



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:11 AM UTC

PDB ID : 8SET / pdb_00008set
EMDB ID : EMD-40428
Title : Cryo-EM Structure of RyR1 + cAMP
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.42 Å(reported)

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:

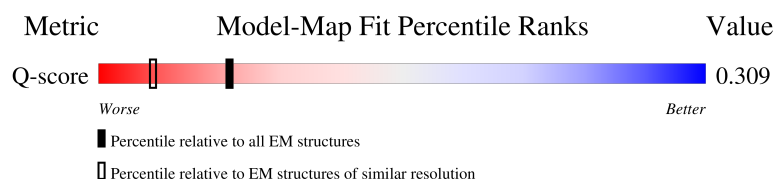
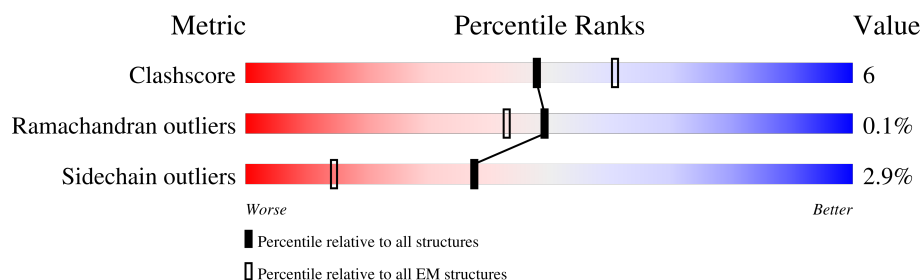
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.42 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	13959 (2.92 - 3.92)

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	17% 71% 15% • 13%
1	B	5037	17% 71% 16% 13%
1	C	5037	17% 71% 15% • 13%
1	D	5037	17% 71% 15% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	350	24%6%69%
2	F	350	24%7%69%
2	G	350	24%7%69%
2	H	350	23%7%69%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 143048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		
1	B	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		
1	C	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		
1	D	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

Continued on next page...

Continued from previous page...

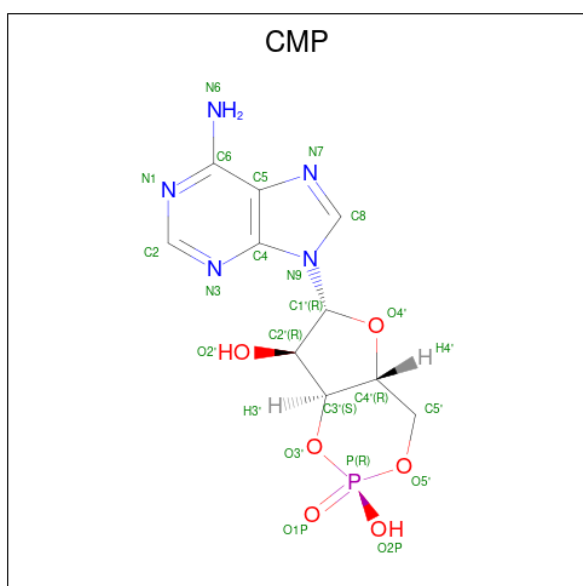
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: $C_{10}H_{12}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	B	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	D	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

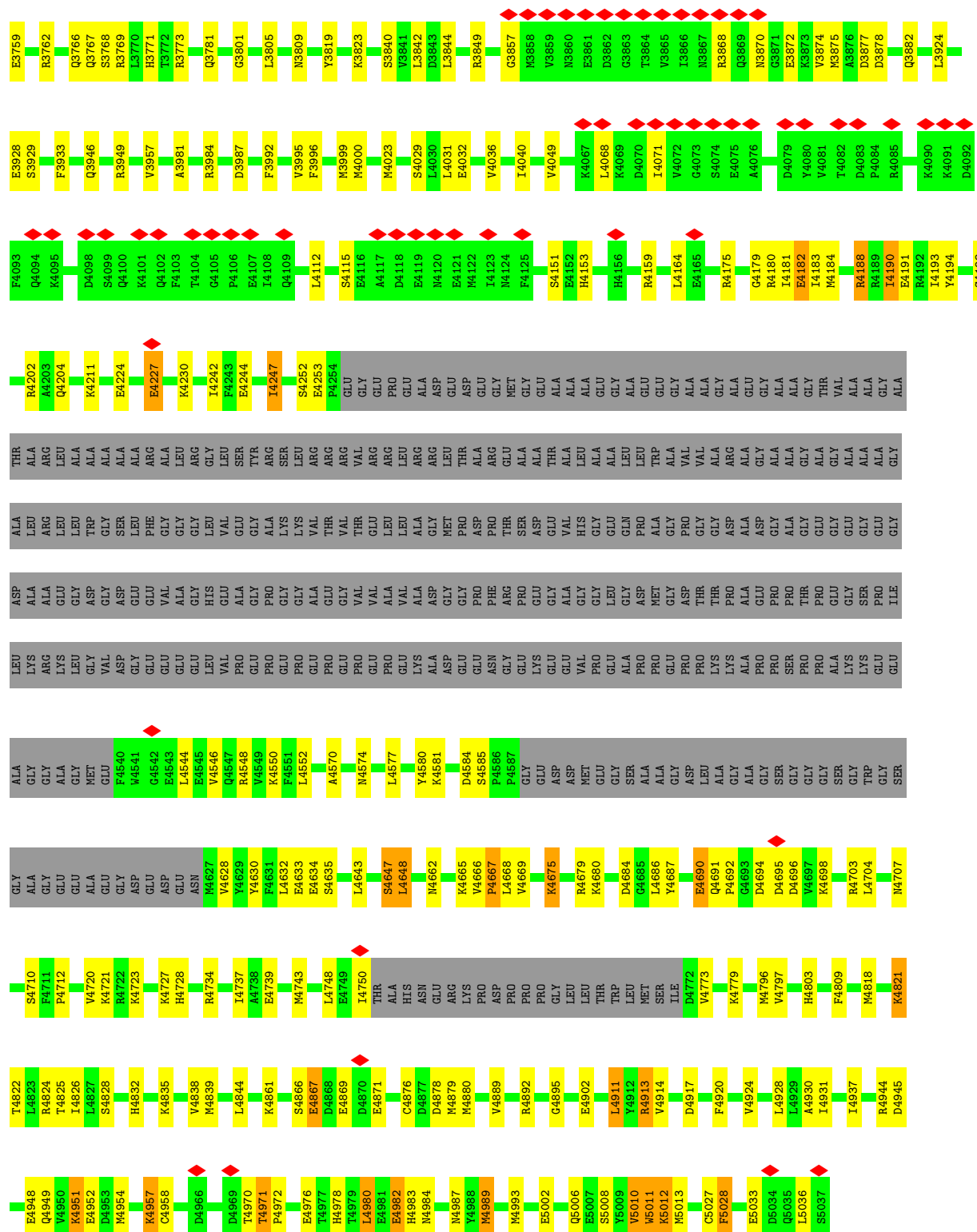
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





L3624	S3625	K3626	Q3627	R3628	R3629	K3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	L3641	L3644	E3655	K3658	A3680	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	D3719	Y3722	E3736	GLU	GLY	GLY	GLU	ASN	GLY	GLU	ALA	GLU	GLU	GLU	V3749	E3750	F3753												
D3546	E3547	E3548	E3551	F3552	N3555	N3556	L3557	H3558	L3559	L3560	G3561	K3562	V3563	E3564	G3565	L3569	M3573	Y3576	L3579	P3580	G3581	R3582	E3583	E3584	V3585	A3586	D3587	D3588	P3589	K3590	K3591	L3592	V3593	R3594	H3605	L3606	E3607	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	H3620	H3621	K3622	L3623								
D3473	S3474	K3475	S3476	K3477	N3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	Q3506	V3511	K3515	R3516	M3517	L3520	N3523	M3524	D3531	M3534	L3535	A3536	K3537	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	T3545								
L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	V3400	R3403	I3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	A3421	H3422	Y3423	L3424	T3425	E3432	F3435	R3436	M3437	V3438	G3439	E3440	I3441	F3442	I3443	Y3444	W3445	S3446	K3447	S3448	N3457	Q3461	N3465	N3466	K3467	S3468	F3469	L3470	T3471	A3472								
A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	S3309	D3310	L3315	L3316	I3322	L3323	N3326	L3327	G3328	L3329	K3332	T3333	K3334	M3335	K3336	R3337	V3340	L3345	V3346	S3347	R3348	E3352	L3353	L3354	H3355	S3356	H3357	F3358	I3359	L3362	R3366	K3371	E3377	Q3378	L3379	R3380												
Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	L3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	K3239	L3243	L3246	D3247	R3248	L3249	M3250	E3258	S3259	E3265	L3277	L3281	W3284	W3285	E3286	R3287	Q3288	P3289	E3290	A3291	P3292	P3293	P3294							
K3123	G3124	N3128	Y3131	T3132	T3133	V3134	A3135	L3136	V3139	F3144	H3146	I3147	A3148	Q3149	H3150	F3152	G3153	D3154	R3155	V3156	L3157	L3158	D3159	Q3162	R3167	T3168	S3171	I3172	Y3173	S3174	T3177	T3178	K3179	T3181	Y3182	V3183	E3184	K3185	L3194	L3197	M3201	F3205	P3208																
K3036	E3037	K3045	R3051	H3052	R3053	V3054	S3055	A3056	F3057	G3058	T3059	P3062	I3065	L3068	L3075	D3076	A3077	R3078	T3079	V3080	K3081	K3082	S3083	G3084	P3085	E3086	L3087	K3088	K3089	R3093	S3094	F3095	S3098	T3103	E3104	K3105	K3106	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL										
D2947	T2948	S2949	S2950	L2960	L2963	L2963	M2967	Q2371	L2974	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	E2993	E2994	F2998	L3002	I3006	N3007	F3010	T3011	F3017	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	N3033	K3034	E3035												
G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	Y2909	D2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	S2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	P2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946
R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	ALA	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	G2880	A2881	Y2882	H2883	N2884	T2885	W2886			
A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	N2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	E2824	K2825	A2826	
H2688	K2689	K2690	Y2691	D2692	L2710	P2711	P2712	D2716	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	K2738	P2739	V2740	E2741	T2742	L2743	K2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	K2756	K2757	A2759	V2761	T2762	H2763	K2765	W2766						



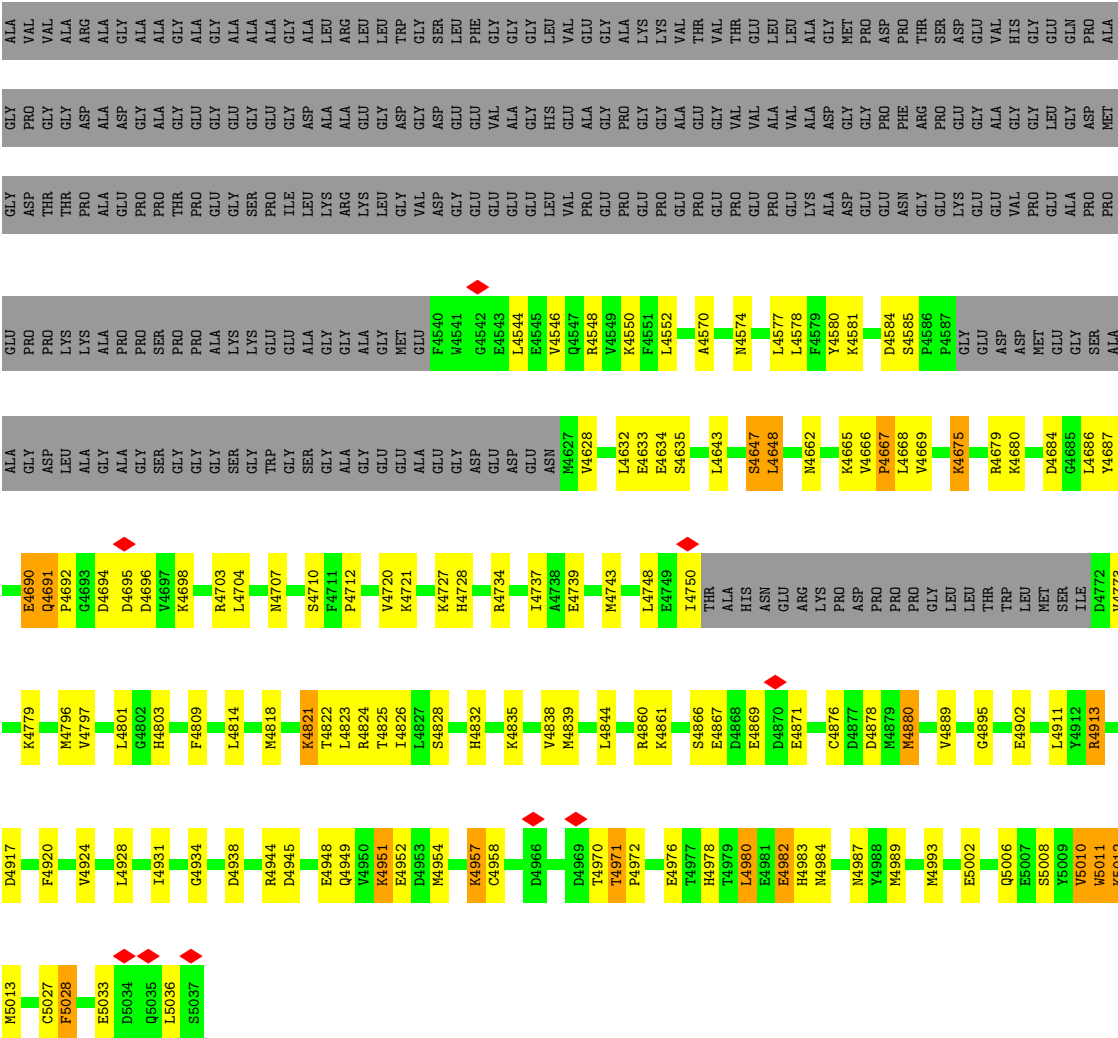
• Molecule 1: Ryanodine receptor 1



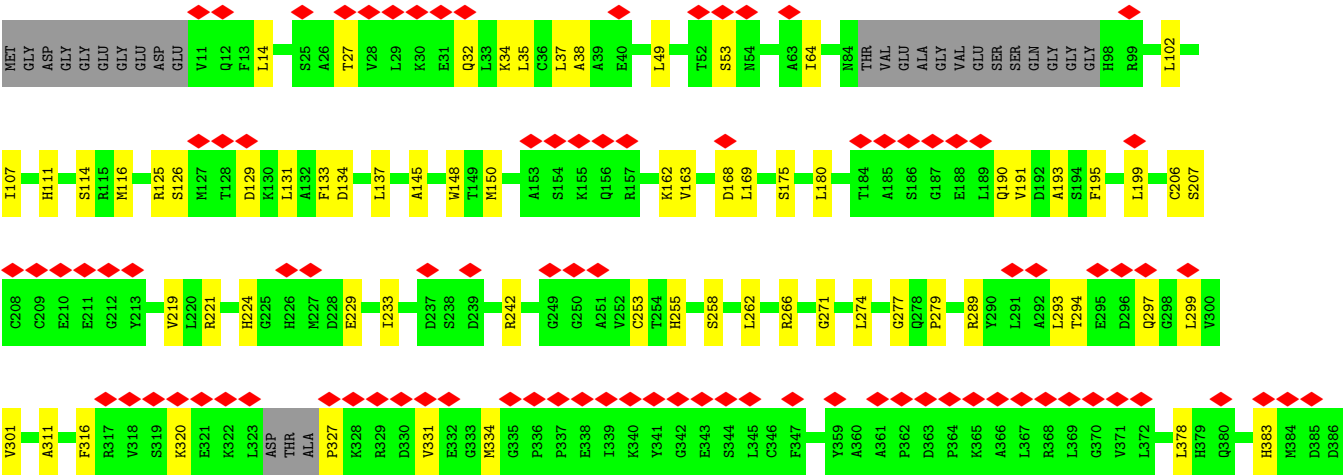


T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	L2947	L2948	S2949	S2950	L2960	L2963	L2967	Q2971	L2974	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	L2991	H2991	E2992	Q2993	E2994	F2998	L3002	N3006	N3007	F3010	T3011	F3017	T3020	F3021	A3022	K3023	V3024	L3025																																																																																																																																																																																																																																																																																																																																																																																																												
L2878	A2879	E2880	N2881	L2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	T2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	M2932	N2933	G2934	Y2935	A2936	V2937																																																																																																																																																																																																																																																																																																																																																																																																			
A2818	N2819	E2820	N2821	T2822	L2823	E2824	K2825	R2826	A2827	E2828	G2829	E2830	GLU	GLY	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	LYS	ASP	PRO	ARG	GLY	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	A2875	E2876	Q2877																																																																																																																																																																																																																																																																																																																																																																																																		
F2758	A2759	E2760	Y2761	L2762	H2763	E2764	K2765	A2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	M2780	V2781	D2782	L2783	E2784	L2785	K2786	H2788	P2789	M2790	L2791	K2792	T2793	Y2794	K2795	L2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	K2806	Q2807	L2808	S2808	R2809	L2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817																																																																																																																																																																																																																																																																																																																																																																																																	
M2546	T2562	T2563	K2564	C2565	A2570	G2571	T2572	E2573	H2574	K2575	A2576	L2577	M2582	L2583	H2584	T2585	R2591	G2592	R2593	S2594	C2611	L2614	R2615	P2616	L2619	R2624	R2625	L2626	V2627	F2628	F2636	P2640	H2647	R2650	Y2655	P2658	T2659	N2663	V2666	T2667	S2668	E2669	E2670	K2757																																																																																																																																																																																																																																																																																																																																																																																																																
E2671	L2672	H2673	L2674	L2678	F2679	W2680	D2684	H2688	K2689	K2690	L2710	P2711	P2712	D2716	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	L2743	T2742	L2744	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	F2753	L2754	I2755	N2756	K2757																																																																																																																																																																																																																																																																																																																																																																																																							
R2415	L2418	I2430	A2437	R2458	V2461	D2464	I2470	S2471	L2474	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	K2489	M2490	F2494	R2508	V2509	Y2510	G2511	L2512	E2513	D2516	F2517	L2518	L2519	H2520	V2521	L2522	D2523	V2524	Q2525	R2531	S2535	T2538	A2539	T2540	F2541	P2410	P2411	E2412	E2413	N2414																																																																																																																																																																																																																																																																																																																																																																																																													
M2312	L2313	L2314	A2315	R2316	G2317	Y2318	P2319	D2320	L2321	R2330	V2354	R2355	L2356	L2357	I2358	F2364	R2369	G2370	E2371	G2372	E2381	E2382	A2383	I2384	R2385	I2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	G2396	ARG	ARG	ARG	ARG	GLY	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	N2414																																																																																																																																																																																																																																																																																																																																																																																																										
C2158	I2162	R2163	S2164	L2165	M2170	Q2173	E2174	E2175	N2176	L2177	M2208	M2211	L2215	G2216	G2217	G2218	F2219	T2220	SER	LEU	K2221	M2228	V2229	R2248	H2253	M2260	I2263	G2264	M2267	V2280	L2286	A2287	L2288	A2289	L2290	V2299	L2302	A2303	G2304	L2307	C2310	P2311																																																																																																																																																																																																																																																																																																																																																																																																																		
D2020	C2021	E2025	R2028	L2046	GLY	GLY	GLU	GLU	GLU	GLU	PRO	GLY	LYS	GLU	THR	SER	SER	SER	ARG	ARG	ARG	VAL	VAL	LEU	LEU	GLU	THR	VAL	ARG	VAL	LYS	LYS	LYS	GLY	GLY	PRO	ALA	GLU	E2088	Q2095	L2098	M2101	D2109	Q2127																																																																																																																																																																																																																																																																																																																																																																																																																
A1784	A1785	L1786	P1787	A1788	L1789	G1790	V1791	A1792	E1793	A1801	R1808	L1815	D1828	P1829	V1830	Q1837	L1842	V1845	L1849	I1853	E1874	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

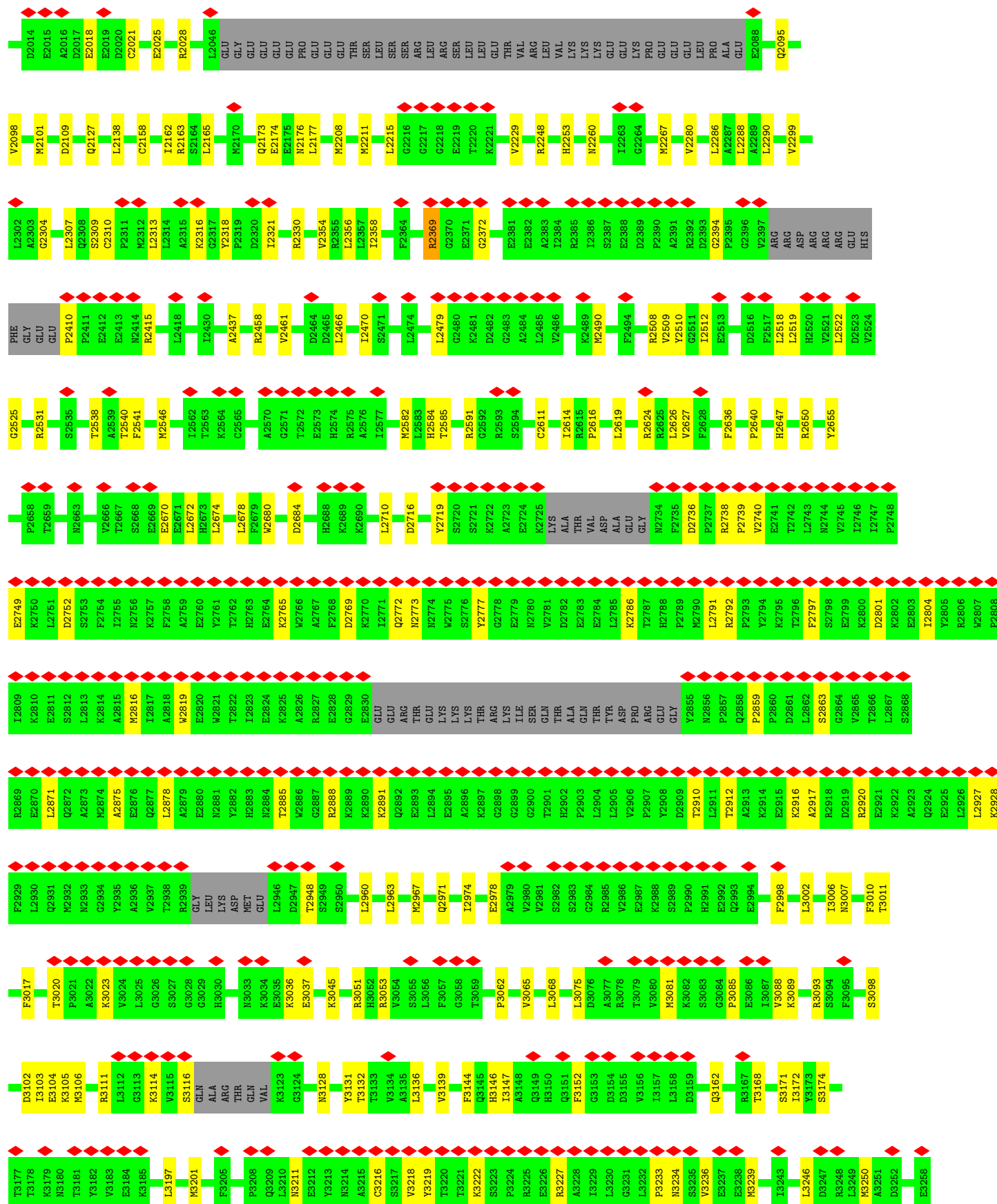
GLY	G4179	G3026	R3111	E3184	L3281	F3358	Q3461	L3536	P3612	GLU	N3870	G4073	G4179	GLY
ALA	R4180	S3027	L3112	K3185	W3284	I3359	N3465	A3536	Y3612	ASN	G3871	S4074	R4180	ALA
ALA	I4181	G3028	G3113	L3197	W3285	I3362	N3466	K3537	K3614	GLY	E3872	E4075	I4181	GLY
ALA	E4182	G3029	K3114	L3197	E3286	R3366	N3467	T3538	S3615	ALA	K3873	E4075	E4182	GLY
GLU	M4184	H3030	V3115	M3201	E3287	R3366	N3467	Y3540	K3616	GLU	V3874	A4076	I4183	ALA
GLY			S3116		G3288		N3468	T3540	K3617	GLU	M3875		M4184	GLY
ALA	R4188	N3033	GLN	F3205	P3289	K3371	F3469	T3540	K3618	GLU	A3876	D4079	R4188	ALA
ALA	R4189	K3034	ALA	P3208	E3290	E3377	F3469	L3542	A3618	GLU	D3877	Y4080	R4189	ALA
THR	I4190	E3035	ARG	Q3209	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4081	R4189	ALA
THR	E4191	K3036	THR	L3210	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4082	R4189	ALA
VAL	R4192	E3037	GLN	N3211	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4083	R4192	VAL
ALA	I4193		VAL	N3211	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4084	R4193	ALA
ALA	Y4194	K3045		N3211	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
GLY	S4198	R3051	G3124	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	GLY
THR	R4202	H3052	N3128	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	THR
ALA	R4202	H3052	N3128	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
ARG	A4203	R3053		E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
LEU	Q4204	V3054	Y3131	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
ALA	K4211	L3056	T3132	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
ALA	E4224	F3057	T3133	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
ALA	E4227	K3058	V3134	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
ARG		T3059	A3135	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
ALA	K4230	P3062	L3136	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
ARG	E4237	V3065	V3139	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
LEU	K4240	L3068	F3144	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
GLY	I4242	L3075	Q3144	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	GLY
LEU	F4243	A3077	H3146	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
SER	E4244	K3078	Q3147	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	SER
TYR	I4247	T3079	A3148	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	TYR
ARG		V3080	Q3149	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
SER	E4252	K3081	Q3150	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	SER
LEU	E4253	R3082	Q3151	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
ARG	P4254	K3083	Q3152	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
ARG	GLU	G3084	Q3153	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
VAL	GLU	P3085	Q3154	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	VAL
ARG	GLU	E3086	Q3155	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
PRO	GLU	I3087	Q3162	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	PRO
ARG	GLU	V3088	Q3167	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
LEU	GLU	K3089	T3168	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
ARG	GLU	K3090	S3171	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
ARG	GLU	G3091	L3172	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ARG
MET	GLY	R3093	Y3173	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	MET
ALA	GLU	S3094	S3174	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
THR	ALA	F3095		E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	THR
ALA	ALA	S3098		E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	ALA
LEU	ALA	D3102	T3177	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
LEU	GLY	T3103	K3179	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
LEU	GLY	E3104	N3180	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
LEU	GLY	K3105	T3181	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	LEU
TRP		M3106	Y3182	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	TRP
			V3183	E3212	A3291	E3377	F3469	L3542	A3618	GLU	D3878	Y4085	R4194	



