



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 06:34 pm BST

PDB ID : 9S5C / pdb_00009s5c
EMDB ID : EMD-54594
Title : Up class, Apo-state RyR1 in the native membrane solved by StA
Authors : Mikirtumov, V.
Deposited on : 2025-07-29
Resolution : 5.98 Å(reported)
Based on initial model : 7tzc

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:

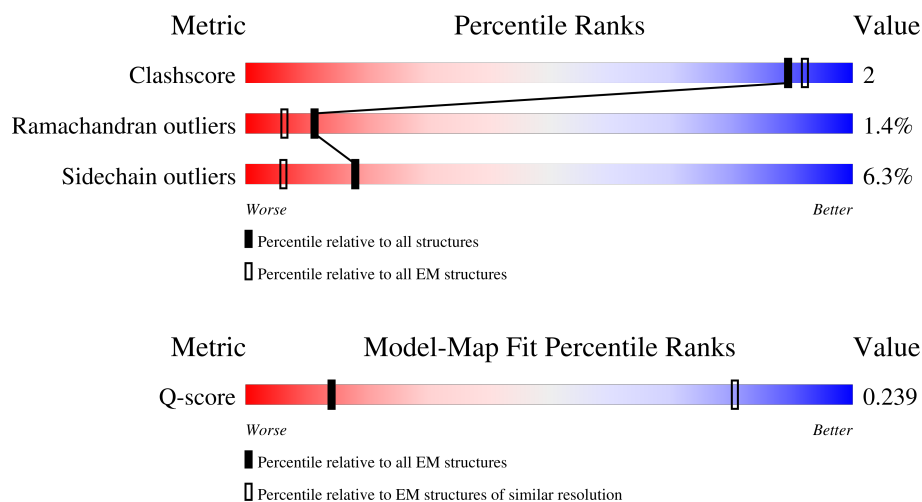
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 5.98 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	474 (5.48 - 6.48)

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	A	5037	15% 76% 10% 13%
1	B	5037	14% 76% 10% 13%
1	C	5037	15% 76% 10% 13%
1	D	5037	15% 76% 10% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	108	24% 91% 7% ..
2	F	108	25% 86% 12% ..
2	G	108	23% 90% 9% .
2	H	108	23% 89% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 285956 atoms, of which 142276 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		

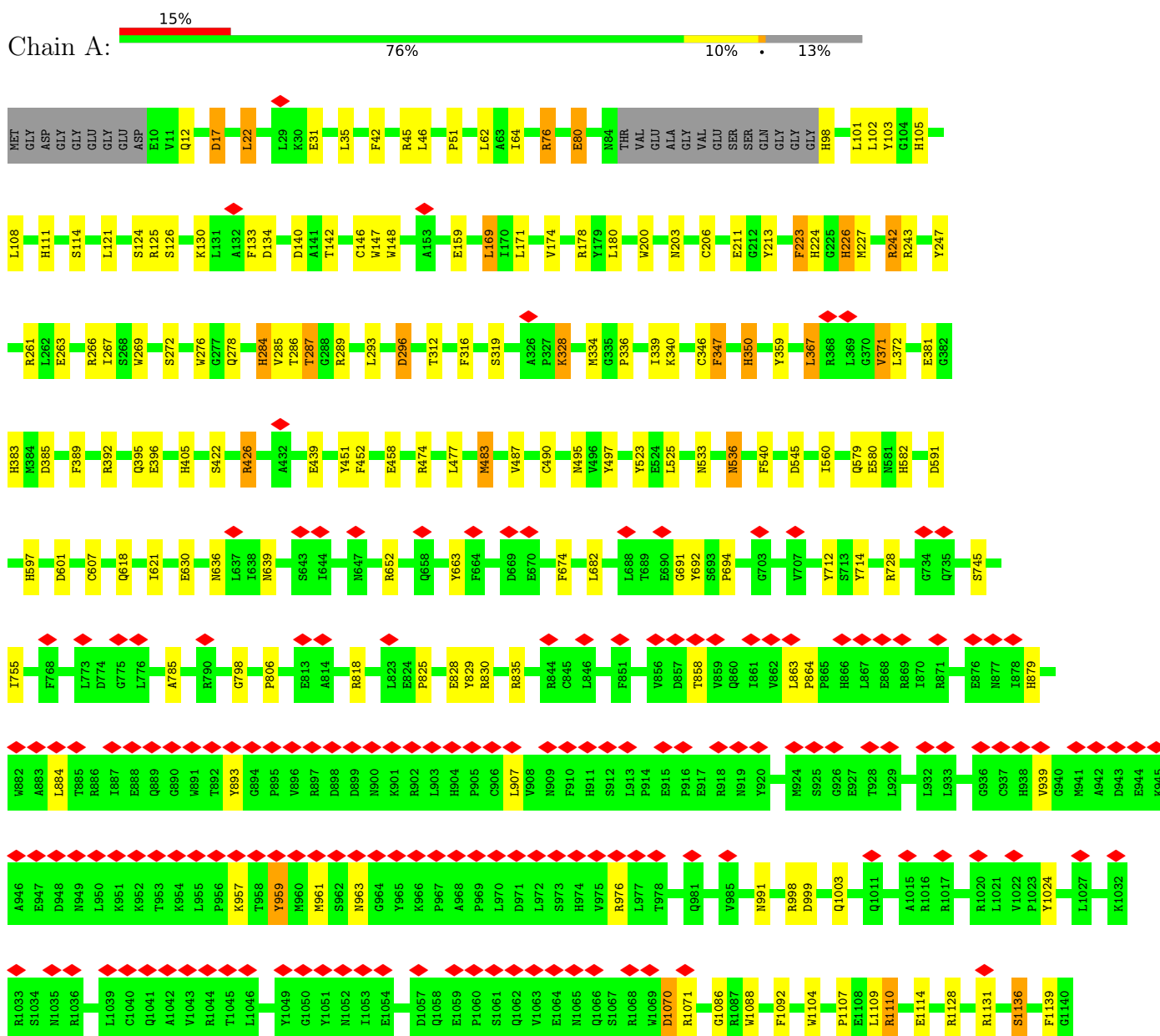
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

3 Residue-property plots

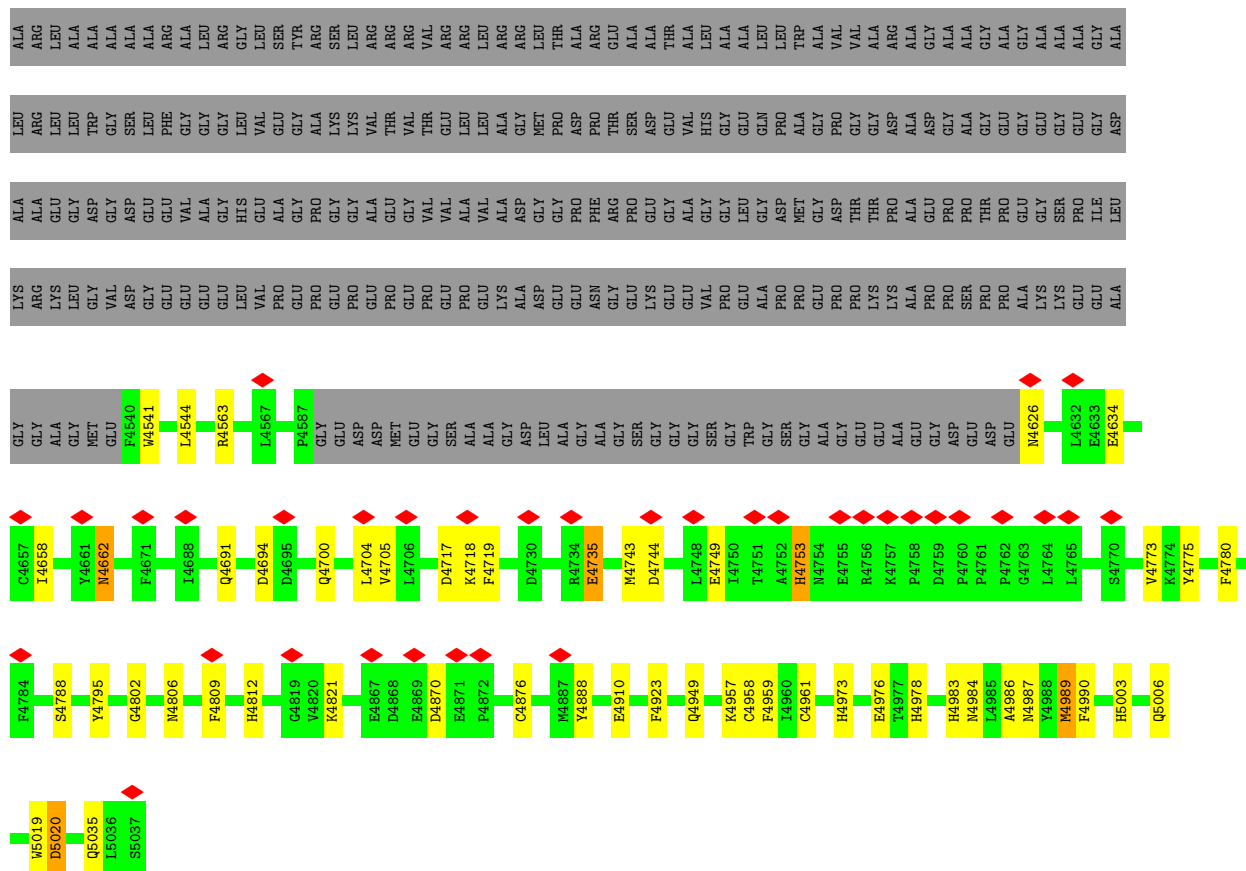
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 1

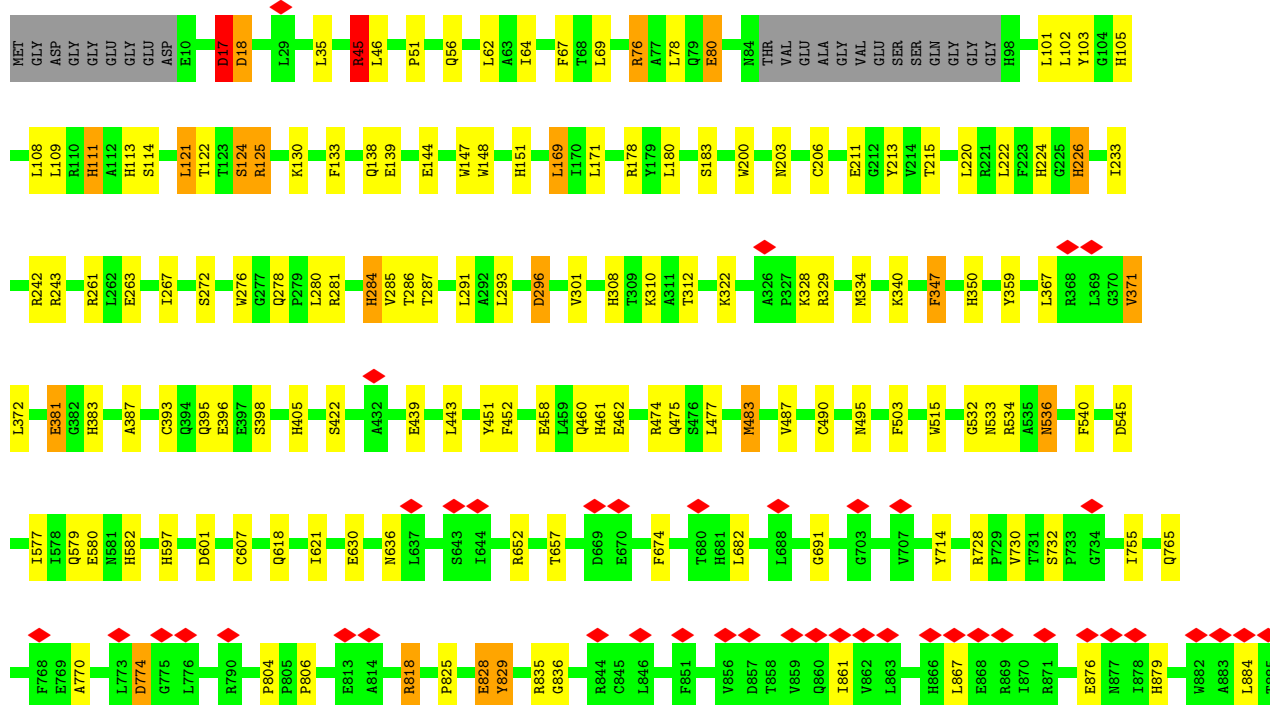
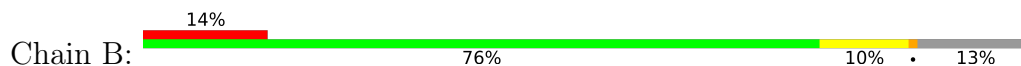


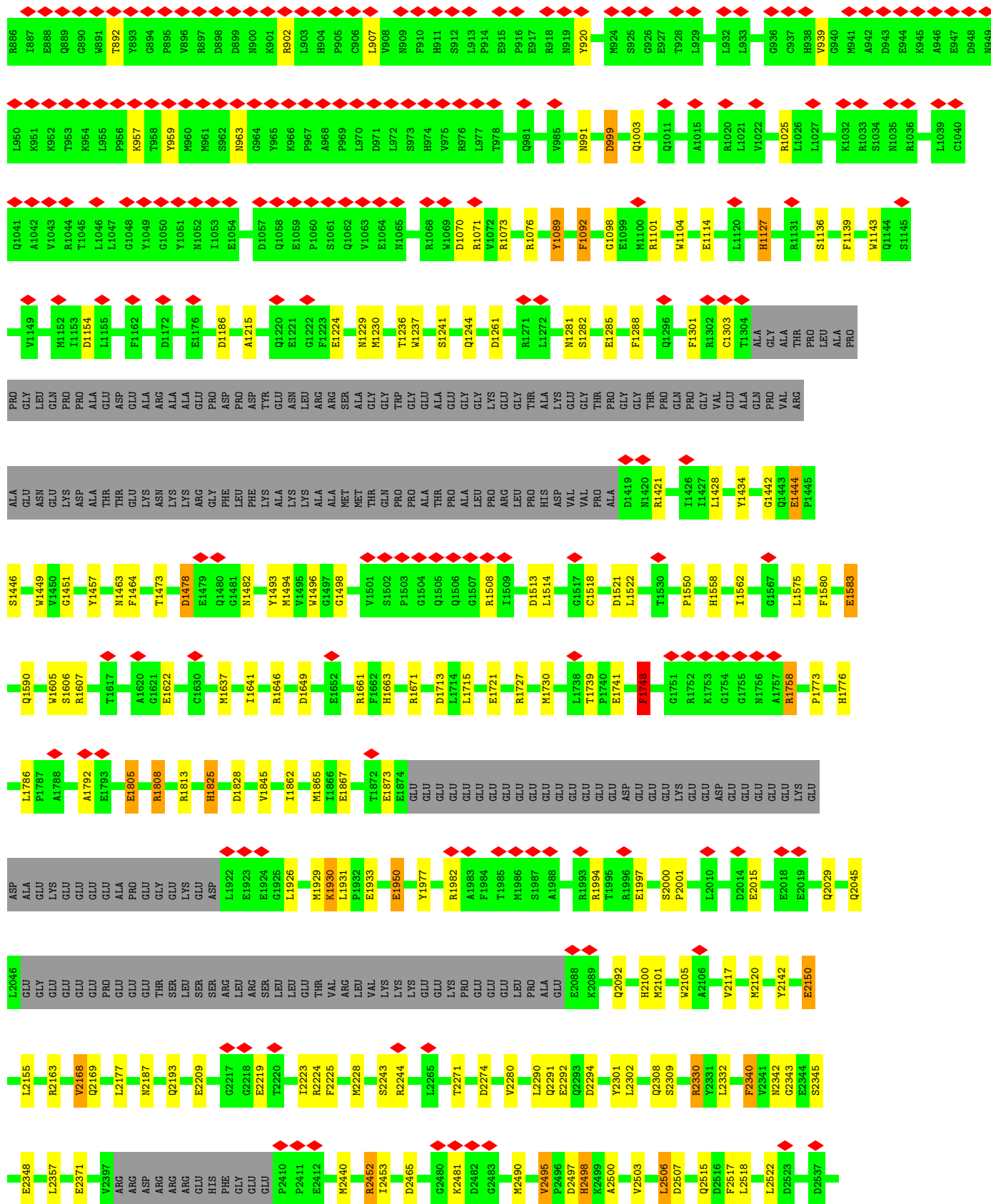




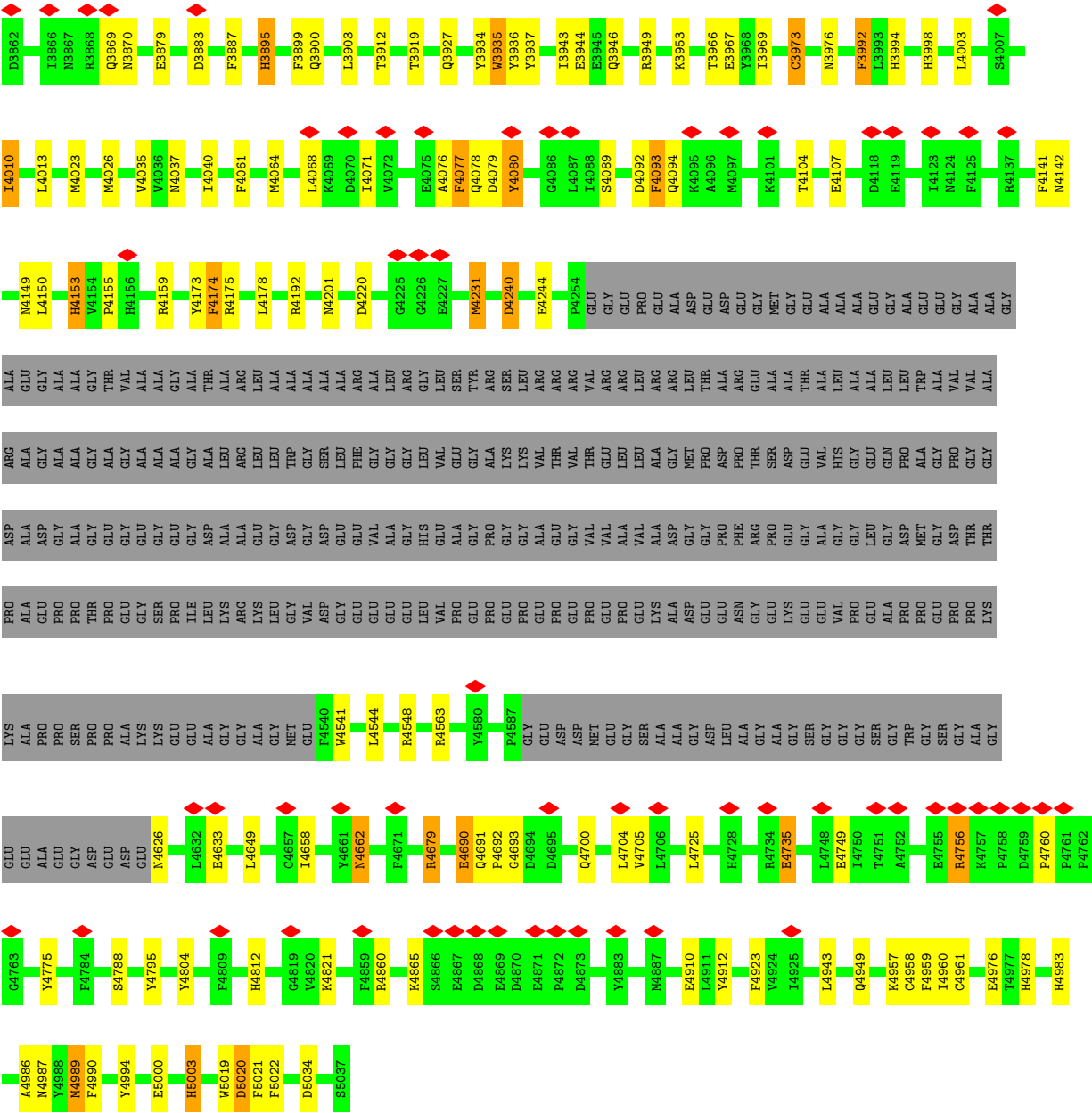


• Molecule 1: Ryanodine receptor 1

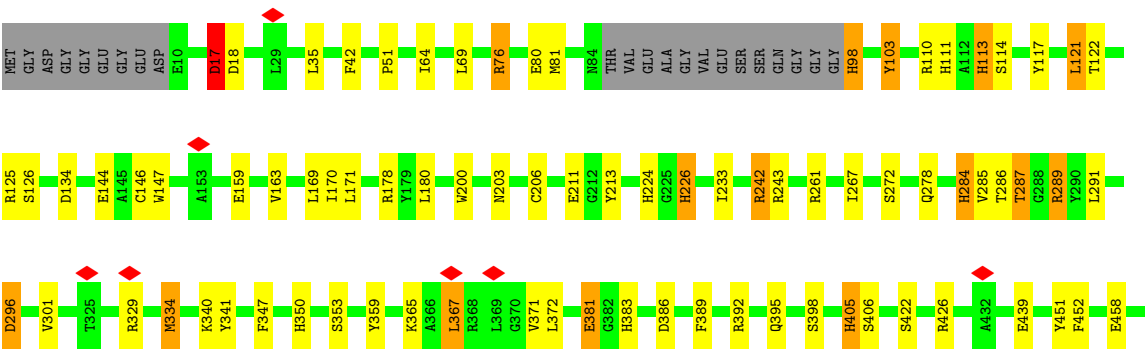
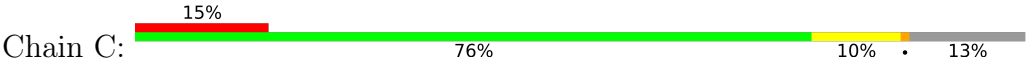


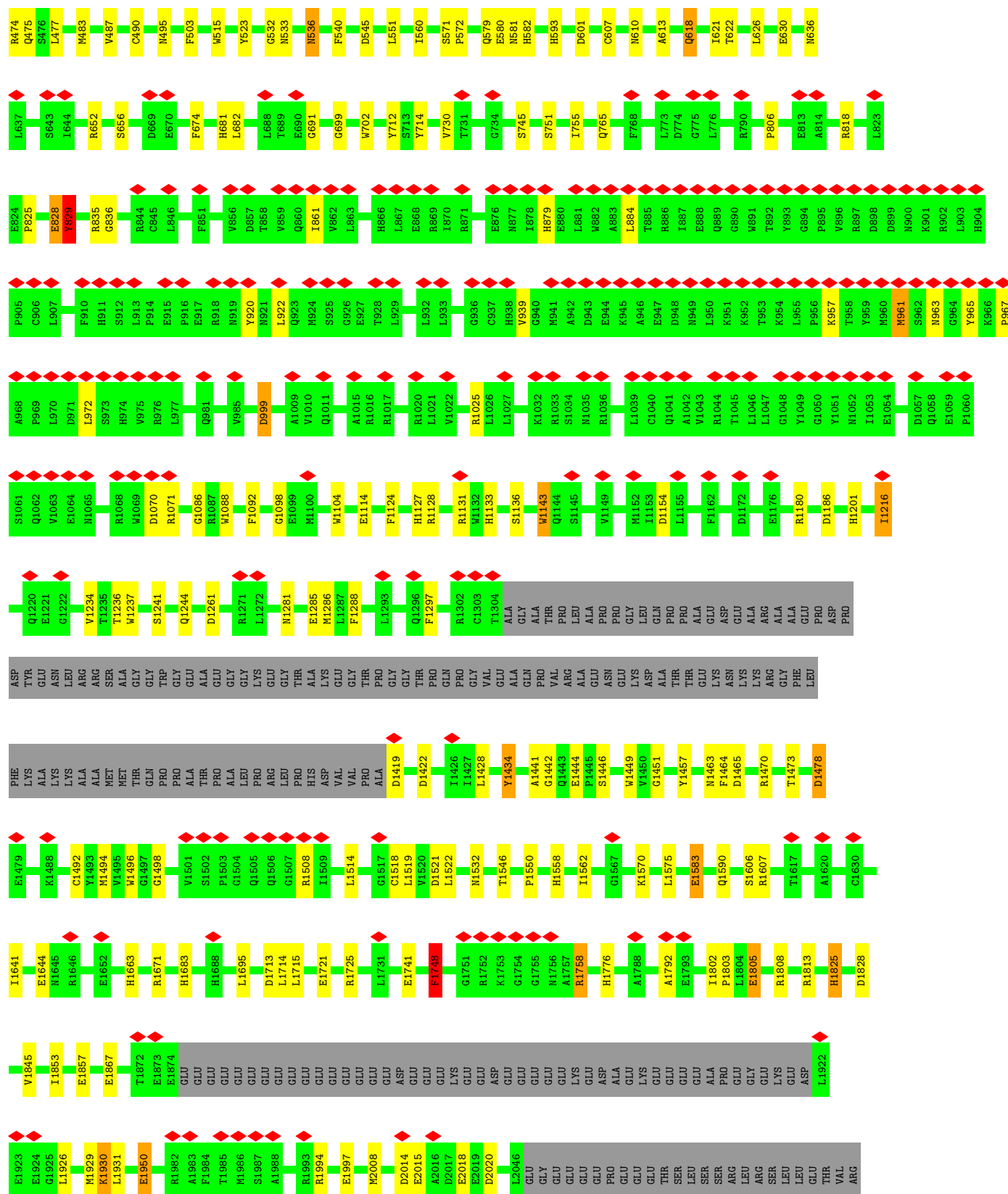


E3689	E3684	E3685	E3686	E3687	E3690	R3595	H3605	H3606	E3607	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	K3628	R3629	R3630	A3631	V3632	V3633	A3634	R3637	F3653	D3666	H3667	E3670	D3675	K3679	Q3683	E3684	E3685	E3686	E3687	E3688																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L3365	R3366	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	E3390	E3391	L3392	L3393	V3394	R3395	F3398	L3405	R3420	E3426	P3427	F3435	G3439	Y3444	F3451	E3463	I3464	K3465	K3466	M3467	L3470	T3471	A3472	D3473	S3474	K3475	R3476	R3477	Y3481																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	ALA	LYS	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	Q3506	M3517	C3525	A3541	L3542	K3543	D3544	T3545	D3546	V3549	R3550	F3551	F3552	L3553	Q3554	N3555	N3556	L3559	K3562	V3563	E3564	G3565	L3575	T3576	R3577	Y3581																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
E3689	D3713	Y2714	A2717	S2718	Y2719	S2720	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2734	R2738	P2739	V2740	E2741	T2742	L2743	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	L2751	D2752	S2753	E2811	S2812	I2755	N2756	K2757	F2758	I2817	E2761	Y2761	T2762	H2763	E2764	W2765	A2767	F2768	D2769	I2771	Q2772	N2773	W2774	W2775	S2776																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
E2544	E2545	N2551	L2556	T2572	E2573	H2574	I2577	N2578	R2588	L2595	T2596	A2609	L2614	Q2620	F2628	D2629	N2634	H2647	Y2654	G2660	W2661	A2662	N2663	T2667	S2668	E2669	R2673	R2676	K2677	I2682	L2686	Q2693	M2700	P2701	A2709	P2712	Y2777	G2778	E2779	N2780	D2781	E2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	Y2793	F2794	K2795	T2796	F2797	S2798	E2799	K2800	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	I2817	E2818	W2819	T2762	H2763	E2764	W2765	A2767	F2768	D2769	E2825	R2827	K2770	I2771	Q2772	N2773	W2774	W2775	S2776																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	Y2883	W2886	G2887	R2888	K2889	L2890	E2891	Q2892	E2893	L2894	I2895	A2896	K2897	G2898	GLU	GLU	ARG	THR	GLU	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G2899	Q2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	E2951	E2952	K2953	R2954	F2955	L2956																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
W2966	M2967	D2968	S2970	F2973	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982	S2983	Q2984	G2984	R2985	V2986	E2987	Y2988	E2994	T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	G3014	L3015	V3016	F3017	T3020	L3025	G3028	R3033	I3039	R3051	H3052	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	T3078	T3079	V3080	L3092	F3095	E3101	E3104	K3105	M3106	V3107	S2982

