



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 5TAV / pdb_00005tav
EMDB ID : EMD-8386
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.80 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:

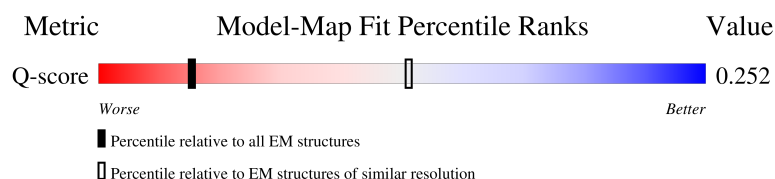
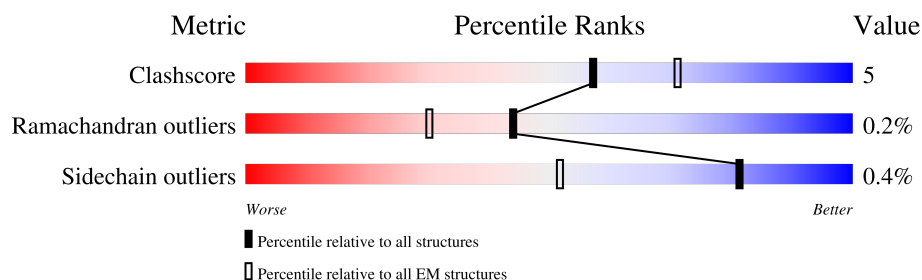
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
2	B	4416	39%			
			84%11%5%			
2	E	4416	39%			
			84%11%5%			
2	G	4416	39%			
			84%10%5%			
2	I	4416	39%			
			84%11%5%			

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

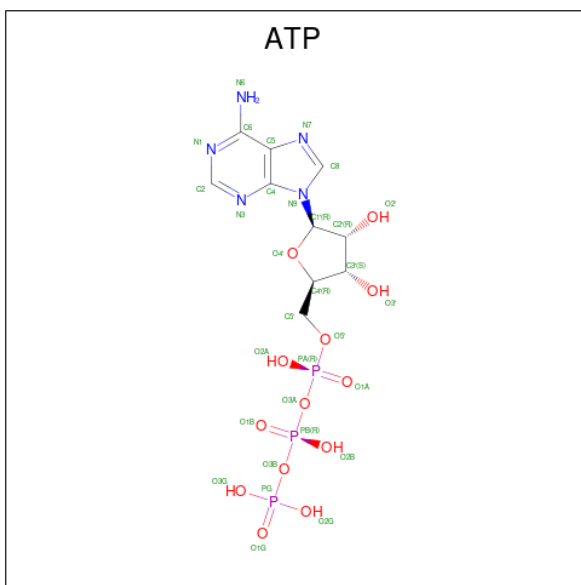
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

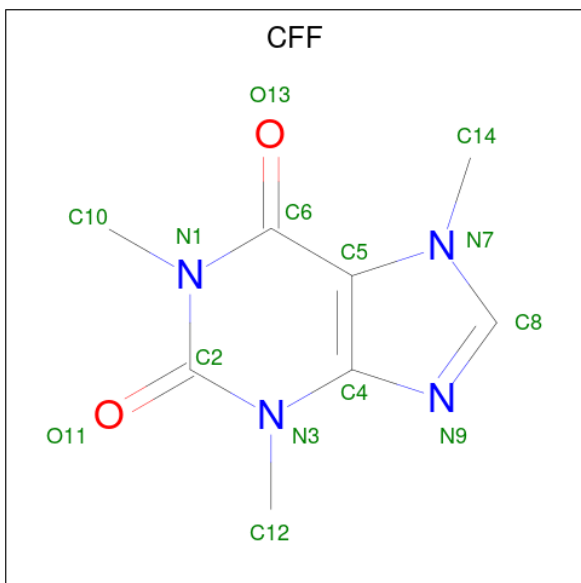
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

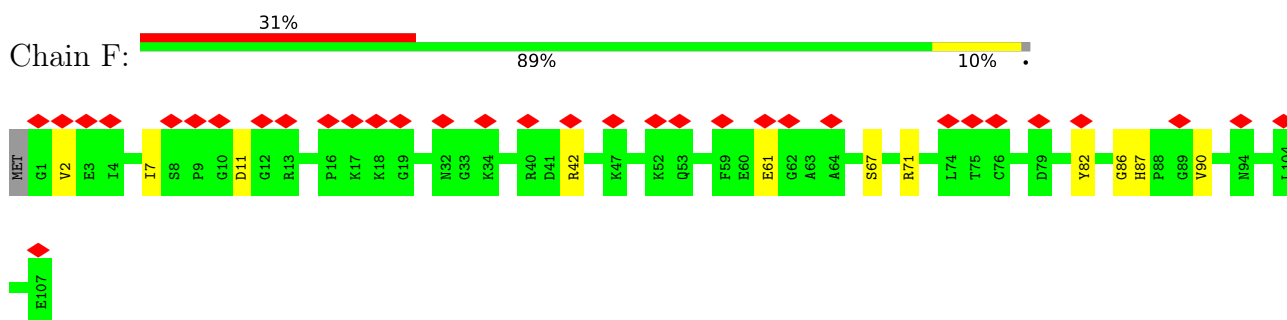
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

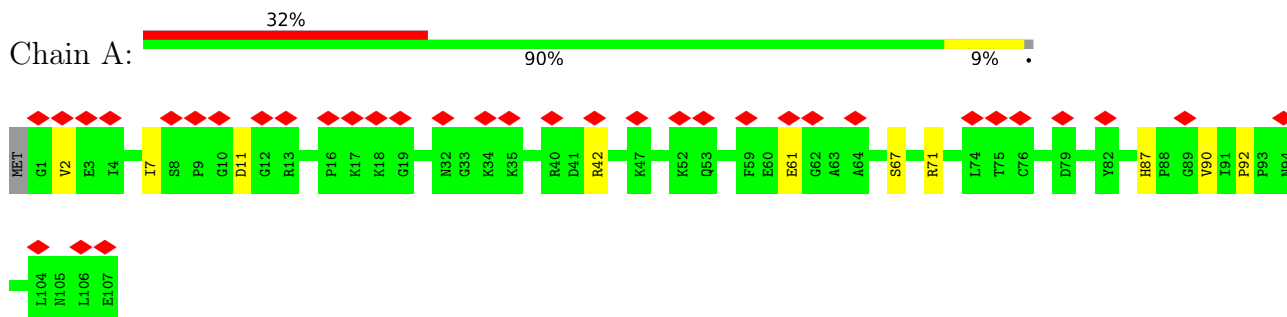
3 Residue-property plots [i](#)

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

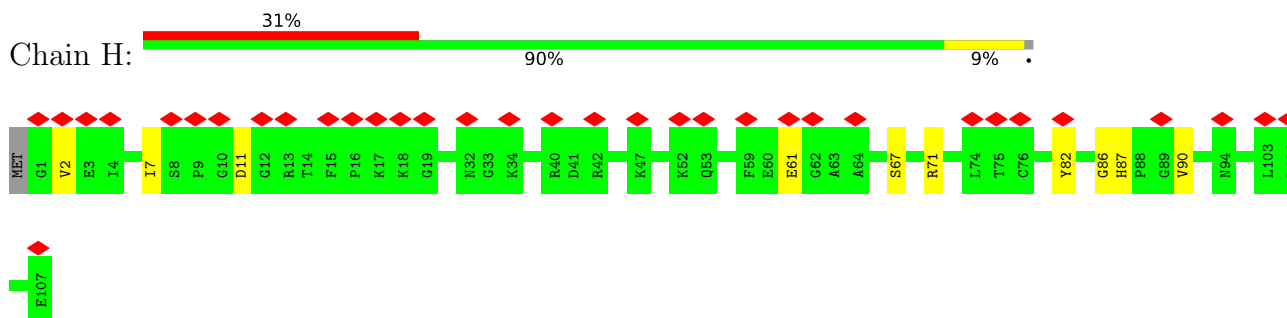
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

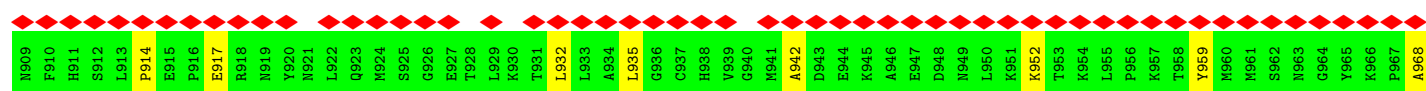


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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







