



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 06:08 pm BST

PDB ID : 9S5Y / pdb_00009s5y
EMDB ID : EMD-54616
Title : Up class, Primed-state RyR1 with activating ligand mixture (Calcium/ACP/Caffeine) in the native membrane solved by StA
Authors : Mikirtumov, V.
Deposited on : 2025-07-30
Resolution : 6.82 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:

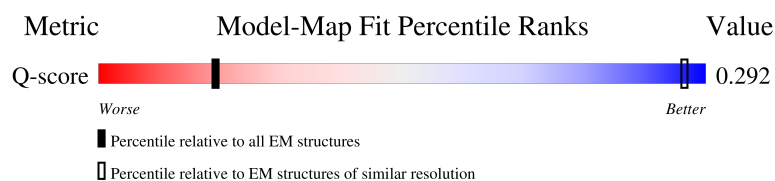
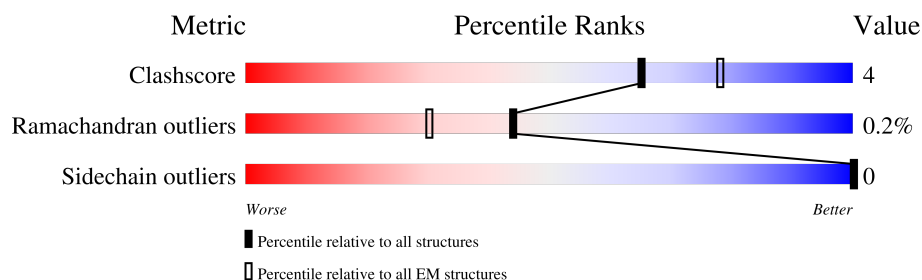
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.82 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	462 (6.32 - 7.30)

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	24% 80% 8% 13%
1	B	5037	24% 80% 8% 13%
1	C	5037	24% 80% 8% 13%
1	D	5037	24% 80% 8% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	108	29% 89% 10%
2	F	108	28% 89% 10%
2	G	108	28% 86% 13%
2	H	108	28% 87% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 285956 atoms, of which 142272 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
			69827	22323	34739	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	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		

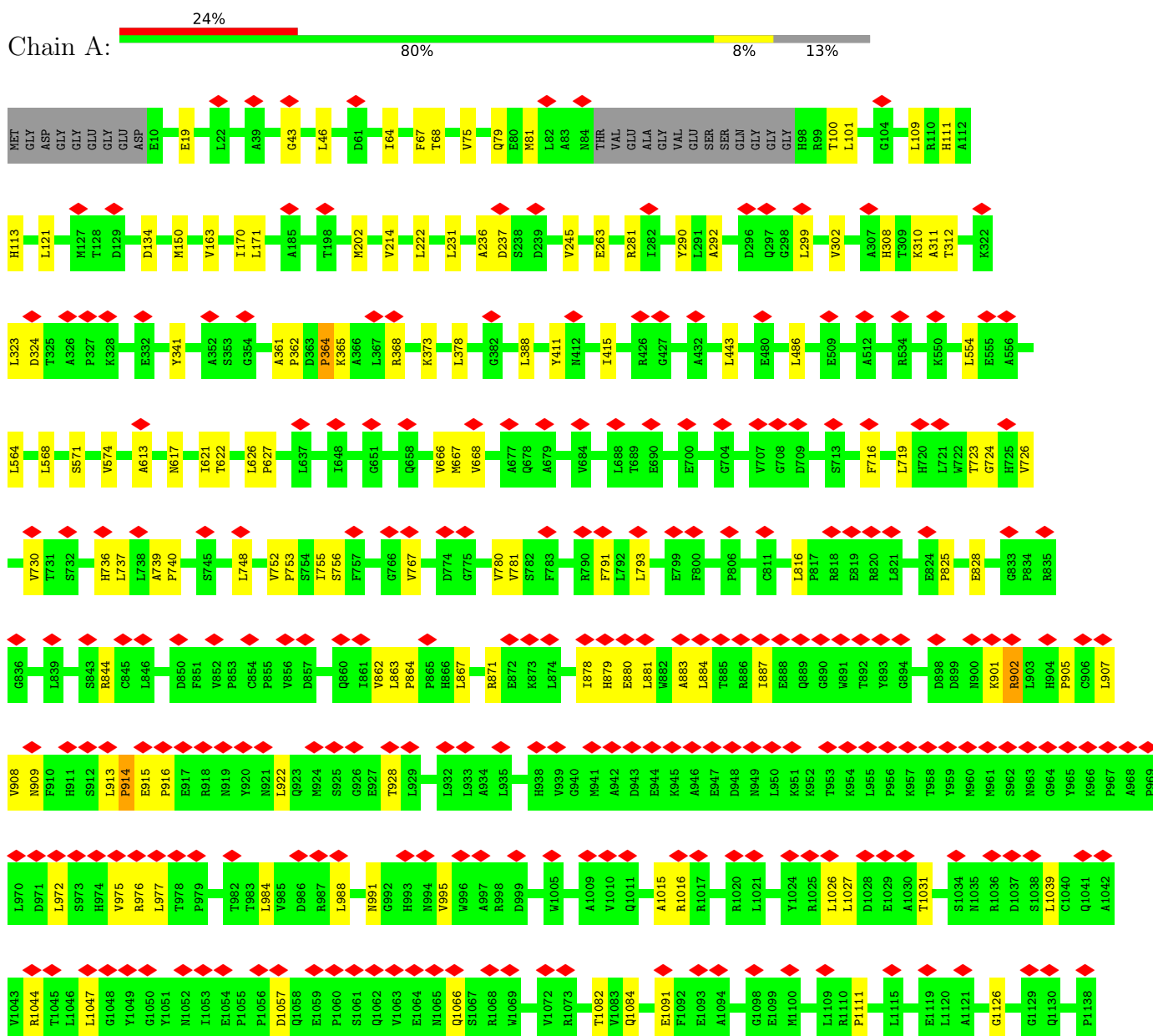
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

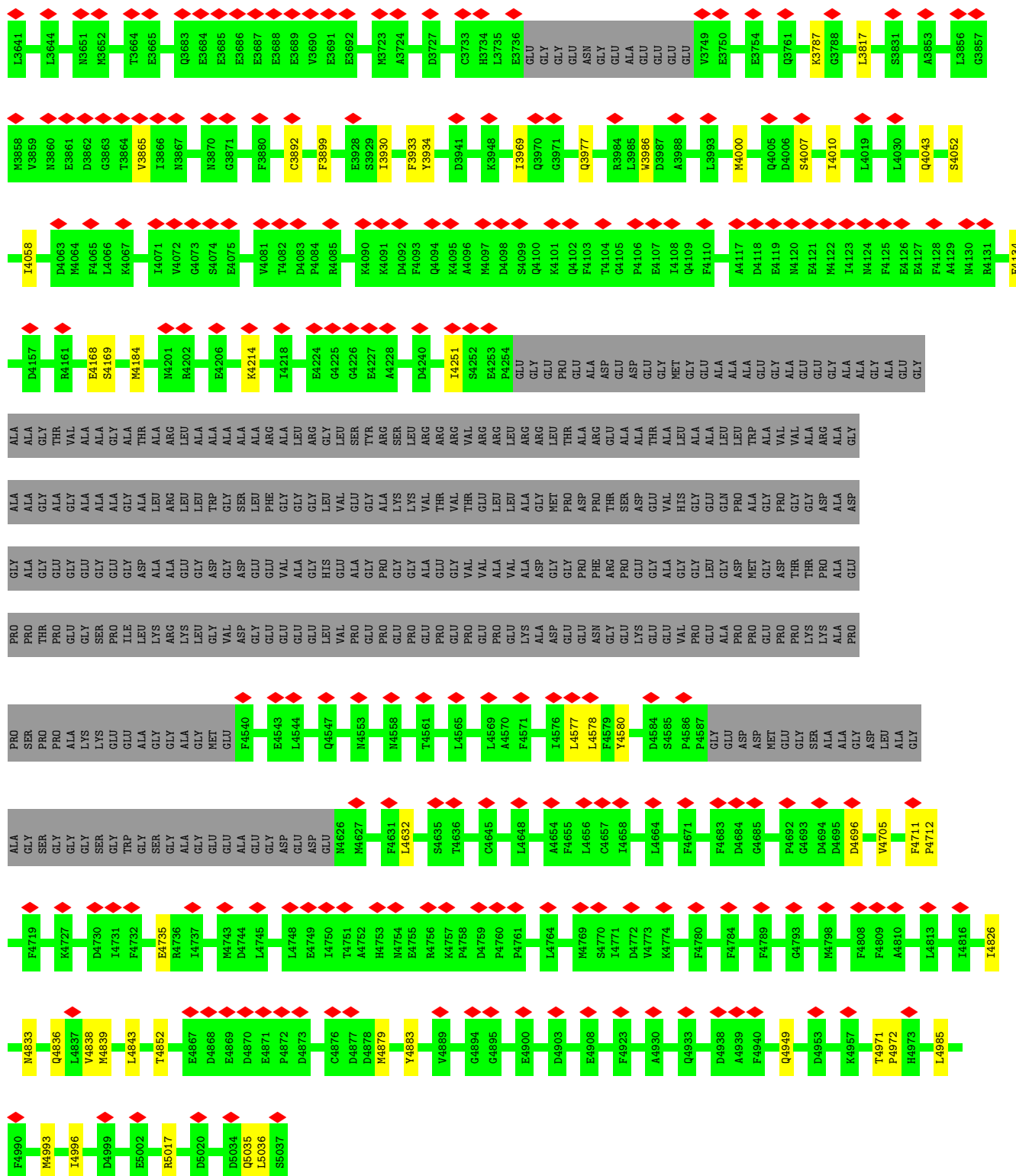
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





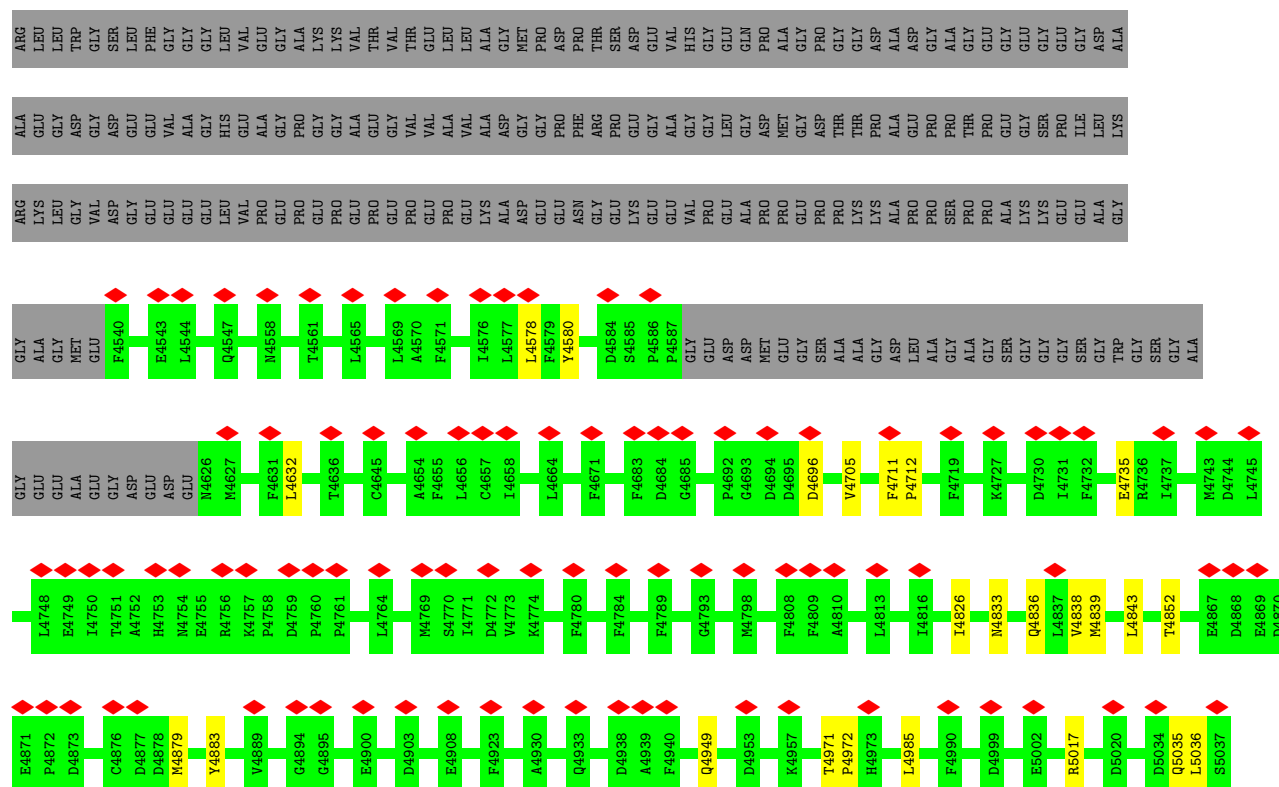




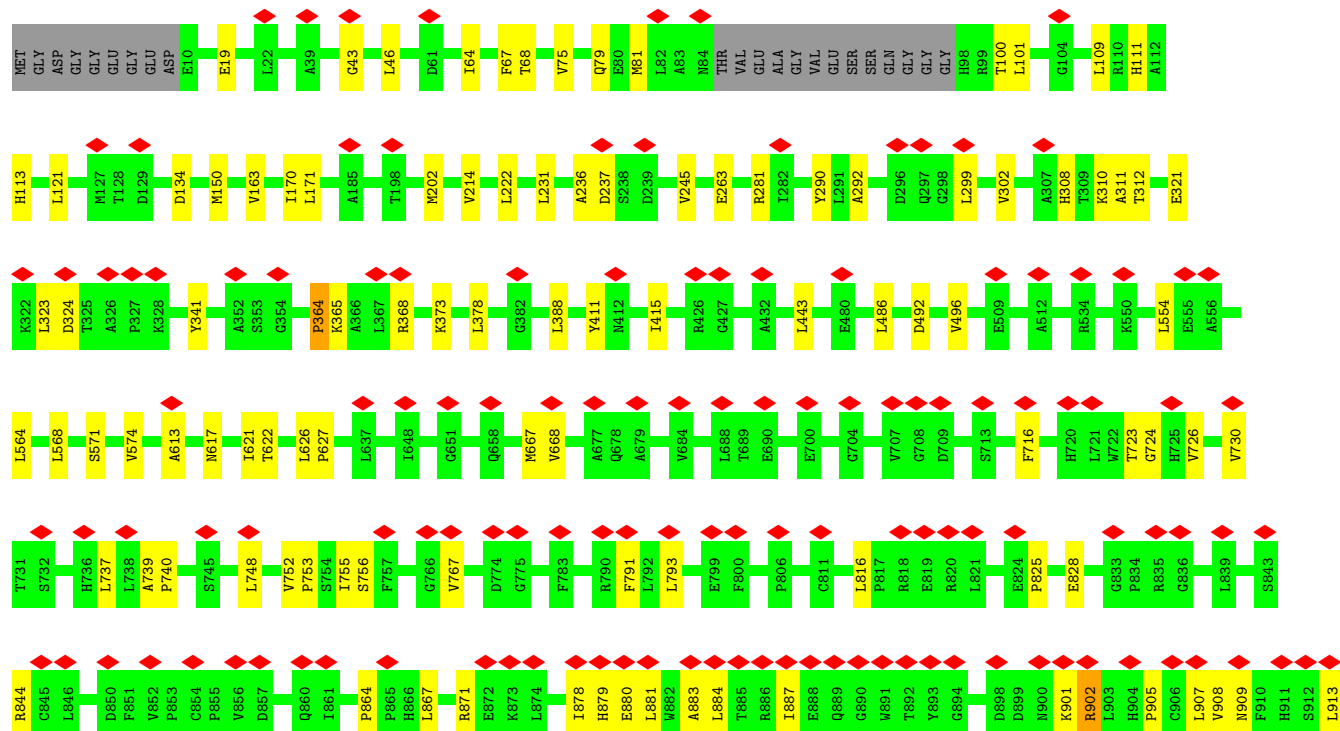
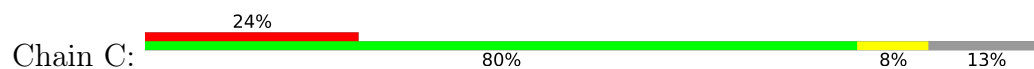




ARG	L3075	F3152	K3222	P3292	A3369	V3438	Q3506	D3585	E3684	N3870	E4075	R4202
LEU	D3076	G3153	S3223	P3293	A3374	T3441	T3507	A3586	E3685	G3871	V4081	E4206
ALA	A3077	D3154	P3224	P3294	G3370	T3444	S3508	D3587	E3686	F3880	T4082	
ALA	R3078	D3155	R3225	A3295	K3371	V3444	T3513	D3588	E3687	F3889	D4083	K4214
ALA	T3079	V3156	L3230	L3296	A3375	K3447	L3514	P3589	E3688	C3892	T4083	
ARG	V3080	I3157	G3231	P3297	E3375	S3448	K3515	E3590	E3689	F3899	F4084	
ALA	K3081	L3158	L3232	A3298	E3376	H3449	K3516	V3593	V3690	F3899	R4085	
ALA	K3082	D3159	L3233	G3299	E3377	H3449	N3517	R3594	E3691	F3899		
ARG	S3083	D3160	N3234	A3300	E3378	E3455	G3521	E3598	E3692	E3928		
ARG		Q3162	N3235	P3301	Q3378	Q3456	G3521	E3598	E3692	S3929		
GLY	T3087	V3161	S3236	P3302	L3379	V3459	C3525	L3603	K3723	I3930	K4090	E4224
LEU	V3088	V3163	V3236	P3303	R3380	Q3461	A3526	H3604	A3724	F3933	K4091	G4225
LEU	K3089	S3164	E3237	P3304	L3381	Q3462	P3527	H3605	A3724	Y3934	D4092	G4226
SER	A3090	C3165	E3238	C3304	E3382	E3463	P3527	L3606	D3727	F3934	F4093	E4227
ARG	G3091	Y3166	E3239	T3305	E3383	E3464	E3532	E3607	C3733	D3941	Q4094	A4228
ARG	L3092	L3169	N3239	A3306	K3384	E3465	I3533	E3608	H3734	K3948	K4095	
ARG		C3170	C3240	V3307	A3385	N3466	M3534	E3609	H3735	I3949	A4096	
ARG	F3096	S3171	P3241	D3310	E3386	N3467	K3537	E3610	E3736	I3969	M4097	
ARG		I3172	D3242	H3311	E3387	S3468	T3538	H3611	GLU	Q3970	D4098	I4251
ARG	S3100	G3177	I3243	L3312	E3388	E3468	R3539	H3612	GLY	G3971	S4099	S4252
ARG	E3101	T3177	R3248	L3315	E3389	F3469	Y3540	K3614	GLY	Q3977	Q4100	E4253
ARG	E3104	T3178	L3249	L3316	G3390	L3470	E3540	S3615	ASN		Q4101	P4254
ALA	K3105	K3179	G3255	L3320	E3391	T3471	K3543	K3616	GLU		Q4102	
ALA	K3106	N3180	L3256	K3321	L3392	T3472	D3544	K3617	GLY		T4103	
ALA	V3107	Y3182	A3257	I3322	L3393	A3472	E3547	A3618	GLU		T4104	
ALA	L3110	V3183	E3258	I3323	V3394	S3473	E3548	V3619	GLU		G4105	
ALA	R3111	E3184	S3259	V3324	R3395	S3474	E3549	W3620	GLU		P4106	
ALA	L3112	K3185	G3260	N3325	E3396	K3475	V3549	K3622	GLY		E4107	
ALA	G3113	L3186	A3261	N3326	F3398	S3476	R3560	L3623	GLY		I4108	
ALA	K3114	R3187	R3262	L3327	C3402	K3477	E3560	L3624	GLY		Q4109	
ALA	V3115	L3190	Y3263	G3328	L3405	A3479	L3553	S3625	GLY		Q4110	
ALA	S3116	G3191	T3264	I3329	Y3406	LYS	Q3554	K3626	GLY		A4117	
ALA	GLN	E3192	E3265	D3330	Y3407	ALA	N3555	K3627	GLY		D4118	
ALA	ALA	C3193	M3266	E3331	A3408	GLY	N3556	Q3627	GLY		E4119	
ALA	ARG	L3194	P3267	A3332	L3408	ASP	E3559	R3628	GLY		N4120	
ALA	THR	A3195	H3268	T3333	Y3409	GLN	Q3560	R3629	GLY		I4121	
ALA	VAL	R3196	V3269	T3334	P3410	GLY	G3561	A3631	GLY		A4122	
ALA	K3123	L3197	I3270	M3335	L3411	GLY	K3562	V3632	GLY		I4123	
ALA		A3198	E3271	L3338	L3412	SER	V3563	R3629	GLY		N4124	
ALA	G3126	A3199	T3272	L3339	Y3415	ASP	E3564	K3630	GLY		F4125	
ALA	Q3127	A3200	L3274	F3341	V3416	GLU	E3565	A3634	GLY		E4126	
ALA	N3128	M3201	P3275	A3342	V3416	THR	S3566	F3636	GLY		E4127	
ALA		V3203	M3276	Q3343	M3419	LYS	P3567	R3637	GLY		A4128	
ALA	Y3131	A3204	L3277	P3344	R3420	LYS	E3570	M3638	GLY		N4130	
ALA	T3132	F3205	C3278	T3345	L3424	LYS	R3573	T3639	GLY		R4131	
ALA	A3135	L3206	S3279	V3346	T3425	LYS	M3573	P3640	GLY		E4134	
ALA	L3136	L3210	Y3280	A3349	E3426	R3498	Y3576	K3644	GLY		D4157	
ALA	L3137	L3281	L3281	L3354	E3427	G3500	E3576	L3644	GLY		R4161	
ALA	F3138	Y3213	P3282	L3354	R3427	R3499	E3577	L3644	GLY		E4168	
ALA	V3139	N3214	R3283	L3354	N3428	G3501	E3578	M3651	GLY		S4169	
ALA		S3217	W3284	L3354	A3429	R3502	E3579	M3652	GLY		I4170	
ALA	F3144	T3220	E3286	L3359	E3432	R3503	E3580	M3652	GLY		I4171	
ALA	A3148	T3221	R3287	P3360	E3433	S3504	E3581	T3664	GLY		N4184	
ALA	Q3149		G3288	R3364	L3434	S3504	E3583	E3665	GLY		M4201	
ALA			E3290	L3365	R3436	V3505	E3584	Q3683	GLY			
ALA			A3291	R3366	M3437							