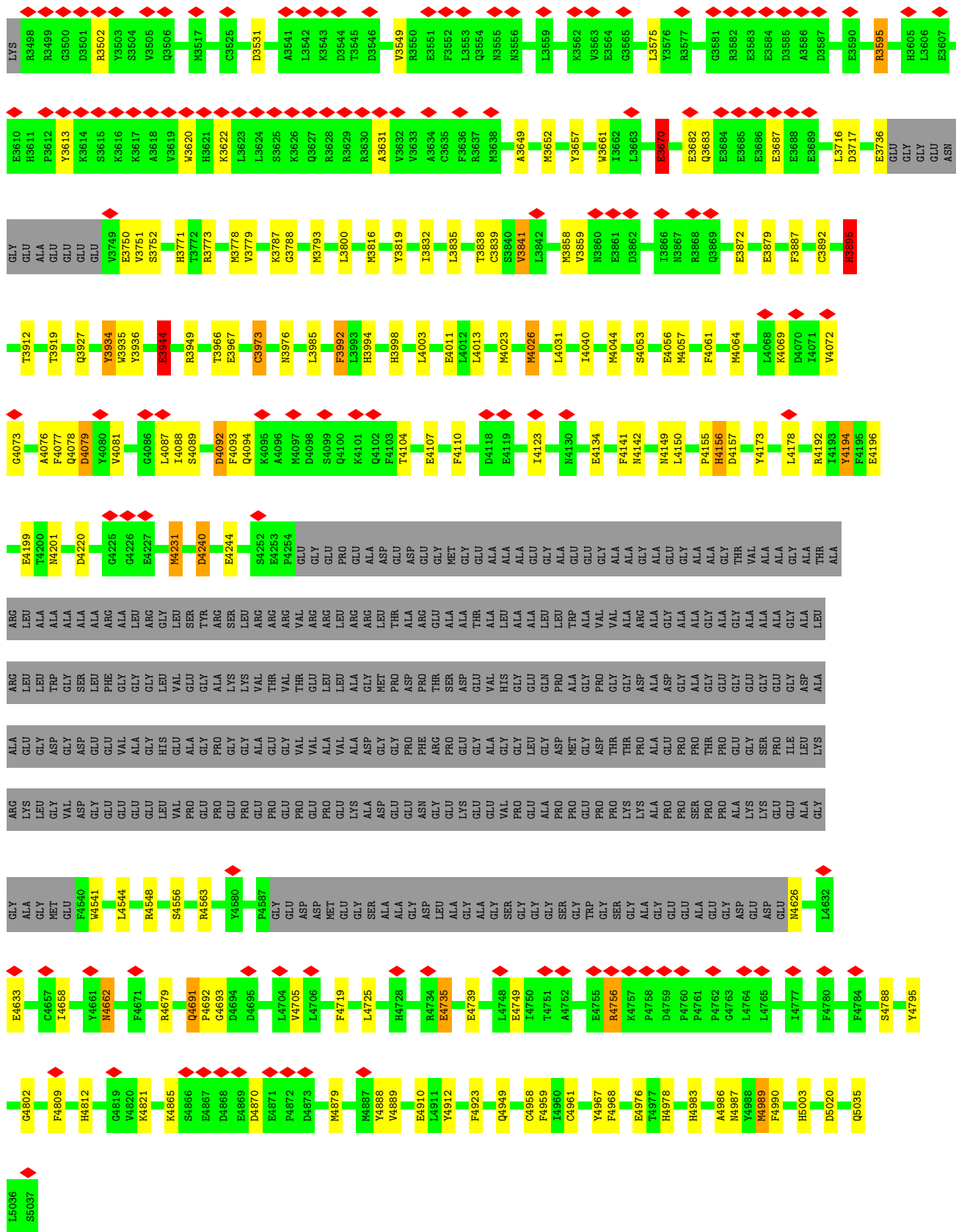


● Molecule 1: Ryanodine receptor 1



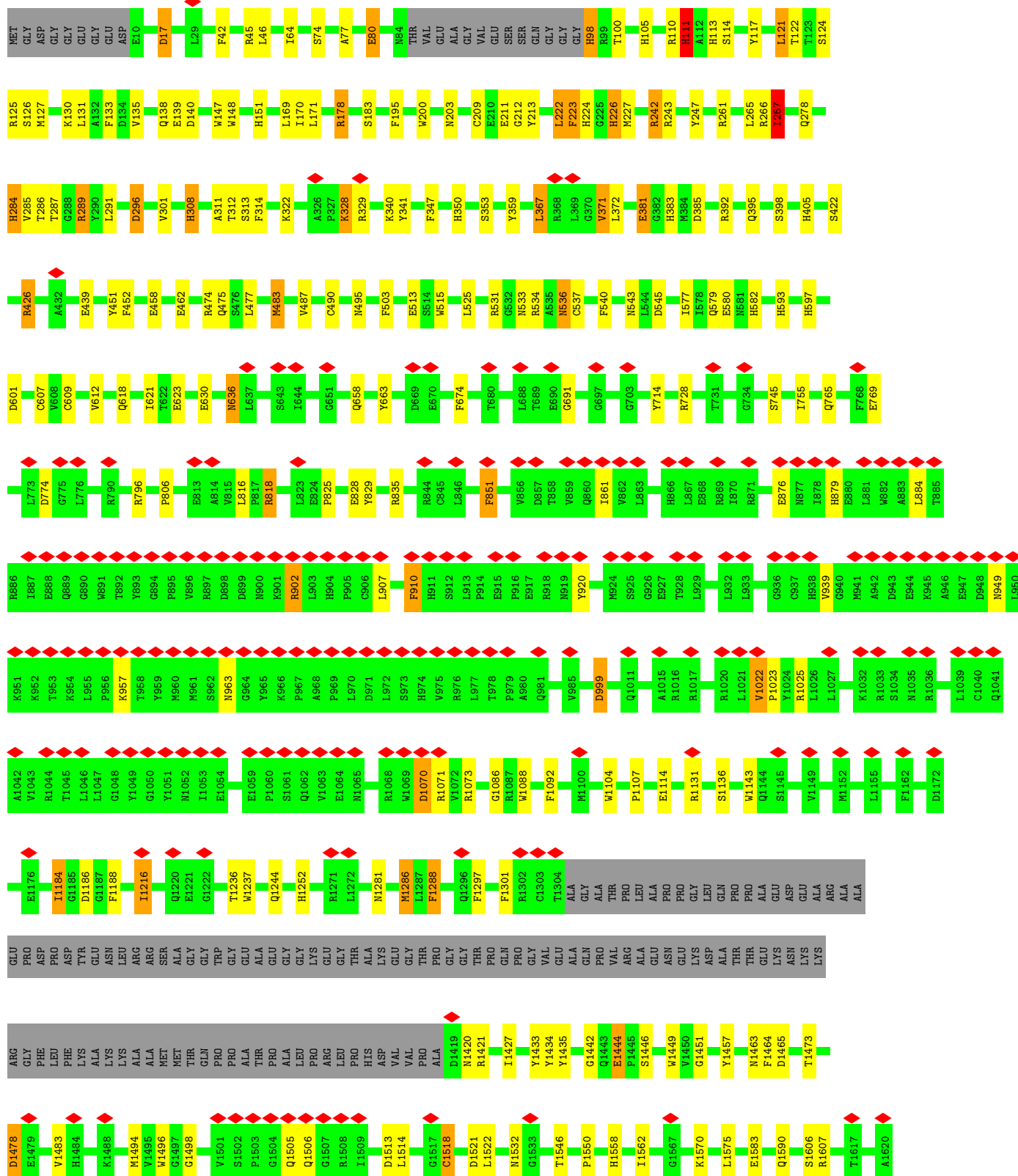


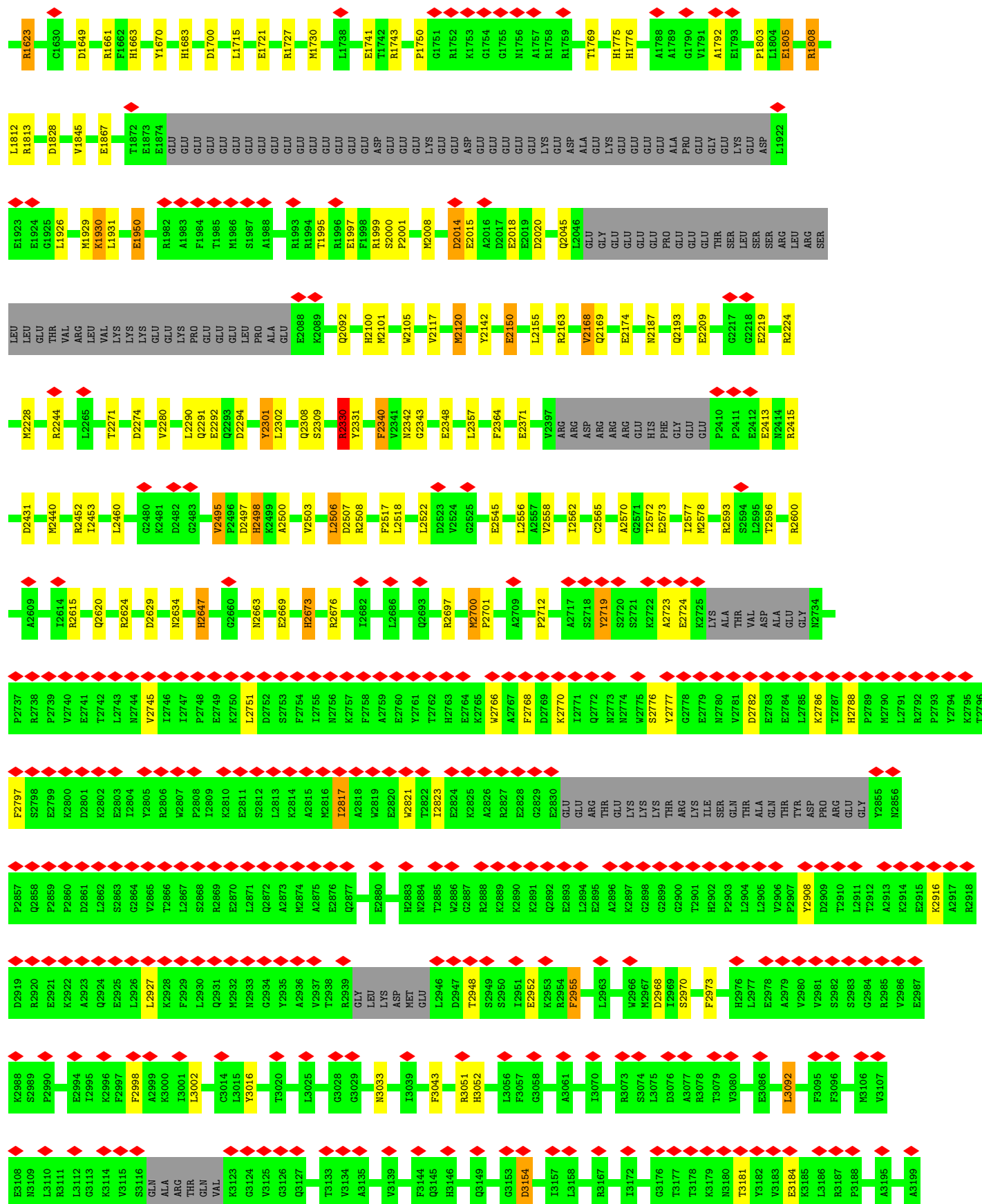
E3389	G3390	E3391	L3392	L3393	L3394	R3395	F3396	L3405	R3420	E3426	P3427	F3435	R3436	F3437	F3438	G3439	Y3444	F3451	E3463	I3464	I3465	N3466	M3467	L3470	T3471	A3472	D3473	S3474	K3475	K3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	GLU	THR	LYS															
R3283	W3284	W3285	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3303	A3306	D3310	R3321	V3324	L3327	G3328	I3329	D3330	M3335	K3336	F3341	A3342	Q3343	P3344	I3345	R3350	I3359	R3366	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	E3381	E3382	A3383	K3384	A3385	A3386	A3387	E3388												
A3199	A3204	F3205	L3206	E3207	Y3213	N3214	A3215	Y3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	N3239	G3240	P3241	D3242	I3243	P3244	D3247	R3248	D3252	I3253	L3256	A3257	G3260	A3261	R3262	Y3263	T3264	E3265	N3266	I3270	E3271	I3272	T3273	C3278									
V3107	E3108	M3109	L3110	L3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	V3134	A3135	V3139	F3144	K3145	H3146	Q3149	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	R3167	I3172	T3177	K3178	K3179	M3180	T3181	V3182	E3184	K3185	L3186	R3187	P3188	A3195								
T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	C3014	L3015	Y3016	F3017	T3020	L3025	G3028	G3029	N3033	I3039	F3043	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	K3078	T3079	V3080	P3085	L3092	F3095	E3101	M3106															
L2862	S2863	G2864	V2865	T2866	L2867	S2868	L2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	L2884	T2885	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	E2920	K2922
A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	I2951	K2952	K2953	R2954	F2955	L2963	W2966	S2970	F2973	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	L2985	V2986	E2987	K2988	S2989	P2990	H2991	E2994				
T2995	K2996	F2997	F2998	A2999	K3000	I3001	L3002	F3010	C3014	L3015	Y3016	F3017	T3020	L3025	G3028	G3029	N3033	I3039	F3043	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	A3061	I3070	R3073	S3074	L3075	D3076	A3077	K3078	T3079	V3080	P3085	L3092	F3095	E3101	M3106															
V3107	E3108	M3109	L3110	L3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	V3134	A3135	V3139	F3144	K3145	H3146	Q3149	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	R3167	I3172	T3177	K3178	K3179	M3180	T3181	V3182	E3184	K3185	L3186	R3187	P3188	A3195								
A3199	A3204	F3205	L3206	E3207	Y3213	N3214	A3215	Y3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	N3239	G3240	P3241	D3242	I3243	P3244	D3247	R3248	D3252	I3253	L3256	A3257	G3260	A3261	R3262	Y3263	T3264	E3265	N3266	I3270	E3271	I3272	T3273	C3278									
R3283	W3284	W3285	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3303	A3306	D3310	R3321	V3324	L3327	G3328	I3329	D3330	M3335	K3336	F3341	A3342	Q3343	P3344	I3345	R3350	I3359	R3366	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	E3381	E3382	A3383	K3384	A3385	A3386	A3387	E3388												



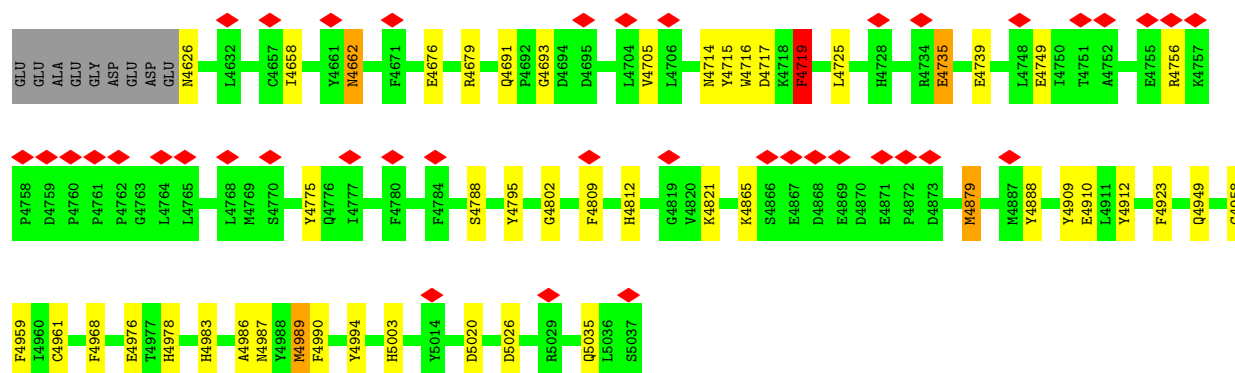
- Molecule 1: Ryanodine receptor 1

Chain D: 15% 76% 10% 13%

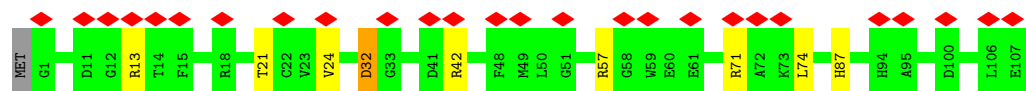




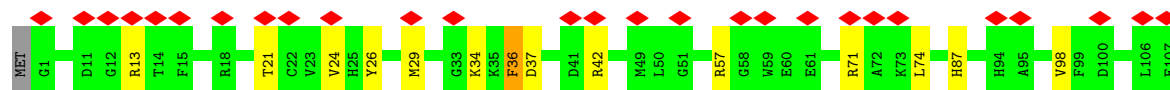
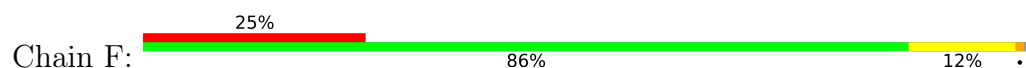




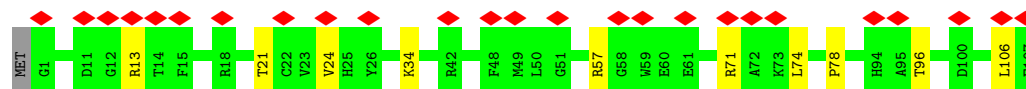
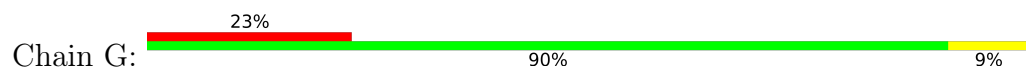
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



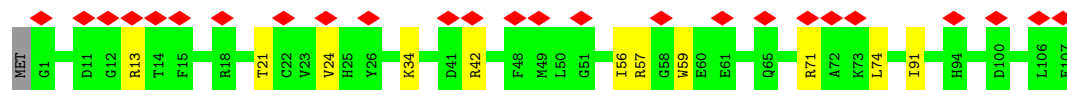
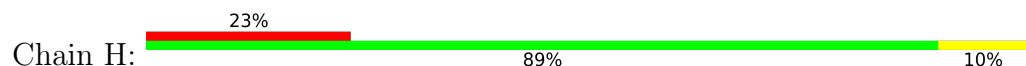
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of subtomograms used	3555	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	132	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	64000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.624	Depositor
Minimum map value	-0.306	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.0893	Depositor
Map size (Å)	496.74, 496.74, 496.74	wwPDB
Map dimensions	170, 170, 170	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.922, 2.922, 2.922	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	0.79	0/35885	1.41	161/48603 (0.3%)
1	B	0.78	0/35885	1.40	176/48603 (0.4%)
1	C	0.78	0/35885	1.40	136/48603 (0.3%)
1	D	0.78	0/35885	1.40	153/48603 (0.3%)
2	E	0.76	0/851	1.37	4/1146 (0.3%)
2	F	0.75	0/851	1.37	3/1146 (0.3%)
2	G	0.76	0/851	1.32	1/1146 (0.1%)
2	H	0.75	0/851	1.30	2/1146 (0.2%)
All	All	0.78	0/146944	1.40	636/198996 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	37
1	B	0	35
1	C	0	36
1	D	0	36
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	152

There are no bond length outliers.