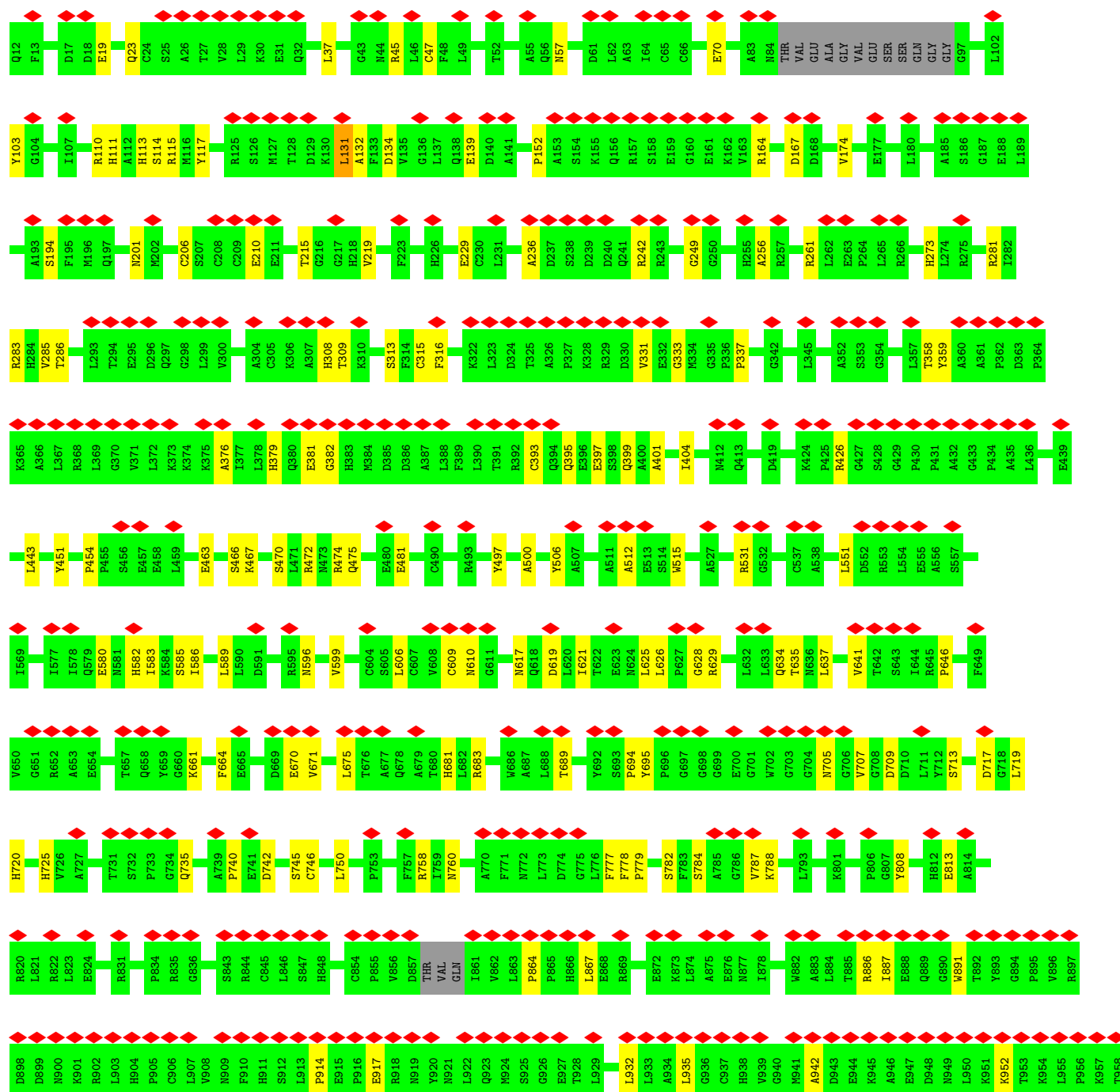
X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3594	X3595	X3596	X3599	X3607	X3608	X3609	X3610	X3611						
X3414	X3417	X3423	X3427	X3431	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3443	X3449	X3453	X3454	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536												
X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3295	X3296	X3297	X3298	X3301	X3302	X3303	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338														
X3196	X3197	X3200	X3206	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3227	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266															
X3034	X3035	X3036	X3037	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3143	X3144	X3149	X3152	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3175	X3176	X3179	X3183	X3189	X3190	X3191	X3192	X3193	X3194	X3195											
L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	S2940	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2961	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2999	X3005	X3006	X3014	X3019	X3022	X3023	X3027	X3028	X3029	X3032	X3033									
L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	E2875	A2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	T2884	T2885	W2886	G2887	T2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	X2896	K2897	G2898	G2899	G2900	T2901	H2902	F2903	L2904	L2905	V2906	P2907	V2908	V2909	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2917	R2918	D2919	X3028	X3029	E2921	K2922	A2923	Q2924	E2925	L2926
W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	LYS	LYS	THR	ARG	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	GLU	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866				
I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	E2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	T2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	
X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2648	X2649	X2650	X2651	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2680	X2681	X2687	X2688	X2689	X2690	X2691	X2692	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746						
R2435	P2438	H2441	G2446	K2447	G2448	E2449	L2453	L2460	D2464	D2465	L2466	L2469	I2470	S2471	L2472	Q2475	L2476	P2477	T2478	L2479	X2491	X2492	X2493	Y2502	X2511	X2512	X2513	X2529	X2534	X2535	X2561	X2562	X2569	X2581	X2582	X2583	X2584	X2585	X2597	X2606																				
E2347	E2348	N2349	K2350	N2351	V2352	R2355	I2358	R2359	E2362	L2368	E2371	G2372	G2373	S2374	A2378	A2379	I2380	E2381	E2382	I2389	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	R2415	T2426	T2430	D2431	G2434												



35037

• Molecule 2: Ryanodine receptor 1

Chain E: 39% 84% 11% 5%



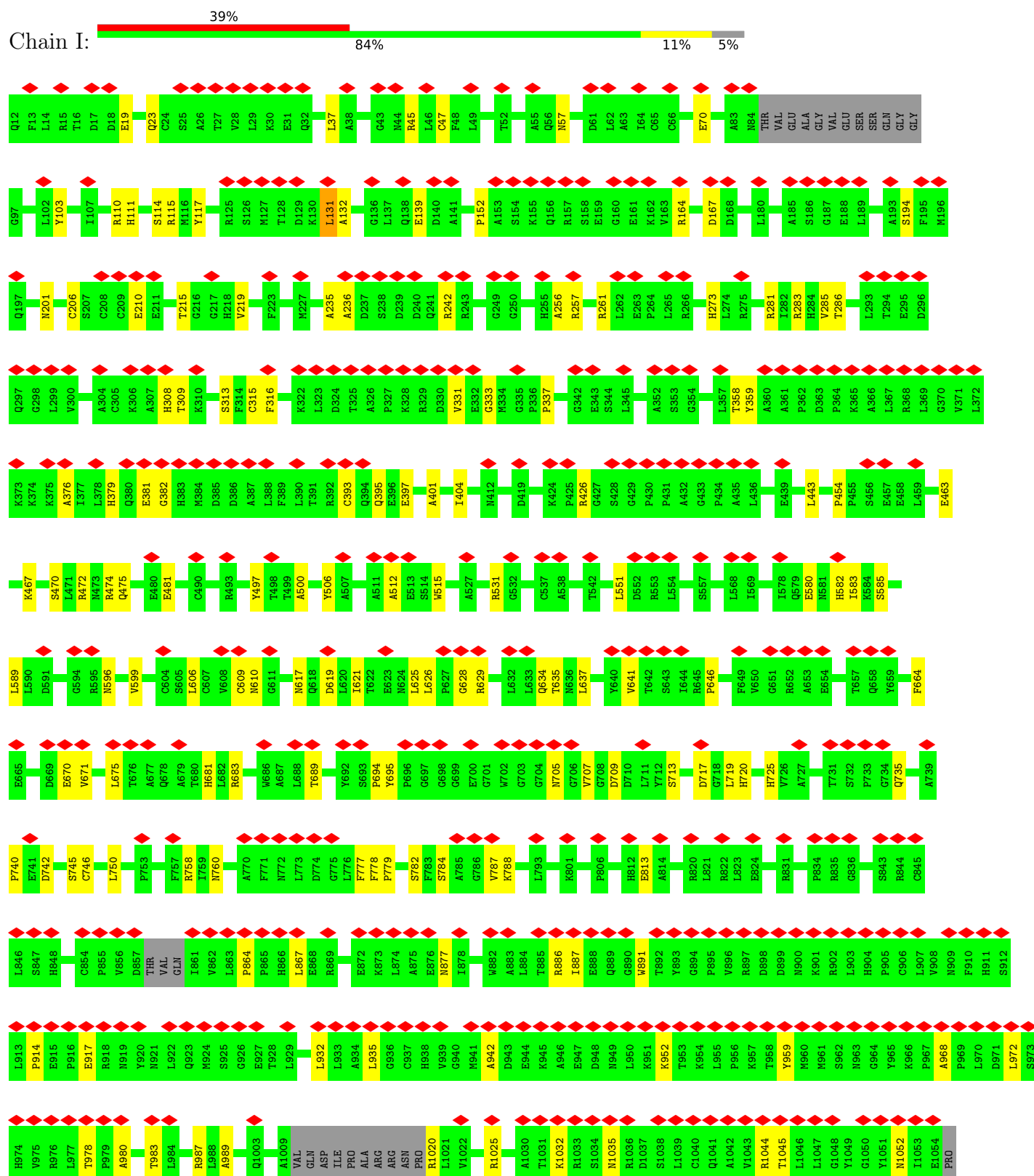


C2326	C2327	C2328	E2329	R2330	V2331	L2332	F2337	F2340	V2341	N2342	G2343	E2347	E2348	N2349	A2350	N2351	V2352	R2355	I2358	R2359	E2362	E2371	G2372	G2373	S2374	I2380	D2389	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU									
N2414	R2415	F2425	F2426	I2430	D2431	G2434	R2435	P2438	H2441	G2446	K2447	G2448	E2449	R2452	I2453	L2460	D2464	D2465	L2466	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	I2476	P2477	T2478	X2491	X2492	X2493	X2502	X2511	X2512	X2513	X2534	X2535	X2561	X2562	X2569	X2581																
X2582	X2583	X2584	X2585	X2597	X2606	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2648	X2649	X2650	X2651	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2734	P2735	D2736	P2737						
R2738	P2739	V2740	E2741	T2742	L2743	M2744	V2745	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	M2756	K2757	F2758	A2759	E2760	V2761	T2762	H2763	E2764	K2765	M2766	G2767	F2768	D2769	K2770	L2771	Q2772	N2773	M2774	S2775	S2776	V2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797
S2798	E2799	K2800	D2801	E2802	E2803	L2804	R2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	G2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	PRO	ARG	GLU	GLY	Y2855	N2856	P2857
Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	E2880	N2881	T2882	H2883	N2884	T2885	G2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	E2915	K2916	A2917	
R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2961	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X3000	X3001	X3006	X3007	X3014	X3022					
X3027	X3028	X3029	X3034	X3035	X3036	X3037	X3040	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3057	X3058	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3143	X3144	X3149	X3152	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3175	X3176	X3177	X3178	X3179	X3183	X3189	X3190												
X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3206	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3268	X3269				
X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3301	X3302	X3311	X3312	X3313	X3314	X3315	X3316	X3319	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3341	X3342	X3343			
X3344	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3369	X3372	X3376	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3408	X3409	X3410	X3411					
X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3423	X3427	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3440	X3441	X3442	X3453	X3454	X3455	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533							
X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3599	