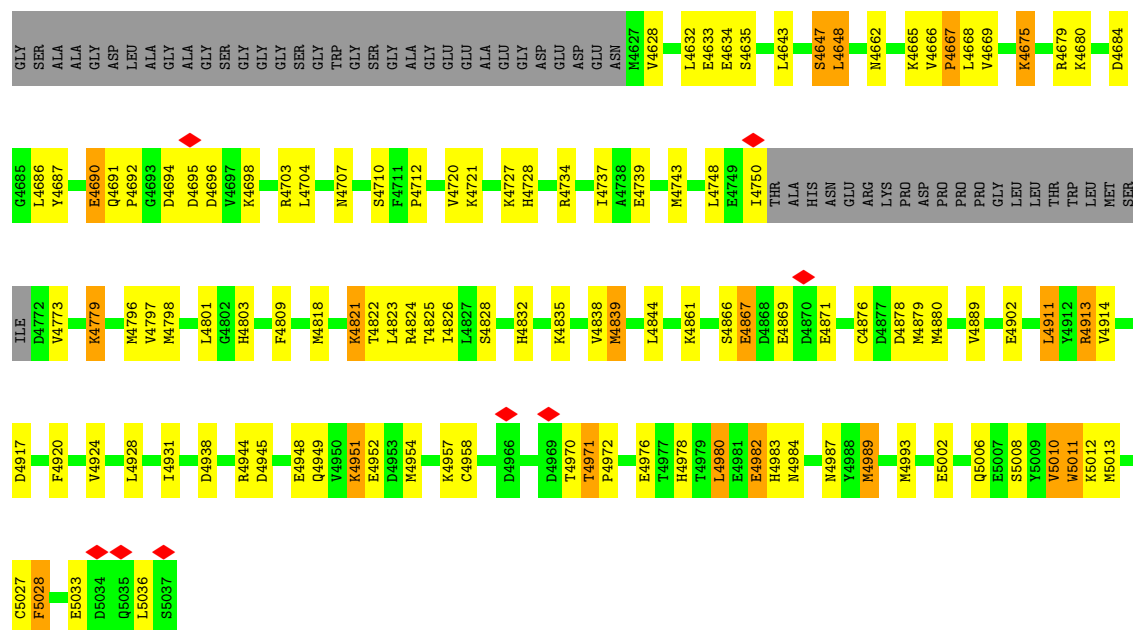
● Molecule 1: Ryanodine receptor 1



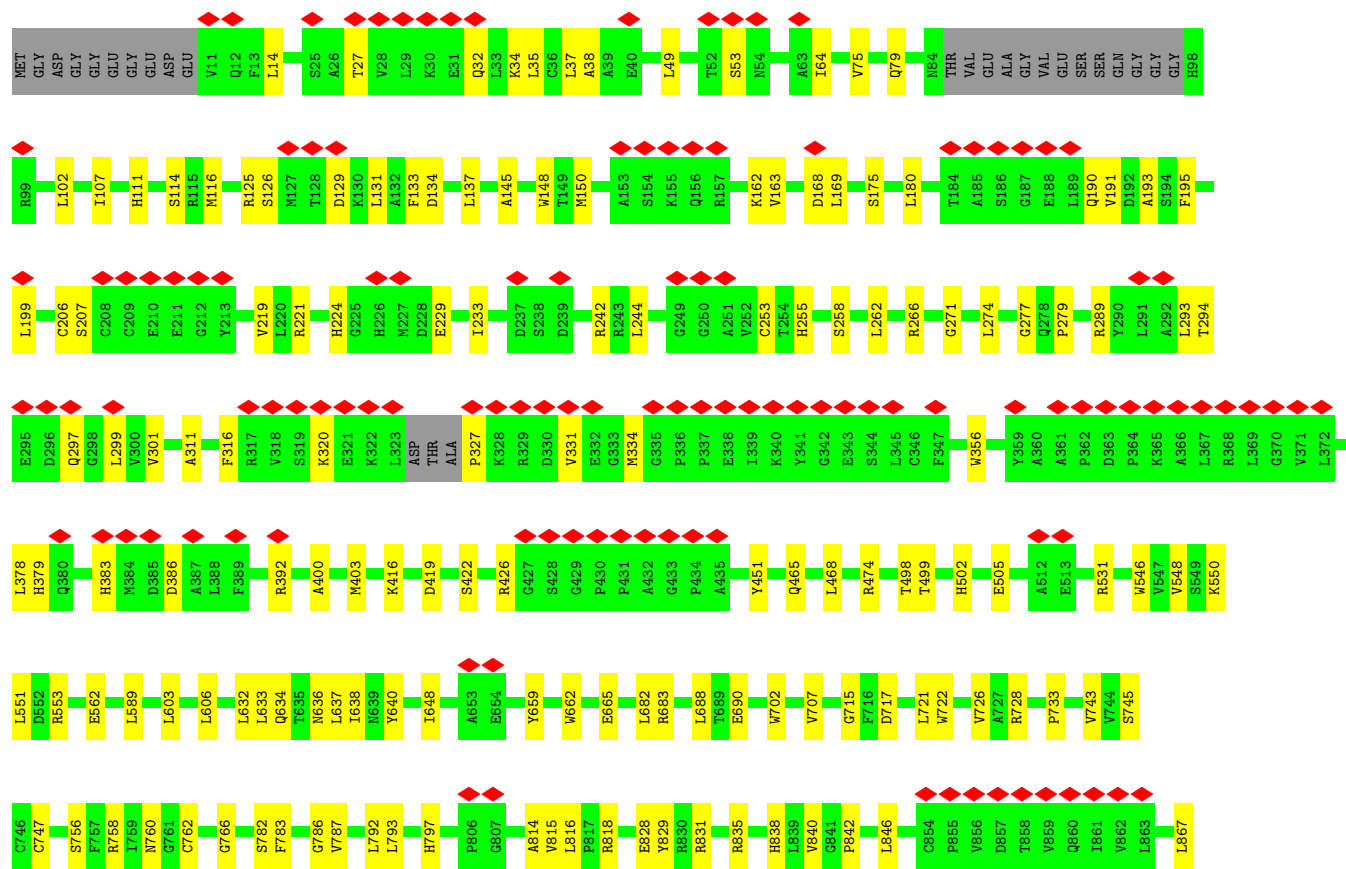




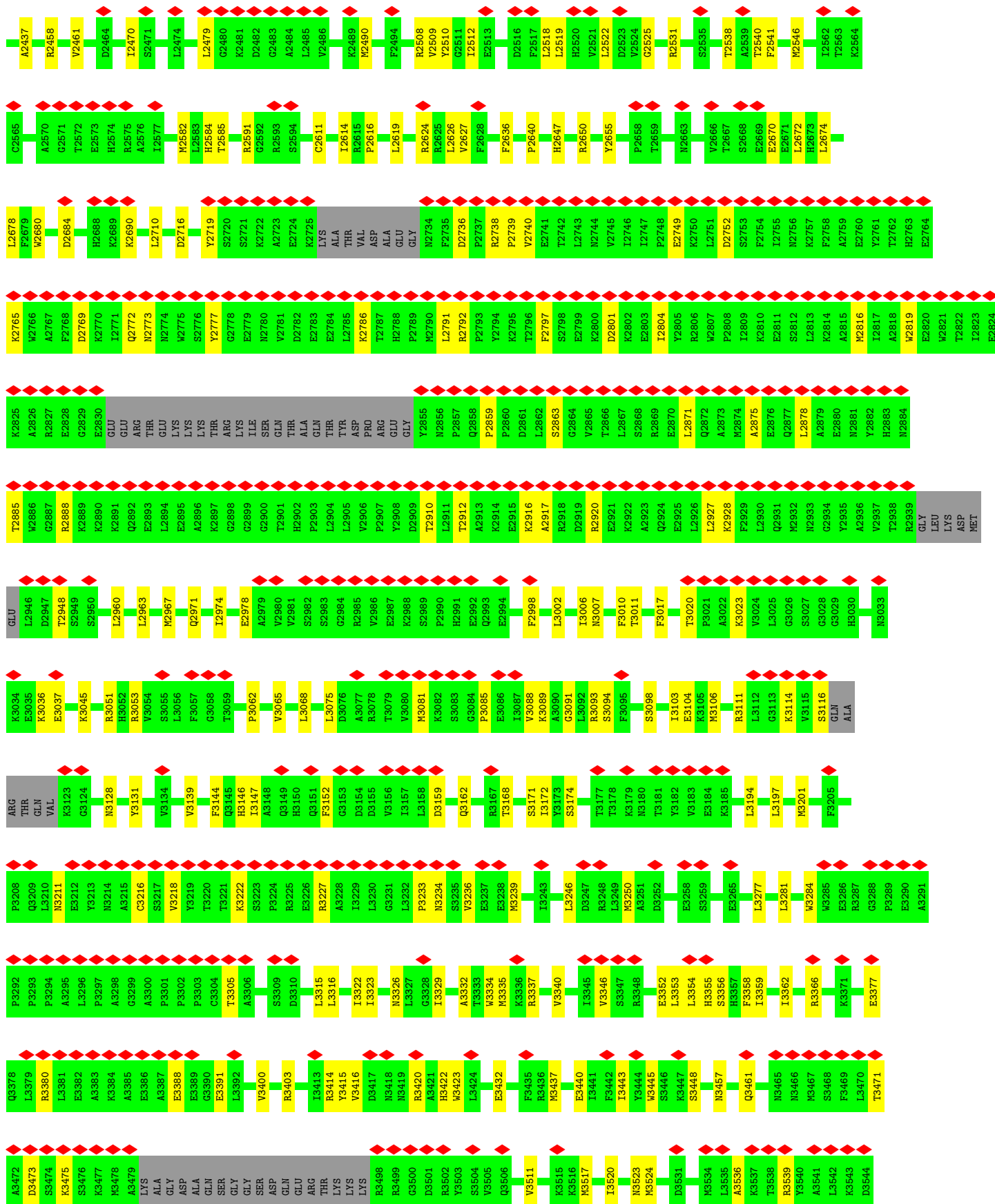
ALA	PRO	PRO	GLY	ASP	GLY	ALA	GLY	LEU	ALA	R4175	S4074	T3864	E3736	E3607	N3523	N3445	E352	S3259	◆
PRO	PRO	GLY	MET	GLY	GLY	ALA	GLY	TRP	GLY	G4179	E4076	V3865	GLU	Q3608	N3524	S3446	L3353	L3353	◆
PRO	PRO	VAL	ASP	PRO	VAL	ALA	GLY	ALA	GLY	R4180	D4079	I3866	GLY	T3609	D3531	S3447	L3354	E3265	◆
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	I4181	V4081	N3867	GLY	H3610	N3534	S3448	H3355	L3277	◆
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	E4182	T4082	Q3868	ASN	P3611	N3535	N3457	H3357	L3281	◆
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	M4184	V4081	Q3869	GLY	Y3613	A3536	Q3461	F3358	L3359	◆
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	R4188	D4082	N3870	ALA	Y3614	N3537	K3371	K3284	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	R4189	D4083	Q3871	GLU	S3615	K3537	N3465	W3285	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	I4190	D4084	E3872	GLU	K3616	T3538	N3466	E3286	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V4191	P4084	V3874	GLU	K3617	R3539	N3467	K3287	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	E4191	R4085	M3875	GLU	A3618	Y3540	S3468	G3288	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	R4192	K4090	A3876	GLU	V3619	A3541	F3469	F3289	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	I4193	K4091	D3877	GLU	W3620	L3542	L3470	E3290	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	D4092	D4092	D3878	GLU	K3621	K3543	T3471	A3291	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	F4093	F4093	Q3882	GLU	H3622	D3544	A3472	P3292	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	Q4094	Q4094	Y3751	GLU	L3623	E3547	D3473	P3293	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	K4095	K4095	E3754	GLU	S3625	E3551	S3474	P3294	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	D4098	D4098	E3755	GLU	K3626	F3552	K3475	L3296	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	Q4100	Q4100	E3759	GLU	Q3627	N3555	S3476	P3297	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	K4101	K4101	R3762	GLU	R3628	N3556	K3477	A3298	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	Q4102	F4103	Q3946	GLU	R3629	N3557	M3478	G3299	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	R3949	T4104	R3949	GLU	H3630	H3558	A3300	A3300	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V3957	C4105	V3957	GLU	A3631	L3559	E3386	G3299	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	A3981	F4106	A3981	GLU	V3632	L3560	A3385	A3298	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	R3984	E4107	R3984	GLU	V3633	G3561	E3386	A3300	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	D3987	I4108	D3987	GLU	A3634	K3562	SER	A3300	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	F3992	Q4109	F3992	GLU	C3635	V3563	GLY	T3305	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V3995	L4112	V3995	GLU	R3636	E3564	ASP	A3306	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	F3996	L4115	F3996	GLU	R3637	G3565	ASP	S3309	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	M3999	E4116	M3999	GLU	M3638	G3565	GLN	D3310	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	M4000	A4117	M4000	GLU	L3641	L3569	GLN	L3315	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	M4023	D4118	M4023	GLU	L3644	K3573	ARG	L3316	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V4036	E4119	V4036	GLU	Y3819	Y3576	THR	L3322	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	M4122	E4121	M4122	GLU	E3655	L3579	LYS	I3323	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V4123	F4125	V4123	GLU	K3658	P3580	R3498	K3326	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	M4124	E4126	M4124	GLU	G3581	R3499	N3418	L3327	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	F4125	E4126	F4125	GLU	R3582	G3500	N3419	G3328	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	E4126	E4127	E4126	GLU	D3583	D3501	A3421	I3329	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V4049	E4127	V4049	GLU	E3584	R3502	W3423	L3329	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	K4067	E4127	K4067	GLU	R3584	R3503	L3424	A3332	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	L4068	R4131	L4068	GLU	D3585	S3504	E3432	T3333	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	K4069	E4131	K4069	GLU	D3586	V3505	F3435	K3334	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	D4070	E4151	D4070	GLU	D3587	R3506	R3436	K3335	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	I4071	E4152	I4071	GLU	D3588	Q3506	K3336	K3336	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	V4072	E4153	V4072	GLU	P3589	V3511	R3337	R3337	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	E4073	H4156	E4073	GLU	E3590	K3515	V3340	V3340	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	C4073	H4156	C4073	GLU	K3591	I3441	I3345	I3345	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	R4159	H4156	R4159	GLU	M3517	F3442	V3346	V3346	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	L4164	H4156	L4164	GLU	I3520	I3443	S3347	S3347	◆	
PRO	PRO	VAL	THR	GLY	ALA	ALA	GLY	VAL	ALA	E4165	H4156	E4165	GLU	L3606	Y3604	R3348	R3348	◆	



• Molecule 1: Ryanodine receptor 1

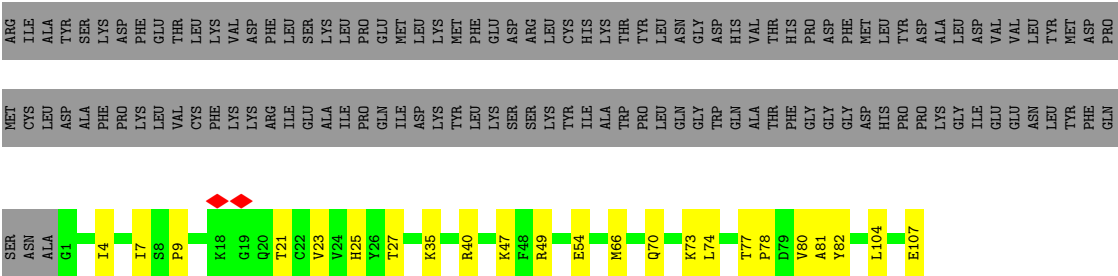




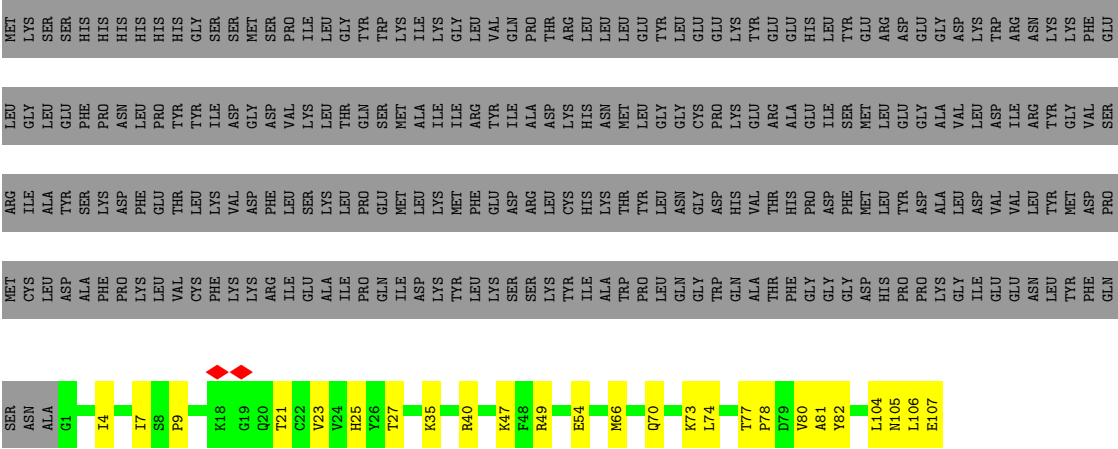








● Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	206618	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.725	Depositor
Minimum map value	-0.299	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.126	Depositor
Map size ($\text{\AA}$)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.288, 1.288, 1.288	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, CMP

