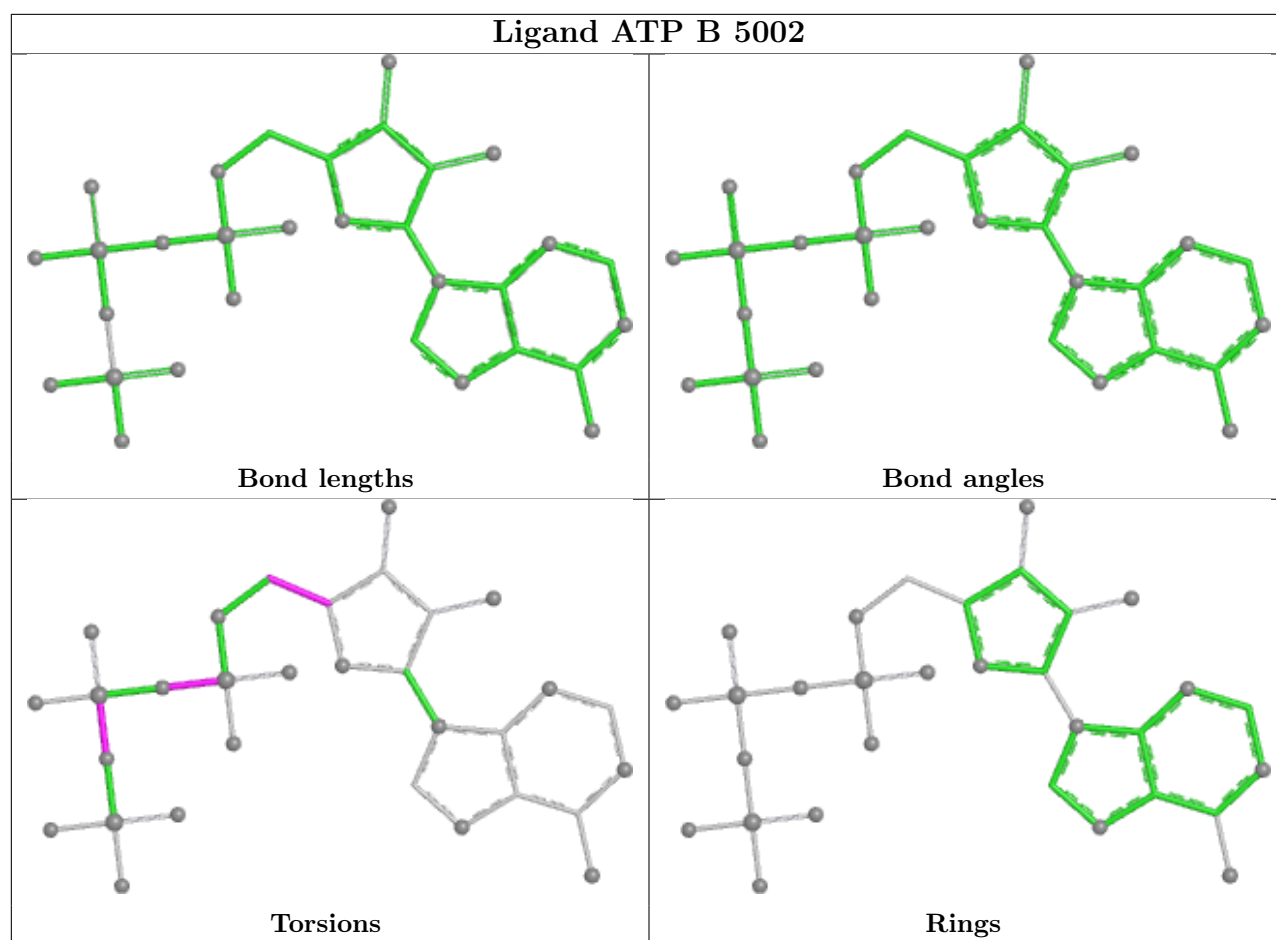












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

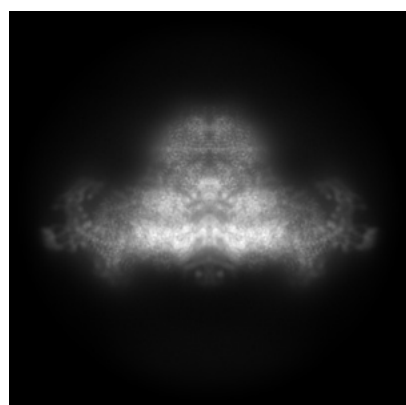
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26405. These allow visual inspection of the internal detail of the map and identification of artifacts.