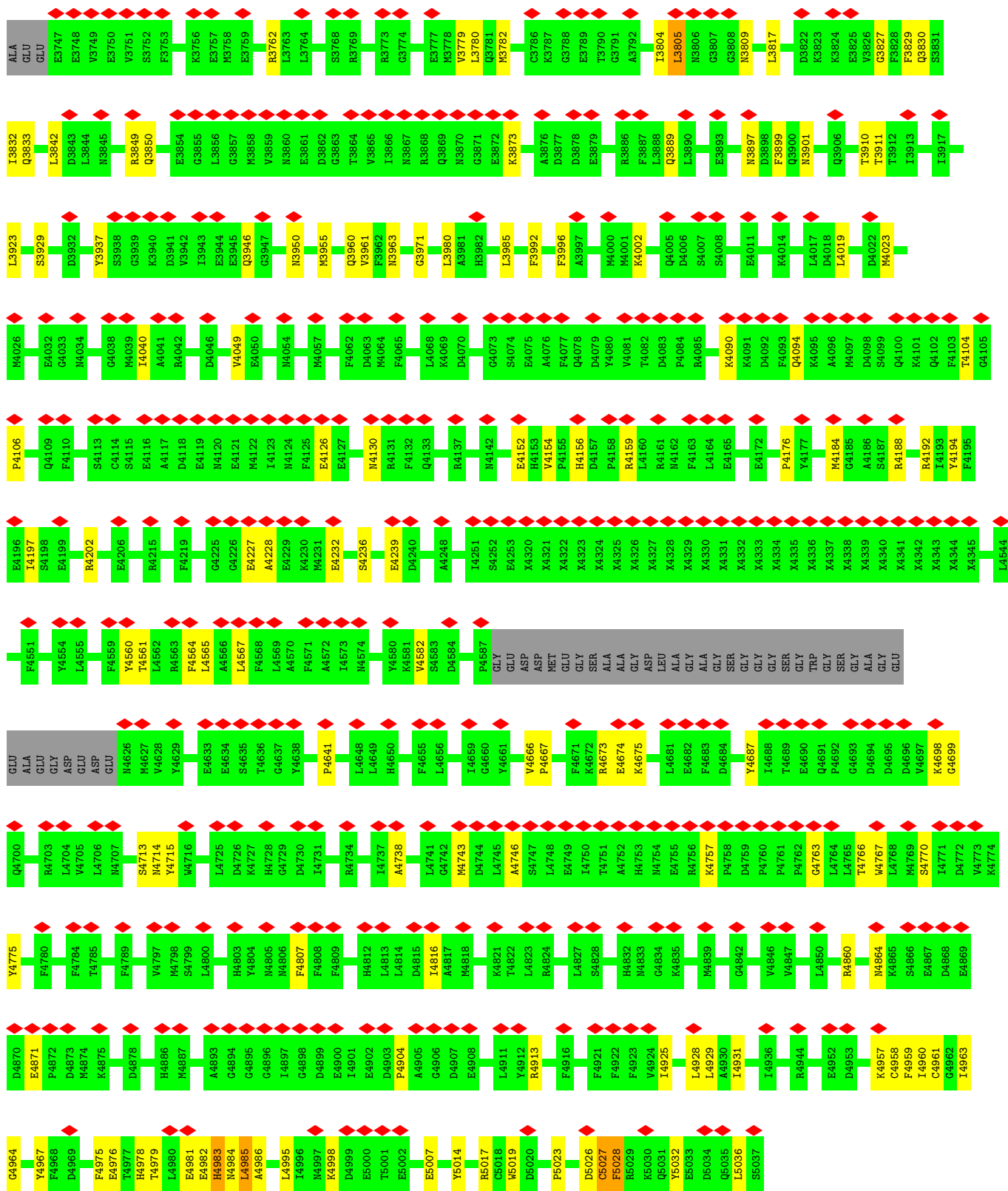
• Molecule 2: Ryanodine receptor 1

Chain I:

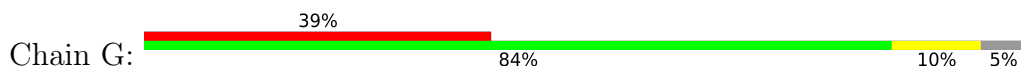




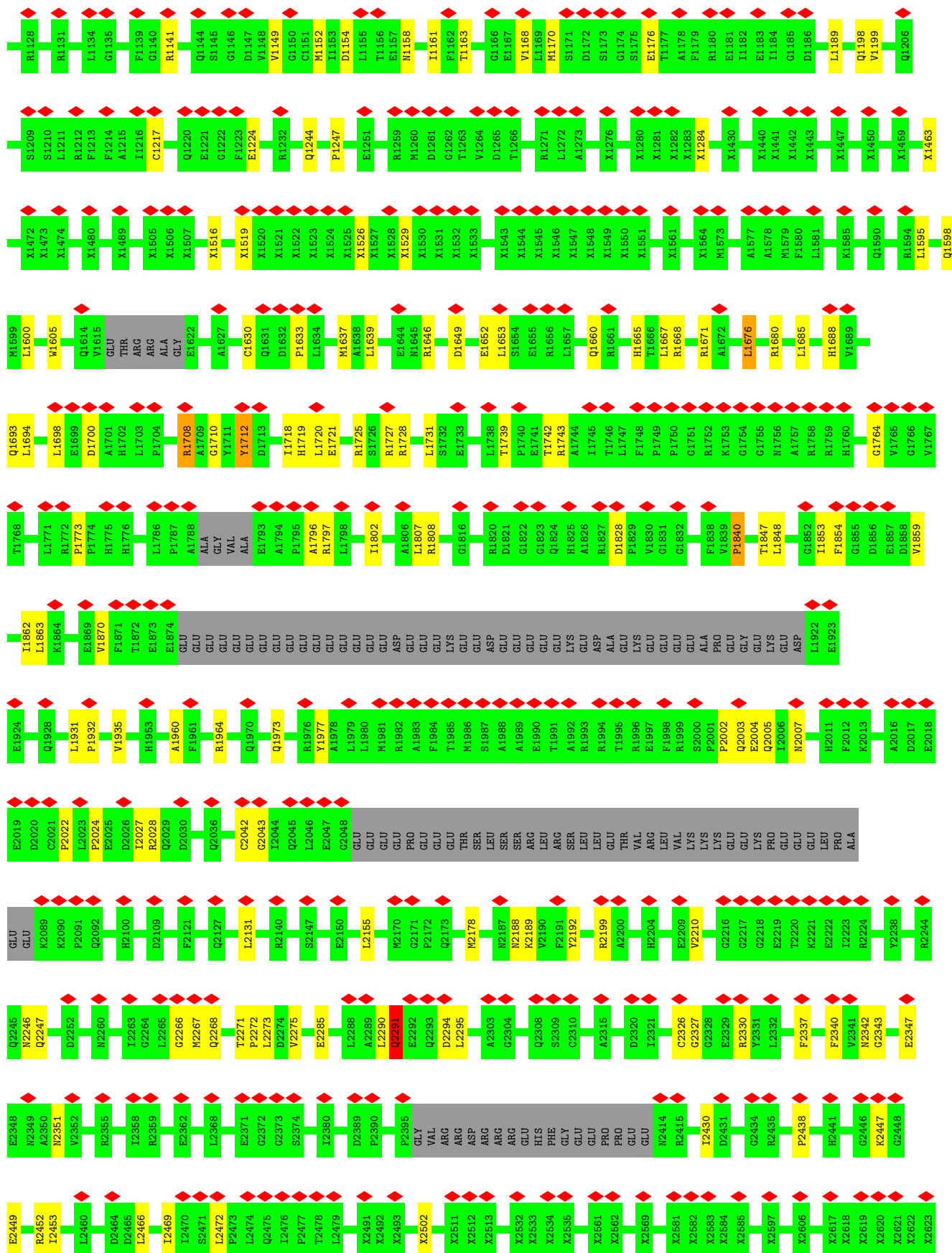




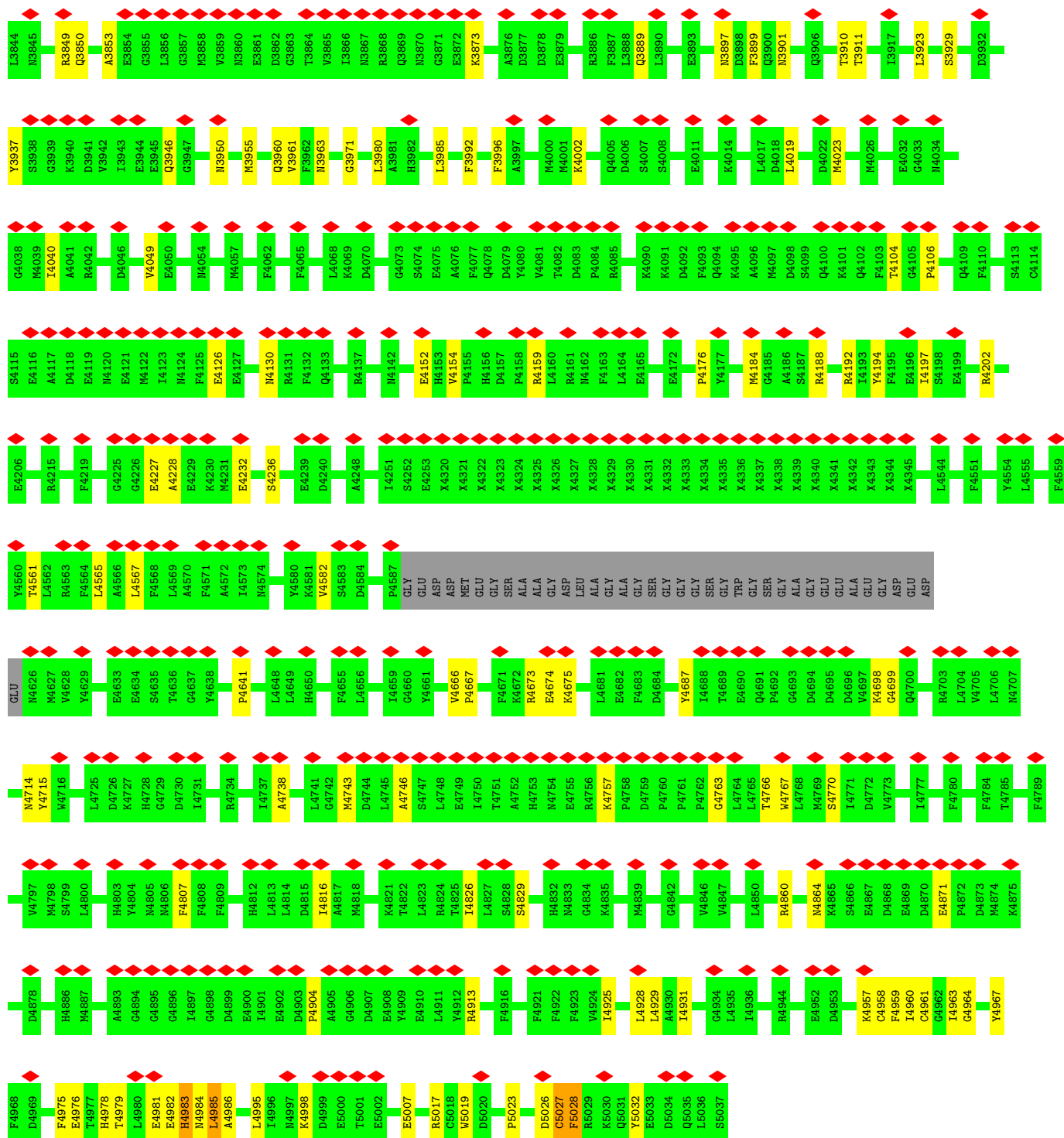
• Molecule 2: Ryanodine receptor 1



PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	R1109	P1111	D1112	L1115	G1116	A1117	D1118	E1119	L1120	V1123
S973	H974	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	ASN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	Y1089	F1092	V1095	T1096	E1099	M1100	G1103	W1104	A1105	R1106												