All (636) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4077	PHE	N-CA-C	10.19	122.47	111.36
1	A	4077	PHE	N-CA-C	9.42	121.63	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3934	TYR	N-CA-C	9.35	121.08	111.07
1	C	1748	PHE	CA-CB-CG	8.84	122.64	113.80
1	C	3992	PHE	CA-CB-CG	8.77	122.57	113.80
1	B	3992	PHE	CA-CB-CG	8.76	122.56	113.80
1	D	3992	PHE	CA-CB-CG	8.30	122.10	113.80
1	D	999	ASP	CA-CB-CG	8.13	120.73	112.60
1	B	999	ASP	CA-CB-CG	8.03	120.63	112.60
1	A	2869	ARG	N-CA-C	8.01	120.02	111.28
1	A	3992	PHE	CA-CB-CG	7.96	121.76	113.80
1	C	540	PHE	CA-CB-CG	-7.95	105.85	113.80
1	C	3206	LEU	CA-C-N	7.93	129.26	122.28
1	C	3206	LEU	C-N-CA	7.93	129.26	122.28
1	C	999	ASP	CA-CB-CG	7.89	120.49	112.60
1	D	536	ASN	CA-CB-CG	7.80	120.40	112.60
1	D	4240	ASP	CA-CB-CG	7.73	120.33	112.60
1	C	1478	ASP	CA-CB-CG	7.63	120.23	112.60
1	A	4240	ASP	CA-CB-CG	7.60	120.20	112.60
1	B	4240	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	4923	PHE	CA-CB-CG	-7.36	106.44	113.80
1	A	1478	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	3969	ILE	N-CA-C	7.34	121.43	113.43
1	A	42	PHE	CA-CB-CG	-7.34	106.46	113.80
1	B	1478	ASP	CA-CB-CG	7.33	119.94	112.60
1	A	17	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	426	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	D	42	PHE	CA-CB-CG	-7.27	106.53	113.80
1	C	4240	ASP	CA-CB-CG	7.22	119.83	112.60
1	C	42	PHE	CA-CB-CG	-7.18	106.62	113.80
1	B	4093	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	1261	ASP	CA-CB-CG	7.13	119.73	112.60
1	C	536	ASN	CA-CB-CG	7.11	119.71	112.60
1	B	636	ASN	CA-CB-CG	7.11	119.71	112.60
1	B	536	ASN	CA-CB-CG	7.10	119.70	112.60
1	C	613	ALA	N-CA-C	7.09	119.85	109.07
1	D	1288	PHE	CA-CB-CG	7.09	120.89	113.80
1	A	4201	ASN	CB-CA-C	7.08	122.89	110.85
1	A	728	ARG	CA-C-N	7.08	127.07	119.78
1	A	728	ARG	C-N-CA	7.08	127.07	119.78
1	D	540	PHE	CA-CB-CG	-7.02	106.78	113.80
1	B	3051	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	D	4153	HIS	CA-CB-CG	-6.99	106.81	113.80
1	B	3109	ASN	CA-CB-CG	6.96	119.56	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3969	ILE	N-CA-C	6.91	120.96	113.43
1	B	1070	ASP	CA-CB-CG	6.88	119.48	112.60
1	D	111	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	C	4201	ASN	CB-CA-C	6.82	122.11	110.79
1	D	2517	PHE	CA-CB-CG	-6.81	106.99	113.80
1	D	426	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	C	3051	ARG	NE-CZ-NH2	6.77	125.30	119.20
1	A	2517	PHE	CA-CB-CG	-6.76	107.04	113.80
1	B	4174	PHE	CA-CB-CG	-6.76	107.04	113.80
1	A	2000	SER	N-CA-C	6.76	114.30	108.22
1	B	804	PRO	N-CA-CB	6.76	106.73	103.22
1	B	4959	PHE	CA-CB-CG	-6.69	107.11	113.80
1	B	2629	ASP	CA-C-N	6.69	124.45	120.24
1	B	2629	ASP	C-N-CA	6.69	124.45	120.24
1	A	3051	ARG	NE-CZ-NH2	6.68	125.21	119.20
1	C	4959	PHE	CA-CB-CG	-6.67	107.13	113.80
1	B	4201	ASN	CB-CA-C	6.64	122.14	110.85
1	C	284	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	D	4078	GLN	CA-C-N	6.63	129.83	120.28
1	D	4078	GLN	C-N-CA	6.63	129.83	120.28
1	D	3502	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	B	3502	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	C	296	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	296	ASP	CA-CB-CG	6.55	119.16	112.60
1	D	296	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	2870	GLU	N-CA-C	6.54	118.21	111.14
1	C	1288	PHE	CA-CB-CG	6.54	120.34	113.80
1	A	4662	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	4959	PHE	CA-CB-CG	-6.49	107.31	113.80
1	B	2517	PHE	CA-CB-CG	-6.49	107.31	113.80
1	B	4077	PHE	N-CA-C	6.49	119.67	111.69
1	D	4959	PHE	CA-CB-CG	-6.44	107.36	113.80
1	C	134	ASP	CA-CB-CG	6.42	119.02	112.60
2	E	32	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	284	HIS	CB-CG-CD2	-6.38	122.90	131.20
1	A	540	PHE	CA-CB-CG	-6.36	107.44	113.80
1	A	3502	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	A	296	ASP	CA-CB-CG	6.35	118.95	112.60
1	D	3987	ASP	CA-CB-CG	6.35	118.95	112.60
1	D	17	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	1288	PHE	CA-CB-CG	6.33	120.13	113.80
1	D	284	HIS	CB-CG-CD2	-6.30	123.01	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3987	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	533	ASN	CA-C-N	6.28	128.98	120.38
1	A	533	ASN	C-N-CA	6.28	128.98	120.38
1	C	3502	ARG	NE-CZ-NH2	6.27	124.85	119.20
1	A	3998	HIS	CA-CB-CG	-6.26	107.54	113.80
1	D	4174	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	636	ASN	CA-CB-CG	6.25	118.85	112.60
1	B	1748	PHE	CA-CB-CG	6.25	120.05	113.80
1	D	1521	ASP	CA-CB-CG	-6.24	106.36	112.60
1	A	3465	ASN	CA-CB-CG	6.24	118.84	112.60
1	D	4201	ASN	CB-CA-C	6.24	121.45	110.85
1	C	4156	HIS	CA-CB-CG	-6.23	107.57	113.80
1	D	4142	ASN	CA-CB-CG	-6.23	106.37	112.60
1	A	284	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	D	4923	PHE	CA-CB-CG	-6.22	107.58	113.80
1	B	261	ARG	NE-CZ-NH2	6.22	124.80	119.20
1	C	203	ASN	CB-CA-C	6.21	119.48	109.41
1	D	4662	ASN	CA-CB-CG	6.21	118.81	112.60
1	D	4031	LEU	N-CA-C	6.21	120.86	113.16
1	D	4192	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	4078	GLN	CA-C-N	6.20	129.21	120.28
1	A	4078	GLN	C-N-CA	6.20	129.21	120.28
1	A	389	PHE	N-CA-C	6.20	120.03	110.42
1	A	536	ASN	CA-CB-CG	6.20	118.80	112.60
1	C	4923	PHE	CA-CB-CG	-6.20	107.60	113.80
1	D	601	ASP	CA-CB-CG	-6.16	106.44	112.60
1	A	991	ASN	CA-CB-CG	-6.16	106.44	112.60
1	B	540	PHE	CA-CB-CG	-6.15	107.65	113.80
1	A	4153	HIS	CA-CB-CG	-6.15	107.65	113.80
1	B	4153	HIS	CA-CB-CG	-6.14	107.66	113.80
1	B	393	CYS	N-CA-CB	-6.14	101.91	110.38
1	A	621	ILE	CB-CA-C	-6.14	104.11	111.97
1	B	111	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	D	1808	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	C	636	ASN	CA-CB-CG	6.12	118.72	112.60
1	C	2291	GLN	CA-C-N	6.12	128.40	120.44
1	C	2291	GLN	C-N-CA	6.12	128.40	120.44
1	B	4662	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	3933	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	3973	CYS	CA-CB-SG	-6.10	100.36	114.40
1	B	1288	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	4093	PHE	CA-CB-CG	6.10	119.90	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4662	ASN	CA-CB-CG	6.08	118.67	112.60
1	B	4080	TYR	N-CA-C	6.06	120.54	113.20
1	A	350	HIS	CA-CB-CG	-6.06	107.74	113.80
1	D	178	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	D	1575	LEU	N-CA-C	6.05	117.96	111.36
1	D	3154	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	17	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	3207	GLU	CA-C-N	6.04	125.73	119.82
1	A	3207	GLU	C-N-CA	6.04	125.73	119.82
1	D	3934	TYR	N-CA-C	6.04	123.65	110.80
1	D	4079	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	242	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	A	3670	GLU	N-CA-C	6.02	117.65	111.14
1	A	284	HIS	CA-CB-CG	-6.02	107.78	113.80
1	B	2869	ARG	N-CA-C	6.02	117.84	111.28
1	B	4142	ASN	CA-CB-CG	-6.01	106.59	112.60
1	C	243	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	B	2291	GLN	CA-C-N	5.99	128.31	120.28
1	B	2291	GLN	C-N-CA	5.99	128.31	120.28
1	B	2869	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	D	1478	ASP	CA-CB-CG	5.99	118.59	112.60
1	D	243	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	B	4192	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	D	835	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	B	284	HIS	CA-CB-CG	-5.97	107.83	113.80
1	B	3771	HIS	CB-CG-CD2	-5.97	123.43	131.20
1	C	2126	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	B	1808	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	C	178	ARG	NE-CZ-NH2	5.95	124.56	119.20
1	B	1575	LEU	N-CA-C	5.95	117.84	111.36
1	C	879	HIS	CA-CB-CG	5.95	119.75	113.80
1	B	835	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	C	4142	ASN	CA-CB-CG	-5.91	106.69	112.60
1	B	621	ILE	CB-CA-C	-5.91	104.40	111.97
1	A	169	LEU	N-CA-C	5.88	118.64	109.52
1	A	4192	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	D	3051	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	D	3935	TRP	N-CA-C	5.86	119.25	111.75
1	B	2163	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	601	ASP	CA-CB-CG	-5.85	106.75	112.60
1	A	1813	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	A	111	HIS	CB-CG-CD2	-5.85	123.60	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1813	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	B	178	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	336	PRO	N-CA-CB	5.83	106.25	103.22
1	D	1813	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	D	2647	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	B	2676	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	3287	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	A	3010	PHE	CA-CB-CG	-5.81	107.99	113.80
1	D	879	HIS	CA-CB-CG	5.80	119.60	113.80
1	C	2187	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	243	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	D	621	ILE	CB-CA-C	-5.80	104.55	111.97
1	D	266	ARG	N-CA-C	5.80	117.06	108.60
1	B	1663	HIS	CA-CB-CG	-5.79	108.01	113.80
2	F	42	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	C	226	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	C	426	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	B	243	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	D	1828	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	17	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	1671	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	C	835	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	C	1671	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	D	3687	GLU	N-CA-C	5.76	119.61	112.47
1	D	1216	ILE	CA-CB-CG1	5.74	120.17	110.40
2	F	24	VAL	N-CA-C	5.74	116.63	108.42
2	H	42	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	C	200	TRP	N-CA-C	5.74	118.00	108.99
1	A	1110	ARG	CB-CA-C	5.74	117.50	108.84
1	B	1813	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	B	461	HIS	N-CA-C	5.73	117.53	111.28
1	B	601	ASP	CA-CB-CG	-5.73	106.87	112.60
1	B	169	LEU	N-CA-C	5.72	118.39	109.52
1	A	389	PHE	CA-C-N	5.72	131.06	122.99
1	A	389	PHE	C-N-CA	5.72	131.06	122.99
1	B	3115	VAL	N-CA-C	5.72	117.14	110.62
1	B	1101	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	4923	PHE	CA-CB-CG	-5.71	108.09	113.80
1	A	5020	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	261	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	835	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	3246	LEU	N-CA-C	5.70	117.30	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3870	ASN	CA-CB-CG	5.69	118.29	112.60
1	C	3595	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	A	206	CYS	N-CA-C	5.68	117.75	108.55
1	C	289	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	3054	VAL	N-CA-C	5.68	116.33	110.36
1	D	98	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	3994	HIS	CA-CB-CG	-5.68	108.12	113.80
1	D	261	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	1663	HIS	CA-CB-CG	-5.68	108.12	113.80
1	C	2647	HIS	CB-CG-CD2	-5.68	123.82	131.20
2	E	24	VAL	N-CA-C	5.67	116.53	108.42
1	D	2817	ILE	CB-CA-C	5.67	119.65	111.88
1	A	350	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	B	732	SER	N-CA-C	5.66	113.11	108.07
1	A	2542	SER	CA-C-N	5.66	128.42	120.28
1	A	2542	SER	C-N-CA	5.66	128.42	120.28
1	C	98	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	D	3246	LEU	N-CA-C	5.65	117.11	111.07
1	A	3321	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	A	863	LEU	CA-C-N	5.64	123.72	119.66
1	A	863	LEU	C-N-CA	5.64	123.72	119.66
1	D	4563	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	1641	ILE	N-CA-CB	-5.64	104.66	111.31
1	B	203	ASN	CA-C-N	5.64	125.61	120.03
1	B	203	ASN	C-N-CA	5.64	125.61	120.03
1	C	621	ILE	CB-CA-C	-5.64	104.75	111.97
2	H	24	VAL	N-CA-C	5.63	116.48	108.42
1	D	308	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	D	226	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	1828	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	4078	GLN	CA-C-N	5.62	128.37	120.28
1	B	4078	GLN	C-N-CA	5.62	128.37	120.28
1	D	3670	GLU	N-CA-C	5.62	117.20	111.14
1	A	2330	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	D	3465	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	3973	CYS	CA-CB-SG	-5.61	101.51	114.40
1	A	2136	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	C	1422	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	1994	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	D	1186	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	5034	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	1558	HIS	CB-CG-CD2	-5.59	123.94	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	TRP	N-CA-C	5.58	117.88	109.23
1	D	1558	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	4037	ASN	CA-CB-CG	-5.58	107.03	112.60
1	B	4079	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	2647	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	C	2768	PHE	CA-CB-CG	5.57	119.37	113.80
1	C	3858	MET	N-CA-C	5.57	117.52	110.33
1	B	200	TRP	N-CA-C	5.57	117.73	108.99
1	D	3973	CYS	CA-CB-SG	-5.57	101.59	114.40
1	A	4142	ASN	CA-CB-CG	-5.57	107.03	112.60
1	D	636	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	2495	VAL	N-CA-C	5.56	113.75	109.19
1	A	2187	ASN	CA-CB-CG	-5.56	107.04	112.60
1	C	3973	CYS	CA-CB-SG	-5.56	101.62	114.40
1	D	45	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	C	601	ASP	CA-CB-CG	-5.55	107.05	112.60
1	A	2785	LEU	CA-C-N	5.55	132.14	121.54
1	A	2785	LEU	C-N-CA	5.55	132.14	121.54
1	B	3998	HIS	CA-CB-CG	-5.55	108.25	113.80
1	A	3883	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	2014	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	328	LYS	N-CA-C	5.54	116.69	108.60
1	A	1558	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	3010	PHE	CA-CB-CG	-5.54	108.26	113.80
1	B	1580	PHE	CA-CB-CG	-5.54	108.26	113.80
1	C	1216	ILE	CA-CB-CG1	5.54	119.81	110.40
1	D	658	GLN	N-CA-C	5.54	117.60	109.24
1	A	818	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	C	3670	GLU	N-CA-C	5.53	117.12	111.14
1	A	203	ASN	CA-C-N	5.53	125.51	120.03
1	A	203	ASN	C-N-CA	5.53	125.51	120.03
1	C	4756	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	D	3771	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	5019	TRP	CA-C-N	5.53	128.45	120.38
1	A	5019	TRP	C-N-CA	5.53	128.45	120.38
1	C	284	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	2647	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	D	3994	HIS	CA-CB-CG	-5.51	108.29	113.80
1	D	1070	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	4159	ARG	NE-CZ-NH2	5.51	124.16	119.20
2	E	87	HIS	CA-CB-CG	-5.51	108.29	113.80
1	D	1999	ARG	NE-CZ-NH2	5.50	124.15	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3945	GLU	N-CA-C	5.50	117.28	111.28
1	D	4879	MET	N-CA-CB	5.50	118.21	110.12
1	B	203	ASN	CB-CA-C	5.50	118.32	109.41
1	D	284	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	774	ASP	CA-CB-CG	5.50	118.09	112.60
1	B	2515	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	C	2588	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	D	2776	SER	N-CA-C	5.49	118.61	110.48
1	C	4192	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	C	1828	ASP	CA-CB-CG	5.49	118.08	112.60
1	D	4968	PHE	CA-CB-CG	-5.48	108.32	113.80
1	D	289	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	B	3883	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	2136	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	C	4092	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	1748	PHE	CA-CB-CG	5.47	119.27	113.80
1	C	2621	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	D	2821	TRP	CA-CB-CG	5.47	124.00	113.60
1	C	2498	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	C	2517	PHE	CA-CB-CG	-5.47	108.33	113.80
1	C	1713	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	1641	ILE	N-CA-CB	-5.46	104.86	111.31
1	B	2556	LEU	N-CA-CB	-5.46	103.32	110.59
1	B	3670	GLU	N-CA-C	5.46	117.04	111.14
1	D	3984	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	2014	ASP	CA-CB-CG	5.46	118.06	112.60
1	D	2000	SER	N-CA-C	5.46	114.58	108.25
1	C	2452	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	D	242	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	B	474	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	A	2676	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	D	2676	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	2621	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	C	2014	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	1558	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	D	533	ASN	CA-C-N	5.43	127.81	120.38
1	D	533	ASN	C-N-CA	5.43	127.81	120.38
1	D	4756	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	C	3010	PHE	CA-CB-CG	-5.42	108.38	113.80
1	D	2545	GLU	N-CA-C	5.42	116.87	111.07
1	B	2588	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	1186	ASP	CA-CB-CG	5.42	118.02	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	818	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	4753	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	B	226	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	C	2487	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	C	2330	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	1131	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	4744	ASP	CA-C-N	5.39	127.51	120.28
1	A	4744	ASP	C-N-CA	5.39	127.51	120.28
1	C	1683	HIS	CA-CB-CG	-5.39	108.41	113.80
1	B	4756	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	D	140	ASP	N-CA-C	5.39	116.47	108.60
1	B	4010	ILE	N-CA-C	5.39	117.78	111.05
1	C	4110	PHE	CA-CB-CG	5.38	119.18	113.80
1	C	1575	LEU	N-CA-C	5.38	117.22	111.36
1	A	5003	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	C	3283	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	D	3667	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	D	3033	ASN	CA-CB-CG	5.38	117.97	112.60
1	B	3033	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	4679	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	1580	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	3246	LEU	N-CA-C	5.37	116.94	111.14
1	D	2673	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	B	2330	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	851	PHE	CA-CB-CG	5.36	119.16	113.80
1	D	2615	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	D	2600	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	A	3368	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	1186	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	2498	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	C	2415	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	D	2291	GLN	CA-C-N	5.36	127.46	120.28
1	D	2291	GLN	C-N-CA	5.36	127.46	120.28
1	D	2163	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	69	LEU	N-CA-CB	-5.35	103.34	110.57
1	C	3994	HIS	CA-CB-CG	-5.35	108.45	113.80
1	C	4548	ARG	N-CA-C	-5.35	105.36	111.14
1	A	1845	VAL	CB-CA-C	-5.34	105.13	111.97
1	D	350	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	A	226	HIS	CA-CB-CG	-5.34	108.46	113.80
1	A	2498	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	C	4879	MET	N-CA-CB	5.34	117.97	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2415	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	2738	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	3895	HIS	CB-CG-CD2	-5.34	124.26	131.20
2	G	24	VAL	N-CA-C	5.34	116.05	108.42
1	A	3868	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	3878	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	226	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	C	2673	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	4070	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	5003	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	B	3994	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	4092	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	1828	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	1550	PRO	N-CA-CB	5.30	108.05	103.27
1	B	3895	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	B	2498	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	C	1143	TRP	N-CA-C	5.30	116.76	110.19
1	B	1825	HIS	CA-CB-CG	5.30	119.10	113.80
1	C	1776	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	C	350	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	C	4087	LEU	CA-C-N	5.29	130.21	122.69
1	C	4087	LEU	C-N-CA	5.29	130.21	122.69
1	A	2673	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	B	2029	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	C	2542	SER	CA-C-N	5.29	127.36	120.28
1	C	2542	SER	C-N-CA	5.29	127.36	120.28
1	A	3683	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	A	134	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	2187	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	347	PHE	CA-CB-CG	5.28	119.08	113.80
1	B	3207	GLU	CA-C-N	5.28	124.99	119.82
1	B	3207	GLU	C-N-CA	5.28	124.99	119.82
1	A	45	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	B	2673	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	C	3266	MET	CA-C-N	5.26	124.87	119.56
1	C	3266	MET	C-N-CA	5.26	124.87	119.56
1	D	2187	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	1994	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	2000	SER	N-CA-C	5.25	114.34	108.25
2	E	42	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	1550	PRO	N-CA-CB	5.25	107.99	103.27
1	B	350	HIS	CA-CB-CG	-5.25	108.56	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1201	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	D	3287	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	B	124	SER	CA-C-N	5.24	131.55	121.54
1	B	124	SER	C-N-CA	5.24	131.55	121.54
1	B	4076	ALA	CA-C-N	5.24	129.54	120.58
1	B	4076	ALA	C-N-CA	5.24	129.54	120.58
1	B	2544	THR	CA-C-N	5.23	127.24	120.44
1	B	2544	THR	C-N-CA	5.23	127.24	120.44
1	D	1845	VAL	CB-CA-C	-5.23	105.27	111.97
1	C	618	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	C	4658	ILE	CB-CA-C	-5.23	105.08	112.14
1	C	1180	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	C	1641	ILE	N-CA-CB	-5.23	105.14	111.31
1	C	3895	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	A	4131	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	3343	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	B	2001	PRO	N-CA-CB	5.22	106.11	103.19
1	A	1070	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	2168	VAL	N-CA-C	5.22	115.49	107.77
1	A	3292	PRO	CA-C-N	5.22	125.75	120.38
1	A	3292	PRO	C-N-CA	5.22	125.75	120.38
1	B	2000	SER	CA-C-N	5.22	123.47	119.66
1	B	2000	SER	C-N-CA	5.22	123.47	119.66
1	D	1683	HIS	CA-CB-CG	-5.22	108.58	113.80
1	D	4658	ILE	CB-CA-C	-5.21	105.10	112.14
1	A	1141	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	B	1825	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	C	3944	GLU	CA-C-N	5.21	127.26	120.28
1	C	3944	GLU	C-N-CA	5.21	127.26	120.28
1	B	151	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	C	4556	SER	CA-C-N	5.21	127.78	120.28
1	C	4556	SER	C-N-CA	5.21	127.78	120.28
1	D	2452	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	3167	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	1139	PHE	CA-CB-CG	-5.21	108.59	113.80
1	B	533	ASN	CA-C-N	5.21	127.51	120.38
1	B	533	ASN	C-N-CA	5.21	127.51	120.38
1	D	2495	VAL	N-CA-C	5.21	113.46	109.19
1	D	4056	GLU	CB-CA-C	-5.21	102.71	110.88
1	B	2168	VAL	N-CA-C	5.20	115.47	107.77
1	D	267	ILE	CA-C-N	5.20	129.06	121.31
1	D	267	ILE	C-N-CA	5.20	129.06	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4658	ILE	CB-CA-C	-5.20	105.31	111.97
1	D	2768	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	3357	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	D	4131	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	879	HIS	CA-CB-CG	5.20	119.00	113.80
1	A	4076	ALA	CA-C-N	5.19	127.66	120.29
1	A	4076	ALA	C-N-CA	5.19	127.66	120.29
1	C	3773	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	C	5003	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	D	4676	GLU	CB-CA-C	-5.19	102.17	110.79
1	C	533	ASN	CA-C-N	5.19	127.49	120.38
1	C	533	ASN	C-N-CA	5.19	127.49	120.38
1	A	2291	GLN	CA-C-N	5.19	127.48	120.38
1	A	2291	GLN	C-N-CA	5.19	127.48	120.38
1	D	1131	ARG	NE-CZ-NH2	5.18	123.87	119.20
1	A	1663	HIS	CA-CB-CG	-5.18	108.62	113.80
1	B	4548	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	4174	PHE	CB-CA-C	5.18	119.34	110.01
1	C	1186	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	2330	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	3773	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	D	2629	ASP	CA-C-N	5.17	123.50	120.24
1	D	2629	ASP	C-N-CA	5.17	123.50	120.24
1	B	4079	ASP	N-CA-CB	-5.17	102.26	110.22
1	B	263	GLU	CA-C-N	5.17	125.45	119.92
1	B	263	GLU	C-N-CA	5.17	125.45	119.92
1	B	4563	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	D	4080	TYR	N-CA-C	5.17	119.58	113.28
1	A	2345	SER	N-CA-C	5.16	117.37	110.35
1	A	4563	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	C	3716	LEU	N-CA-CB	-5.16	103.32	110.38
1	D	226	HIS	CA-CB-CG	-5.16	108.64	113.80
1	D	203	ASN	CB-CA-C	5.15	117.76	109.41
1	A	1580	PHE	N-CA-C	5.15	118.14	110.52
1	A	2274	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	4548	ARG	NE-CZ-NH2	5.15	123.83	119.20
2	F	87	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	879	HIS	CA-CB-CG	5.15	118.95	113.80
1	B	475	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	B	3667	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	C	1825	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	C	3892	CYS	CA-CB-SG	-5.14	102.57	114.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4153	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	B	1521	ASP	N-CA-C	5.14	116.89	108.52
1	A	1131	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	C	3985	LEU	N-CA-C	5.13	117.54	111.33
1	B	1127	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	4658	ILE	CB-CA-C	-5.13	105.22	112.14
1	C	836	GLY	CA-C-N	5.13	125.34	120.31
1	C	836	GLY	C-N-CA	5.13	125.34	120.31
1	B	203	ASN	CA-CB-CG	-5.13	107.47	112.60
1	B	350	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	D	4548	ARG	N-CA-C	-5.12	105.78	111.36
1	B	1646	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	5019	TRP	CA-C-N	5.12	127.85	120.38
1	B	5019	TRP	C-N-CA	5.12	127.85	120.38
1	B	2345	SER	N-CA-C	5.11	117.31	110.35
1	B	3595	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	5003	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	C	4679	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	728	ARG	CA-C-N	5.11	125.04	119.78
1	D	728	ARG	C-N-CA	5.11	125.04	119.78
1	A	2713	ASP	CA-CB-CG	5.11	117.70	112.60
1	C	242	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	B	1303	CYS	N-CA-C	5.10	116.68	110.41
1	B	4220	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	1143	TRP	N-CA-C	5.09	117.10	110.53
1	A	5006	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	C	261	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	1623	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	3716	LEU	N-CA-CB	-5.09	102.98	110.26
1	B	460	GLN	CA-C-N	5.09	127.10	120.28
1	B	460	GLN	C-N-CA	5.09	127.10	120.28
1	B	2773	ASN	CA-CB-CG	5.09	117.69	112.60
1	B	4760	PRO	N-CA-C	5.09	116.91	110.70
1	C	1201	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	C	1124	PHE	CA-CB-CG	-5.09	108.71	113.80
1	C	2827	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	3771	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	D	3368	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	4870	ASP	CA-CB-CG	5.08	117.69	112.60
1	B	1092	PHE	CA-CB-CG	-5.08	108.72	113.80
1	B	1580	PHE	N-CA-C	5.08	118.05	110.52
1	D	1301	PHE	CA-CB-CG	5.08	118.89	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	D	2168	VAL	N-CA-C	5.08	115.30	107.77
1	D	4163	PHE	CA-CB-CG	-5.08	108.72	113.80
1	D	1775	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	B	1776	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	D	151	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	D	593	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	B	836	GLY	CA-C-N	5.07	125.28	120.31
1	B	836	GLY	C-N-CA	5.07	125.28	120.31
1	C	2385	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	B	4548	ARG	N-CA-C	-5.07	105.83	111.36
1	B	18	ASP	N-CA-C	5.07	117.07	110.43
1	C	1663	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	1423	ASP	CA-C-N	5.06	125.34	119.47
1	A	1423	ASP	C-N-CA	5.06	125.34	119.47
1	B	1139	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	3343	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	1136	SER	N-CA-C	5.06	117.07	109.23
1	C	1521	ASP	N-CA-C	5.06	116.77	108.52
1	C	4870	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	4968	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	178	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	B	215	THR	CA-C-N	5.06	125.14	120.34
1	B	215	THR	C-N-CA	5.06	125.14	120.34
1	D	1252	HIS	CA-CB-CG	-5.06	108.74	113.80
1	D	2001	PRO	CA-C-N	5.06	124.23	118.97
1	D	2001	PRO	C-N-CA	5.06	124.23	118.97
1	D	2697	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	D	2508	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	D	2556	LEU	N-CA-CB	-5.05	103.87	110.59
1	B	3266	MET	CA-C-N	5.05	124.66	119.56
1	B	3266	MET	C-N-CA	5.05	124.66	119.56
1	A	4163	PHE	CA-CB-CG	-5.05	108.75	113.80
1	B	69	LEU	N-CA-CB	-5.05	103.75	110.57
1	C	4220	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	4563	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A	4773	VAL	N-CA-C	5.05	117.36	111.05
1	C	475	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	D	1743	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	B	280	LEU	N-CA-C	5.04	116.19	108.42
1	B	1713	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	4056	GLU	CB-CA-C	-5.04	102.75	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2508	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	1143	TRP	N-CA-C	5.04	116.43	110.19
1	B	2291	GLN	CA-C-O	5.03	126.80	121.11
1	D	5026	ASP	N-CA-C	5.03	115.94	108.60
1	B	991	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	751	SER	CA-C-N	5.03	124.35	120.33
1	C	751	SER	C-N-CA	5.03	124.35	120.33
1	A	3966	THR	CB-CA-C	-5.03	102.99	110.88
1	C	4079	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	774	ASP	CA-CB-CG	5.03	117.62	112.60
1	D	2788	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	B	818	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	C	1550	PRO	N-CA-CB	5.02	107.79	103.27
1	D	910	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	12	GLN	N-CA-C	5.02	117.18	109.95
1	B	2821	TRP	CA-CB-CG	5.02	123.14	113.60
1	C	3998	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	200	TRP	N-CA-C	5.02	117.01	109.23
1	A	864	PRO	N-CA-CB	5.02	105.83	103.22
1	B	45	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	D	1776	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	C	3321	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	5020	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	728	ARG	CA-C-N	5.01	124.94	119.78
1	B	728	ARG	C-N-CA	5.01	124.94	119.78
1	B	1301	PHE	CA-CB-CG	5.01	118.81	113.80
1	B	1845	VAL	CB-CA-C	-5.01	105.56	111.97
1	B	2465	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	1845	VAL	CB-CA-C	-5.01	105.56	111.97
1	B	1994	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	C	2615	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	1772	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	263	GLU	CA-C-N	5.01	125.28	119.92
1	A	263	GLU	C-N-CA	5.01	125.28	119.92
1	C	551	LEU	N-CA-C	5.01	118.88	112.87
1	D	1506	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	D	1550	PRO	N-CA-CB	5.00	107.77	103.36
1	A	3686	GLU	CA-C-N	5.00	131.10	121.54
1	A	3686	GLU	C-N-CA	5.00	131.10	121.54
1	B	281	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	C	593	HIS	CB-CG-CD2	-5.00	124.70	131.20
1	D	133	PHE	CA-C-N	5.00	127.97	120.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	PHE	C-N-CA	5.00	127.97	120.87
1	D	203	ASN	CA-CB-CG	-5.00	107.60	112.60
1	D	816	LEU	CA-C-N	5.00	124.78	119.28
1	D	816	LEU	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