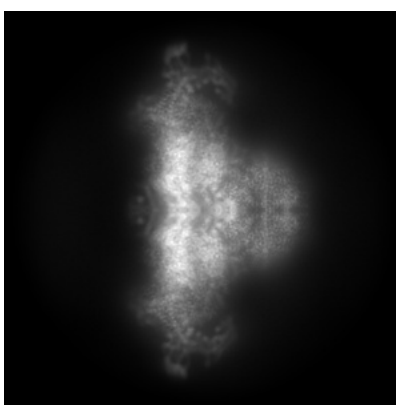
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

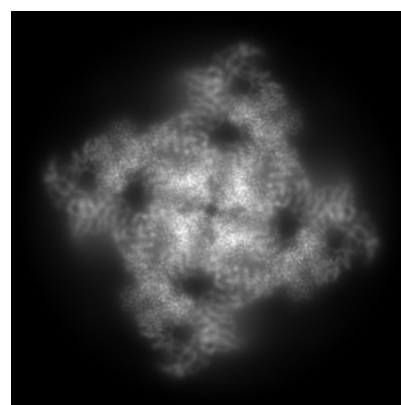
6.1.1 Primary map



X



Y

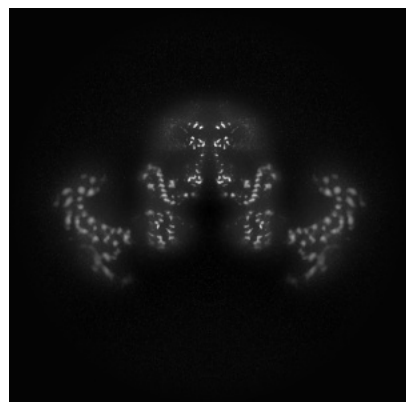


Z

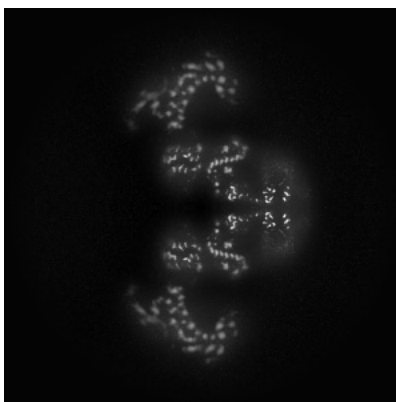
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