V3749	E3670	X3440	X3289	X3217	X3049	G2934	M2874	K2814	F2754	X2624
E3750	D3671	X3443	X3290	X3218	X3050	Y2935	M2875	A2815	I2755	X2625
V3751	X3672	X3449	X3291	X3219	X3051	A2936	E2876	A2816	N2756	X2626
S3752	X3673	X3449	X3292	X3220	X3052	V2937	Q2877	I2817	K2757	X2627
F3753	D3675	X3453	X3295	X3221	X3059	V2938	L2878	A2818	F2758	X2628
K3756	D3676	X3454	X3296	X3222	X3060	R2939	A2879	W2819	A2759	X2629
K3679	K3679	X3455	X3297	X3223	X3061	X2942	E2880	E2820	E2760	X2630
A3680	A3680	X3457	X3301	X3224	X3062	X2943	N2881	W2821	Y2761	X2648
G3681	G3681	X3458	X3302	X3227	X3063	X2944	H2882	T2822	T2762	X2649
E3682	E3682	X3463	X3303	X3230	X3134	X2945	H2883	E2824	H2763	X2650
E3683	E3683	X3466	X3312	X3231	X3135	X2946	N2884	E2825	E2764	X2651
E3685	E3685	X3467	X3313	X3232	X3136	X2947	T2885	K2826	K2765	
E3686	E3686	X3468	X3314	X3233	X3137	X2948	W2886	A2827	W2766	X2669
E3687	E3687	X3511	X3315	X3234	X3138	X2949	Q2887	R2827	A2767	X2670
E3688	E3688	X3512	X3316	X3235	X3139	X2950	R2888	E2828	F2768	X2671
E3689	E3689	X3513	X3317	X3236	X3143	X2951	K2889	Q2829	D2769	X2672
V3690	V3690	X3514	X3318	X3241	X3144	X2952	K2890	E2830	K2770	X2673
E3691	E3691	X3515	X3323	X3242	X3149	X2961	K2891	GLU	I2771	X2674
E3692	E3692	X3515	X3324	X3243	X3152	X2966	Q2892	ARG	Q2772	X2675
K3693	K3693	X3518	X3325	X3244	X3158	X2967	E2893	THR	N2773	X2676
K3694	K3694	X3519	X3326	X3245	X3159	X2968	L2894	GLU	N2774	
P3695	P3695	X3520	X3327	X3246	X3160	X2969	E2895	LYS	W2775	X2680
R3707	R3707	X3521	X3328	X3247	X3161	X2970	A2896	LYS	S2776	X2681
E3712	E3712	X3522	X3329	X3248	X3162	X2971	K2897	THR	S2777	X2687
K3713	K3713	X3523	X3330	X3249	X3163	X2972	G2898	ARG	G2778	X2688
S3714	S3714	X3524	X3331	X3250	X3166	X2973	G2899	LYS	E2779	X2689
K3715	K3715	X3525	X3332	X3251	X3170	X2974	G2900	ILE	N2780	X2690
L3716	L3716	X3526	X3333	X3252	X3171	X2975	T2901	SER	V2781	X2691
D3717	D3717	X3527	X3334	X3253	X3176	X2976	H2902	GLN	D2782	X2692
E3718	E3718	X3528	X3335	X3254	X3175	X2977	P2903	ALA	E2783	
E3719	E3719	X3529	X3336	X3255	X3176	X2978	L2904	THR	E2784	X2696
Y3720	Y3720	X3530	X3337	X3256	X3179	X2979	L2905	TYR	L2785	X2697
Y3722	Y3722	X3531	X3338	X3257	X3183	X2996	P2906	ASP	K2786	X2698
I3728	I3728	X3532	X3341	X3258	X3189	X2999	P2907	PRO	T2787	X2699
M3729	M3729	X3533	X3342	X3259	X3190	X3005	Y2908	ARG	H2788	X2700
A3730	A3730	X3534	X3343	X3260	X3191	X3006	D2909	GLU	H2789	X2701
K3731	K3731	X3535	X3344	X3261	X3192	X3014	T2910	GLY	P2789	X2702
H3734	H3734	X3536	X3345	X3262	X3193	X3019	L2911		M2790	X2703
L3735	L3735	X3537	X3346	X3263	X3194	X3022	T2912		L2791	X2734
E3736	E3736	X3538	X3347	X3264	X3195	X3023	T2913		R2792	X2735
E3737	E3737	X3539	X3348	X3265	X3196	X3027	K2914		P2793	D2736
G3738	G3738	X3540	X3349	X3266	X3197	X3034	E2915		Y2794	D2737
F3829	F3829	X3541	X3350	X3267	X3200	X3035	K2916		K2795	R2738
F3829	F3829	X3542	X3351	X3268	X3206	X3036	A2917		T2796	P2739
Q3830	Q3830	X3543	X3352	X3269	X3211	X3037	S2918		F2797	
Q3831	Q3831	X3544	X3353	X3270	X3212	X3043	D2919		S2798	W2740
Q3832	Q3832	X3545	X3354	X3271	X3213	X3044	R2920		E2799	E2741
Q3833	Q3833	X3546	X3355	X3272	X3214	X3045	E2921		K2800	T2742
L3842	L3842	X3547	X3356	X3273	X3215	X3046	E2922		L2801	L2743
D3843	D3843	X3548	X3357	X3274	X3216	X3047	K2923		L2802	L2744
		X3549	X3358	X3275	X3217	X3048	A2924		E2803	V2745
		X3550	X3359	X3276	X3218		Q2924		I2804	L2746
		X3551	X3360	X3277	X3219		E2925		L2805	L2747
		X3552	X3361	X3278	X3220		L2926		W2806	P2748
		X3553	X3362	X3279	X3221		L2927		P2807	E2749
		X3554	X3363	X3280	X3222		L2928		P2808	K2750
		X3555	X3364	X3281	X3223		Q2929		L2810	L2751
		X3556	X3365	X3282	X3224		Q2930		E2811	D2752
		X3557	X3366	X3283	X3225		L2931		S2812	
		X3558	X3367	X3284	X3226		Q2932		L2813	
		X3559	X3368	X3285	X3227		L2933			
		X3560	X3369	X3286	X3228					
		X3561	X3370	X3287	X3229					
		X3562	X3371	X3288	X3230					
		X3563	X3372	X3289	X3231					
		X3564	X3373	X3290	X3232					
		X3565	X3374	X3291	X3233					
		X3566	X3375	X3292	X3234					
		X3567	X3376	X3293	X3235					
		X3568	X3377	X3294	X3236					
		X3569	X3378	X3295	X3237					
		X3570	X3379	X3296	X3238					
		X3571	X3380	X3297	X3239					
		X3572	X3381	X3298	X3240					
		X3573	X3382	X3299	X3241					
		X3574	X3383	X3300	X3242					
		X3575	X3384	X3301	X3243					
		X3576	X3385	X3302	X3244					
		X3577	X3386	X3303	X3245					
		X3578	X3387	X3304	X3246					
		X3579	X3388	X3305	X3247					
		X3580	X3389	X3306	X3248					
		X3581	X3390	X3307	X3249					
		X3582	X3391	X3308	X3250					
		X3583	X3392	X3309	X3251					
		X3584	X3393	X3310	X3252					
		X3585	X3394	X3311	X3253					
		X3586	X3395	X3312	X3254					
		X3587	X3396	X3313	X3255					
		X3588	X3397	X3314	X3256					
		X3589	X3398	X3315	X3257					
		X3590	X3399	X3316	X3258					
		X3591	X3400	X3317	X3259					
		X3592	X3401	X3318	X3260					
		X3593	X3402	X3319	X3261					
		X3594	X3403	X3320	X3262					
		X3595	X3404	X3321	X3263					
		X3596	X3405	X3322	X3264					
		X3597	X3406	X3323	X3265					
		X3598	X3407	X3324	X3266					
		X3599	X3408	X3325	X3267					
		X3600	X3409	X3326	X3268					
		X3601	X3410	X3327	X3269					
		X3602	X3411	X3328	X3270					
		X3603	X3412	X3329	X3271					
		X3604	X3413	X3330	X3272					
		X3605	X3414	X3331	X3273					
		X3606	X3415	X3332	X3274					
		X3607	X3416	X3333	X3275					
		X3608	X3417	X3334	X3276					
		X3609	X3418	X3335	X3277					
		X3610	X3419	X3336	X3278					
		X3611	X3420	X3337	X3279					
		X3612	X3421	X3338	X3280					
		X3613	X3422	X3339	X3281					
		X3614	X3423	X3340	X3282					
		X3615	X3424	X3341	X3283					
		X3616	X3425	X3342	X3284					
		X3617	X3426	X3343	X3285					
		X3618	X3427	X3344	X3286					
		X3619	X3428	X3345	X3287					
		X3620	X3429	X3346	X3288					
		X3621	X3430	X3347	X3289					
		X3622	X3431	X3348	X3290					
		X3623	X3432	X3349	X3291					
		X3624	X3433	X3350	X3292					
		X3625	X3434	X3351	X3293					
		X3626	X3435	X3352	X3294					
		X3627	X3436	X3353	X3295					
		X3628	X3437	X3354	X3296					
		X3629	X3438	X3355	X3297					
		X3630	X3439	X3356	X3298					
		X3631	X3440	X3357	X3299					
		X3632	X3441	X3358	X3300					
		X3633	X3442	X3359	X3301					
		X3634	X3443	X3360	X3302					
		X3635	X3444	X3361	X3303					
		X3636	X3445	X3362	X3304					
		X3637	X3446	X3363	X3305					
		X3638	X3447	X3364	X3306					
		X3639	X3448	X3365	X3307					
		X3640	X3449	X3366	X3308					
		X3641	X3450	X3367	X3309					
		X3642	X3451	X3368	X3310					
		X3643	X3452	X3369	X3311					
		X3644	X3453	X3370	X3312					
		X3645	X3454	X3371	X3313					
		X3646	X3455	X3372	X3314					
		X3647	X3456	X3373	X3315					
		X3648	X3457	X3374	X3316					
		X3649	X3458	X3375	X3317					
		X3650	X3459	X3376	X3318					
		X3651	X3460	X3377	X3319					
		X3652	X3461	X3378	X3320					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/834	0.44	0/1123
1	F	0.18	0/834	0.44	0/1123
1	H	0.18	0/834	0.44	0/1123
1	J	0.18	0/834	0.45	0/1123
2	B	0.20	0/25428	0.52	6/34534 (0.0%)
2	E	0.20	0/25428	0.52	6/34534 (0.0%)
2	G	0.20	0/25428	0.52	6/34534 (0.0%)
2	I	0.20	0/25428	0.52	6/34534 (0.0%)
All	All	0.20	0/105048	0.52	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2807	TRP	CA-C-N	-7.39	112.52	120.94
2	I	2807	TRP	C-N-CA	-7.39	112.52	120.94
2	B	2807	TRP	CA-C-N	-7.38	112.53	120.94
2	B	2807	TRP	C-N-CA	-7.38	112.53	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2807	TRP	CA-C-N	-7.38	112.53	120.94
2	G	2807	TRP	C-N-CA	-7.38	112.53	120.94
2	E	2807	TRP	CA-C-N	-7.35	112.56	120.94
2	E	2807	TRP	C-N-CA	-7.35	112.56	120.94
2	G	131	LEU	CA-CB-CG	5.25	134.66	116.30
2	B	131	LEU	CA-CB-CG	5.24	134.65	116.30
2	E	131	LEU	CA-CB-CG	5.24	134.63	116.30
2	I	131	LEU	CA-CB-CG	5.23	134.60	116.30
2	E	4040	ILE	N-CA-C	-5.19	106.61	111.48
2	B	4040	ILE	N-CA-C	-5.15	106.64	111.48
2	G	4040	ILE	N-CA-C	-5.15	106.64	111.48
2	I	4040	ILE	N-CA-C	-5.12	106.67	111.48
2	I	3642	TYR	CA-C-N	5.11	129.66	122.46
2	I	3642	TYR	C-N-CA	5.11	129.66	122.46
2	G	3642	TYR	CA-C-N	5.11	129.66	122.46
2	G	3642	TYR	C-N-CA	5.11	129.66	122.46
2	E	3642	TYR	CA-C-N	5.10	129.65	122.46
2	E	3642	TYR	C-N-CA	5.10	129.65	122.46
2	B	3642	TYR	CA-C-N	5.09	129.64	122.46
2	B	3642	TYR	C-N-CA	5.09	129.64	122.46