All (152) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1024	TYR	Sidechain
1	A	1607	ARG	Sidechain
1	A	1670	TYR	Sidechain
1	A	1725	ARG	Sidechain
1	A	2110	TYR	Sidechain
1	A	2142	TYR	Sidechain
1	A	2244	ARG	Sidechain
1	A	226	HIS	Sidechain
1	A	2301	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	2452	ARG	Sidechain
1	A	2624	ARG	Sidechain
1	A	2777	TYR	Sidechain
1	A	2855	TYR	Sidechain
1	A	2935	TYR	Sidechain
1	A	3219	TYR	Sidechain
1	A	3263	TYR	Sidechain
1	A	3350	ARG	Sidechain
1	A	350	HIS	Sidechain
1	A	3613	TYR	Sidechain
1	A	3819	TYR	Sidechain
1	A	3895	HIS	Sidechain
1	A	392	ARG	Sidechain
1	A	3933	PHE	Sidechain
1	A	3936	TYR	Sidechain
1	A	3937	TYR	Sidechain
1	A	3949	ARG	Sidechain
1	A	4080	TYR	Sidechain
1	A	4177	TYR	Sidechain
1	A	426	ARG	Sidechain
1	A	474	ARG	Sidechain
1	A	4888	TYR	Sidechain
1	A	497	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	714	TYR	Sidechain
1	A	76	ARG	Sidechain
1	A	893	TYR	Sidechain
1	A	959	TYR	Sidechain
1	B	1025	ARG	Sidechain
1	B	1073	ARG	Sidechain
1	B	1089	TYR	Sidechain
1	B	1607	ARG	Sidechain
1	B	1748	PHE	Sidechain
1	B	1977	TYR	Sidechain
1	B	2142	TYR	Sidechain
1	B	2244	ARG	Sidechain
1	B	226	HIS	Sidechain
1	B	2301	TYR	Sidechain
1	B	2340	PHE	Sidechain
1	B	242	ARG	Sidechain
1	B	2452	ARG	Sidechain
1	B	2935	TYR	Sidechain
1	B	2954	ARG	Sidechain
1	B	3213	TYR	Sidechain
1	B	3219	TYR	Sidechain
1	B	3280	TYR	Sidechain
1	B	3350	ARG	Sidechain
1	B	347	PHE	Sidechain
1	B	3765	TYR	Sidechain
1	B	3819	TYR	Sidechain
1	B	3937	TYR	Sidechain
1	B	3949	ARG	Sidechain
1	B	4080	TYR	Sidechain
1	B	4153	HIS	Sidechain
1	B	45	ARG	Sidechain
1	B	4775	TYR	Sidechain
1	B	4804	TYR	Sidechain
1	B	4860	ARG	Sidechain
1	B	4912	TYR	Sidechain
1	B	4994	TYR	Sidechain
1	B	714	TYR	Sidechain
1	B	818	ARG	Sidechain
1	B	920	TYR	Sidechain
1	C	1025	ARG	Sidechain
1	C	103	TYR	Sidechain
1	C	1071	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	1434	TYR	Sidechain
1	C	1607	ARG	Sidechain
1	C	1725	ARG	Sidechain
1	C	1808	ARG	Sidechain
1	C	2110	TYR	Sidechain
1	C	2142	TYR	Sidechain
1	C	226	HIS	Sidechain
1	C	2301	TYR	Sidechain
1	C	2340	PHE	Sidechain
1	C	242	ARG	Sidechain
1	C	3213	TYR	Sidechain
1	C	3219	TYR	Sidechain
1	C	3263	TYR	Sidechain
1	C	3350	ARG	Sidechain
1	C	3380	ARG	Sidechain
1	C	341	TYR	Sidechain
1	C	347	PHE	Sidechain
1	C	3613	TYR	Sidechain
1	C	3819	TYR	Sidechain
1	C	3895	HIS	Sidechain
1	C	392	ARG	Sidechain
1	C	3934	TYR	Sidechain
1	C	3949	ARG	Sidechain
1	C	4194	TYR	Sidechain
1	C	4719	PHE	Sidechain
1	C	474	ARG	Sidechain
1	C	4888	TYR	Sidechain
1	C	4912	TYR	Sidechain
1	C	4967	TYR	Sidechain
1	C	714	TYR	Sidechain
1	C	76	ARG	Sidechain
1	C	818	ARG	Sidechain
1	C	829	TYR	Sidechain
1	D	1025	ARG	Sidechain
1	D	1071	ARG	Sidechain
1	D	111	HIS	Sidechain
1	D	1607	ARG	Sidechain
1	D	1670	TYR	Sidechain
1	D	2142	TYR	Sidechain
1	D	2244	ARG	Sidechain
1	D	226	HIS	Sidechain
1	D	2301	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	2340	PHE	Sidechain
1	D	242	ARG	Sidechain
1	D	247	TYR	Sidechain
1	D	2624	ARG	Sidechain
1	D	2777	TYR	Sidechain
1	D	3350	ARG	Sidechain
1	D	341	TYR	Sidechain
1	D	347	PHE	Sidechain
1	D	3613	TYR	Sidechain
1	D	3819	TYR	Sidechain
1	D	392	ARG	Sidechain
1	D	3937	TYR	Sidechain
1	D	3949	ARG	Sidechain
1	D	4080	TYR	Sidechain
1	D	4153	HIS	Sidechain
1	D	426	ARG	Sidechain
1	D	4719	PHE	Sidechain
1	D	474	ARG	Sidechain
1	D	4775	TYR	Sidechain
1	D	4888	TYR	Sidechain
1	D	4909	TYR	Sidechain
1	D	4912	TYR	Sidechain
1	D	4994	TYR	Sidechain
1	D	714	TYR	Sidechain
1	D	818	ARG	Sidechain
1	D	902	ARG	Sidechain
1	D	920	TYR	Sidechain
2	E	57	ARG	Sidechain
2	E	71	ARG	Sidechain
2	F	57	ARG	Sidechain
2	F	71	ARG	Sidechain
2	G	57	ARG	Sidechain
2	G	71	ARG	Sidechain
2	H	57	ARG	Sidechain
2	H	71	ARG	Sidechain

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	35088	34740	34717	123	0
1	B	35088	34740	34717	121	0
1	C	35088	34740	34717	127	0
1	D	35088	34740	34717	129	0
2	E	832	829	831	0	0
2	F	832	829	831	3	0
2	G	832	829	831	2	0
2	H	832	829	831	1	0
All	All	143680	142276	142192	500	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 2.