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	0.28	1/35738 (0.0%)	0.60	2/48398 (0.0%)
1	B	0.28	1/35738 (0.0%)	0.60	1/48398 (0.0%)
1	C	0.28	1/35738 (0.0%)	0.60	1/48398 (0.0%)
1	D	0.28	1/35738 (0.0%)	0.60	1/48398 (0.0%)
2	E	0.22	0/834	0.54	0/1123
2	F	0.22	0/834	0.53	0/1123
2	G	0.22	0/834	0.53	0/1123
2	H	0.22	0/834	0.54	0/1123
All	All	0.28	4/146288 (0.0%)	0.60	5/198084 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4175	ARG	C-N	5.76	1.39	1.34
1	A	4175	ARG	C-N	5.67	1.39	1.34
1	D	4175	ARG	C-N	5.62	1.39	1.34
1	B	4175	ARG	C-N	5.62	1.39	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5028	PHE	CA-CB-CG	5.76	119.56	113.80
1	D	5028	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	5028	PHE	CA-CB-CG	5.74	119.54	113.80
1	C	5028	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	905	PRO	N-CA-C	5.01	122.80	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34921	0	34546	409	0
1	B	34921	0	34546	419	0
1	C	34921	0	34546	414	0
1	D	34921	0	34546	413	0
2	E	818	0	824	13	0
2	F	818	0	824	14	0
2	G	818	0	824	14	0
2	H	818	0	824	15	0
3	A	22	0	11	2	0
3	B	22	0	11	2	0
3	C	22	0	11	2	0
3	D	22	0	11	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	143048	0	141524	1689	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1689) 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)
3:B:5101:CMP:H2	3:B:5101:CMP:C2	0.97	1.49
3:A:5101:CMP:C2	3:A:5101:CMP:H2	0.97	1.49
3:C:5101:CMP:H2	3:C:5101:CMP:C2	0.97	1.48
3:D:5101:CMP:H2	3:D:5101:CMP:C2	0.97	1.47
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.61	0.74
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.61	0.74
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.61	0.73
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.61	0.73
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.71	0.72
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.71	0.72
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.71	0.71
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.73	0.70
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.73	0.70
1:C:3106:MET:SD	1:C:3128:ASN:ND2	2.66	0.69
1:B:3106:MET:SD	1:B:3128:ASN:ND2	2.66	0.69
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.73	0.69
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.73	0.69
1:D:3106:MET:SD	1:D:3128:ASN:ND2	2.66	0.68
1:B:3634:ALA:O	1:B:3638:MET:HB3	1.94	0.68
1:B:4686:LEU:HA	1:B:4690:GLU:HG3	1.76	0.68
1:A:3634:ALA:O	1:A:3638:MET:HB3	1.94	0.68
1:C:3680:ALA:HB1	1:C:3683:GLN:HE22	1.59	0.68
1:A:3106:MET:SD	1:A:3128:ASN:ND2	2.66	0.67
1:C:4686:LEU:HA	1:C:4690:GLU:HG3	1.76	0.67
1:D:224:HIS:HB3	1:D:229:GLU:HB3	1.77	0.67
1:D:3634:ALA:O	1:D:3638:MET:HB3	1.94	0.67
1:A:4686:LEU:HA	1:A:4690:GLU:HG3	1.76	0.67
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.76	0.67
1:A:224:HIS:HB3	1:A:229:GLU:HB3	1.77	0.67
1:D:3680:ALA:HB1	1:D:3683:GLN:HE22	1.59	0.67
1:C:3420:ARG:HG3	1:C:3520:ILE:HD11	1.77	0.67
1:C:3634:ALA:O	1:C:3638:MET:HB3	1.94	0.67
1:A:3680:ALA:HB1	1:A:3683:GLN:HE22	1.59	0.67
1:C:224:HIS:HB3	1:C:229:GLU:HB3	1.77	0.67
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.78	0.66
1:B:3420:ARG:HG3	1:B:3520:ILE:HD11	1.77	0.66
1:D:4686:LEU:HA	1:D:4690:GLU:HG3	1.76	0.66
1:B:636:ASN:HD21	2:F:35:LYS:HE3	1.60	0.66
1:C:636:ASN:HD21	2:G:35:LYS:HE3	1.60	0.66
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.76	0.66
1:B:224:HIS:HB3	1:B:229:GLU:HB3	1.77	0.66
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.78	0.66
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.76	0.65
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.76	0.65
1:B:3680:ALA:HB1	1:B:3683:GLN:HE22	1.59	0.65
1:D:636:ASN:HD21	2:H:35:LYS:HE3	1.60	0.65
1:D:3420:ARG:HG3	1:D:3520:ILE:HD11	1.77	0.65
1:A:3332:ALA:HB3	1:A:3403:ARG:HD2	1.79	0.65
1:C:3332:ALA:HB3	1:C:3403:ARG:HD2	1.79	0.65
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.78	0.65
1:B:3332:ALA:HB3	1:B:3403:ARG:HD2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:PRO:HA	2:F:70:GLN:HG2	1.79	0.65
1:A:3420:ARG:HG3	1:A:3520:ILE:HD11	1.77	0.65
2:E:9:PRO:HA	2:E:70:GLN:HG2	1.79	0.65
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.78	0.64
1:D:3332:ALA:HB3	1:D:3403:ARG:HD2	1.79	0.64
1:B:688:LEU:HD23	1:B:690:GLU:H	1.63	0.64
1:B:2531:ARG:HH12	1:B:2582:MET:HA	1.63	0.64
1:A:2531:ARG:HH12	1:A:2582:MET:HA	1.63	0.64
2:H:9:PRO:HA	2:H:70:GLN:HG2	1.79	0.64
1:C:2531:ARG:HH12	1:C:2582:MET:HA	1.63	0.64
1:C:688:LEU:HD23	1:C:690:GLU:H	1.63	0.63
1:C:1449:TRP:HB2	1:C:1553:PHE:HB2	1.80	0.63
2:G:9:PRO:HA	2:G:70:GLN:HG2	1.79	0.63
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.80	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.80	0.63
1:B:1449:TRP:HB2	1:B:1553:PHE:HB2	1.80	0.63
1:B:2007:ASN:O	1:B:2011:HIS:HB2	1.99	0.63
1:C:2007:ASN:O	1:C:2011:HIS:HB2	1.99	0.63
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.80	0.63
1:A:2007:ASN:O	1:A:2011:HIS:HB2	1.99	0.63
1:D:2007:ASN:O	1:D:2011:HIS:HB2	1.99	0.63
1:D:688:LEU:HD23	1:D:690:GLU:H	1.63	0.63
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.80	0.63
2:F:25:HIS:HB2	2:F:104:LEU:HD22	1.81	0.63
1:B:219:VAL:O	1:B:392:ARG:NH2	2.32	0.63
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.17	0.63
1:C:219:VAL:O	1:C:392:ARG:NH2	2.32	0.62
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.80	0.62
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.81	0.62
1:A:219:VAL:O	1:A:392:ARG:NH2	2.32	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.17	0.62
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.17	0.62
2:G:25:HIS:HB2	2:G:104:LEU:HD22	1.81	0.62
1:A:688:LEU:HD23	1:A:690:GLU:H	1.62	0.62
1:D:219:VAL:O	1:D:392:ARG:NH2	2.32	0.62
1:D:2531:ARG:HH12	1:D:2582:MET:HA	1.63	0.62
1:A:3103:ILE:HG21	1:A:3168:THR:HG23	1.82	0.62
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.80	0.62
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.80	0.62
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.17	0.62
1:D:3103:ILE:HG21	1:D:3168:THR:HG23	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1449:TRP:HB2	1:A:1553:PHE:HB2	1.80	0.62
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.80	0.62
1:C:835:ARG:NH1	1:C:1093:GLU:OE1	2.33	0.62
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.64	0.62
1:B:3103:ILE:HG21	1:B:3168:THR:HG23	1.82	0.61
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.33	0.61
1:D:835:ARG:NH1	1:D:1093:GLU:OE1	2.33	0.61
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.64	0.61
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.81	0.61
1:A:3416:VAL:HG21	1:A:3517:MET:HE1	1.82	0.61
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.81	0.61
2:E:25:HIS:HB2	2:E:104:LEU:HD22	1.81	0.61
1:A:835:ARG:NH1	1:A:1093:GLU:OE1	2.33	0.61
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.81	0.61
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.82	0.61
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.65	0.61
1:C:3416:VAL:HG21	1:C:3517:MET:HE1	1.83	0.61
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.65	0.61
1:D:1449:TRP:HB2	1:D:1553:PHE:HB2	1.80	0.61
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.33	0.61
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.65	0.61
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.82	0.61
2:H:25:HIS:HB2	2:H:104:LEU:HD22	1.81	0.61
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.82	0.61
1:B:3416:VAL:HG21	1:B:3517:MET:HE1	1.83	0.61
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.83	0.61
1:C:3103:ILE:HG21	1:C:3168:THR:HG23	1.82	0.61
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.33	0.61
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.65	0.61
1:B:835:ARG:NH1	1:B:1093:GLU:OE1	2.33	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.34	0.61
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.64	0.61
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.66	0.61
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.66	0.61
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.34	0.60
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.34	0.60
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.83	0.60
1:D:3416:VAL:HG21	1:D:3517:MET:HE1	1.83	0.60
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.34	0.60
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.33	0.60
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.83	0.60
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.65	0.60
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.84	0.60
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.66	0.60
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.82	0.60
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.83	0.60
1:C:4049:VAL:HG21	1:C:4159:ARG:HE	1.67	0.60
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.84	0.59
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.66	0.59
1:D:4049:VAL:HG21	1:D:4159:ARG:HE	1.67	0.59
1:C:125:ARG:HH22	1:C:190:GLN:HB3	1.67	0.59
1:B:4049:VAL:HG21	1:B:4159:ARG:HE	1.67	0.59
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.84	0.59
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.83	0.59
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.84	0.59
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.85	0.59
1:C:34:LYS:H	1:C:53:SER:HB3	1.68	0.59
1:D:34:LYS:H	1:D:53:SER:HB3	1.68	0.59
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.33	0.59
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.85	0.59
1:D:125:ARG:HH22	1:D:190:GLN:HB3	1.67	0.59
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.83	0.59
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.85	0.59
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.84	0.59
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.33	0.59
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.84	0.59
1:A:125:ARG:HH22	1:A:190:GLN:HB3	1.67	0.59
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.85	0.59
1:A:4049:VAL:HG21	1:A:4159:ARG:HE	1.67	0.59
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.85	0.59
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.85	0.59
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.85	0.59
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.33	0.59
1:D:3162:GLN:NE2	1:D:3216:CYS:SG	2.76	0.59
1:A:34:LYS:H	1:A:53:SER:HB3	1.68	0.58
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.85	0.58
1:B:4920:PHE:O	1:B:4924:VAL:HB	2.03	0.58
1:C:4920:PHE:O	1:C:4924:VAL:HB	2.03	0.58
1:B:125:ARG:HH22	1:B:190:GLN:HB3	1.67	0.58
1:A:3162:GLN:NE2	1:A:3216:CYS:SG	2.76	0.58
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3457:ASN:O	1:B:3461:GLN:NE2	2.37	0.58
1:C:3162:GLN:NE2	1:C:3216:CYS:SG	2.76	0.58
1:D:3457:ASN:O	1:D:3461:GLN:NE2	2.37	0.58
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.86	0.58
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.37	0.58
1:C:3457:ASN:O	1:C:3461:GLN:NE2	2.37	0.58
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.83	0.58
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.86	0.58
1:D:4928:LEU:HD23	1:D:4931:ILE:HD12	1.85	0.58
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.68	0.58
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.85	0.58
1:D:4920:PHE:O	1:D:4924:VAL:HB	2.03	0.58
1:A:3946:GLN:OE1	1:A:3949:ARG:NH2	2.36	0.58
1:B:34:LYS:H	1:B:53:SER:HB3	1.68	0.58
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.84	0.58
1:B:1476:MET:HB2	1:B:1485:SER:HB3	1.86	0.58
1:B:2885:THR:HG22	1:B:2888:ARG:HH12	1.69	0.58
1:C:2885:THR:HG22	1:C:2888:ARG:HH12	1.69	0.58
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.84	0.58
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.85	0.58
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.85	0.58
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.86	0.58
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.36	0.58
1:D:2885:THR:HG22	1:D:2888:ARG:HH12	1.69	0.58
1:A:2885:THR:HG22	1:A:2888:ARG:HH12	1.69	0.57
1:A:4920:PHE:O	1:A:4924:VAL:HB	2.04	0.57
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.37	0.57
1:B:3162:GLN:NE2	1:B:3216:CYS:SG	2.76	0.57
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.37	0.57
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.68	0.57
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.68	0.57
2:G:27:THR:OG1	2:G:40:ARG:NH1	2.37	0.57
1:B:632:LEU:O	1:B:634:GLN:NE2	2.38	0.57
1:C:632:LEU:O	1:C:634:GLN:NE2	2.38	0.57
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.86	0.57
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.36	0.57
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.37	0.57
1:B:4928:LEU:HD23	1:B:4931:ILE:HD12	1.85	0.57
1:D:1476:MET:HB2	1:D:1485:SER:HB3	1.86	0.57
2:F:27:THR:OG1	2:F:40:ARG:NH1	2.37	0.57
1:A:37:LEU:HD21	1:A:191:VAL:HG21	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2490:MET:HE1	1:A:2546:MET:HG2	1.87	0.57
1:B:2765:LYS:NZ	1:B:2859:PRO:O	2.38	0.57
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.68	0.57
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.37	0.57
2:E:27:THR:OG1	2:E:40:ARG:NH1	2.37	0.57
1:C:1476:MET:HB2	1:C:1485:SER:HB3	1.86	0.57
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	1.85	0.57
1:D:3562:LYS:HE3	1:D:3564:GLU:HB2	1.87	0.57
1:A:2765:LYS:NZ	1:A:2859:PRO:O	2.38	0.57
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.87	0.57
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.37	0.57
1:A:3457:ASN:O	1:A:3461:GLN:NE2	2.37	0.57
1:B:37:LEU:HD21	1:B:191:VAL:HG21	1.87	0.57
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.86	0.57
1:B:2670:GLU:HG2	1:B:2912:THR:HA	1.87	0.57
1:B:3562:LYS:HE3	1:B:3564:GLU:HB2	1.87	0.57
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.37	0.57
2:H:27:THR:OG1	2:H:40:ARG:NH1	2.37	0.57
1:B:2490:MET:HE1	1:B:2546:MET:HG2	1.87	0.57
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.37	0.56
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.85	0.56
1:C:3081:MET:HG2	1:C:3089:LYS:HE3	1.87	0.56
1:D:632:LEU:O	1:D:634:GLN:NE2	2.38	0.56
2:E:66:MET:HE1	2:E:74:LEU:HD11	1.86	0.56
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.87	0.56
1:A:636:ASN:HD21	2:E:35:LYS:HE3	1.70	0.56
1:A:1476:MET:HB2	1:A:1485:SER:HB3	1.86	0.56
1:A:2670:GLU:HG2	1:A:2912:THR:HA	1.87	0.56
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.38	0.56
1:B:3081:MET:HG2	1:B:3089:LYS:HE3	1.87	0.56
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.86	0.56
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.86	0.56
1:C:3562:LYS:HE3	1:C:3564:GLU:HB2	1.87	0.56
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.38	0.56
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.38	0.56
1:D:2490:MET:HE1	1:D:2546:MET:HG2	1.87	0.56
1:D:2655:TYR:HB3	1:D:2672:LEU:HD21	1.88	0.56
1:D:3147:ILE:HG23	1:D:3152:PHE:HB2	1.88	0.56
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.87	0.56
2:F:66:MET:HE1	2:F:74:LEU:HD11	1.86	0.56
1:A:35:LEU:HB3	1:A:49:LEU:HD22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.38	0.56
1:A:1291:LEU:HB3	1:A:1595:LEU:HD11	1.88	0.56
1:A:2655:TYR:HB3	1:A:2672:LEU:HD21	1.88	0.56
1:B:882:TRP:O	1:B:886:ARG:NH1	2.39	0.56
1:C:37:LEU:HD21	1:C:191:VAL:HG21	1.87	0.56
1:A:632:LEU:O	1:A:634:GLN:NE2	2.38	0.56
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.86	0.56
1:A:3562:LYS:HE3	1:A:3564:GLU:HB2	1.87	0.56
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.38	0.56
1:A:207:SER:OG	1:A:334:MET:SD	2.64	0.56
1:B:35:LEU:HB3	1:B:49:LEU:HD22	1.87	0.56
1:B:207:SER:OG	1:B:334:MET:SD	2.64	0.56
1:C:882:TRP:O	1:C:886:ARG:NH1	2.39	0.56
1:B:3524:MET:HA	1:B:3582:ARG:HH12	1.71	0.56
1:C:2670:GLU:HG2	1:C:2912:THR:HA	1.87	0.56
1:D:2765:LYS:NZ	1:D:2859:PRO:O	2.38	0.56
2:G:66:MET:HE1	2:G:74:LEU:HD11	1.86	0.56
1:A:882:TRP:O	1:A:886:ARG:NH1	2.39	0.56
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.38	0.56
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.88	0.56
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.39	0.56
1:C:2490:MET:HE1	1:C:2546:MET:HG2	1.87	0.56
1:D:35:LEU:HB3	1:D:49:LEU:HD22	1.87	0.56
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.88	0.56
1:A:3081:MET:HG2	1:A:3089:LYS:HE3	1.87	0.56
1:A:3524:MET:HA	1:A:3582:ARG:HH12	1.71	0.56
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.39	0.56
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.36	0.56
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.24	0.56
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.87	0.56
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.88	0.56
1:D:2670:GLU:HG2	1:D:2912:THR:HA	1.87	0.56
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.88	0.56
1:D:37:LEU:HD21	1:D:191:VAL:HG21	1.87	0.56
2:H:66:MET:HE1	2:H:74:LEU:HD11	1.86	0.56
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.39	0.55
1:A:3147:ILE:HG23	1:A:3152:PHE:HB2	1.88	0.55
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.88	0.55
1:C:3147:ILE:HG23	1:C:3152:PHE:HB2	1.88	0.55
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.23	0.55
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.36	0.55
1:B:1291:LEU:HB3	1:B:1595:LEU:HD11	1.88	0.55
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.24	0.55
1:B:3766:GLN:OE1	1:B:3769:ARG:NH2	2.40	0.55
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.89	0.55
1:C:4976:GLU:O	1:C:4980:LEU:HB2	2.06	0.55
1:D:882:TRP:O	1:D:886:ARG:NH1	2.39	0.55
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.39	0.55
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.88	0.55
1:B:2777:TYR:HB3	1:B:2791:LEU:HD23	1.89	0.55
1:C:207:SER:OG	1:C:334:MET:SD	2.64	0.55
1:C:1291:LEU:HB3	1:C:1595:LEU:HD11	1.88	0.55
1:C:2655:TYR:HB3	1:C:2672:LEU:HD21	1.88	0.55
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.88	0.55
1:D:3081:MET:HG2	1:D:3089:LYS:HE3	1.87	0.55
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.88	0.55
1:D:3524:MET:HA	1:D:3582:ARG:HH12	1.71	0.55
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.40	0.55
1:B:4976:GLU:O	1:B:4980:LEU:HB2	2.06	0.55
1:C:35:LEU:HB3	1:C:49:LEU:HD22	1.87	0.55
1:C:3524:MET:O	1:C:3576:TYR:OH	2.24	0.55
1:D:1579:MET:HE1	1:D:1595:LEU:HD22	1.89	0.55
1:D:3766:GLN:OE1	1:D:3769:ARG:NH2	2.40	0.55
1:A:1579:MET:HE1	1:A:1595:LEU:HD22	1.89	0.55
1:B:27:THR:OG1	1:B:32:GLN:OE1	2.23	0.55
1:B:1579:MET:HE1	1:B:1595:LEU:HD22	1.89	0.55
1:B:3147:ILE:HG23	1:B:3152:PHE:HB2	1.88	0.55
1:C:1579:MET:HE1	1:C:1595:LEU:HD22	1.89	0.55
1:C:2777:TYR:HB3	1:C:2791:LEU:HD23	1.89	0.55
1:A:2777:TYR:HB3	1:A:2791:LEU:HD23	1.89	0.55
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.89	0.55
1:C:2765:LYS:NZ	1:C:2859:PRO:O	2.38	0.55
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.88	0.55
1:D:1291:LEU:HB3	1:D:1595:LEU:HD11	1.88	0.55
1:D:2394:GLY:HA3	1:D:2415:ARG:HH21	1.72	0.55
1:D:2777:TYR:HB3	1:D:2791:LEU:HD23	1.89	0.55
1:D:4976:GLU:O	1:D:4980:LEU:HB2	2.06	0.55
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.88	0.55
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.89	0.55
1:B:4983:HIS:O	3:B:5101:CMP:N6	2.40	0.55
1:C:4151:SER:HB3	1:C:4164:LEU:HD21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4151:SER:HB3	1:D:4164:LEU:HD21	1.88	0.55
1:A:2394:GLY:HA3	1:A:2415:ARG:HH21	1.72	0.55
1:A:4983:HIS:O	3:A:5101:CMP:N6	2.40	0.55
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.33	0.55
1:C:3766:GLN:OE1	1:C:3769:ARG:NH2	2.40	0.55
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.89	0.55
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.40	0.54
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.88	0.54
1:B:1784:ALA:O	2:F:82:TYR:OH	2.26	0.54
1:B:2655:TYR:HB3	1:B:2672:LEU:HD21	1.88	0.54
1:C:3524:MET:HA	1:C:3582:ARG:HH12	1.71	0.54
1:D:207:SER:OG	1:D:334:MET:SD	2.64	0.54
1:D:1089:TYR:HE2	1:D:1211:LEU:HD13	1.72	0.54
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.89	0.54
1:D:3524:MET:O	1:D:3576:TYR:OH	2.24	0.54
1:A:659:TYR:O	1:A:662:TRP:NE1	2.40	0.54
1:A:1089:TYR:HE2	1:A:1211:LEU:HD13	1.72	0.54
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.75	0.54
1:A:3766:GLN:OE1	1:A:3769:ARG:NH2	2.40	0.54
1:B:3445:TRP:HZ3	1:B:3511:VAL:HG13	1.73	0.54
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.89	0.54
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.40	0.54
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.89	0.54
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.90	0.54
1:D:4983:HIS:O	3:D:5101:CMP:N6	2.40	0.54
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.39	0.54
1:A:4913:ARG:NH2	1:D:4888:TYR:OH	2.40	0.54
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.89	0.54
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.88	0.54
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.89	0.54
1:C:3946:GLN:OE1	1:C:3949:ARG:NH2	2.36	0.54
1:A:4976:GLU:O	1:A:4980:LEU:HB2	2.06	0.54
1:B:2394:GLY:HA3	1:B:2415:ARG:HH21	1.72	0.54
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.36	0.54
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.88	0.54
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.40	0.54
1:C:4983:HIS:O	3:C:5101:CMP:N6	2.40	0.54
1:B:3246:LEU:HG	1:B:3250:MET:HE2	1.90	0.54
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.90	0.54
1:C:2519:LEU:HD13	1:C:2522:LEU:HD23	1.90	0.54
1:C:3445:TRP:HZ3	1:C:3511:VAL:HG13	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.41	0.54
1:D:3445:TRP:HZ3	1:D:3511:VAL:HG13	1.73	0.54
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.89	0.54
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.90	0.54
1:C:2394:GLY:HA3	1:C:2415:ARG:HH21	1.72	0.54
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.88	0.54
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.88	0.54
1:C:1089:TYR:HE2	1:C:1211:LEU:HD13	1.72	0.54
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.89	0.54
1:A:2280:VAL:HG11	1:A:2290:LEU:HD12	1.90	0.54
1:A:3984:ARG:NH2	1:A:3987:ASP:OD2	2.41	0.54
1:A:4151:SER:HB3	1:A:4164:LEU:HD21	1.88	0.54
1:C:828:GLU:O	1:C:1073:ARG:NH1	2.40	0.54
1:D:125:ARG:NH1	1:D:126:SER:OG	2.41	0.54
1:D:2280:VAL:HG11	1:D:2290:LEU:HD12	1.90	0.54
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.89	0.54
1:D:3995:VAL:O	1:D:3999:MET:HB2	2.08	0.54
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.41	0.54
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.90	0.54
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.90	0.54
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.90	0.54
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.90	0.54
1:C:3246:LEU:HG	1:C:3250:MET:HE2	1.90	0.54
1:D:27:THR:OG1	1:D:32:GLN:OE1	2.23	0.54
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.90	0.53
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.41	0.53
1:B:659:TYR:O	1:B:662:TRP:NE1	2.40	0.53
1:B:2458:ARG:NH2	1:B:2509:VAL:O	2.41	0.53
1:C:1784:ALA:O	2:G:82:TYR:OH	2.26	0.53
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.88	0.53
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.42	0.53
1:B:4151:SER:HB3	1:B:4164:LEU:HD21	1.88	0.53
1:C:659:TYR:O	1:C:662:TRP:NE1	2.40	0.53
1:D:2458:ARG:NH2	1:D:2509:VAL:O	2.41	0.53
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.08	0.53
1:B:3995:VAL:O	1:B:3999:MET:HB2	2.08	0.53
1:C:125:ARG:NH1	1:C:126:SER:OG	2.41	0.53
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.90	0.53
1:C:2458:ARG:NH2	1:C:2509:VAL:O	2.41	0.53
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.91	0.53
1:D:2519:LEU:HD13	1:D:2522:LEU:HD23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.89	0.53
1:B:1089:TYR:HE2	1:B:1211:LEU:HD13	1.72	0.53
1:B:3524:MET:O	1:B:3576:TYR:OH	2.24	0.53
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.41	0.53
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.91	0.53
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.75	0.53
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.90	0.53
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.90	0.53
1:D:1784:ALA:O	2:H:82:TYR:OH	2.26	0.53
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.39	0.53
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.89	0.53
1:A:3246:LEU:HG	1:A:3250:MET:HE2	1.90	0.53
1:A:4630:TYR:OH	1:B:4860:ARG:NH1	2.38	0.53
1:B:2519:LEU:HD13	1:B:2522:LEU:HD23	1.90	0.53
1:B:3984:ARG:NH2	1:B:3987:ASP:OD2	2.41	0.53
1:C:27:THR:OG1	1:C:32:GLN:OE1	2.23	0.53
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.90	0.53
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.90	0.53
1:A:2458:ARG:NH2	1:A:2509:VAL:O	2.41	0.53
1:B:2280:VAL:HG11	1:B:2290:LEU:HD12	1.90	0.53
1:D:659:TYR:O	1:D:662:TRP:NE1	2.40	0.53
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.40	0.53
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.24	0.53
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.42	0.53
1:C:111:HIS:ND1	1:C:114:SER:OG	2.37	0.53
1:C:3995:VAL:O	1:C:3999:MET:HB2	2.08	0.53
1:D:3984:ARG:NH2	1:D:3987:ASP:OD2	2.41	0.53
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.53
1:B:277:GLY:N	1:B:316:PHE:O	2.39	0.53
1:B:3111:ARG:NH2	1:B:3174:SER:OG	2.42	0.53
1:C:2267:MET:O	1:C:2330:ARG:NH1	2.41	0.53
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.39	0.53
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.40	0.53
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.90	0.53
1:D:3111:ARG:NH2	1:D:3174:SER:OG	2.42	0.53
1:D:3246:LEU:HG	1:D:3250:MET:HE2	1.90	0.53
1:A:3445:TRP:HZ3	1:A:3511:VAL:HG13	1.73	0.53
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.38	0.53
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.91	0.53
1:C:3111:ARG:NH2	1:C:3174:SER:OG	2.42	0.53
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLY:N	1:A:316:PHE:O	2.39	0.53
1:A:2917:ALA:HA	1:A:2920:ARG:HB3	1.91	0.53
1:C:3984:ARG:NH2	1:C:3987:ASP:OD2	2.41	0.53
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.35	0.53
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.89	0.53
1:A:747:CYS:HB2	1:A:756:SER:HB2	1.91	0.52
1:A:818:ARG:HH12	1:A:1026:LEU:HA	1.74	0.52
1:B:125:ARG:NH1	1:B:126:SER:OG	2.41	0.52
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.41	0.52
1:C:1728:ARG:HA	1:C:1731:LEU:HD23	1.91	0.52
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.42	0.52
1:C:2280:VAL:HG11	1:C:2290:LEU:HD12	1.90	0.52
1:C:2736:ASP:O	1:C:2738:ARG:NH1	2.42	0.52
1:D:2917:ALA:HA	1:D:2920:ARG:HB3	1.91	0.52
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.91	0.52
1:A:2519:LEU:HD13	1:A:2522:LEU:HD23	1.90	0.52
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.40	0.52
1:A:1728:ARG:HA	1:A:1731:LEU:HD23	1.91	0.52
1:A:2736:ASP:O	1:A:2738:ARG:NH1	2.42	0.52
1:A:3524:MET:O	1:A:3576:TYR:OH	2.24	0.52
1:B:747:CYS:HB2	1:B:756:SER:HB2	1.91	0.52
1:D:2736:ASP:O	1:D:2738:ARG:NH1	2.42	0.52
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.33	0.52
1:C:2369[A]:ARG:NH2	1:C:2372:GLY:O	2.39	0.52
1:D:818:ARG:HH12	1:D:1026:LEU:HA	1.74	0.52
1:A:1547:LYS:NZ	1:A:1642:PRO:O	2.43	0.52
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.42	0.52
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.38	0.52
1:D:277:GLY:N	1:D:316:PHE:O	2.39	0.52
1:D:2369[A]:ARG:NH2	1:D:2372:GLY:O	2.39	0.52
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.41	0.52
1:C:320:LYS:NZ	1:C:383:HIS:O	2.43	0.52
1:D:747:CYS:HB2	1:D:756:SER:HB2	1.91	0.52
1:A:125:ARG:NH1	1:A:126:SER:OG	2.41	0.52
1:D:1547:LYS:NZ	1:D:1642:PRO:O	2.43	0.52
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.90	0.52
1:A:3111:ARG:NH2	1:A:3174:SER:OG	2.42	0.52
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.39	0.52
1:B:3569:LEU:HB3	1:B:3573:MET:HE2	1.92	0.52
1:B:818:ARG:HH12	1:B:1026:LEU:HA	1.74	0.52
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1547:LYS:NZ	1:B:1642:PRO:O	2.43	0.52
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.43	0.52
1:C:1547:LYS:NZ	1:C:1642:PRO:O	2.43	0.52
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	1.91	0.52
1:C:3414:ARG:HH21	1:C:3473:ASP:HB2	1.75	0.52
1:B:2736:ASP:O	1:B:2738:ARG:NH1	2.42	0.51
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.75	0.51
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.90	0.51
1:B:3414:ARG:HH21	1:B:3473:ASP:HB2	1.75	0.51
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.43	0.51
1:C:451:TYR:O	1:C:474:ARG:NH1	2.44	0.51
1:A:168:ASP:HB3	1:A:199:LEU:HD11	1.93	0.51
1:A:3569:LEU:HB3	1:A:3573:MET:HE2	1.92	0.51
1:A:4913:ARG:NH2	1:A:4917:ASP:OD2	2.44	0.51
1:B:168:ASP:HB3	1:B:199:LEU:HD11	1.93	0.51
1:B:1728:ARG:HA	1:B:1731:LEU:HD23	1.91	0.51
1:C:1674:CYS:HG	1:C:1717:SER:HG	1.56	0.51
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.92	0.51
1:D:168:ASP:HB3	1:D:199:LEU:HD11	1.93	0.51
1:D:1728:ARG:HA	1:D:1731:LEU:HD23	1.91	0.51
1:D:2267:MET:O	1:D:2330:ARG:NH1	2.41	0.51
1:D:3414:ARG:HH21	1:D:3473:ASP:HB2	1.75	0.51
1:A:320:LYS:NZ	1:A:383:HIS:O	2.43	0.51
1:A:451:TYR:O	1:A:474:ARG:NH1	2.44	0.51
1:B:451:TYR:O	1:B:474:ARG:NH1	2.44	0.51
1:C:168:ASP:HB3	1:C:199:LEU:HD11	1.93	0.51
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.41	0.51
1:D:150:MET:HB2	1:D:169:LEU:HD12	1.93	0.51
2:F:7:ILE:HD11	2:F:73:LYS:HB2	1.93	0.51
1:A:150:MET:HB2	1:A:169:LEU:HD12	1.93	0.51
1:C:747:CYS:HB2	1:C:756:SER:HB2	1.91	0.51
1:D:131:LEU:HD13	1:D:195:PHE:HE2	1.76	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:A:3414:ARG:HH21	1:A:3473:ASP:HB2	1.75	0.51
1:C:818:ARG:HH12	1:C:1026:LEU:HA	1.74	0.51
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.43	0.51
1:A:2369[A]:ARG:NH2	1:A:2372:GLY:O	2.39	0.51
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.92	0.51
1:B:3352:GLU:O	1:B:3356:SER:OG	2.29	0.51
1:C:3062:PRO:HA	1:C:3065:VAL:HG12	1.93	0.51
1:D:320:LYS:NZ	1:D:383:HIS:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.93	0.51
1:B:2917:ALA:HA	1:B:2920:ARG:HB3	1.91	0.51
1:B:3359:ILE:HD13	1:B:3362:ILE:HD11	1.93	0.51
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.29	0.51
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.36	0.51
1:A:221:ARG:NH2	1:A:255:HIS:O	2.40	0.51
1:B:150:MET:HB2	1:B:169:LEU:HD12	1.93	0.51
1:B:320:LYS:NZ	1:B:383:HIS:O	2.43	0.51
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.33	0.51
1:A:1927:LEU:HD13	1:A:2101:MET:HG3	1.93	0.50
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.93	0.50
1:B:1243:PRO:O	1:B:1458:HIS:ND1	2.41	0.50
1:B:3089:LYS:HE2	1:B:3093:ARG:HH21	1.76	0.50
1:B:4913:ARG:NH2	1:B:4917:ASP:OD2	2.44	0.50
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.94	0.50
1:D:1674:CYS:HG	1:D:1717:SER:HG	1.58	0.50
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.92	0.50
1:A:3359:ILE:HD13	1:A:3362:ILE:HD11	1.93	0.50
1:D:3062:PRO:HA	1:D:3065:VAL:HG12	1.93	0.50
2:G:7:ILE:HD11	2:G:73:LYS:HB2	1.93	0.50
1:A:131:LEU:HD13	1:A:195:PHE:HE2	1.76	0.50
1:B:3068:LEU:HD23	1:B:3139:VAL:HG21	1.93	0.50
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.50
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.36	0.50
1:D:1927:LEU:HD13	1:D:2101:MET:HG3	1.93	0.50
1:D:3068:LEU:HD23	1:D:3139:VAL:HG21	1.93	0.50
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.94	0.50
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.47	0.50
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.50
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.93	0.50
1:D:451:TYR:O	1:D:474:ARG:NH1	2.44	0.50
1:A:3068:LEU:HD23	1:A:3139:VAL:HG21	1.93	0.50
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.41	0.50
1:C:131:LEU:HD13	1:C:195:PHE:HE2	1.76	0.50
1:C:221:ARG:NH2	1:C:255:HIS:O	2.40	0.50
1:C:2614:ILE:O	1:C:2650:ARG:NH2	2.45	0.50
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.94	0.50
1:C:3068:LEU:HD23	1:C:3139:VAL:HG21	1.93	0.50
1:D:3569:LEU:HB3	1:D:3573:MET:HE2	1.92	0.50
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.93	0.50
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3359:ILE:HD13	1:C:3362:ILE:HD11	1.93	0.50
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.50
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.41	0.50
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.47	0.50
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.47	0.50
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.47	0.50
1:C:3089:LYS:HE2	1:C:3093:ARG:HH21	1.76	0.50
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.36	0.49
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.36	0.49
1:B:2267:MET:O	1:B:2330:ARG:NH1	2.41	0.49
1:C:150:MET:HB2	1:C:169:LEU:HD12	1.93	0.49
1:A:3062:PRO:HA	1:A:3065:VAL:HG12	1.93	0.49
1:A:4917:ASP:HB2	1:D:4888:TYR:HE1	1.78	0.49
1:D:786:GLY:N	1:D:1630:CYS:O	2.46	0.49
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.46	0.49
1:D:3359:ILE:HD13	1:D:3362:ILE:HD11	1.93	0.49
1:A:116:MET:HB2	1:A:137:LEU:HD13	1.94	0.49
1:A:3089:LYS:HE2	1:A:3093:ARG:HH21	1.76	0.49
1:D:2614:ILE:O	1:D:2650:ARG:NH2	2.45	0.49
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.93	0.49
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.46	0.49
1:B:426:ARG:N	1:B:505:GLU:O	2.45	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.93	0.49
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.45	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.49
1:D:815:VAL:O	1:D:1007:TYR:OH	2.29	0.49
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.94	0.49
1:B:131:LEU:HD13	1:B:195:PHE:HE2	1.76	0.49
1:B:134:ASP:OD1	1:B:134:ASP:N	2.46	0.49
1:C:1927:LEU:HD13	1:C:2101:MET:HG3	1.93	0.49
1:C:3569:LEU:HB3	1:C:3573:MET:HE2	1.92	0.49
1:D:111:HIS:ND1	1:D:114:SER:OG	2.37	0.49
1:A:2267:MET:O	1:A:2330:ARG:NH1	2.41	0.49
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.46	0.49
1:B:3062:PRO:HA	1:B:3065:VAL:HG12	1.93	0.49
1:C:116:MET:HB2	1:C:137:LEU:HD13	1.94	0.49
1:C:277:GLY:N	1:C:316:PHE:O	2.39	0.49
1:A:111:HIS:ND1	1:A:114:SER:OG	2.37	0.49
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2309:SER:OG	1:A:2321:ILE:O	2.30	0.49
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.46	0.49
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.45	0.49
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.46	0.49
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.29	0.49
1:C:815:VAL:O	1:C:1007:TYR:OH	2.29	0.49
1:C:2002:PRO:HB3	1:C:3641:LEU:HD13	1.95	0.49
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.46	0.49
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.95	0.49
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.95	0.49
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.45	0.49
1:A:4247:ILE:HD11	1:A:4667:PRO:HB2	1.95	0.49
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.94	0.49
1:A:1422:ASP:OD2	1:A:1568:LYS:NZ	2.36	0.49
1:B:266:ARG:NH2	1:B:331:VAL:O	2.39	0.49
1:B:2369[A]:ARG:NH2	1:B:2372:GLY:O	2.39	0.49
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.46	0.49
1:C:1422:ASP:OD2	1:C:1568:LYS:NZ	2.36	0.49
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.95	0.49
1:C:2309:SER:OG	1:C:2321:ILE:O	2.30	0.49
1:C:3380:ARG:HH22	1:C:3448:SER:HA	1.78	0.49
1:D:3089:LYS:HE2	1:D:3093:ARG:HH21	1.76	0.49
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.44	0.49
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.95	0.48
1:A:2002:PRO:HB3	1:A:3641:LEU:HD13	1.95	0.48
1:B:116:MET:HB2	1:B:137:LEU:HD13	1.94	0.48
1:C:38:ALA:HB1	1:C:64:ILE:HG13	1.95	0.48
1:D:221:ARG:NH2	1:D:255:HIS:O	2.40	0.48
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.95	0.48
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.46	0.48
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.46	0.48
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.29	0.48
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.46	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:D:38:ALA:HB1	1:D:64:ILE:HG13	1.95	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.48
1:D:2309:SER:OG	1:D:2321:ILE:O	2.30	0.48
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.41	0.48
1:A:1287:LEU:HD11	1:A:1599:MET:HE3	1.96	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.46	0.48
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3380:ARG:HH22	1:D:3448:SER:HA	1.78	0.48
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.45	0.48
2:H:4:ILE:HG22	2:H:74:LEU:HG	1.96	0.48
1:A:38:ALA:HB1	1:A:64:ILE:HG13	1.95	0.48
1:A:637:LEU:HD12	1:A:1692:ALA:HB1	1.96	0.48
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.46	0.48
1:B:4247:ILE:HD11	1:B:4667:PRO:HB2	1.95	0.48
1:C:786:GLY:N	1:C:1630:CYS:O	2.46	0.48
1:C:1733:GLU:OE2	1:C:2163:ARG:NH2	2.46	0.48
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.95	0.48
1:B:637:LEU:HD12	1:B:1692:ALA:HB1	1.96	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:B:3323:ILE:HD12	1:B:3335:MET:HE3	1.95	0.48
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.43	0.48
2:E:4:ILE:HG22	2:E:74:LEU:HG	1.96	0.48
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.96	0.48
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.94	0.48
1:A:3323:ILE:HD12	1:A:3335:MET:HE3	1.96	0.48
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.95	0.48
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.96	0.48
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.95	0.48
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.96	0.48
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	1.95	0.48
1:D:134:ASP:OD1	1:D:134:ASP:N	2.46	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.48
1:D:2002:PRO:HB3	1:D:3641:LEU:HD13	1.95	0.48
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.95	0.48
2:F:4:ILE:HG22	2:F:74:LEU:HG	1.96	0.48
2:G:4:ILE:HG22	2:G:74:LEU:HG	1.96	0.48
1:A:875:ALA:O	1:A:879:HIS:ND1	2.46	0.48
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.95	0.48
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.75	0.48
1:B:3380:ARG:HH22	1:B:3448:SER:HA	1.78	0.48
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.96	0.48
1:A:3380:ARG:HH22	1:A:3448:SER:HA	1.78	0.48
1:B:221:ARG:NH2	1:B:255:HIS:O	2.40	0.48
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.95	0.48
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.95	0.48
1:C:3352:GLU:O	1:C:3356:SER:OG	2.29	0.48
1:C:3443:ILE:HG12	1:C:3605:HIS:HD2	1.79	0.48
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.95	0.48
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.95	0.48
1:A:1733:GLU:OE2	1:A:2163:ARG:NH2	2.46	0.48
1:A:2614:ILE:O	1:A:2650:ARG:NH2	2.45	0.48
1:B:38:ALA:HB1	1:B:64:ILE:HG13	1.95	0.48
1:B:1287:LEU:HD11	1:B:1599:MET:HE3	1.96	0.48
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.47	0.48
1:D:1733:GLU:OE2	1:D:2163:ARG:NH2	2.46	0.48
1:D:1996:ARG:HA	1:D:1999:ARG:HG2	1.96	0.48
1:D:3037:GLU:HG2	1:D:3085:PRO:HD2	1.96	0.48
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.96	0.48
1:B:815:VAL:O	1:B:1007:TYR:OH	2.29	0.48
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.43	0.48
1:D:116:MET:HB2	1:D:137:LEU:HD13	1.94	0.48
1:D:3443:ILE:HG12	1:D:3605:HIS:HD2	1.79	0.48
1:D:5011:TRP:HD1	1:D:5011:TRP:HA	1.66	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.46	0.47
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.96	0.47
1:B:3233:PRO:HG2	1:B:3239:MET:HA	1.96	0.47
1:C:637:LEU:HD12	1:C:1692:ALA:HB1	1.96	0.47
1:C:3037:GLU:HG2	1:C:3085:PRO:HD2	1.96	0.47
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.96	0.47
1:D:4247:ILE:HD11	1:D:4667:PRO:HB2	1.95	0.47
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.96	0.47
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.33	0.47
1:C:4112:LEU:O	1:C:4115:SER:OG	2.32	0.47
1:D:4190:ILE:H	1:D:4190:ILE:HG12	1.49	0.47
1:A:816:LEU:HD23	1:A:818:ARG:H	1.79	0.47
1:A:3037:GLU:HG2	1:A:3085:PRO:HD2	1.96	0.47
1:A:3277:LEU:HD23	1:A:3315:LEU:HD13	1.96	0.47
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.41	0.47
1:B:3277:LEU:HD23	1:B:3315:LEU:HD13	1.96	0.47
1:C:1287:LEU:HD11	1:C:1599:MET:HE3	1.95	0.47
1:C:3323:ILE:HD12	1:C:3335:MET:HE3	1.96	0.47
1:B:1733:GLU:OE2	1:B:2163:ARG:NH2	2.46	0.47
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.96	0.47
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.45	0.47
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.47
1:A:4892:ARG:NH1	1:B:4895:GLY:O	2.45	0.47
1:C:2248:ARG:HG2	1:C:2286:LEU:HD21	1.97	0.47
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.80	0.47
1:C:4913:ARG:NH2	1:C:4917:ASP:OD2	2.44	0.47
1:D:133:PHE:O	1:D:193:ALA:N	2.40	0.47
1:D:1287:LEU:HD11	1:D:1599:MET:HE3	1.95	0.47
1:D:2248:ARG:HG2	1:D:2286:LEU:HD21	1.97	0.47
1:A:1996:ARG:HA	1:A:1999:ARG:HG2	1.96	0.47
1:A:4112:LEU:O	1:A:4115:SER:OG	2.32	0.47
1:B:133:PHE:O	1:B:193:ALA:N	2.40	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.95	0.47
1:B:1996:ARG:HA	1:B:1999:ARG:HG2	1.96	0.47
1:B:2002:PRO:HB3	1:B:3641:LEU:HD13	1.95	0.47
1:B:2248:ARG:HG2	1:B:2286:LEU:HD21	1.97	0.47
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.45	0.47
1:B:3443:ILE:HG12	1:B:3605:HIS:HD2	1.79	0.47
1:C:134:ASP:N	1:C:134:ASP:OD1	2.46	0.47
1:C:426:ARG:N	1:C:505:GLU:O	2.45	0.47
1:C:682:LEU:HD13	1:C:787:VAL:HG11	1.97	0.47
1:C:816:LEU:HD23	1:C:818:ARG:H	1.80	0.47
1:C:1996:ARG:HA	1:C:1999:ARG:HG2	1.96	0.47
1:C:3233:PRO:HG2	1:C:3239:MET:HA	1.96	0.47
1:C:3277:LEU:HD23	1:C:3315:LEU:HD13	1.96	0.47
1:C:4948:GLU:HA	1:C:4951:LYS:HE3	1.97	0.47
1:D:816:LEU:HD23	1:D:818:ARG:H	1.80	0.47
1:D:2719:TYR:HB3	1:D:2948:THR:HG21	1.97	0.47
1:A:1577:ALA:HB1	1:A:1584:ARG:HD3	1.97	0.47
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.96	0.47
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.96	0.47
1:C:1577:ALA:HB1	1:C:1584:ARG:HD3	1.97	0.47
1:D:682:LEU:HD13	1:D:787:VAL:HG11	1.97	0.47
2:H:21:THR:N	2:H:107:GLU:OE2	2.48	0.47
1:A:1674:CYS:SG	1:A:1717:SER:OG	2.73	0.47
1:A:2248:ARG:HG2	1:A:2286:LEU:HD21	1.97	0.47
1:B:3037:GLU:HG2	1:B:3085:PRO:HD2	1.96	0.47
1:C:2095:GLN:HG3	1:C:2127:GLN:HB3	1.97	0.47
1:D:637:LEU:HD12	1:D:1692:ALA:HB1	1.96	0.47
1:D:2531:ARG:NH1	1:D:2585:THR:OG1	2.48	0.47
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.97	0.47
1:A:2531:ARG:NH1	1:A:2585:THR:OG1	2.48	0.47
1:B:111:HIS:ND1	1:B:114:SER:OG	2.37	0.47
1:C:499:THR:HG23	1:C:502:HIS:H	1.80	0.47
1:C:715:GLY:O	1:C:722:TRP:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1782:PHE:O	2:G:82:TYR:OH	2.28	0.47
1:C:4867:GLU:H	1:C:4867:GLU:HG2	1.50	0.47
1:D:1577:ALA:HB1	1:D:1584:ARG:HD3	1.97	0.47
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.96	0.47
1:D:3233:PRO:HG2	1:D:3239:MET:HA	1.96	0.47
1:D:4948:GLU:HA	1:D:4951:LYS:HE3	1.97	0.47
2:E:23:VAL:HG22	2:E:47:LYS:HG2	1.97	0.47
1:A:1640:HIS:HA	1:A:1647:CYS:HA	1.97	0.46
1:A:2095:GLN:HG3	1:A:2127:GLN:HB3	1.97	0.46
1:A:3443:ILE:HG12	1:A:3605:HIS:HD2	1.79	0.46
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.47	0.46
1:B:1782:PHE:O	2:F:82:TYR:OH	2.28	0.46
1:B:2531:ARG:NH1	1:B:2585:THR:OG1	2.48	0.46
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.80	0.46
1:D:499:THR:HG23	1:D:502:HIS:H	1.80	0.46
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.98	0.46
1:A:786:GLY:N	1:A:1630:CYS:O	2.46	0.46
1:A:1784:ALA:O	2:E:82:TYR:OH	2.25	0.46
1:A:4948:GLU:HA	1:A:4951:LYS:HE3	1.97	0.46
1:B:786:GLY:N	1:B:1630:CYS:O	2.46	0.46
1:B:1577:ALA:HB1	1:B:1584:ARG:HD3	1.97	0.46
1:B:1674:CYS:SG	1:B:1717:SER:OG	2.73	0.46
1:B:2719:TYR:HB3	1:B:2948:THR:HG21	1.97	0.46