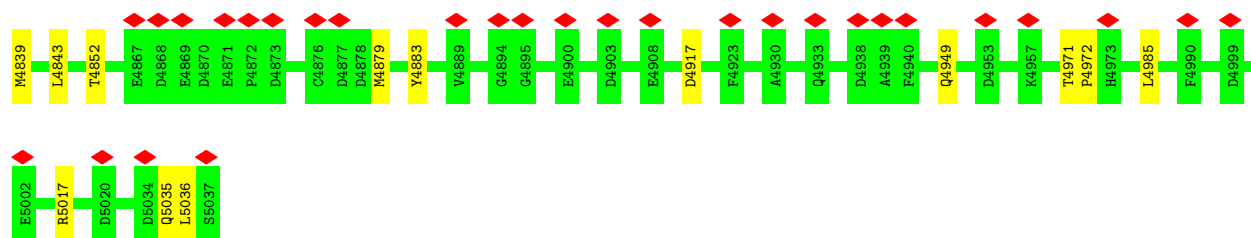
• Molecule 1: Ryanodine receptor 1



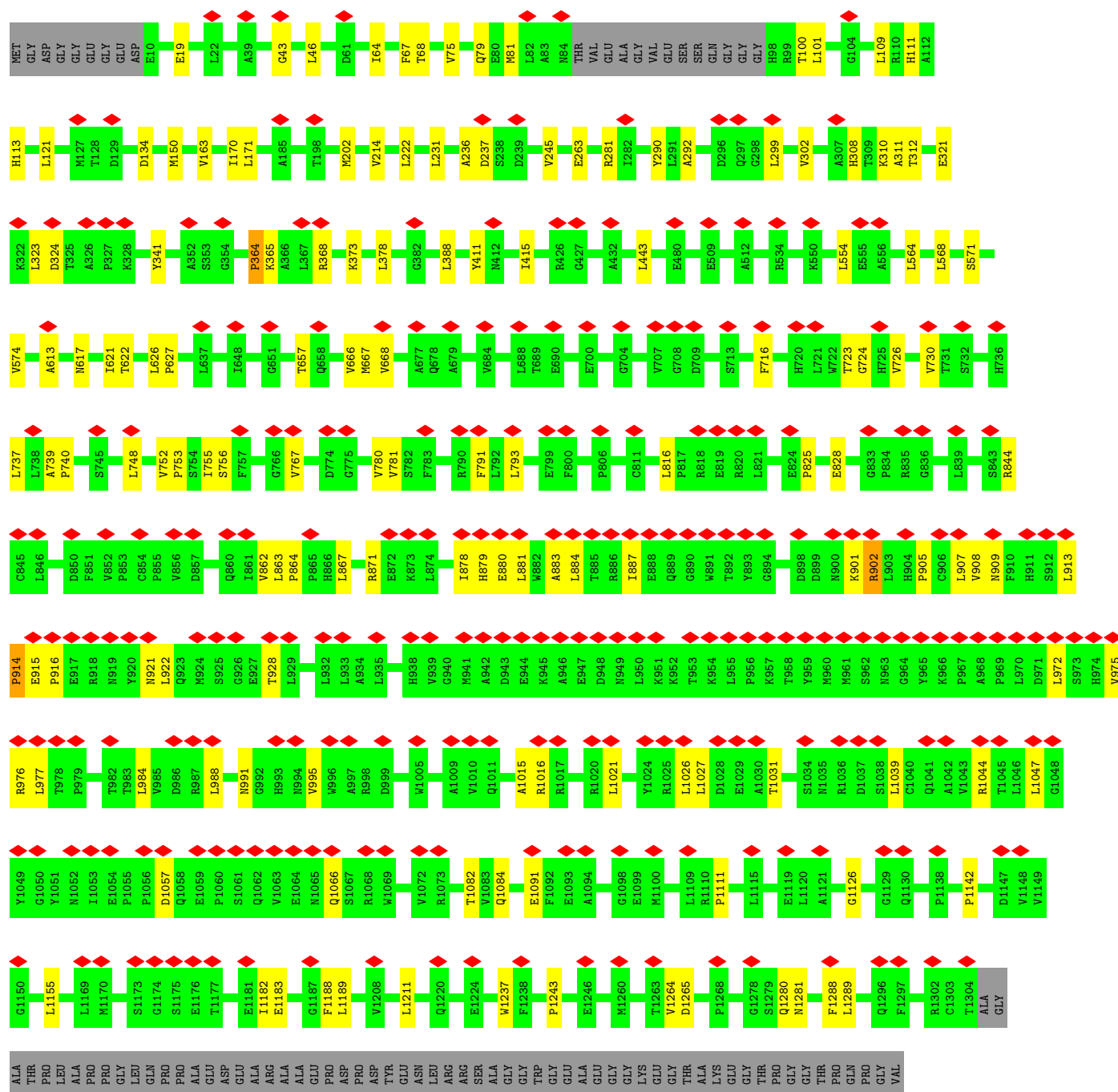
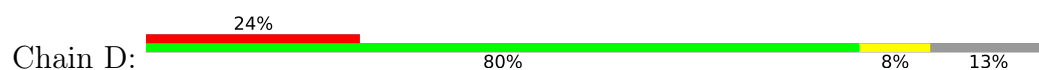


L3365	R3366	A3369	G3370	K3371	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	F3398	C3402	L3405	Y3406	A3407	L3408	Y3409	F3410	L3411	L3412	Y3415	V3416	N3419	R3420	L3424	P3427	N3428	A3429	E3432	E3433	L3434	F3435	R3436								
E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	V3307	D3310	H3311	L3312	L3315	L3316	R3320	R3321	I3322	I3323	V3324	N3325	N3326	L3327	G3328	I3329	D3330	E3331	A3332	T3333	W3334	M3335	L3338	F3341	A3342	Q3343	P3344	I3345	V3346	A3349	L3354	I3359	P3360	R3364							
S3217	T3220	T3221	K3222	S3223	P3224	R3225	L3230	G3231	L3232	P3233	N3234	S3235	S3236	E3237	E3238	M3239	C3240	P3241	D3242	I3243	R3248	L3249	G3255	L3256	A3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	M3266	P3267	H3268	V3269	I3270	E3271	I3272	T3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	G3288	P3289			
L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	I3087	V3088	K3089	A3090	G3091	L3092	F3096	S3100	E3101	E3104	K3105	M3106	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	ALA	ARG	THR	GLN	VAL	K3123	G3126	Q3127	N3128	Y3131	T3132	A3135	L3136	L3137	P3138	V3139	F3144								
E2994	I2995	K2996	F2997	F2998	L3005	I3006	N3007	Q3008	Y3009	F3010	T3011	N3012	L3018	S3019	T3020	P3021	A3022	K3023	V3024	G3026	S3027	G3028	A3031	S3032	N3033	K3034	E3035	K3036	E3037	M3038	I3039	F3043	C3044	K3045	L3046	A3047	A3048	L3049	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	A3061	P3062	A3063	V3064	I3070						
L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	I2951	E2952	K2953	A2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	
L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	A2875	E2876	Q2877	L2878	A2879	E2880	Y2881	Y2882	H2883	N2884	T2885	W2886	G2887	K2890	K2891	Q2892	A2896	K2897	K2898	G2899	G2900	T2901	H2902	L2903	L2904	L2905	V2906	F2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	K2928	F2929	
R2806	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	GLU	GLY	ARG	THR	GLU	LYS	LYS	LYS	THR	M2967	D2968	I2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993
I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	K2756	W2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	I2768	D2769	K2770	I2771	Y2714	Y2715	D2716	A2717	S2718	W2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	TYR	ASP	PRO	ALA	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745
E2545	R2552	L2556	A2557	V2558	L2559	P2560	HIS	PHE	GLY	GLU	P2410	G2571	T2572	E2573	A2576	L2583	V2586	R2589	D2601	E2604	D2605	R2615	P2616	R2624	V2627	F2628	D2629	I2632	A2637	M2502	V2503	L2504	E2513	Y2648	E2649	R2650	C2656	A2662	N2663	F2664	G2665	S2668	L2536	D2537	S2535	L2543	T2544										
L2672	L2678	I2682	F2683	D2684	S2685	L2686	S2753	L2562	A2570	G2571	T2572	E2573	A2576	L2583	V2586	R2589	D2601	E2604	D2605	R2615	P2616	R2624	V2627	F2628	D2629	I2632	A2637	M2502	V2503	L2504	E2513	Y2648	E2649	R2650	C2656	A2662	N2663	F2664	G2665	S2668	L2536	D2537	S2535	L2543	T2544												



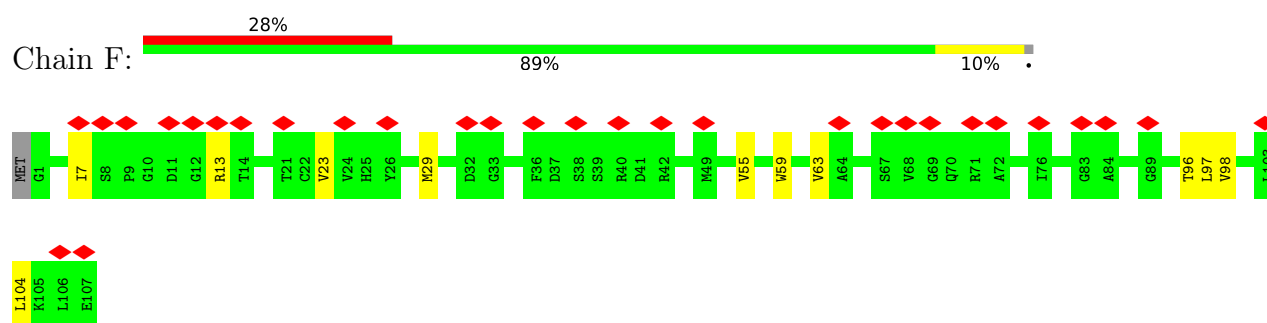


• Molecule 1: Ryanodine receptor 1

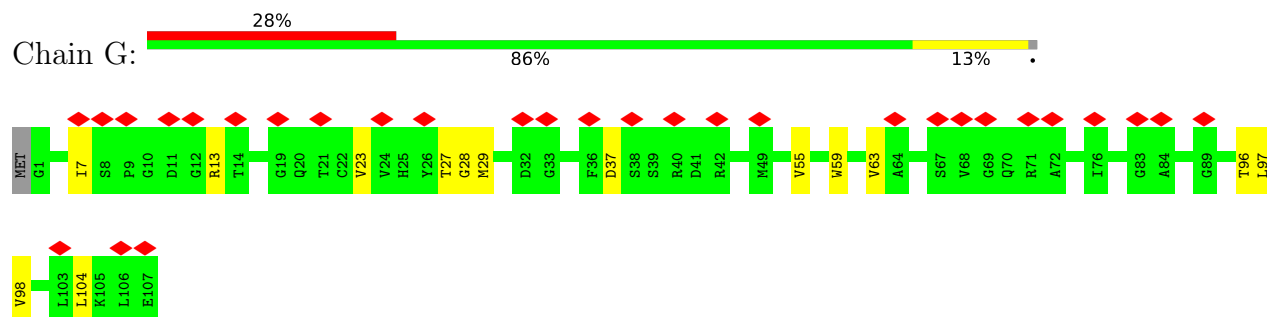




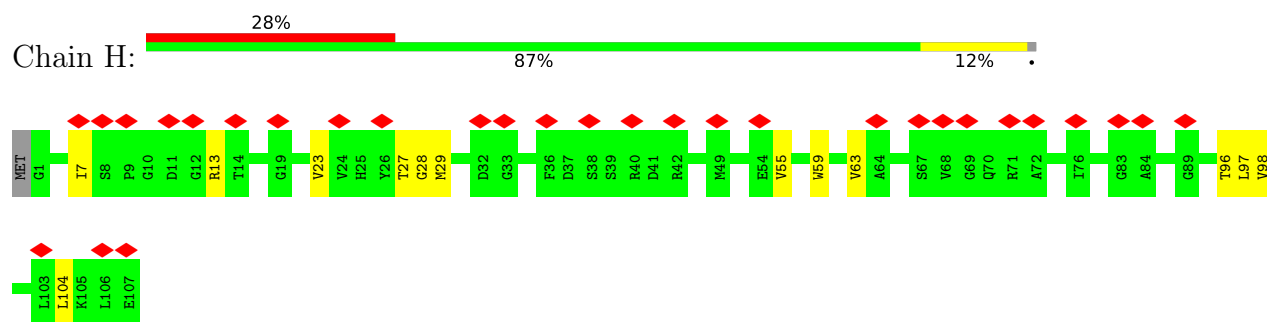
L2871	Q2872	A2873	W2874	A2875	Q2876	Q2877	L2878	A2879	E2880	W2881	Y2882	H2883	L2884	T2885	W2886	Q2887	K2890	K2891	Q2892	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	F2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	K2918	D2919	K2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	W2933
G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	I2951	E2952	K2953	A2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	V2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	L2995	K2996	F2997
F2998	L3005	I3006	N3007	Q3008	Y3009	F3010	T3011	N3012	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	A3031	S3032	N3033	K3034	E3035	K3036	E3037	N3038	I3039	F3043	G3044	K3045	L3046	A3047	A3048	L3049	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	A3063	V3064	I3070	L3071	A3072	K3073	S3074			
L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	I3087	V3088	K3089	A3090	G3091	L3092	F3096	S3100	E3101	E3104	K3105	M3106	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3126	Q3127	N3128	Y3131	T3132	A3135	L3136	L3137	F3138	V3139	F3144	A3148	Q3149								
F3152	G3153	D3154	L3155	V3156	I3157	L3158	D3159	L3160	V3161	Q3162	V3163	S3164	C3165	Y3166	L3169	S3171	I3172	T3177	T3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3185	L3186	R3187	L3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	V3202	V3203	A3204	F3205	L3206	L3210	Y3213	N3214	S3217	T3220	T3221					
K3222	S3223	P3224	R3225	L3230	Q3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	N3239	C3240	P3241	D3242	I3243	R3248	L3249	G3255	L3256	A3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	K3266	P3267	H3268	V3269	I3270	E3271	P3275	M3276	L3277	C3278	S3279	V3280	L3281	P3282	R3283	W3284	G3288	P3289	E3290	A3291	P3292	F3293	P3294	A3295		
L3296	P3297	A3298	G3299	A3300	P3301	P3302	F3303	C3304	T3305	A3306	V3307	D3310	H3311	L3312	L3315	L3316	L3320	R3321	I3322	I3323	N3325	N3326	L3327	G3328	I3329	D3330	E3331	A3332	T3333	W3334	M3335	L3338	F3341	A3342	Q3343	P3344	I3345	V3346	A3349	L3354	I3359	P3360	R3364	L3365	R3366	A3369	G3370	K3371								
A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	F3398	C3402	L3405	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	Y3415	V3416	N3419	R3420	L3424	P3427	N3428	A3429	E3432	E3433	L3434	F3435	R3436	M3437	V3438	I3441	Y3444								
K3447	S3448	H3449	E3455	Q3456	V3459	V3460	Q3461	N3462	E3463	I3464	N3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	SER	ASP	GLN	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	V3503	S3504	V3505	S3506	T3507	S3508	T3513				
L3514	K3515	K3516	M3517	G3521	C3525	A3526	P3527	I3532	L3533	M3534	K3537	T3538	R3539	Y3540	K3543	D3544	E3547	E3548	V3549	R3550	L3553	Q3554	N3555	N3556	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	S3566	P3567	R3570	M3573	Y3576	L3579	P3580	C3581	K3582	E3583	E3584	D3585	A3586	D3587	L3588	P3589									
E3590	V3593	R3594	E3598	L3603	H3604	L3606	E3607	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	A3630	A3631	V3632	V3633	A3634	G3635	F3636	R3637	K3638	T3639	L3641	L3644	N3651	N3652	T3664	E3665	Q3683	E3684	E3685	E3686	E3687	E3688							
E3689	V3690	E3691	E3692	M3723	A3724	D3727	C3733	H3734	L3735	E3736	GLU	GLY	GLY	GLU	ASN	GLY	ALA	GLU	GLU	GLU	GLU	W3749	E3750	E3754	Q3761	K3787	G3788	L3817	S3831	R3849	A3853	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871									
F3880	C3892	F3899	E3928	S3929	I3930	F3933	Y3934	D3941	K3948	I3969	Q3970	G3971	Q3977	R3984	L3985	K3986	S3987	A3988	L3993	D4005	P4006	S4007	L4010	L4019	L4030	Q4043	S4052	D4063	M4064	F4065	L4066	K4067	T4071	V4072	G4073	S4074	E4075	V4081	T4082																	



- 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	1541	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 ($e^-/\text{\AA}^2$)	117	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00458	Depositor
Map size (Å)	430.08, 430.08, 430.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.68, 1.68, 1.68	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/35885	0.37	0/48603
1	B	0.13	0/35885	0.37	0/48603
1	C	0.12	0/35885	0.37	0/48603
1	D	0.13	0/35885	0.37	0/48603
2	E	0.17	0/851	0.42	0/1146
2	F	0.18	0/851	0.42	0/1146
2	G	0.17	0/851	0.42	0/1146
2	H	0.18	0/851	0.42	0/1146
All	All	0.13	0/146944	0.37	0/198996

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	34739	34716	286	0
1	B	35088	34739	34716	280	0
1	C	35088	34739	34716	282	0
1	D	35088	34739	34716	284	0
2	E	832	829	831	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	832	829	831	10	0
2	G	832	829	831	10	0
2	H	832	829	831	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	143684	142272	142188	1133	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 4.