All (500) 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:D:171:LEU:HD23	1:D:171:LEU:H	1.53	0.71
1:C:171:LEU:H	1:C:171:LEU:HD23	1.57	0.70
1:B:171:LEU:HD23	1:B:171:LEU:H	1.57	0.69
1:B:284:HIS:ND1	1:B:287:THR:HG22	2.07	0.69
1:A:171:LEU:H	1:A:171:LEU:HD23	1.57	0.69
1:C:2719:TYR:CE2	1:C:2948:THR:HG21	2.31	0.65
1:A:22:LEU:HD23	1:A:22:LEU:H	1.61	0.64
1:D:2948:THR:HG23	1:D:2952:GLU:HB2	1.82	0.62
1:C:2948:THR:HG23	1:C:2952:GLU:HB2	1.83	0.60
1:A:22:LEU:H	1:A:22:LEU:CD2	2.14	0.60
1:D:1930:LYS:C	1:D:1931:LEU:HD22	2.29	0.58
1:C:169:LEU:HD23	1:C:170:ILE:N	2.19	0.57
1:D:2719:TYR:CE2	1:D:2948:THR:HG21	2.39	0.57
1:B:284:HIS:CE1	1:B:286:THR:H	2.23	0.57
1:D:1022:VAL:HG22	1:D:1023:PRO:HD2	1.87	0.57
1:D:2117:VAL:HA	1:D:2120:MET:SD	2.45	0.57
1:B:1496:TRP:CD1	1:B:1498:GLY:H	2.22	0.56
1:B:2948:THR:HG23	1:B:2952:GLU:HB2	1.86	0.56
1:B:1930:LYS:C	1:B:1931:LEU:HD22	2.32	0.55
1:A:2948:THR:HG23	1:A:2952:GLU:HB2	1.87	0.55
1:B:458:GLU:CD	1:B:458:GLU:H	2.14	0.55
1:B:4690:GLU:C	1:B:4692:PRO:HD3	2.32	0.55
1:D:169:LEU:HD23	1:D:170:ILE:N	2.21	0.54
1:B:2117:VAL:HA	1:B:2120:MET:SD	2.48	0.54
1:A:213:TYR:CD2	1:A:340:LYS:HE3	2.43	0.54
1:A:483:MET:HA	1:A:483:MET:HE3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:VAL:HA	1:A:2120:MET:SD	2.48	0.54
1:A:1297:PHE:CE2	1:A:1546:THR:HB	2.43	0.53
1:C:1930:LYS:C	1:C:1931:LEU:HD22	2.33	0.53
1:D:1496:TRP:CD1	1:D:1498:GLY:H	2.26	0.53
1:A:4978:HIS:CE1	1:A:4983:HIS:CG	2.96	0.53
1:C:213:TYR:CD2	1:C:340:LYS:HE3	2.44	0.53
1:D:4199:GLU:H	1:D:4199:GLU:CD	2.16	0.53
1:C:4031:LEU:HD21	1:C:4044:MET:HE1	1.91	0.53
1:B:2719:TYR:CE2	1:B:2948:THR:HG21	2.43	0.53
1:D:284:HIS:ND1	1:D:287:THR:HG22	2.23	0.53
1:B:2495:VAL:H	1:B:2498:HIS:CD2	2.27	0.53
1:B:3899:PHE:CE1	1:B:3903:LEU:HD21	2.44	0.52
1:C:2117:VAL:HA	1:C:2120:MET:SD	2.48	0.52
1:D:111:HIS:CE1	1:D:114:SER:H	2.28	0.52
1:C:1496:TRP:CD1	1:C:1498:GLY:H	2.28	0.52
1:C:2495:VAL:H	1:C:2498:HIS:CD2	2.27	0.52
1:B:483:MET:HE3	1:B:483:MET:HA	1.91	0.52
1:B:1076:ARG:HH11	1:B:1605:TRP:CG	2.27	0.52
1:D:483:MET:HE3	1:D:483:MET:HA	1.90	0.52
1:C:4989:MET:SD	1:C:4989:MET:C	2.93	0.52
1:B:213:TYR:CD2	1:B:340:LYS:HE3	2.45	0.52
1:C:76:ARG:NH1	1:D:3936:TYR:H	2.06	0.52
1:B:4987:ASN:HA	1:B:4990:PHE:CD2	2.45	0.52
1:A:458:GLU:CD	1:A:458:GLU:H	2.18	0.51
1:C:2777:TYR:HA	1:C:2787:THR:HG23	1.91	0.51
1:D:287:THR:HG23	1:D:289:ARG:H	1.74	0.51
1:D:227:MET:HE2	1:D:227:MET:H	1.75	0.51
1:D:1715:LEU:C	1:D:1715:LEU:HD23	2.35	0.51
1:A:1496:TRP:CD1	1:A:1498:GLY:H	2.28	0.51
1:B:359:TYR:CZ	1:B:383:HIS:CE1	2.98	0.51
1:C:146:CYS:HG	1:C:147:TRP:CD1	2.28	0.51
1:C:4023:MET:SD	1:C:4023:MET:C	2.94	0.51
1:C:4958:CYS:CB	1:C:4961:CYS:HG	2.23	0.51
1:C:1127:HIS:CE1	1:C:1128:ARG:HH11	2.29	0.51
1:D:213:TYR:CD2	1:D:340:LYS:HE3	2.46	0.51
1:A:359:TYR:CE2	1:A:383:HIS:CE1	3.00	0.50
1:B:2150:GLU:CD	1:B:2150:GLU:H	2.19	0.50
1:D:2495:VAL:H	1:D:2498:HIS:CD2	2.30	0.50
1:D:3936:TYR:CD1	1:D:3936:TYR:C	2.88	0.50
1:D:4989:MET:SD	1:D:4989:MET:C	2.94	0.50
1:B:3936:TYR:CD1	1:B:3936:TYR:C	2.90	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:TYR:CZ	1:C:383:HIS:CE1	2.99	0.50
1:D:4023:MET:SD	1:D:4023:MET:C	2.95	0.50
1:A:4986:ALA:HB1	1:A:4990:PHE:CZ	2.47	0.50
1:B:1741:GLU:CD	1:B:1741:GLU:H	2.20	0.50
1:B:4978:HIS:CE1	1:B:4983:HIS:CG	3.00	0.50
1:C:3936:TYR:CD1	1:C:3936:TYR:C	2.90	0.50
1:D:2700:MET:SD	1:D:2701:PRO:HD3	2.52	0.50
1:D:4986:ALA:HB1	1:D:4990:PHE:CZ	2.47	0.49
1:A:2700:MET:SD	1:A:2701:PRO:HD3	2.52	0.49
1:A:1715:LEU:C	1:A:1715:LEU:HD23	2.37	0.49
1:C:4003:LEU:HD22	1:C:4013:LEU:HB2	1.93	0.49
1:A:2719:TYR:CE2	1:A:2948:THR:HG21	2.47	0.49
1:A:2875:ALA:HA	1:A:2927:LEU:HD13	1.94	0.49
1:B:2101:MET:SD	1:B:2105:TRP:CE2	3.06	0.49
1:A:284:HIS:CE1	1:A:287:THR:H	2.31	0.49
1:A:2495:VAL:H	1:A:2498:HIS:CD2	2.31	0.49
1:B:1715:LEU:HD23	1:B:1715:LEU:C	2.38	0.49
1:B:1730:MET:HE3	1:B:1773:PRO:HD2	1.94	0.49
1:C:4987:ASN:HA	1:C:4990:PHE:CD2	2.48	0.49
1:A:1930:LYS:C	1:A:1931:LEU:HD22	2.38	0.49
1:D:609:CYS:H	1:D:612:VAL:HB	1.78	0.49
1:D:1184:ILE:H	1:D:1184:ILE:HD12	1.78	0.49
1:D:2101:MET:SD	1:D:2105:TRP:CE2	3.06	0.49
1:A:4989:MET:SD	1:A:4989:MET:C	2.95	0.49
1:B:828:GLU:HG2	1:B:829:TYR:H	1.77	0.49
1:A:227:MET:H	1:A:227:MET:HE2	1.76	0.48
1:C:1805:GLU:H	1:C:1805:GLU:CD	2.20	0.48
1:D:308:HIS:CD2	1:D:311:ALA:H	2.31	0.48
1:B:359:TYR:CE2	1:B:383:HIS:CE1	3.02	0.48
1:C:2150:GLU:H	1:C:2150:GLU:CD	2.21	0.48
1:D:487:VAL:HA	1:D:490:CYS:SG	2.53	0.48
1:D:2292:GLU:CD	1:D:2292:GLU:H	2.21	0.48
1:D:4958:CYS:SG	1:D:4961:CYS:SG	3.06	0.48
1:A:579:GLN:H	1:A:582:HIS:CE1	2.32	0.48
1:B:347:PHE:CE1	1:B:387:ALA:HB2	2.48	0.48
1:B:4989:MET:SD	1:B:4989:MET:C	2.96	0.48
1:C:287:THR:HG23	1:C:289:ARG:H	1.78	0.48
1:D:4978:HIS:CE1	1:D:4983:HIS:CG	3.02	0.48
1:A:319:SER:HA	1:A:347:PHE:CE1	2.48	0.48
1:D:1741:GLU:CD	1:D:1741:GLU:H	2.22	0.48
1:A:35:LEU:HD23	1:A:51:PRO:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1741:GLU:CD	1:C:1741:GLU:H	2.22	0.48
1:B:147:TRP:C	1:B:148:TRP:CD1	2.92	0.47
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.49	0.47
1:C:359:TYR:CE2	1:C:383:HIS:CE1	3.02	0.47
1:B:4986:ALA:HB1	1:B:4990:PHE:CZ	2.50	0.47
1:C:4735:GLU:CD	1:C:4735:GLU:H	2.22	0.47
1:D:2348:GLU:CD	1:D:2348:GLU:H	2.22	0.47
1:D:4064:MET:HE2	1:D:4064:MET:HA	1.96	0.47
1:A:2150:GLU:CD	1:A:2150:GLU:H	2.21	0.47
1:A:4003:LEU:HD22	1:A:4013:LEU:HB2	1.95	0.47
1:A:4987:ASN:HA	1:A:4990:PHE:CD2	2.50	0.47
1:B:3653:PHE:CD1	1:B:3653:PHE:C	2.92	0.47
1:A:2506:LEU:HD23	1:A:2507:ASP:N	2.30	0.47
1:C:1715:LEU:C	1:C:1715:LEU:HD23	2.40	0.47
1:C:3092:LEU:C	1:C:3092:LEU:HD23	2.40	0.47
1:A:3631:ALA:HB2	1:A:3859:VAL:HG11	1.97	0.47
1:A:4795:TYR:CZ	1:A:4812:HIS:CD2	3.03	0.47
1:C:2178:MET:SD	1:C:2182:ILE:HD11	2.54	0.47
1:C:4978:HIS:CE1	1:C:4983:HIS:CG	3.02	0.47
1:D:458:GLU:CD	1:D:458:GLU:H	2.23	0.47
1:D:579:GLN:H	1:D:582:HIS:CE1	2.32	0.47
1:C:2712:PRO:HA	1:C:2955:PHE:CE2	2.50	0.47
1:C:4194:TYR:CD2	1:C:4194:TYR:N	2.82	0.47
1:D:359:TYR:CZ	1:D:383:HIS:CE1	3.03	0.47
1:A:4023:MET:SD	1:A:4023:MET:C	2.98	0.47
1:D:4003:LEU:HD22	1:D:4013:LEU:HB2	1.96	0.47
1:A:4735:GLU:CD	1:A:4735:GLU:H	2.23	0.46
1:C:2101:MET:SD	1:C:2105:TRP:CE2	3.08	0.46
1:D:2970:SER:HA	1:D:2973:PHE:CE2	2.50	0.46
1:A:76:ARG:HD3	1:B:3935:TRP:CD2	2.49	0.46
1:B:2908:TYR:CZ	1:B:2916:LYS:HE2	2.50	0.46
1:B:3670:GLU:CD	1:B:3670:GLU:H	2.23	0.46
1:B:4795:TYR:CZ	1:B:4812:HIS:CD2	3.03	0.46
1:D:113:HIS:H	1:D:113:HIS:CD2	2.34	0.46
1:D:2150:GLU:CD	1:D:2150:GLU:H	2.23	0.46
1:D:213:TYR:CD1	1:D:340:LYS:HG2	2.50	0.46
1:D:1926:LEU:HA	1:D:1929:MET:SD	2.55	0.46
1:D:4231:MET:SD	1:D:4231:MET:N	2.89	0.46
1:B:101:LEU:C	1:B:102:LEU:HD12	2.41	0.46
1:C:4231:MET:SD	1:C:4231:MET:N	2.89	0.46
1:D:2497:ASP:O	1:D:2500:ALA:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4987:ASN:HA	1:D:4990:PHE:CD2	2.50	0.46
1:A:1741:GLU:H	1:A:1741:GLU:CD	2.24	0.46
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.50	0.46
1:C:2348:GLU:H	1:C:2348:GLU:CD	2.24	0.46
1:C:2700:MET:SD	1:C:2701:PRO:HD3	2.56	0.46
1:C:4986:ALA:HB1	1:C:4990:PHE:CZ	2.51	0.46
1:A:2348:GLU:CD	1:A:2348:GLU:H	2.24	0.46
1:A:3092:LEU:C	1:A:3092:LEU:HD23	2.41	0.46
1:B:2545:GLU:CD	1:B:2545:GLU:H	2.24	0.46
1:C:111:HIS:CE1	1:C:114:SER:H	2.33	0.46
1:C:487:VAL:HA	1:C:490:CYS:SG	2.55	0.46
1:B:67:PHE:CD1	1:B:109:LEU:HB3	2.51	0.46
1:B:2700:MET:SD	1:B:2701:PRO:HD3	2.55	0.46
1:A:4958:CYS:CB	1:A:4961:CYS:HG	2.29	0.46
1:B:4003:LEU:HD22	1:B:4013:LEU:HB2	1.97	0.46
1:B:4231:MET:SD	1:B:4231:MET:N	2.89	0.46
1:A:4984:ASN:HD21	1:A:4986:ALA:HB3	1.81	0.46
1:B:487:VAL:HA	1:B:490:CYS:SG	2.56	0.46
1:B:1237:TRP:CE3	1:B:1606:SER:C	2.94	0.46
1:D:138:GLN:HG2	1:D:139:GLU:H	1.81	0.46
1:B:4064:MET:HA	1:B:4064:MET:HE2	1.98	0.45
1:A:284:HIS:ND1	1:A:287:THR:HG22	2.31	0.45
1:A:487:VAL:HA	1:A:490:CYS:SG	2.56	0.45
1:B:579:GLN:H	1:B:582:HIS:CE1	2.34	0.45
1:B:1727:ARG:HD3	1:B:1730:MET:HE1	1.98	0.45
1:C:81:MET:SD	1:C:81:MET:C	2.99	0.45
1:C:3657:TYR:CD1	1:C:3661:TRP:CD1	3.04	0.45
1:D:1805:GLU:CD	1:D:1805:GLU:H	2.23	0.45
1:D:2330:ARG:HA	1:D:2330:ARG:NE	2.32	0.45
1:A:1805:GLU:CD	1:A:1805:GLU:H	2.25	0.45
1:B:138:GLN:HG2	1:B:139:GLU:H	1.80	0.45
1:B:3675:ASP:C	1:B:3679:LYS:HE2	2.41	0.45
1:C:579:GLN:H	1:C:582:HIS:CE1	2.34	0.45
1:C:2292:GLU:H	1:C:2292:GLU:CD	2.24	0.45
1:D:222:LEU:N	1:D:222:LEU:HD12	2.31	0.45
1:A:2819:TRP:CG	1:A:2877:GLN:HE22	2.35	0.45
1:C:2970:SER:HA	1:C:2973:PHE:CE2	2.52	0.45
1:B:3290:GLU:CD	1:B:3309:SER:H	2.25	0.45
1:D:74:SER:O	1:D:77:ALA:HB3	2.16	0.45
1:D:4795:TYR:CZ	1:D:4812:HIS:CD2	3.04	0.45
1:B:111:HIS:CE1	1:B:113:HIS:CD2	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:CE1	1:D:286:THR:H	2.34	0.45
1:D:1421:ARG:CZ	1:D:1421:ARG:HA	2.47	0.45
1:A:284:HIS:CE1	1:A:286:THR:H	2.35	0.45
1:B:3092:LEU:C	1:B:3092:LEU:HD23	2.42	0.45
1:C:2481:LYS:HE2	1:C:2481:LYS:HA	1.99	0.45
1:D:2506:LEU:HD23	1:D:2507:ASP:N	2.31	0.45
1:D:3670:GLU:CD	1:D:3670:GLU:H	2.25	0.45
1:A:4173:TYR:CD1	1:A:4173:TYR:C	2.94	0.45
1:A:4194:TYR:CD2	1:A:4194:TYR:N	2.84	0.45
1:B:2292:GLU:CD	1:B:2292:GLU:H	2.25	0.45
1:C:2497:ASP:O	1:C:2500:ALA:HB3	2.17	0.45
1:C:4173:TYR:CD1	1:C:4173:TYR:C	2.94	0.45
1:D:1237:TRP:CE3	1:D:1606:SER:C	2.95	0.45
1:B:451:TYR:CD2	1:B:452:PHE:CE1	3.05	0.45
1:B:3973:CYS:SG	1:B:3976:ASN:CG	3.00	0.45
1:D:2340:PHE:CZ	1:D:2343:GLY:C	2.95	0.45
1:A:1237:TRP:CE3	1:A:1606:SER:C	2.95	0.45
1:A:2330:ARG:HA	1:A:2330:ARG:NE	2.32	0.45
1:A:2497:ASP:O	1:A:2500:ALA:HB3	2.17	0.45
1:B:2481:LYS:HE2	1:B:2481:LYS:HA	1.98	0.45
1:C:4795:TYR:CZ	1:C:4812:HIS:CD2	3.05	0.45
1:D:3902:TYR:CZ	1:D:3906:GLN:HA	2.52	0.45
1:B:2340:PHE:CZ	1:B:2343:GLY:C	2.95	0.44
1:B:4068:LEU:HA	1:B:4071:ILE:HG22	1.99	0.44
1:C:213:TYR:CD1	1:C:340:LYS:HG2	2.51	0.44
1:C:2110:TYR:CD1	1:C:2110:TYR:C	2.95	0.44
1:D:451:TYR:CD2	1:D:452:PHE:CZ	3.05	0.44
1:B:1748:PHE:CD1	1:B:1758:ARG:HB3	2.52	0.44
1:B:4978:HIS:CE1	1:B:4983:HIS:CD2	3.06	0.44
1:C:2955:PHE:CD1	1:C:2955:PHE:C	2.95	0.44
1:C:3778:MET:SD	1:C:3778:MET:C	3.00	0.44
1:C:3934:TYR:CD1	1:C:3934:TYR:C	2.95	0.44
1:C:4691:GLN:N	1:C:4692:PRO:HD3	2.33	0.44
1:D:121:LEU:HD23	1:D:122:THR:H	1.83	0.44
1:A:287:THR:HG23	1:A:289:ARG:H	1.82	0.44
1:A:2364:PHE:CD1	1:A:2364:PHE:N	2.85	0.44
1:A:3973:CYS:SG	1:A:3976:ASN:CG	3.00	0.44
1:A:4231:MET:SD	1:A:4231:MET:N	2.90	0.44
1:C:2228:MET:SD	1:C:2228:MET:C	3.00	0.44
1:C:483:MET:SD	1:C:483:MET:N	2.90	0.44
1:C:1237:TRP:CE3	1:C:1606:SER:C	2.95	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1926:LEU:C	1:A:1926:LEU:HD23	2.43	0.44
1:B:45:ARG:C	1:B:46:LEU:HD12	2.43	0.44
1:C:103:TYR:CZ	1:C:163:VAL:HG22	2.51	0.44
1:C:3973:CYS:SG	1:C:3976:ASN:CG	3.01	0.44
1:D:1286:MET:C	1:D:1286:MET:SD	3.00	0.44
1:A:1857:GLU:CD	1:A:1857:GLU:H	2.24	0.44
1:B:2712:PRO:HA	1:B:2955:PHE:CE2	2.52	0.44
1:C:110:ARG:HB2	1:C:117:TYR:CE2	2.53	0.44
1:C:4023:MET:HG2	1:C:4026:MET:HE3	2.00	0.44
1:D:3778:MET:SD	1:D:3778:MET:C	3.00	0.44
1:A:140:ASP:CG	1:A:142:THR:H	2.26	0.44
1:A:663:TYR:CE1	1:A:745:SER:HB3	2.53	0.44
1:B:76:ARG:HD3	1:C:3935:TRP:CE3	2.53	0.44
1:C:451:TYR:CD2	1:C:452:PHE:CZ	3.05	0.44
1:C:1926:LEU:HA	1:C:1929:MET:CE	2.47	0.44
1:D:3899:PHE:CE1	1:D:3903:LEU:HD21	2.52	0.44
1:D:4059:LEU:HA	1:D:4062:PHE:CZ	2.53	0.44
1:A:3934:TYR:CD1	1:A:3934:TYR:C	2.96	0.44
1:A:3937:TYR:CE1	1:A:3943:ILE:HA	2.53	0.44
1:B:1127:HIS:HA	1:B:1143:TRP:CZ2	2.53	0.44
1:B:2348:GLU:H	1:B:2348:GLU:CD	2.26	0.44
1:C:284:HIS:ND1	1:C:287:THR:HG22	2.33	0.44
1:D:503:PHE:CD2	1:D:515:TRP:CD1	3.05	0.44
1:A:1434:TYR:CD1	1:A:1434:TYR:C	2.94	0.43
1:B:2955:PHE:CD1	1:B:2955:PHE:C	2.96	0.43
1:C:1562:ILE:C	1:C:1562:ILE:HD12	2.43	0.43
1:D:1086:GLY:HA3	1:D:1088:TRP:CZ2	2.53	0.43
1:A:146:CYS:HG	1:A:147:TRP:CD1	2.36	0.43
1:A:171:LEU:HD21	1:A:180:LEU:HB3	2.00	0.43
1:A:483:MET:SD	1:A:483:MET:N	2.90	0.43
1:A:3657:TYR:CD1	1:A:3661:TRP:CD1	3.06	0.43
1:B:503:PHE:CD2	1:B:515:TRP:CD1	3.06	0.43
1:B:1926:LEU:HA	1:B:1929:MET:CE	2.48	0.43
1:B:4735:GLU:H	1:B:4735:GLU:CD	2.27	0.43
1:C:2506:LEU:HD23	1:C:2507:ASP:N	2.32	0.43
1:C:3649:ALA:HA	1:C:3652:MET:HG2	1.99	0.43
1:D:3653:PHE:CD1	1:D:3653:PHE:C	2.95	0.43
1:D:3819:TYR:CE2	1:D:3823:LYS:HE2	2.53	0.43
1:A:2481:LYS:HE2	1:A:2481:LYS:HA	2.00	0.43
1:B:3838:THR:C	1:B:3839:CYS:SG	3.01	0.43
1:C:503:PHE:CD2	1:C:515:TRP:CD1	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1127:HIS:HA	1:C:1143:TRP:CZ2	2.54	0.43
1:B:2506:LEU:HD23	1:B:2507:ASP:N	2.32	0.43
1:C:80:GLU:C	1:C:80:GLU:CD	2.86	0.43
1:D:1092:PHE:CD2	1:D:1092:PHE:C	2.96	0.43
1:A:3899:PHE:CE1	1:A:3903:LEU:HD21	2.52	0.43
1:B:171:LEU:HD21	1:B:180:LEU:HB3	1.99	0.43
1:B:1562:ILE:C	1:B:1562:ILE:HD12	2.44	0.43
1:B:1950:GLU:C	1:B:1950:GLU:CD	2.87	0.43
1:C:2875:ALA:HA	1:C:2927:LEU:HD13	2.00	0.43
1:D:4104:THR:HG23	1:D:4107:GLU:HB2	2.00	0.43
1:A:607:CYS:SG	1:A:618:GLN:N	2.92	0.43
1:A:2223:ILE:H	1:A:2223:ILE:HD12	1.83	0.43
1:B:2150:GLU:CD	1:B:2150:GLU:N	2.77	0.43
1:C:3670:GLU:H	1:C:3670:GLU:CD	2.26	0.43
1:D:663:TYR:CE1	1:D:745:SER:HB3	2.54	0.43
2:H:56:ILE:HD11	2:H:59:TRP:CD1	2.53	0.43
1:B:1805:GLU:CD	1:B:1805:GLU:H	2.26	0.43
1:C:284:HIS:CE1	1:C:286:THR:H	2.36	0.43
1:D:1286:MET:HE1	1:D:1288:PHE:CD1	2.53	0.43
1:A:1109:LEU:HD12	1:A:1110:ARG:H	1.83	0.43
1:D:2712:PRO:HA	1:D:2955:PHE:CE2	2.54	0.43
2:F:26:TYR:CD1	2:F:26:TYR:C	2.97	0.43
1:A:147:TRP:C	1:A:148:TRP:CD1	2.97	0.43
1:A:1286:MET:SD	1:A:1286:MET:C	3.02	0.43
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	2.00	0.43
1:C:1419:ASP:HA	1:C:1570:LYS:HE2	2.01	0.43
1:C:4064:MET:HE2	1:C:4064:MET:HA	2.01	0.43
1:D:223:PHE:CE1	1:D:227:MET:HA	2.54	0.43
1:D:367:LEU:C	1:D:367:LEU:HD12	2.43	0.43
1:D:2364:PHE:CD1	1:D:2364:PHE:N	2.86	0.43
1:A:4717:ASP:C	1:A:4719:PHE:H	2.27	0.43
1:B:1229:ASN:C	1:B:1230:MET:HG3	2.44	0.43
1:D:313:SER:C	1:D:314:PHE:CD1	2.97	0.43
1:D:2562:ILE:HA	1:D:2565:CYS:SG	2.59	0.43
1:D:4199:GLU:CD	1:D:4199:GLU:N	2.76	0.43
2:G:106:LEU:HD23	2:G:106:LEU:H	1.83	0.43
1:A:1936:LYS:HZ3	1:A:2105:TRP:CG	2.37	0.42
1:B:291:LEU:HA	1:B:301:VAL:HG12	2.00	0.42
1:D:1727:ARG:HA	1:D:1730:MET:HE1	2.01	0.42
1:D:2228:MET:SD	1:D:2228:MET:C	3.02	0.42
1:D:4717:ASP:C	1:D:4719:PHE:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3778:MET:SD	1:B:3778:MET:C	3.03	0.42
1:B:4173:TYR:C	1:B:4173:TYR:CD1	2.97	0.42
1:B:4958:CYS:CB	1:B:4961:CYS:HG	2.33	0.42
1:C:35:LEU:HD23	1:C:51:PRO:HA	2.00	0.42
1:C:284:HIS:CE1	1:C:287:THR:H	2.37	0.42
1:C:458:GLU:CD	1:C:458:GLU:H	2.27	0.42
1:A:276:TRP:CD2	1:A:339:ILE:HD11	2.54	0.42
1:A:1421:ARG:CZ	1:A:1421:ARG:HA	2.49	0.42
1:A:3778:MET:SD	1:A:3778:MET:C	3.02	0.42
1:C:1583:GLU:CD	1:C:1583:GLU:N	2.78	0.42
1:D:483:MET:SD	1:D:483:MET:N	2.91	0.42
1:D:3092:LEU:C	1:D:3092:LEU:HD23	2.44	0.42
1:D:4715:TYR:CE1	1:D:4716:TRP:CZ2	3.08	0.42
1:A:108:LEU:HB2	1:A:147:TRP:CZ3	2.55	0.42
1:A:1092:PHE:CD2	1:A:1092:PHE:C	2.97	0.42
1:A:1107:PRO:HD3	1:A:1188:PHE:HA	2.00	0.42
1:A:2228:MET:SD	1:A:2228:MET:C	3.02	0.42
1:B:121:LEU:HD23	1:B:122:THR:H	1.85	0.42
1:B:483:MET:SD	1:B:483:MET:N	2.93	0.42
1:C:1297:PHE:CE2	1:C:1546:THR:HB	2.55	0.42
1:C:3838:THR:C	1:C:3839:CYS:SG	3.02	0.42
1:D:284:HIS:CE1	1:D:287:THR:H	2.38	0.42
1:D:291:LEU:HA	1:D:301:VAL:HG12	2.02	0.42
1:D:3838:THR:C	1:D:3839:CYS:SG	3.03	0.42
1:A:523:TYR:CE2	1:A:560:ILE:HG12	2.55	0.42
1:A:2654:TYR:CZ	1:A:2667:THR:HA	2.55	0.42
1:B:2228:MET:C	1:B:2228:MET:SD	3.02	0.42
1:C:1950:GLU:C	1:C:1950:GLU:CD	2.87	0.42
1:D:147:TRP:C	1:D:148:TRP:CD1	2.98	0.42
1:D:3290:GLU:CD	1:D:3309:SER:H	2.28	0.42
1:D:3973:CYS:SG	1:D:3976:ASN:CG	3.02	0.42
1:D:4053:SER:O	1:D:4057:MET:HE2	2.20	0.42
1:B:108:LEU:HB2	1:B:147:TRP:CZ3	2.55	0.42
1:B:1451:GLY:HA3	1:B:1494:MET:HG2	2.01	0.42
1:B:1583:GLU:N	1:B:1583:GLU:CD	2.78	0.42
1:C:291:LEU:HA	1:C:301:VAL:HG12	2.01	0.42
1:C:1286:MET:SD	1:C:1286:MET:C	3.03	0.42
1:D:1457:TYR:CD1	1:D:1457:TYR:C	2.97	0.42
1:D:1562:ILE:HD12	1:D:1562:ILE:C	2.44	0.42
1:A:101:LEU:C	1:A:102:LEU:HD12	2.45	0.42
1:A:2506:LEU:HD23	1:A:2506:LEU:C	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4023:MET:SD	1:B:4023:MET:C	3.02	0.42
1:B:4679:ARG:HH21	1:B:4679:ARG:HG3	1.85	0.42
1:C:2150:GLU:CD	1:C:2150:GLU:N	2.78	0.42
1:A:124:SER:HB3	1:A:133:PHE:HA	2.02	0.42
1:C:1092:PHE:CD2	1:C:1092:PHE:C	2.97	0.42
1:D:4679:ARG:HH21	1:D:4679:ARG:HG3	1.84	0.42
1:A:597:HIS:CG	1:A:1661:ARG:HH22	2.37	0.42
1:A:1950:GLU:CD	1:A:1950:GLU:C	2.88	0.42
1:A:2150:GLU:CD	1:A:2150:GLU:N	2.77	0.42
1:B:4173:TYR:CD1	1:B:4174:PHE:CZ	3.08	0.42
1:C:2506:LEU:HD23	1:C:2506:LEU:C	2.45	0.42
1:D:1464:PHE:CE2	1:D:1465:ASP:HA	2.55	0.42
1:D:3906:GLN:CD	1:D:3906:GLN:H	2.27	0.42
1:A:367:LEU:C	1:A:367:LEU:HD12	2.45	0.42
1:A:3670:GLU:CD	1:A:3670:GLU:H	2.28	0.42
1:A:3989:VAL:HA	1:A:3992:PHE:CD2	2.55	0.42
1:B:2770:LYS:HA	1:B:2770:LYS:HE2	2.01	0.42
1:D:4036:VAL:HG13	1:D:4153:HIS:O	2.20	0.42
1:B:35:LEU:HD23	1:B:51:PRO:HA	2.02	0.41
1:B:222:LEU:N	1:B:222:LEU:HD12	2.34	0.41
1:C:2364:PHE:CD1	1:C:2364:PHE:N	2.84	0.41
1:D:1297:PHE:CE2	1:D:1546:THR:HB	2.54	0.41
1:A:174:VAL:HG12	1:B:2452:ARG:HH22	1.85	0.41
1:A:451:TYR:CD2	1:A:452:PHE:CZ	3.08	0.41
1:A:597:HIS:CD2	1:A:1661:ARG:HH22	2.39	0.41
1:A:2756:ASN:C	1:A:2756:ASN:HD22	2.28	0.41
1:B:18:ASP:CG	1:B:206:CYS:H	2.28	0.41
1:C:712:TYR:CZ	1:C:1470:ARG:HD2	2.55	0.41
1:C:828:GLU:HA	1:C:829:TYR:CD2	2.55	0.41
1:C:3934:TYR:CD2	1:C:3935:TRP:CD1	3.08	0.41
1:C:4053:SER:O	1:C:4057:MET:HE2	2.21	0.41
1:C:4077:PHE:CG	1:C:4078:GLN:N	2.87	0.41
1:D:1950:GLU:C	1:D:1950:GLU:CD	2.88	0.41
1:D:4735:GLU:H	1:D:4735:GLU:CD	2.28	0.41
1:A:76:ARG:NH1	1:B:3936:TYR:H	2.18	0.41
1:A:1086:GLY:HA3	1:A:1088:TRP:CZ2	2.55	0.41
1:A:2908:TYR:CZ	1:A:2916:LYS:HE2	2.55	0.41
1:C:571:SER:HA	1:C:572:PRO:HD2	1.96	0.41
1:C:2770:LYS:HD3	1:C:2787:THR:HG22	2.01	0.41
1:D:1449:TRP:CE2	1:D:1464:PHE:CE2	3.08	0.41
1:D:2955:PHE:CD1	1:D:2955:PHE:C	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4173:TYR:CD1	1:D:4173:TYR:C	2.97	0.41
1:A:213:TYR:CD1	1:A:340:LYS:HG2	2.56	0.41
1:A:4978:HIS:CE1	1:A:4983:HIS:CD2	3.08	0.41
1:B:1092:PHE:CD2	1:B:1092:PHE:C	2.97	0.41
1:B:1421:ARG:CZ	1:B:1421:ARG:HA	2.49	0.41
1:B:1449:TRP:CE2	1:B:1464:PHE:CE2	3.09	0.41
1:B:2497:ASP:O	1:B:2500:ALA:HB3	2.20	0.41
1:C:76:ARG:HD3	1:D:3935:TRP:CE3	2.55	0.41
1:C:1451:GLY:HA3	1:C:1494:MET:HG2	2.02	0.41
1:C:1457:TYR:CD1	1:C:1457:TYR:C	2.99	0.41
1:C:1464:PHE:CE2	1:C:1465:ASP:HA	2.55	0.41
1:D:1107:PRO:HD3	1:D:1188:PHE:HA	2.02	0.41
1:A:1457:TYR:CD1	1:A:1457:TYR:C	2.98	0.41
1:A:2955:PHE:CD1	1:A:2955:PHE:C	2.98	0.41
1:C:4802:GLY:HA3	1:C:4809:PHE:CE1	2.56	0.41
1:B:597:HIS:CG	1:B:1661:ARG:HH22	2.38	0.41
1:B:2654:TYR:CZ	1:B:2667:THR:HA	2.55	0.41
1:C:607:CYS:SG	1:C:618:GLN:N	2.93	0.41
1:C:1449:TRP:CE2	1:C:1464:PHE:CE2	3.08	0.41
1:C:2340:PHE:CZ	1:C:2343:GLY:C	2.98	0.41
1:D:451:TYR:CD2	1:D:452:PHE:CE1	3.09	0.41
2:F:36:PHE:CZ	2:F:37:ASP:HB2	2.56	0.41
1:A:692:TYR:CE2	1:A:694:PRO:HD3	2.56	0.41
1:A:1449:TRP:CE2	1:A:1464:PHE:CE2	3.08	0.41
1:A:2290:LEU:HD23	1:A:2291:GLN:H	1.85	0.41
1:C:111:HIS:CD2	1:C:113:HIS:H	2.39	0.41
1:C:367:LEU:HD12	1:C:367:LEU:C	2.46	0.41
1:C:961:MET:HE3	1:C:965:TYR:H	1.85	0.41
1:C:972:LEU:HD23	1:C:972:LEU:H	1.85	0.41
1:C:1492:CYS:SG	1:C:1494:MET:HG3	2.60	0.41
1:C:2301:TYR:HB3	1:C:2331:TYR:CZ	2.56	0.41
1:C:2562:ILE:HA	1:C:2565:CYS:SG	2.60	0.41
1:D:359:TYR:CE2	1:D:383:HIS:CE1	3.09	0.41
1:D:2908:TYR:CZ	1:D:2916:LYS:HE2	2.56	0.41
1:A:451:TYR:CD2	1:A:452:PHE:CE1	3.09	0.41
1:A:712:TYR:CZ	1:A:1470:ARG:HD2	2.55	0.41
1:B:3935:TRP:H	1:B:3935:TRP:CD1	2.39	0.41
1:B:4958:CYS:SG	1:B:4960:ILE:HB	2.61	0.41
1:C:622:THR:HG23	1:C:626:LEU:HD12	2.02	0.41
1:D:80:GLU:CD	1:D:80:GLU:C	2.89	0.41
1:D:111:HIS:CE1	1:D:114:SER:N	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:MET:HB2	2:F:98:VAL:HG13	2.03	0.41
1:A:1286:MET:HE1	1:A:1288:PHE:CD1	2.56	0.41
1:A:2687:ALA:HA	1:A:2997:PHE:CE2	2.55	0.41
1:A:4802:GLY:HA3	1:A:4809:PHE:CE1	2.56	0.41
1:B:213:TYR:CD1	1:B:340:LYS:HG2	2.56	0.41
1:B:607:CYS:SG	1:B:618:GLN:N	2.93	0.41
1:B:1457:TYR:CD1	1:B:1457:TYR:C	2.99	0.41
1:B:1730:MET:HE2	1:B:1730:MET:HB2	1.93	0.41
1:B:3365:LEU:HD12	1:B:3365:LEU:HA	1.95	0.41
1:B:5000:GLU:HA	1:B:5003:HIS:CD2	2.56	0.41
1:C:121:LEU:HD23	1:C:122:THR:H	1.86	0.41
1:C:171:LEU:HD21	1:C:180:LEU:HB3	2.02	0.41
1:D:597:HIS:CG	1:D:1661:ARG:HH22	2.38	0.41
1:D:1451:GLY:HA3	1:D:1494:MET:HG2	2.02	0.41
1:D:2770:LYS:HE2	1:D:2770:LYS:HA	2.03	0.41
1:D:4879:MET:HE3	1:D:4879:MET:HB3	1.93	0.41
1:A:223:PHE:CE1	1:A:227:MET:HA	2.56	0.41
1:A:1435:TYR:CE2	1:A:1518:CYS:SG	3.13	0.41
1:B:2506:LEU:HD23	1:B:2506:LEU:C	2.46	0.41
1:B:2661:TRP:CD1	1:B:2662:ALA:H	2.39	0.41
1:C:405:HIS:CG	1:C:406:SER:N	2.88	0.41
1:C:1748:PHE:CG	1:C:1758:ARG:HB2	2.56	0.41
1:D:178:ARG:CZ	1:D:195:PHE:CZ	3.04	0.41
1:D:4115:SER:HA	1:D:4128:PHE:CZ	2.56	0.41
1:A:266:ARG:HH11	1:A:269:TRP:HB2	1.86	0.40
1:A:316:PHE:CB	1:A:346:CYS:HG	2.34	0.40
1:C:523:TYR:CE2	1:C:560:ILE:HG12	2.56	0.40
1:D:1435:TYR:CE2	1:D:1518:CYS:SG	3.14	0.40
1:D:2150:GLU:CD	1:D:2150:GLU:N	2.79	0.40
1:D:2174:GLU:N	1:D:2174:GLU:CD	2.79	0.40
1:D:2301:TYR:HB3	1:D:2331:TYR:CZ	2.56	0.40
1:D:4802:GLY:HA3	1:D:4809:PHE:CE1	2.56	0.40
1:A:2997:PHE:CD1	1:A:2997:PHE:C	2.99	0.40
1:A:3838:THR:C	1:A:3839:CYS:SG	3.04	0.40
1:B:124:SER:HB3	1:B:133:PHE:HA	2.02	0.40
1:B:1493:TYR:CD1	1:B:1493:TYR:N	2.89	0.40
1:D:328:LYS:H	1:D:328:LYS:HD2	1.85	0.40
1:A:80:GLU:C	1:A:80:GLU:CD	2.88	0.40
1:B:2551:ASN:HB3	1:B:2595:LEU:HD21	2.04	0.40
1:C:18:ASP:CG	1:C:206:CYS:H	2.28	0.40
1:C:2223:ILE:H	1:C:2223:ILE:HD12	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4978:HIS:CE1	1:C:4983:HIS:CD2	3.09	0.40
1:A:3653:PHE:CD1	1:A:3653:PHE:C	2.98	0.40
1:A:4026:MET:HG2	1:A:4027:LEU:N	2.36	0.40
1:B:111:HIS:CE1	1:B:114:SER:N	2.90	0.40
1:B:1862:ILE:HA	1:B:1865:MET:SD	2.62	0.40
1:C:1086:GLY:HA3	1:C:1088:TRP:CZ2	2.56	0.40
1:C:1127:HIS:HA	1:C:1143:TRP:CE2	2.55	0.40
1:C:3631:ALA:HB2	1:C:3859:VAL:HG11	2.03	0.40
1:C:4149:ASN:ND2	1:C:4194:TYR:CE2	2.90	0.40
1:D:110:ARG:HB2	1:D:117:TYR:CE2	2.57	0.40
1:D:607:CYS:SG	1:D:618:GLN:HG3	2.60	0.40
1:D:3657:TYR:CE1	1:D:3661:TRP:CG	3.10	0.40
1:D:4173:TYR:CD1	1:D:4174:PHE:CZ	3.10	0.40
2:G:78:PRO:HD3	2:G:96:THR:HG22	2.03	0.40
1:A:785:ALA:HA	1:A:1630:CYS:SG	2.61	0.40
1:A:1493:TYR:CD1	1:A:1493:TYR:N	2.90	0.40
1:B:78:LEU:HD12	1:B:78:LEU:HA	2.02	0.40
1:B:80:GLU:CD	1:B:80:GLU:C	2.89	0.40
1:B:3817:LEU:C	1:B:3821:LYS:HE2	2.47	0.40
1:B:5021:PHE:CZ	1:B:5022:PHE:HB2	2.56	0.40
1:C:681:HIS:CD2	1:C:681:HIS:C	2.98	0.40
1:C:1926:LEU:C	1:C:1926:LEU:HD23	2.46	0.40
1:D:2712:PRO:HD2	1:D:3016:TYR:CZ	2.57	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	4376/5037 (87%)	4032 (92%)	287 (7%)	57 (1%)	9	41
1	B	4376/5037 (87%)	4028 (92%)	295 (7%)	53 (1%)	10	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	4376/5037 (87%)	4010 (92%)	299 (7%)	67 (2%)	8	39
1	D	4376/5037 (87%)	4019 (92%)	292 (7%)	65 (2%)	8	39
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
All	All	17924/20580 (87%)	16489 (92%)	1193 (7%)	242 (1%)	11	40