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	6	0
1	F	818	0	824	6	0
1	H	818	0	824	5	0
1	J	818	0	824	4	0
2	B	29499	0	24746	267	0
2	E	29499	0	24746	272	0
2	G	29499	0	24746	264	0
2	I	29499	0	24746	269	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1082	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 5.

All (1082) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.58	0.92
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.58	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.58	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.58	0.91
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.99	0.81
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.99	0.80
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.99	0.79
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.99	0.79
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.99	0.79
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.99	0.79
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.63	0.79
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.63	0.78
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.64	0.78
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.00	0.77
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.00	0.76
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.69
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.75	0.69
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.68
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.75	0.68
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.75	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.59	0.68
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.59	0.68
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.95	0.67
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.59	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.77	0.66
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.95	0.66
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.95	0.66
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.78	0.66
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.66
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.66
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.95	0.65
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.78	0.65
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.13	0.65
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.13	0.65
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.59	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.65
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.13	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.64
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.13	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.62	0.64
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.62	0.64
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.63	0.63
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.31	0.63
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.31	0.63
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.31	0.63
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.63	0.62
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.82	0.62
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.61
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.33	0.61
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:I:4192:ARG:HD2	2:I:5028:PHE:CD2	2.35	0.61
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.82	0.61
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.33	0.61
2:B:4192:ARG:HD2	2:B:5028:PHE:CD2	2.35	0.61
2:E:4192:ARG:HD2	2:E:5028:PHE:CD2	2.35	0.61
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.33	0.61
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.60
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.60
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.60
2:G:4192:ARG:HD2	2:G:5028:PHE:CD2	2.35	0.60
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.33	0.60
2:G:683:ARG:NH1	2:G:707:VAL:O	2.35	0.60
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.67	0.60
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.59
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:B:683:ARG:NH1	2:B:707:VAL:O	2.35	0.59
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.84	0.59
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.85	0.59
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.88	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.35	0.59
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.67	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.59
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.59
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.59
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.85	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.58
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.84	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.58
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.58
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.67	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.58
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.85	0.58
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.58
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.84	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.58
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.58
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.85	0.58
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.58
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.86	0.58
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	1.86	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.58
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.58
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.37	0.58
2:I:683:ARG:NH1	2:I:707:VAL:O	2.35	0.57
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.57
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	1.86	0.57
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.86	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.77	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.86	0.57
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.87	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.37	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.57
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.38	0.57
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.37	0.57
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.37	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.57
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.38	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.77	0.57
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.38	0.57
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.38	0.57
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.57
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.86	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.37	0.57
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.38	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.67	0.57
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.86	0.57
2:B:132:ALA:HA	2:B:194:SER:HB2	1.86	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.77	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:I:359:TYR:HA	2:I:376:ALA:HA	1.86	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.38	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.38	0.57
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.39	0.56
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	1.86	0.56
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.87	0.56
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.56
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.56
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.56
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	1.86	0.56
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.86	0.56
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.39	0.56
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.87	0.56
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.87	0.56
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.86	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.87	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.86	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.38	0.56
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.56
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.39	0.56
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.56
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.86	0.56
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.39	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.71	0.56
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.38	0.56
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.86	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.86	0.56
2:E:111:HIS:HD2	2:E:114:SER:H	1.54	0.56
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.86	0.56
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.37	0.56
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.38	0.56
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.39	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.39	0.56
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.37	0.55
2:B:111:HIS:HD2	2:B:114:SER:H	1.54	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.86	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.55
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.55
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.55
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.39	0.55
2:G:111:HIS:HD2	2:G:114:SER:H	1.54	0.55
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.89	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.55
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.55
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.55
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.39	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.55
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.89	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.79	0.55
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.89	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.71	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.54
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.90	0.54
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.90	0.54
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.37	0.54
2:I:2868:SER:O	2:I:2872:GLN:N	2.38	0.54
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.39	0.54
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.71	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.54
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.39	0.54
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.54
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.89	0.54
2:I:111:HIS:HD2	2:I:114:SER:H	1.54	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.89	0.54
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.54
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.90	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.54
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.89	0.54
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.90	0.54
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.39	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.54
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.90	0.54
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.90	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.41	0.54
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.88	0.54
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.90	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.54
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.89	0.53
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.42	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.53
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.53
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.73	0.53
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.42	0.53
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.73	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.42	0.53
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.90	0.53
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.42	0.53
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.53
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.39	0.53
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.42	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.41	0.53
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.42	0.53
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.42	0.53
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.38	0.53
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.53
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.42	0.53
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.52
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.52
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.73	0.52
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.42	0.52
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.41	0.52
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.90	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.38	0.52
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.52
2:E:689:THR:H	2:E:778:PHE:HE2	1.58	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.52
2:B:689:THR:H	2:B:778:PHE:HE2	1.58	0.52
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.90	0.52
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.40	0.52
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.73	0.52
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.92	0.52
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.42	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.88	0.52
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.91	0.52
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.92	0.52
2:G:3842:LEU:O	2:G:3929:SER:OG	2.26	0.52
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.42	0.52
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.90	0.52
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.42	0.52
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.92	0.52
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.92	0.52
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.91	0.52
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.90	0.52
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.92	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.52
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.91	0.52
2:B:3842:LEU:O	2:B:3929:SER:OG	2.26	0.51
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.51
2:I:689:THR:H	2:I:778:PHE:HE2	1.58	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.43	0.51
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.88	0.51
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.91	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.43	0.51
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.91	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.51
2:E:3842:LEU:O	2:E:3929:SER:OG	2.27	0.51
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.92	0.51
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.51
2:E:2868:SER:O	2:E:2872:GLN:N	2.38	0.51
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.44	0.51
2:G:689:THR:H	2:G:778:PHE:HE2	1.58	0.51
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.92	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.51
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.91	0.51
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.41	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.51
2:I:3842:LEU:O	2:I:3929:SER:OG	2.27	0.51
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.92	0.51
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.44	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.51
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.44	0.51
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.91	0.51
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.40	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.43	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.40	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.92	0.51
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.84	0.51
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.44	0.51
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.76	0.51
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.93	0.51
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.84	0.51
2:I:626:LEU:HG	2:I:628:GLY:H	1.76	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.44	0.51
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.51
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.51
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.93	0.51
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.93	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.93	0.50
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.44	0.50
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.44	0.50
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.44	0.50
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.44	0.50
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.41	0.50
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.91	0.50
2:G:626:LEU:HG	2:G:628:GLY:H	1.76	0.50
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.76	0.50
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.76	0.50
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.93	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.93	0.50
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.45	0.50