All (1133) 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:C:3467:MET:O	1:C:3471:THR:HG22	1.81	0.80
1:D:3467:MET:O	1:D:3471:THR:HG22	1.81	0.80
1:B:3467:MET:O	1:B:3471:THR:HG22	1.81	0.79
1:A:3467:MET:O	1:A:3471:THR:HG22	1.81	0.79
1:C:816:LEU:HD12	1:C:1026:LEU:HD21	1.64	0.79
1:A:816:LEU:HD12	1:A:1026:LEU:HD21	1.64	0.78
1:D:816:LEU:HD12	1:D:1026:LEU:HD21	1.64	0.78
1:B:816:LEU:HD12	1:B:1026:LEU:HD21	1.64	0.78
1:C:791:PHE:CZ	1:C:793:LEU:HD21	2.23	0.74
1:D:791:PHE:CZ	1:D:793:LEU:HD21	2.23	0.74
1:A:791:PHE:CZ	1:A:793:LEU:HD21	2.23	0.74
1:B:791:PHE:CZ	1:B:793:LEU:HD21	2.23	0.73
1:A:1449:TRP:NE1	1:A:1466:LEU:HD21	2.04	0.73
1:C:1449:TRP:NE1	1:C:1466:LEU:HD21	2.04	0.73
1:D:1449:TRP:NE1	1:D:1466:LEU:HD21	2.04	0.72
1:B:1449:TRP:NE1	1:B:1466:LEU:HD21	2.04	0.72
1:B:724:GLY:O	1:B:726:VAL:HG23	1.90	0.72
1:C:724:GLY:O	1:C:726:VAL:HG23	1.90	0.72
1:A:724:GLY:O	1:A:726:VAL:HG23	1.90	0.71
1:D:724:GLY:O	1:D:726:VAL:HG23	1.90	0.70
1:A:3787:LYS:O	1:A:3787:LYS:HG3	1.92	0.69
1:C:3787:LYS:O	1:C:3787:LYS:HG3	1.92	0.69
1:C:214:VAL:HG22	1:C:341:TYR:CE2	2.29	0.68
1:D:214:VAL:HG22	1:D:341:TYR:CE2	2.29	0.68
1:D:3787:LYS:O	1:D:3787:LYS:HG3	1.92	0.68
1:B:214:VAL:HG22	1:B:341:TYR:CE2	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG22	1:A:341:TYR:CE2	2.29	0.67
1:B:3787:LYS:HG3	1:B:3787:LYS:O	1.92	0.67
1:A:67:PHE:HB3	1:A:109:LEU:HD11	1.79	0.64
1:B:67:PHE:HB3	1:B:109:LEU:HD11	1.79	0.64
1:C:716:PHE:CE1	1:C:730:VAL:HG11	2.33	0.64
1:C:5017:ARG:O	1:C:5017:ARG:HD3	1.97	0.64
1:D:716:PHE:CE1	1:D:730:VAL:HG11	2.33	0.64
1:A:5017:ARG:O	1:A:5017:ARG:HD3	1.97	0.63
1:D:67:PHE:HB3	1:D:109:LEU:HD11	1.79	0.63
1:A:2678:LEU:O	1:A:2682:ILE:HD12	1.99	0.63
1:B:2678:LEU:O	1:B:2682:ILE:HD12	1.99	0.63
1:C:67:PHE:HB3	1:C:109:LEU:HD11	1.79	0.63
1:D:2678:LEU:O	1:D:2682:ILE:HD12	1.99	0.63
1:D:5017:ARG:O	1:D:5017:ARG:HD3	1.98	0.63
1:B:2572:THR:HG22	1:B:2572:THR:O	1.98	0.62
1:B:5017:ARG:O	1:B:5017:ARG:HD3	1.98	0.62
1:B:913:LEU:HD23	1:B:914:PRO:O	1.99	0.62
1:C:2572:THR:HG22	1:C:2572:THR:O	1.98	0.62
1:A:716:PHE:CE1	1:A:730:VAL:HG11	2.33	0.62
1:A:2572:THR:HG22	1:A:2572:THR:O	1.98	0.62
1:C:2678:LEU:O	1:C:2682:ILE:HD12	1.99	0.62
1:D:2572:THR:HG22	1:D:2572:THR:O	1.98	0.62
1:B:716:PHE:CE1	1:B:730:VAL:HG11	2.33	0.62
1:A:913:LEU:HD23	1:A:914:PRO:O	1.99	0.62
1:C:913:LEU:HD23	1:C:914:PRO:O	1.99	0.62
1:D:913:LEU:HD23	1:D:914:PRO:O	1.99	0.62
1:D:908:VAL:HG13	1:D:909:ASN:H	1.65	0.61
1:D:3532:LEU:HD21	1:D:3553:LEU:HD22	1.82	0.61
1:A:1091:GLU:OE2	1:A:1211:LEU:HD22	2.01	0.61
1:B:908:VAL:HG13	1:B:909:ASN:H	1.65	0.61
1:C:3532:LEU:HD21	1:C:3553:LEU:HD22	1.82	0.61
1:D:3416:VAL:HG21	1:D:3517:MET:HE1	1.83	0.61
1:D:1091:GLU:OE2	1:D:1211:LEU:HD22	2.01	0.60
1:A:908:VAL:HG13	1:A:909:ASN:H	1.66	0.60
1:A:1651:LEU:HD21	1:A:1703:LEU:HD22	1.84	0.60
1:A:3532:LEU:HD21	1:A:3553:LEU:HD22	1.82	0.60
1:C:908:VAL:HG13	1:C:909:ASN:H	1.66	0.60
1:C:3416:VAL:HG21	1:C:3517:MET:HE1	1.83	0.60
1:C:622:THR:HG23	1:C:626:LEU:HD12	1.84	0.60
1:A:3416:VAL:HG21	1:A:3517:MET:HE1	1.83	0.60
1:B:1091:GLU:OE2	1:B:1211:LEU:HD22	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3532:LEU:HD21	1:B:3553:LEU:HD22	1.82	0.60
1:D:1651:LEU:HD21	1:D:1703:LEU:HD22	1.84	0.60
1:B:3416:VAL:HG21	1:B:3517:MET:HE1	1.83	0.60
2:F:13:ARG:HE	2:F:13:ARG:C	2.10	0.60
1:B:1651:LEU:HD21	1:B:1703:LEU:HD22	1.84	0.59
1:C:2214:VAL:HG11	1:C:2228:MET:HE2	1.84	0.59
1:D:622:THR:HG23	1:D:626:LEU:HD12	1.84	0.59
2:E:13:ARG:HE	2:E:13:ARG:C	2.11	0.59
1:A:2214:VAL:HG11	1:A:2228:MET:HE2	1.85	0.59
1:A:3359:ILE:HG23	1:A:3437:MET:HE3	1.85	0.59
1:C:1651:LEU:HD21	1:C:1703:LEU:HD22	1.84	0.59
1:B:622:THR:HG23	1:B:626:LEU:HD12	1.84	0.59
1:C:1091:GLU:OE2	1:C:1211:LEU:HD22	2.01	0.59
1:A:214:VAL:HG22	1:A:341:TYR:CD2	2.38	0.59
1:A:622:THR:HG23	1:A:626:LEU:HD12	1.84	0.59
1:D:3359:ILE:HG23	1:D:3437:MET:HE3	1.85	0.59
1:B:2214:VAL:HG11	1:B:2228:MET:HE2	1.84	0.59
1:D:3096:PHE:CE2	1:D:3161:VAL:HG13	2.38	0.59
2:H:13:ARG:HE	2:H:13:ARG:C	2.10	0.59
1:B:3096:PHE:CE2	1:B:3161:VAL:HG13	2.38	0.59
1:B:214:VAL:HG22	1:B:341:TYR:CD2	2.38	0.59
1:C:3359:ILE:HG23	1:C:3437:MET:HE3	1.85	0.59
1:D:2214:VAL:HG11	1:D:2228:MET:HE2	1.84	0.59
1:C:3096:PHE:CE2	1:C:3161:VAL:HG13	2.38	0.59
1:C:214:VAL:HG22	1:C:341:TYR:CD2	2.38	0.59
1:D:214:VAL:HG22	1:D:341:TYR:CD2	2.38	0.59
1:A:3096:PHE:CE2	1:A:3161:VAL:HG13	2.37	0.58
1:B:883:ALA:O	1:B:887:ILE:HG22	2.03	0.58
1:C:883:ALA:O	1:C:887:ILE:HG22	2.03	0.58
2:G:13:ARG:HE	2:G:13:ARG:C	2.10	0.58
1:D:883:ALA:O	1:D:887:ILE:HG22	2.04	0.58
1:D:737:LEU:HD23	2:H:7:ILE:CG2	2.34	0.58
1:B:3359:ILE:HG23	1:B:3437:MET:HE3	1.84	0.58
1:A:1449:TRP:CD1	1:A:1466:LEU:HD21	2.39	0.58
1:B:1449:TRP:CD1	1:B:1466:LEU:HD21	2.39	0.58
1:C:1449:TRP:CD1	1:C:1466:LEU:HD21	2.39	0.58
1:A:883:ALA:O	1:A:887:ILE:HG22	2.03	0.58
1:D:878:ILE:HA	1:D:881:LEU:HD23	1.86	0.58
1:D:1449:TRP:CD1	1:D:1466:LEU:HD21	2.39	0.58
1:A:878:ILE:HA	1:A:881:LEU:HD23	1.86	0.57
1:A:1280:GLN:O	1:A:1281:ASN:OD1	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1544:PRO:O	1:C:1545:ASN:OD1	2.22	0.57
1:C:3232:LEU:HD22	1:C:3239:MET:CE	2.35	0.57
1:B:1188:PHE:O	1:B:1189:LEU:HD23	2.05	0.57
1:C:1280:GLN:O	1:C:1281:ASN:OD1	2.22	0.57
1:D:1280:GLN:O	1:D:1281:ASN:OD1	2.22	0.57
1:D:3232:LEU:HD22	1:D:3239:MET:CE	2.35	0.57
1:C:1188:PHE:O	1:C:1189:LEU:HD23	2.05	0.57
1:A:1188:PHE:O	1:A:1189:LEU:HD23	2.05	0.57
1:B:1544:PRO:O	1:B:1545:ASN:OD1	2.22	0.57
2:F:29:MET:O	2:F:98:VAL:HG22	2.05	0.57
1:C:878:ILE:HA	1:C:881:LEU:HD23	1.86	0.56
1:C:2558:VAL:O	1:C:2562:ILE:HD12	2.05	0.56
1:B:1280:GLN:O	1:B:1281:ASN:OD1	2.22	0.56
2:H:29:MET:O	2:H:98:VAL:HG22	2.05	0.56
1:A:1544:PRO:O	1:A:1545:ASN:OD1	2.22	0.56
1:D:1188:PHE:O	1:D:1189:LEU:HD23	2.05	0.56
1:B:3232:LEU:HD22	1:B:3239:MET:CE	2.35	0.56
1:A:3232:LEU:HD22	1:A:3239:MET:CE	2.35	0.56
1:D:2558:VAL:O	1:D:2562:ILE:HD12	2.05	0.56
2:G:29:MET:O	2:G:98:VAL:HG22	2.05	0.56
1:B:878:ILE:HA	1:B:881:LEU:HD23	1.86	0.56
2:E:29:MET:O	2:E:98:VAL:HG22	2.05	0.56
1:D:1243:PRO:CB	1:D:1600:LEU:HD11	2.36	0.56
1:D:1544:PRO:O	1:D:1545:ASN:OD1	2.22	0.56
1:A:2558:VAL:O	1:A:2562:ILE:HD12	2.05	0.56
1:B:2558:VAL:O	1:B:2562:ILE:HD12	2.05	0.56
1:D:3930:ILE:HG23	1:D:3933:PHE:HE1	1.71	0.56
1:A:3930:ILE:HG23	1:A:3933:PHE:HE1	1.71	0.55
1:B:908:VAL:HG13	1:B:909:ASN:N	2.22	0.55
1:C:3930:ILE:HG23	1:C:3933:PHE:HE1	1.71	0.55
1:B:1243:PRO:CB	1:B:1600:LEU:HD11	2.36	0.55
1:B:3930:ILE:HG23	1:B:3933:PHE:HE1	1.71	0.55
1:C:281:ARG:HG3	1:C:312:THR:HG21	1.88	0.55
1:C:299:LEU:HD22	1:C:378:LEU:CD2	2.37	0.55
1:C:1936:LYS:HZ3	1:C:2105:TRP:CD1	2.25	0.55
1:D:3043:PHE:CZ	1:D:3075:LEU:HD13	2.42	0.55
1:B:2977:LEU:HD23	1:B:3056:LEU:HD11	1.89	0.55
1:C:1288:PHE:C	1:C:1289:LEU:HD22	2.32	0.55
1:D:299:LEU:HD22	1:D:378:LEU:CD2	2.37	0.55
1:A:1243:PRO:CB	1:A:1600:LEU:HD11	2.36	0.55
1:A:1936:LYS:HZ3	1:A:2105:TRP:CD1	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3455:GLU:O	1:A:3459:VAL:HG23	2.07	0.55
1:B:3043:PHE:CZ	1:B:3075:LEU:HD13	2.42	0.55
1:A:3043:PHE:CZ	1:A:3075:LEU:HD13	2.42	0.55
1:A:2977:LEU:HD23	1:A:3056:LEU:HD11	1.89	0.55
1:B:1288:PHE:C	1:B:1289:LEU:HD22	2.32	0.55
1:B:3455:GLU:O	1:B:3459:VAL:HG23	2.07	0.55
1:D:1288:PHE:C	1:D:1289:LEU:HD22	2.32	0.55
1:B:2781:VAL:O	1:B:2781:VAL:HG13	2.07	0.55
1:D:2159:LEU:HD12	1:D:2203:MET:HE1	1.89	0.55
1:B:2159:LEU:HD12	1:B:2203:MET:HE1	1.89	0.55
1:C:1243:PRO:CB	1:C:1600:LEU:HD11	2.36	0.55
1:C:4838:VAL:HG12	1:C:4839:MET:HE2	1.89	0.55
1:C:4971:THR:OG1	1:C:4972:PRO:HD2	2.08	0.55
1:D:3455:GLU:O	1:D:3459:VAL:HG23	2.07	0.55
1:A:908:VAL:HG13	1:A:909:ASN:N	2.22	0.54
1:A:2159:LEU:HD12	1:A:2203:MET:HE1	1.89	0.54
1:C:2781:VAL:HG13	1:C:2781:VAL:O	2.07	0.54
1:D:281:ARG:HG3	1:D:312:THR:HG21	1.88	0.54
1:A:1288:PHE:C	1:A:1289:LEU:HD22	2.32	0.54
1:C:3043:PHE:CZ	1:C:3075:LEU:HD13	2.42	0.54
1:D:1936:LYS:HZ3	1:D:2105:TRP:CD1	2.25	0.54
1:C:3455:GLU:O	1:C:3459:VAL:HG23	2.07	0.54
1:A:2781:VAL:O	1:A:2781:VAL:HG13	2.07	0.54
1:B:1936:LYS:HZ3	1:B:2105:TRP:CD1	2.25	0.54
1:C:2159:LEU:HD12	1:C:2203:MET:HE1	1.89	0.54
1:C:2977:LEU:HD23	1:C:3056:LEU:HD11	1.89	0.54
1:D:908:VAL:HG13	1:D:909:ASN:N	2.22	0.54
1:D:2977:LEU:HD23	1:D:3056:LEU:HD11	1.89	0.54
1:D:4971:THR:OG1	1:D:4972:PRO:HD2	2.08	0.54
1:A:299:LEU:HD22	1:A:378:LEU:CD2	2.37	0.54
1:A:4971:THR:OG1	1:A:4972:PRO:HD2	2.07	0.54
1:B:299:LEU:HD22	1:B:378:LEU:CD2	2.37	0.54
1:B:2742:THR:O	1:B:2742:THR:HG22	2.07	0.54
1:A:1082:THR:OG1	1:A:1189:LEU:HD21	2.08	0.54
1:B:281:ARG:CG	1:B:312:THR:HG21	2.38	0.54
1:B:281:ARG:HG3	1:B:312:THR:HG21	1.88	0.54
1:B:1082:THR:OG1	1:B:1189:LEU:HD21	2.08	0.54
1:C:908:VAL:HG13	1:C:909:ASN:N	2.22	0.54
1:C:739:ALA:HB1	1:C:740:PRO:HD2	1.90	0.54
1:A:3614:LYS:HD2	1:A:3614:LYS:O	2.08	0.54
1:B:4838:VAL:HG12	1:B:4839:MET:HE2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLU:HG2	1:A:263:GLU:O	2.08	0.54
1:A:281:ARG:CG	1:A:312:THR:HG21	2.38	0.54
1:D:3614:LYS:HD2	1:D:3614:LYS:O	2.08	0.54
1:C:1927:LEU:HD22	1:C:2101:MET:HE1	1.90	0.54
1:D:1082:THR:OG1	1:D:1189:LEU:HD21	2.08	0.54
1:D:1430:THR:HG23	1:D:1430:THR:O	2.09	0.54
1:D:1927:LEU:HD22	1:D:2101:MET:HE1	1.90	0.54
1:D:2781:VAL:HG13	1:D:2781:VAL:O	2.07	0.54
1:A:2552:ARG:O	1:A:2556:LEU:HD23	2.08	0.53
1:A:4580:TYR:HA	1:A:4632:LEU:HD13	1.90	0.53
1:C:263:GLU:O	1:C:263:GLU:HG2	2.08	0.53
1:B:2502:MET:N	1:B:2502:MET:HE2	2.24	0.53
1:B:4971:THR:OG1	1:B:4972:PRO:HD2	2.08	0.53
1:C:281:ARG:CG	1:C:312:THR:HG21	2.38	0.53
1:C:2502:MET:N	1:C:2502:MET:HE2	2.24	0.53
1:C:2742:THR:HG22	1:C:2742:THR:O	2.06	0.53
1:C:4580:TYR:HA	1:C:4632:LEU:HD13	1.90	0.53
1:C:2552:ARG:O	1:C:2556:LEU:HD23	2.08	0.53
1:A:739:ALA:HB1	1:A:740:PRO:HD2	1.90	0.53
1:A:2742:THR:HG22	1:A:2742:THR:O	2.07	0.53
1:B:3614:LYS:HD2	1:B:3614:LYS:O	2.08	0.53
1:C:1082:THR:OG1	1:C:1189:LEU:HD21	2.08	0.53
1:C:3614:LYS:HD2	1:C:3614:LYS:O	2.08	0.53
1:D:739:ALA:HB1	1:D:740:PRO:CD	2.39	0.53
1:D:4838:VAL:HG12	1:D:4839:MET:HE2	1.89	0.53
1:A:1927:LEU:HD22	1:A:2101:MET:HE1	1.90	0.53
1:A:2502:MET:HE2	1:A:2502:MET:N	2.24	0.53
1:D:263:GLU:O	1:D:263:GLU:HG2	2.08	0.53
1:D:281:ARG:CG	1:D:312:THR:HG21	2.38	0.53
1:D:2552:ARG:O	1:D:2556:LEU:HD23	2.08	0.53
1:A:281:ARG:HG3	1:A:312:THR:HG21	1.89	0.53
1:A:1430:THR:HG23	1:A:1430:THR:O	2.09	0.53
1:B:1927:LEU:HD22	1:B:2101:MET:HE1	1.90	0.53
1:C:739:ALA:HB1	1:C:740:PRO:CD	2.39	0.53
1:B:263:GLU:O	1:B:263:GLU:HG2	2.08	0.53
1:D:4214:LYS:NZ	1:D:4985:LEU:HD21	2.24	0.53
1:C:2986:VAL:HG13	1:C:2986:VAL:O	2.09	0.53
1:D:739:ALA:HB1	1:D:740:PRO:HD2	1.90	0.53
1:D:2742:THR:HG22	1:D:2742:THR:O	2.07	0.53
1:A:2214:VAL:HG11	1:A:2228:MET:CE	2.39	0.53
1:A:4838:VAL:HG12	1:A:4839:MET:HE2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:ALA:HB1	1:B:740:PRO:CD	2.39	0.53
1:C:1430:THR:O	1:C:1430:THR:HG23	2.09	0.53
1:D:4580:TYR:HA	1:D:4632:LEU:HD13	1.90	0.53
1:A:231:LEU:HD11	1:A:245:VAL:CG1	2.39	0.53
1:A:613:ALA:HB3	1:A:1676:LEU:HD12	1.90	0.53
1:A:739:ALA:HB1	1:A:740:PRO:CD	2.39	0.53
1:B:2098:VAL:O	1:B:2102:VAL:HG23	2.10	0.52
1:B:2552:ARG:O	1:B:2556:LEU:HD23	2.08	0.52
1:B:2986:VAL:HG13	1:B:2986:VAL:O	2.09	0.52
1:B:4214:LYS:NZ	1:B:4985:LEU:HD21	2.24	0.52
1:C:2098:VAL:O	1:C:2102:VAL:HG23	2.10	0.52
1:D:1289:LEU:HD12	1:D:1597:VAL:HG12	1.92	0.52
1:B:231:LEU:HD11	1:B:245:VAL:CG1	2.39	0.52
1:B:739:ALA:HB1	1:B:740:PRO:HD2	1.90	0.52
1:B:3930:ILE:O	1:B:3933:PHE:CE1	2.62	0.52
1:B:4580:TYR:HA	1:B:4632:LEU:HD13	1.90	0.52
1:C:1289:LEU:HD12	1:C:1597:VAL:HG12	1.91	0.52
1:C:1714:LEU:HD11	1:C:1718:ILE:HD11	1.92	0.52
1:D:3930:ILE:O	1:D:3933:PHE:CE1	2.62	0.52
1:C:2214:VAL:HG11	1:C:2228:MET:CE	2.39	0.52
1:D:613:ALA:HB3	1:D:1676:LEU:HD12	1.90	0.52
1:A:2986:VAL:HG13	1:A:2986:VAL:O	2.09	0.52
1:A:3603:LEU:O	1:A:3607:GLU:OE1	2.28	0.52
1:B:1714:LEU:HD11	1:B:1718:ILE:HD11	1.92	0.52
1:B:2214:VAL:HG11	1:B:2228:MET:CE	2.39	0.52
1:C:3930:ILE:O	1:C:3933:PHE:CE1	2.62	0.52
1:A:1714:LEU:HD11	1:A:1718:ILE:HD11	1.92	0.52
1:A:4214:LYS:NZ	1:A:4985:LEU:HD21	2.24	0.52
1:C:3603:LEU:O	1:C:3607:GLU:OE1	2.28	0.52
1:D:2502:MET:HE2	1:D:2502:MET:N	2.24	0.52
1:D:3603:LEU:O	1:D:3607:GLU:OE1	2.28	0.52
1:C:3438:VAL:HG21	1:C:3517:MET:HG2	1.92	0.52
1:D:1714:LEU:HD11	1:D:1718:ILE:HD11	1.92	0.52
1:B:613:ALA:HB3	1:B:1676:LEU:HD12	1.90	0.52
1:B:1289:LEU:HD12	1:B:1597:VAL:HG12	1.92	0.52
1:D:231:LEU:HD11	1:D:245:VAL:CG1	2.39	0.52
1:A:2858:GLN:O	1:A:2859:PRO:C	2.53	0.52
1:B:2858:GLN:O	1:B:2859:PRO:C	2.53	0.52
1:B:3603:LEU:O	1:B:3607:GLU:OE1	2.28	0.52
1:C:613:ALA:HB3	1:C:1676:LEU:HD12	1.90	0.52
1:C:748:LEU:HD13	1:C:755:ILE:HG12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:LEU:HD12	1:A:1597:VAL:HG12	1.91	0.52
1:C:231:LEU:HD11	1:C:245:VAL:CG1	2.39	0.52
1:C:368:ARG:CD	1:C:2307:LEU:HD12	2.40	0.52
1:D:3438:VAL:HG21	1:D:3517:MET:HG2	1.92	0.52
1:A:3930:ILE:O	1:A:3933:PHE:CE1	2.62	0.51
1:D:737:LEU:HD23	2:H:7:ILE:HG22	1.91	0.51
1:D:2214:VAL:HG11	1:D:2228:MET:CE	2.39	0.51
1:D:3323:ILE:HG23	1:D:3335:MET:CE	2.41	0.51
1:A:2098:VAL:O	1:A:2102:VAL:HG23	2.10	0.51
1:A:3323:ILE:HG23	1:A:3335:MET:HE3	1.92	0.51
1:B:748:LEU:HD13	1:B:755:ILE:HG12	1.92	0.51
1:C:3323:ILE:HG23	1:C:3335:MET:HE3	1.92	0.51
1:D:64:ILE:O	1:D:64:ILE:HG22	2.10	0.51
1:D:748:LEU:HD13	1:D:755:ILE:HG12	1.92	0.51
1:B:368:ARG:CD	1:B:2307:LEU:HD12	2.40	0.51
1:D:2986:VAL:HG13	1:D:2986:VAL:O	2.09	0.51
1:A:748:LEU:HD13	1:A:755:ILE:HG12	1.92	0.51
1:A:3323:ILE:HG23	1:A:3335:MET:CE	2.41	0.51
1:B:64:ILE:HG22	1:B:64:ILE:O	2.10	0.51
1:D:816:LEU:HD12	1:D:1026:LEU:CD2	2.39	0.51
1:A:3006:ILE:HD11	1:A:3010:PHE:CE2	2.46	0.51
1:C:2416:VAL:HG23	1:C:2416:VAL:O	2.11	0.51
1:D:2098:VAL:O	1:D:2102:VAL:HG23	2.10	0.51
1:D:2858:GLN:N	1:D:2859:PRO:CD	2.74	0.51
1:D:2858:GLN:O	1:D:2859:PRO:C	2.52	0.51
1:B:3323:ILE:HG23	1:B:3335:MET:HE3	1.92	0.51
1:B:3438:VAL:HG21	1:B:3517:MET:HG2	1.92	0.51
1:C:905:PRO:O	1:C:908:VAL:HG12	2.11	0.51
1:C:4214:LYS:NZ	1:C:4985:LEU:HD21	2.24	0.51
1:B:816:LEU:HD12	1:B:1026:LEU:CD2	2.39	0.51
1:B:3323:ILE:HG23	1:B:3335:MET:CE	2.41	0.51
1:C:3266:MET:O	1:C:3266:MET:HG2	2.11	0.51
1:A:905:PRO:O	1:A:908:VAL:HG12	2.11	0.51
1:A:928:THR:CG2	1:A:1039:LEU:HD12	2.41	0.51
1:B:3266:MET:HG2	1:B:3266:MET:O	2.11	0.51
1:C:1735:ILE:HG23	1:C:1735:ILE:O	2.11	0.51
1:D:368:ARG:CD	1:D:2307:LEU:HD12	2.40	0.51
1:B:864:PRO:HD2	1:B:867:LEU:HD13	1.93	0.51
1:B:928:THR:CG2	1:B:1039:LEU:HD12	2.41	0.51
1:C:3006:ILE:HD11	1:C:3010:PHE:CE2	2.46	0.51
1:A:3438:VAL:HG21	1:A:3517:MET:HG2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2858:GLN:O	1:C:2859:PRO:C	2.53	0.50
1:D:737:LEU:C	1:D:737:LEU:HD12	2.37	0.50
1:D:3006:ILE:HD11	1:D:3010:PHE:CE2	2.46	0.50
1:A:368:ARG:CD	1:A:2307:LEU:HD12	2.40	0.50
1:A:737:LEU:HD12	1:A:737:LEU:C	2.37	0.50
1:A:2858:GLN:N	1:A:2859:PRO:CD	2.74	0.50
1:B:1430:THR:HG23	1:B:1430:THR:O	2.09	0.50
1:B:2858:GLN:N	1:B:2859:PRO:CD	2.74	0.50
1:B:3166:TYR:O	1:B:3170:CYS:HB2	2.12	0.50
1:C:3323:ILE:HG23	1:C:3335:MET:CE	2.41	0.50
1:D:928:THR:CG2	1:D:1039:LEU:HD12	2.41	0.50
1:D:3266:MET:O	1:D:3266:MET:HG2	2.11	0.50
1:D:3323:ILE:HG23	1:D:3335:MET:HE3	1.92	0.50
1:B:1762:LEU:HD11	1:B:1873:GLU:OE2	2.11	0.50
1:B:2416:VAL:HG23	1:B:2416:VAL:O	2.11	0.50
1:C:928:THR:CG2	1:C:1039:LEU:HD12	2.41	0.50
1:B:3006:ILE:HD11	1:B:3010:PHE:CE2	2.46	0.50
1:A:3166:TYR:O	1:A:3170:CYS:HB2	2.12	0.50
1:C:2858:GLN:N	1:C:2859:PRO:CD	2.74	0.50
1:D:2251:PHE:CG	1:D:2286:LEU:HD22	2.47	0.50
1:A:292:ALA:HB1	1:A:311:ALA:HB1	1.94	0.50
1:A:1762:LEU:HD11	1:A:1873:GLU:OE2	2.11	0.50
1:A:2416:VAL:O	1:A:2416:VAL:HG23	2.11	0.50
1:B:905:PRO:O	1:B:908:VAL:HG12	2.11	0.50
1:B:2251:PHE:CG	1:B:2286:LEU:HD22	2.47	0.50
1:B:3969:ILE:HG23	1:B:3977:GLN:HG3	1.94	0.50
1:C:2629:ASP:O	1:C:2632:ILE:HG22	2.12	0.50
1:C:3166:TYR:O	1:C:3170:CYS:HB2	2.12	0.50
1:D:1735:ILE:O	1:D:1735:ILE:HG23	2.11	0.50
1:D:3166:TYR:O	1:D:3170:CYS:HB2	2.12	0.50
1:A:3054:VAL:HG13	1:A:3055:SER:N	2.27	0.50
1:C:3043:PHE:CE1	1:C:3075:LEU:HD22	2.47	0.50
1:D:3969:ILE:HG23	1:D:3977:GLN:HG3	1.94	0.50
1:B:3043:PHE:CE1	1:B:3075:LEU:HD22	2.47	0.50
1:C:1762:LEU:HD11	1:C:1873:GLU:OE2	2.11	0.50
1:C:2251:PHE:CG	1:C:2286:LEU:HD22	2.47	0.50
1:D:2416:VAL:HG23	1:D:2416:VAL:O	2.11	0.50
1:C:64:ILE:HG22	1:C:64:ILE:O	2.10	0.50
1:C:972:LEU:HD12	1:C:1044:ARG:HE	1.77	0.50
1:C:2440:MET:HE3	1:C:2440:MET:HA	1.94	0.50
1:C:3054:VAL:HG13	1:C:3055:SER:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:ALA:HB1	1:D:311:ALA:HB1	1.94	0.50
1:A:2629:ASP:O	1:A:2632:ILE:HG22	2.12	0.49
1:A:3043:PHE:CE1	1:A:3075:LEU:HD22	2.47	0.49
1:B:2629:ASP:O	1:B:2632:ILE:HG22	2.12	0.49
1:C:4879:MET:HE2	1:D:4578:LEU:HD22	1.94	0.49
1:D:905:PRO:O	1:D:908:VAL:HG12	2.11	0.49
1:A:3266:MET:O	1:A:3266:MET:HG2	2.11	0.49
1:B:719:LEU:HD11	2:F:7:ILE:HG23	1.94	0.49
1:B:737:LEU:C	1:B:737:LEU:HD12	2.36	0.49
1:B:1735:ILE:HG23	1:B:1735:ILE:O	2.11	0.49
1:B:3054:VAL:HG13	1:B:3055:SER:N	2.27	0.49
1:C:3969:ILE:HG23	1:C:3977:GLN:HG3	1.94	0.49
1:D:2440:MET:HE3	1:D:2440:MET:HA	1.94	0.49
1:A:2251:PHE:CG	1:A:2286:LEU:HD22	2.47	0.49
1:C:816:LEU:HD12	1:C:1026:LEU:CD2	2.39	0.49
1:D:972:LEU:HD12	1:D:1044:ARG:HE	1.77	0.49
1:A:4578:LEU:HD22	1:D:4879:MET:HE2	1.94	0.49
1:B:928:THR:HG21	1:B:1039:LEU:HD12	1.94	0.49
1:C:928:THR:HG21	1:C:1039:LEU:HD12	1.94	0.49
1:C:3532:LEU:HD21	1:C:3553:LEU:CD2	2.43	0.49
1:D:1280:GLN:CD	1:D:1281:ASN:H	2.20	0.49
1:A:864:PRO:HD2	1:A:867:LEU:HD13	1.93	0.49
1:A:2440:MET:HE3	1:A:2440:MET:HA	1.94	0.49