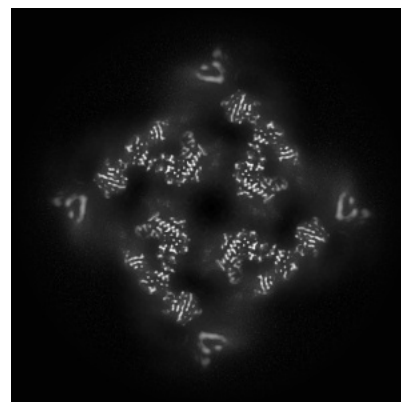
6.2.1 Primary map



X Index: 256



Y Index: 256

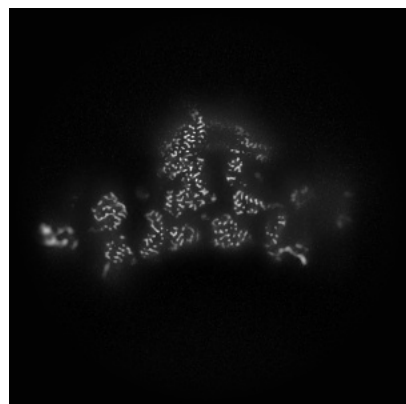


Z Index: 256

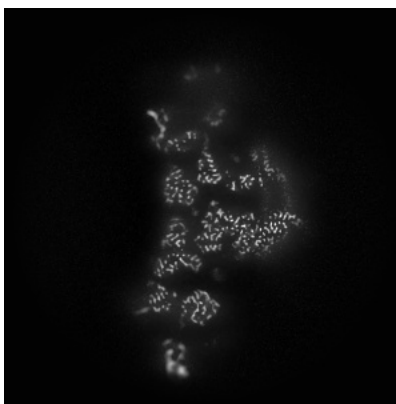
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

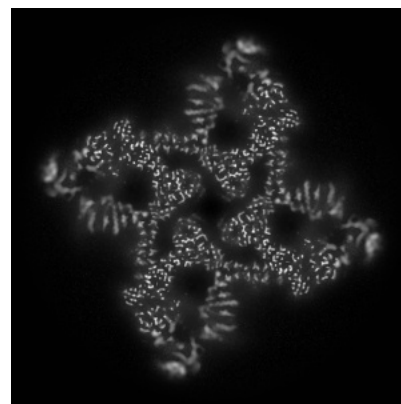
6.3.1 Primary map



X Index: 219



Y Index: 293

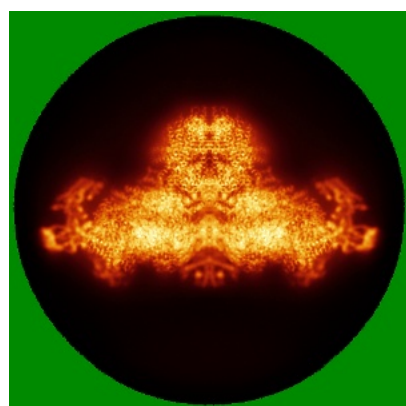


Z Index: 224

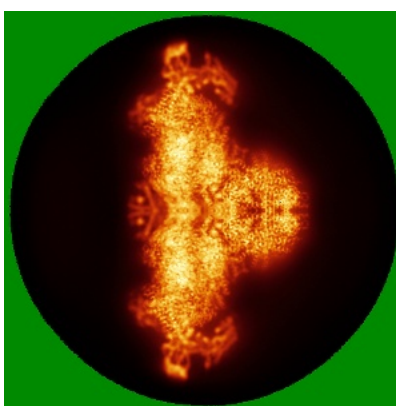
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