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.50
2:I:3992:PHE:O	2:I:3996:PHE:N	2.40	0.50
2:E:626:LEU:HG	2:E:628:GLY:H	1.76	0.50
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.50
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.93	0.50
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.77	0.50
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.50
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.27	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.93	0.50
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.45	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:E:4176:PRO:O	2:E:4202:ARG:NH2	2.45	0.50
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.93	0.50
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.44	0.50
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.41	0.50
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.45	0.50
2:B:626:LEU:HG	2:B:628:GLY:H	1.76	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.93	0.49
2:E:621:ILE:O	2:E:625:LEU:N	2.45	0.49
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.45	0.49
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.77	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.94	0.49
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.49
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.45	0.49
2:G:621:ILE:O	2:G:625:LEU:N	2.45	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.49
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.49
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.78	0.49
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.45	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.79	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.44	0.49
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.93	0.49
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.45	0.49
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.49
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.84	0.49
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.95	0.49
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.78	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.78	0.49
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.45	0.49
2:B:4228:ALA:O	2:B:4232:GLU:N	2.46	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:I:621:ILE:O	2:I:625:LEU:N	2.45	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.46	0.49
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.95	0.49
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.45	0.49
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.95	0.49
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.27	0.49
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.49
2:I:4228:ALA:O	2:I:4232:GLU:N	2.46	0.49
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.77	0.48
2:I:4976:GLU:HA	2:I:4979:THR:HG23	1.95	0.48
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.95	0.48
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.95	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:B:4176:PRO:O	2:B:4202:ARG:NH2	2.45	0.48
2:B:4976:GLU:HA	2:B:4979:THR:HG23	1.95	0.48
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.46	0.48
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.84	0.48
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.46	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.95	0.48
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.95	0.48
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.95	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.46	0.48
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.48
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.95	0.48
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.46	0.48
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.95	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.93	0.48
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.78	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.95	0.48
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.48
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.78	0.48
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.48
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.95	0.48
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.96	0.48
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.48
2:G:37:LEU:HD11	2:G:47:CYS:HB3	1.96	0.48
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.95	0.48
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.46	0.48
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.77	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.46	0.48
2:E:4228:ALA:O	2:E:4232:GLU:N	2.46	0.48
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.48
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.45	0.48
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.78	0.48
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.96	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.48
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.47	0.48
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.96	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.38	0.48
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.45	0.48
2:G:4228:ALA:O	2:G:4232:GLU:N	2.46	0.48
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.78	0.48
2:I:37:LEU:HD11	2:I:47:CYS:HB3	1.96	0.48
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.96	0.48
2:I:4963:ILE:HG21	2:I:4967:TYR:HD2	1.79	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.95	0.48
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.95	0.48
2:I:4176:PRO:O	2:I:4202:ARG:NH2	2.45	0.48
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.45	0.48
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.96	0.48
2:E:4976:GLU:HA	2:E:4979:THR:HG23	1.95	0.48
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.96	0.48
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.95	0.47
2:E:4963:ILE:HG21	2:E:4967:TYR:HD2	1.79	0.47
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.96	0.47
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.78	0.47
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.47	0.47
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.79	0.47
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.95	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.78	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.97	0.47
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.95	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.47
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.79	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.96	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.47
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.47
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4976:GLU:HA	2:G:4979:THR:HG23	1.95	0.47
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.95	0.47
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.78	0.47
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.96	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.79	0.47
2:G:4192:ARG:HD2	2:G:5028:PHE:CE2	2.50	0.47
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.46	0.47
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.96	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.47	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.97	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.38	0.47
2:B:3992:PHE:O	2:B:3996:PHE:N	2.40	0.47
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.96	0.47
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.47
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.47
2:E:5023:PRO:HB3	2:E:5026:ASP:O	2.14	0.47
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.47
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.47	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.47
2:G:5023:PRO:HB3	2:G:5026:ASP:O	2.15	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.97	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.97	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:B:4192:ARG:HD2	2:B:5028:PHE:CE2	2.50	0.47
2:B:4963:ILE:HG21	2:B:4967:TYR:HD2	1.79	0.47
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.80	0.47
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.47	0.47
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.96	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.97	0.47
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.44	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.78	0.47
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.96	0.47
2:G:4963:ILE:HG21	2:G:4967:TYR:HD2	1.79	0.47
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.96	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.97	0.47
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.96	0.47
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.80	0.47
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.96	0.47
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:463:GLU:O	2:E:466:SER:OG	2.30	0.47
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.79	0.47
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.97	0.47
2:B:5023:PRO:HB3	2:B:5026:ASP:O	2.15	0.47
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.96	0.47
2:E:4192:ARG:HD2	2:E:5028:PHE:CE2	2.50	0.47
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.96	0.47
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.80	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.97	0.47
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.80	0.47
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.47	0.46
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.80	0.46
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.97	0.46
2:I:5023:PRO:HB3	2:I:5026:ASP:O	2.15	0.46
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.79	0.46
2:B:472:ARG:HA	2:B:475:GLN:HB2	1.98	0.46
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.46
2:E:37:LEU:HD11	2:E:47:CYS:HB3	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.96	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.79	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.47	0.46
2:G:70:GLU:HG3	2:G:117:TYR:HE1	1.80	0.46
2:E:4561:THR:O	2:E:4565:LEU:N	2.46	0.46
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.46
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.46
2:B:37:LEU:HD11	2:B:47:CYS:HB3	1.96	0.46
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.46
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.96	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.49	0.46
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.81	0.46
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.98	0.46
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.79	0.46
2:I:4192:ARG:HD2	2:I:5028:PHE:CE2	2.50	0.46
2:I:4713:SER:HG	2:I:4775:TYR:HH	1.63	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.81	0.46
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.46
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.81	0.46
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.97	0.46
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.81	0.46
2:B:621:ILE:O	2:B:625:LEU:N	2.45	0.46
2:I:512:ALA:HA	2:I:515:TRP:HB2	1.98	0.46
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.97	0.46
2:I:4561:THR:O	2:I:4565:LEU:N	2.46	0.46
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.46
2:E:472:ARG:HA	2:E:475:GLN:HB2	1.98	0.46
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.46
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.97	0.46
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.80	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.46
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.98	0.46
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.46
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.97	0.46
2:I:472:ARG:HA	2:I:475:GLN:HB2	1.98	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.46
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.80	0.46
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.97	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.46
1:A:11:ASP:OD1	1:A:67:SER:OG	2.34	0.46
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.81	0.46
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.97	0.46
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.98	0.46
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.97	0.46
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.79	0.46
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.46
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.46
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.46
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.81	0.46
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.80	0.45
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.96	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.97	0.45
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.45
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.81	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.49	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.45
2:G:512:ALA:HA	2:G:515:TRP:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.45
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.41	0.45
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.80	0.45
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.99	0.45
2:E:3992:PHE:O	2:E:3996:PHE:N	2.40	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.98	0.45
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.99	0.45
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.30	0.45
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.98	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.45
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.97	0.45
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.97	0.45
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.98	0.45
2:E:914:PRO:HD2	2:E:917:GLU:HB2	1.98	0.45
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.99	0.45
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.99	0.45
2:G:472:ARG:HA	2:G:475:GLN:HB2	1.98	0.45
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.97	0.45
2:B:4561:THR:O	2:B:4565:LEU:N	2.46	0.45
2:E:932:LEU:HA	2:E:935:LEU:HD12	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.99	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.49	0.45
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.45
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.99	0.45
2:E:512:ALA:HA	2:E:515:TRP:HB2	1.98	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.99	0.45
2:B:932:LEU:HA	2:B:935:LEU:HD12	1.98	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.98	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.34	0.45
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.50	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.44	0.45
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.45
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.70	0.45
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.99	0.45
2:I:5028:PHE:O	2:I:5028:PHE:CD1	2.70	0.45
2:G:215:THR:HG22	2:G:273:HIS:HA	1.99	0.45
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:B:914:PRO:HD2	2:B:917:GLU:HB2	1.98	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.81	0.45
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.99	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.98	0.45
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.45
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.45
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.70	0.45
2:B:512:ALA:HA	2:B:515:TRP:HB2	1.98	0.44
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.34	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:I:914:PRO:HD2	2:I:917:GLU:HB2	1.98	0.44
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.44
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.99	0.44
2:G:914:PRO:HD2	2:G:917:GLU:HB2	1.98	0.44
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.98	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CD1	2.70	0.44
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.98	0.44
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.50	0.44
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.99	0.44
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.99	0.44
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.83	0.44
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.44
2:E:4959:PHE:O	2:E:4959:PHE:CD1	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.44
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.00	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.98	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.99	0.44
2:B:4959:PHE:CG	2:B:4959:PHE:O	2.70	0.44
2:E:580:GLU:HG2	2:E:583:ILE:HD11	2.00	0.44
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.99	0.44
2:E:3762:ARG:NH2	2:E:4757:LYS:O	2.51	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.45	0.44
2:I:932:LEU:HA	2:I:935:LEU:HD12	1.98	0.44
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.50	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:G:3762:ARG:NH2	2:G:4757:LYS:O	2.51	0.44
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.00	0.44
2:B:983:THR:O	2:B:987:ARG:N	2.50	0.44
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.50	0.44
2:E:983:THR:O	2:E:987:ARG:N	2.50	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.00	0.44
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.44
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.99	0.44
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.50	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.44
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.44
2:B:3762:ARG:NH2	2:B:4757:LYS:O	2.51	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.70	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	1.99	0.44