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.46	0.46
1:B:3781:GLN:NE2	1:B:3819:TYR:OH	2.41	0.46
1:C:1780:PRO:HD3	1:C:1801:ALA:H	1.81	0.46
1:C:2739:PRO:HB3	1:C:2888:ARG:HH11	1.81	0.46
1:C:4643:LEU:O	1:C:4647:SER:HB3	2.15	0.46
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.96	0.46
1:D:2739:PRO:HB3	1:D:2888:ARG:HH11	1.81	0.46
2:F:21:THR:N	2:F:107:GLU:OE2	2.48	0.46
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.97	0.46
1:A:262:LEU:HD13	1:A:274:LEU:HD11	1.97	0.46
1:A:4643:LEU:O	1:A:4647:SER:HB3	2.15	0.46
1:B:499:THR:HG23	1:B:502:HIS:H	1.81	0.46
1:B:3103:ILE:HD11	1:B:3172:ILE:HB	1.98	0.46
1:B:3432:GLU:HG3	1:B:3524:MET:HE3	1.97	0.46
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.33	0.46
1:A:2479:LEU:HB2	1:A:2541:PHE:HZ	1.81	0.46
1:A:2591:ARG:HG2	1:A:2636:PHE:HB3	1.98	0.46
1:B:1640:HIS:HA	1:B:1647:CYS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.81	0.46
1:C:2461:VAL:O	1:C:2510:TYR:OH	2.30	0.46
1:C:2719:TYR:HB3	1:C:2948:THR:HG21	1.97	0.46
2:G:23:VAL:HG22	2:G:47:LYS:HG2	1.97	0.46
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.97	0.46
1:A:3233:PRO:HG2	1:A:3239:MET:HA	1.96	0.46
1:B:2739:PRO:HB3	1:B:2888:ARG:HH11	1.81	0.46
1:B:4643:LEU:O	1:B:4647:SER:HB3	2.15	0.46
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.80	0.46
1:C:3432:GLU:HG3	1:C:3524:MET:HE3	1.97	0.46
1:D:1423:ASP:HB2	1:D:1426:ILE:HG22	1.98	0.46
1:D:2479:LEU:HB2	1:D:2541:PHE:HZ	1.81	0.46
1:D:2591:ARG:HG2	1:D:2636:PHE:HB3	1.98	0.46
1:D:3103:ILE:HD11	1:D:3172:ILE:HB	1.98	0.46
1:D:3323:ILE:HD12	1:D:3335:MET:HE3	1.96	0.46
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.45	0.46
2:E:21:THR:N	2:E:107:GLU:OE2	2.48	0.46
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.97	0.46
1:A:4188:ARG:HA	1:A:4188:ARG:HD2	1.58	0.46
1:B:715:GLY:O	1:B:722:TRP:N	2.48	0.46
1:B:3981:ALA:HB2	1:B:4040:ILE:HG12	1.97	0.46
1:B:4675:LYS:HG3	1:B:4679:ARG:HE	1.81	0.46
1:C:1291:LEU:HD13	1:C:1595:LEU:HD21	1.98	0.46
1:C:2025:GLU:OE2	1:C:2028:ARG:NH1	2.49	0.46
1:C:2531:ARG:NH1	1:C:2585:THR:OG1	2.48	0.46
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.46	0.46
1:D:1640:HIS:HA	1:D:1647:CYS:HA	1.97	0.46
1:A:134:ASP:OD1	1:A:134:ASP:N	2.46	0.46
1:A:4179:GLY:O	1:A:4194:TYR:HA	2.16	0.46
1:A:4989:MET:HE2	1:A:4989:MET:HB2	1.71	0.46
1:B:148:TRP:CZ3	1:B:180:LEU:HB2	2.51	0.46
1:B:682:LEU:HD13	1:B:787:VAL:HG11	1.97	0.46
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.98	0.46
1:B:1780:PRO:HD3	1:B:1801:ALA:H	1.81	0.46
1:B:2461:VAL:O	1:B:2510:TYR:OH	2.30	0.46
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.97	0.46
1:C:426:ARG:NH1	1:C:429:GLY:O	2.41	0.46
1:C:1640:HIS:HA	1:C:1647:CYS:HA	1.97	0.46
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.97	0.46
1:C:2538:THR:HG23	1:C:2540:THR:H	1.81	0.46
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:LYS:HB3	1:D:416:LYS:HE2	1.76	0.46
1:D:715:GLY:O	1:D:722:TRP:N	2.48	0.46
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.97	0.46
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.80	0.46
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.98	0.46
1:D:4643:LEU:O	1:D:4647:SER:HB3	2.15	0.46
1:A:4930:ALA:HB2	1:D:4933:GLN:HG2	1.97	0.46
1:B:816:LEU:HD23	1:B:818:ARG:H	1.80	0.46
1:B:2002:PRO:HD3	1:B:3638:MET:HE1	1.97	0.46
1:B:2025:GLU:OE2	1:B:2028:ARG:NH1	2.49	0.46
1:B:2670:GLU:HG3	1:B:2674:LEU:HD13	1.98	0.46
1:B:4179:GLY:O	1:B:4194:TYR:HA	2.16	0.46
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.98	0.46
1:C:2002:PRO:HD3	1:C:3638:MET:HE1	1.97	0.46
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.98	0.46
1:D:2025:GLU:OE2	1:D:2028:ARG:NH1	2.49	0.46
1:D:2538:THR:HG23	1:D:2540:THR:H	1.81	0.46
1:D:3352:GLU:O	1:D:3356:SER:OG	2.29	0.46
1:A:2025:GLU:OE2	1:A:2028:ARG:NH1	2.49	0.46
1:A:2719:TYR:HB3	1:A:2948:THR:HG21	1.97	0.46
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.98	0.46
1:B:3536:ALA:HA	1:B:3539:ARG:HG2	1.98	0.46
1:C:262:LEU:HD13	1:C:274:LEU:HD11	1.97	0.46
1:C:3233:PRO:HD2	1:C:3239:MET:HG2	1.98	0.46
1:C:4675:LYS:HG3	1:C:4679:ARG:HE	1.81	0.46
1:D:266:ARG:NH2	1:D:331:VAL:O	2.39	0.46
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.16	0.46
1:A:426:ARG:N	1:A:505:GLU:O	2.45	0.46
1:A:1291:LEU:HD13	1:A:1595:LEU:HD21	1.98	0.46
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.16	0.46
1:A:4675:LYS:HG3	1:A:4679:ARG:HE	1.81	0.46
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.98	0.46
1:B:2479:LEU:HB2	1:B:2541:PHE:HZ	1.81	0.46
1:C:548:VAL:HA	1:C:551:LEU:HG	1.98	0.46
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.41	0.46
1:C:3981:ALA:HB2	1:C:4040:ILE:HG12	1.97	0.46
1:C:4188:ARG:HD2	1:C:4188:ARG:HA	1.58	0.46
1:D:548:VAL:HA	1:D:551:LEU:HG	1.98	0.46
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.81	0.46
1:A:1780:PRO:HD3	1:A:1801:ALA:H	1.81	0.45
1:A:2002:PRO:HD3	1:A:3638:MET:HE1	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3536:ALA:HA	1:A:3539:ARG:HG2	1.98	0.45
1:A:3981:ALA:HB2	1:A:4040:ILE:HG12	1.97	0.45
1:B:4948:GLU:HA	1:B:4951:LYS:HE3	1.97	0.45
1:C:253:CYS:O	1:C:258:SER:OG	2.34	0.45
1:C:2479:LEU:HB2	1:C:2541:PHE:HZ	1.81	0.45
1:C:3731:LYS:HA	1:C:3731:LYS:HD3	1.76	0.45
1:D:426:ARG:N	1:D:505:GLU:O	2.45	0.45
1:D:4179:GLY:O	1:D:4194:TYR:HA	2.16	0.45
1:D:4648:LEU:HD12	1:D:4803:HIS:HE1	1.81	0.45
1:D:4971:THR:HG22	1:D:4972:PRO:HD2	1.98	0.45
1:A:2680:TRP:O	1:A:2684:ASP:HB2	2.17	0.45
1:A:4971:THR:HG22	1:A:4972:PRO:HD2	1.98	0.45
1:B:2591:ARG:HG2	1:B:2636:PHE:HB3	1.98	0.45
1:C:107:ILE:N	1:C:148:TRP:O	2.40	0.45
1:D:2095:GLN:HG3	1:D:2127:GLN:HB3	1.97	0.45
1:D:3277:LEU:HD23	1:D:3315:LEU:HD13	1.96	0.45
1:D:4675:LYS:HG3	1:D:4679:ARG:HE	1.81	0.45
1:A:499:THR:HG23	1:A:502:HIS:H	1.80	0.45
1:A:682:LEU:HD13	1:A:787:VAL:HG11	1.97	0.45
1:A:4648:LEU:HD12	1:A:4803:HIS:HE1	1.81	0.45
1:B:1422:ASP:OD2	1:B:1568:LYS:NZ	2.35	0.45
1:B:2095:GLN:HG3	1:B:2127:GLN:HB3	1.97	0.45
1:B:3233:PRO:HD2	1:B:3239:MET:HG2	1.98	0.45
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.98	0.45
1:B:5011:TRP:HD1	1:B:5011:TRP:HA	1.66	0.45
1:C:2670:GLU:HG3	1:C:2674:LEU:HD13	1.98	0.45
1:D:2670:GLU:HG3	1:D:2674:LEU:HD13	1.98	0.45
1:D:3981:ALA:HB2	1:D:4040:ILE:HG12	1.97	0.45
1:A:148:TRP:CZ3	1:A:180:LEU:HB2	2.51	0.45
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.98	0.45
1:A:2769:ASP:HA	1:A:2772:GLN:HB2	1.98	0.45
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.52	0.45
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.81	0.45
1:B:1423:ASP:HB2	1:B:1426:ILE:HG22	1.97	0.45
1:B:2680:TRP:O	1:B:2684:ASP:HB2	2.17	0.45
1:B:4648:LEU:HD12	1:B:4803:HIS:HE1	1.81	0.45
1:C:266:ARG:NH2	1:C:331:VAL:O	2.39	0.45
1:C:1434:TYR:HA	1:C:1518:CYS:O	2.17	0.45
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.33	0.45
1:C:3719:ASP:HB2	1:C:3722:TYR:HB3	1.98	0.45
1:C:4179:GLY:O	1:C:4194:TYR:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:TRP:CZ3	1:D:180:LEU:HB2	2.51	0.45
1:D:1992:ALA:HA	1:D:1995:THR:HG22	1.98	0.45
1:D:4984:ASN:HB3	1:D:4987:ASN:HB2	1.99	0.45
1:A:831:ARG:HG3	1:A:840:VAL:HG21	1.99	0.45
1:A:2670:GLU:HG3	1:A:2674:LEU:HD13	1.98	0.45
1:B:2538:THR:HG23	1:B:2540:THR:H	1.81	0.45
1:C:831:ARG:HG3	1:C:840:VAL:HG21	1.99	0.45
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.80	0.45
1:C:2591:ARG:HG2	1:C:2636:PHE:HB3	1.98	0.45
1:C:3536:ALA:HA	1:C:3539:ARG:HG2	1.98	0.45
1:C:4989:MET:HB2	1:C:4989:MET:HE2	1.70	0.45
1:D:1434:TYR:HA	1:D:1518:CYS:O	2.17	0.45
1:D:2916:LYS:HD3	1:D:2920:ARG:HH21	1.82	0.45
1:D:3432:GLU:HG3	1:D:3524:MET:HE3	1.97	0.45
1:D:4036:VAL:HG12	1:D:4153:HIS:HA	1.99	0.45
1:A:2916:LYS:HD3	1:A:2920:ARG:HH21	1.82	0.45
1:A:3233:PRO:HD2	1:A:3239:MET:HG2	1.98	0.45
1:A:4190:ILE:H	1:A:4190:ILE:HG12	1.49	0.45
1:B:3219:TYR:OH	1:B:3239:MET:SD	2.73	0.45
1:B:4112:LEU:O	1:B:4115:SER:OG	2.32	0.45
1:B:4984:ASN:HB3	1:B:4987:ASN:HB2	1.99	0.45
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.98	0.45
1:C:1423:ASP:HB2	1:C:1426:ILE:HG22	1.98	0.45
1:C:1992:ALA:HA	1:C:1995:THR:HG22	1.98	0.45
1:C:2967:MET:HE2	1:C:3045:LYS:HB3	1.99	0.45
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.52	0.45
1:D:831:ARG:HG3	1:D:840:VAL:HG21	1.99	0.45
1:D:1291:LEU:HD13	1:D:1595:LEU:HD21	1.98	0.45
2:G:21:THR:N	2:G:107:GLU:OE2	2.48	0.45
1:A:133:PHE:O	1:A:193:ALA:N	2.40	0.45
1:A:3352:GLU:HA	1:A:3355:HIS:HE1	1.82	0.45
1:A:4957:LYS:HB2	1:A:4957:LYS:HE2	1.64	0.45
1:B:1291:LEU:HD13	1:B:1595:LEU:HD21	1.98	0.45
1:B:4828:SER:O	1:B:4832:HIS:HB2	2.17	0.45
1:C:148:TRP:CZ3	1:C:180:LEU:HB2	2.51	0.45
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.52	0.45
1:C:3103:ILE:HD11	1:C:3172:ILE:HB	1.98	0.45
1:D:145:ALA:HA	1:D:175:SER:HB3	1.99	0.45
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.17	0.45
1:D:2002:PRO:HD3	1:D:3638:MET:HE1	1.97	0.45
1:D:3536:ALA:HA	1:D:3539:ARG:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3759:GLU:OE1	1:D:3762:ARG:NH2	2.50	0.45
1:A:253:CYS:O	1:A:258:SER:OG	2.34	0.45
1:A:266:ARG:NH2	1:A:331:VAL:O	2.39	0.45
1:A:2739:PRO:HB3	1:A:2888:ARG:HH11	1.81	0.45
1:A:3103:ILE:HD11	1:A:3172:ILE:HB	1.98	0.45
1:A:4984:ASN:HB3	1:A:4987:ASN:HB2	1.99	0.45
1:B:726:VAL:HB	1:B:728:ARG:HH21	1.82	0.45
1:B:4971:THR:HG22	1:B:4972:PRO:HD2	1.98	0.45
1:C:133:PHE:O	1:C:193:ALA:N	2.40	0.45
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.17	0.45
1:C:4036:VAL:HG12	1:C:4153:HIS:HA	1.99	0.45
1:C:4648:LEU:HD12	1:C:4803:HIS:HE1	1.81	0.45
1:C:4879:MET:HE3	1:C:4879:MET:HB3	1.83	0.45
1:C:4971:THR:HG22	1:C:4972:PRO:HD2	1.98	0.45
1:D:253:CYS:O	1:D:258:SER:OG	2.34	0.45
1:D:2769:ASP:HA	1:D:2772:GLN:HB2	1.99	0.45
1:A:548:VAL:HA	1:A:551:LEU:HG	1.98	0.45
1:A:1423:ASP:HB2	1:A:1426:ILE:HG22	1.98	0.45
1:A:1434:TYR:HA	1:A:1518:CYS:O	2.17	0.45
1:A:1780:PRO:O	2:E:42:ARG:NH1	2.28	0.45
1:A:1992:ALA:HA	1:A:1995:THR:HG22	1.98	0.45
1:A:3432:GLU:HG3	1:A:3524:MET:HE3	1.97	0.45
1:A:3759:GLU:OE1	1:A:3762:ARG:NH2	2.50	0.45
1:A:4036:VAL:HG12	1:A:4153:HIS:HA	1.99	0.45
1:A:4867:GLU:H	1:A:4867:GLU:HG2	1.50	0.45
1:B:831:ARG:HG3	1:B:840:VAL:HG21	1.99	0.45
1:B:1992:ALA:HA	1:B:1995:THR:HG22	1.98	0.45
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.46	0.45
1:B:2916:LYS:HD3	1:B:2920:ARG:HH21	1.82	0.45
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.16	0.45
1:C:2680:TRP:O	1:C:2684:ASP:HB2	2.17	0.45
1:D:1780:PRO:HD3	1:D:1801:ALA:H	1.81	0.45
1:D:2165:LEU:HD21	1:D:2177:LEU:HD23	1.99	0.45
1:D:2967:MET:HE2	1:D:3045:LYS:HB3	1.99	0.45
1:D:3352:GLU:HA	1:D:3355:HIS:HE1	1.82	0.45
1:A:294:THR:HG23	1:A:297:GLN:H	1.82	0.45
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.52	0.45
1:A:715:GLY:O	1:A:722:TRP:N	2.48	0.45
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.81	0.45
1:A:5011:TRP:HD1	1:A:5011:TRP:HA	1.66	0.45
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.17	0.45
1:B:3051:ARG:CZ	1:B:3098:SER:HB3	2.47	0.45
1:B:4188:ARG:HA	1:B:4188:ARG:HD2	1.58	0.45
1:C:498:THR:HA	1:C:553:ARG:HH22	1.82	0.45
1:C:3352:GLU:HA	1:C:3355:HIS:HE1	1.82	0.45
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.84	0.45
1:D:294:THR:HG23	1:D:297:GLN:H	1.82	0.45
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.82	0.45
1:D:4687:TYR:HE2	1:D:4703:ARG:HG2	1.82	0.45
1:A:640:TYR:HD2	1:A:1634:LEU:HB3	1.83	0.44
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.50	0.44
1:A:3326:ASN:HB3	1:A:3329:ILE:HD13	1.99	0.44
1:B:548:VAL:HA	1:B:551:LEU:HG	1.98	0.44
1:C:726:VAL:HB	1:C:728:ARG:HH21	1.82	0.44
1:C:1568:LYS:HE2	1:C:1574:PRO:HD3	1.99	0.44
1:C:4984:ASN:HB3	1:C:4987:ASN:HB2	1.99	0.44
1:D:3719:ASP:HB2	1:D:3722:TYR:HB3	1.98	0.44
1:D:4828:SER:O	1:D:4832:HIS:HB2	2.17	0.44
1:A:145:ALA:HA	1:A:175:SER:HB3	1.99	0.44
1:A:2165:LEU:HD21	1:A:2177:LEU:HD23	1.99	0.44
1:A:2541:PHE:O	1:A:2544:THR:OG1	2.31	0.44
1:A:3051:ARG:CZ	1:A:3098:SER:HB3	2.47	0.44
1:A:3329:ILE:HD11	1:A:3332:ALA:HB2	1.99	0.44
1:B:3719:ASP:HB2	1:B:3722:TYR:HB3	1.98	0.44
1:C:4828:SER:O	1:C:4832:HIS:HB2	2.17	0.44
1:D:262:LEU:HD13	1:D:274:LEU:HD11	1.98	0.44
1:A:76:ARG:HH12	1:D:3936:TYR:HB2	1.82	0.44
1:A:129:ASP:OD1	1:A:129:ASP:N	2.50	0.44
1:A:726:VAL:HB	1:A:728:ARG:HH21	1.82	0.44
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.82	0.44
1:B:145:ALA:HA	1:B:175:SER:HB3	1.99	0.44
1:B:1256:GLU:HB3	1:B:1275:ARG:HD2	2.00	0.44
1:B:2967:MET:HE2	1:B:3045:LYS:HB3	1.99	0.44
1:B:3759:GLU:OE1	1:B:3762:ARG:NH2	2.50	0.44
1:C:294:THR:HG23	1:C:297:GLN:H	1.82	0.44
1:C:2916:LYS:HD3	1:C:2920:ARG:HH21	1.82	0.44
1:C:3281:LEU:HD12	1:C:3315:LEU:HD22	1.99	0.44
1:D:726:VAL:HB	1:D:728:ARG:HH21	1.82	0.44
1:D:3233:PRO:HD2	1:D:3239:MET:HG2	1.98	0.44
1:A:877:ASN:HA	1:A:970:LEU:H	1.83	0.44
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:THR:HG23	1:A:2540:THR:H	1.81	0.44
1:B:3329:ILE:HD11	1:B:3332:ALA:HB2	1.99	0.44
1:B:4036:VAL:HG12	1:B:4153:HIS:HA	1.99	0.44
1:C:665:GLU:HB2	1:C:792:LEU:HB2	2.00	0.44
1:C:858:THR:OG1	1:C:927:GLU:OE2	2.33	0.44
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.99	0.44
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.50	0.44
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	2.00	0.44
1:C:3051:ARG:CZ	1:C:3098:SER:HB3	2.47	0.44
1:D:102:LEU:HA	1:D:162:LYS:HA	2.00	0.44
1:D:665:GLU:HB2	1:D:792:LEU:HB2	2.00	0.44
1:D:2680:TRP:O	1:D:2684:ASP:HB2	2.17	0.44
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	2.00	0.44
1:D:3281:LEU:HD12	1:D:3315:LEU:HD22	1.99	0.44
1:A:603:LEU:HA	1:A:606:LEU:HD12	2.00	0.44
1:A:884:LEU:HD13	1:A:968:ALA:H	1.83	0.44
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	2.00	0.44
1:A:2967:MET:HE2	1:A:3045:LYS:HB3	1.99	0.44
1:B:102:LEU:HA	1:B:162:LYS:HA	2.00	0.44
1:B:2769:ASP:HA	1:B:2772:GLN:HB2	1.99	0.44
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	2.00	0.44
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	2.00	0.44
1:B:3352:GLU:HA	1:B:3355:HIS:HE1	1.82	0.44
1:C:640:TYR:HD2	1:C:1634:LEU:HB3	1.82	0.44
1:C:884:LEU:HD13	1:C:968:ALA:H	1.83	0.44
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	2.00	0.44
1:C:3759:GLU:OE1	1:C:3762:ARG:NH2	2.50	0.44
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.98	0.44
1:D:2461:VAL:O	1:D:2510:TYR:OH	2.30	0.44
1:D:4867:GLU:H	1:D:4867:GLU:HG2	1.50	0.44
1:A:102:LEU:HA	1:A:162:LYS:HA	2.00	0.44
1:B:640:TYR:HD2	1:B:1634:LEU:HB3	1.82	0.44
1:B:1434:TYR:HA	1:B:1518:CYS:O	2.17	0.44
1:B:4880:MET:HE2	1:B:4880:MET:HB2	1.74	0.44
1:B:5012:LYS:HE3	1:B:5012:LYS:HB3	1.69	0.44
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.87	0.44
1:C:3388:GLU:HA	1:C:3391:GLU:HB3	1.99	0.44
1:D:3051:ARG:CZ	1:D:3098:SER:HB3	2.47	0.44
1:D:3996:PHE:O	1:D:4000:MET:HG2	2.18	0.44
1:D:4879:MET:HE3	1:D:4879:MET:HB3	1.83	0.44
1:A:1256:GLU:HB3	1:A:1275:ARG:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3006:ILE:HD12	1:A:3010:PHE:HE2	1.83	0.44
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	2.00	0.44
1:A:3996:PHE:O	1:A:4000:MET:HG2	2.18	0.44
1:A:4828:SER:O	1:A:4832:HIS:HB2	2.17	0.44
1:B:426:ARG:NH1	1:B:429:GLY:O	2.41	0.44
1:B:498:THR:HA	1:B:553:ARG:HH22	1.82	0.44
1:B:877:ASN:HA	1:B:970:LEU:H	1.83	0.44
1:B:2215:LEU:HD23	1:B:2260:ASN:HB3	2.00	0.44
1:B:3316:LEU:HD11	1:B:3353:LEU:HD11	2.00	0.44
1:B:3366:ARG:NH1	1:B:3440:GLU:OE1	2.47	0.44
1:B:4687:TYR:HE2	1:B:4703:ARG:HG2	1.82	0.44
1:C:129:ASP:OD1	1:C:129:ASP:N	2.50	0.44
1:C:869:ARG:HE	1:C:869:ARG:HB3	1.64	0.44
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	2.00	0.44
1:C:2215:LEU:HD23	1:C:2260:ASN:HB3	2.00	0.44
1:C:4839:MET:HE3	1:C:4839:MET:HB3	1.91	0.44
1:D:498:THR:HA	1:D:553:ARG:HH22	1.82	0.44
1:D:603:LEU:HA	1:D:606:LEU:HD12	2.00	0.44
1:D:3992:PHE:HB2	1:D:4023:MET:HE1	2.00	0.44
1:A:3719:ASP:HB2	1:A:3722:TYR:HB3	1.98	0.44
1:B:603:LEU:HA	1:B:606:LEU:HD12	2.00	0.44
1:B:884:LEU:HD13	1:B:968:ALA:H	1.83	0.44
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.50	0.44
1:B:1849:LEU:HD23	1:B:1849:LEU:HA	1.87	0.44
1:B:2165:LEU:HD21	1:B:2177:LEU:HD23	1.99	0.44
1:B:3326:ASN:HB3	1:B:3329:ILE:HD13	1.99	0.44
1:C:3316:LEU:HD11	1:C:3353:LEU:HD11	2.00	0.44
1:C:4687:TYR:HE2	1:C:4703:ARG:HG2	1.82	0.44
1:D:3006:ILE:HD12	1:D:3010:PHE:HE2	1.83	0.44
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.90	0.44
1:A:793:LEU:HB2	1:A:797:HIS:HB2	2.00	0.44
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	2.00	0.44
1:C:877:ASN:HA	1:C:970:LEU:H	1.83	0.44
1:D:129:ASP:N	1:D:129:ASP:OD1	2.50	0.44
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.49	0.44
1:D:2211:MET:HE1	1:D:2229:VAL:HA	2.00	0.44
1:D:4112:LEU:O	1:D:4115:SER:OG	2.32	0.44
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.99	0.43
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.43	0.43
1:A:3219:TYR:OH	1:A:3239:MET:SD	2.73	0.43
1:A:4687:TYR:HE2	1:A:4703:ARG:HG2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3006:ILE:HD12	1:B:3010:PHE:HE2	1.83	0.43
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.83	0.43
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.99	0.43
1:D:2215:LEU:HD23	1:D:2260:ASN:HB3	2.00	0.43
1:D:4244:GLU:HG2	1:D:4668:LEU:HD13	2.01	0.43
1:D:4989:MET:HE2	1:D:4989:MET:HB2	1.70	0.43
1:A:2215:LEU:HD23	1:A:2260:ASN:HB3	2.00	0.43
1:A:3992:PHE:HB2	1:A:4023:MET:HE1	2.00	0.43
1:B:766:GLY:HA2	1:B:1475:THR:O	2.18	0.43
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.99	0.43
1:B:1568:LYS:HE2	1:B:1574:PRO:HD3	1.99	0.43
1:C:145:ALA:HA	1:C:175:SER:HB3	1.99	0.43
1:C:766:GLY:HA2	1:C:1475:THR:O	2.18	0.43
1:C:1256:GLU:HB3	1:C:1275:ARG:HD2	2.00	0.43
1:C:3366:ARG:NH1	1:C:3440:GLU:OE1	2.47	0.43
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	2.01	0.43
1:C:5011:TRP:HD1	1:C:5011:TRP:HA	1.66	0.43
1:D:3388:GLU:HA	1:D:3391:GLU:HB3	1.99	0.43
1:A:498:THR:HA	1:A:553:ARG:HH22	1.82	0.43
1:B:1221:GLU:HG3	1:B:1223:PHE:HD1	1.83	0.43
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	2.00	0.43
1:B:3334:TRP:CD1	1:B:3334:TRP:H	2.37	0.43
1:B:4957:LYS:HB2	1:B:4957:LYS:HE2	1.64	0.43
1:C:2165:LEU:HD21	1:C:2177:LEU:HD23	1.99	0.43
1:C:4190:ILE:H	1:C:4190:ILE:HG12	1.49	0.43
1:D:640:TYR:HD2	1:D:1634:LEU:HB3	1.82	0.43
1:D:766:GLY:HA2	1:D:1475:THR:O	2.18	0.43
1:D:1256:GLU:HB3	1:D:1275:ARG:HD2	2.00	0.43
1:D:1568:LYS:HE2	1:D:1574:PRO:HD3	1.99	0.43
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.29	0.43
1:A:465:GLN:HA	1:A:468:LEU:HB2	2.00	0.43
1:A:2211:MET:HE1	1:A:2229:VAL:HA	2.00	0.43
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.33	0.43
1:A:4879:MET:HE3	1:A:4879:MET:HB3	1.83	0.43
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	2.00	0.43
1:D:2716:ASP:N	1:D:2716:ASP:OD1	2.50	0.43
1:D:3316:LEU:HD11	1:D:3353:LEU:HD11	2.00	0.43
1:B:294:THR:HG23	1:B:297:GLN:H	1.82	0.43
1:C:102:LEU:HA	1:C:162:LYS:HA	2.00	0.43
1:C:603:LEU:HA	1:C:606:LEU:HD12	2.00	0.43
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3006:ILE:HD12	1:C:3010:PHE:HE2	1.83	0.43
1:C:4944:ARG:NE	1:D:4938:ASP:OD1	2.51	0.43
1:D:3844:LEU:HD21	1:D:3933:PHE:HA	2.01	0.43
1:A:766:GLY:HA2	1:A:1475:THR:O	2.18	0.43
1:A:1221:GLU:HG3	1:A:1223:PHE:HD1	1.83	0.43
1:A:1737:PRO:HD3	1:A:1771:LEU:HG	2.00	0.43
1:A:3281:LEU:HD12	1:A:3315:LEU:HD22	1.99	0.43
1:A:3366:ARG:NH1	1:A:3440:GLU:OE1	2.47	0.43
1:B:721:LEU:HD23	1:B:721:LEU:HA	1.90	0.43
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.83	0.43
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.82	0.43
1:B:3388:GLU:HA	1:B:3391:GLU:HB3	1.99	0.43
1:C:1221:GLU:HG3	1:C:1223:PHE:HD1	1.83	0.43
1:C:3992:PHE:HB2	1:C:4023:MET:HE1	2.00	0.43
1:C:4184:MET:HE2	1:C:4184:MET:HB2	1.81	0.43
1:C:4244:GLU:HG2	1:C:4668:LEU:HD13	2.01	0.43
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.83	0.43
1:D:3326:ASN:HB3	1:D:3329:ILE:HD13	1.99	0.43
1:D:4880:MET:HB2	1:D:4880:MET:HE2	1.74	0.43
1:A:400:ALA:HA	1:A:403:MET:HG2	2.01	0.43
1:A:665:GLU:HB2	1:A:792:LEU:HB2	2.00	0.43
1:A:3388:GLU:HA	1:A:3391:GLU:HB3	1.99	0.43
1:B:400:ALA:HA	1:B:403:MET:HG2	2.01	0.43
1:B:4244:GLU:HG2	1:B:4668:LEU:HD13	2.01	0.43
1:C:793:LEU:HB2	1:C:797:HIS:HB2	2.00	0.43
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	2.01	0.43
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.43
1:C:2769:ASP:HA	1:C:2772:GLN:HB2	1.99	0.43
1:C:3329:ILE:HD11	1:C:3332:ALA:HB2	1.99	0.43
1:C:3996:PHE:O	1:C:4000:MET:HG2	2.18	0.43
1:D:877:ASN:HA	1:D:970:LEU:H	1.83	0.43
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	2.01	0.43
1:D:1737:PRO:HD3	1:D:1771:LEU:HG	2.01	0.43
1:D:3329:ILE:HD11	1:D:3332:ALA:HB2	1.99	0.43
1:D:3471:THR:O	1:D:3475:LYS:HG3	2.19	0.43
1:A:893:TYR:HB3	1:A:960:MET:HE2	2.01	0.43
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	2.01	0.43
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	2.01	0.43
1:B:893:TYR:HB3	1:B:960:MET:HE2	2.01	0.43
1:B:2354:VAL:O	1:B:2358:ILE:HG12	2.19	0.43
1:B:3211:ASN:HB3	1:B:3236:VAL:HG21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3731:LYS:HA	1:B:3731:LYS:HD3	1.76	0.43
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	2.01	0.43
1:B:3996:PHE:O	1:B:4000:MET:HG2	2.18	0.43
1:C:3037:GLU:HG3	1:C:3088:VAL:HG21	2.01	0.43
1:C:3211:ASN:HB3	1:C:3236:VAL:HG21	2.01	0.43
1:C:3844:LEU:HD21	1:C:3933:PHE:HA	2.01	0.43
1:D:1782:PHE:O	2:H:82:TYR:OH	2.28	0.43
1:A:279:PRO:HD3	1:A:327:PRO:HB3	2.01	0.43
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.47	0.43
1:A:3346:VAL:HG22	1:A:3415:TYR:HB2	2.01	0.43
1:A:3471:THR:O	1:A:3475:LYS:HG3	2.19	0.43
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	2.01	0.43
1:B:1792:ALA:O	1:B:2176:ASN:ND2	2.52	0.43
1:B:3281:LEU:HD12	1:B:3315:LEU:HD22	1.99	0.43
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.54	0.43
1:C:2354:VAL:O	1:C:2358:ILE:HG12	2.19	0.43
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	2.00	0.43
1:D:1830:VAL:HB	1:D:1837:GLN:HG3	2.01	0.43
1:D:3366:ARG:NH1	1:D:3440:GLU:OE1	2.47	0.43
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.84	0.43
1:A:1568:LYS:HE2	1:A:1574:PRO:HD3	1.99	0.43
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.52	0.43
1:A:2354:VAL:O	1:A:2358:ILE:HG12	2.19	0.43
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.83	0.43
1:B:665:GLU:HB2	1:B:792:LEU:HB2	2.00	0.43
1:B:783:PHE:HB2	1:B:787:VAL:HG21	2.01	0.43
1:B:793:LEU:HB2	1:B:797:HIS:HB2	2.00	0.43
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.84	0.43
1:C:3326:ASN:HB3	1:C:3329:ILE:HD13	1.99	0.43
1:C:3801:GLY:O	1:C:3805:LEU:HB2	2.19	0.43
1:D:721:LEU:HD23	1:D:721:LEU:HA	1.90	0.43
1:D:793:LEU:HB2	1:D:797:HIS:HB2	2.00	0.43
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.54	0.43
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.84	0.43
1:D:3346:VAL:HG22	1:D:3415:TYR:HB2	2.01	0.43
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	2.00	0.42
1:A:3334:TRP:CD1	1:A:3334:TRP:H	2.37	0.42
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.80	0.42
1:B:3844:LEU:HD21	1:B:3933:PHE:HA	2.01	0.42
1:C:400:ALA:HA	1:C:403:MET:HG2	2.01	0.42
1:C:783:PHE:HB2	1:C:787:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1248:VAL:HG12	1:C:1599:MET:HG3	2.01	0.42
1:C:2466:LEU:HD23	1:C:2466:LEU:HA	1.88	0.42
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.50	0.42
1:C:3334:TRP:CD1	1:C:3334:TRP:H	2.37	0.42
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.41	0.42
1:D:884:LEU:HD13	1:D:968:ALA:H	1.83	0.42
1:D:2354:VAL:O	1:D:2358:ILE:HG12	2.19	0.42
1:D:3211:ASN:HB3	1:D:3236:VAL:HG21	2.01	0.42
2:G:49:ARG:N	2:G:54:GLU:OE2	2.52	0.42
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.54	0.42
1:A:3211:ASN:HB3	1:A:3236:VAL:HG21	2.01	0.42
1:A:3316:LEU:HD11	1:A:3353:LEU:HD11	2.00	0.42
1:A:3875:MET:HB3	1:A:3878:ASP:HB3	2.02	0.42
1:B:416:LYS:HB3	1:B:416:LYS:HE2	1.76	0.42
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.54	0.42
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.84	0.42
1:B:1689:VAL:HG21	1:B:1714:LEU:HD21	2.01	0.42
1:B:3799:LYS:HE3	1:B:3799:LYS:HB2	1.94	0.42
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.45	0.42
1:B:4578:LEU:HD23	1:C:4879:MET:HE3	2.01	0.42
1:C:465:GLN:HA	1:C:468:LEU:HB2	2.00	0.42
1:C:3471:THR:O	1:C:3475:LYS:HG3	2.19	0.42
1:D:2165:LEU:HD22	1:D:2174:GLU:HG2	2.01	0.42
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.46	0.42
1:A:3162:GLN:HG2	1:A:3201:MET:HE1	2.01	0.42
1:A:3801:GLY:O	1:A:3805:LEU:HB2	2.19	0.42
1:B:253:CYS:O	1:B:258:SER:OG	2.34	0.42
1:B:3471:THR:O	1:B:3475:LYS:HG3	2.19	0.42
1:D:244:LEU:HD23	1:D:244:LEU:HA	1.90	0.42
1:D:1792:ALA:O	1:D:2176:ASN:ND2	2.52	0.42
1:D:2611:CYS:HA	1:D:2614:ILE:HG22	2.02	0.42
1:D:3162:GLN:HG2	1:D:3201:MET:HE1	2.01	0.42
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	2.00	0.42
2:H:49:ARG:N	2:H:54:GLU:OE2	2.52	0.42
1:A:815:VAL:O	1:A:1007:TYR:OH	2.29	0.42
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	2.00	0.42
1:A:2927:LEU:HD12	1:A:2927:LEU:HA	1.87	0.42
1:A:4244:GLU:HG2	1:A:4668:LEU:HD13	2.01	0.42
1:B:129:ASP:N	1:B:129:ASP:OD1	2.50	0.42
1:B:3362:ILE:HG13	1:B:3437:MET:HG2	2.01	0.42
1:B:3801:GLY:O	1:B:3805:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3992:PHE:HB2	1:B:4023:MET:HE1	2.00	0.42
1:C:1634:LEU:HD23	1:C:1634:LEU:HA	1.91	0.42
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.53	0.42
1:C:3875:MET:HB3	1:C:3878:ASP:HB3	2.02	0.42
1:D:279:PRO:HD3	1:D:327:PRO:HB3	2.01	0.42
1:D:400:ALA:HA	1:D:403:MET:HG2	2.01	0.42
1:D:1221:GLU:HG3	1:D:1223:PHE:HD1	1.83	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.54	0.42
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.19	0.42
1:A:743:VAL:HB	1:A:760:ASN:HA	2.02	0.42
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.53	0.42
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	2.02	0.42
1:B:3037:GLU:HG3	1:B:3088:VAL:HG21	2.01	0.42
1:B:3875:MET:HB3	1:B:3878:ASP:HB3	2.02	0.42
1:C:206:CYS:HB2	1:C:271:GLY:HA3	2.01	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.54	0.42
1:C:1689:VAL:HG21	1:C:1714:LEU:HD21	2.01	0.42
1:C:2138:LEU:HD23	1:C:2138:LEU:HA	1.90	0.42
1:C:2616:PRO:HA	1:C:2619:LEU:HD12	2.02	0.42
1:D:1248:VAL:HG12	1:D:1599:MET:HG3	2.01	0.42
1:D:2616:PRO:HA	1:D:2619:LEU:HD12	2.02	0.42
1:A:1248:VAL:HG12	1:A:1599:MET:HG3	2.01	0.42
1:A:4182:GLU:HA	1:A:4191:GLU:O	2.20	0.42
1:A:5012:LYS:HB3	1:A:5012:LYS:HE3	1.69	0.42
1:B:743:VAL:HB	1:B:760:ASN:HA	2.02	0.42
1:B:1248:VAL:HG12	1:B:1599:MET:HG3	2.01	0.42
1:B:1830:VAL:HB	1:B:1837:GLN:HG3	2.01	0.42
1:B:2624:ARG:HG3	1:B:2910:THR:HB	2.02	0.42
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.50	0.42
1:B:3641:LEU:HA	1:B:3644:LEU:HD23	2.01	0.42
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.52	0.42
1:C:2611:CYS:HA	1:C:2614:ILE:HG22	2.02	0.42
1:D:107:ILE:N	1:D:148:TRP:O	2.40	0.42
1:D:206:CYS:HB2	1:D:271:GLY:HA3	2.01	0.42
1:D:893:TYR:HB3	1:D:960:MET:HE2	2.01	0.42
1:D:1689:VAL:HG21	1:D:1714:LEU:HD21	2.02	0.42
1:D:3037:GLU:HG3	1:D:3088:VAL:HG21	2.01	0.42
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.45	0.42
1:D:3875:MET:HB3	1:D:3878:ASP:HB3	2.02	0.42
1:D:4188:ARG:HD2	1:D:4188:ARG:HA	1.58	0.42
1:A:1689:VAL:HG21	1:A:1714:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	2.01	0.42
1:A:5006:GLN:O	1:A:5010:VAL:HG12	2.20	0.42
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.54	0.42
1:B:2165:LEU:HD22	1:B:2174:GLU:HG2	2.01	0.42
1:B:2211:MET:HE1	1:B:2229:VAL:HA	2.00	0.42
1:B:2816:MET:HE3	1:B:2878:LEU:HD22	2.01	0.42
1:B:4944:ARG:NE	1:C:4938:ASP:OD1	2.51	0.42
1:C:1737:PRO:HD3	1:C:1771:LEU:HG	2.01	0.42
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	2.01	0.42
1:C:2165:LEU:HD22	1:C:2174:GLU:HG2	2.01	0.42
1:C:2211:MET:HE1	1:C:2229:VAL:HA	2.00	0.42
1:C:2316:LYS:HD3	1:C:2318:TYR:HE1	1.84	0.42
1:C:2624:ARG:HG3	1:C:2910:THR:HB	2.02	0.42
1:C:3641:LEU:HA	1:C:3644:LEU:HD23	2.01	0.42
1:D:1674:CYS:SG	1:D:1717:SER:OG	2.73	0.42
1:D:2816:MET:HE3	1:D:2878:LEU:HD22	2.01	0.42
1:D:5012:LYS:HB3	1:D:5012:LYS:HE3	1.69	0.42
2:F:49:ARG:N	2:F:54:GLU:OE2	2.52	0.42
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.54	0.42
1:A:2611:CYS:HA	1:A:2614:ILE:HG22	2.02	0.42
1:A:3641:LEU:HA	1:A:3644:LEU:HD23	2.01	0.42
1:A:3844:LEU:HD21	1:A:3933:PHE:HA	2.01	0.42
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.55	0.42
1:B:206:CYS:SG	1:B:207:SER:N	2.93	0.42
1:C:3353:LEU:HD23	1:C:3358:PHE:HE2	1.85	0.42
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.88	0.42
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	2.00	0.42
1:D:5006:GLN:O	1:D:5010:VAL:HG12	2.20	0.42
1:A:2316:LYS:HD3	1:A:2318:TYR:HE1	1.85	0.42
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	2.01	0.42
1:B:3346:VAL:HG22	1:B:3415:TYR:HB2	2.01	0.42
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.20	0.42
1:C:279:PRO:HD3	1:C:327:PRO:HB3	2.01	0.42
1:C:419:ASP:HA	1:C:422:SER:HB3	2.02	0.42
1:C:743:VAL:HB	1:C:760:ASN:HA	2.02	0.42
1:C:846:LEU:HD22	1:C:846:LEU:HA	1.89	0.42
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.38	0.42
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.43	0.42
1:C:2672:LEU:HD23	1:C:2672:LEU:HA	1.83	0.42
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	2.01	0.42
1:C:3337:ARG:HA	1:C:3340:VAL:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3346:VAL:HG22	1:C:3415:TYR:HB2	2.01	0.42
1:C:4727:LYS:HG2	1:C:4728:HIS:CD2	2.55	0.42
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.02	0.42
1:D:3334:TRP:CD1	1:D:3334:TRP:H	2.37	0.42
1:D:3353:LEU:HD23	1:D:3358:PHE:HE2	1.85	0.42
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.53	0.42
1:D:3781:GLN:NE2	1:D:3819:TYR:OH	2.41	0.42
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	2.01	0.42
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.20	0.42
1:A:4727:LYS:HG2	1:A:4728:HIS:CD2	2.55	0.42
1:B:465:GLN:HA	1:B:468:LEU:HB2	2.00	0.42
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.50	0.42
1:B:1737:PRO:HD3	1:B:1771:LEU:HG	2.01	0.42
1:B:2891:LYS:HA	1:B:2891:LYS:HD3	1.97	0.42
1:B:3091:GLY:O	1:B:3094:SER:OG	2.36	0.42
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.53	0.42
1:B:4227:GLU:H	1:B:4227:GLU:HG3	1.55	0.42
1:C:3219:TYR:OH	1:C:3239:MET:SD	2.73	0.42
1:C:3362:ILE:HG13	1:C:3437:MET:HG2	2.01	0.42
1:C:5006:GLN:O	1:C:5010:VAL:HG12	2.20	0.42
1:D:743:VAL:HB	1:D:760:ASN:HA	2.02	0.42
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	2.02	0.42
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.47	0.42
1:D:2863:SER:HA	1:D:2928:LYS:HG3	2.02	0.42
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.55	0.42
1:A:783:PHE:HB2	1:A:787:VAL:HG21	2.01	0.41
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.02	0.41
1:A:1097:THR:HA	1:A:1143:TRP:HE1	1.85	0.41
1:A:2624:ARG:HG3	1:A:2910:THR:HB	2.02	0.41
1:A:3144:PHE:CZ	1:A:3197:LEU:HD13	2.55	0.41
1:A:3352:GLU:O	1:A:3356:SER:OG	2.29	0.41
1:B:206:CYS:HB2	1:B:271:GLY:HA3	2.01	0.41
1:B:279:PRO:HD3	1:B:327:PRO:HB3	2.01	0.41
1:B:293:LEU:HB3	1:B:311:ALA:HB1	2.02	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HB2	2.55	0.41
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.41
1:B:4727:LYS:HG2	1:B:4728:HIS:CD2	2.55	0.41
1:C:4578:LEU:HD23	1:D:4879:MET:HE3	2.01	0.41
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.20	0.41
1:D:465:GLN:HA	1:D:468:LEU:HB2	2.00	0.41
1:D:638:ILE:HD11	1:D:702:TRP:HE3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	2.03	0.41
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.89	0.41
1:D:3641:LEU:HA	1:D:3644:LEU:HD23	2.01	0.41
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.90	0.41
1:D:3924:LEU:O	1:D:3928:GLU:HG2	2.20	0.41
1:D:4182:GLU:HA	1:D:4191:GLU:O	2.20	0.41
1:A:356:TRP:O	1:A:379:HIS:N	2.53	0.41
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.41	0.41
1:A:4031:LEU:HD23	1:A:4031:LEU:HA	1.88	0.41
1:B:1097:THR:HA	1:B:1143:TRP:HE1	1.85	0.41
1:B:2616:PRO:HB3	1:B:2647:HIS:HE1	1.85	0.41
1:B:3144:PHE:CZ	1:B:3197:LEU:HD13	2.56	0.41
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.02	0.41
1:C:1097:THR:HA	1:C:1143:TRP:HE1	1.85	0.41
1:C:2891:LYS:HA	1:C:2891:LYS:HD3	1.97	0.41
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.33	0.41
1:C:3162:GLN:HG2	1:C:3201:MET:HE1	2.01	0.41
1:D:2672:LEU:HD22	1:D:2710:LEU:HD23	2.02	0.41
2:E:49:ARG:N	2:E:54:GLU:OE2	2.52	0.41
1:A:75:VAL:O	1:A:79:GLN:HG2	2.21	0.41
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.89	0.41
1:A:1830:VAL:HB	1:A:1837:GLN:HG3	2.01	0.41
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	2.03	0.41
1:A:2816:MET:HE3	1:A:2878:LEU:HD22	2.01	0.41
1:A:3037:GLU:HG3	1:A:3088:VAL:HG21	2.01	0.41
1:A:3353:LEU:HD23	1:A:3358:PHE:HE2	1.85	0.41
1:A:3924:LEU:O	1:A:3928:GLU:HG2	2.20	0.41
1:B:75:VAL:O	1:B:79:GLN:HG2	2.21	0.41
1:C:893:TYR:HB3	1:C:960:MET:HE2	2.01	0.41
1:C:2616:PRO:HB3	1:C:2647:HIS:HE1	1.85	0.41
1:C:2816:MET:HE3	1:C:2878:LEU:HD22	2.01	0.41
1:D:75:VAL:O	1:D:79:GLN:HG2	2.21	0.41
1:D:2624:ARG:HG3	1:D:2910:THR:HB	2.02	0.41
1:D:4029:SER:HA	1:D:4032:GLU:HG3	2.02	0.41
1:A:426:ARG:NH1	1:A:429:GLY:O	2.41	0.41
1:A:2165:LEU:HD22	1:A:2174:GLU:HG2	2.01	0.41
1:A:2208:MET:HE1	1:A:2253:HIS:CE1	2.56	0.41
1:A:2863:SER:HA	1:A:2928:LYS:HG3	2.02	0.41
1:A:3362:ILE:HG13	1:A:3437:MET:HG2	2.02	0.41
1:B:1842:LEU:HD23	1:B:1842:LEU:HA	1.87	0.41
1:B:2616:PRO:HA	1:B:2619:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3162:GLN:HG2	1:B:3201:MET:HE1	2.01	0.41
1:B:3416:VAL:O	1:B:3420:ARG:N	2.53	0.41
1:B:3924:LEU:O	1:B:3928:GLU:HG2	2.20	0.41
1:B:4182:GLU:HA	1:B:4191:GLU:O	2.20	0.41
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.50	0.41
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.02	0.41
1:C:2773:ASN:OD1	1:C:2786:LYS:NZ	2.48	0.41
1:C:4779:LYS:HB3	1:C:4779:LYS:HE3	1.87	0.41
1:C:4911:LEU:HA	1:C:4914:VAL:HG22	2.03	0.41
1:D:206:CYS:SG	1:D:207:SER:N	2.93	0.41
1:D:3416:VAL:O	1:D:3420:ARG:N	2.53	0.41
1:D:3944:GLU:OE1	1:D:3946:GLN:N	2.50	0.41
1:D:4993:MET:HE2	1:D:4993:MET:HB3	1.86	0.41
1:A:206:CYS:HB2	1:A:271:GLY:HA3	2.01	0.41
1:A:419:ASP:HA	1:A:422:SER:HB3	2.02	0.41
1:A:638:ILE:HD11	1:A:702:TRP:HE3	1.85	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.02	0.41
1:A:3823:LYS:HA	1:A:3823:LYS:HD3	1.90	0.41
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.38	0.41
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.91	0.41
1:B:2672:LEU:HD23	1:B:2672:LEU:HA	1.83	0.41
1:B:4031:LEU:HD23	1:B:4031:LEU:HA	1.88	0.41
1:C:4798:MET:HE3	1:C:4798:MET:HB3	1.98	0.41
1:D:783:PHE:HB2	1:D:787:VAL:HG21	2.01	0.41
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.38	0.41
1:A:2616:PRO:HA	1:A:2619:LEU:HD12	2.01	0.41
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.20	0.41
1:A:4917:ASP:OD2	1:D:4888:TYR:OH	2.29	0.41
1:A:4937:ILE:HG12	1:B:4934:GLY:HA2	2.02	0.41
1:B:2208:MET:HE1	1:B:2253:HIS:CE1	2.56	0.41
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	2.02	0.41
1:B:3353:LEU:HD23	1:B:3358:PHE:HE2	1.85	0.41
1:C:638:ILE:HD11	1:C:702:TRP:HE3	1.85	0.41
1:D:293:LEU:HB3	1:D:311:ALA:HB1	2.02	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.50	0.41
1:D:3091:GLY:O	1:D:3094:SER:OG	2.36	0.41
1:D:3888:LEU:HD23	1:D:3888:LEU:HA	1.89	0.41
1:D:4727:LYS:HG2	1:D:4728:HIS:CD2	2.55	0.41
1:D:4911:LEU:HA	1:D:4914:VAL:HG22	2.03	0.41
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.38	0.41
1:A:2716:ASP:N	1:A:2716:ASP:OD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3354:LEU:HD22	1:A:3423:TRP:HE1	1.86	0.41
1:A:3655:GLU:HA	1:A:3658:LYS:HG2	2.03	0.41
1:B:4801:LEU:HD23	1:B:4801:LEU:HA	1.88	0.41
1:C:394:GLN:HE22	1:C:396:GLU:HB2	1.86	0.41
1:C:733:PRO:HG2	1:C:762:CYS:HB3	2.03	0.41
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.56	0.41
1:C:2304:GLY:HA2	1:C:2307:LEU:HG	2.02	0.41
1:D:733:PRO:HG2	1:D:762:CYS:HB3	2.03	0.41
1:D:1097:THR:HA	1:D:1143:TRP:HE1	1.85	0.41
1:D:2304:GLY:HA2	1:D:2307:LEU:HG	2.02	0.41
1:D:2616:PRO:HB3	1:D:2647:HIS:HE1	1.85	0.41
2:H:105:ASN:OD1	2:H:106:LEU:N	2.54	0.41
1:A:293:LEU:HB3	1:A:311:ALA:HB1	2.02	0.41
1:A:1634:LEU:HD23	1:A:1634:LEU:HA	1.91	0.41
1:A:2672:LEU:HD22	1:A:2710:LEU:HD23	2.02	0.41
1:A:3132:THR:HG23	1:A:3136:LEU:HD22	2.03	0.41
1:B:2316:LYS:HD3	1:B:2318:TYR:HE1	1.84	0.41
1:B:3337:ARG:HA	1:B:3340:VAL:HG22	2.02	0.41
1:B:4814:LEU:HD23	1:B:4814:LEU:HA	1.91	0.41
1:C:206:CYS:SG	1:C:207:SER:N	2.93	0.41
1:C:1792:ALA:HA	1:C:2173:GLN:HA	2.03	0.41
1:C:1929:MET:HE2	1:C:1929:MET:HB3	1.98	0.41
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	2.02	0.41
1:C:2672:LEU:HD22	1:C:2710:LEU:HD23	2.02	0.41
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	2.01	0.41
1:D:3589:PRO:HA	1:D:3592:ILE:HG22	2.03	0.41
1:D:3677:LEU:HD23	1:D:3677:LEU:HA	1.91	0.41
1:D:4823:LEU:HA	1:D:4823:LEU:HD23	1.84	0.41
1:D:4957:LYS:HE2	1:D:4957:LYS:HB2	1.64	0.41
1:A:383:HIS:N	1:A:386:ASP:OD2	2.54	0.41
1:A:2616:PRO:HB3	1:A:2647:HIS:HE1	1.85	0.41
1:A:3337:ARG:HA	1:A:3340:VAL:HG22	2.02	0.41
1:A:3589:PRO:HA	1:A:3592:ILE:HG22	2.03	0.41
1:A:3882:GLN:HG3	1:A:3957:VAL:HG22	2.03	0.41
1:A:4895:GLY:O	1:D:4892:ARG:NH1	2.46	0.41
1:A:4911:LEU:HA	1:A:4914:VAL:HG22	2.03	0.41
1:A:4944:ARG:NE	1:B:4938:ASP:OD1	2.51	0.41
1:B:356:TRP:O	1:B:379:HIS:N	2.54	0.41
1:B:638:ILE:HD11	1:B:702:TRP:HE3	1.85	0.41
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.02	0.41
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:GLU:HB2	1:B:1203:ASN:HB3	2.03	0.41
1:B:1792:ALA:HA	1:B:2173:GLN:HA	2.03	0.41
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.21	0.41
1:B:2228:MET:HE3	1:B:2228:MET:HB3	1.95	0.41
1:B:2304:GLY:HA2	1:B:2307:LEU:HG	2.02	0.41
1:B:3102:ASP:HA	1:B:3105:LYS:HE2	2.03	0.41
1:B:3104:GLU:HG2	1:B:3171:SER:HB3	2.03	0.41
1:B:5006:GLN:O	1:B:5010:VAL:HG12	2.20	0.41
1:C:293:LEU:HB3	1:C:311:ALA:HB1	2.02	0.41
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	2.03	0.41
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.54	0.41
1:C:2208:MET:HE1	1:C:2253:HIS:CE1	2.56	0.41
1:C:2863:SER:HA	1:C:2928:LYS:HG3	2.02	0.41
1:C:3102:ASP:HA	1:C:3105:LYS:HE2	2.03	0.41
1:C:3104:GLU:HG2	1:C:3171:SER:HB3	2.03	0.41
1:C:3400:VAL:HG23	1:C:3403:ARG:HE	1.86	0.41
1:C:3655:GLU:HA	1:C:3658:LYS:HG2	2.03	0.41
1:C:4182:GLU:HA	1:C:4191:GLU:O	2.20	0.41
1:D:356:TRP:O	1:D:379:HIS:N	2.54	0.41
1:D:383:HIS:N	1:D:386:ASP:OD2	2.54	0.41
1:D:2109:ASP:N	1:D:2109:ASP:OD1	2.54	0.41
1:D:2208:MET:HE1	1:D:2253:HIS:CE1	2.56	0.41
1:D:3144:PHE:CZ	1:D:3197:LEU:HD13	2.55	0.41
1:D:3337:ARG:HA	1:D:3340:VAL:HG22	2.02	0.41
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.39	0.41
2:F:105:ASN:OD1	2:F:106:LEU:N	2.54	0.41
1:A:4993:MET:HE2	1:A:4993:MET:HB3	1.86	0.41
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.02	0.41
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.54	0.41
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.33	0.41
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.90	0.41
1:B:4686:LEU:O	1:B:4691:GLN:N	2.50	0.41
1:C:416:LYS:HB3	1:C:416:LYS:HE2	1.76	0.41
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.21	0.41
1:C:3144:PHE:CZ	1:C:3197:LEU:HD13	2.56	0.41
1:C:4675:LYS:HD2	1:C:4679:ARG:HH21	1.86	0.41
1:D:2690:LYS:HA	1:D:2690:LYS:HD2	1.90	0.41
2:G:77:THR:HG22	2:G:80:VAL:HG22	2.03	0.41
1:A:733:PRO:HG2	1:A:762:CYS:HB3	2.03	0.40
1:A:838:HIS:CE1	1:A:1201:HIS:HB2	2.55	0.40
1:A:4029:SER:HA	1:A:4032:GLU:HG3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4675:LYS:HD2	1:A:4679:ARG:HH21	1.86	0.40
1:A:4723:LYS:HB3	1:A:4723:LYS:HE2	1.98	0.40
1:B:383:HIS:N	1:B:386:ASP:OD2	2.54	0.40
1:B:2711:PRO:HA	1:B:2712:PRO:HD3	1.94	0.40
1:B:3589:PRO:HA	1:B:3592:ILE:HG22	2.03	0.40
1:B:4029:SER:HA	1:B:4032:GLU:HG3	2.02	0.40
1:D:419:ASP:HA	1:D:422:SER:HB3	2.02	0.40
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.55	0.40
1:D:3362:ILE:HG13	1:D:3437:MET:HG2	2.02	0.40
1:A:1128:ARG:HB2	1:A:1130:GLN:HE22	1.87	0.40
1:A:2461:VAL:O	1:A:2510:TYR:OH	2.30	0.40
1:A:3172:ILE:HG21	1:A:3194:LEU:HD13	2.03	0.40
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.87	0.40
1:B:733:PRO:HG2	1:B:762:CYS:HB3	2.03	0.40
1:B:3545:THR:HG23	1:B:3548:GLU:H	1.87	0.40
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.57	0.40
1:B:3882:GLN:HG3	1:B:3957:VAL:HG22	2.03	0.40
1:C:660:GLY:O	1:C:750:LEU:N	2.53	0.40
1:C:3354:LEU:HD22	1:C:3423:TRP:HE1	1.86	0.40
1:C:3604:TYR:O	1:C:3608:GLN:HG2	2.22	0.40
1:C:3862:ASP:OD1	1:C:3862:ASP:N	2.45	0.40
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	2.03	0.40
1:D:2773:ASN:OD1	1:D:2786:LYS:NZ	2.48	0.40
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.46	0.40
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.86	0.40
1:D:3604:TYR:O	1:D:3608:GLN:HG2	2.22	0.40
1:D:3882:GLN:HG3	1:D:3957:VAL:HG22	2.03	0.40
1:D:4686:LEU:O	1:D:4691:GLN:N	2.50	0.40
1:A:22:LEU:HD23	1:A:202:MET:HE1	2.04	0.40
1:A:869:ARG:CZ	1:A:870:ILE:HB	2.50	0.40
1:A:2304:GLY:HA2	1:A:2307:LEU:HG	2.02	0.40
1:A:3438:VAL:HG21	1:A:3517:MET:HG3	2.03	0.40
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.56	0.40
1:B:676:THR:HG22	1:B:677:ALA:H	1.87	0.40
1:B:846:LEU:HD22	1:B:846:LEU:HA	1.89	0.40
1:B:1128:ARG:HB2	1:B:1130:GLN:HE22	1.87	0.40
1:B:3132:THR:HG23	1:B:3136:LEU:HD22	2.03	0.40
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.39	0.40
1:B:3354:LEU:HD22	1:B:3423:TRP:HE1	1.86	0.40
1:B:3438:VAL:HG21	1:B:3517:MET:HG3	2.04	0.40
1:C:3132:THR:HG23	1:C:3136:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.57	0.40
1:C:3924:LEU:O	1:C:3928:GLU:HG2	2.20	0.40
1:C:4127:GLU:O	1:C:4131:ARG:HB2	2.22	0.40
1:D:2316:LYS:HD3	1:D:2318:TYR:HE1	1.85	0.40
1:D:3104:GLU:HG2	1:D:3171:SER:HB3	2.03	0.40
1:D:3354:LEU:HD22	1:D:3423:TRP:HE1	1.86	0.40
2:H:77:THR:HG22	2:H:80:VAL:HG22	2.03	0.40
1:A:183:SER:O	1:A:183:SER:OG	2.38	0.40
1:A:206:CYS:SG	1:A:207:SER:N	2.93	0.40
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.03	0.40
1:A:1792:ALA:HA	1:A:2173:GLN:HA	2.03	0.40
1:A:2711:PRO:HA	1:A:2712:PRO:HD3	1.94	0.40
1:A:3104:GLU:HG2	1:A:3171:SER:HB3	2.03	0.40
1:A:3400:VAL:HG23	1:A:3403:ARG:HE	1.86	0.40
1:B:2672:LEU:HD22	1:B:2710:LEU:HD23	2.02	0.40
1:B:3152:PHE:HB3	1:B:3156:VAL:HG23	2.03	0.40
1:B:3301:PRO:HA	1:B:3302:PRO:HD3	1.92	0.40
1:B:3511:VAL:HG12	1:B:3514:LEU:HD12	2.04	0.40
1:B:3655:GLU:HA	1:B:3658:LYS:HG2	2.03	0.40
1:B:4823:LEU:HA	1:B:4823:LEU:HD23	1.84	0.40
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.04	0.40
1:C:1091:GLU:HB2	1:C:1203:ASN:HB3	2.03	0.40
1:C:3589:PRO:HA	1:C:3592:ILE:HG22	2.03	0.40
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.39	0.40
1:D:932:LEU:HD22	1:D:984:LEU:HD21	2.04	0.40
1:D:3172:ILE:HG21	1:D:3194:LEU:HD13	2.03	0.40
1:D:3400:VAL:HG23	1:D:3403:ARG:HE	1.86	0.40
1:D:4127:GLU:O	1:D:4131:ARG:HB2	2.22	0.40
1:A:4821:LYS:H	1:A:4821:LYS:HG2	1.75	0.40
1:B:394:GLN:HE22	1:B:396:GLU:HB2	1.86	0.40
1:B:2863:SER:HA	1:B:2928:LYS:HG3	2.02	0.40
1:B:4675:LYS:HD2	1:B:4679:ARG:HH21	1.86	0.40
1:C:676:THR:HG22	1:C:677:ALA:H	1.87	0.40
1:C:3302:PRO:HA	1:C:3303:PRO:HD3	1.98	0.40
1:C:3882:GLN:HG3	1:C:3957:VAL:HG22	2.03	0.40
1:D:1000:ARG:HA	1:D:1000:ARG:HD3	1.80	0.40
1:D:1091:GLU:HB2	1:D:1203:ASN:HB3	2.03	0.40
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.41	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	4355/5037 (86%)	4218 (97%)	133 (3%)	4 (0%)	48	78
1	B	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	48	78
1	C	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	48	78
1	D	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	48	78
2	E	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	F	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	G	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	H	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
All	All	17840/21548 (83%)	17287 (97%)	537 (3%)	16 (0%)	49	78