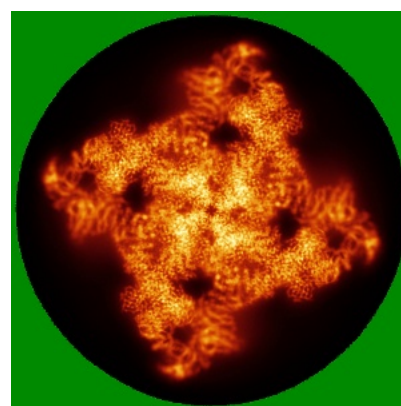
6.4.1 Primary map



X



Y



Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

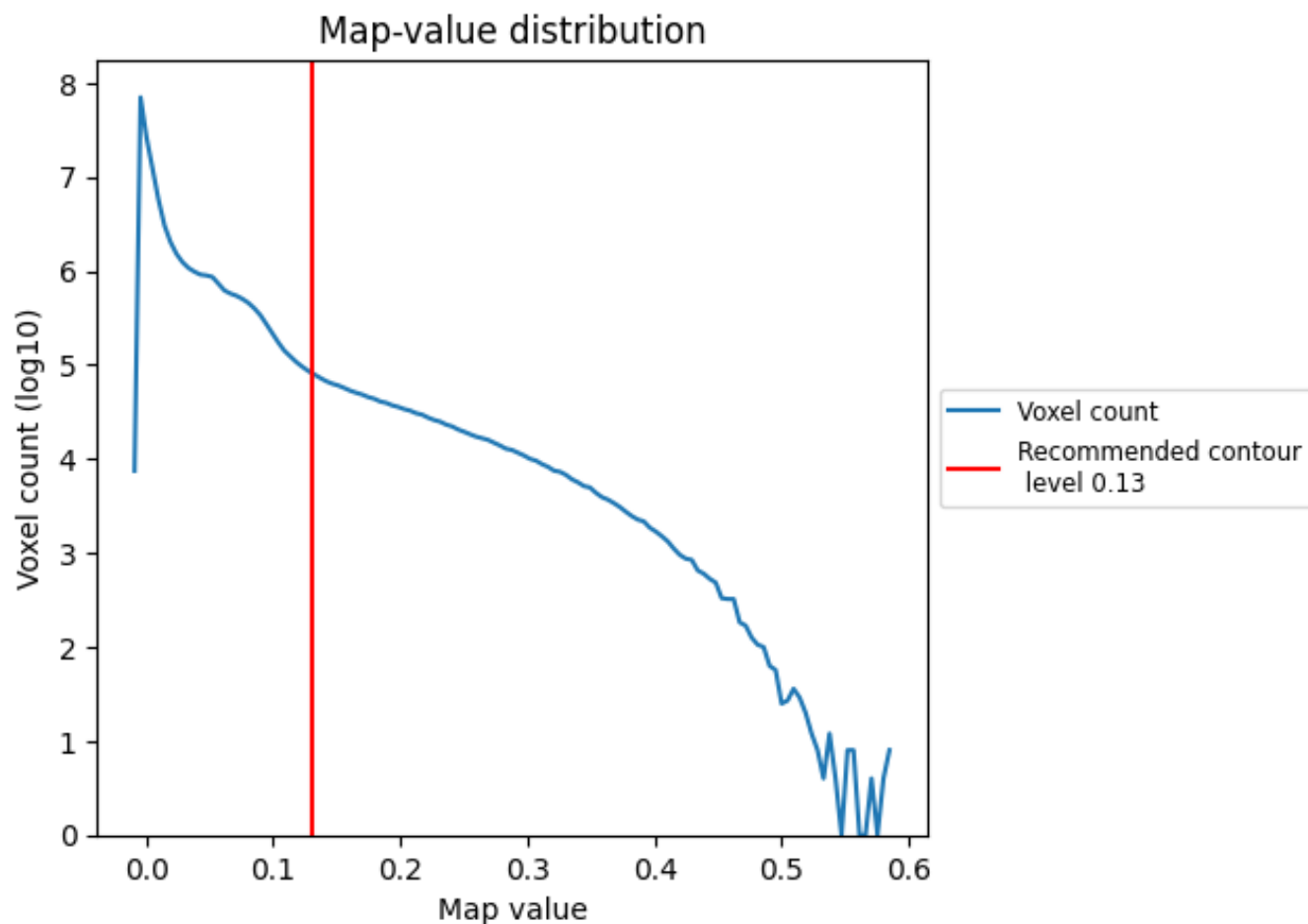
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