1:B:3343:GLN:O	1:B:3346:VAL:HG12	2.13	0.49
1:C:864:PRO:HD2	1:C:867:LEU:HD13	1.93	0.49
1:D:3043:PHE:CE1	1:D:3075:LEU:HD22	2.47	0.49
1:A:1280:GLN:CD	1:A:1281:ASN:H	2.20	0.49
1:A:3969:ILE:HG23	1:A:3977:GLN:HG3	1.94	0.49
1:B:716:PHE:CZ	1:B:730:VAL:HG11	2.48	0.49
1:C:292:ALA:HB1	1:C:311:ALA:HB1	1.94	0.49
1:C:737:LEU:HD12	1:C:737:LEU:C	2.37	0.49
1:C:3343:GLN:O	1:C:3346:VAL:HG12	2.13	0.49
1:D:716:PHE:CZ	1:D:730:VAL:HG11	2.48	0.49
1:A:64:ILE:HG22	1:A:64:ILE:O	2.10	0.49
1:A:81:MET:HA	1:A:81:MET:HE3	1.94	0.49
1:A:1735:ILE:HG23	1:A:1735:ILE:O	2.11	0.49
1:A:2212:VAL:HG11	1:A:2256:TYR:CE2	2.48	0.49
1:B:81:MET:HE3	1:B:81:MET:HA	1.94	0.49
1:D:3343:GLN:O	1:D:3346:VAL:HG12	2.13	0.49
1:A:236:ALA:O	1:A:237:ASP:OD1	2.31	0.49
1:B:2212:VAL:HG11	1:B:2256:TYR:CE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2254:LEU:C	1:B:2254:LEU:HD23	2.38	0.49
1:C:2212:VAL:HG11	1:C:2256:TYR:CE2	2.48	0.49
1:D:2629:ASP:O	1:D:2632:ILE:HG22	2.12	0.49
1:D:3054:VAL:HG13	1:D:3055:SER:N	2.27	0.49
1:B:972:LEU:HD12	1:B:1044:ARG:HE	1.77	0.49
1:C:81:MET:HE3	1:C:81:MET:HA	1.94	0.49
1:C:3071:LEU:O	1:C:3075:LEU:HD21	2.13	0.49
1:C:3540:TYR:CE1	1:C:3549:VAL:HG11	2.48	0.49
1:D:887:ILE:HB	1:D:907:LEU:HD12	1.95	0.49
1:D:2212:VAL:HG11	1:D:2256:TYR:CE2	2.48	0.49
1:A:1439:VAL:HG12	1:A:1562:ILE:HG22	1.95	0.48
1:A:2882:TYR:HA	1:A:2885:THR:HG22	1.95	0.48
1:A:3343:GLN:O	1:A:3346:VAL:HG12	2.13	0.48
1:B:1439:VAL:HG12	1:B:1562:ILE:HG22	1.95	0.48
1:C:1280:GLN:CD	1:C:1281:ASN:H	2.20	0.48
1:C:1439:VAL:HG12	1:C:1562:ILE:HG22	1.95	0.48
1:C:2882:TYR:HA	1:C:2885:THR:HG22	1.95	0.48
1:D:236:ALA:O	1:D:237:ASP:OD1	2.31	0.48
1:D:290:TYR:O	1:D:302:VAL:HG22	2.13	0.48
1:D:1762:LEU:HD11	1:D:1873:GLU:OE2	2.11	0.48
1:D:3071:LEU:O	1:D:3075:LEU:HD21	2.13	0.48
1:D:4184:MET:HA	1:D:4184:MET:HE2	1.95	0.48
1:A:2254:LEU:HD23	1:A:2254:LEU:C	2.38	0.48
1:B:292:ALA:HB1	1:B:311:ALA:HB1	1.94	0.48
1:B:1280:GLN:CD	1:B:1281:ASN:H	2.20	0.48
1:D:1439:VAL:HG12	1:D:1562:ILE:HG22	1.95	0.48
1:A:716:PHE:CZ	1:A:730:VAL:HG11	2.48	0.48
1:A:3532:LEU:HD21	1:A:3553:LEU:CD2	2.43	0.48
1:B:236:ALA:O	1:B:237:ASP:OD1	2.31	0.48
1:B:1289:LEU:HD12	1:B:1597:VAL:CG1	2.43	0.48
1:C:236:ALA:O	1:C:237:ASP:OD1	2.31	0.48
1:C:290:TYR:O	1:C:302:VAL:HG22	2.13	0.48
1:D:81:MET:HE3	1:D:81:MET:HA	1.94	0.48
1:D:864:PRO:HD2	1:D:867:LEU:HD13	1.93	0.48
1:A:928:THR:HG21	1:A:1039:LEU:HD12	1.94	0.48
1:A:4007:SER:O	1:A:4010:ILE:HG22	2.13	0.48
1:C:737:LEU:HD23	2:G:7:ILE:HG22	1.95	0.48
1:C:4184:MET:HE2	1:C:4184:MET:HA	1.95	0.48
1:D:3540:TYR:CE1	1:D:3549:VAL:HG11	2.48	0.48
1:B:4007:SER:O	1:B:4010:ILE:HG22	2.13	0.48
1:C:756:SER:HA	1:C:767:VAL:HG12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:TYR:O	1:A:302:VAL:HG22	2.13	0.48
1:C:3300:ALA:HB3	1:C:3301:PRO:HD3	1.96	0.48
1:D:4007:SER:O	1:D:4010:ILE:HG22	2.13	0.48
1:A:1289:LEU:HD12	1:A:1597:VAL:CG1	2.43	0.48
1:A:2240:CYS:SG	1:A:2250:MET:HE3	2.54	0.48
1:B:4879:MET:HE2	1:C:4578:LEU:HD22	1.96	0.48
1:C:4705:VAL:O	1:C:4705:VAL:HG22	2.14	0.48
1:D:3532:LEU:HD21	1:D:3553:LEU:CD2	2.43	0.48
1:A:231:LEU:HD11	1:A:245:VAL:HG11	1.95	0.48
1:A:3434:LEU:HA	1:A:3437:MET:HE2	1.96	0.48
1:A:4184:MET:HA	1:A:4184:MET:HE2	1.95	0.48
1:B:3434:LEU:HA	1:B:3437:MET:HE2	1.96	0.48
1:C:1289:LEU:HD12	1:C:1597:VAL:CG1	2.43	0.48
1:C:4007:SER:O	1:C:4010:ILE:HG22	2.13	0.48
1:D:928:THR:HG21	1:D:1039:LEU:HD12	1.94	0.48
1:A:3071:LEU:O	1:A:3075:LEU:HD21	2.13	0.48
1:A:3540:TYR:CE1	1:A:3549:VAL:HG11	2.48	0.48
1:B:2440:MET:HE3	1:B:2440:MET:HA	1.94	0.48
1:C:3638:MET:HE3	1:C:3639:THR:O	2.14	0.48
1:D:1015:ALA:C	1:D:1016:ARG:HD3	2.39	0.48
1:D:2254:LEU:C	1:D:2254:LEU:HD23	2.38	0.48
1:D:4705:VAL:HG22	1:D:4705:VAL:O	2.14	0.48
1:A:972:LEU:HD12	1:A:1044:ARG:HE	1.77	0.48
1:B:3300:ALA:HB3	1:B:3301:PRO:HD3	1.96	0.48
1:B:3540:TYR:CE1	1:B:3549:VAL:HG11	2.48	0.48
1:B:3638:MET:HE3	1:B:3639:THR:O	2.14	0.48
1:C:231:LEU:HD11	1:C:245:VAL:HG11	1.95	0.48
1:C:2254:LEU:HD23	1:C:2254:LEU:C	2.38	0.48
1:D:1289:LEU:HD12	1:D:1597:VAL:CG1	2.43	0.48
1:A:887:ILE:HB	1:A:907:LEU:HD12	1.95	0.47
1:A:2201:LEU:HB2	1:A:2203:MET:SD	2.55	0.47
1:B:3071:LEU:O	1:B:3075:LEU:HD21	2.13	0.47
1:B:4711:PHE:HB3	1:B:4712:PRO:HD3	1.96	0.47
1:B:290:TYR:O	1:B:302:VAL:HG22	2.13	0.47
1:B:1015:ALA:C	1:B:1016:ARG:HD3	2.39	0.47
1:D:571:SER:OG	1:D:574:VAL:HG23	2.14	0.47
1:D:2240:CYS:SG	1:D:2250:MET:HE3	2.54	0.47
1:D:2882:TYR:HA	1:D:2885:THR:HG22	1.95	0.47
1:B:202:MET:C	1:B:202:MET:SD	2.98	0.47
1:B:571:SER:OG	1:B:574:VAL:HG23	2.14	0.47
1:B:2240:CYS:SG	1:B:2250:MET:HE3	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4184:MET:HE2	1:B:4184:MET:HA	1.95	0.47
1:C:737:LEU:HD23	2:G:7:ILE:CG2	2.44	0.47
1:D:756:SER:HA	1:D:767:VAL:HG12	1.96	0.47
2:G:23:VAL:HG23	2:G:104:LEU:HB3	1.96	0.47
1:A:1652:GLU:OE1	1:A:1652:GLU:HA	2.15	0.47
1:A:3295:ALA:HB1	1:A:3299:GLY:HA3	1.97	0.47
1:A:3621:HIS:O	1:A:3622:LYS:HG3	2.14	0.47
1:A:3638:MET:HE3	1:A:3639:THR:O	2.14	0.47
1:B:3532:LEU:HD21	1:B:3553:LEU:CD2	2.43	0.47
1:C:2201:LEU:HB2	1:C:2203:MET:SD	2.55	0.47
1:D:3300:ALA:HB3	1:D:3301:PRO:HD3	1.96	0.47
1:A:719:LEU:HD11	2:E:7:ILE:HG23	1.96	0.47
1:A:4879:MET:HE2	1:B:4578:LEU:HD22	1.96	0.47
1:B:2882:TYR:HA	1:B:2885:THR:HG22	1.95	0.47
1:B:3621:HIS:O	1:B:3622:LYS:HG3	2.14	0.47
1:C:887:ILE:HB	1:C:907:LEU:HD12	1.95	0.47
1:C:1652:GLU:OE1	1:C:1652:GLU:HA	2.15	0.47
1:D:3295:ALA:HB1	1:D:3299:GLY:HA3	1.97	0.47
1:D:3434:LEU:HA	1:D:3437:MET:HE2	1.96	0.47
1:D:4711:PHE:HB3	1:D:4712:PRO:HD3	1.96	0.47
1:A:202:MET:SD	1:A:202:MET:C	2.98	0.47
1:C:2240:CYS:SG	1:C:2250:MET:HE3	2.54	0.47
1:A:2303:ALA:O	1:A:2307:LEU:HD23	2.15	0.47
1:A:4705:VAL:O	1:A:4705:VAL:HG22	2.14	0.47
1:B:231:LEU:HD11	1:B:245:VAL:HG11	1.95	0.47
1:B:756:SER:HA	1:B:767:VAL:HG12	1.96	0.47
1:B:3295:ALA:HB1	1:B:3299:GLY:HA3	1.97	0.47
1:B:4705:VAL:HG22	1:B:4705:VAL:O	2.14	0.47
1:C:202:MET:SD	1:C:202:MET:C	2.98	0.47
1:C:571:SER:OG	1:C:574:VAL:HG23	2.14	0.47
1:D:2212:VAL:HG12	1:D:2260:ASN:HD22	1.80	0.47
1:D:3638:MET:HE3	1:D:3639:THR:O	2.14	0.47
1:A:4833:ASN:OD1	1:A:4836:GLN:HB2	2.15	0.47
1:B:2205:GLU:OE2	1:B:2205:GLU:N	2.48	0.47
1:C:3434:LEU:HA	1:C:3437:MET:HE2	1.96	0.47
1:D:1652:GLU:HA	1:D:1652:GLU:OE1	2.15	0.47
2:F:23:VAL:HG23	2:F:104:LEU:HB3	1.96	0.47
1:A:756:SER:HA	1:A:767:VAL:HG12	1.96	0.47
1:B:1264:VAL:HG13	1:B:1265:ASP:N	2.30	0.47
1:C:716:PHE:CZ	1:C:730:VAL:HG11	2.48	0.47
1:C:2212:VAL:HG12	1:C:2260:ASN:HD22	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1737:PRO:HG3	1:A:1771:LEU:HD11	1.97	0.47
1:B:2303:ALA:O	1:B:2307:LEU:HD23	2.15	0.47
1:B:3197:LEU:C	1:B:3197:LEU:HD23	2.40	0.47
1:C:1015:ALA:C	1:C:1016:ARG:HD3	2.39	0.47
1:C:1737:PRO:HG3	1:C:1771:LEU:HD11	1.97	0.47
1:A:1015:ALA:C	1:A:1016:ARG:HD3	2.39	0.46
1:A:4578:LEU:HA	1:D:4879:MET:SD	2.56	0.46
1:B:2201:LEU:HB2	1:B:2203:MET:SD	2.54	0.46
1:B:3434:LEU:HD21	1:B:3517:MET:HE3	1.97	0.46
1:B:4833:ASN:OD1	1:B:4836:GLN:HB2	2.15	0.46
1:C:3295:ALA:HB1	1:C:3299:GLY:HA3	1.97	0.46
1:C:4833:ASN:OD1	1:C:4836:GLN:HB2	2.15	0.46
1:D:2201:LEU:HB2	1:D:2203:MET:SD	2.55	0.46
1:D:2205:GLU:N	1:D:2205:GLU:OE2	2.48	0.46
1:D:2303:ALA:O	1:D:2307:LEU:HD23	2.15	0.46
1:D:4843:LEU:C	1:D:4843:LEU:HD23	2.40	0.46
1:A:571:SER:OG	1:A:574:VAL:HG23	2.14	0.46
1:A:3300:ALA:HB3	1:A:3301:PRO:HD3	1.96	0.46
1:A:4836:GLN:OE1	1:B:4826:ILE:HD11	2.14	0.46
1:B:887:ILE:HB	1:B:907:LEU:HD12	1.95	0.46
1:B:1931:LEU:HB3	1:B:1932:PRO:HD2	1.97	0.46
1:C:4711:PHE:HB3	1:C:4712:PRO:HD3	1.97	0.46
1:D:170:ILE:C	1:D:171:LEU:HD12	2.41	0.46
1:A:4251:ILE:HG22	1:A:4251:ILE:O	2.15	0.46
1:C:2303:ALA:O	1:C:2307:LEU:HD23	2.15	0.46
1:D:202:MET:SD	1:D:202:MET:C	2.98	0.46
1:A:2188:ASN:CG	1:A:2190:VAL:HG12	2.41	0.46
1:A:2212:VAL:HG12	1:A:2260:ASN:HD22	1.80	0.46
1:A:3197:LEU:C	1:A:3197:LEU:HD23	2.40	0.46
1:A:4852:THR:HG21	1:A:4883:TYR:HA	1.97	0.46
1:C:1931:LEU:HB3	1:C:1932:PRO:HD2	1.97	0.46
1:D:231:LEU:HD11	1:D:245:VAL:HG11	1.95	0.46
1:D:3621:HIS:O	1:D:3622:LYS:HG3	2.14	0.46
1:D:4833:ASN:OD1	1:D:4836:GLN:HB2	2.15	0.46
1:A:323:LEU:O	1:A:324:ASP:C	2.59	0.46
1:A:737:LEU:HD23	2:E:7:ILE:HG22	1.98	0.46
1:A:3232:LEU:HD22	1:A:3239:MET:HE1	1.98	0.46
1:B:170:ILE:C	1:B:171:LEU:HD12	2.41	0.46
1:B:1737:PRO:HG3	1:B:1771:LEU:HD11	1.97	0.46
1:B:3232:LEU:HD22	1:B:3239:MET:HE1	1.98	0.46
1:B:3263:TYR:CE1	1:B:3270:ILE:HD13	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4843:LEU:HD23	1:B:4843:LEU:C	2.40	0.46
1:C:3197:LEU:C	1:C:3197:LEU:HD23	2.40	0.46
1:D:2390:PRO:O	1:D:2391:ALA:HB3	2.16	0.46
2:E:23:VAL:HG23	2:E:104:LEU:HB3	1.96	0.46
1:A:2205:GLU:N	1:A:2205:GLU:OE2	2.48	0.46
1:A:4711:PHE:HB3	1:A:4712:PRO:HD3	1.96	0.46
1:B:323:LEU:O	1:B:324:ASP:C	2.59	0.46
1:B:2212:VAL:HG12	1:B:2260:ASN:HD22	1.80	0.46
1:C:43:GLY:O	1:C:443:LEU:HD21	2.16	0.46
1:C:3621:HIS:O	1:C:3622:LYS:HG3	2.14	0.46
1:D:975:VAL:HG13	1:D:1047:LEU:HB3	1.97	0.46
1:D:4852:THR:HG21	1:D:4883:TYR:HA	1.97	0.46
1:A:170:ILE:C	1:A:171:LEU:HD12	2.41	0.46
1:A:1264:VAL:HG13	1:A:1265:ASP:N	2.31	0.46
1:A:3930:ILE:HG23	1:A:3933:PHE:CE1	2.51	0.46
1:B:880:GLU:O	1:B:884:LEU:HD13	2.15	0.46
1:B:1652:GLU:HA	1:B:1652:GLU:OE1	2.15	0.46
1:B:2188:ASN:CG	1:B:2190:VAL:HG12	2.41	0.46
1:B:2583:LEU:HA	1:B:2586:VAL:HG12	1.98	0.46
1:C:170:ILE:C	1:C:171:LEU:HD12	2.41	0.46
1:C:2188:ASN:CG	1:C:2190:VAL:HG12	2.41	0.46
1:D:1264:VAL:HG13	1:D:1265:ASP:N	2.31	0.46
1:A:411:TYR:O	1:A:415:ILE:HG12	2.16	0.46
1:B:2390:PRO:O	1:B:2391:ALA:HB3	2.16	0.46
1:B:3061:ALA:N	1:B:3062:PRO:CD	2.79	0.46
1:C:880:GLU:O	1:C:884:LEU:HD13	2.15	0.46
1:D:880:GLU:O	1:D:884:LEU:HD13	2.15	0.46
1:D:2583:LEU:HA	1:D:2586:VAL:HG12	1.98	0.46
2:H:23:VAL:HG23	2:H:104:LEU:HB3	1.96	0.46
1:A:880:GLU:O	1:A:884:LEU:HD13	2.15	0.46
1:A:2390:PRO:O	1:A:2391:ALA:HB3	2.16	0.46
1:B:2306:GLY:C	1:B:2307:LEU:HD22	2.41	0.46
1:B:4214:LYS:HZ2	1:B:4985:LEU:HD21	1.81	0.46
1:C:3061:ALA:N	1:C:3062:PRO:CD	2.79	0.46
1:D:4251:ILE:HG22	1:D:4251:ILE:O	2.16	0.46
1:A:975:VAL:HG13	1:A:1047:LEU:HB3	1.97	0.46
1:C:2205:GLU:OE2	1:C:2205:GLU:N	2.48	0.46
1:C:2583:LEU:HA	1:C:2586:VAL:HG12	1.98	0.46
1:C:4843:LEU:C	1:C:4843:LEU:HD23	2.40	0.46
1:D:43:GLY:O	1:D:443:LEU:HD21	2.16	0.46
1:D:323:LEU:O	1:D:324:ASP:C	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3061:ALA:N	1:D:3062:PRO:CD	2.79	0.46
1:D:3197:LEU:C	1:D:3197:LEU:HD23	2.40	0.46
1:D:3930:ILE:HG23	1:D:3933:PHE:CE1	2.50	0.46
1:A:222:LEU:HD23	1:A:388:LEU:HD13	1.98	0.45
1:A:2583:LEU:HA	1:A:2586:VAL:HG12	1.98	0.45
1:A:3061:ALA:N	1:A:3062:PRO:CD	2.79	0.45
1:A:4843:LEU:C	1:A:4843:LEU:HD23	2.40	0.45
1:B:4836:GLN:OE1	1:C:4826:ILE:HD11	2.15	0.45
1:B:4852:THR:HG21	1:B:4883:TYR:HA	1.97	0.45
1:C:3434:LEU:HD21	1:C:3517:MET:HE3	1.98	0.45
1:C:4852:THR:HG21	1:C:4883:TYR:HA	1.97	0.45
1:D:1931:LEU:HB3	1:D:1932:PRO:HD2	1.97	0.45
1:D:2188:ASN:CG	1:D:2190:VAL:HG12	2.41	0.45
1:D:2306:GLY:C	1:D:2307:LEU:HD22	2.41	0.45
1:A:3263:TYR:CE1	1:A:3270:ILE:HD13	2.51	0.45
1:B:411:TYR:O	1:B:415:ILE:HG12	2.16	0.45
1:C:915:GLU:O	1:C:916:PRO:C	2.59	0.45
1:C:2306:GLY:C	1:C:2307:LEU:HD22	2.41	0.45
1:C:2390:PRO:O	1:C:2391:ALA:HB3	2.16	0.45
1:C:3263:TYR:CE1	1:C:3270:ILE:HD13	2.51	0.45
1:C:4251:ILE:O	1:C:4251:ILE:HG22	2.15	0.45
1:D:3263:TYR:CE1	1:D:3270:ILE:HD13	2.51	0.45
1:A:1931:LEU:HB3	1:A:1932:PRO:HD2	1.97	0.45
1:A:3434:LEU:HD21	1:A:3517:MET:HE3	1.97	0.45
1:B:4251:ILE:HG22	1:B:4251:ILE:O	2.15	0.45
1:C:4836:GLN:OE1	1:D:4826:ILE:HD11	2.16	0.45
1:D:411:TYR:O	1:D:415:ILE:HG12	2.16	0.45
1:D:977:LEU:HD21	1:D:1044:ARG:HH12	1.82	0.45
1:A:3389:GLU:O	1:A:3389:GLU:CD	2.60	0.45
1:B:1111:PRO:HB2	1:B:1603:VAL:HG11	1.98	0.45
1:D:915:GLU:O	1:D:916:PRO:C	2.59	0.45
1:D:1783:VAL:HG23	2:H:55:VAL:HG23	1.97	0.45
1:A:1057:ASP:OD2	1:B:2951:ILE:HG13	2.17	0.45
1:A:3416:VAL:CG2	1:A:3517:MET:HE1	2.46	0.45
1:B:222:LEU:HD23	1:B:388:LEU:HD13	1.98	0.45
1:C:975:VAL:HG13	1:C:1047:LEU:HB3	1.97	0.45
1:C:2504:LEU:HD23	1:C:2504:LEU:O	2.17	0.45
1:C:3389:GLU:CD	1:C:3389:GLU:O	2.60	0.45
1:A:150:MET:HE1	1:A:163:VAL:HG21	1.99	0.45
1:A:5035:GLN:C	1:A:5036:LEU:HD22	2.42	0.45
1:B:5035:GLN:C	1:B:5036:LEU:HD22	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HD23	1:C:388:LEU:HD13	1.98	0.45
1:C:1264:VAL:HG13	1:C:1265:ASP:N	2.31	0.45
1:C:3434:LEU:CD2	1:C:3517:MET:HE3	2.47	0.45
1:C:5035:GLN:C	1:C:5036:LEU:HD22	2.42	0.45
1:D:1737:PRO:HG3	1:D:1771:LEU:HD11	1.97	0.45
1:D:3416:VAL:CG2	1:D:3517:MET:HE1	2.47	0.45
1:A:977:LEU:HD21	1:A:1044:ARG:HH12	1.82	0.45
1:B:2504:LEU:HD23	1:B:2504:LEU:O	2.16	0.45
1:B:3434:LEU:CD2	1:B:3517:MET:HE3	2.47	0.45
1:C:411:TYR:O	1:C:415:ILE:HG12	2.16	0.45
1:C:3232:LEU:HD22	1:C:3239:MET:HE1	1.98	0.45
1:D:864:PRO:HD2	1:D:867:LEU:HD22	1.99	0.45
1:D:1111:PRO:HB2	1:D:1603:VAL:HG11	1.98	0.45
1:D:4580:TYR:CA	1:D:4632:LEU:HD13	2.47	0.45
1:A:816:LEU:HD12	1:A:1026:LEU:CD2	2.39	0.45
1:A:1111:PRO:HB2	1:A:1603:VAL:HG11	1.98	0.45
1:A:2306:GLY:C	1:A:2307:LEU:HD22	2.41	0.45
1:B:977:LEU:HD21	1:B:1044:ARG:HH12	1.82	0.45
1:C:902:ARG:HG2	1:C:902:ARG:O	2.17	0.45
1:A:43:GLY:O	1:A:443:LEU:HD21	2.16	0.45
1:A:1027:LEU:HD11	1:A:1031:THR:CG2	2.47	0.45
1:B:150:MET:HE1	1:B:163:VAL:HG21	1.99	0.45
1:C:323:LEU:O	1:C:324:ASP:C	2.59	0.45
1:C:3201:MET:SD	1:C:3203:VAL:HG22	2.57	0.45
1:D:3232:LEU:HD22	1:D:3239:MET:HE1	1.98	0.45
1:A:68:THR:O	1:A:109:LEU:HD12	2.17	0.45
1:A:554:LEU:HD12	1:A:554:LEU:H	1.82	0.45
1:A:864:PRO:HD2	1:A:867:LEU:HD22	1.99	0.45
1:B:43:GLY:O	1:B:443:LEU:HD21	2.16	0.45
1:B:975:VAL:HG13	1:B:1047:LEU:HB3	1.97	0.45
1:B:3930:ILE:HG23	1:B:3933:PHE:CE1	2.51	0.45
1:C:554:LEU:H	1:C:554:LEU:HD12	1.81	0.45
1:C:1525:GLY:C	1:C:1526:LEU:HD12	2.42	0.45
1:D:1509:ILE:H	1:D:1509:ILE:HD12	1.82	0.45
1:D:2970:SER:O	1:D:2974:ILE:HD12	2.17	0.45
1:D:3389:GLU:O	1:D:3389:GLU:CD	2.60	0.45
1:A:902:ARG:O	1:A:902:ARG:HG2	2.17	0.44
1:A:4580:TYR:CA	1:A:4632:LEU:HD13	2.47	0.44
1:B:915:GLU:O	1:B:916:PRO:C	2.59	0.44
1:C:150:MET:HE1	1:C:163:VAL:HG21	1.99	0.44
1:A:4735:GLU:N	1:A:4735:GLU:OE1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:LEU:N	1:C:627:PRO:HD2	2.33	0.44
1:C:977:LEU:HD21	1:C:1044:ARG:HH12	1.82	0.44
1:C:3593:VAL:HG23	1:C:3594:ARG:HD2	1.99	0.44
1:D:3434:LEU:CD2	1:D:3517:MET:HE3	2.47	0.44
1:D:3434:LEU:HD21	1:D:3517:MET:HE3	1.98	0.44
1:D:5035:GLN:C	1:D:5036:LEU:HD22	2.42	0.44
2:F:96:THR:C	2:F:97:LEU:HD12	2.43	0.44
1:A:46:LEU:HD12	1:A:46:LEU:H	1.82	0.44
1:B:554:LEU:HD12	1:B:554:LEU:H	1.82	0.44
1:B:1509:ILE:HD12	1:B:1509:ILE:H	1.82	0.44
1:B:1525:GLY:C	1:B:1526:LEU:HD12	2.42	0.44
1:C:1111:PRO:HB2	1:C:1603:VAL:HG11	1.98	0.44
2:E:96:THR:C	2:E:97:LEU:HD12	2.42	0.44
2:G:96:THR:C	2:G:97:LEU:HD12	2.42	0.44
1:A:3434:LEU:CD2	1:A:3517:MET:HE3	2.47	0.44
1:A:4879:MET:SD	1:B:4580:TYR:CE1	3.11	0.44
1:B:1027:LEU:HD11	1:B:1031:THR:CG2	2.47	0.44
1:B:3201:MET:SD	1:B:3203:VAL:HG22	2.57	0.44
1:B:3389:GLU:CD	1:B:3389:GLU:O	2.60	0.44
1:C:1027:LEU:HD11	1:C:1031:THR:CG2	2.47	0.44
1:C:2977:LEU:O	1:C:2981:VAL:HG12	2.18	0.44
1:D:222:LEU:HD23	1:D:388:LEU:HD13	1.98	0.44
1:D:554:LEU:HD12	1:D:554:LEU:H	1.82	0.44
1:D:723:THR:HG23	1:D:723:THR:O	2.18	0.44
1:D:902:ARG:O	1:D:902:ARG:HG2	2.17	0.44
1:D:991:ASN:O	1:D:995:VAL:HG23	2.17	0.44
1:D:2977:LEU:O	1:D:2981:VAL:HG12	2.18	0.44
1:B:68:THR:O	1:B:109:LEU:HD12	2.17	0.44
1:B:723:THR:HG23	1:B:723:THR:O	2.18	0.44
1:B:2504:LEU:HD23	1:B:2504:LEU:C	2.43	0.44
1:B:3593:VAL:HG23	1:B:3594:ARG:HD2	1.99	0.44
1:C:1084:GLN:C	1:C:1155:LEU:HD13	2.43	0.44
1:C:3416:VAL:CG2	1:C:3517:MET:HE1	2.46	0.44
1:C:3930:ILE:HG23	1:C:3933:PHE:CE1	2.50	0.44
1:C:4696:ASP:OD1	1:C:4696:ASP:O	2.36	0.44
1:D:68:THR:O	1:D:109:LEU:HD12	2.18	0.44
1:D:2504:LEU:C	1:D:2504:LEU:HD23	2.43	0.44
1:A:723:THR:O	1:A:723:THR:HG23	2.17	0.44
1:A:2504:LEU:O	1:A:2504:LEU:HD23	2.17	0.44
1:B:4696:ASP:OD1	1:B:4696:ASP:O	2.36	0.44
1:C:991:ASN:O	1:C:995:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2504:LEU:HD23	1:D:2504:LEU:O	2.17	0.44
2:H:96:THR:C	2:H:97:LEU:HD12	2.43	0.44
1:A:2504:LEU:HD23	1:A:2504:LEU:C	2.43	0.44
1:A:2970:SER:O	1:A:2974:ILE:HD12	2.17	0.44
1:B:737:LEU:HD23	2:F:7:ILE:HG22	1.99	0.44
1:B:902:ARG:O	1:B:902:ARG:HG2	2.17	0.44
1:D:1084:GLN:C	1:D:1155:LEU:HD13	2.43	0.44
1:D:1525:GLY:C	1:D:1526:LEU:HD12	2.42	0.44
1:D:3201:MET:SD	1:D:3203:VAL:HG22	2.57	0.44
1:D:3277:LEU:HD23	1:D:3315:LEU:HD13	2.00	0.44
1:A:825:PRO:HG2	1:A:828:GLU:HG2	2.00	0.44
1:A:2715:VAL:HG13	1:A:2719:TYR:OH	2.18	0.44
1:B:991:ASN:O	1:B:995:VAL:HG23	2.17	0.44
1:B:2174:GLU:OE2	1:B:2174:GLU:N	2.51	0.44
1:B:3277:LEU:HD23	1:B:3315:LEU:HD13	2.00	0.44
1:C:2938:THR:HG22	1:C:2939:ARG:N	2.33	0.44
1:C:4735:GLU:N	1:C:4735:GLU:OE1	2.50	0.44
1:D:1027:LEU:HD11	1:D:1031:THR:CG2	2.47	0.44
1:A:626:LEU:N	1:A:627:PRO:HD2	2.33	0.44
1:A:991:ASN:O	1:A:995:VAL:HG23	2.18	0.44
1:A:1509:ILE:HD12	1:A:1509:ILE:H	1.83	0.44
1:A:2977:LEU:O	1:A:2981:VAL:HG12	2.18	0.44
1:B:626:LEU:N	1:B:627:PRO:HD2	2.33	0.44
1:B:3416:VAL:CG2	1:B:3517:MET:HE1	2.46	0.44
1:B:4580:TYR:CA	1:B:4632:LEU:HD13	2.47	0.44
1:C:46:LEU:HD12	1:C:46:LEU:H	1.83	0.44
1:C:4580:TYR:CA	1:C:4632:LEU:HD13	2.47	0.44
1:D:2715:VAL:HG13	1:D:2719:TYR:OH	2.18	0.44
1:A:915:GLU:O	1:A:916:PRO:C	2.59	0.43
1:A:2886:TRP:CH2	1:A:2904:LEU:HD23	2.53	0.43
1:A:3438:VAL:O	1:A:3441:ILE:HG22	2.18	0.43
1:B:825:PRO:HG2	1:B:828:GLU:HG2	2.00	0.43
1:B:1783:VAL:HG23	2:F:55:VAL:HG23	2.00	0.43
1:B:1951:LEU:C	1:B:1951:LEU:HD23	2.43	0.43
1:B:2715:VAL:HG13	1:B:2719:TYR:OH	2.18	0.43