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	B	3615	SER
1	C	3615	SER
1	D	3615	SER
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	842	PRO
1	B	842	PRO
1	C	842	PRO
1	D	842	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	3807/4276 (89%)	3689 (97%)	118 (3%)	35	58
1	B	3807/4276 (89%)	3689 (97%)	118 (3%)	35	58
1	C	3807/4276 (89%)	3689 (97%)	118 (3%)	35	58
1	D	3807/4276 (89%)	3689 (97%)	118 (3%)	35	58
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15580/18320 (85%)	15108 (97%)	472 (3%)	38	59

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	LEU
1	A	1072	VAL
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2584[A]	HIS
1	A	2584[B]	HIS
1	A	3422[A]	HIS
1	A	3422[B]	HIS
1	A	4180	ARG
1	A	4181	ILE
1	A	4182	GLU
1	A	4183	ILE
1	A	4184	MET
1	A	4188	ARG
1	A	4190	ILE
1	A	4193	ILE
1	A	4198	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4202	ARG
1	A	4204	GLN
1	A	4211	LYS
1	A	4224	GLU
1	A	4227	GLU
1	A	4230	LYS
1	A	4247	ILE
1	A	4252	SER
1	A	4253	GLU
1	A	4544	LEU
1	A	4546	VAL
1	A	4548	ARG
1	A	4550	LYS
1	A	4552	LEU
1	A	4577	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4584	ASP
1	A	4585	SER
1	A	4628	VAL
1	A	4632	LEU
1	A	4633	GLU
1	A	4634	GLU
1	A	4635	SER
1	A	4647	SER
1	A	4648	LEU
1	A	4662	ASN
1	A	4665	LYS
1	A	4666	VAL
1	A	4667	PRO
1	A	4669	VAL
1	A	4675	LYS
1	A	4680	LYS
1	A	4684	ASP
1	A	4690	GLU
1	A	4692	PRO
1	A	4694	ASP
1	A	4695	ASP
1	A	4696	ASP
1	A	4698	LYS
1	A	4704	LEU
1	A	4707	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4710	SER
1	A	4720	VAL
1	A	4721	LYS
1	A	4734	ARG
1	A	4737	ILE
1	A	4739	GLU
1	A	4743	MET
1	A	4748	LEU
1	A	4750	ILE
1	A	4773	VAL
1	A	4779	LYS
1	A	4796	MET
1	A	4797	VAL
1	A	4809	PHE
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4824	ARG
1	A	4826	ILE
1	A	4835	LYS
1	A	4838	VAL
1	A	4839	MET
1	A	4844	LEU
1	A	4861	LYS
1	A	4866	SER
1	A	4867	GLU
1	A	4869	GLU
1	A	4871	GLU
1	A	4876	CYS
1	A	4878	ASP
1	A	4880	MET
1	A	4889	VAL
1	A	4902	GLU
1	A	4911	LEU
1	A	4913	ARG
1	A	4945	ASP
1	A	4949	GLN
1	A	4951	LYS
1	A	4952	GLU
1	A	4954	MET
1	A	4957	LYS
1	A	4958	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4970	THR
1	A	4971	THR
1	A	4980	LEU
1	A	4982	GLU
1	A	4989	MET
1	A	5002	GLU
1	A	5008	SER
1	A	5010	VAL
1	A	5011	TRP
1	A	5012	LYS
1	A	5013	MET
1	A	5027	CYS
1	A	5028	PHE
1	A	5033	GLU
1	A	5036	LEU
1	B	846	LEU
1	B	1072	VAL
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2584[A]	HIS
1	B	2584[B]	HIS
1	B	3422[A]	HIS
1	B	3422[B]	HIS
1	B	4180	ARG
1	B	4181	ILE
1	B	4182	GLU
1	B	4183	ILE
1	B	4184	MET
1	B	4188	ARG
1	B	4190	ILE
1	B	4193	ILE
1	B	4198	SER
1	B	4202	ARG
1	B	4204	GLN
1	B	4211	LYS
1	B	4224	GLU
1	B	4227	GLU
1	B	4230	LYS
1	B	4247	ILE
1	B	4252	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4253	GLU
1	B	4544	LEU
1	B	4546	VAL
1	B	4548	ARG
1	B	4550	LYS
1	B	4552	LEU
1	B	4577	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4584	ASP
1	B	4585	SER
1	B	4628	VAL
1	B	4632	LEU
1	B	4633	GLU
1	B	4634	GLU
1	B	4635	SER
1	B	4647	SER
1	B	4648	LEU
1	B	4662	ASN
1	B	4665	LYS
1	B	4666	VAL
1	B	4667	PRO
1	B	4669	VAL
1	B	4675	LYS
1	B	4680	LYS
1	B	4684	ASP
1	B	4690	GLU
1	B	4692	PRO
1	B	4694	ASP
1	B	4695	ASP
1	B	4696	ASP
1	B	4698	LYS
1	B	4704	LEU
1	B	4707	ASN
1	B	4710	SER
1	B	4720	VAL
1	B	4721	LYS
1	B	4734	ARG
1	B	4737	ILE
1	B	4739	GLU
1	B	4743	MET
1	B	4748	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4750	ILE
1	B	4773	VAL
1	B	4779	LYS
1	B	4796	MET
1	B	4797	VAL
1	B	4809	PHE
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4824	ARG
1	B	4826	ILE
1	B	4835	LYS
1	B	4838	VAL
1	B	4839	MET
1	B	4844	LEU
1	B	4861	LYS
1	B	4866	SER
1	B	4867	GLU
1	B	4869	GLU
1	B	4871	GLU
1	B	4876	CYS
1	B	4878	ASP
1	B	4880	MET
1	B	4889	VAL
1	B	4902	GLU
1	B	4911	LEU
1	B	4913	ARG
1	B	4945	ASP
1	B	4949	GLN
1	B	4951	LYS
1	B	4952	GLU
1	B	4954	MET
1	B	4957	LYS
1	B	4958	CYS
1	B	4970	THR
1	B	4971	THR
1	B	4980	LEU
1	B	4982	GLU
1	B	4989	MET
1	B	5002	GLU
1	B	5008	SER
1	B	5010	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	5011	TRP
1	B	5012	LYS
1	B	5013	MET
1	B	5027	CYS
1	B	5028	PHE
1	B	5033	GLU
1	B	5036	LEU
1	C	846	LEU
1	C	1072	VAL
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2584[A]	HIS
1	C	2584[B]	HIS
1	C	3422[A]	HIS
1	C	3422[B]	HIS
1	C	4180	ARG
1	C	4181	ILE
1	C	4182	GLU
1	C	4183	ILE
1	C	4184	MET
1	C	4188	ARG
1	C	4190	ILE
1	C	4193	ILE
1	C	4198	SER
1	C	4202	ARG
1	C	4204	GLN
1	C	4211	LYS
1	C	4224	GLU
1	C	4227	GLU
1	C	4230	LYS
1	C	4247	ILE
1	C	4252	SER
1	C	4253	GLU
1	C	4544	LEU
1	C	4546	VAL
1	C	4548	ARG
1	C	4550	LYS
1	C	4552	LEU
1	C	4577	LEU
1	C	4580	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4581	LYS
1	C	4584	ASP
1	C	4585	SER
1	C	4628	VAL
1	C	4632	LEU
1	C	4633	GLU
1	C	4634	GLU
1	C	4635	SER
1	C	4647	SER
1	C	4648	LEU
1	C	4662	ASN
1	C	4665	LYS
1	C	4666	VAL
1	C	4667	PRO
1	C	4669	VAL
1	C	4675	LYS
1	C	4680	LYS
1	C	4684	ASP
1	C	4690	GLU
1	C	4692	PRO
1	C	4694	ASP
1	C	4695	ASP
1	C	4696	ASP
1	C	4698	LYS
1	C	4704	LEU
1	C	4707	ASN
1	C	4710	SER
1	C	4720	VAL
1	C	4721	LYS
1	C	4734	ARG
1	C	4737	ILE
1	C	4739	GLU
1	C	4743	MET
1	C	4748	LEU
1	C	4750	ILE
1	C	4773	VAL
1	C	4779	LYS
1	C	4796	MET
1	C	4797	VAL
1	C	4809	PHE
1	C	4818	MET
1	C	4821	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4822	THR
1	C	4824	ARG
1	C	4826	ILE
1	C	4835	LYS
1	C	4838	VAL
1	C	4839	MET
1	C	4844	LEU
1	C	4861	LYS
1	C	4866	SER
1	C	4867	GLU
1	C	4869	GLU
1	C	4871	GLU
1	C	4876	CYS
1	C	4878	ASP
1	C	4880	MET
1	C	4889	VAL
1	C	4902	GLU
1	C	4911	LEU
1	C	4913	ARG
1	C	4945	ASP
1	C	4949	GLN
1	C	4951	LYS
1	C	4952	GLU
1	C	4954	MET
1	C	4957	LYS
1	C	4958	CYS
1	C	4970	THR
1	C	4971	THR
1	C	4980	LEU
1	C	4982	GLU
1	C	4989	MET
1	C	5002	GLU
1	C	5008	SER
1	C	5010	VAL
1	C	5011	TRP
1	C	5012	LYS
1	C	5013	MET
1	C	5027	CYS
1	C	5028	PHE
1	C	5033	GLU
1	C	5036	LEU
1	D	846	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1072	VAL
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2584[A]	HIS
1	D	2584[B]	HIS
1	D	3422[A]	HIS
1	D	3422[B]	HIS
1	D	4180	ARG
1	D	4181	ILE
1	D	4182	GLU
1	D	4183	ILE
1	D	4184	MET
1	D	4188	ARG
1	D	4190	ILE
1	D	4193	ILE
1	D	4198	SER
1	D	4202	ARG
1	D	4204	GLN
1	D	4211	LYS
1	D	4224	GLU
1	D	4227	GLU
1	D	4230	LYS
1	D	4247	ILE
1	D	4252	SER
1	D	4253	GLU
1	D	4544	LEU
1	D	4546	VAL
1	D	4548	ARG
1	D	4550	LYS
1	D	4552	LEU
1	D	4577	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4584	ASP
1	D	4585	SER
1	D	4628	VAL
1	D	4632	LEU
1	D	4633	GLU
1	D	4634	GLU
1	D	4635	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4647	SER
1	D	4648	LEU
1	D	4662	ASN
1	D	4665	LYS
1	D	4666	VAL
1	D	4667	PRO
1	D	4669	VAL
1	D	4675	LYS
1	D	4680	LYS
1	D	4684	ASP
1	D	4690	GLU
1	D	4692	PRO
1	D	4694	ASP
1	D	4695	ASP
1	D	4696	ASP
1	D	4698	LYS
1	D	4704	LEU
1	D	4707	ASN
1	D	4710	SER
1	D	4720	VAL
1	D	4721	LYS
1	D	4734	ARG
1	D	4737	ILE
1	D	4739	GLU
1	D	4743	MET
1	D	4748	LEU
1	D	4750	ILE
1	D	4773	VAL
1	D	4779	LYS
1	D	4796	MET
1	D	4797	VAL
1	D	4809	PHE
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4824	ARG
1	D	4826	ILE
1	D	4835	LYS
1	D	4838	VAL
1	D	4839	MET
1	D	4844	LEU
1	D	4861	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4866	SER
1	D	4867	GLU
1	D	4869	GLU
1	D	4871	GLU
1	D	4876	CYS
1	D	4878	ASP
1	D	4880	MET
1	D	4889	VAL
1	D	4902	GLU
1	D	4911	LEU
1	D	4913	ARG
1	D	4945	ASP
1	D	4949	GLN
1	D	4951	LYS
1	D	4952	GLU
1	D	4954	MET
1	D	4957	LYS
1	D	4958	CYS
1	D	4970	THR
1	D	4971	THR
1	D	4980	LEU
1	D	4982	GLU
1	D	4989	MET
1	D	5002	GLU
1	D	5008	SER
1	D	5010	VAL
1	D	5011	TRP
1	D	5012	LYS
1	D	5013	MET
1	D	5027	CYS
1	D	5028	PHE
1	D	5033	GLU
1	D	5036	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	297	GLN
1	A	383	HIS
1	A	636	ASN
1	A	720	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	765	GLN
1	A	877	ASN
1	A	1058	GLN
1	A	1066	GLN
1	A	1084	GLN
1	A	1158	ASN
1	A	1229	ASN
1	A	1558	HIS
1	A	1611	HIS
1	A	1631	GLN
1	A	2092	GLN
1	A	2173	GLN
1	A	2260	ASN
1	A	2284	ASN
1	A	2351	ASN
1	A	2772	GLN
1	A	3150	HIS
1	A	3162	GLN
1	A	3313	ASN
1	A	3418	ASN
1	A	3466	ASN
1	A	3555	ASN
1	A	3683	GLN
1	A	3896	ASN
1	A	4043	GLN
1	A	4162	ASN
1	A	4201	ASN
1	A	4246	GLN
1	A	4558	ASN
1	A	4707	ASN
1	A	4832	HIS
1	A	4836	GLN
1	A	4949	GLN
1	A	4973	HIS
1	A	4984	ASN
1	A	5003	HIS
1	A	5006	GLN
1	A	5035	GLN
1	B	56	GLN
1	B	383	HIS
1	B	636	ASN
1	B	720	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	765	GLN
1	B	838	HIS
1	B	877	ASN
1	B	1058	GLN
1	B	1066	GLN
1	B	1084	GLN
1	B	1158	ASN
1	B	1229	ASN
1	B	1558	HIS
1	B	1611	HIS
1	B	1631	GLN
1	B	1640	HIS
1	B	1691	GLN
1	B	1756	ASN
1	B	2092	GLN
1	B	2173	GLN
1	B	2260	ASN
1	B	2284	ASN
1	B	2351	ASN
1	B	2772	GLN
1	B	3150	HIS
1	B	3162	GLN
1	B	3313	ASN
1	B	3418	ASN
1	B	3466	ASN
1	B	3555	ASN
1	B	3683	GLN
1	B	3896	ASN
1	B	4043	GLN
1	B	4201	ASN
1	B	4246	GLN
1	B	4558	ASN
1	B	4707	ASN
1	B	4728	HIS
1	B	4832	HIS
1	B	4836	GLN
1	B	4973	HIS
1	B	4984	ASN
1	B	5003	HIS
1	B	5006	GLN
1	B	5035	GLN
1	C	56	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	203	ASN
1	C	383	HIS
1	C	636	ASN
1	C	720	HIS
1	C	765	GLN
1	C	877	ASN
1	C	1066	GLN
1	C	1084	GLN
1	C	1158	ASN
1	C	1229	ASN
1	C	1558	HIS
1	C	1559	GLN
1	C	1611	HIS
1	C	1631	GLN
1	C	1756	ASN
1	C	2092	GLN
1	C	2173	GLN
1	C	2260	ASN
1	C	2284	ASN
1	C	2351	ASN
1	C	2772	GLN
1	C	3007	ASN
1	C	3150	HIS
1	C	3162	GLN
1	C	3313	ASN
1	C	3418	ASN
1	C	3466	ASN
1	C	3555	ASN
1	C	3683	GLN
1	C	3896	ASN
1	C	4043	GLN
1	C	4201	ASN
1	C	4246	GLN
1	C	4558	ASN
1	C	4707	ASN
1	C	4728	HIS
1	C	4832	HIS
1	C	4973	HIS
1	C	4984	ASN
1	C	5003	HIS
1	C	5006	GLN
1	C	5035	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	56	GLN
1	D	297	GLN
1	D	383	HIS
1	D	636	ASN
1	D	765	GLN
1	D	877	ASN
1	D	1066	GLN
1	D	1084	GLN
1	D	1158	ASN
1	D	1229	ASN
1	D	1558	HIS
1	D	1611	HIS
1	D	1631	GLN
1	D	1756	ASN
1	D	2092	GLN
1	D	2173	GLN
1	D	2260	ASN
1	D	2284	ASN
1	D	2351	ASN
1	D	2772	GLN
1	D	3007	ASN
1	D	3150	HIS
1	D	3162	GLN
1	D	3313	ASN
1	D	3418	ASN
1	D	3466	ASN
1	D	3555	ASN
1	D	3683	GLN
1	D	3896	ASN
1	D	3960	GLN
1	D	4043	GLN
1	D	4201	ASN
1	D	4246	GLN
1	D	4558	ASN
1	D	4650	HIS
1	D	4707	ASN
1	D	4728	HIS
1	D	4832	HIS
1	D	4984	ASN
1	D	5003	HIS
1	D	5006	GLN
1	D	5035	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	87	HIS
2	F	87	HIS
2	G	43	ASN
2	G	87	HIS
2	H	87	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CMP	D	5101	-	25,25,25	1.70	7 (28%)	37,39,39	2.10	10 (27%)
3	CMP	B	5101	-	25,25,25	1.70	7 (28%)	37,39,39	2.10	10 (27%)
3	CMP	C	5101	-	25,25,25	1.70	7 (28%)	37,39,39	2.10	10 (27%)
3	CMP	A	5101	-	25,25,25	1.70	7 (28%)	37,39,39	2.10	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CMP	D	5101	-	-	0/4/31/31	0/4/4/4
3	CMP	B	5101	-	-	0/4/31/31	0/4/4/4
3	CMP	C	5101	-	-	0/4/31/31	0/4/4/4
3	CMP	A	5101	-	-	0/4/31/31	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	CMP	C5-C4	4.45	1.47	1.39
3	B	5101	CMP	C5-C4	4.45	1.47	1.39
3	C	5101	CMP	C5-C4	4.45	1.47	1.39
3	D	5101	CMP	C5-C4	4.45	1.47	1.39
3	D	5101	CMP	P-O3'	3.21	1.63	1.57
3	B	5101	CMP	P-O3'	3.21	1.63	1.57
3	C	5101	CMP	P-O3'	3.21	1.63	1.57
3	A	5101	CMP	P-O3'	3.21	1.63	1.57
3	C	5101	CMP	C5-C6	2.58	1.48	1.41
3	A	5101	CMP	C5-C6	2.58	1.48	1.41
3	B	5101	CMP	C5-C6	2.58	1.48	1.41
3	D	5101	CMP	C5-C6	2.58	1.48	1.41
3	D	5101	CMP	O5'-C5'	-2.57	1.42	1.46
3	C	5101	CMP	O5'-C5'	-2.56	1.42	1.46
3	B	5101	CMP	O5'-C5'	-2.56	1.42	1.46
3	A	5101	CMP	O5'-C5'	-2.55	1.42	1.46
3	C	5101	CMP	C5-N7	-2.53	1.34	1.39
3	D	5101	CMP	C5-N7	-2.53	1.34	1.39
3	A	5101	CMP	C5-N7	-2.53	1.34	1.39
3	B	5101	CMP	C5-N7	-2.53	1.34	1.39
3	C	5101	CMP	C8-N7	2.19	1.35	1.31
3	D	5101	CMP	C8-N7	2.19	1.35	1.31
3	A	5101	CMP	C8-N7	2.19	1.35	1.31
3	B	5101	CMP	C8-N7	2.18	1.35	1.31
3	C	5101	CMP	P-O5'	2.08	1.60	1.57
3	D	5101	CMP	P-O5'	2.08	1.60	1.57
3	A	5101	CMP	P-O5'	2.08	1.60	1.57
3	B	5101	CMP	P-O5'	2.07	1.60	1.57