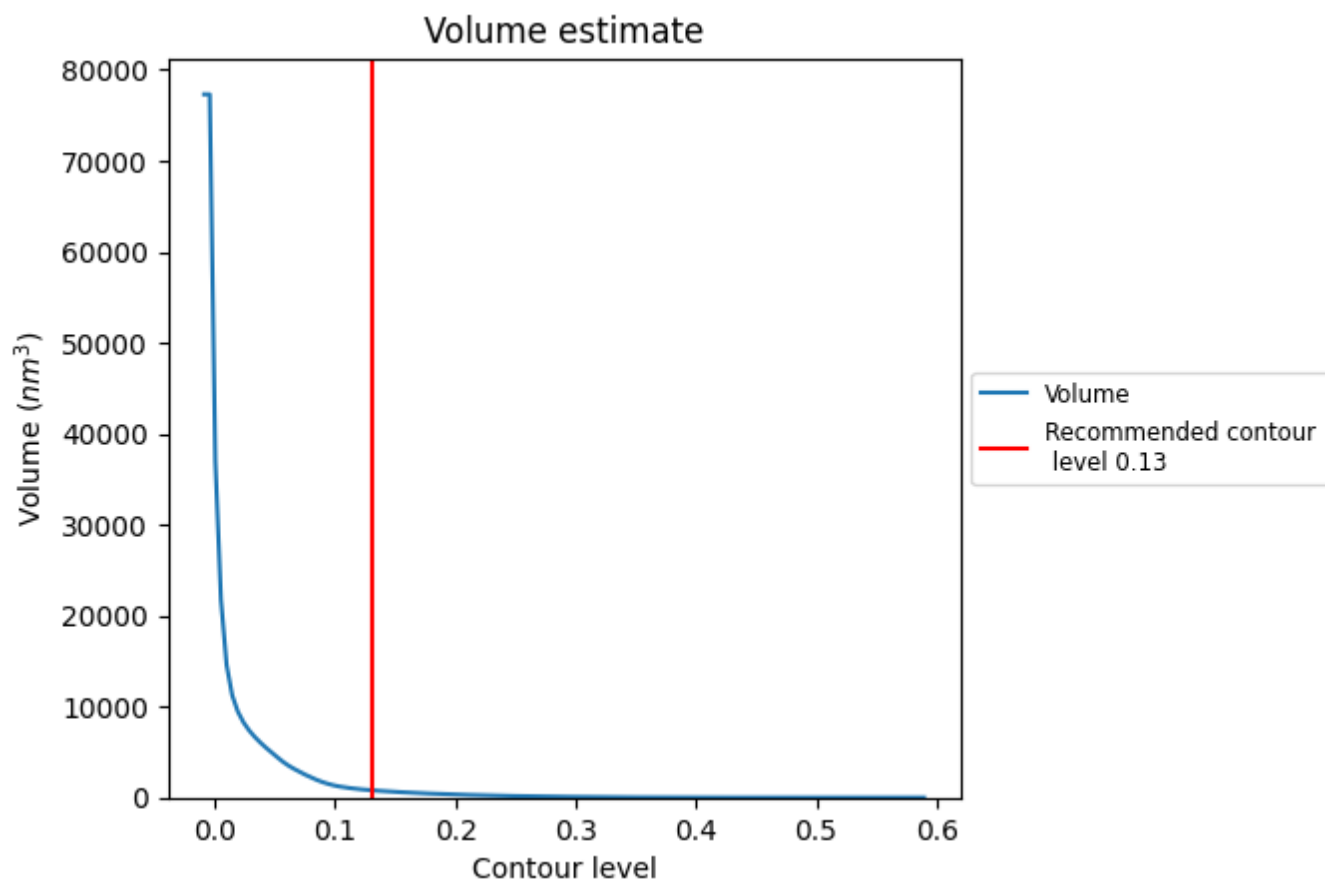
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