1:B:2977:LEU:O	1:B:2981:VAL:HG12	2.18	0.43
1:B:4735:GLU:N	1:B:4735:GLU:OE1	2.50	0.43
1:C:723:THR:HG23	1:C:723:THR:O	2.18	0.43
1:C:1237:TRP:HA	1:C:1607:ARG:HA	2.00	0.43
1:C:1951:LEU:C	1:C:1951:LEU:HD23	2.43	0.43
1:C:2715:VAL:HG13	1:C:2719:TYR:OH	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3365:LEU:HD21	1:C:3408:LEU:HD12	2.00	0.43
1:D:626:LEU:N	1:D:627:PRO:HD2	2.33	0.43
1:D:4696:ASP:OD1	1:D:4696:ASP:O	2.36	0.43
1:A:737:LEU:HD23	2:E:7:ILE:CG2	2.48	0.43
1:A:3201:MET:SD	1:A:3203:VAL:HG22	2.57	0.43
1:A:3622:LYS:O	1:A:3623:LEU:C	2.62	0.43
1:B:864:PRO:HD2	1:B:867:LEU:HD22	1.99	0.43
1:B:1237:TRP:HA	1:B:1607:ARG:HA	2.00	0.43
1:B:2970:SER:O	1:B:2974:ILE:HD12	2.17	0.43
1:C:864:PRO:HD2	1:C:867:LEU:HD22	1.99	0.43
1:C:1509:ILE:HD12	1:C:1509:ILE:H	1.82	0.43
1:C:2886:TRP:CH2	1:C:2904:LEU:HD23	2.53	0.43
1:C:2970:SER:O	1:C:2974:ILE:HD12	2.17	0.43
1:D:150:MET:HE1	1:D:163:VAL:HG21	1.99	0.43
1:A:1084:GLN:C	1:A:1155:LEU:HD13	2.43	0.43
1:A:1525:GLY:C	1:A:1526:LEU:HD12	2.42	0.43
1:A:1951:LEU:C	1:A:1951:LEU:HD23	2.43	0.43
1:A:2662:ALA:O	1:A:2663:ASN:OD1	2.37	0.43
1:A:3593:VAL:HG23	1:A:3594:ARG:HD2	1.99	0.43
1:B:626:LEU:HD22	1:B:1688:HIS:CE1	2.53	0.43
1:B:2559:LEU:N	1:B:2560:PRO:HD2	2.33	0.43
1:B:2938:THR:HG22	1:B:2939:ARG:N	2.33	0.43
1:B:3365:LEU:HD21	1:B:3408:LEU:HD12	2.00	0.43
1:C:68:THR:O	1:C:109:LEU:HD12	2.18	0.43
1:C:2174:GLU:N	1:C:2174:GLU:OE2	2.51	0.43
1:C:2504:LEU:HD23	1:C:2504:LEU:C	2.43	0.43
1:C:2662:ALA:O	1:C:2663:ASN:OD1	2.37	0.43
1:C:3438:VAL:O	1:C:3441:ILE:HG22	2.18	0.43
1:D:46:LEU:HD12	1:D:46:LEU:H	1.83	0.43
1:D:1465:ASP:OD1	1:D:1468:LYS:HG2	2.18	0.43
1:D:1607:ARG:HH22	1:D:1651:LEU:HD13	1.84	0.43
1:D:2886:TRP:CH2	1:D:2904:LEU:HD23	2.53	0.43
1:D:3438:VAL:O	1:D:3441:ILE:HG22	2.18	0.43
1:A:2174:GLU:N	1:A:2174:GLU:OE2	2.51	0.43
1:A:3277:LEU:HD23	1:A:3315:LEU:HD13	2.00	0.43
1:B:736:HIS:HA	2:F:7:ILE:O	2.19	0.43
1:B:1084:GLN:C	1:B:1155:LEU:HD13	2.43	0.43
1:C:1607:ARG:HH22	1:C:1651:LEU:HD13	1.84	0.43
1:C:4879:MET:SD	1:D:4578:LEU:HA	2.59	0.43
1:D:2174:GLU:OE2	1:D:2174:GLU:N	2.51	0.43
1:D:2559:LEU:N	1:D:2560:PRO:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:HIS:NE2	1:B:913:LEU:HD22	2.34	0.43
1:B:1607:ARG:HH22	1:B:1651:LEU:HD13	1.84	0.43
1:B:3438:VAL:O	1:B:3441:ILE:HG22	2.18	0.43
1:D:3622:LYS:O	1:D:3623:LEU:C	2.61	0.43
1:B:46:LEU:HD12	1:B:46:LEU:H	1.82	0.43
1:B:1465:ASP:OD1	1:B:1468:LYS:HG2	2.19	0.43
1:B:3865:VAL:O	1:B:3865:VAL:HG13	2.19	0.43
1:C:111:HIS:CE1	1:C:113:HIS:HB3	2.54	0.43
1:C:626:LEU:HD22	1:C:1688:HIS:CE1	2.53	0.43
1:C:1465:ASP:OD1	1:C:1468:LYS:HG2	2.18	0.43
1:C:2559:LEU:N	1:C:2560:PRO:HD2	2.33	0.43
1:D:308:HIS:CD2	1:D:310:LYS:HB2	2.54	0.43
1:D:825:PRO:HG2	1:D:828:GLU:HG2	2.00	0.43
1:D:879:HIS:NE2	1:D:913:LEU:HD22	2.34	0.43
1:D:3593:VAL:HG23	1:D:3594:ARG:HD2	1.99	0.43
1:A:364:PRO:O	1:A:365:LYS:HB3	2.19	0.43
1:A:1237:TRP:HA	1:A:1607:ARG:HA	2.00	0.43
1:A:1465:ASP:OD1	1:A:1468:LYS:HG2	2.19	0.43
1:A:2951:ILE:HG13	1:D:1057:ASP:OD2	2.19	0.43
1:A:3930:ILE:HA	1:A:3933:PHE:CE1	2.54	0.43
1:A:4826:ILE:HD11	1:D:4836:GLN:OE1	2.19	0.43
1:B:3622:LYS:O	1:B:3623:LEU:C	2.61	0.43
1:C:308:HIS:CD2	1:C:310:LYS:HB2	2.54	0.43
1:C:825:PRO:HG2	1:C:828:GLU:HG2	2.00	0.43
1:C:3277:LEU:HD23	1:C:3315:LEU:HD13	2.00	0.43
1:D:1237:TRP:HA	1:D:1607:ARG:HA	2.01	0.43
1:D:2490:MET:HE3	1:D:2545:GLU:HG2	2.01	0.43
1:A:626:LEU:HD22	1:A:1688:HIS:CE1	2.53	0.43
1:A:1607:ARG:HH22	1:A:1651:LEU:HD13	1.84	0.43
1:B:308:HIS:CD2	1:B:310:LYS:HB2	2.54	0.43
1:B:2886:TRP:CH2	1:B:2904:LEU:HD23	2.53	0.43
1:C:2624:ARG:O	1:C:2627:VAL:HG12	2.18	0.43
1:C:3930:ILE:HA	1:C:3933:PHE:CE1	2.54	0.43
1:D:4735:GLU:N	1:D:4735:GLU:OE1	2.50	0.43
1:A:111:HIS:CE1	1:A:113:HIS:HB3	2.54	0.43
1:A:373:LYS:O	1:A:373:LYS:HG3	2.19	0.43
1:A:3934:TYR:CD2	1:A:3934:TYR:C	2.97	0.43
1:B:364:PRO:O	1:B:365:LYS:HB3	2.19	0.43
1:B:1182:ILE:HG22	1:B:1183:GLU:N	2.34	0.43
1:C:368:ARG:HD2	1:C:2307:LEU:HD12	2.01	0.43
1:C:617:ASN:O	1:C:621:ILE:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:HIS:CE1	1:D:113:HIS:HB3	2.54	0.43
1:D:1126:GLY:O	1:D:1142:PRO:HA	2.19	0.43
1:D:1951:LEU:C	1:D:1951:LEU:HD23	2.43	0.43
1:D:3865:VAL:HG13	1:D:3865:VAL:O	2.19	0.43
1:A:2559:LEU:N	1:A:2560:PRO:HD2	2.33	0.43
1:B:368:ARG:HD2	1:B:2307:LEU:HD12	2.01	0.43
1:B:2819:TRP:O	1:B:2820:GLU:HG3	2.19	0.43
1:C:2819:TRP:O	1:C:2820:GLU:HG3	2.19	0.43
1:D:617:ASN:O	1:D:621:ILE:HG22	2.19	0.43
1:A:2938:THR:HG22	1:A:2939:ARG:N	2.33	0.42
1:A:4696:ASP:OD1	1:A:4696:ASP:O	2.36	0.42
1:C:976:ARG:O	1:C:977:LEU:HD23	2.19	0.42
1:C:2974:ILE:HD13	1:C:3049:LEU:HD11	2.01	0.42
1:C:3934:TYR:CD2	1:C:3934:TYR:C	2.97	0.42
1:D:1434:TYR:CD1	1:D:1569:GLN:HB2	2.54	0.42
1:D:2662:ALA:O	1:D:2663:ASN:OD1	2.37	0.42
1:D:2938:THR:HG22	1:D:2939:ARG:N	2.33	0.42
1:A:2624:ARG:O	1:A:2627:VAL:HG12	2.18	0.42
1:B:373:LYS:HG3	1:B:373:LYS:O	2.19	0.42
1:B:2624:ARG:O	1:B:2627:VAL:HG12	2.18	0.42
1:C:364:PRO:O	1:C:365:LYS:HB3	2.19	0.42
1:C:1603:VAL:HG12	1:C:1604:SER:N	2.34	0.42
1:D:626:LEU:HD22	1:D:1688:HIS:CE1	2.53	0.42
1:A:901:LYS:O	1:A:902:ARG:HD3	2.19	0.42
1:A:1603:VAL:HG12	1:A:1604:SER:N	2.35	0.42
1:B:976:ARG:O	1:B:977:LEU:HD23	2.19	0.42
1:B:1472:VAL:HG22	1:B:1473:THR:N	2.35	0.42
1:B:1603:VAL:HG12	1:B:1604:SER:N	2.34	0.42
1:B:2251:PHE:CD2	1:B:2286:LEU:HD22	2.55	0.42
1:B:2662:ALA:O	1:B:2663:ASN:OD1	2.37	0.42
1:B:3934:TYR:CD2	1:B:3934:TYR:C	2.97	0.42
1:C:1057:ASP:OD2	1:D:2951:ILE:HG13	2.19	0.42
1:C:1783:VAL:HG23	2:G:55:VAL:HG23	2.01	0.42
1:D:368:ARG:HD2	1:D:2307:LEU:HD12	2.01	0.42
1:D:976:ARG:O	1:D:977:LEU:HD23	2.19	0.42
1:D:1182:ILE:HG22	1:D:1183:GLU:N	2.34	0.42
1:D:2819:TRP:O	1:D:2820:GLU:HG3	2.19	0.42
1:D:3969:ILE:HG23	1:D:3977:GLN:CG	2.49	0.42
1:A:1126:GLY:O	1:A:1142:PRO:HA	2.19	0.42
1:B:111:HIS:CE1	1:B:113:HIS:HB3	2.54	0.42
1:C:3559:LEU:O	1:C:3559:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2251:PHE:CD2	1:D:2286:LEU:HD22	2.55	0.42
1:D:2624:ARG:O	1:D:2627:VAL:HG12	2.18	0.42
1:D:3930:ILE:HA	1:D:3933:PHE:CE1	2.54	0.42
1:D:3934:TYR:CD2	1:D:3934:TYR:C	2.97	0.42
1:A:75:VAL:O	1:A:79:GLN:HG2	2.20	0.42
1:A:368:ARG:HD2	1:A:2307:LEU:HD12	2.01	0.42
1:A:736:HIS:HA	2:E:7:ILE:O	2.20	0.42
1:A:1434:TYR:CD1	1:A:1569:GLN:HB2	2.55	0.42
1:A:1472:VAL:HG22	1:A:1473:THR:N	2.35	0.42
1:A:4580:TYR:CE1	1:D:4879:MET:SD	3.13	0.42
1:B:1434:TYR:CD1	1:B:1569:GLN:HB2	2.55	0.42
1:C:901:LYS:O	1:C:902:ARG:HD3	2.20	0.42
1:C:1243:PRO:HB2	1:C:1600:LEU:HD11	2.01	0.42
1:D:1243:PRO:HB2	1:D:1600:LEU:HD11	2.01	0.42
1:D:3986:TRP:CD2	1:D:4043:GLN:NE2	2.88	0.42
1:A:308:HIS:CD2	1:A:310:LYS:HB2	2.54	0.42
1:A:1182:ILE:HG22	1:A:1183:GLU:N	2.34	0.42
1:A:2819:TRP:O	1:A:2820:GLU:HG3	2.19	0.42
1:A:3986:TRP:CD2	1:A:4043:GLN:NE2	2.88	0.42
1:B:2490:MET:HE3	1:B:2545:GLU:HG2	2.01	0.42
1:C:373:LYS:O	1:C:373:LYS:HG3	2.19	0.42
1:C:879:HIS:NE2	1:C:913:LEU:HD22	2.34	0.42
1:D:4214:LYS:HZ1	1:D:4985:LEU:HD21	1.85	0.42
1:A:2490:MET:HE3	1:A:2545:GLU:HG2	2.01	0.42
1:B:19:GLU:HA	1:B:68:THR:HG22	2.02	0.42
1:B:901:LYS:O	1:B:902:ARG:HD3	2.19	0.42
1:B:3817:LEU:HB2	1:B:3899:PHE:CZ	2.55	0.42
1:B:4879:MET:SD	1:C:4580:TYR:CE1	3.13	0.42
1:C:667:MET:HG2	1:C:668:VAL:N	2.35	0.42
1:C:1434:TYR:CD1	1:C:1569:GLN:HB2	2.54	0.42
1:A:976:ARG:O	1:A:977:LEU:HD23	2.19	0.42
1:B:4168:GLU:HG2	1:B:4169:SER:N	2.35	0.42
1:C:1182:ILE:HG22	1:C:1183:GLU:N	2.34	0.42
1:C:3137:LEU:C	1:C:3137:LEU:HD23	2.45	0.42
1:C:4949:GLN:OE1	1:C:4949:GLN:HA	2.20	0.42
1:D:871:ARG:HG2	1:D:922:LEU:HD11	2.02	0.42
1:D:3365:LEU:HD21	1:D:3408:LEU:HD12	2.00	0.42
2:G:59:TRP:O	2:G:63:VAL:HG12	2.19	0.42
1:A:3865:VAL:O	1:A:3865:VAL:HG13	2.19	0.42
1:A:4577:LEU:O	1:D:4879:MET:SD	2.78	0.42
1:B:3986:TRP:CD2	1:B:4043:GLN:NE2	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1126:GLY:O	1:C:1142:PRO:HA	2.19	0.42
1:C:2251:PHE:CD2	1:C:2286:LEU:HD22	2.55	0.42
1:C:2490:MET:HE3	1:C:2545:GLU:HG2	2.01	0.42
1:C:2967:MET:SD	1:C:3045:LYS:HG3	2.60	0.42
1:C:3817:LEU:HB2	1:C:3899:PHE:CZ	2.55	0.42
1:D:373:LYS:O	1:D:373:LYS:HG3	2.19	0.42
1:D:3559:LEU:HG	1:D:3559:LEU:O	2.19	0.42
1:D:4949:GLN:HA	1:D:4949:GLN:OE1	2.20	0.42
1:A:1782:PHE:CD2	2:E:37:ASP:HB3	2.55	0.42
1:A:2251:PHE:CD2	1:A:2286:LEU:HD22	2.55	0.42
1:A:3365:LEU:HD21	1:A:3408:LEU:HD12	2.00	0.42
1:A:3969:ILE:HG23	1:A:3977:GLN:CG	2.49	0.42
1:B:75:VAL:O	1:B:79:GLN:HG2	2.20	0.42
1:B:617:ASN:O	1:B:621:ILE:HG22	2.19	0.42
1:B:3930:ILE:HA	1:B:3933:PHE:CE1	2.54	0.42
1:C:364:PRO:O	1:C:365:LYS:CB	2.68	0.42
1:C:2290:LEU:CD2	1:C:2295:LEU:HD21	2.50	0.42
1:C:3346:VAL:HG22	1:C:3346:VAL:O	2.20	0.42
1:C:3865:VAL:O	1:C:3865:VAL:HG13	2.19	0.42
1:D:364:PRO:O	1:D:365:LYS:HB3	2.19	0.42
1:D:3232:LEU:HD22	1:D:3239:MET:HE3	2.02	0.42
2:H:59:TRP:O	2:H:63:VAL:HG12	2.19	0.42
1:A:667:MET:HG2	1:A:668:VAL:N	2.35	0.41
1:B:3057:PHE:CZ	1:B:3064:VAL:HG11	2.55	0.41
1:B:3346:VAL:O	1:B:3346:VAL:HG22	2.20	0.41
1:B:3969:ILE:HG23	1:B:3977:GLN:CG	2.49	0.41
1:C:2995:ILE:HA	1:C:2998:PHE:CE1	2.55	0.41
1:C:3622:LYS:O	1:C:3623:LEU:C	2.62	0.41
1:C:3986:TRP:CD2	1:C:4043:GLN:NE2	2.87	0.41
1:D:2290:LEU:CD2	1:D:2295:LEU:HD21	2.50	0.41
1:D:3639:THR:O	1:D:3639:THR:HG23	2.20	0.41
1:A:752:VAL:HB	1:A:753:PRO:C	2.46	0.41
1:A:871:ARG:HG2	1:A:922:LEU:HD11	2.02	0.41
1:A:879:HIS:NE2	1:A:913:LEU:HD22	2.34	0.41
1:A:3057:PHE:CZ	1:A:3064:VAL:HG11	2.55	0.41
1:A:4949:GLN:HA	1:A:4949:GLN:OE1	2.20	0.41
1:B:2920:ARG:C	1:B:2920:ARG:HD2	2.46	0.41
1:C:121:LEU:HD13	1:C:134:ASP:HB2	2.02	0.41
1:C:3639:THR:O	1:C:3639:THR:HG23	2.21	0.41
1:C:3969:ILE:HG23	1:C:3977:GLN:CG	2.49	0.41
1:C:4168:GLU:HG2	1:C:4169:SER:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LEU:HD13	1:D:134:ASP:CB	2.51	0.41
1:D:3137:LEU:HD23	1:D:3137:LEU:C	2.45	0.41
1:A:3559:LEU:O	1:A:3559:LEU:HG	2.19	0.41
1:B:667:MET:HG2	1:B:668:VAL:N	2.35	0.41
1:B:871:ARG:HG2	1:B:922:LEU:HD11	2.02	0.41
1:B:2967:MET:SD	1:B:3045:LYS:HG3	2.60	0.41
1:B:2974:ILE:HD13	1:B:3049:LEU:HD11	2.01	0.41
1:C:3232:LEU:HD22	1:C:3239:MET:HE3	2.02	0.41
1:D:364:PRO:O	1:D:365:LYS:CB	2.68	0.41
1:D:780:VAL:HG22	1:D:781:VAL:N	2.35	0.41
1:D:2920:ARG:C	1:D:2920:ARG:HD2	2.45	0.41
1:D:3343:GLN:N	1:D:3344:PRO:CD	2.83	0.41
1:D:4168:GLU:HG2	1:D:4169:SER:N	2.35	0.41
1:B:121:LEU:HD13	1:B:134:ASP:HB2	2.02	0.41
1:B:486:LEU:O	1:B:486:LEU:HD23	2.21	0.41
1:B:2102:VAL:HG21	1:B:2124:LEU:HD13	2.02	0.41
1:B:3137:LEU:HD23	1:B:3137:LEU:C	2.45	0.41
1:B:3343:GLN:N	1:B:3344:PRO:CD	2.83	0.41
1:B:3559:LEU:HG	1:B:3559:LEU:O	2.19	0.41
1:B:4879:MET:SD	1:C:4578:LEU:HA	2.59	0.41
1:B:4949:GLN:OE1	1:B:4949:GLN:HA	2.20	0.41
1:C:1472:VAL:HG22	1:C:1473:THR:N	2.35	0.41
1:D:667:MET:HG2	1:D:668:VAL:N	2.35	0.41
1:D:984:LEU:HD21	1:D:988:LEU:HD12	2.03	0.41
1:D:3346:VAL:HG22	1:D:3346:VAL:O	2.20	0.41
1:A:100:THR:HG22	1:A:101:LEU:H	1.86	0.41
1:A:984:LEU:HD21	1:A:988:LEU:HD12	2.03	0.41
1:A:1243:PRO:HB2	1:A:1600:LEU:HD11	2.02	0.41
1:A:2974:ILE:HD13	1:A:3049:LEU:HD11	2.01	0.41
1:A:3343:GLN:N	1:A:3344:PRO:CD	2.83	0.41
1:A:3468:SER:O	1:A:3472:ALA:HB3	2.21	0.41
1:B:1126:GLY:O	1:B:1142:PRO:HA	2.19	0.41
1:B:3892:CYS:SG	1:B:3899:PHE:HB2	2.61	0.41
1:C:2920:ARG:HD2	1:C:2920:ARG:C	2.45	0.41
1:C:3096:PHE:CE2	1:C:3164:SER:HB2	2.56	0.41
1:D:901:LYS:O	1:D:902:ARG:HD3	2.20	0.41
1:A:121:LEU:HD13	1:A:134:ASP:CB	2.50	0.41
1:A:364:PRO:O	1:A:365:LYS:CB	2.68	0.41
1:A:2102:VAL:HG21	1:A:2124:LEU:HD13	2.02	0.41
1:A:3137:LEU:C	1:A:3137:LEU:HD23	2.45	0.41
1:A:4168:GLU:HG2	1:A:4169:SER:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4580:TYR:HE2	1:D:4856:PHE:CZ	2.38	0.41
1:B:121:LEU:HD13	1:B:134:ASP:CB	2.51	0.41
1:B:737:LEU:HD23	2:F:7:ILE:CG2	2.50	0.41
1:B:3096:PHE:CE2	1:B:3164:SER:HB2	2.56	0.41
1:C:752:VAL:HB	1:C:753:PRO:C	2.45	0.41
1:C:1782:PHE:CD2	2:G:37:ASP:HB3	2.56	0.41
1:C:2562:ILE:HD12	1:C:2562:ILE:H	1.86	0.41
1:C:3892:CYS:SG	1:C:3899:PHE:HB2	2.61	0.41
1:D:1472:VAL:HG22	1:D:1473:THR:N	2.35	0.41
1:D:2722:LYS:O	1:D:2723:ALA:C	2.64	0.41
1:D:2974:ILE:HD13	1:D:3049:LEU:HD11	2.01	0.41
1:A:2225:PHE:N	1:A:2226:PRO:CD	2.84	0.41
1:B:752:VAL:HB	1:B:753:PRO:C	2.45	0.41
1:B:862:VAL:O	1:B:863:LEU:C	2.64	0.41
1:C:19:GLU:HA	1:C:68:THR:HG22	2.02	0.41
1:C:75:VAL:O	1:C:79:GLN:HG2	2.20	0.41
1:C:564:LEU:HD11	1:C:568:LEU:HD11	2.03	0.41
1:C:871:ARG:HG2	1:C:922:LEU:HD11	2.02	0.41
1:C:3057:PHE:CZ	1:C:3064:VAL:HG11	2.55	0.41
1:D:1603:VAL:HG12	1:D:1604:SER:N	2.34	0.41
1:D:2995:ILE:HA	1:D:2998:PHE:CE1	2.55	0.41
1:D:3817:LEU:HB2	1:D:3899:PHE:CZ	2.55	0.41
2:E:59:TRP:O	2:E:63:VAL:HG12	2.19	0.41
1:A:486:LEU:HD23	1:A:486:LEU:O	2.21	0.41
1:A:617:ASN:O	1:A:621:ILE:HG22	2.19	0.41
1:B:2290:LEU:CD2	1:B:2295:LEU:HD21	2.50	0.41
1:D:100:THR:HG22	1:D:101:LEU:H	1.86	0.41
1:D:2669:GLU:HA	1:D:2672:LEU:HD12	2.02	0.41
1:D:3468:SER:O	1:D:3472:ALA:HB3	2.21	0.41
1:A:2562:ILE:HD12	1:A:2562:ILE:H	1.86	0.41
1:A:2669:GLU:HA	1:A:2672:LEU:HD12	2.02	0.41
1:A:2722:LYS:O	1:A:2723:ALA:C	2.64	0.41
1:A:2995:ILE:HA	1:A:2998:PHE:CE1	2.55	0.41
1:A:3163:VAL:HG13	1:A:3164:SER:N	2.36	0.41
1:A:3817:LEU:HB2	1:A:3899:PHE:CZ	2.55	0.41
1:A:3892:CYS:SG	1:A:3899:PHE:HB2	2.61	0.41
1:A:4879:MET:SD	1:B:4578:LEU:HA	2.61	0.41
1:B:364:PRO:O	1:B:365:LYS:CB	2.68	0.41
1:B:492:ASP:O	1:B:496:VAL:HG13	2.21	0.41
1:B:1243:PRO:HB2	1:B:1600:LEU:HD11	2.01	0.41
1:C:321:GLU:OE2	1:C:321:GLU:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:LEU:O	1:C:486:LEU:HD23	2.21	0.41
1:C:844:ARG:CG	1:C:1066:GLN:HG2	2.51	0.41
1:C:901:LYS:C	1:C:902:ARG:HD3	2.46	0.41
1:C:2102:VAL:HG21	1:C:2124:LEU:HD13	2.02	0.41
1:C:3163:VAL:HG13	1:C:3164:SER:N	2.36	0.41
1:C:3343:GLN:N	1:C:3344:PRO:CD	2.83	0.41
1:D:75:VAL:O	1:D:79:GLN:HG2	2.20	0.41
1:D:321:GLU:HA	1:D:321:GLU:OE2	2.21	0.41
1:D:752:VAL:HB	1:D:753:PRO:C	2.46	0.41
1:D:3892:CYS:SG	1:D:3899:PHE:HB2	2.61	0.41
2:F:59:TRP:O	2:F:63:VAL:HG12	2.20	0.41
1:A:564:LEU:HD11	1:A:568:LEU:HD11	2.03	0.41
1:A:780:VAL:HG22	1:A:781:VAL:N	2.36	0.41
1:A:3096:PHE:CE2	1:A:3164:SER:HB2	2.56	0.41
1:B:100:THR:HG22	1:B:101:LEU:H	1.86	0.41
1:B:3468:SER:O	1:B:3472:ALA:HB3	2.21	0.41
1:D:19:GLU:HA	1:D:68:THR:HG22	2.02	0.41
1:D:878:ILE:HD11	1:D:921:ASN:O	2.21	0.41
1:D:2967:MET:SD	1:D:3045:LYS:HG3	2.60	0.41
1:D:3057:PHE:CZ	1:D:3064:VAL:HG11	2.55	0.41
1:A:19:GLU:HA	1:A:68:THR:HG22	2.02	0.40
1:A:2244:ARG:HH11	1:A:2244:ARG:HG3	1.86	0.40
1:A:2920:ARG:HD2	1:A:2920:ARG:C	2.46	0.40
1:B:564:LEU:HD11	1:B:568:LEU:HD11	2.03	0.40
1:B:2225:PHE:N	1:B:2226:PRO:CD	2.84	0.40
1:B:3163:VAL:HG13	1:B:3164:SER:N	2.36	0.40
1:C:121:LEU:HD13	1:C:134:ASP:CB	2.51	0.40
1:C:2225:PHE:N	1:C:2226:PRO:CD	2.84	0.40
1:C:2669:GLU:HA	1:C:2672:LEU:HD12	2.02	0.40
1:C:2722:LYS:O	1:C:2723:ALA:C	2.64	0.40
1:D:564:LEU:HD11	1:D:568:LEU:HD11	2.03	0.40
1:D:657:THR:HB	1:D:1021:LEU:HD21	2.03	0.40
1:D:862:VAL:O	1:D:863:LEU:C	2.64	0.40
1:D:901:LYS:C	1:D:902:ARG:HD3	2.46	0.40
1:A:361:ALA:N	1:A:362:PRO:HD3	2.37	0.40
1:A:666:VAL:HG22	1:A:667:MET:N	2.37	0.40
1:A:862:VAL:O	1:A:863:LEU:C	2.64	0.40
1:A:2290:LEU:CD2	1:A:2295:LEU:HD21	2.50	0.40
1:A:3346:VAL:HG22	1:A:3346:VAL:O	2.20	0.40
1:B:780:VAL:HG22	1:B:781:VAL:N	2.35	0.40
1:B:844:ARG:CG	1:B:1066:GLN:HG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2562:ILE:HD12	1:B:2562:ILE:H	1.86	0.40
1:B:2722:LYS:O	1:B:2723:ALA:C	2.64	0.40
1:C:100:THR:HG22	1:C:101:LEU:H	1.86	0.40
1:C:2244:ARG:HH11	1:C:2244:ARG:HG3	1.87	0.40
1:C:3468:SER:O	1:C:3472:ALA:HB3	2.21	0.40
1:C:4917:ASP:OD1	1:D:4892:ARG:NE	2.54	0.40
1:D:121:LEU:HD13	1:D:134:ASP:HB2	2.02	0.40
1:D:2102:VAL:HG21	1:D:2124:LEU:HD13	2.02	0.40
1:A:121:LEU:HD13	1:A:134:ASP:HB2	2.02	0.40
1:A:844:ARG:CG	1:A:1066:GLN:HG2	2.51	0.40
1:A:1562:ILE:HD12	1:A:1564:PHE:HE1	1.87	0.40
1:A:2967:MET:SD	1:A:3045:LYS:HG3	2.60	0.40
1:A:3416:VAL:HG21	1:A:3517:MET:CE	2.51	0.40
1:A:4214:LYS:HZ2	1:A:4985:LEU:HD21	1.84	0.40
1:D:1562:ILE:HD12	1:D:1564:PHE:HE1	1.87	0.40
1:D:2225:PHE:N	1:D:2226:PRO:CD	2.84	0.40
1:D:2244:ARG:HH11	1:D:2244:ARG:HG3	1.87	0.40
1:D:3096:PHE:CE2	1:D:3164:SER:HB2	2.56	0.40
1:D:3163:VAL:HG13	1:D:3164:SER:N	2.36	0.40
2:G:27:THR:HG22	2:G:28:GLY:N	2.37	0.40
1:A:3639:THR:O	1:A:3639:THR:HG23	2.20	0.40
1:B:486:LEU:HD23	1:B:486:LEU:C	2.46	0.40
1:B:666:VAL:HG22	1:B:667:MET:N	2.36	0.40
1:B:2244:ARG:HH11	1:B:2244:ARG:HG3	1.87	0.40
1:C:492:ASP:O	1:C:496:VAL:HG13	2.21	0.40
1:D:666:VAL:HG22	1:D:667:MET:N	2.36	0.40
2:H:27:THR:HG22	2:H:28:GLY:N	2.37	0.40
1:A:4000:MET:HE1	1:A:4058:ILE:CD1	2.52	0.40
1:A:4993:MET:CE	1:A:4996:ILE:HD12	2.52	0.40
1:B:1562:ILE:HD12	1:B:1564:PHE:HE1	1.87	0.40
1:B:2576:ALA:HB1	1:B:2618:MET:CG	2.52	0.40
1:B:2995:ILE:HA	1:B:2998:PHE:CE1	2.55	0.40
1:B:4031:LEU:HD11	1:B:4044:MET:HE2	2.03	0.40
1:C:984:LEU:HD21	1:C:988:LEU:HD12	2.03	0.40
1:C:1562:ILE:HD12	1:C:1564:PHE:HE1	1.87	0.40
1:C:4000:MET:HE1	1:C:4058:ILE:CD1	2.52	0.40
1:C:4031:LEU:HD11	1:C:4044:MET:HE2	2.03	0.40
1:C:4149:ASN:OD1	1:C:4149:ASN:C	2.65	0.40
1:C:4640:GLU:O	1:C:4643:LEU:HG	2.22	0.40
1:D:844:ARG:CG	1:D:1066:GLN:HG2	2.51	0.40
1:D:1016:ARG:O	1:D:1016:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4376/5037 (87%)	3978 (91%)	390 (9%)	8 (0%)	43	78
1	B	4376/5037 (87%)	3978 (91%)	390 (9%)	8 (0%)	43	78
1	C	4376/5037 (87%)	3979 (91%)	389 (9%)	8 (0%)	43	78
1	D	4376/5037 (87%)	3979 (91%)	389 (9%)	8 (0%)	43	78
2	E	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	G	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
All	All	17924/20580 (87%)	16282 (91%)	1610 (9%)	32 (0%)	44	78