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	825	PRO
1	A	2719	TYR
1	A	3687	GLU
1	B	3687	GLU
1	B	3869	GLN
1	B	4155	PRO
1	B	4691	GLN
1	C	126	SER
1	C	825	PRO
1	C	3239	MET
1	C	3687	GLU
1	D	267	ILE
1	D	825	PRO
1	D	3239	MET
1	D	3682	GLU
1	D	3869	GLN
1	D	4691	GLN
1	A	385	ASP
1	A	422	SER
1	A	2786	LYS
1	A	3227	ARG
1	A	3682	GLU
1	A	3787	LYS
1	A	3869	GLN
1	B	125	ARG
1	B	285	VAL
1	B	329	ARG
1	B	532	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	825	PRO
1	B	1241	SER
1	B	2719	TYR
1	B	3787	LYS
1	B	4693	GLY
1	C	285	VAL
1	C	329	ARG
1	C	699	GLY
1	C	829	TYR
1	C	1241	SER
1	C	1532	ASN
1	C	1930	LYS
1	C	2572	THR
1	C	2865	VAL
1	C	3293	PRO
1	C	3478	MET
1	C	3787	LYS
1	D	353	SER
1	D	385	ASP
1	D	1930	LYS
1	D	2719	TYR
1	D	3787	LYS
1	D	4155	PRO
1	D	4693	GLY
1	A	272	SER
1	A	285	VAL
1	A	691	GLY
1	A	1792	ALA
1	A	1997	GLU
1	A	2570	ALA
1	A	2572	THR
1	A	2723	ALA
1	A	2748	PRO
1	A	3052	HIS
1	A	3293	PRO
1	A	3465	ASN
1	A	3478	MET
1	A	4155	PRO
1	A	4694	ASP
1	B	62	LEU
1	B	272	SER
1	B	691	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	861	ILE
1	B	1215	ALA
1	B	1281	ASN
1	B	1792	ALA
1	B	1930	LYS
1	B	2572	THR
1	B	2663	ASN
1	B	2748	PRO
1	B	3052	HIS
1	C	144	GLU
1	C	272	SER
1	C	353	SER
1	C	532	GLY
1	C	691	GLY
1	C	1281	ASN
1	C	1508	ARG
1	C	1792	ALA
1	C	2020	ASP
1	C	2783	GLU
1	C	3052	HIS
1	C	3682	GLU
1	C	4072	VAL
1	C	4155	PRO
1	D	285	VAL
1	D	329	ARG
1	D	691	GLY
1	D	1792	ALA
1	D	2020	ASP
1	D	2570	ALA
1	D	2572	THR
1	D	2723	ALA
1	D	2786	LYS
1	D	3052	HIS
1	D	3465	ASN
1	A	62	LEU
1	A	114	SER
1	A	858	THR
1	A	1281	ASN
1	A	1508	ARG
1	A	1770	SER
1	A	2663	ASN
1	A	2868	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3622	LYS
1	A	3735	LEU
1	A	3788	GLY
1	B	17	ASP
1	B	276	TRP
1	B	334	MET
1	B	422	SER
1	B	770	ALA
1	B	902	ARG
1	B	1508	ARG
1	B	1997	GLU
1	B	3427	PRO
1	B	3666	ASP
1	B	3735	LEU
1	B	3788	GLY
1	C	17	ASP
1	C	334	MET
1	C	365	LYS
1	C	371	VAL
1	C	422	SER
1	C	806	PRO
1	C	861	ILE
1	C	1442	GLY
1	C	1997	GLU
1	C	2574	HIS
1	C	2663	ASN
1	C	3944	GLU
1	D	127	MET
1	D	1281	ASN
1	D	1420	ASN
1	D	1505	GLN
1	D	1750	PRO
1	D	1997	GLU
1	D	2342	ASN
1	D	2663	ASN
1	D	3206	LEU
1	D	3622	LYS
1	D	3692	GLU
1	D	3788	GLY
1	A	371	VAL
1	A	806	PRO
1	A	1420	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1700	ASP
1	A	1930	LYS
1	A	3734	HIS
1	A	3858	MET
1	B	371	VAL
1	B	381	GLU
1	B	1482	ASN
1	B	1786	LEU
1	B	2342	ASN
1	B	2750	LYS
1	B	3622	LYS
1	C	381	GLU
1	C	1133	HIS
1	C	1441	ALA
1	C	2413	GLU
1	C	3620	TRP
1	C	3622	LYS
1	C	3788	GLY
1	C	4076	ALA
1	C	4693	GLY
1	D	64	ILE
1	D	126	SER
1	D	371	VAL
1	D	381	GLU
1	D	422	SER
1	D	531	ARG
1	D	543	ASN
1	D	796	ARG
1	D	806	PRO
1	D	861	ILE
1	D	902	ARG
1	D	1532	ASN
1	D	1700	ASP
1	D	2092	GLN
1	D	2413	GLU
1	D	3427	PRO
1	D	3620	TRP
1	D	3666	ASP
1	D	3734	HIS
1	A	64	ILE
1	A	1456	ASP
1	A	1767	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3466	ASN
1	A	4691	GLN
1	A	4718	LYS
1	B	64	ILE
1	B	1282	SER
1	B	1442	GLY
1	C	386	ASP
1	C	2342	ASN
1	C	2719	TYR
1	C	2748	PRO
1	C	3233	PRO
1	C	3427	PRO
1	C	4073	GLY
1	C	4691	GLN
1	D	3293	PRO
1	D	3466	ASN
1	A	798	GLY
1	A	1442	GLY
1	A	4072	VAL
1	B	1098	GLY
1	B	3293	PRO
1	C	64	ILE
1	C	1098	GLY
1	A	1783	VAL
1	A	1853	ILE
1	B	3841	VAL
1	C	1853	ILE
1	C	3841	VAL
1	D	1444	GLU
1	D	3233	PRO
1	D	3841	VAL
1	A	1444	GLU
1	A	3581	GLY
1	B	806	PRO
1	B	3581	GLY
1	C	4081	VAL
1	D	1803	PRO
1	B	1444	GLU
1	C	1803	PRO
1	D	1442	GLY
1	D	3581	GLY
1	C	967	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3751	VAL
1	D	212	GLY
1	D	3751	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3827/4276 (90%)	3588 (94%)	239 (6%)	16	38
1	B	3827/4276 (90%)	3571 (93%)	256 (7%)	15	36
1	C	3827/4276 (90%)	3597 (94%)	230 (6%)	17	38
1	D	3827/4276 (90%)	3576 (93%)	251 (7%)	15	37
2	E	89/90 (99%)	85 (96%)	4 (4%)	24	46
2	F	89/90 (99%)	84 (94%)	5 (6%)	19	40
2	G	89/90 (99%)	85 (96%)	4 (4%)	24	46
2	H	89/90 (99%)	84 (94%)	5 (6%)	19	40
All	All	15664/17464 (90%)	14670 (94%)	994 (6%)	18	37

All (994) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	22	LEU
1	A	31	GLU
1	A	46	LEU
1	A	80	GLU
1	A	98	HIS
1	A	103	TYR
1	A	105	HIS
1	A	121	LEU
1	A	125	ARG
1	A	130	LYS
1	A	159	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	169	LEU
1	A	211	GLU
1	A	223	PHE
1	A	224	HIS
1	A	247	TYR
1	A	267	ILE
1	A	278	GLN
1	A	287	THR
1	A	293	LEU
1	A	296	ASP
1	A	312	THR
1	A	328	LYS
1	A	334	MET
1	A	367	LEU
1	A	371	VAL
1	A	372	LEU
1	A	381	GLU
1	A	395	GLN
1	A	396	GLU
1	A	405	HIS
1	A	439	GLU
1	A	477	LEU
1	A	483	MET
1	A	495	ASN
1	A	525	LEU
1	A	536	ASN
1	A	545	ASP
1	A	580	GLU
1	A	591	ASP
1	A	630	GLU
1	A	639	ASN
1	A	652	ARG
1	A	674	PHE
1	A	682	LEU
1	A	755	ILE
1	A	828	GLU
1	A	829	TYR
1	A	830	ARG
1	A	884	LEU
1	A	907	LEU
1	A	939	VAL
1	A	957	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	959	TYR
1	A	961	MET
1	A	963	ASN
1	A	976	ARG
1	A	998	ARG
1	A	999	ASP
1	A	1003	GLN
1	A	1070	ASP
1	A	1071	ARG
1	A	1104	TRP
1	A	1114	GLU
1	A	1128	ARG
1	A	1136	SER
1	A	1143	TRP
1	A	1216	ILE
1	A	1234	VAL
1	A	1236	THR
1	A	1244	GLN
1	A	1285	GLU
1	A	1428	LEU
1	A	1433	TYR
1	A	1434	TYR
1	A	1444	GLU
1	A	1446	SER
1	A	1463	ASN
1	A	1473	THR
1	A	1478	ASP
1	A	1480	GLN
1	A	1513	ASP
1	A	1514	LEU
1	A	1518	CYS
1	A	1583	GLU
1	A	1637	MET
1	A	1649	ASP
1	A	1651	LEU
1	A	1702	HIS
1	A	1721	GLU
1	A	1758	ARG
1	A	1805	GLU
1	A	1857	GLU
1	A	1872	THR
1	A	1933	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1950	GLU
1	A	1952	GLN
1	A	1984	PHE
1	A	2008	MET
1	A	2045	GLN
1	A	2100	HIS
1	A	2150	GLU
1	A	2155	LEU
1	A	2168	VAL
1	A	2193	GLN
1	A	2209	GLU
1	A	2219	GLU
1	A	2234	ARG
1	A	2271	THR
1	A	2274	ASP
1	A	2280	VAL
1	A	2290	LEU
1	A	2302	LEU
1	A	2308	GLN
1	A	2309	SER
1	A	2330	ARG
1	A	2340	PHE
1	A	2357	LEU
1	A	2371	GLU
1	A	2415	ARG
1	A	2440	MET
1	A	2453	ILE
1	A	2460	LEU
1	A	2503	VAL
1	A	2506	LEU
1	A	2513	GLU
1	A	2518	LEU
1	A	2522	LEU
1	A	2558	VAL
1	A	2573	GLU
1	A	2577	ILE
1	A	2578	MET
1	A	2582	MET
1	A	2596	THR
1	A	2647	HIS
1	A	2669	GLU
1	A	2673	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2690	LYS
1	A	2700	MET
1	A	2724	GLU
1	A	2747	ILE
1	A	2751	LEU
1	A	2755	ILE
1	A	2855	TYR
1	A	2869	ARG
1	A	2894	LEU
1	A	2933	ASN
1	A	2955	PHE
1	A	2968	ASP
1	A	2998	PHE
1	A	3033	ASN
1	A	3043	PHE
1	A	3051	ARG
1	A	3173	TYR
1	A	3184	GLU
1	A	3205	PHE
1	A	3263	TYR
1	A	3310	ASP
1	A	3324	VAL
1	A	3329	ILE
1	A	3531	ASP
1	A	3549	VAL
1	A	3550	ARG
1	A	3670	GLU
1	A	3683	GLN
1	A	3687	GLU
1	A	3717	ASP
1	A	3736	GLU
1	A	3750	GLU
1	A	3752	SER
1	A	3779	VAL
1	A	3793	MET
1	A	3800	LEU
1	A	3816	MET
1	A	3832	ILE
1	A	3835	LEU
1	A	3841	VAL
1	A	3856	LEU
1	A	3870	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3879	GLU
1	A	3887	PHE
1	A	3900	GLN
1	A	3912	THR
1	A	3919	THR
1	A	3927	GLN
1	A	3934	TYR
1	A	3953	LYS
1	A	3966	THR
1	A	3967	GLU
1	A	3987	ASP
1	A	3992	PHE
1	A	4011	GLU
1	A	4026	MET
1	A	4035	VAL
1	A	4040	ILE
1	A	4047	MET
1	A	4061	PHE
1	A	4089	SER
1	A	4092	ASP
1	A	4094	GLN
1	A	4103	PHE
1	A	4130	ASN
1	A	4134	GLU
1	A	4141	PHE
1	A	4150	LEU
1	A	4154	VAL
1	A	4161	ARG
1	A	4178	LEU
1	A	4196	GLU
1	A	4199	GLU
1	A	4240	ASP
1	A	4244	GLU
1	A	4541	TRP
1	A	4544	LEU
1	A	4626	ASN
1	A	4634	GLU
1	A	4662	ASN
1	A	4700	GLN
1	A	4704	LEU
1	A	4705	VAL
1	A	4735	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4743	MET
1	A	4749	GLU
1	A	4753	HIS
1	A	4775	TYR
1	A	4780	PHE
1	A	4788	SER
1	A	4806	ASN
1	A	4821	LYS
1	A	4876	CYS
1	A	4910	GLU
1	A	4949	GLN
1	A	4957	LYS
1	A	4973	HIS
1	A	4976	GLU
1	A	4989	MET
1	A	5020	ASP
1	A	5035	GLN
1	B	17	ASP
1	B	56	GLN
1	B	76	ARG
1	B	80	GLU
1	B	103	TYR
1	B	105	HIS
1	B	121	LEU
1	B	125	ARG
1	B	130	LYS
1	B	144	GLU
1	B	169	LEU
1	B	183	SER
1	B	211	GLU
1	B	220	LEU
1	B	224	HIS
1	B	233	ILE
1	B	267	ILE
1	B	278	GLN
1	B	293	LEU
1	B	296	ASP
1	B	308	HIS
1	B	310	LYS
1	B	312	THR
1	B	322	LYS
1	B	328	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	367	LEU
1	B	371	VAL
1	B	372	LEU
1	B	381	GLU
1	B	395	GLN
1	B	396	GLU
1	B	398	SER
1	B	405	HIS
1	B	439	GLU
1	B	443	LEU
1	B	462	GLU
1	B	477	LEU
1	B	483	MET
1	B	495	ASN
1	B	534	ARG
1	B	536	ASN
1	B	545	ASP
1	B	577	ILE
1	B	580	GLU
1	B	630	GLU
1	B	652	ARG
1	B	657	THR
1	B	674	PHE
1	B	682	LEU
1	B	730	VAL
1	B	755	ILE
1	B	765	GLN
1	B	774	ASP
1	B	828	GLU
1	B	829	TYR
1	B	867	LEU
1	B	876	GLU
1	B	884	LEU
1	B	892	THR
1	B	907	LEU
1	B	939	VAL
1	B	957	LYS
1	B	959	TYR
1	B	963	ASN
1	B	999	ASP
1	B	1003	GLN
1	B	1071	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1089	TYR
1	B	1104	TRP
1	B	1114	GLU
1	B	1136	SER
1	B	1154	ASP
1	B	1224	GLU
1	B	1236	THR
1	B	1244	GLN
1	B	1261	ASP
1	B	1285	GLU
1	B	1428	LEU
1	B	1434	TYR
1	B	1444	GLU
1	B	1446	SER
1	B	1463	ASN
1	B	1473	THR
1	B	1478	ASP
1	B	1513	ASP
1	B	1514	LEU
1	B	1518	CYS
1	B	1522	LEU
1	B	1583	GLU
1	B	1590	GLN
1	B	1622	GLU
1	B	1637	MET
1	B	1649	ASP
1	B	1721	GLU
1	B	1739	THR
1	B	1758	ARG
1	B	1805	GLU
1	B	1808	ARG
1	B	1825	HIS
1	B	1867	GLU
1	B	1873	GLU
1	B	1933	GLU
1	B	1950	GLU
1	B	1982	ARG
1	B	2015	GLU
1	B	2045	GLN
1	B	2092	GLN
1	B	2100	HIS
1	B	2150	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2155	LEU
1	B	2168	VAL
1	B	2169	GLN
1	B	2177	LEU
1	B	2193	GLN
1	B	2209	GLU
1	B	2219	GLU
1	B	2223	ILE
1	B	2224	ARG
1	B	2225	PHE
1	B	2243	SER
1	B	2271	THR
1	B	2274	ASP
1	B	2280	VAL
1	B	2290	LEU
1	B	2294	ASP
1	B	2302	LEU
1	B	2308	GLN
1	B	2309	SER
1	B	2330	ARG
1	B	2332	LEU
1	B	2357	LEU
1	B	2371	GLU
1	B	2440	MET
1	B	2453	ILE
1	B	2490	MET
1	B	2503	VAL
1	B	2506	LEU
1	B	2518	LEU
1	B	2522	LEU
1	B	2574	HIS
1	B	2577	ILE
1	B	2578	MET
1	B	2588	ARG
1	B	2596	THR
1	B	2620	GLN
1	B	2634	ASN
1	B	2647	HIS
1	B	2669	GLU
1	B	2673	HIS
1	B	2700	MET
1	B	2724	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2734	ASN
1	B	2747	ILE
1	B	2782	ASP
1	B	2827	ARG
1	B	2881	ASN
1	B	2892	GLN
1	B	2927	LEU
1	B	2928	LYS
1	B	2955	PHE
1	B	2968	ASP
1	B	2998	PHE
1	B	3002	LEU
1	B	3020	THR
1	B	3051	ARG
1	B	3109	ASN
1	B	3184	GLU
1	B	3205	PHE
1	B	3226	GLU
1	B	3240	CYS
1	B	3263	TYR
1	B	3266	MET
1	B	3290	GLU
1	B	3324	VAL
1	B	3379	LEU
1	B	3380	ARG
1	B	3463	GLU
1	B	3467	MET
1	B	3549	VAL
1	B	3575	LEU
1	B	3595	ARG
1	B	3620	TRP
1	B	3670	GLU
1	B	3683	GLN
1	B	3717	ASP
1	B	3750	GLU
1	B	3752	SER
1	B	3779	VAL
1	B	3793	MET
1	B	3800	LEU
1	B	3822	ASP
1	B	3825	GLU
1	B	3832	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3841	VAL
1	B	3842	LEU
1	B	3856	LEU
1	B	3870	ASN
1	B	3879	GLU
1	B	3887	PHE
1	B	3895	HIS
1	B	3900	GLN
1	B	3912	THR
1	B	3919	THR
1	B	3927	GLN
1	B	3935	TRP
1	B	3943	ILE
1	B	3944	GLU
1	B	3946	GLN
1	B	3953	LYS
1	B	3966	THR
1	B	3967	GLU
1	B	3992	PHE
1	B	4010	ILE
1	B	4026	MET
1	B	4035	VAL
1	B	4040	ILE
1	B	4061	PHE
1	B	4077	PHE
1	B	4089	SER
1	B	4092	ASP
1	B	4093	PHE
1	B	4094	GLN
1	B	4104	THR
1	B	4107	GLU
1	B	4141	PHE
1	B	4149	ASN
1	B	4150	LEU
1	B	4175	ARG
1	B	4178	LEU
1	B	4231	MET
1	B	4240	ASP
1	B	4244	GLU
1	B	4541	TRP
1	B	4544	LEU
1	B	4626	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4633	GLU
1	B	4649	LEU
1	B	4662	ASN
1	B	4690	GLU
1	B	4700	GLN
1	B	4704	LEU
1	B	4705	VAL
1	B	4725	LEU
1	B	4735	GLU
1	B	4749	GLU
1	B	4756	ARG
1	B	4788	SER
1	B	4821	LYS
1	B	4865	LYS
1	B	4910	GLU
1	B	4943	LEU
1	B	4949	GLN
1	B	4957	LYS
1	B	4976	GLU
1	B	4989	MET
1	B	5020	ASP
1	C	17	ASP
1	C	98	HIS
1	C	113	HIS
1	C	121	LEU
1	C	125	ARG
1	C	159	GLU
1	C	211	GLU
1	C	224	HIS
1	C	233	ILE
1	C	267	ILE
1	C	278	GLN
1	C	287	THR
1	C	296	ASP
1	C	334	MET
1	C	367	LEU
1	C	372	LEU
1	C	381	GLU
1	C	389	PHE
1	C	395	GLN
1	C	398	SER
1	C	405	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	439	GLU
1	C	477	LEU
1	C	495	ASN
1	C	536	ASN
1	C	545	ASP
1	C	580	GLU
1	C	581	ASN
1	C	610	ASN
1	C	630	GLU
1	C	652	ARG
1	C	656	SER
1	C	674	PHE
1	C	682	LEU
1	C	702	TRP
1	C	730	VAL
1	C	745	SER
1	C	755	ILE
1	C	765	GLN
1	C	828	GLU
1	C	884	LEU
1	C	920	TYR
1	C	922	LEU
1	C	939	VAL
1	C	957	LYS
1	C	961	MET
1	C	963	ASN
1	C	999	ASP
1	C	1070	ASP
1	C	1104	TRP
1	C	1114	GLU
1	C	1136	SER
1	C	1154	ASP
1	C	1216	ILE
1	C	1234	VAL
1	C	1236	THR
1	C	1244	GLN
1	C	1261	ASP
1	C	1285	GLU
1	C	1428	LEU
1	C	1434	TYR
1	C	1444	GLU
1	C	1446	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1463	ASN
1	C	1473	THR
1	C	1478	ASP
1	C	1514	LEU
1	C	1518	CYS
1	C	1519	LEU
1	C	1522	LEU
1	C	1583	GLU
1	C	1590	GLN
1	C	1644	GLU
1	C	1695	LEU
1	C	1714	LEU
1	C	1721	GLU
1	C	1748	PHE
1	C	1758	ARG
1	C	1802	ILE
1	C	1805	GLU
1	C	1825	HIS
1	C	1857	GLU
1	C	1867	GLU
1	C	1950	GLU
1	C	2008	MET
1	C	2015	GLU
1	C	2018	GLU
1	C	2092	GLN
1	C	2100	HIS
1	C	2109	ASP
1	C	2110	TYR
1	C	2150	GLU
1	C	2155	LEU
1	C	2167	ILE
1	C	2193	GLN
1	C	2209	GLU
1	C	2219	GLU
1	C	2243	SER
1	C	2271	THR
1	C	2274	ASP
1	C	2280	VAL
1	C	2290	LEU
1	C	2294	ASP
1	C	2302	LEU
1	C	2309	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2330	ARG
1	C	2332	LEU
1	C	2357	LEU
1	C	2415	ARG
1	C	2440	MET
1	C	2452	ARG
1	C	2453	ILE
1	C	2464	ASP
1	C	2482	ASP
1	C	2487	GLN
1	C	2503	VAL
1	C	2506	LEU
1	C	2513	GLU
1	C	2518	LEU
1	C	2558	VAL
1	C	2559	LEU
1	C	2573	GLU
1	C	2577	ILE
1	C	2578	MET
1	C	2582	MET
1	C	2588	ARG
1	C	2593	ARG
1	C	2596	THR
1	C	2620	GLN
1	C	2647	HIS
1	C	2666	VAL
1	C	2673	HIS
1	C	2700	MET
1	C	2724	GLU
1	C	2747	ILE
1	C	2768	PHE
1	C	2774	ASN
1	C	2881	ASN
1	C	2892	GLN
1	C	2955	PHE
1	C	2998	PHE
1	C	3002	LEU
1	C	3020	THR
1	C	3033	ASN
1	C	3043	PHE
1	C	3154	ASP
1	C	3184	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3230	LEU
1	C	3243	ILE
1	C	3263	TYR
1	C	3266	MET
1	C	3310	ASP
1	C	3324	VAL
1	C	3379	LEU
1	C	3463	GLU
1	C	3467	MET
1	C	3531	ASP
1	C	3549	VAL
1	C	3575	LEU
1	C	3595	ARG
1	C	3670	GLU
1	C	3683	GLN
1	C	3717	ASP
1	C	3736	GLU
1	C	3750	GLU
1	C	3752	SER
1	C	3779	VAL
1	C	3793	MET
1	C	3800	LEU
1	C	3816	MET
1	C	3832	ILE
1	C	3835	LEU
1	C	3841	VAL
1	C	3872	GLU
1	C	3879	GLU
1	C	3887	PHE
1	C	3895	HIS
1	C	3912	THR
1	C	3919	THR
1	C	3927	GLN
1	C	3944	GLU
1	C	3966	THR
1	C	3967	GLU
1	C	3992	PHE
1	C	4011	GLU
1	C	4026	MET
1	C	4040	ILE
1	C	4061	PHE
1	C	4069	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4079	ASP
1	C	4088	ILE
1	C	4089	SER
1	C	4092	ASP
1	C	4093	PHE
1	C	4094	GLN
1	C	4104	THR
1	C	4107	GLU
1	C	4123	ILE
1	C	4134	GLU
1	C	4141	PHE
1	C	4150	LEU
1	C	4156	HIS
1	C	4157	ASP
1	C	4178	LEU
1	C	4196	GLU
1	C	4199	GLU
1	C	4231	MET
1	C	4240	ASP
1	C	4244	GLU
1	C	4541	TRP
1	C	4544	LEU
1	C	4626	ASN
1	C	4633	GLU
1	C	4662	ASN
1	C	4705	VAL
1	C	4725	LEU
1	C	4735	GLU
1	C	4739	GLU
1	C	4749	GLU
1	C	4756	ARG
1	C	4788	SER
1	C	4821	LYS
1	C	4865	LYS
1	C	4889	VAL
1	C	4910	GLU
1	C	4949	GLN
1	C	4976	GLU
1	C	4989	MET
1	C	5020	ASP
1	C	5035	GLN
1	D	17	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	46	LEU
1	D	80	GLU
1	D	98	HIS
1	D	100	THR
1	D	105	HIS
1	D	111	HIS
1	D	121	LEU
1	D	124	SER
1	D	125	ARG
1	D	130	LYS
1	D	131	LEU
1	D	135	VAL
1	D	183	SER
1	D	209	CYS
1	D	211	GLU
1	D	222	LEU
1	D	223	PHE
1	D	224	HIS
1	D	265	LEU
1	D	267	ILE
1	D	278	GLN
1	D	296	ASP
1	D	312	THR
1	D	322	LYS
1	D	328	LYS
1	D	367	LEU
1	D	371	VAL
1	D	372	LEU
1	D	381	GLU
1	D	395	GLN
1	D	398	SER
1	D	405	HIS
1	D	439	GLU
1	D	462	GLU
1	D	477	LEU
1	D	483	MET
1	D	495	ASN
1	D	513	GLU
1	D	525	LEU
1	D	534	ARG
1	D	536	ASN
1	D	537	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	545	ASP
1	D	577	ILE
1	D	580	GLU
1	D	623	GLU
1	D	630	GLU
1	D	636	ASN
1	D	674	PHE
1	D	755	ILE
1	D	765	GLN
1	D	769	GLU
1	D	828	GLU
1	D	829	TYR
1	D	851	PHE
1	D	876	GLU
1	D	884	LEU
1	D	907	LEU
1	D	910	PHE
1	D	939	VAL
1	D	949	ASN
1	D	957	LYS
1	D	963	ASN
1	D	999	ASP
1	D	1022	VAL
1	D	1070	ASP
1	D	1073	ARG
1	D	1104	TRP
1	D	1114	GLU
1	D	1136	SER
1	D	1184	ILE
1	D	1216	ILE
1	D	1236	THR
1	D	1244	GLN
1	D	1286	MET
1	D	1427	ILE
1	D	1433	TYR
1	D	1434	TYR
1	D	1444	GLU
1	D	1446	SER
1	D	1463	ASN
1	D	1473	THR
1	D	1478	ASP
1	D	1483	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1513	ASP
1	D	1514	LEU
1	D	1518	CYS
1	D	1522	LEU
1	D	1570	LYS
1	D	1583	GLU
1	D	1590	GLN
1	D	1623	ARG
1	D	1649	ASP
1	D	1721	GLU
1	D	1769	THR
1	D	1805	GLU
1	D	1808	ARG
1	D	1812	LEU
1	D	1867	GLU
1	D	1950	GLU
1	D	1995	THR
1	D	2008	MET
1	D	2014	ASP
1	D	2015	GLU
1	D	2018	GLU
1	D	2045	GLN
1	D	2100	HIS
1	D	2120	MET
1	D	2150	GLU
1	D	2155	LEU
1	D	2168	VAL
1	D	2169	GLN
1	D	2193	GLN
1	D	2209	GLU
1	D	2219	GLU
1	D	2224	ARG
1	D	2271	THR
1	D	2274	ASP
1	D	2280	VAL
1	D	2290	LEU
1	D	2294	ASP
1	D	2302	LEU
1	D	2308	GLN
1	D	2309	SER
1	D	2330	ARG
1	D	2357	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2371	GLU
1	D	2415	ARG
1	D	2431	ASP
1	D	2440	MET
1	D	2453	ILE
1	D	2460	LEU
1	D	2503	VAL
1	D	2506	LEU
1	D	2518	LEU
1	D	2522	LEU
1	D	2558	VAL
1	D	2573	GLU
1	D	2577	ILE
1	D	2578	MET
1	D	2593	ARG
1	D	2596	THR
1	D	2620	GLN
1	D	2634	ASN
1	D	2647	HIS
1	D	2669	GLU
1	D	2673	HIS
1	D	2700	MET
1	D	2724	GLU
1	D	2745	VAL
1	D	2751	LEU
1	D	2766	TRP
1	D	2782	ASP
1	D	2797	PHE
1	D	2817	ILE
1	D	2823	ILE
1	D	2927	LEU
1	D	2955	PHE
1	D	2968	ASP
1	D	2998	PHE
1	D	3002	LEU
1	D	3043	PHE
1	D	3092	LEU
1	D	3154	ASP
1	D	3181	THR
1	D	3184	GLU
1	D	3226	GLU
1	D	3238	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3290	GLU
1	D	3324	VAL
1	D	3549	VAL
1	D	3670	GLU
1	D	3683	GLN
1	D	3713	LYS
1	D	3723	MET
1	D	3736	GLU
1	D	3750	GLU
1	D	3779	VAL
1	D	3793	MET
1	D	3794	VAL
1	D	3800	LEU
1	D	3822	ASP
1	D	3825	GLU
1	D	3832	ILE
1	D	3835	LEU
1	D	3841	VAL
1	D	3856	LEU
1	D	3870	ASN
1	D	3879	GLU
1	D	3887	PHE
1	D	3895	HIS
1	D	3900	GLN
1	D	3909	ASN
1	D	3910	THR
1	D	3919	THR
1	D	3927	GLN
1	D	3943	ILE
1	D	3944	GLU
1	D	3953	LYS
1	D	3966	THR
1	D	3967	GLU
1	D	3970	GLN
1	D	3987	ASP
1	D	3989	VAL
1	D	3992	PHE
1	D	4026	MET
1	D	4040	ILE
1	D	4047	MET
1	D	4061	PHE
1	D	4068	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4071	ILE
1	D	4088	ILE
1	D	4089	SER
1	D	4092	ASP
1	D	4094	GLN
1	D	4104	THR
1	D	4123	ILE
1	D	4134	GLU
1	D	4141	PHE
1	D	4149	ASN
1	D	4150	LEU
1	D	4154	VAL
1	D	4156	HIS
1	D	4161	ARG
1	D	4175	ARG
1	D	4199	GLU
1	D	4200	THR
1	D	4231	MET
1	D	4240	ASP
1	D	4244	GLU
1	D	4541	TRP
1	D	4544	LEU
1	D	4626	ASN
1	D	4662	ASN
1	D	4705	VAL
1	D	4714	ASN
1	D	4719	PHE
1	D	4725	LEU
1	D	4735	GLU
1	D	4739	GLU
1	D	4749	GLU
1	D	4788	SER
1	D	4821	LYS
1	D	4865	LYS
1	D	4910	GLU
1	D	4949	GLN
1	D	4976	GLU
1	D	4989	MET
1	D	5020	ASP
1	D	5035	GLN
2	E	13	ARG
2	E	21	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	32	ASP
2	E	74	LEU
2	F	13	ARG
2	F	21	THR
2	F	34	LYS
2	F	36	PHE
2	F	74	LEU
2	G	13	ARG
2	G	21	THR
2	G	34	LYS
2	G	74	LEU
2	H	13	ARG
2	H	21	THR
2	H	34	LYS
2	H	74	LEU
2	H	91	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	308	HIS
1	A	383	HIS
1	A	405	HIS
1	A	520	ASN
1	A	634	GLN
1	A	678	GLN
1	A	720	HIS
1	A	1052	ASN
1	A	1158	ASN
1	A	1459	GLN
1	A	1563	GLN
1	A	1614	GLN
1	A	1691	GLN
1	A	1949	GLN
1	A	2003	GLN
1	A	2007	ASN
1	A	2011	HIS
1	A	2184	ASN
1	A	2475	GLN
1	A	2498	HIS
1	A	2788	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2856	ASN
1	A	2858	GLN
1	A	3109	ASN
1	A	3128	ASN
1	A	3180	ASN
1	A	3378	GLN
1	A	3430	ASN
1	A	3457	ASN
1	A	3461	GLN
1	A	3572	GLN
1	A	3667	HIS
1	A	3766	GLN
1	A	4009	GLN
1	A	4133	GLN
1	A	4662	ASN
1	A	4812	HIS
1	A	4949	GLN
1	A	4984	ASN
1	B	32	GLN
1	B	105	HIS
1	B	113	HIS
1	B	383	HIS
1	B	489	ASN
1	B	520	ASN
1	B	705	ASN
1	B	720	HIS
1	B	866	HIS
1	B	911	HIS
1	B	981	GLN
1	B	1158	ASN
1	B	1459	GLN
1	B	1614	GLN
1	B	1688	HIS
1	B	1696	HIS
1	B	1702	HIS
1	B	1949	GLN
1	B	2029	GLN
1	B	2161	GLN
1	B	2173	GLN
1	B	2184	ASN
1	B	2414	ASN
1	B	2475	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2487	GLN
1	B	2498	HIS
1	B	2744	ASN
1	B	2756	ASN
1	B	2774	ASN
1	B	2877	GLN
1	B	2883	HIS
1	B	2931	GLN
1	B	3013	HIS
1	B	3030	HIS
1	B	3109	ASN
1	B	3128	ASN
1	B	3162	GLN
1	B	3180	ASN
1	B	3326	ASN
1	B	3897	ASN
1	B	3901	ASN
1	B	3927	GLN
1	B	4009	GLN
1	B	4034	ASN
1	B	4094	GLN
1	B	4149	ASN
1	B	4209	GLN
1	B	4662	ASN
1	B	4754	ASN
1	B	4812	HIS
1	B	4832	HIS
1	B	4833	ASN
1	B	5035	GLN
1	C	32	GLN
1	C	57	ASN
1	C	105	HIS
1	C	461	HIS
1	C	520	ASN
1	C	678	GLN
1	C	720	HIS
1	C	877	ASN
1	C	909	ASN
1	C	1125	ASN
1	C	1459	GLN
1	C	1560	ASN
1	C	1611	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1614	GLN
1	C	1688	HIS
1	C	1941	ASN
1	C	1949	GLN
1	C	2011	HIS
1	C	2029	GLN
1	C	2184	ASN
1	C	2414	ASN
1	C	2441	HIS
1	C	2475	GLN
1	C	2498	HIS
1	C	2744	ASN
1	C	2856	ASN
1	C	2858	GLN
1	C	3013	HIS
1	C	3162	GLN
1	C	3180	ASN
1	C	3234	ASN
1	C	3430	ASN
1	C	3572	GLN
1	C	3667	HIS
1	C	3895	HIS
1	C	3901	ASN
1	C	3927	GLN
1	C	3970	GLN
1	C	4009	GLN
1	C	4078	GLN
1	C	4094	GLN
1	C	4100	GLN
1	C	4102	GLN
1	C	4130	ASN
1	C	4149	ASN
1	C	4662	ASN
1	C	4753	HIS
1	C	4832	HIS
1	C	4833	ASN
1	D	32	GLN
1	D	57	ASN
1	D	113	HIS
1	D	201	ASN
1	D	383	HIS
1	D	520	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	636	ASN
1	D	720	HIS
1	D	877	ASN
1	D	911	HIS
1	D	981	GLN
1	D	1011	GLN
1	D	1052	ASN
1	D	1299	GLN
1	D	1459	GLN
1	D	1560	ASN
1	D	1614	GLN
1	D	1688	HIS
1	D	1941	ASN
1	D	1949	GLN
1	D	1952	GLN
1	D	2011	HIS
1	D	2107	GLN
1	D	2351	ASN
1	D	2414	ASN
1	D	2475	GLN
1	D	2498	HIS
1	D	2763	HIS
1	D	2856	ASN
1	D	2924	GLN
1	D	3013	HIS
1	D	3109	ASN
1	D	3162	GLN
1	D	3572	GLN
1	D	3667	HIS
1	D	3870	ASN
1	D	3901	ASN
1	D	3927	GLN
1	D	3946	GLN
1	D	4078	GLN
1	D	4149	ASN
1	D	4662	ASN
1	D	4753	HIS
1	D	4812	HIS
1	D	4832	HIS
1	D	4833	ASN
2	E	94	HIS
2	F	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	3	GLN
2	G	94	HIS
2	H	3	GLN
2	H	87	HIS
2	H	94	HIS