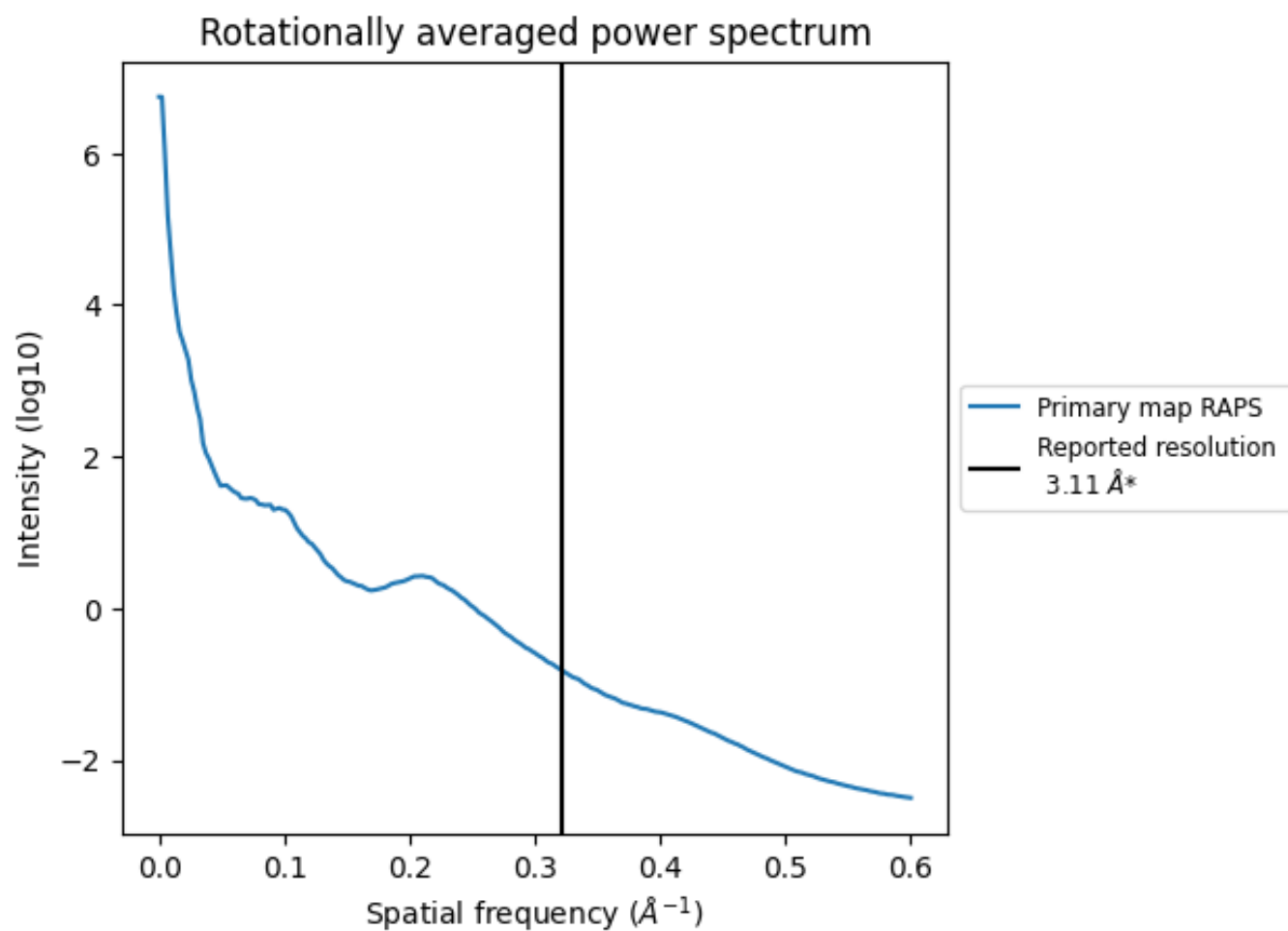
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 805 nm^3 ; this corresponds to an approximate mass of 728 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

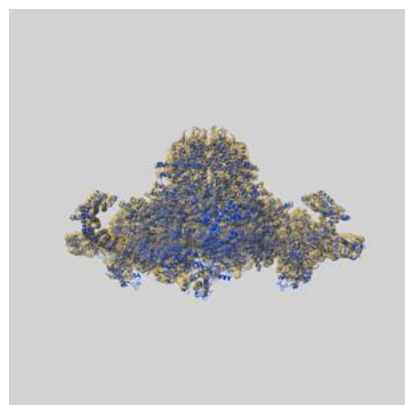
8 Fourier-Shell correlation

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

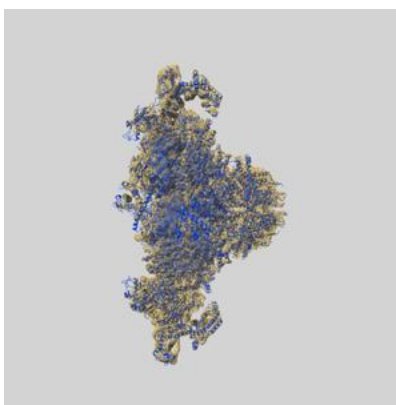
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26405 and PDB model 7U9Q. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