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3300	ALA
1	A	4134	GLU
1	B	3300	ALA
1	B	4134	GLU
1	C	3300	ALA
1	C	4134	GLU
1	D	3300	ALA
1	D	4134	GLU
1	A	3614	LYS
1	B	3614	LYS
1	C	3614	LYS
1	D	3614	LYS
1	A	4052	SER
1	B	4052	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4052	SER
1	D	4052	SER
1	A	902	ARG
1	A	914	PRO
1	B	902	ARG
1	B	914	PRO
1	C	902	ARG
1	C	914	PRO
1	D	902	ARG
1	D	914	PRO
1	A	3623	LEU
1	B	3623	LEU
1	C	3623	LEU
1	D	3623	LEU
1	A	364	PRO
1	B	364	PRO
1	C	364	PRO
1	D	364	PRO

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%)	3827 (100%)	0	100	100
1	B	3827/4276 (90%)	3827 (100%)	0	100	100
1	C	3827/4276 (90%)	3827 (100%)	0	100	100
1	D	3827/4276 (90%)	3827 (100%)	0	100	100
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15664/17464 (90%)	15664 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	156	GLN
1	A	226	HIS
1	A	284	HIS
1	A	383	HIS
1	A	405	HIS
1	A	681	HIS
1	A	736	HIS
1	A	1125	ASN
1	A	1254	HIS
1	A	1298	HIS
1	A	1429	ASN
1	A	1563	GLN
1	A	1953	HIS
1	A	2194	HIS
1	A	2441	HIS
1	A	2584	HIS
1	A	2647	HIS
1	A	2881	ASN
1	A	3456	GLN
1	A	3462	ASN
1	A	3766	GLN
1	A	3895	HIS
1	A	3960	GLN
1	A	4650	HIS
1	A	5015	GLN
1	B	111	HIS
1	B	156	GLN
1	B	226	HIS
1	B	273	HIS
1	B	284	HIS
1	B	405	HIS
1	B	681	HIS
1	B	736	HIS
1	B	1125	ASN
1	B	1254	HIS
1	B	1429	ASN
1	B	1563	GLN
1	B	1571	ASN
1	B	1953	HIS
1	B	2194	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2441	HIS
1	B	2584	HIS
1	B	2647	HIS
1	B	2881	ASN
1	B	3456	GLN
1	B	3462	ASN
1	B	3621	HIS
1	B	3766	GLN
1	B	3895	HIS
1	B	3960	GLN
1	B	3994	HIS
1	B	4009	GLN
1	B	4054	ASN
1	B	4650	HIS
1	B	5015	GLN
1	C	111	HIS
1	C	113	HIS
1	C	156	GLN
1	C	226	HIS
1	C	273	HIS
1	C	284	HIS
1	C	405	HIS
1	C	461	HIS
1	C	681	HIS
1	C	736	HIS
1	C	1125	ASN
1	C	1254	HIS
1	C	1429	ASN
1	C	1563	GLN
1	C	1571	ASN
1	C	1665	HIS
1	C	1683	HIS
1	C	2194	HIS
1	C	2441	HIS
1	C	2584	HIS
1	C	2647	HIS
1	C	2881	ASN
1	C	3456	GLN
1	C	3462	ASN
1	C	3704	HIS
1	C	3766	GLN
1	C	3895	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3960	GLN
1	C	4650	HIS
1	C	5015	GLN
1	D	111	HIS
1	D	156	GLN
1	D	226	HIS
1	D	273	HIS
1	D	284	HIS
1	D	405	HIS
1	D	461	HIS
1	D	681	HIS
1	D	736	HIS
1	D	1125	ASN
1	D	1254	HIS
1	D	1429	ASN
1	D	1563	GLN
1	D	1953	HIS
1	D	2194	HIS
1	D	2441	HIS
1	D	2584	HIS
1	D	2647	HIS
1	D	2881	ASN
1	D	3456	GLN
1	D	3462	ASN
1	D	3766	GLN
1	D	3895	HIS
1	D	3994	HIS
1	D	4054	ASN
1	D	4650	HIS
1	D	5015	GLN
2	E	25	HIS
2	F	25	HIS
2	F	87	HIS
2	G	25	HIS
2	H	25	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