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](#)

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.

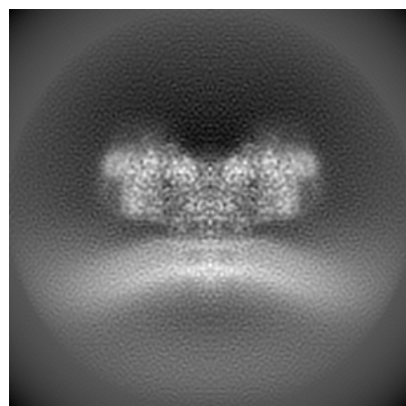
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54594. These allow visual inspection of the internal detail of the map and identification of artifacts.

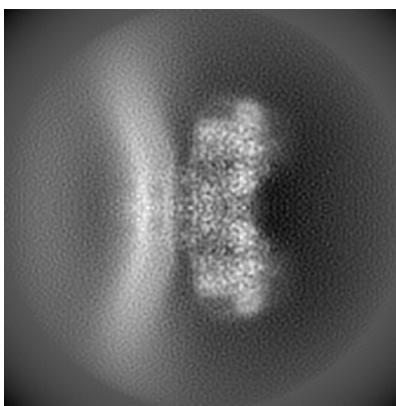
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

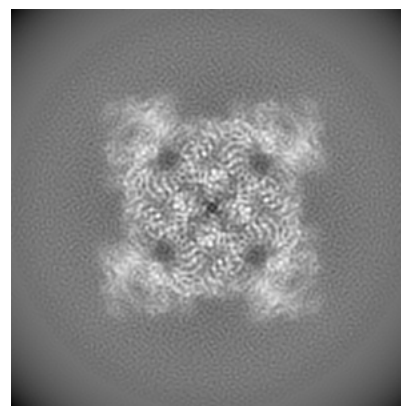
6.1.1 Primary map



X

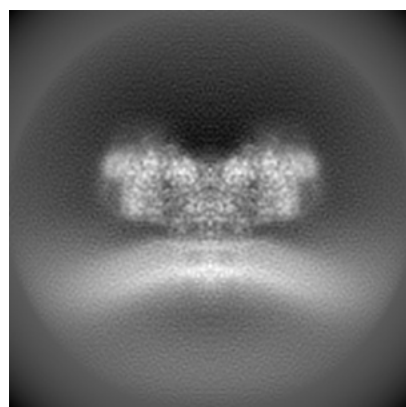


Y

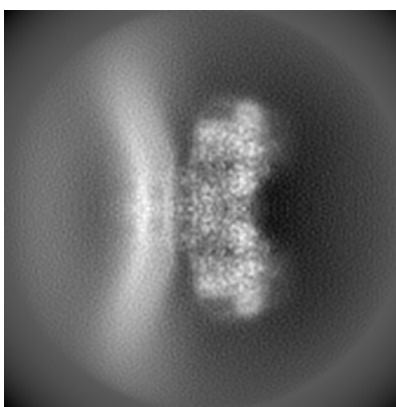


Z

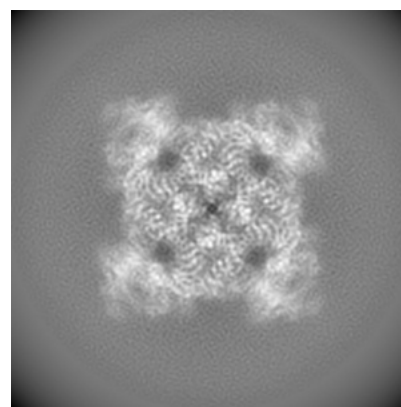
6.1.2 Raw map



X



Y

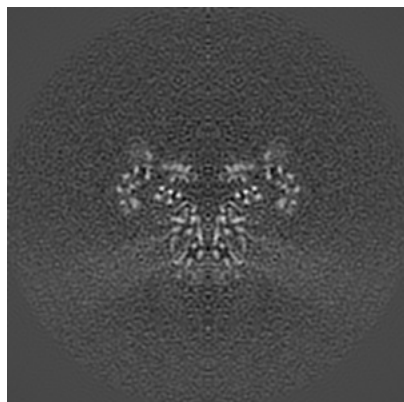


Z

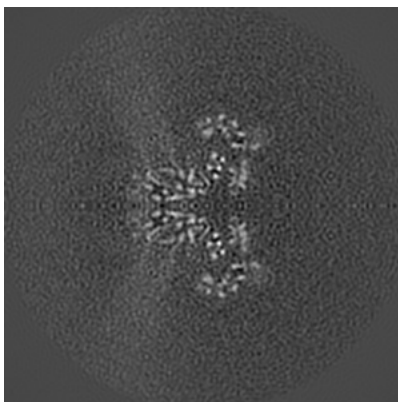
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

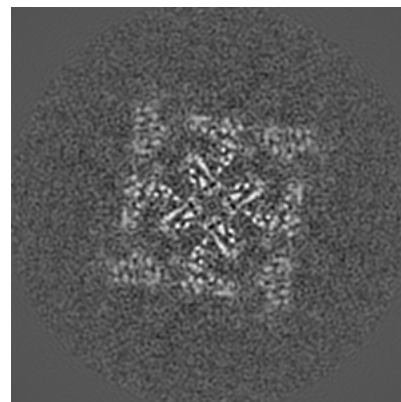
6.2.1 Primary map



X Index: 85

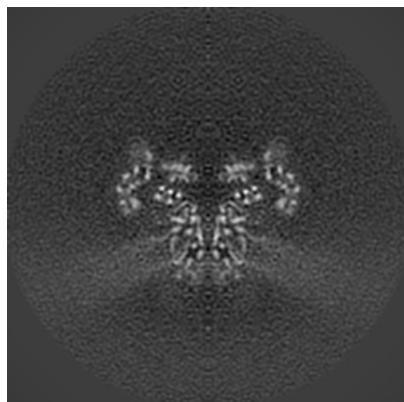


Y Index: 85

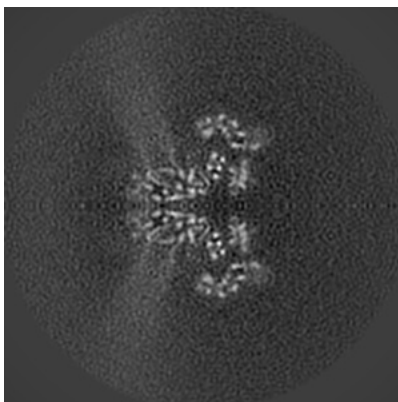


Z Index: 85

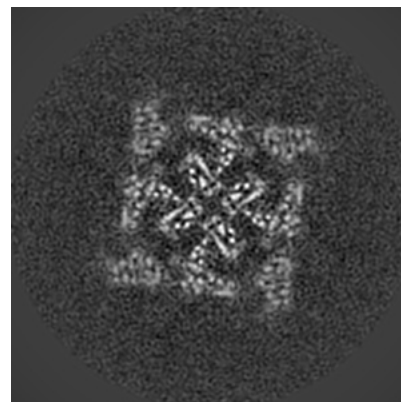
6.2.2 Raw map



X Index: 85



Y Index: 85

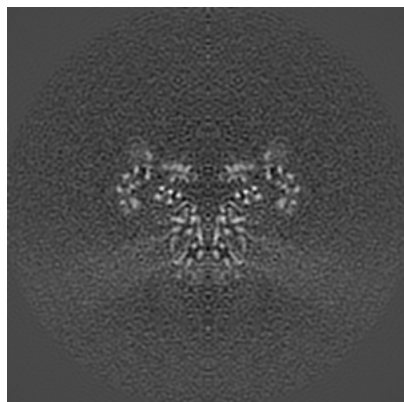


Z Index: 85

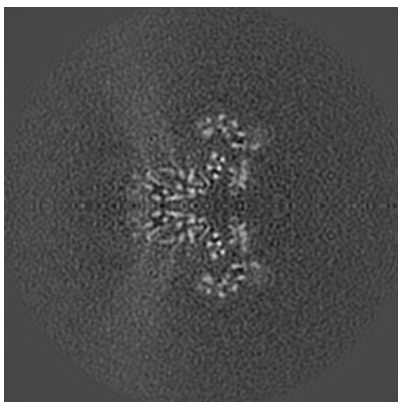
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

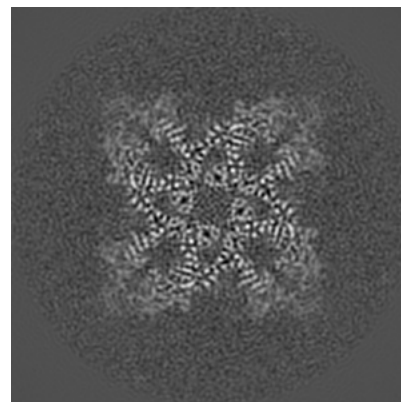
6.3.1 Primary map



X Index: 85

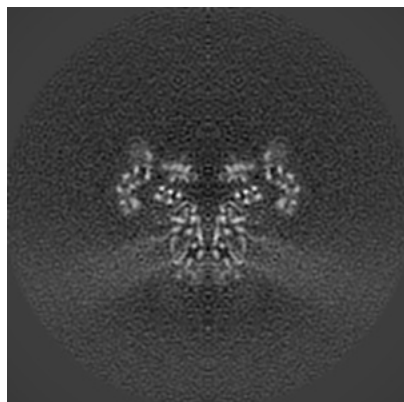


Y Index: 85

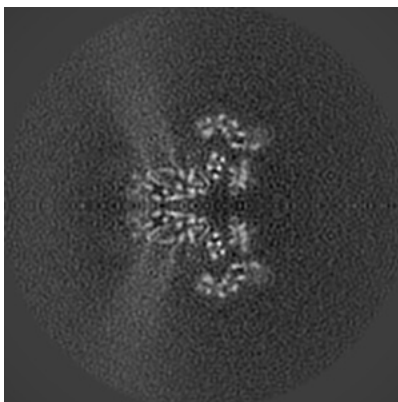


Z Index: 100

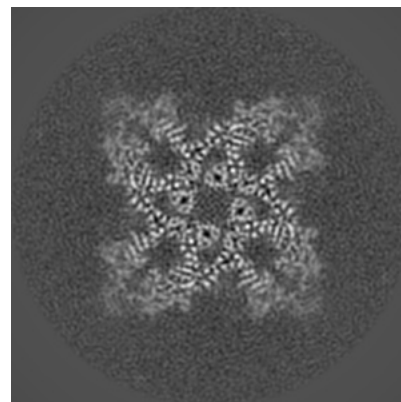
6.3.2 Raw map



X Index: 85



Y Index: 85

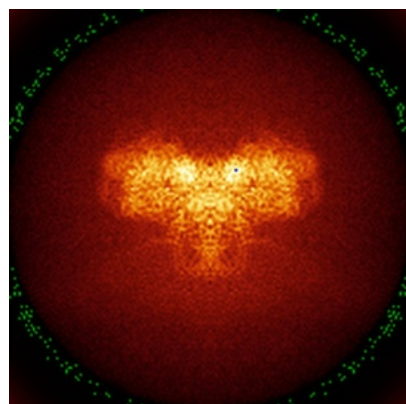


Z Index: 100

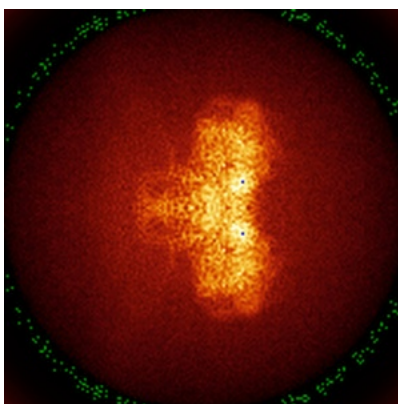
The images above show the largest variance slices of the map in three orthogonal directions.

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

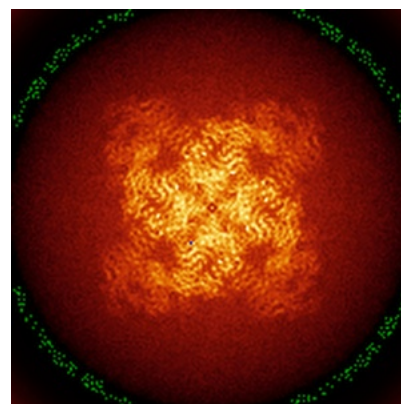
6.4.1 Primary map



X

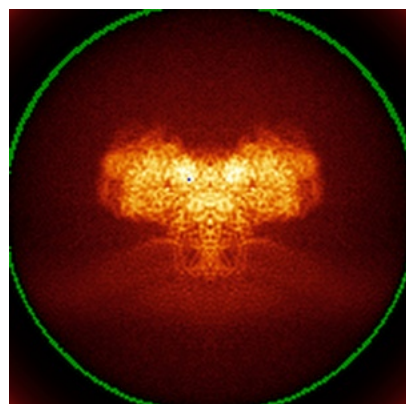


Y

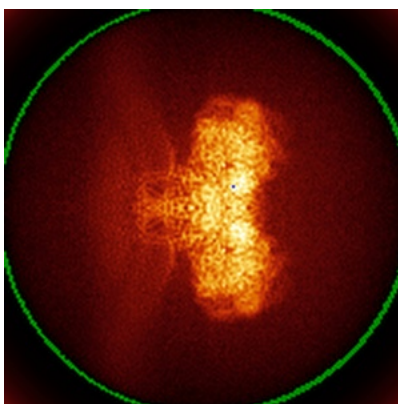


Z

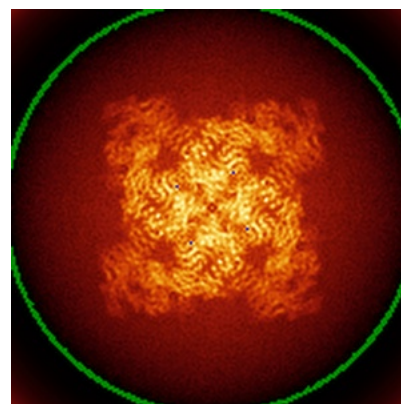
6.4.2 Raw map



X



Y

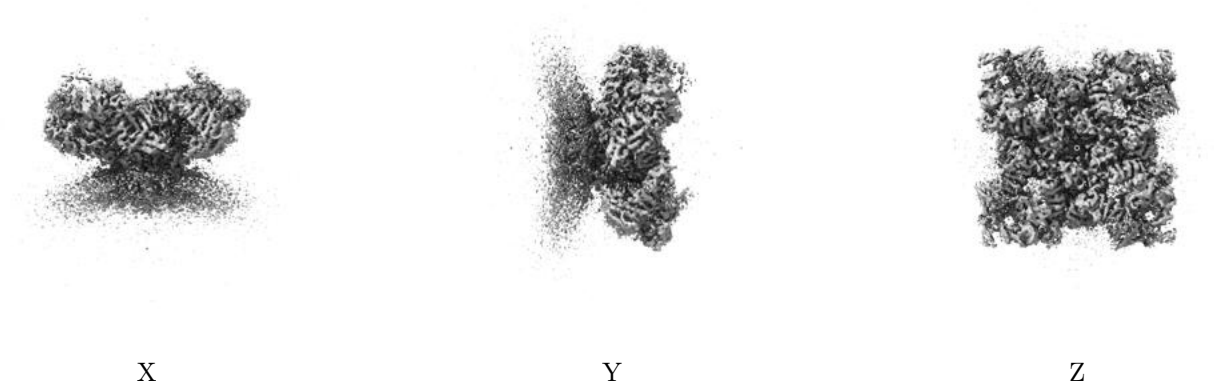


Z

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.