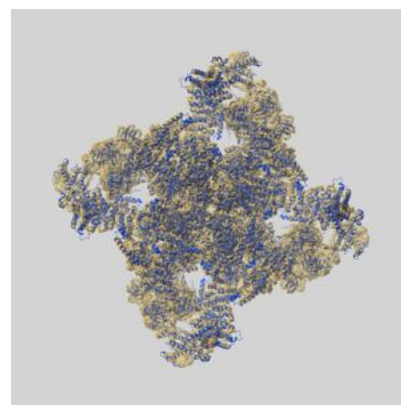
9.1 Map-model overlay [i](#)



X



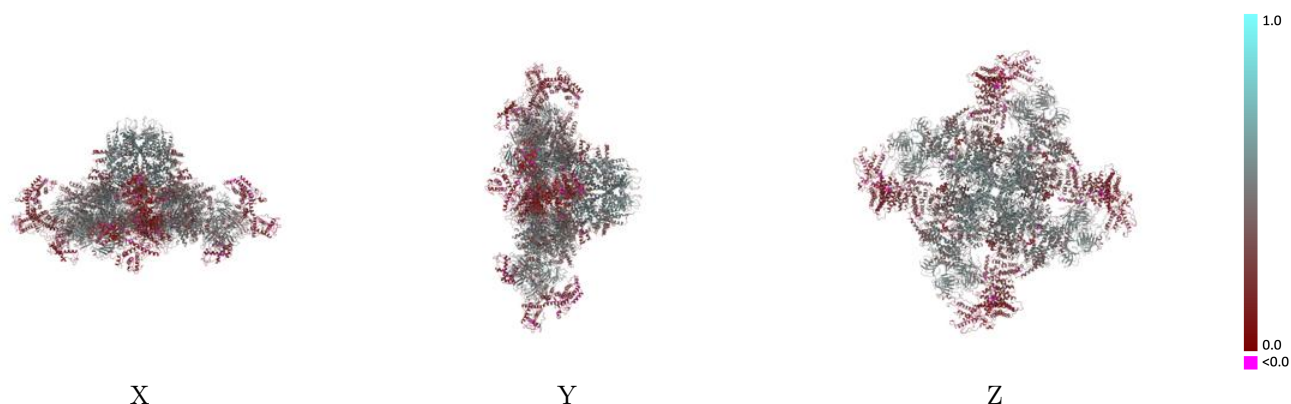
Y



Z

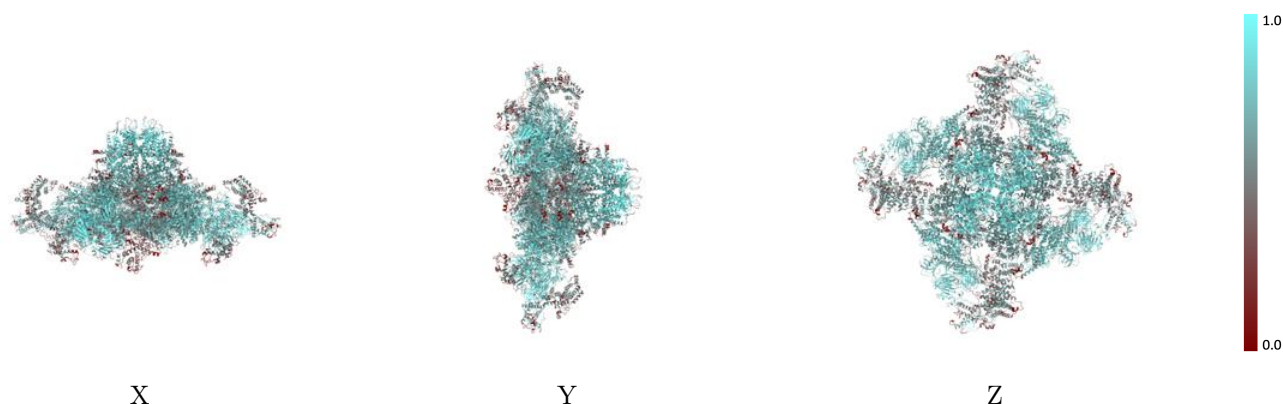
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