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.44
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.99	0.44
2:I:1739:THR:H	2:I:1742:THR:HB	1.83	0.44
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.99	0.44
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CD1	2.70	0.44
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.50	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.70	0.44
2:G:932:LEU:HA	2:G:935:LEU:HD12	1.98	0.44
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.00	0.44
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:PRO:HD2	2:B:867:LEU:HD12	2.00	0.44
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.99	0.44
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.00	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.44
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.44
2:E:5028:PHE:O	2:E:5028:PHE:CD1	2.70	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.99	0.44
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.99	0.44
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.50	0.44
2:G:3992:PHE:HB2	2:G:4023:MET:HE1	2.00	0.44
2:G:4561:THR:O	2:G:4565:LEU:N	2.46	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.43
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.99	0.43
2:E:1739:THR:H	2:E:1742:THR:HB	1.83	0.43
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.50	0.43
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.99	0.43
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.00	0.43
2:I:3762:ARG:NH2	2:I:4757:LYS:O	2.51	0.43
2:I:3992:PHE:HB2	2:I:4023:MET:HE1	2.00	0.43
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.43
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.00	0.43
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.99	0.43
2:B:1154:ASP:O	2:B:1158:ASN:N	2.51	0.43
2:B:1739:THR:H	2:B:1742:THR:HB	1.83	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.99	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.99	0.43
2:G:2780:ASN:O	2:G:2787:THR:OG1	2.30	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.00	0.43
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.43
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.00	0.43
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.43
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.52	0.43
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.99	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.51	0.43
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.43
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.00	0.43
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.43
2:B:3992:PHE:HB2	2:B:4023:MET:HE1	2.00	0.43
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.84	0.43
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.00	0.43
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.32	0.43
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.00	0.43
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:1284:UNK:HA	2:I:1463:UNK:HA	2.00	0.43
2:G:3992:PHE:O	2:G:3996:PHE:N	2.40	0.43
1:H:11:ASP:OD1	1:H:67:SER:OG	2.34	0.43
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.43
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.50	0.43
2:E:864:PRO:HD2	2:E:867:LEU:HD12	2.00	0.43
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.00	0.43
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.43
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.83	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.99	0.43
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.00	0.43
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.00	0.43
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.84	0.43
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.00	0.43
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.99	0.43
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.43
2:E:2290:LEU:HB3	2:E:3849:ARG:HH12	1.84	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.51	0.43
2:G:1739:THR:H	2:G:1742:THR:HB	1.83	0.43
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.99	0.43
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.00	0.43
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.01	0.43
2:E:582:HIS:O	2:E:585:SER:OG	2.31	0.43
2:E:1284:UNK:HA	2:E:1463:UNK:HA	2.00	0.43
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.00	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.43
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.01	0.43
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.84	0.43
2:G:983:THR:O	2:G:987:ARG:N	2.49	0.43
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.84	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	2.01	0.43
2:I:401:ALA:HA	2:I:404:ILE:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:983:THR:O	2:I:987:ARG:N	2.50	0.43
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.84	0.43
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.00	0.43
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.84	0.43
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	2.01	0.43
2:E:1154:ASP:O	2:E:1158:ASN:N	2.51	0.43
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.43
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.43
2:E:3992:PHE:HB2	2:E:4023:MET:HE1	2.00	0.43
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.83	0.43
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	2.01	0.43
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.00	0.43
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.01	0.43
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.43
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	2.01	0.43
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.00	0.43
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.00	0.42
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.00	0.42
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.29	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.42
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.00	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.83	0.42
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	2.01	0.42
2:E:401:ALA:HA	2:E:404:ILE:HD12	2.01	0.42
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	2.01	0.42
2:I:582:HIS:O	2:I:585:SER:OG	2.31	0.42
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.00	0.42
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.53	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.00	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.83	0.42
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.53	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.01	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.52	0.42
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.52	0.42
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.53	0.42
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.46	0.42
2:G:2290:LEU:HB3	2:G:3849:ARG:HH12	1.84	0.42
2:B:2290:LEU:HB3	2:B:3849:ARG:HH12	1.84	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.42
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	2.01	0.42
2:I:2758:PHE:O	2:I:2762:THR:N	2.49	0.42
2:I:3513:UNK:O	2:I:3515:UNK:N	2.53	0.42
2:I:4560:TYR:O	2:I:4564:PHE:N	2.49	0.42
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	2.01	0.42
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.51	0.42
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.42
2:B:401:ALA:HA	2:B:404:ILE:HD12	2.00	0.42
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	2.02	0.42
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.42
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.52	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.53	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:G:1105:ALA:N	2:G:1189:LEU:O	2.53	0.42
1:F:82:TYR:O	1:F:86:GLY:N	2.53	0.42
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.84	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.42
2:E:4984:ASN:C	2:E:4986:ALA:N	2.78	0.42
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.93	0.42
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.44	0.42
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.34	0.42
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	2.01	0.42
2:I:2290:LEU:HB3	2:I:3849:ARG:HH12	1.84	0.42
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.55	0.42
2:I:2902:HIS:CE1	2:I:2904:LEU:HB2	2.55	0.42
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.00	0.42
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.51	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.53	0.42
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.00	0.42
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.51	0.42
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.93	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.42
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	2.02	0.42
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.93	0.42
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.42
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	2.01	0.42
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.52	0.42
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.55	0.42
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4984:ASN:C	2:I:4986:ALA:N	2.78	0.42
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.95	0.42
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	2.01	0.42
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	2.01	0.42
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	2.01	0.42
2:E:3513:UNK:O	2:E:3515:UNK:N	2.53	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.42
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.55	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.42
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	2.02	0.42
2:B:4826:ILE:O	2:B:4829:SER:OG	2.37	0.42
2:E:2902:HIS:CE1	2:E:2904:LEU:HB2	2.55	0.42
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.01	0.42
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	2.01	0.41
2:B:2902:HIS:CE1	2:B:2904:LEU:HB2	2.55	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.01	0.41
2:E:635:THR:HG23	2:E:1693:GLN:HE22	1.85	0.41
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	2.01	0.41
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.55	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:I:1089:TYR:N	2:I:1224:GLU:O	2.53	0.41
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.02	0.41
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	2.02	0.41
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.55	0.41
2:G:3513:UNK:O	2:G:3515:UNK:N	2.53	0.41
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.02	0.41
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.02	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.48	0.41
2:E:1089:TYR:N	2:E:1224:GLU:O	2.53	0.41
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.53	0.41
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.93	0.41
2:E:4197:ILE:HG21	2:E:4202:ARG:HH21	1.85	0.41
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.84	0.41
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	2.02	0.41
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.41
2:I:2883:HIS:NE2	2:I:2906:VAL:O	2.50	0.41
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.85	0.41
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.02	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.41
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.85	0.41
2:B:4984:ASN:C	2:B:4986:ALA:N	2.78	0.41
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.02	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.01	0.41
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.03	0.41
2:I:4197:ILE:HG21	2:I:4202:ARG:HH21	1.85	0.41
2:G:1284:UNK:HA	2:G:1463:UNK:HA	2.00	0.41
2:G:2902:HIS:CE1	2:G:2904:LEU:HB2	2.55	0.41
2:B:261:ARG:HB3	2:B:283:ARG:HB3	2.02	0.41
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.02	0.41
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	2.03	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.93	0.41
2:G:401:ALA:HA	2:G:404:ILE:HD12	2.01	0.41
1:F:11:ASP:OD1	1:F:67:SER:OG	2.34	0.41
2:E:3722:TYR:CZ	2:E:3782:MET:HE3	2.56	0.41
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.32	0.41
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.01	0.41
2:E:4978:HIS:CA	2:E:4982:GLU:HB2	2.43	0.41
2:I:261:ARG:HB3	2:I:283:ARG:HB3	2.02	0.41
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.02	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.03	0.41
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.41
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.54	0.41
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.03	0.41
2:G:1089:TYR:N	2:G:1224:GLU:O	2.54	0.41
2:G:4197:ILE:HG21	2:G:4202:ARG:HH21	1.85	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:B:3513:UNK:O	2:B:3515:UNK:N	2.53	0.41
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.41
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.56	0.41
2:B:3722:TYR:CZ	2:B:3782:MET:HE3	2.56	0.41
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.03	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.56	0.41
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.55	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.49	0.41
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.02	0.41
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.41
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.03	0.41
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.44	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.41
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.55	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.56	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.29	0.41
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.46	0.41
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.02	0.41
2:B:4197:ILE:HG21	2:B:4202:ARG:HH21	1.85	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.84	0.41
2:E:4826:ILE:O	2:E:4829:SER:OG	2.37	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	2.03	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.53	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.31	0.41
2:G:635:THR:HG23	2:G:1693:GLN:HE22	1.85	0.41
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.03	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
2:G:3722:TYR:CZ	2:G:3782:MET:HE3	2.56	0.41
2:B:134:ASP:OD1	2:B:134:ASP:N	2.53	0.41
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.54	0.41
2:B:2378:ALA:O	2:B:2382:GLU:N	2.54	0.41
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	2.03	0.41
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.02	0.41
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.03	0.41
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.02	0.41
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.03	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.02	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.03	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.41
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.02	0.41
2:B:635:THR:HG23	2:B:1693:GLN:HE22	1.85	0.41
2:B:1089:TYR:N	2:B:1224:GLU:O	2.54	0.41
2:B:2103:VAL:O	2:B:2107:GLN:N	2.46	0.41
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.03	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.56	0.41
2:I:1105:ALA:N	2:I:1189:LEU:O	2.53	0.41
2:I:3722:TYR:CZ	2:I:3782:MET:HE3	2.55	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.41
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.02	0.40
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.40
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.03	0.40
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.54	0.40
2:I:683:ARG:HG2	2:I:717:ASP:HB3	2.04	0.40
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	2.03	0.40
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	2.03	0.40
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.93	0.40
2:G:4984:ASN:C	2:G:4986:ALA:N	2.78	0.40
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.02	0.40
2:B:5014:TYR:HE2	4:B:5102:CFF:H102	1.86	0.40
2:E:134:ASP:OD1	2:E:134:ASP:N	2.53	0.40
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.51	0.40
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	2.02	0.40
2:I:635:THR:HG23	2:I:1693:GLN:HE22	1.85	0.40
2:I:4090:LYS:O	2:I:4094:GLN:N	2.53	0.40
2:I:4156:HIS:CE1	2:I:5036:LEU:HD11	2.56	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.40
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.02	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.86	0.40
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	2.02	0.40
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.40
2:G:4826:ILE:O	2:G:4829:SER:OG	2.37	0.40
2:B:229:GLU:HA	2:B:249:GLY:HA2	2.03	0.40
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.03	0.40
2:E:229:GLU:HA	2:E:249:GLY:HA2	2.03	0.40
2:E:261:ARG:HB3	2:E:283:ARG:HB3	2.02	0.40
2:E:1076:ARG:HB3	2:E:1191:VAL:HG23	2.03	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.86	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40
2:G:683:ARG:HG2	2:G:717:ASP:HB3	2.04	0.40
2:E:113:HIS:O	2:E:399:GLN:NE2	2.55	0.40
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.54	0.40
2:G:261:ARG:HB3	2:G:283:ARG:HB3	2.02	0.40
2:B:4156:HIS:CE1	2:B:5036:LEU:HD11	2.56	0.40
2:B:4984:ASN:C	2:B:4986:ALA:H	2.29	0.40
2:E:661:LYS:HB3	2:E:808:TYR:CD1	2.57	0.40
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.80	0.40
2:E:4984:ASN:C	2:E:4986:ALA:H	2.29	0.40
2:I:4984:ASN:C	2:I:4986:ALA:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.03	0.40
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2916 (90%)	311 (10%)	8 (0%)	43	78
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	43	78
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	43	78
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	43	78
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	44	78