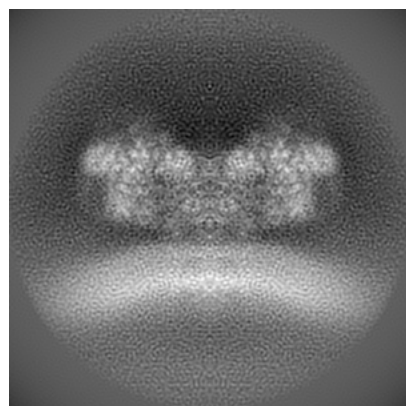
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54616. These allow visual inspection of the internal detail of the map and identification of artifacts.

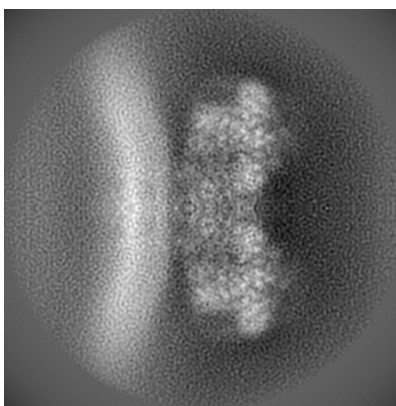
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

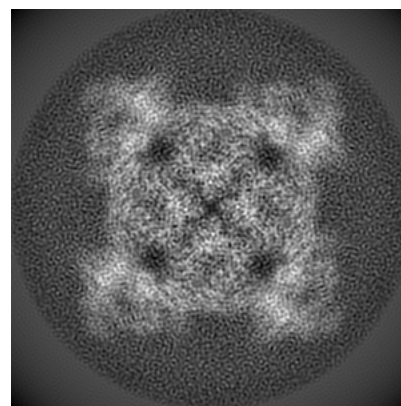
6.1.1 Primary map



X

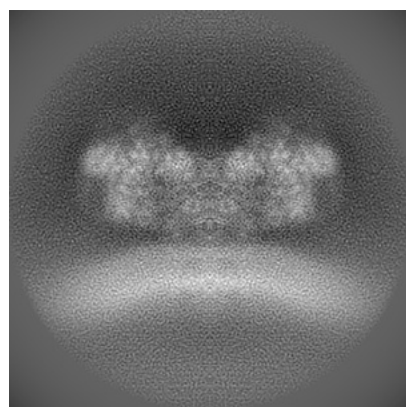


Y

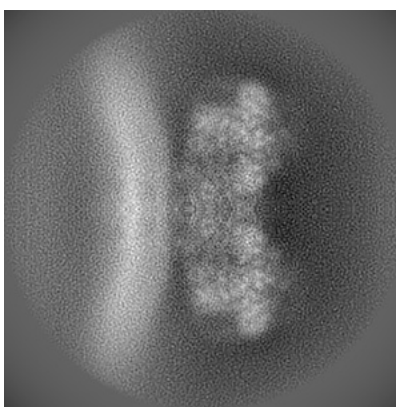


Z

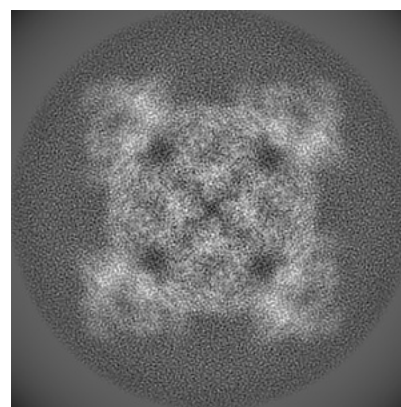
6.1.2 Raw map



X



Y

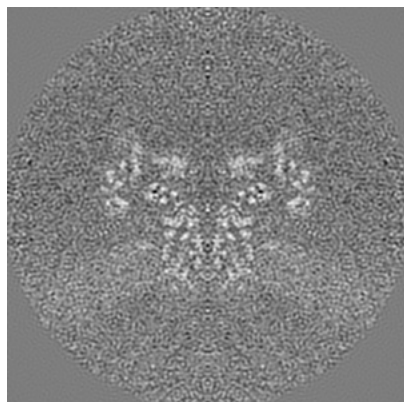


Z

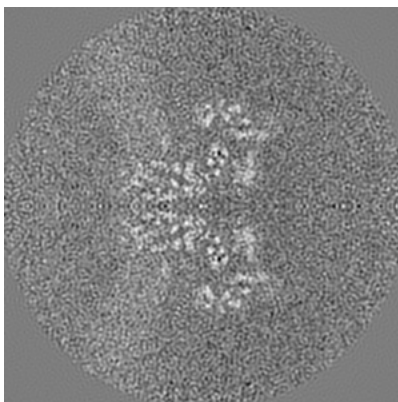
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

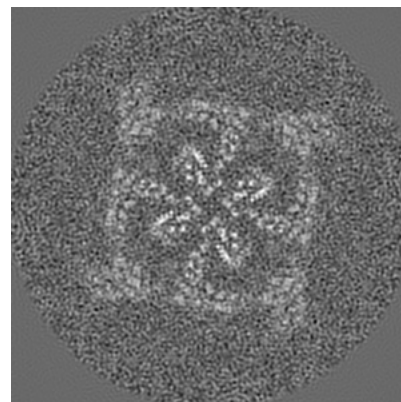
6.2.1 Primary map



X Index: 128

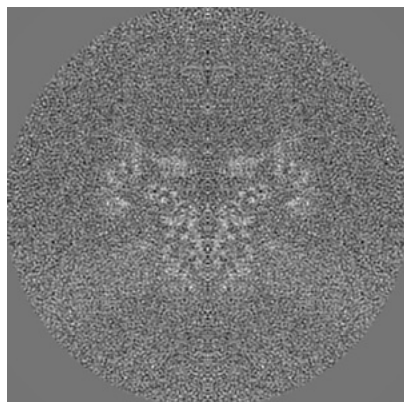


Y Index: 128

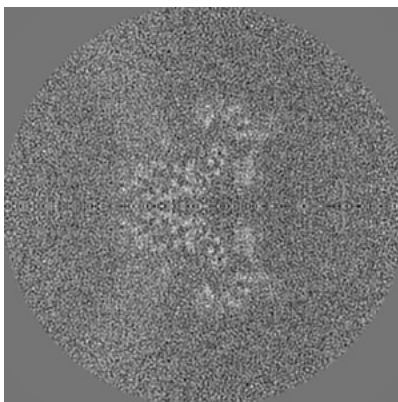


Z Index: 128

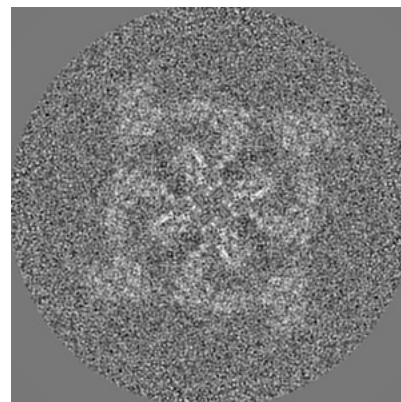
6.2.2 Raw map



X Index: 128



Y Index: 128

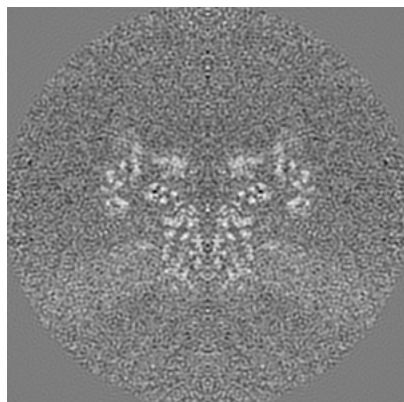


Z Index: 128

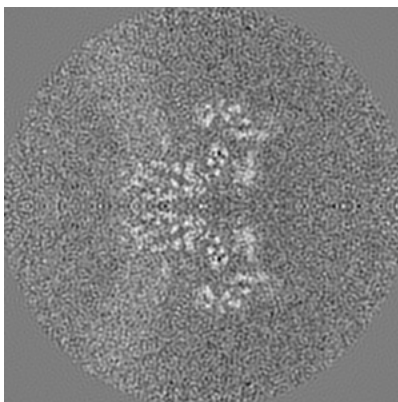
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

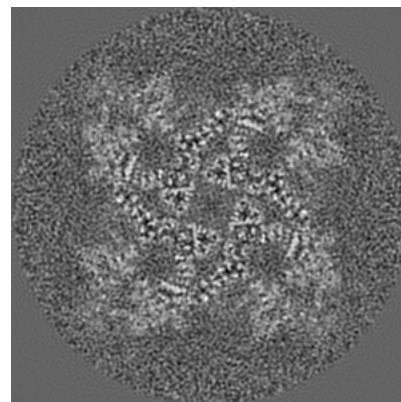
6.3.1 Primary map



X Index: 128

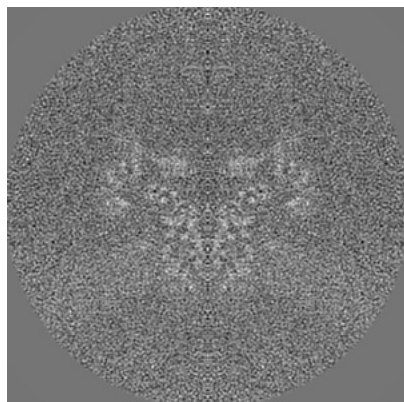


Y Index: 128

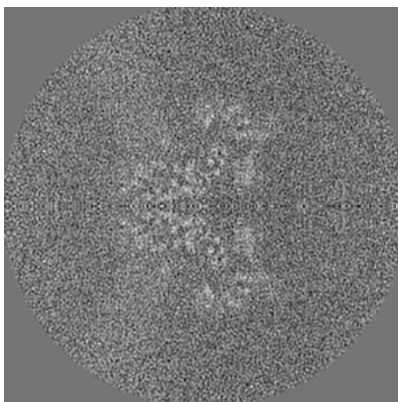


Z Index: 153

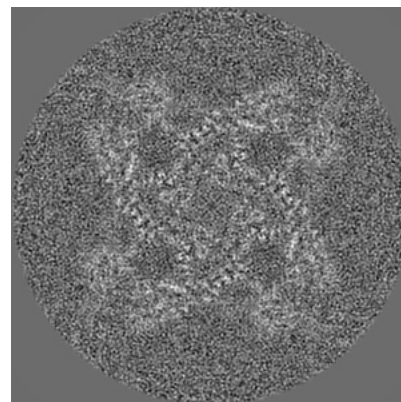
6.3.2 Raw map



X Index: 128



Y Index: 128

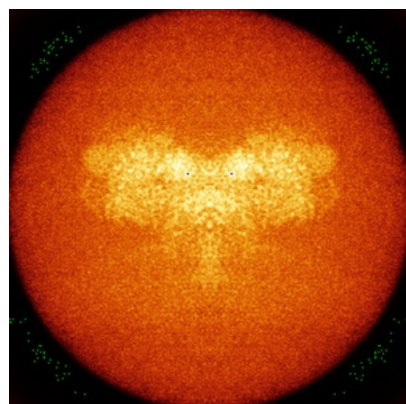


Z Index: 152

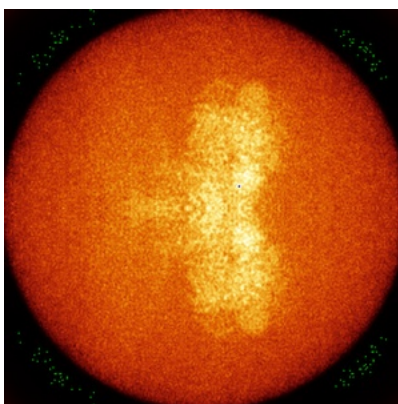
The images above show the largest variance slices of the map in three orthogonal directions.

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

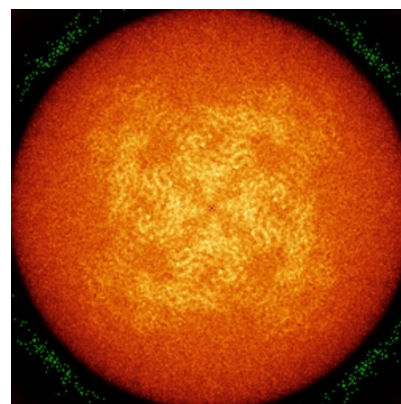
6.4.1 Primary map



X

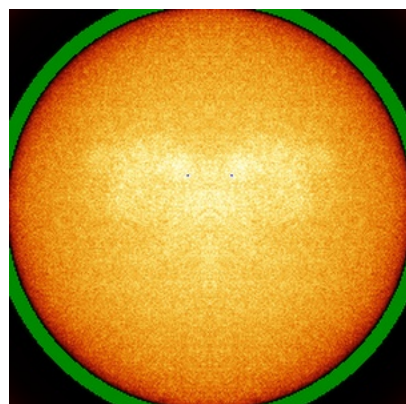


Y

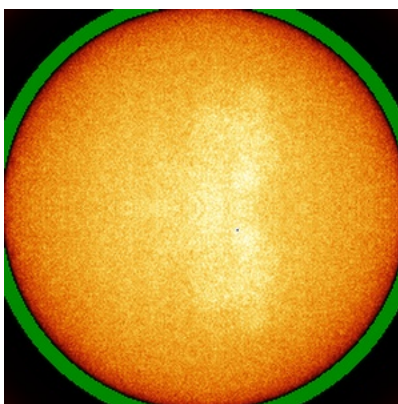


Z

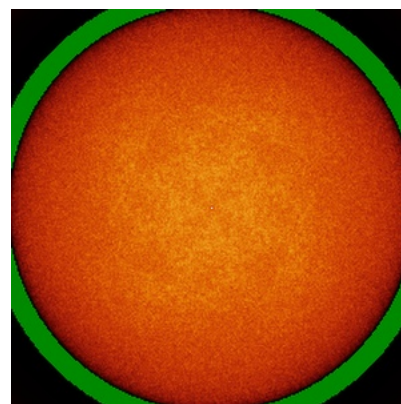
6.4.2 Raw map



X



Y

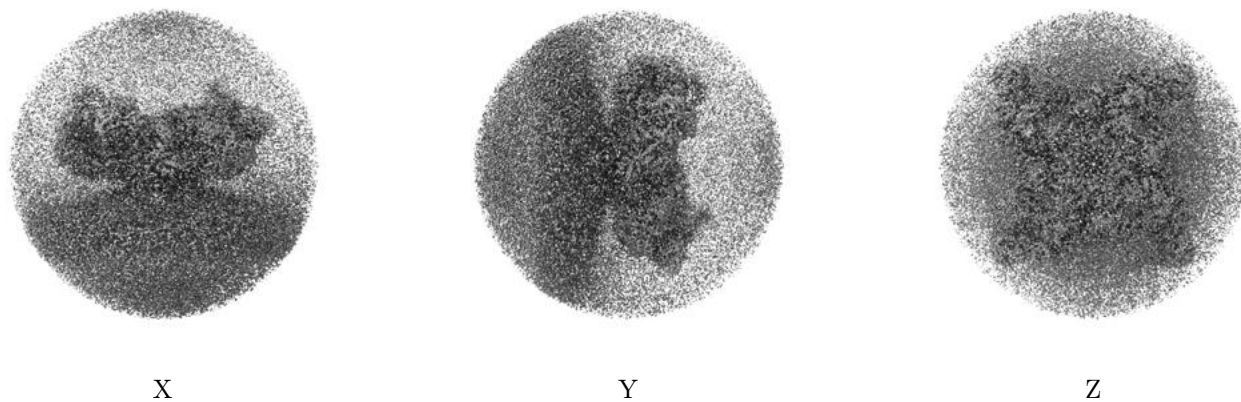


Z

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

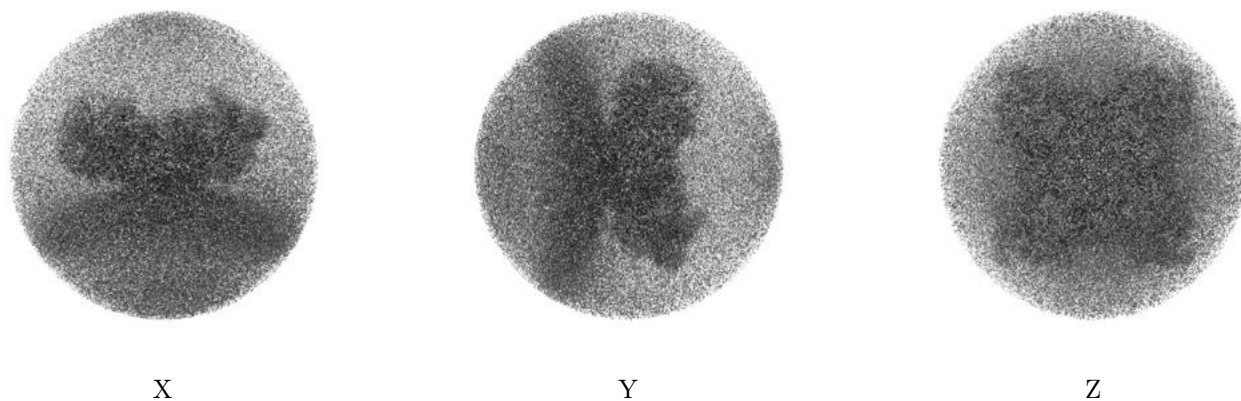
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00458. 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.