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	CMP	C5-C4-N3	-6.42	117.88	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5101	CMP	C5-C4-N3	-6.41	117.88	126.72
3	A	5101	CMP	C5-C4-N3	-6.41	117.89	126.72
3	D	5101	CMP	C5-C4-N3	-6.41	117.89	126.72
3	C	5101	CMP	N3-C4-N9	5.05	135.76	127.17
3	A	5101	CMP	N3-C4-N9	5.05	135.76	127.17
3	B	5101	CMP	N3-C4-N9	5.05	135.76	127.17
3	D	5101	CMP	N3-C4-N9	5.05	135.75	127.17
3	C	5101	CMP	C2-N3-C4	4.09	121.83	111.83
3	B	5101	CMP	C2-N3-C4	4.09	121.82	111.83
3	D	5101	CMP	C2-N3-C4	4.09	121.82	111.83
3	A	5101	CMP	C2-N3-C4	4.09	121.82	111.83
3	D	5101	CMP	N3-C2-N1	-3.40	123.44	128.58
3	C	5101	CMP	N3-C2-N1	-3.39	123.44	128.58
3	A	5101	CMP	N3-C2-N1	-3.39	123.45	128.58
3	B	5101	CMP	N3-C2-N1	-3.39	123.45	128.58
3	C	5101	CMP	O2P-P-O1P	3.35	118.85	108.56
3	B	5101	CMP	O2P-P-O1P	3.35	118.85	108.56
3	D	5101	CMP	O2P-P-O1P	3.35	118.85	108.56
3	A	5101	CMP	O2P-P-O1P	3.35	118.85	108.56
3	B	5101	CMP	C4-C5-N7	-3.17	106.96	110.58
3	A	5101	CMP	C4-C5-N7	-3.17	106.96	110.58
3	D	5101	CMP	C4-C5-N7	-3.17	106.96	110.58
3	C	5101	CMP	C4-C5-N7	-3.16	106.97	110.58
3	D	5101	CMP	O5'-P-O3'	-3.12	101.53	105.70
3	A	5101	CMP	O5'-P-O3'	-3.12	101.53	105.70
3	B	5101	CMP	O5'-P-O3'	-3.12	101.53	105.70
3	C	5101	CMP	O5'-P-O3'	-3.12	101.53	105.70
3	B	5101	CMP	C5-N7-C8	2.28	107.04	103.45
3	D	5101	CMP	C5-N7-C8	2.28	107.04	103.45
3	A	5101	CMP	C5-N7-C8	2.28	107.03	103.45
3	C	5101	CMP	C5-N7-C8	2.28	107.03	103.45
3	A	5101	CMP	C4-N9-C8	2.13	107.97	105.74
3	C	5101	CMP	C4-N9-C8	2.13	107.97	105.74
3	B	5101	CMP	C4-N9-C8	2.13	107.97	105.74
3	D	5101	CMP	C4-N9-C8	2.13	107.97	105.74
3	A	5101	CMP	O3'-C3'-C2'	2.05	117.61	115.61
3	B	5101	CMP	O3'-C3'-C2'	2.05	117.61	115.61
3	D	5101	CMP	O3'-C3'-C2'	2.05	117.61	115.61
3	C	5101	CMP	O3'-C3'-C2'	2.04	117.61	115.61