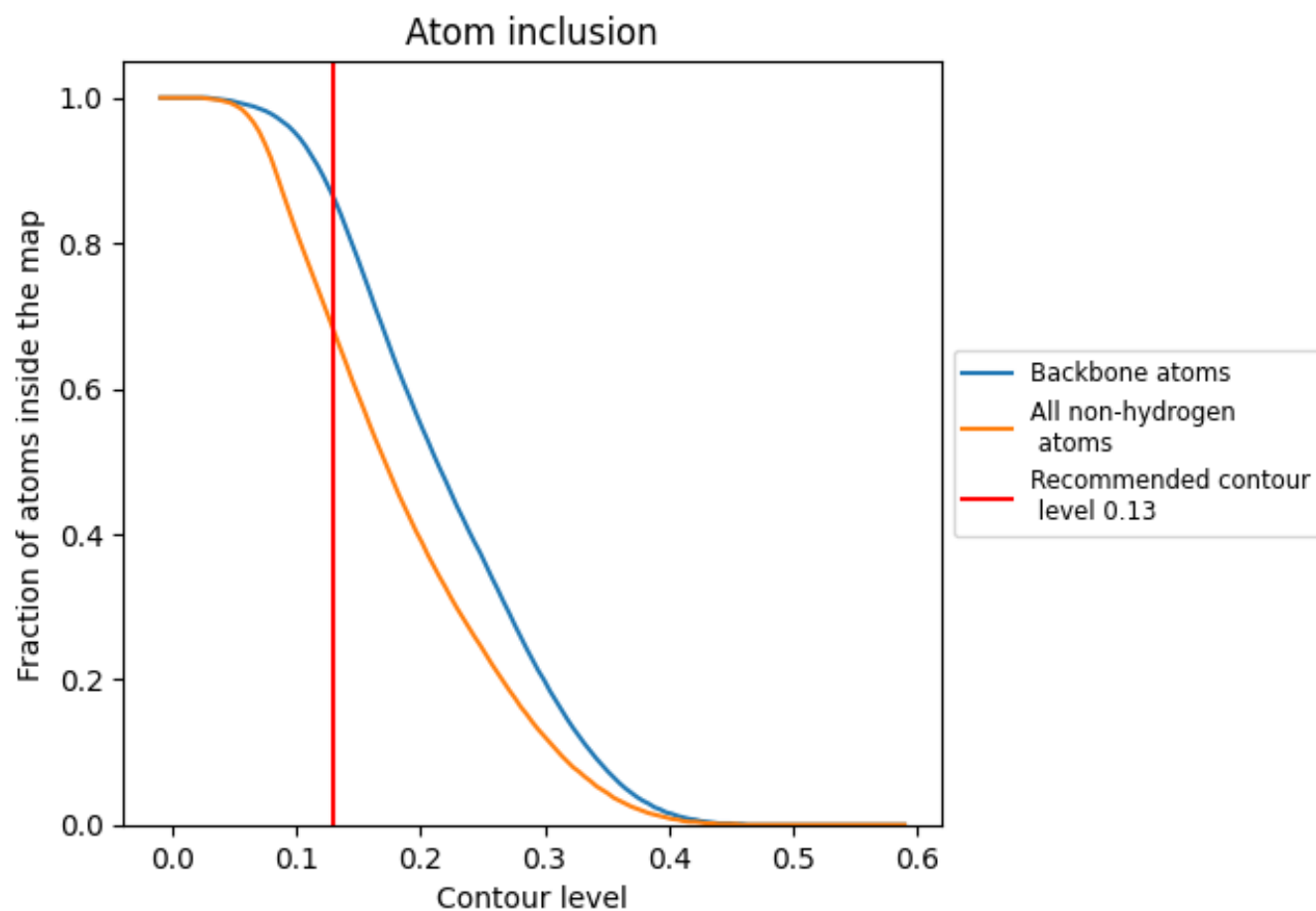
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.3770
A	0.6830	0.3810
B	0.6700	0.3640
C	0.6810	0.3790
D	0.6780	0.3740
E	0.7980	0.4950
F	0.7870	0.4900
G	0.7890	0.5020
H	0.8090	0.5130

1.0

0.0

<0.0