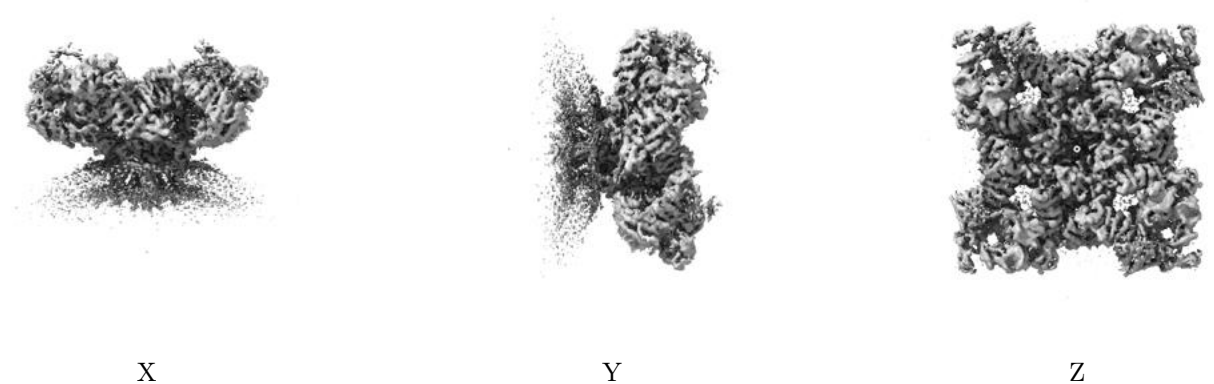
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0893. 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



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.

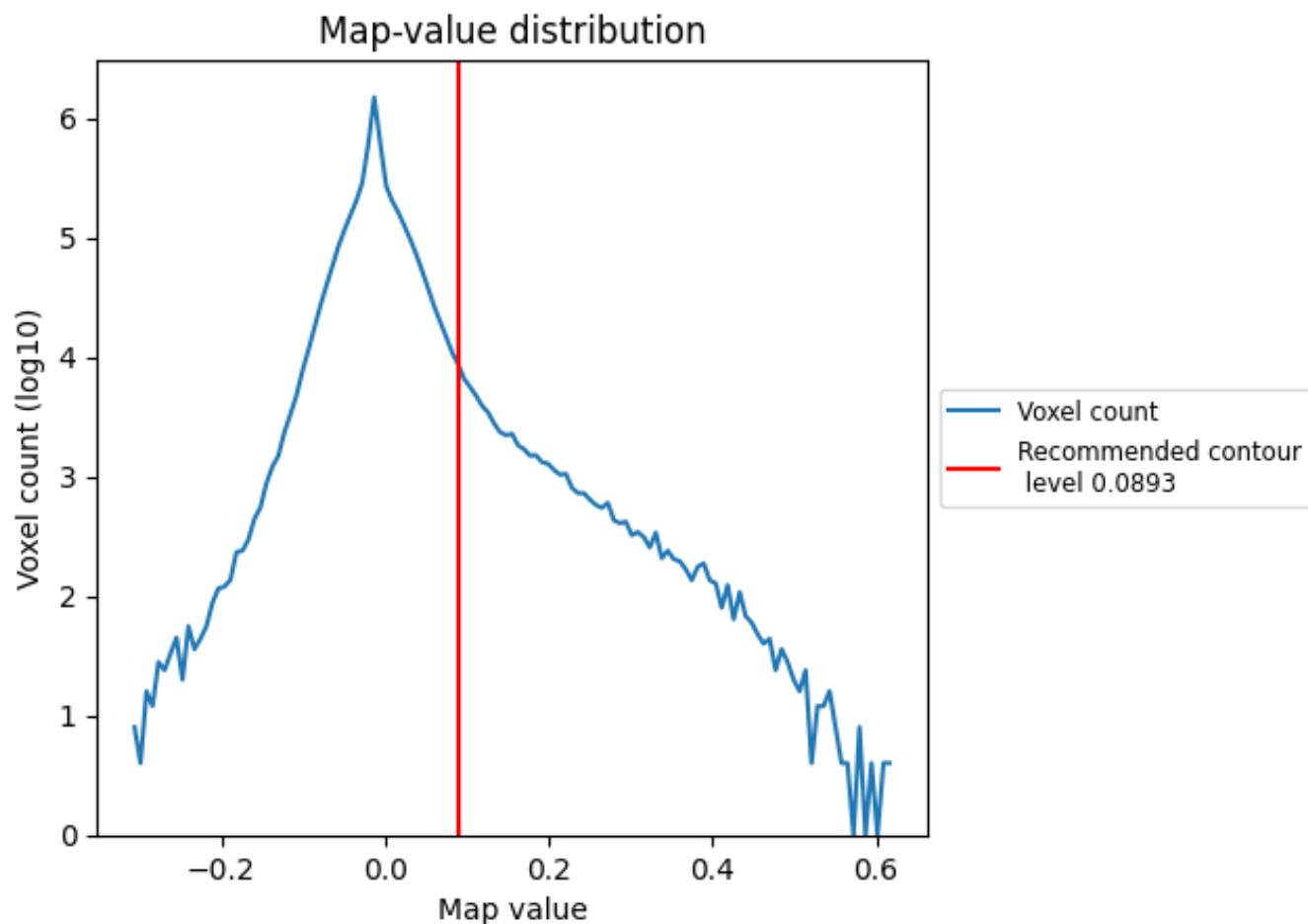
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

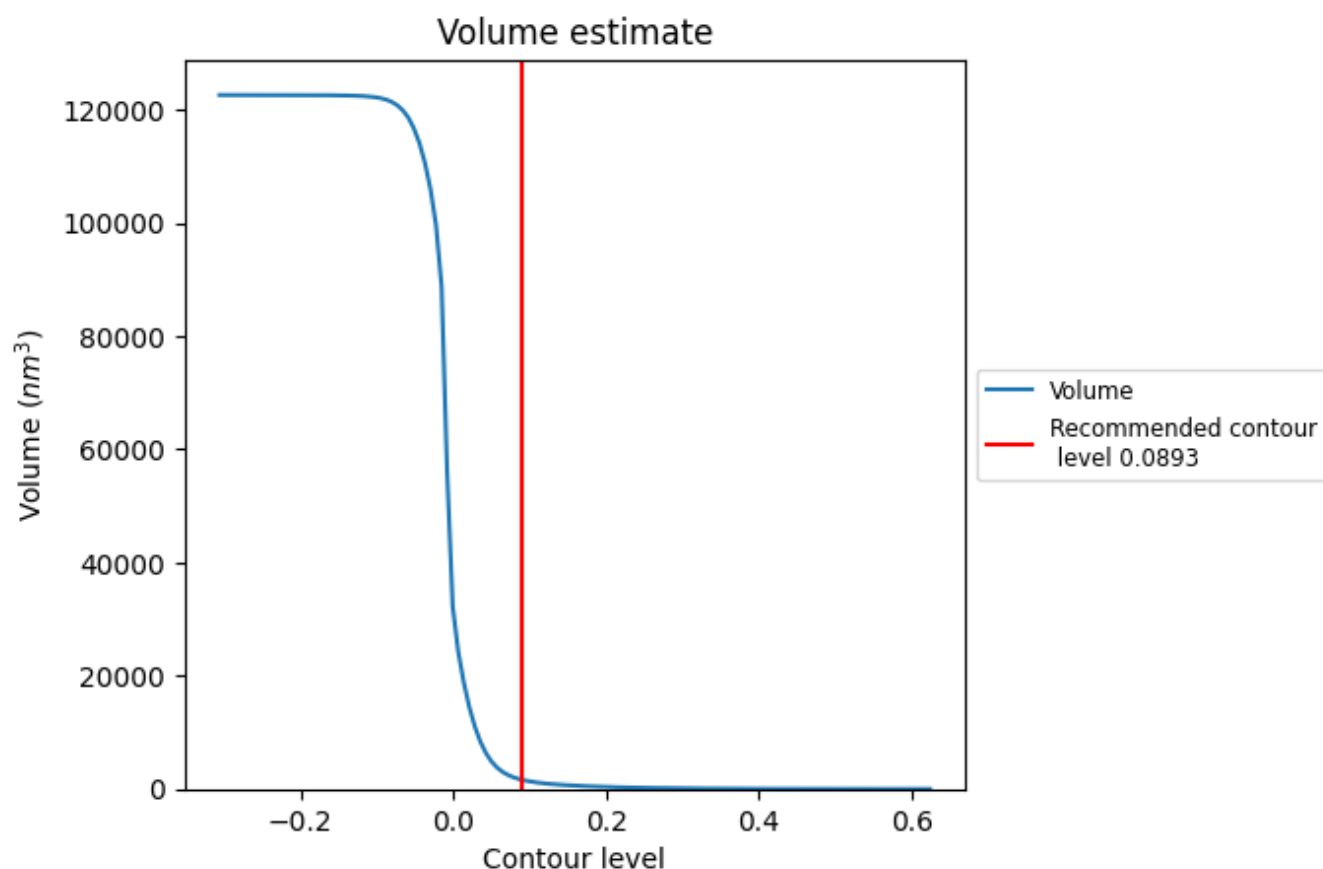
This section contains the results of statistical analysis of the map.

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.

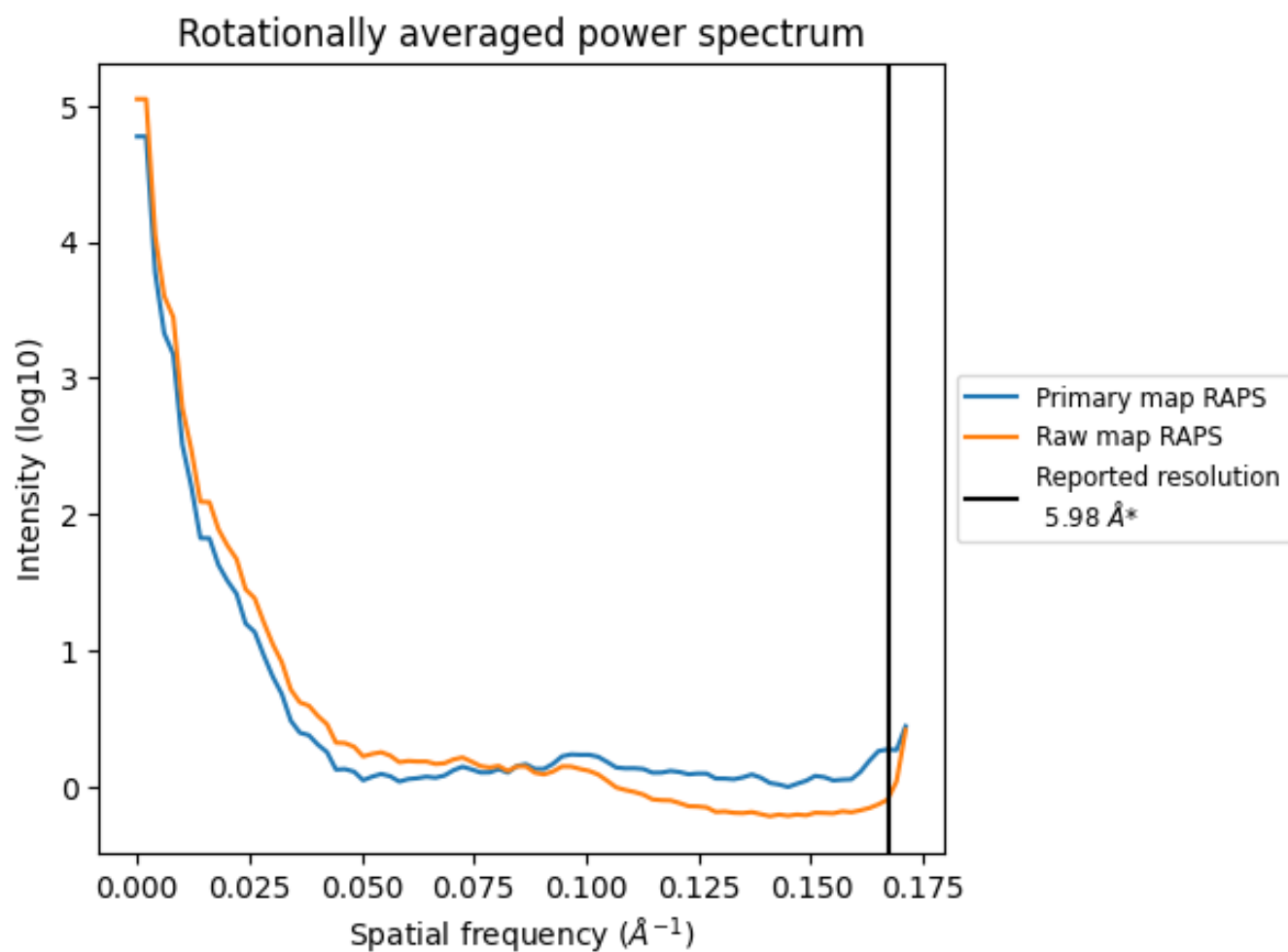
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1630 nm^3 ; this corresponds to an approximate mass of 1473 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 ⓘ

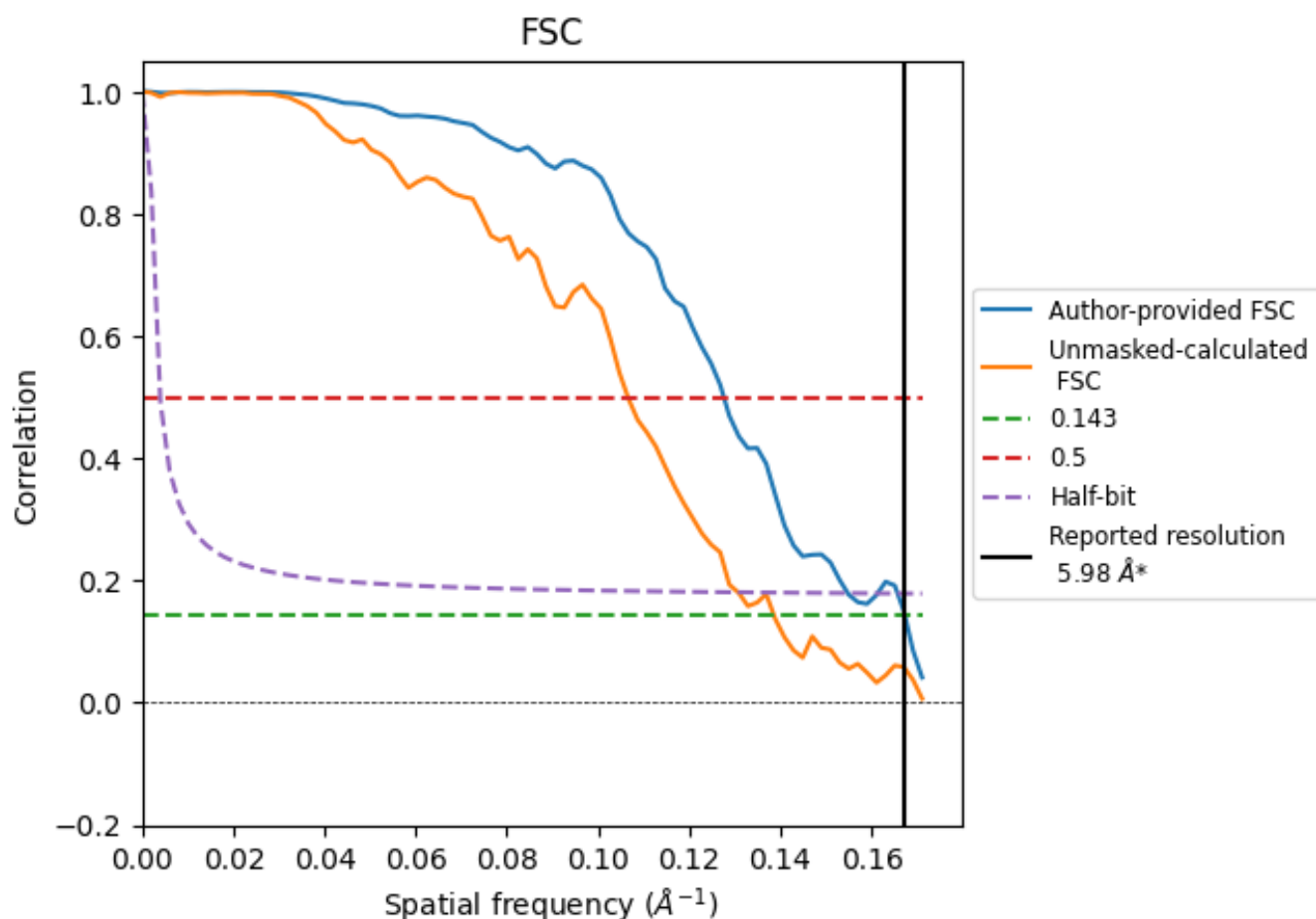


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

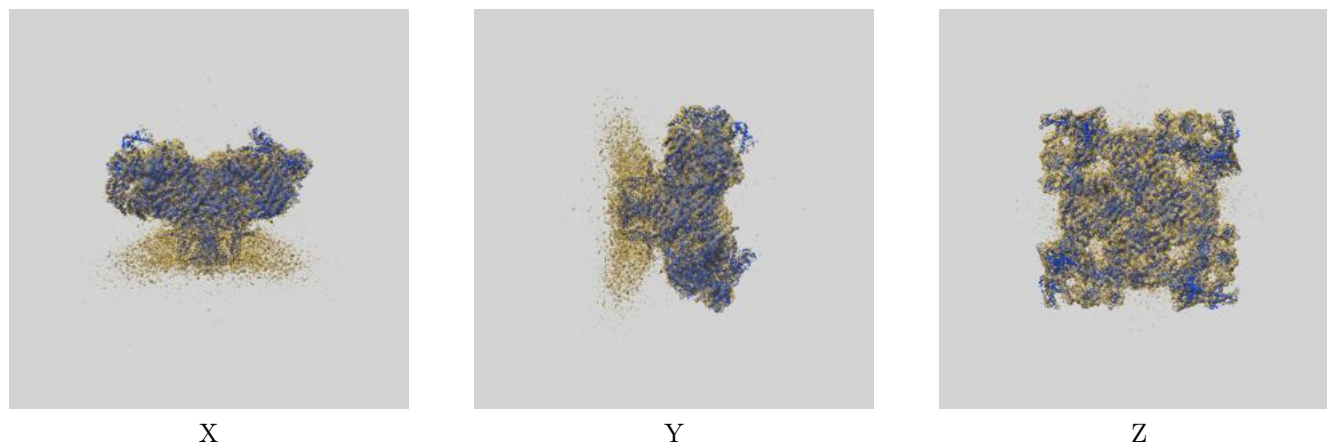
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.98	-	-
Author-provided FSC curve	5.98	7.84	6.46
Unmasked-calculated*	7.22	9.38	7.65

*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 7.22 differs from the reported value 5.98 by more than 10 %

9 Map-model fit [i](#)

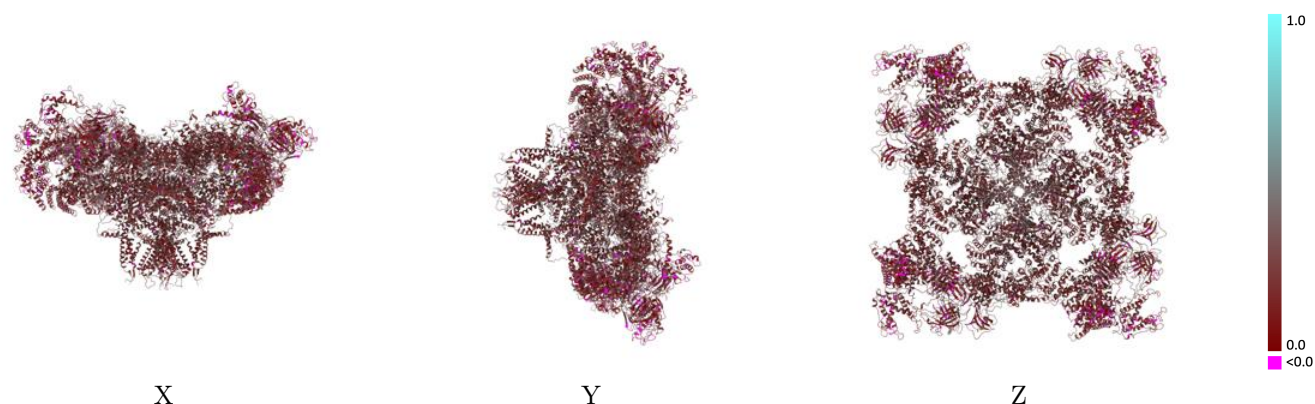
This section contains information regarding the fit between EMDB map EMD-54594 and PDB model 9S5C. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



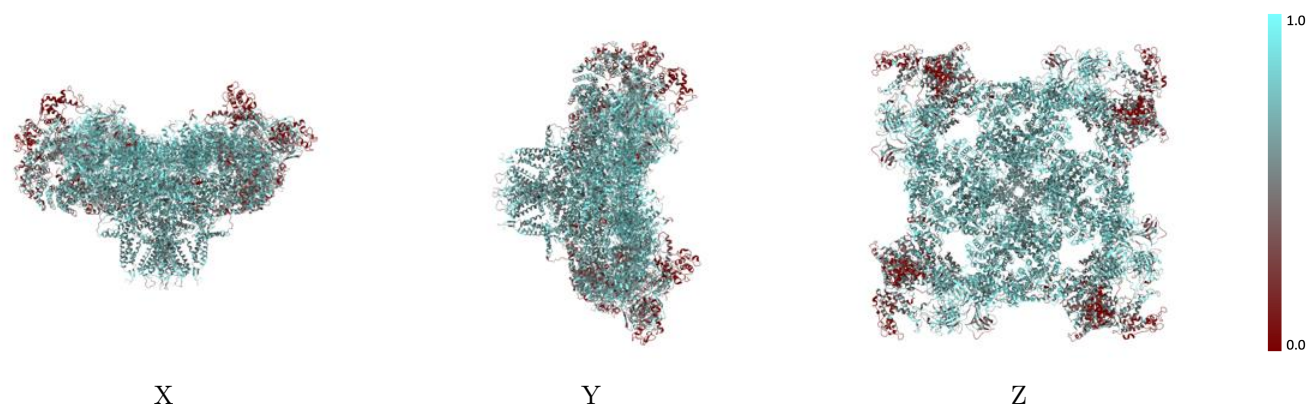
The images above show the 3D surface view of the map at the recommended contour level 0.0893 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



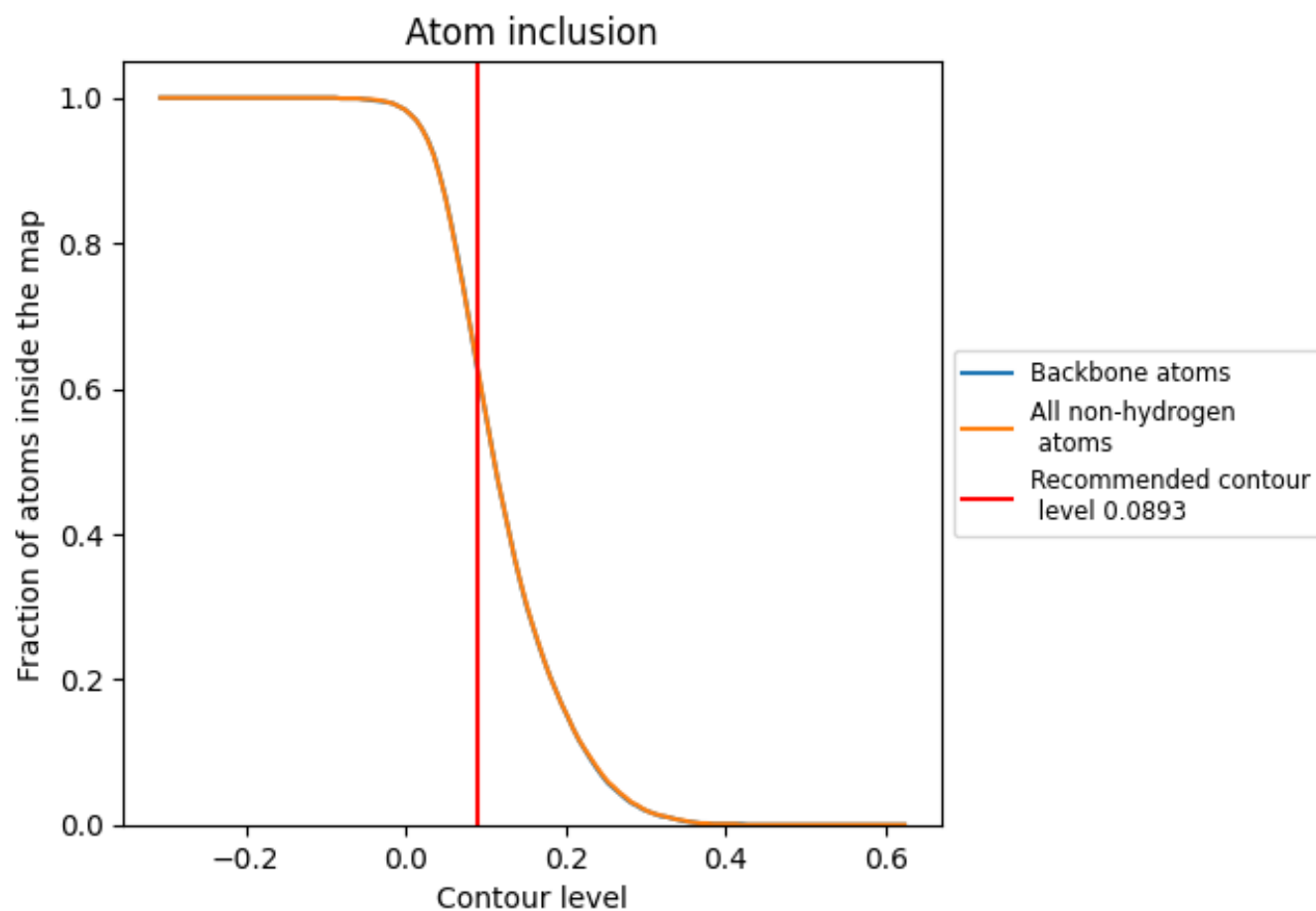
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0893).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.0893) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.2390
A	0.6430	0.2380
B	0.6440	0.2390
C	0.6460	0.2400
D	0.6430	0.2380
E	0.5540	0.2250
F	0.5580	0.2280
G	0.5560	0.2230
H	0.5580	0.2340