There are no chirality outliers.

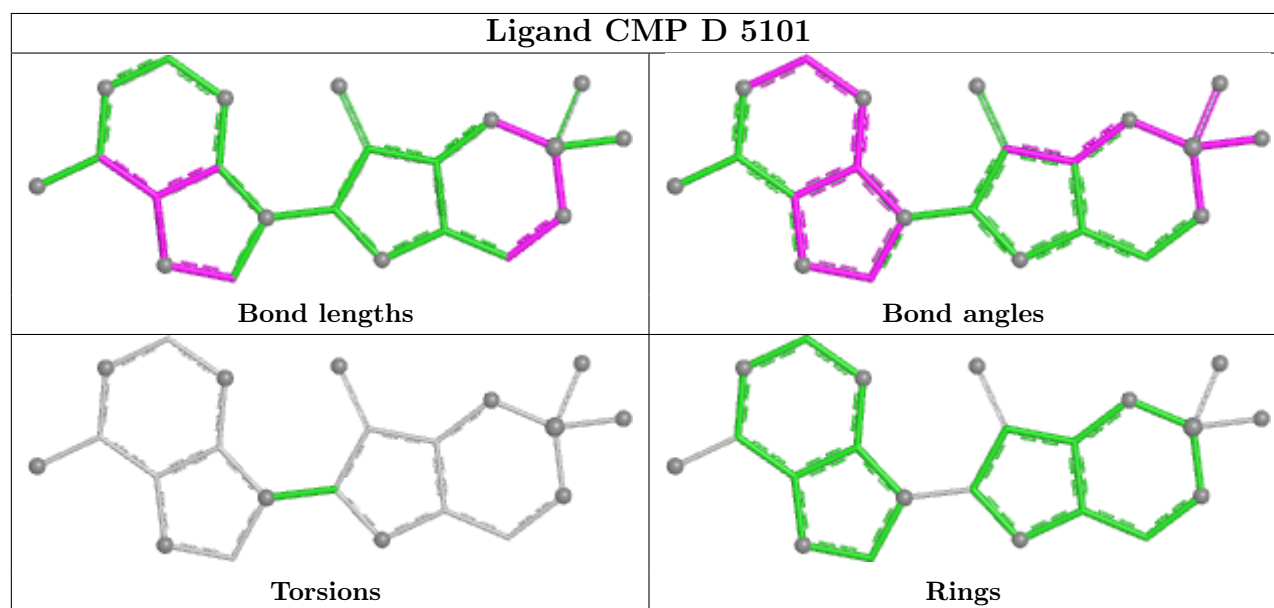
There are no torsion outliers.

There are no ring outliers.

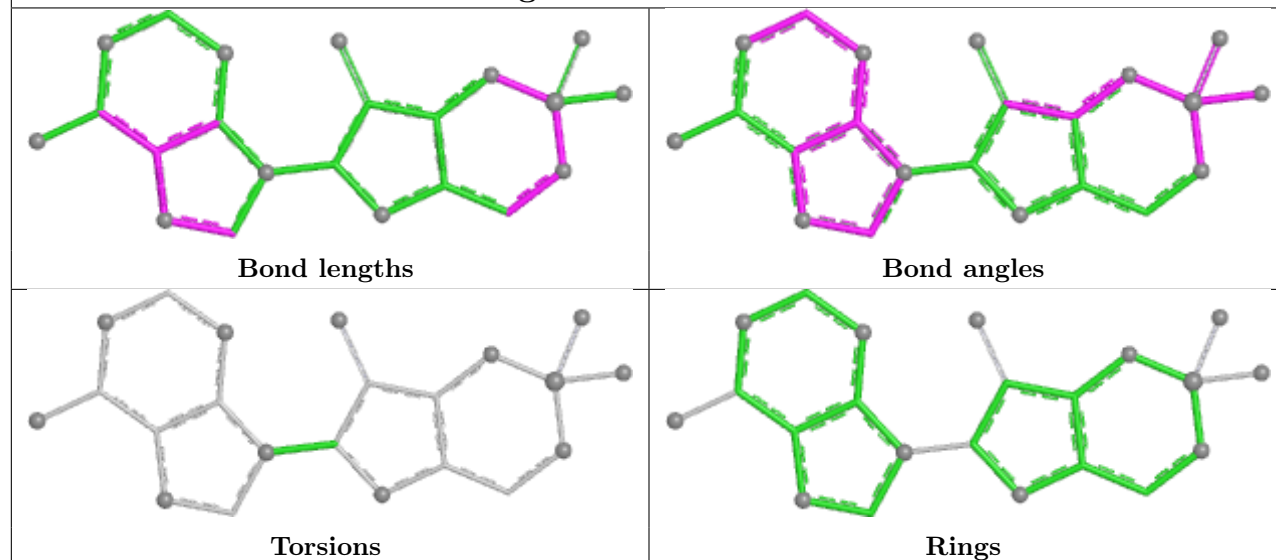
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5101	CMP	2	0
3	B	5101	CMP	2	0
3	C	5101	CMP	2	0
3	A	5101	CMP	2	0

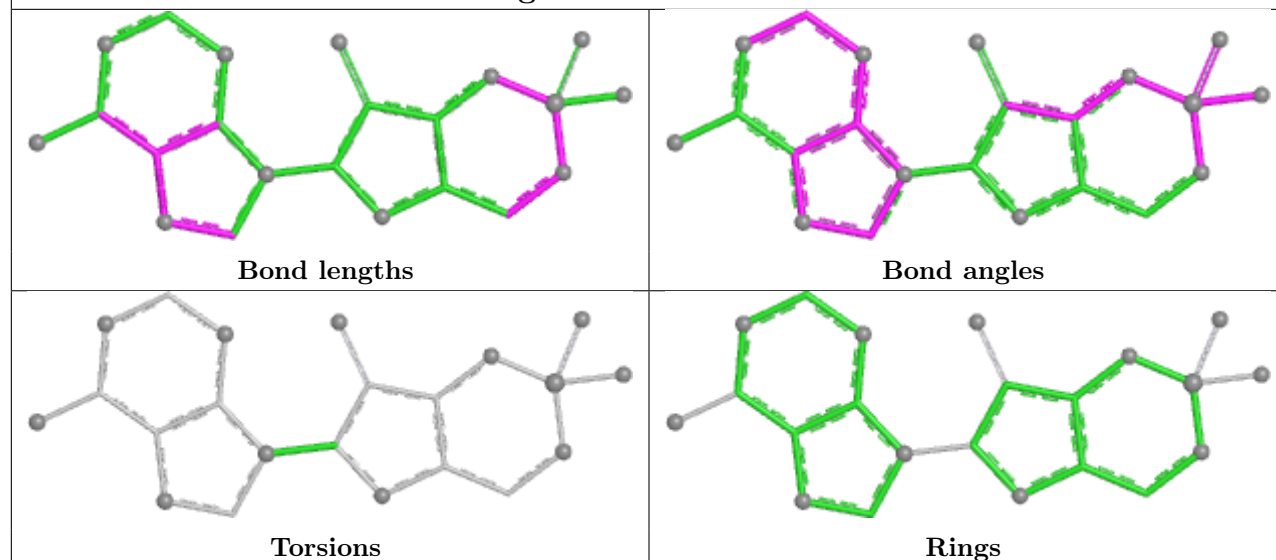
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

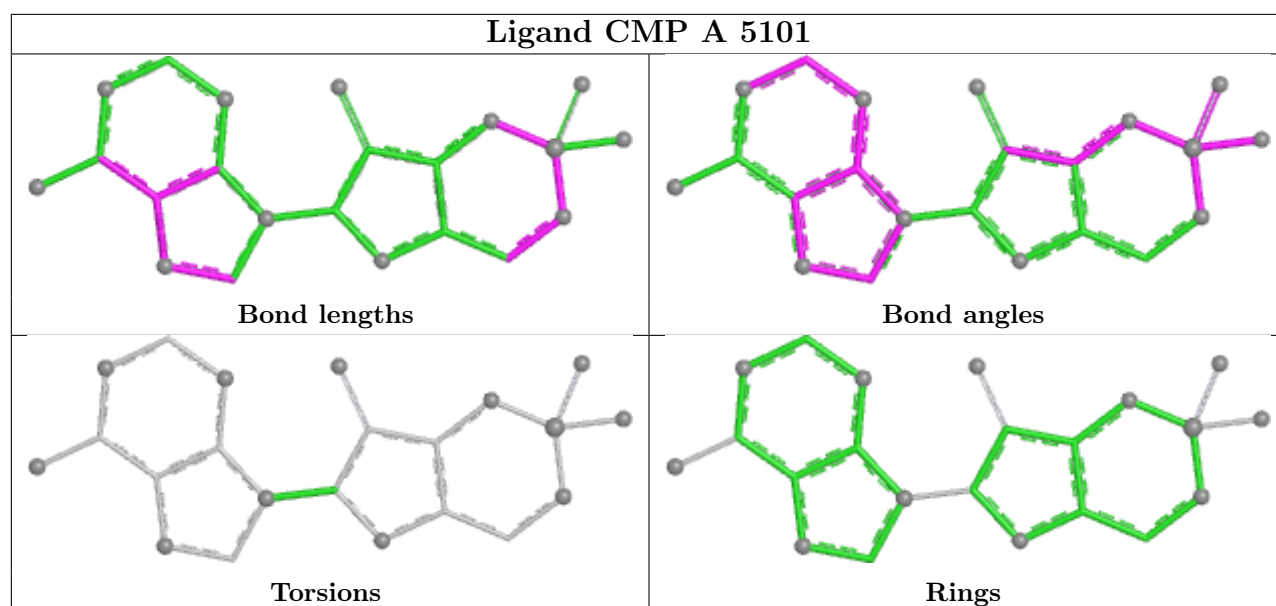


Ligand CMP B 5101



Ligand CMP C 5101





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.

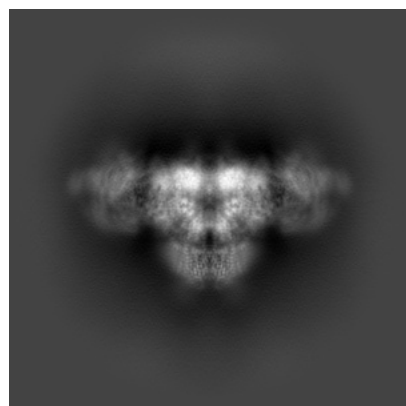
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40428. These allow visual inspection of the internal detail of the map and identification of artifacts.

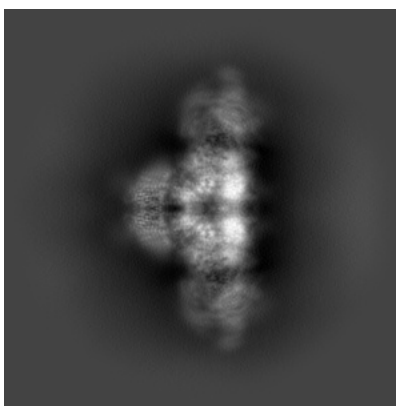
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

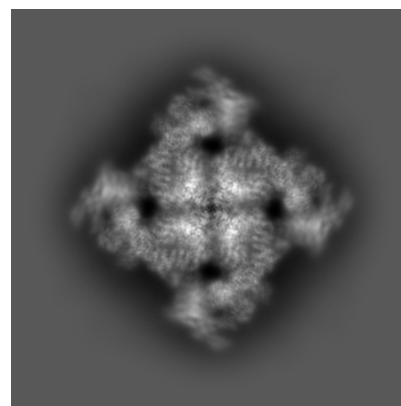
6.1.1 Primary map



X

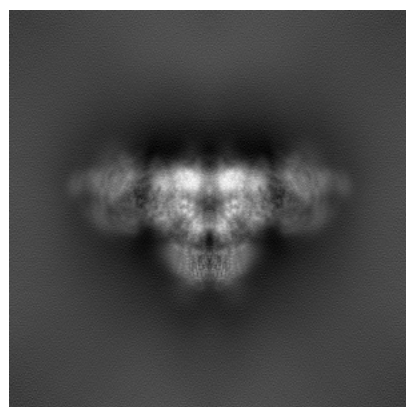


Y

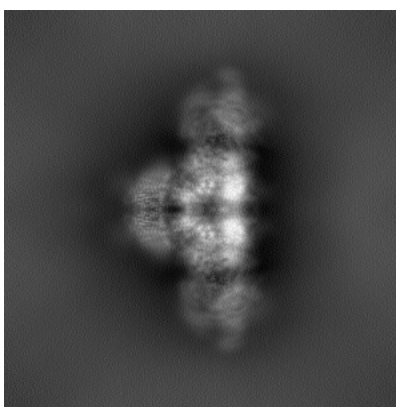


Z

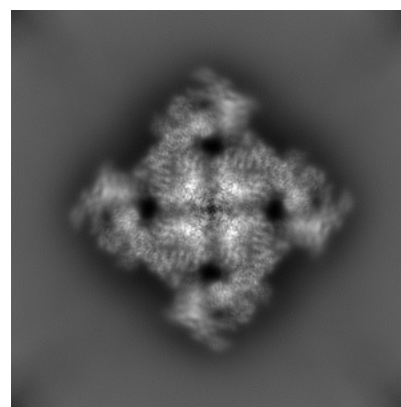
6.1.2 Raw map



X



Y

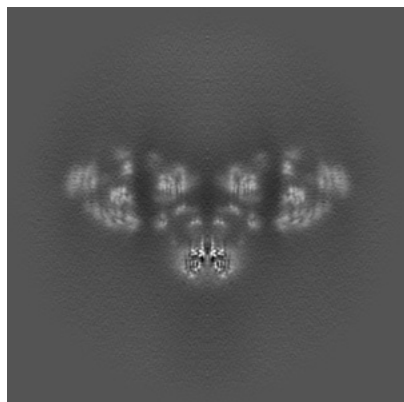


Z

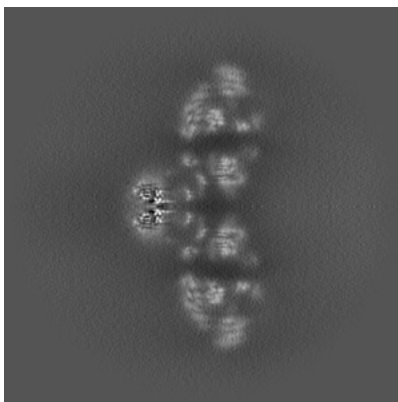
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

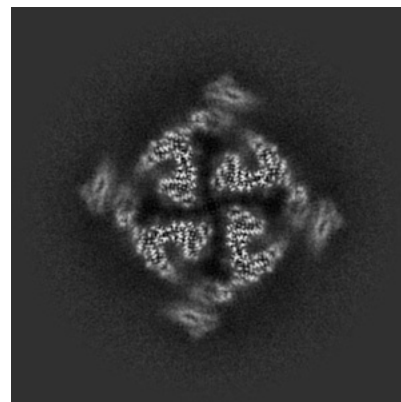
6.2.1 Primary map



X Index: 200

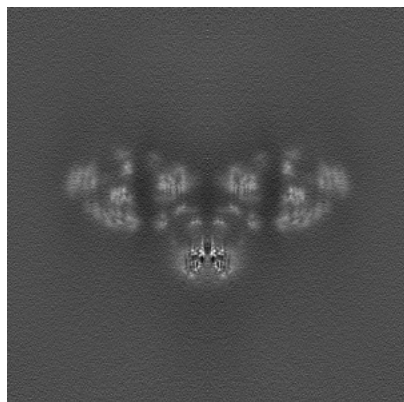


Y Index: 200

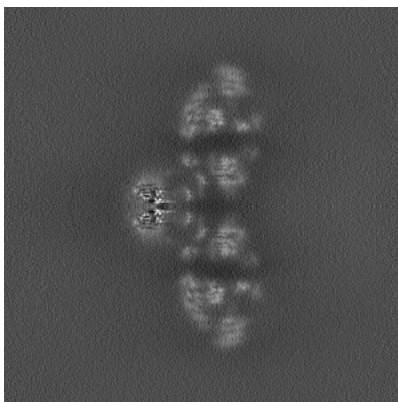


Z Index: 200

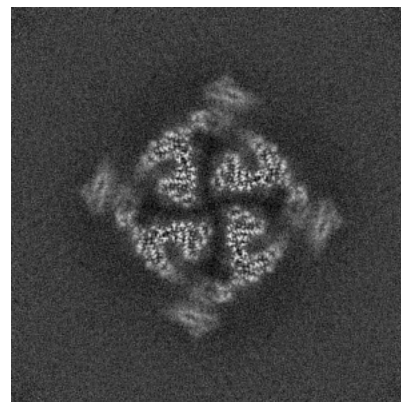
6.2.2 Raw map



X Index: 200



Y Index: 200

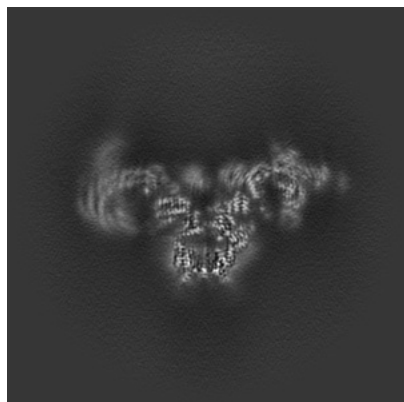


Z Index: 200

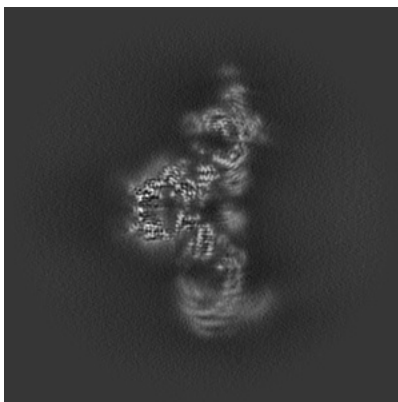
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

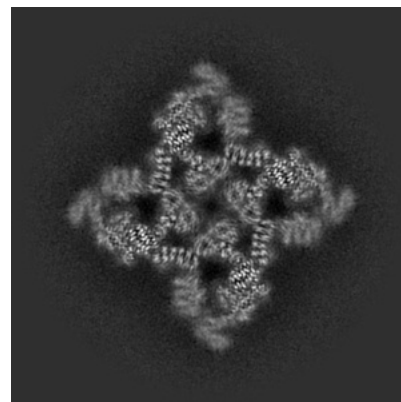
6.3.1 Primary map



X Index: 182

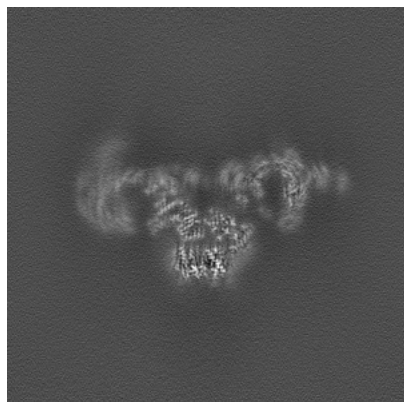


Y Index: 218

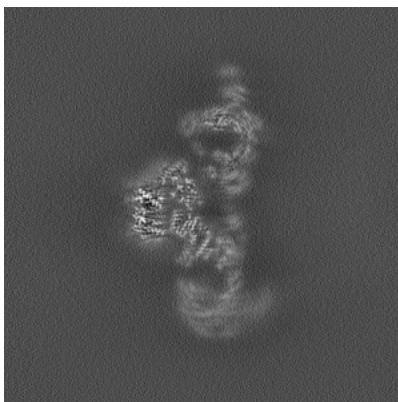


Z Index: 224

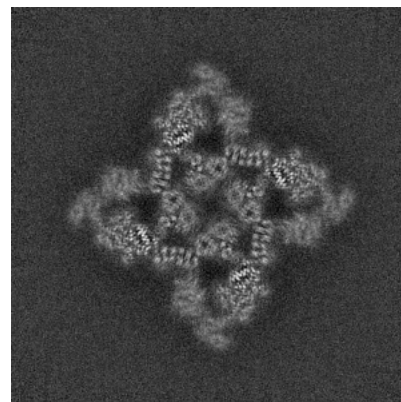
6.3.2 Raw map



X Index: 186



Y Index: 214

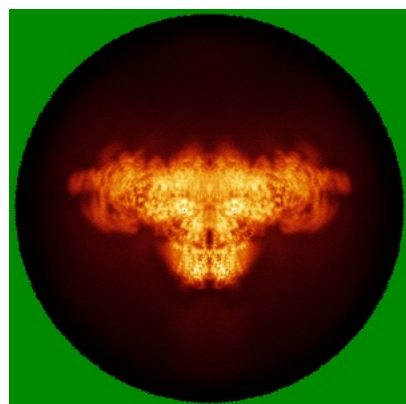


Z Index: 223

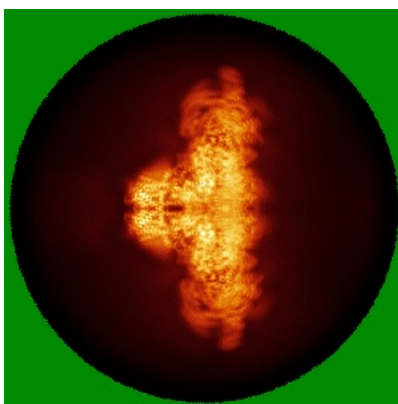
The images above show the largest variance slices of the map in three orthogonal directions.