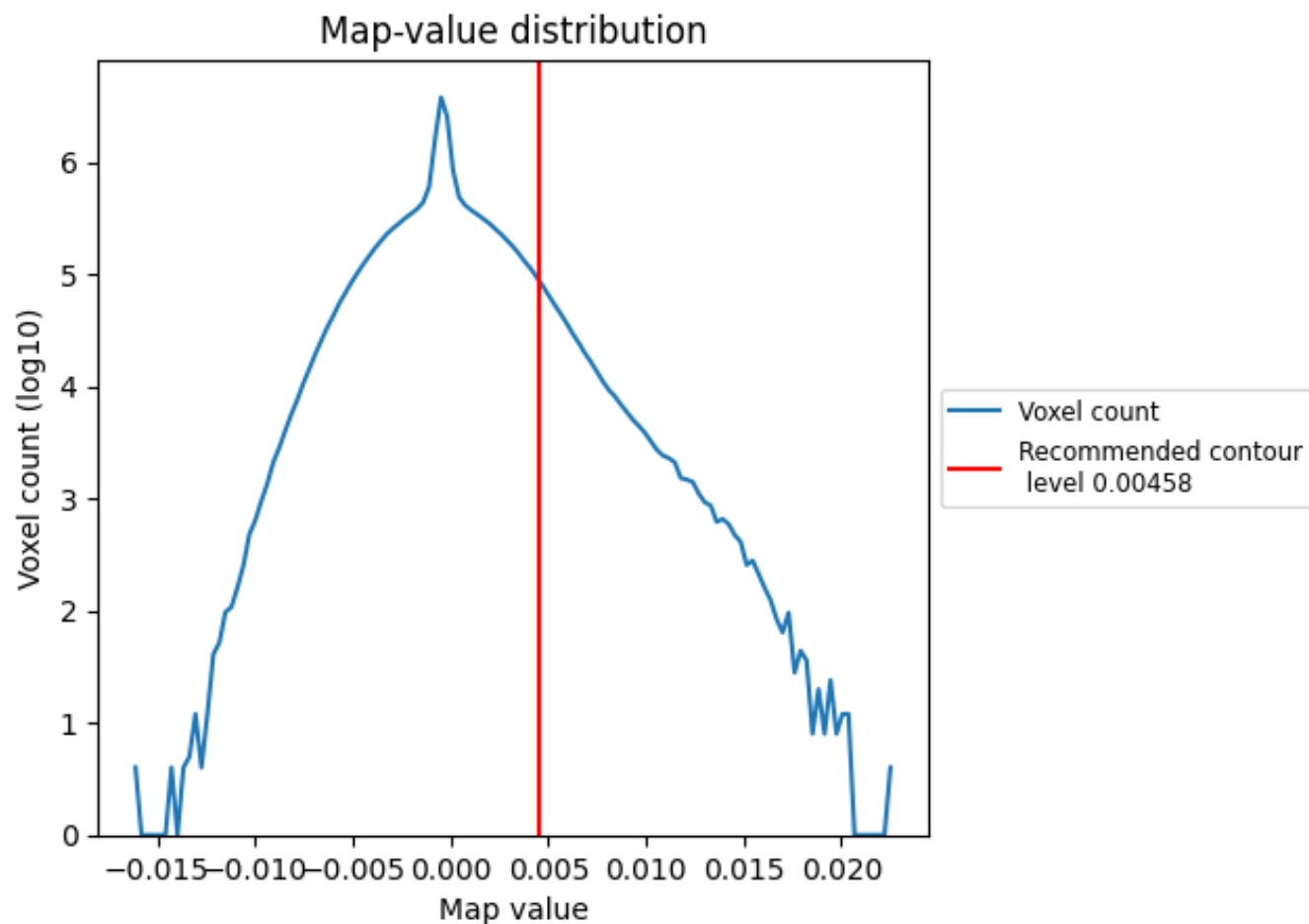
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

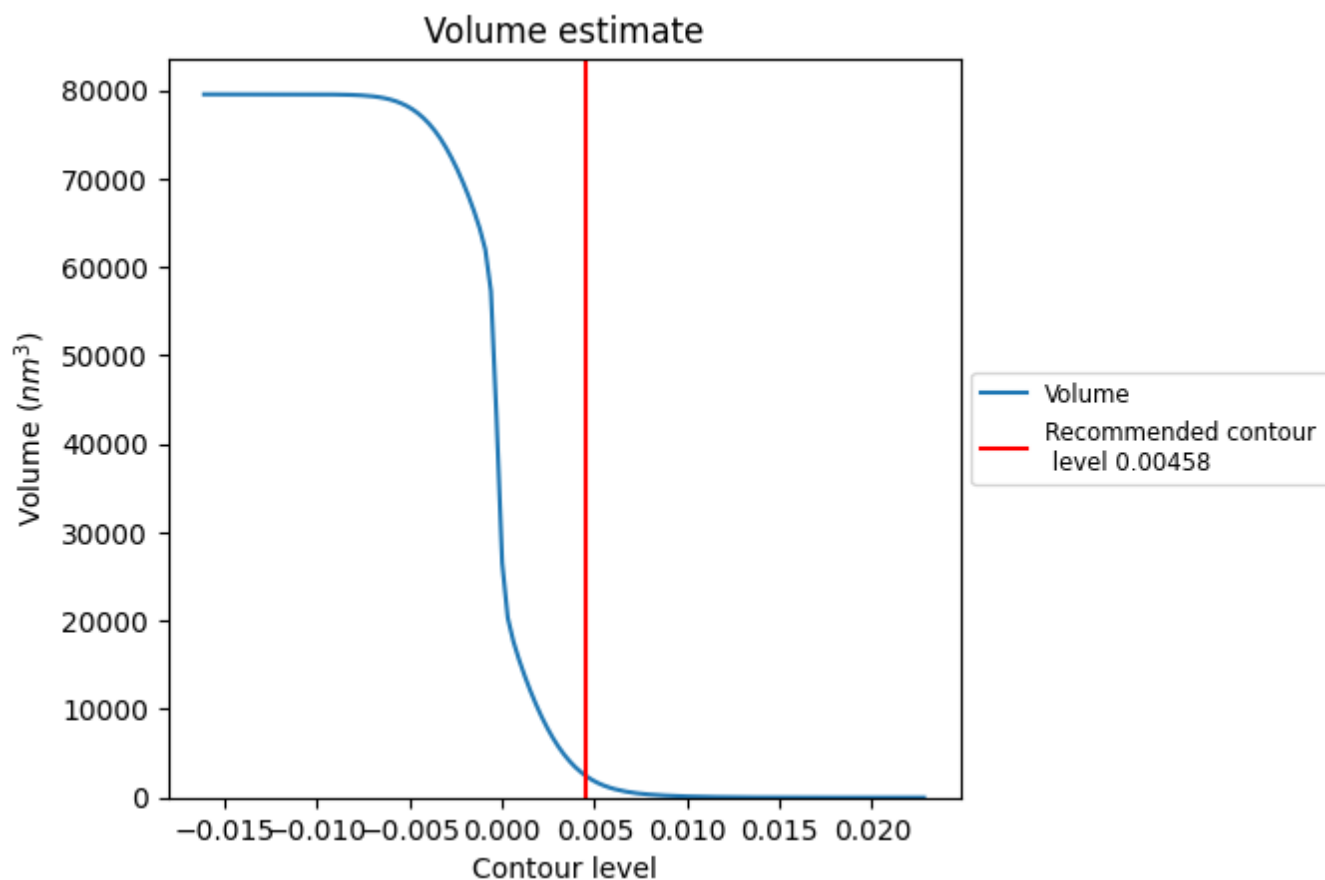
This section contains the results of statistical analysis of the map.

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.

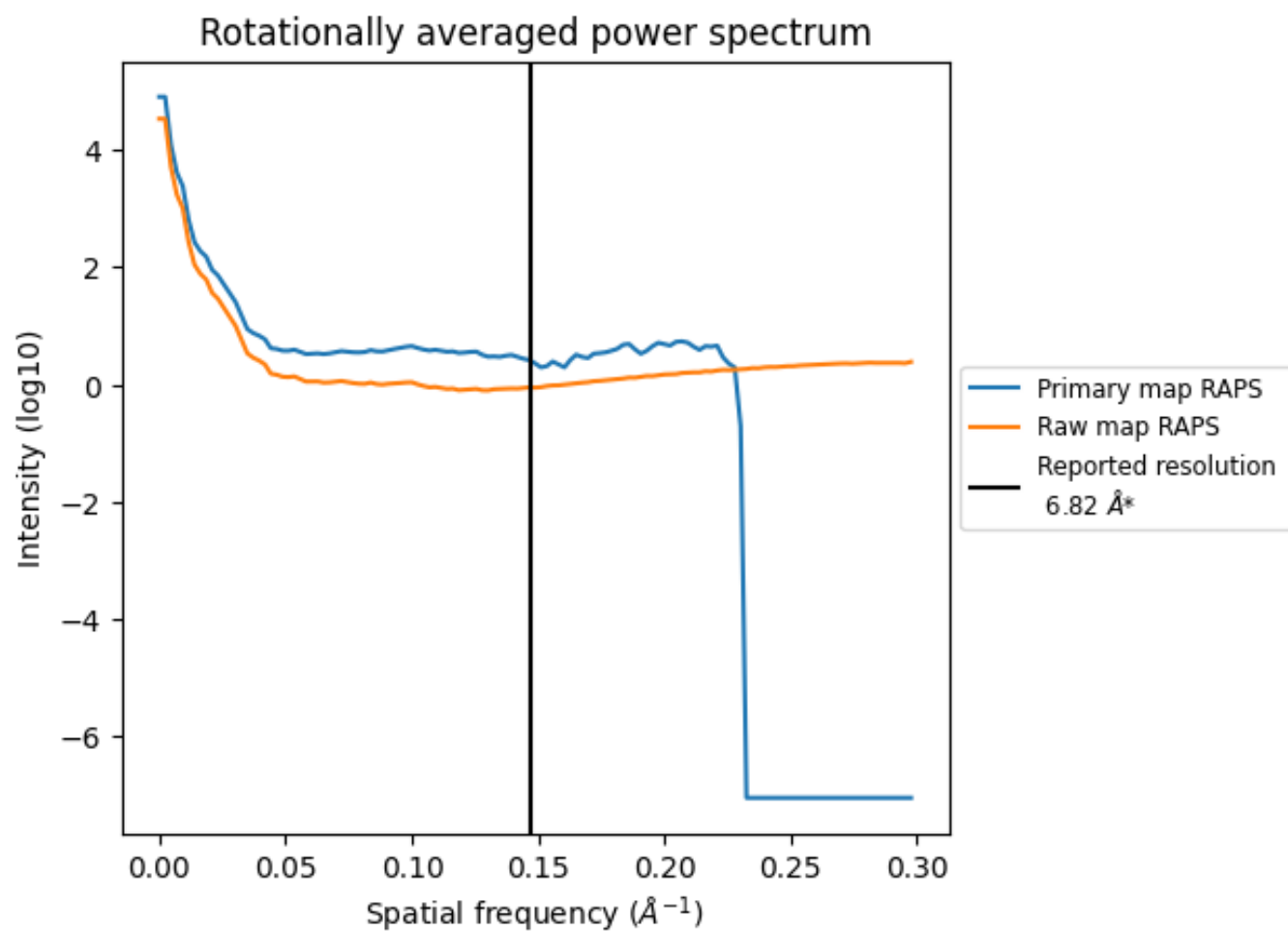
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2387 nm³; this corresponds to an approximate mass of 2156 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 ⓘ

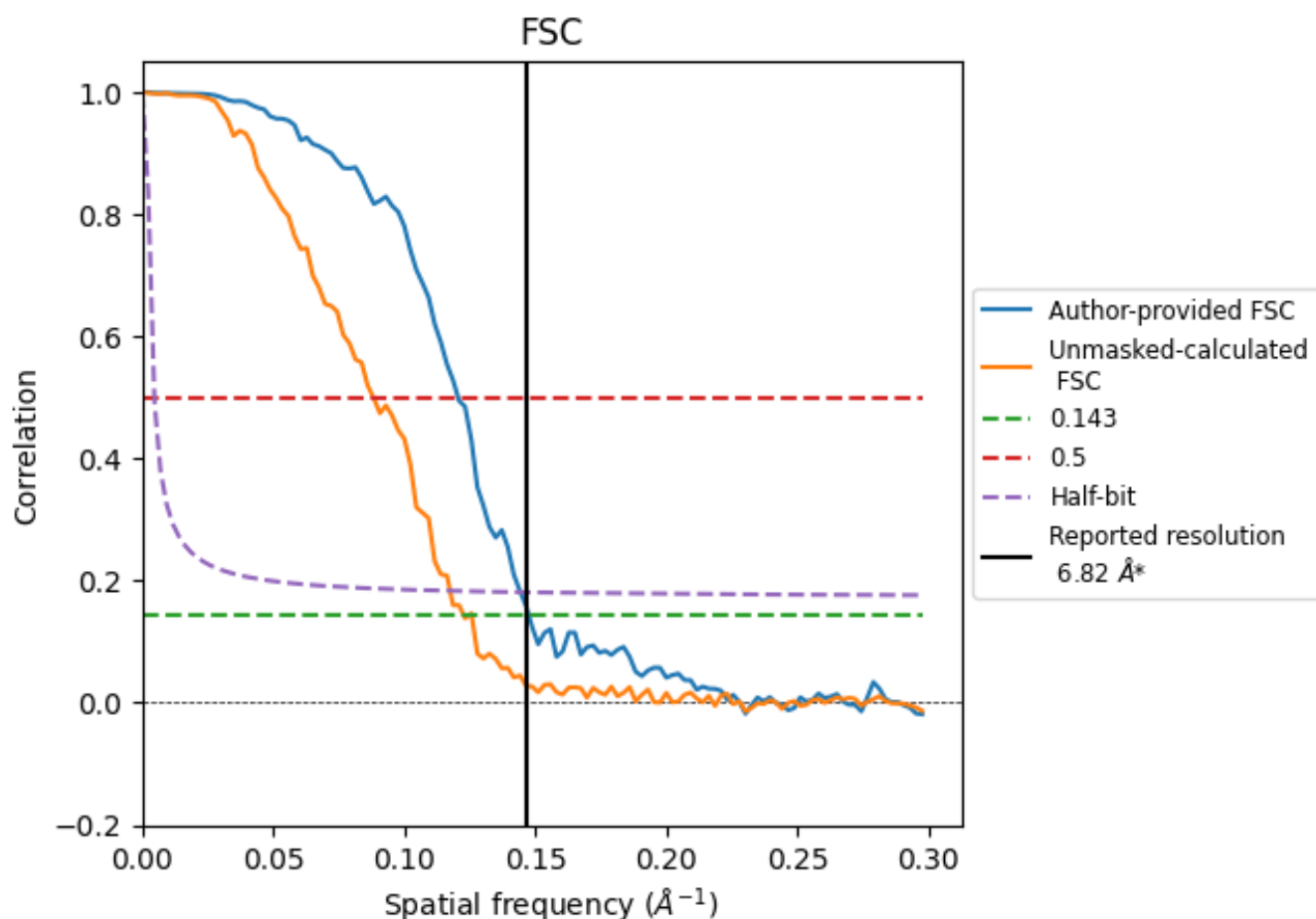


*Reported resolution corresponds to spatial frequency of $0.147 \text{ \AA}^{-1}$

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 0.147 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

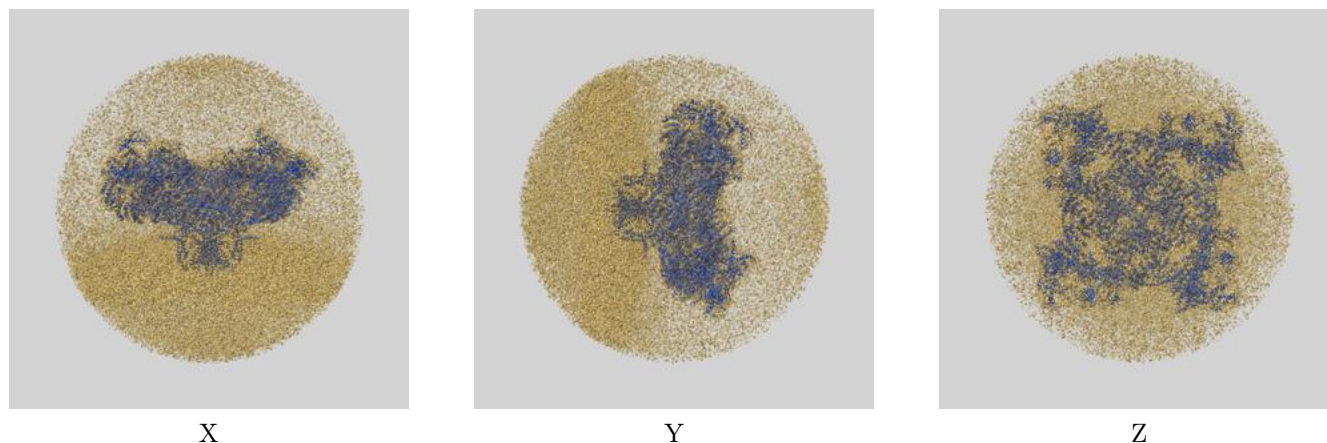
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.82	-	-
Author-provided FSC curve	6.78	8.30	6.93
Unmasked-calculated*	8.15	11.34	8.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.15 differs from the reported value 6.82 by more than 10 %

9 Map-model fit [i](#)

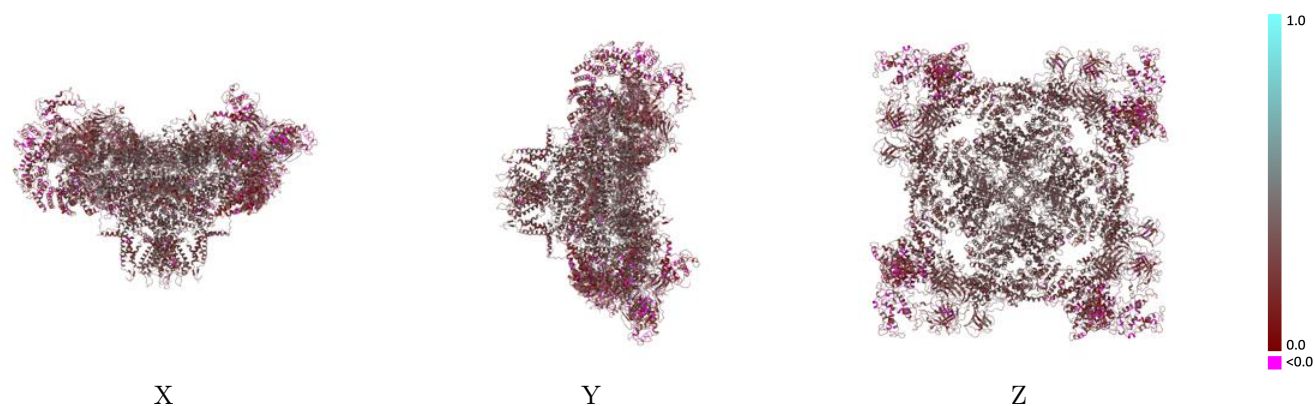
This section contains information regarding the fit between EMDB map EMD-54616 and PDB model 9S5Y. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



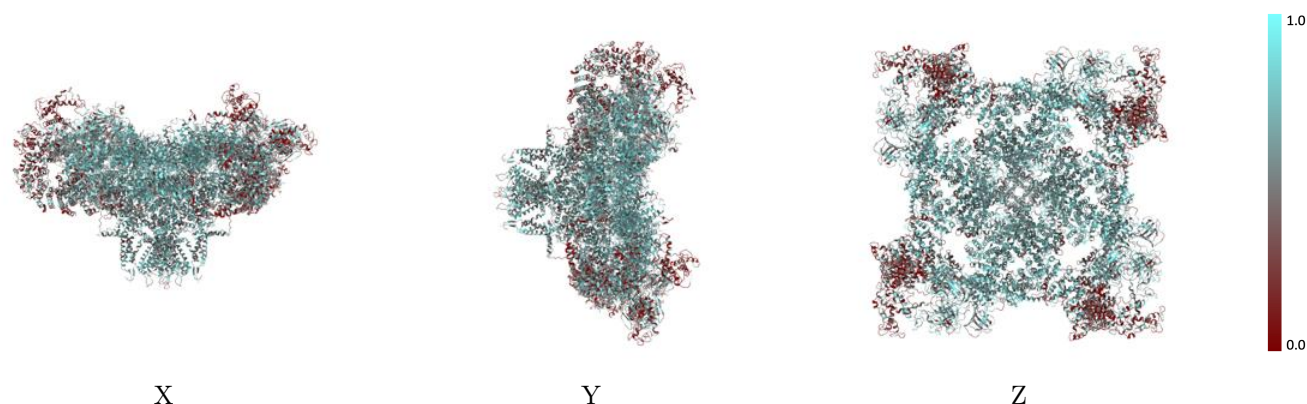
The images above show the 3D surface view of the map at the recommended contour level 0.00458 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



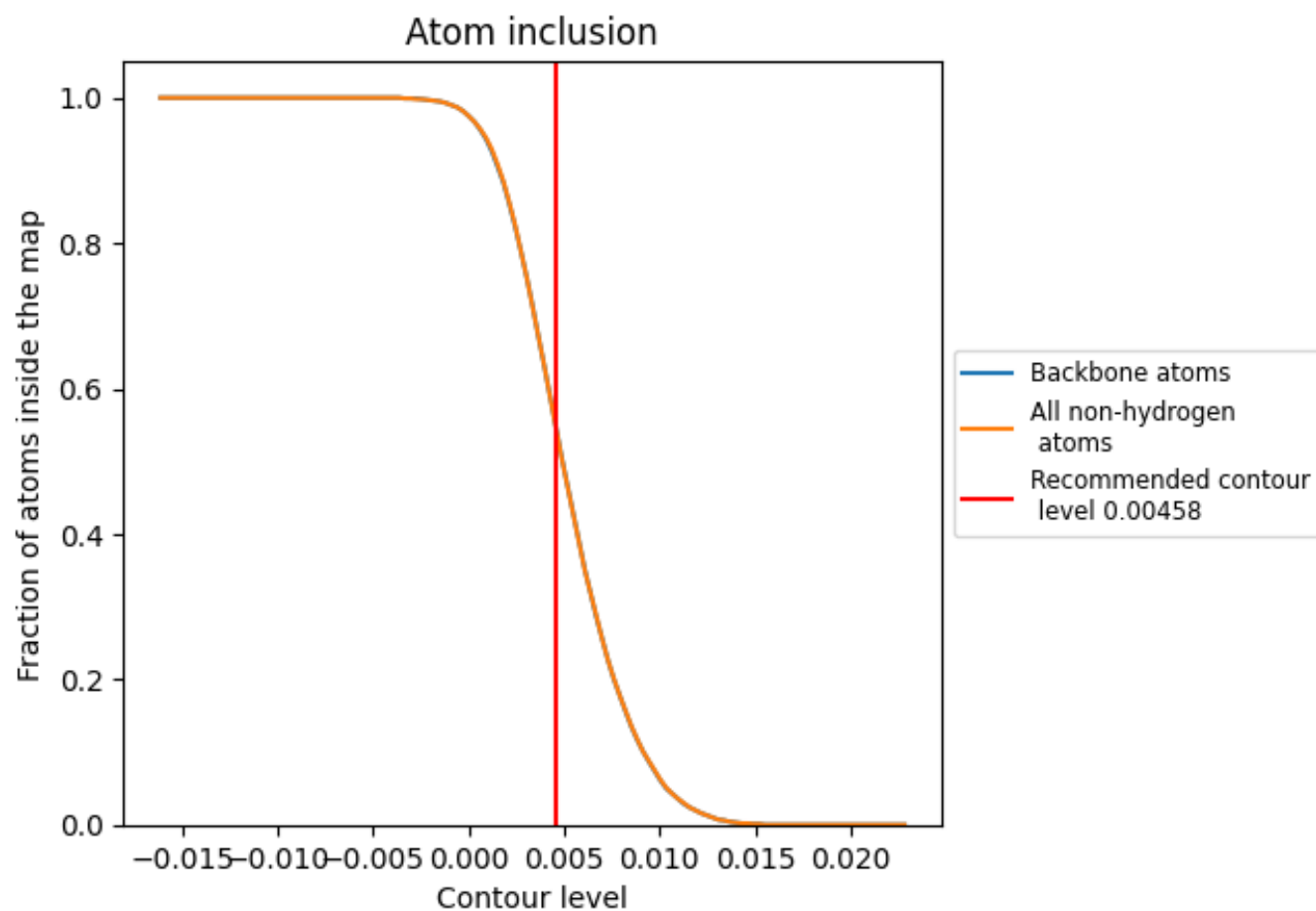
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00458).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (0.00458) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5460	0.2920
A	0.5550	0.2920
B	0.5550	0.2920
C	0.5560	0.2920
D	0.5560	0.2920
E	0.5420	0.3050
F	0.5400	0.3030
G	0.5480	0.3010
H	0.5470	0.2990

1.0

0.0

<0.0