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

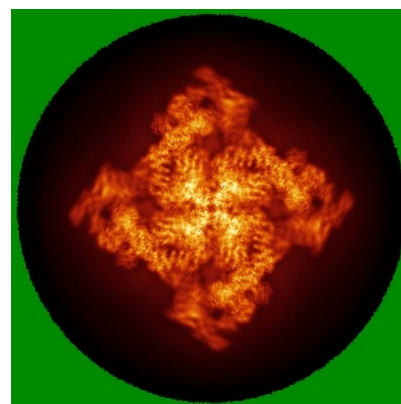
6.4.1 Primary map



X

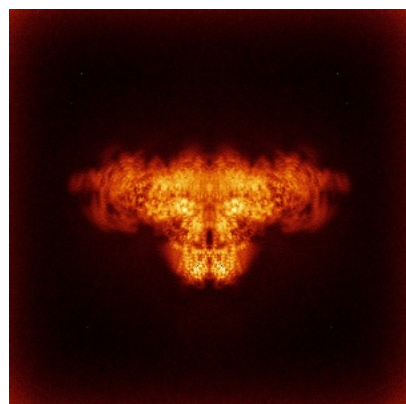


Y

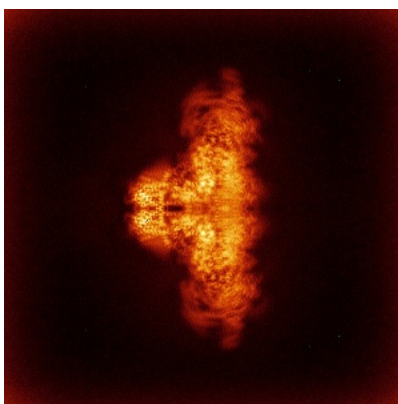


Z

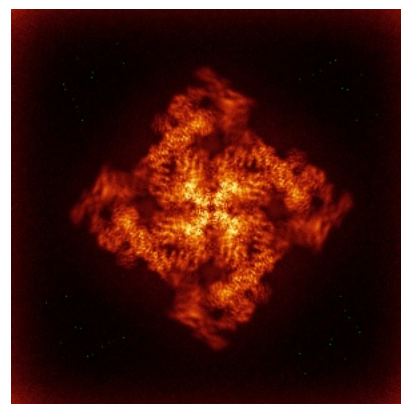
6.4.2 Raw map



X



Y

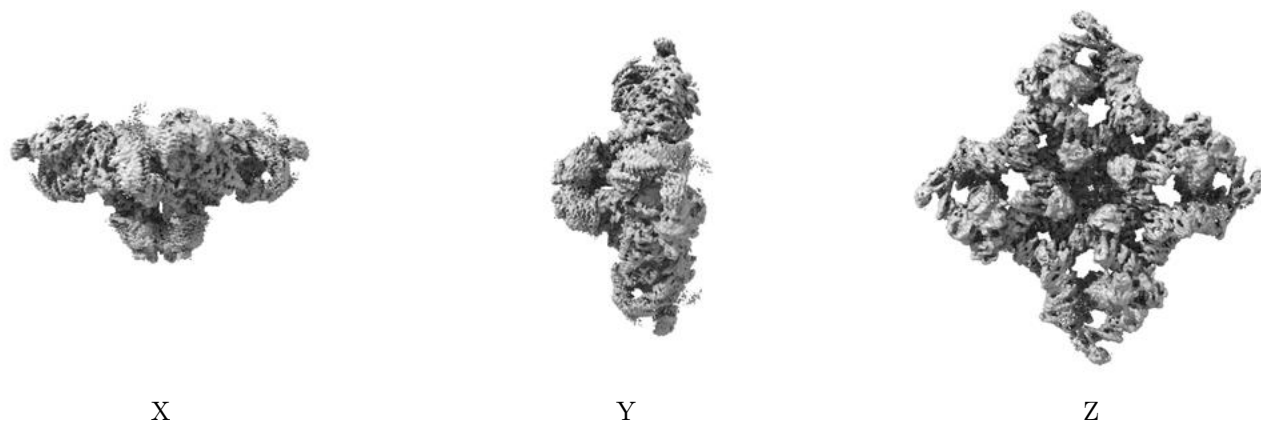


Z

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.

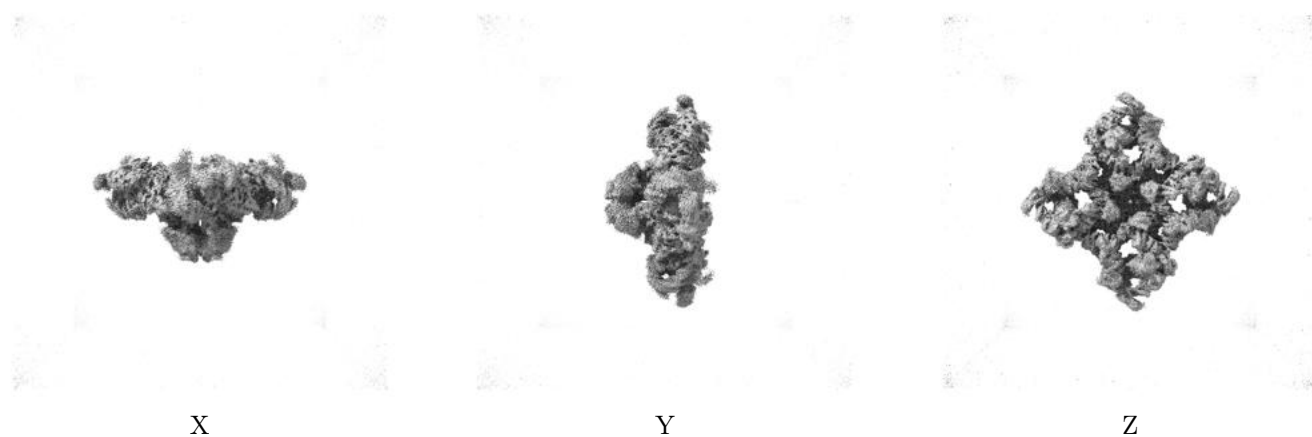
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.126. 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.

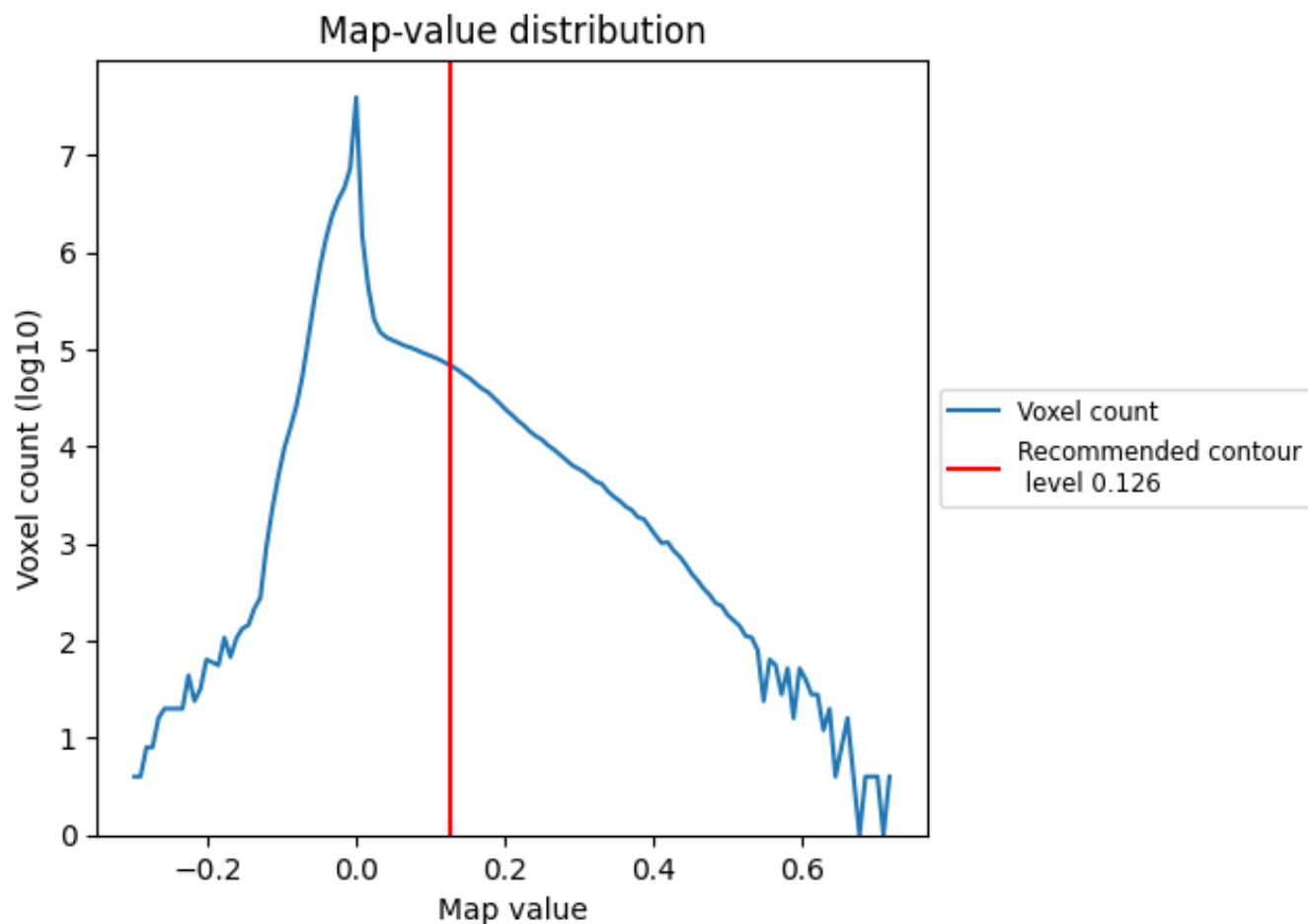
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

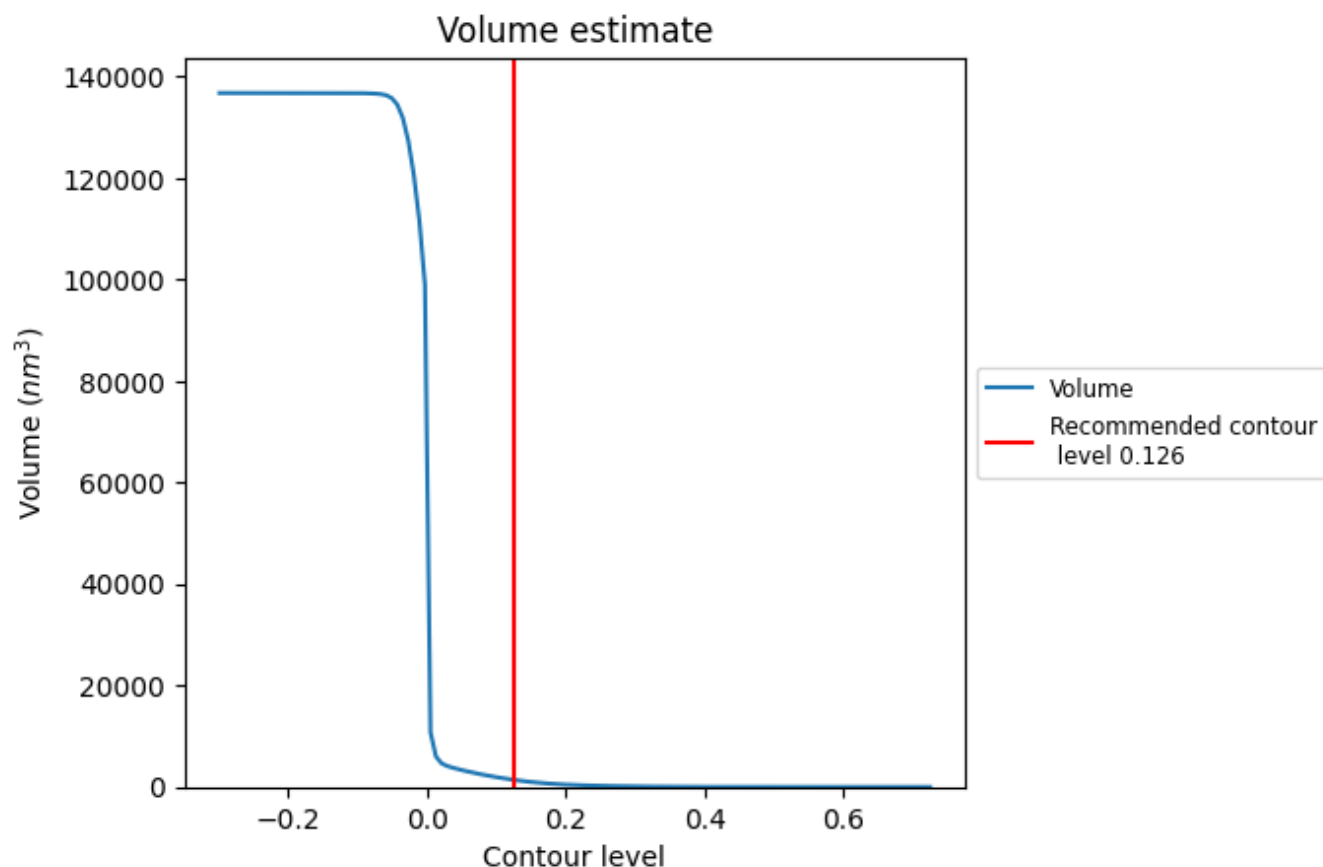
This section contains the results of statistical analysis of the map.

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.

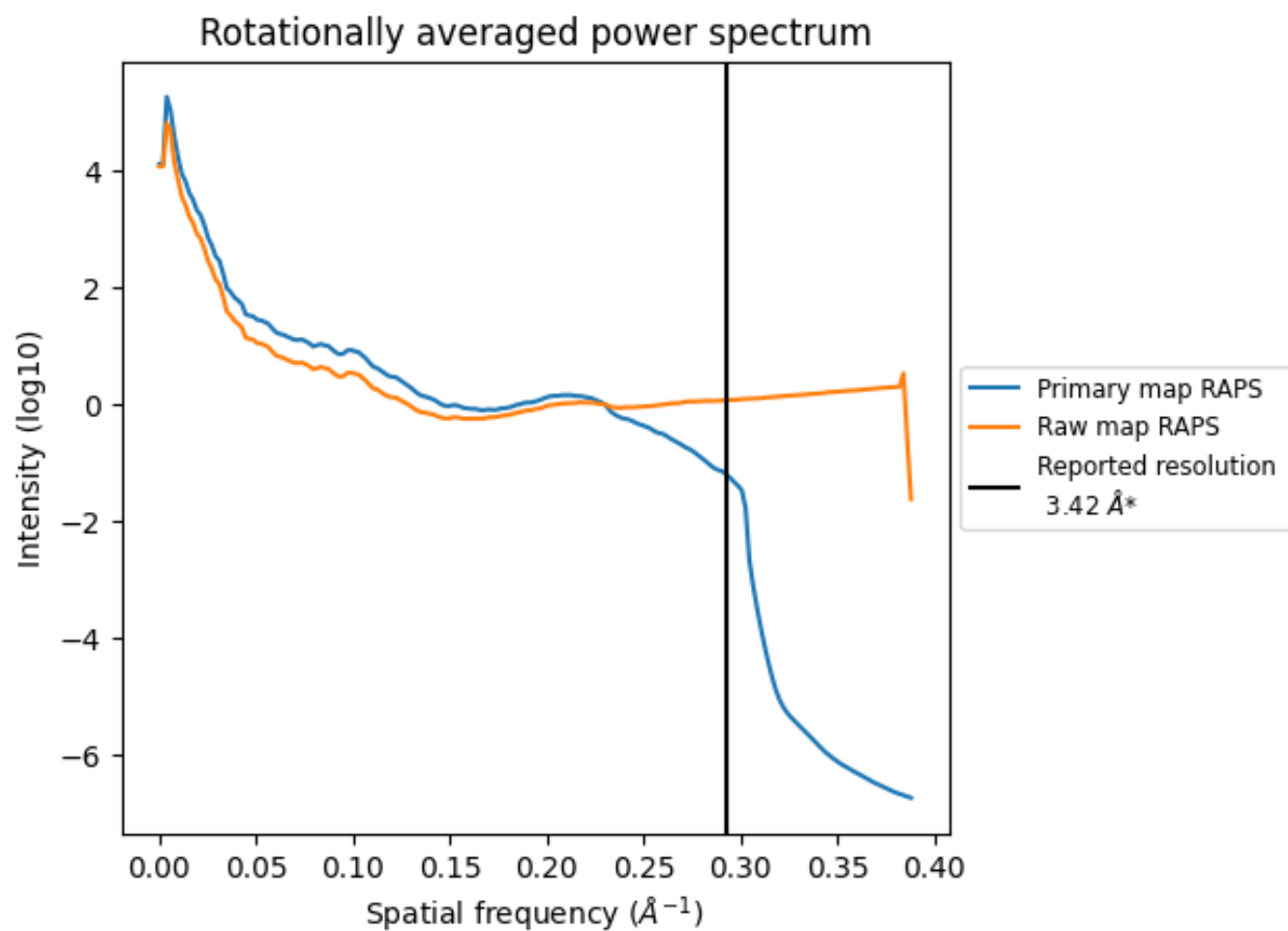
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1379 nm^3 ; this corresponds to an approximate mass of 1246 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 ⓘ

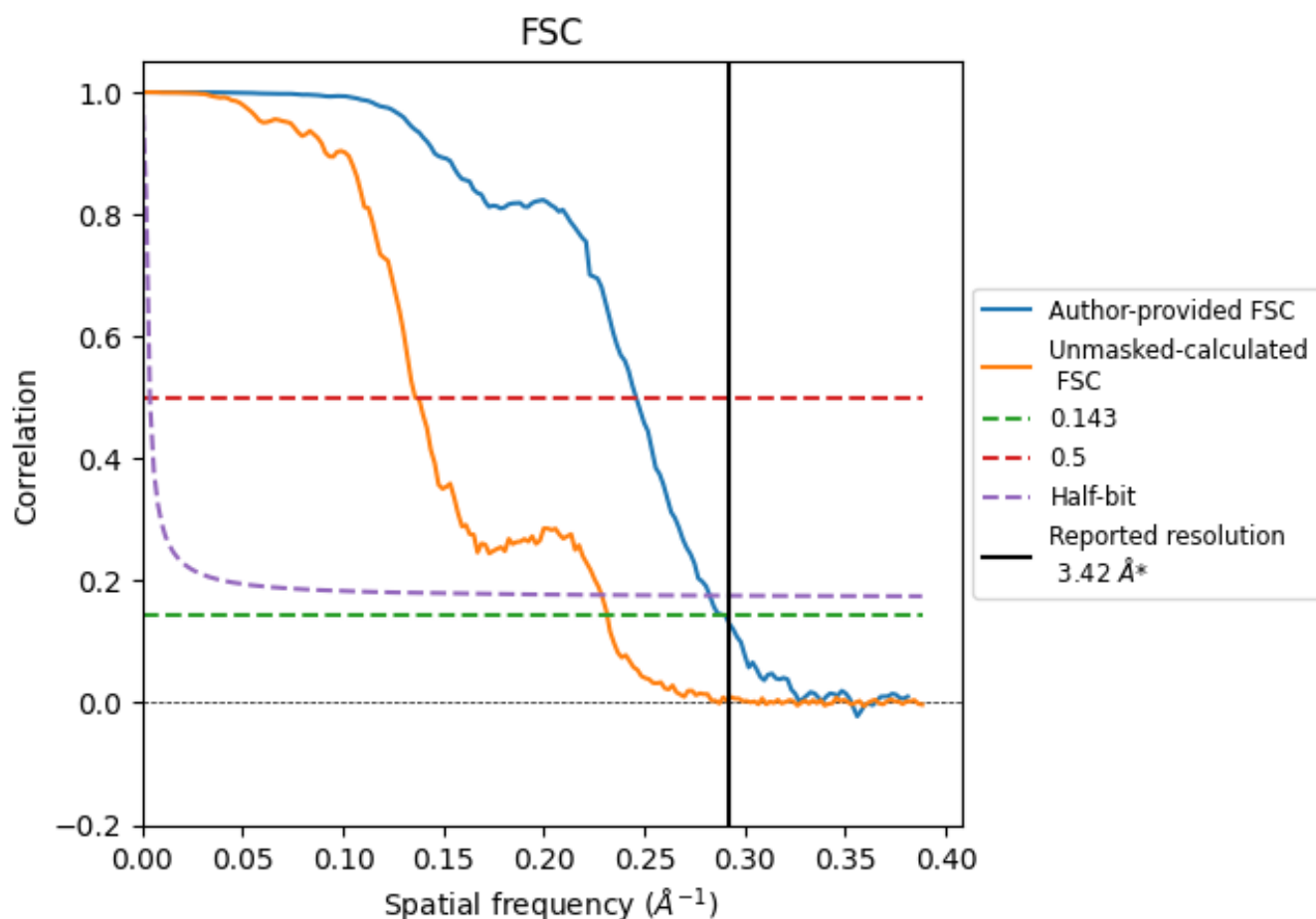


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

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 0.292 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

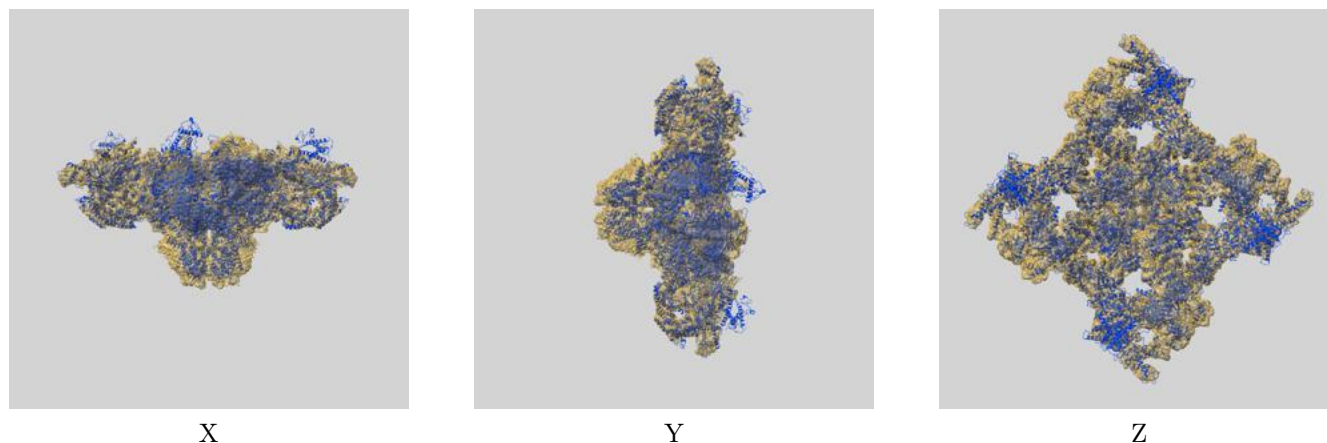
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.45	4.07	3.54
Unmasked-calculated*	4.32	7.36	4.37

*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 4.32 differs from the reported value 3.42 by more than 10 %

9 Map-model fit [i](#)

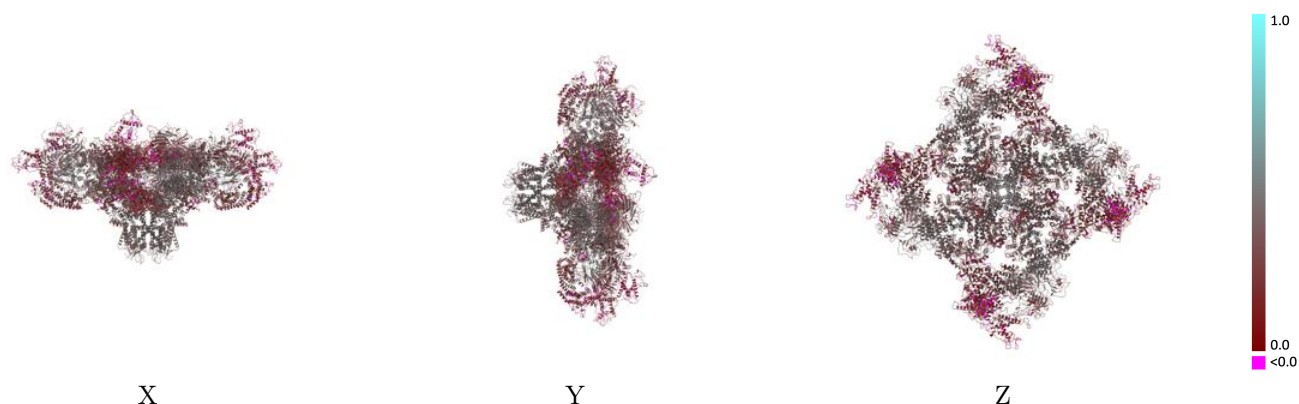
This section contains information regarding the fit between EMDB map EMD-40428 and PDB model 8SET. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



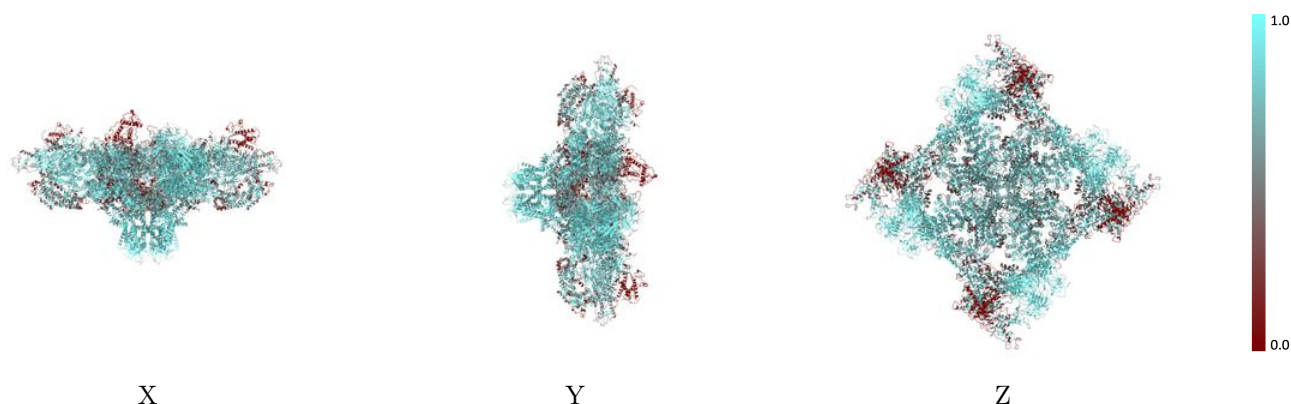
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



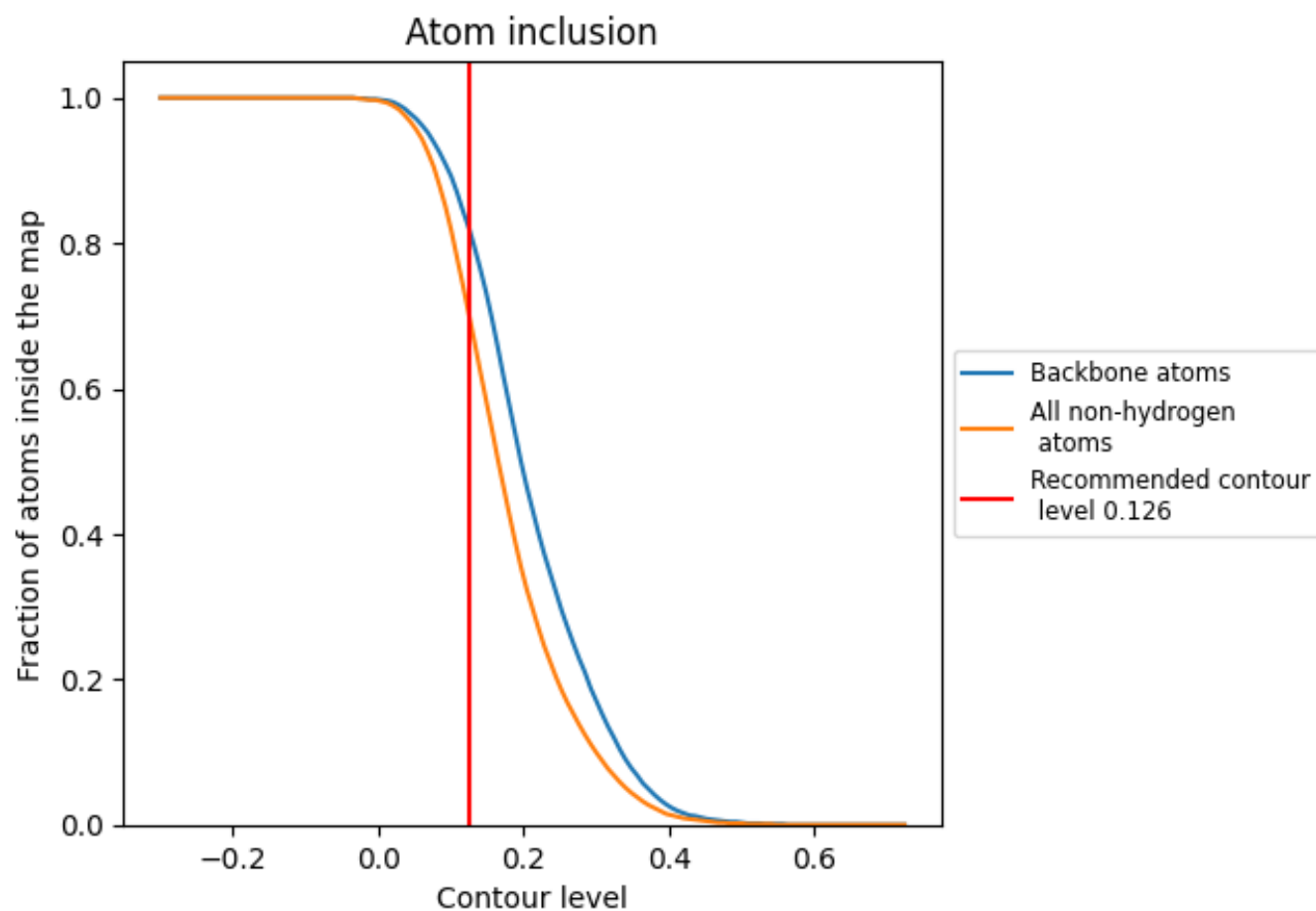
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.3090
A	0.6960	0.3070
B	0.6960	0.3070
C	0.6960	0.3070
D	0.6960	0.3070
E	0.8410	0.3850
F	0.8410	0.3870
G	0.8410	0.3850
H	0.8410	0.3860

1.0

0.0

<0.0