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	4985	LEU
2	E	1708	ARG
2	E	4985	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1708	ARG
2	I	4985	LEU
2	G	1708	ARG
2	G	4985	LEU
2	B	1840	PRO
2	B	2291	GLN
2	E	1840	PRO
2	E	2291	GLN
2	I	1840	PRO
2	I	2291	GLN
2	G	1840	PRO
2	G	2291	GLN
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO
2	B	4667	PRO
2	E	4667	PRO
2	I	4667	PRO
2	G	4667	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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83
2	G	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83
2	I	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83
All	All	10324/12444 (83%)	10284 (100%)	40 (0%)	81	83

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	1600	LEU
2	B	1676	LEU
2	B	3663	LEU
2	B	3805	LEU
2	B	4154	VAL
2	B	4981	GLU
2	B	4983	HIS
2	B	4995	LEU
2	B	5027	CYS
2	E	131	LEU
2	E	1600	LEU
2	E	1676	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4154	VAL
2	E	4981	GLU
2	E	4983	HIS
2	E	4995	LEU
2	E	5027	CYS
2	I	131	LEU
2	I	1600	LEU
2	I	1676	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4154	VAL
2	I	4981	GLU
2	I	4983	HIS
2	I	4995	LEU
2	I	5027	CYS
2	G	131	LEU
2	G	1600	LEU
2	G	1676	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	3663	LEU
2	G	3805	LEU
2	G	4154	VAL
2	G	4981	GLU
2	G	4983	HIS
2	G	4995	LEU
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (227) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	151	HIS
2	B	218	HIS
2	B	224	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	399	GLN
2	B	413	GLN
2	B	582	HIS
2	B	597	HIS
2	B	765	GLN
2	B	797	HIS
2	B	838	HIS
2	B	877	ASN
2	B	1206	GLN
2	B	1598	GLN
2	B	1665	HIS
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1861	GLN
2	B	1973	GLN
2	B	2127	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2194	HIS
2	B	2260	ASN
2	B	2858	GLN
2	B	3761	GLN
2	B	3781	GLN
2	B	3806	ASN
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3970	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4043	GLN
2	B	4054	ASN
2	B	4109	GLN
2	B	4120	ASN
2	B	4133	GLN
2	B	4553	ASN
2	B	4691	GLN
2	B	4776	GLN
2	B	4946	GLN
2	B	4947	GLN
2	B	4949	GLN
2	B	4983	HIS
2	E	57	ASN
2	E	113	HIS
2	E	151	HIS
2	E	218	HIS
2	E	224	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	399	GLN
2	E	413	GLN
2	E	582	HIS
2	E	597	HIS
2	E	765	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	797	HIS
2	E	838	HIS
2	E	877	ASN
2	E	1206	GLN
2	E	1598	GLN
2	E	1665	HIS
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1861	GLN
2	E	1973	GLN
2	E	2127	GLN
2	E	2194	HIS
2	E	2260	ASN
2	E	2773	ASN
2	E	2858	GLN
2	E	3761	GLN
2	E	3806	ASN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3970	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4043	GLN
2	E	4054	ASN
2	E	4109	GLN
2	E	4120	ASN
2	E	4133	GLN
2	E	4553	ASN
2	E	4691	GLN
2	E	4776	GLN
2	E	4806	ASN
2	E	4946	GLN
2	E	4947	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	4949	GLN
2	E	4983	HIS
2	I	57	ASN
2	I	113	HIS
2	I	151	HIS
2	I	201	ASN
2	I	218	HIS
2	I	224	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	399	GLN
2	I	413	GLN
2	I	582	HIS
2	I	765	GLN
2	I	797	HIS
2	I	838	HIS
2	I	877	ASN
2	I	1206	GLN
2	I	1598	GLN
2	I	1665	HIS
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1861	GLN
2	I	1973	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	2858	GLN
2	I	3699	HIS
2	I	3761	GLN
2	I	3781	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	3963	ASN
2	I	3970	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4043	GLN
2	I	4054	ASN
2	I	4109	GLN
2	I	4120	ASN
2	I	4133	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4776	GLN
2	I	4946	GLN
2	I	4947	GLN
2	I	4949	GLN
2	I	4983	HIS
2	G	57	ASN
2	G	113	HIS
2	G	151	HIS
2	G	201	ASN
2	G	218	HIS
2	G	224	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	399	GLN
2	G	413	GLN
2	G	489	ASN
2	G	582	HIS
2	G	597	HIS
2	G	838	HIS
2	G	877	ASN
2	G	1206	GLN
2	G	1598	GLN
2	G	1665	HIS
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1861	GLN
2	G	1973	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	2127	GLN
2	G	2194	HIS
2	G	2260	ASN
2	G	2858	GLN
2	G	3761	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3970	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4043	GLN
2	G	4054	ASN
2	G	4109	GLN
2	G	4120	ASN
2	G	4133	GLN
2	G	4553	ASN
2	G	4691	GLN
2	G	4776	GLN
2	G	4806	ASN
2	G	4947	GLN
2	G	4949	GLN
2	G	4983	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	G	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.80	9 (18%)
4	CFF	B	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.78	9 (39%)
4	CFF	I	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.77	9 (39%)
3	ATP	E	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.81	9 (18%)
3	ATP	I	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.80	9 (18%)
3	ATP	B	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.80	9 (18%)
4	CFF	G	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.79	9 (39%)
4	CFF	E	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.78	9 (39%)

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	ATP	G	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.53	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	4.53	1.47	1.39
3	G	5101	ATP	C5-C4	4.53	1.47	1.39
3	E	5101	ATP	C5-C4	4.52	1.47	1.39
4	I	5102	CFF	C6-N1	-3.89	1.32	1.40
4	E	5102	CFF	C6-N1	-3.88	1.32	1.40
4	B	5102	CFF	C6-N1	-3.87	1.32	1.40
4	G	5102	CFF	C6-N1	-3.87	1.32	1.40
4	B	5102	CFF	C4-N3	-2.58	1.33	1.38
4	I	5102	CFF	C4-N3	-2.58	1.33	1.38
4	G	5102	CFF	C4-N3	-2.58	1.33	1.38
3	B	5101	ATP	C5-N7	-2.57	1.34	1.39
3	G	5101	ATP	C5-N7	-2.57	1.34	1.39
4	E	5102	CFF	C4-N3	-2.57	1.33	1.38
3	E	5101	ATP	C5-N7	-2.56	1.34	1.39
3	I	5101	ATP	C5-N7	-2.53	1.34	1.39
3	E	5101	ATP	C5-C6	2.35	1.47	1.41
3	B	5101	ATP	C5-C6	2.35	1.47	1.41
3	I	5101	ATP	C5-C6	2.35	1.47	1.41
3	G	5101	ATP	C5-C6	2.33	1.47	1.41
3	E	5101	ATP	C8-N7	2.32	1.36	1.31
3	B	5101	ATP	C8-N7	2.31	1.36	1.31
3	G	5101	ATP	C8-N7	2.31	1.36	1.31
3	I	5101	ATP	C8-N7	2.29	1.36	1.31
4	G	5102	CFF	C5-N7	-2.26	1.34	1.38
4	E	5102	CFF	C5-N7	-2.24	1.34	1.38
4	I	5102	CFF	C5-N7	-2.23	1.34	1.38
4	B	5102	CFF	C5-N7	-2.22	1.34	1.38
3	B	5101	ATP	C4-N9	-2.13	1.33	1.37
3	G	5101	ATP	C4-N9	-2.13	1.33	1.37
3	E	5101	ATP	C4-N9	-2.12	1.33	1.37
4	B	5102	CFF	O13-C6	-2.10	1.18	1.23
4	I	5102	CFF	O13-C6	-2.10	1.18	1.23
4	G	5102	CFF	O13-C6	-2.10	1.18	1.23
3	I	5101	ATP	C4-N9	-2.10	1.33	1.37
4	E	5102	CFF	O13-C6	-2.08	1.18	1.23
4	B	5102	CFF	O11-C2	-2.05	1.18	1.22
4	I	5102	CFF	O11-C2	-2.05	1.18	1.22
4	G	5102	CFF	O11-C2	-2.05	1.18	1.22
4	E	5102	CFF	O11-C2	-2.04	1.18	1.22

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.62	112.02	126.28
4	E	5102	CFF	C14-N7-C8	-7.61	112.03	126.28
4	B	5102	CFF	C14-N7-C8	-7.60	112.05	126.28
4	I	5102	CFF	C14-N7-C8	-7.59	112.08	126.28
3	B	5101	ATP	C5-C4-N3	-5.91	118.58	126.72
3	E	5101	ATP	C5-C4-N3	-5.91	118.58	126.72
3	I	5101	ATP	C5-C4-N3	-5.91	118.58	126.72
3	G	5101	ATP	C5-C4-N3	-5.90	118.59	126.72
4	G	5102	CFF	C14-N7-C5	5.04	139.75	127.77
4	E	5102	CFF	C14-N7-C5	5.02	139.71	127.77
4	B	5102	CFF	C14-N7-C5	5.02	139.71	127.77
4	I	5102	CFF	C14-N7-C5	5.00	139.66	127.77
3	I	5101	ATP	N3-C4-N9	4.77	135.28	127.17
3	E	5101	ATP	N3-C4-N9	4.77	135.28	127.17
3	B	5101	ATP	N3-C4-N9	4.76	135.26	127.17
3	G	5101	ATP	N3-C4-N9	4.76	135.26	127.17
4	I	5102	CFF	C5-C6-N1	4.33	120.00	112.06
4	E	5102	CFF	C5-C6-N1	4.32	119.98	112.06
4	G	5102	CFF	C5-C6-N1	4.32	119.98	112.06
4	B	5102	CFF	C5-C6-N1	4.31	119.95	112.06
3	E	5101	ATP	C2-N3-C4	3.78	121.07	111.83
3	I	5101	ATP	C2-N3-C4	3.78	121.06	111.83
3	B	5101	ATP	C2-N3-C4	3.78	121.06	111.83
3	G	5101	ATP	C2-N3-C4	3.78	121.05	111.83
3	E	5101	ATP	N3-C2-N1	-3.58	123.17	128.58
3	I	5101	ATP	N3-C2-N1	-3.54	123.22	128.58
3	B	5101	ATP	N3-C2-N1	-3.54	123.22	128.58
3	G	5101	ATP	N3-C2-N1	-3.54	123.22	128.58
4	G	5102	CFF	C6-N1-C2	-3.38	120.16	125.66
4	E	5102	CFF	C6-N1-C2	-3.37	120.18	125.66
4	B	5102	CFF	C6-N1-C2	-3.36	120.20	125.66
4	I	5102	CFF	C6-N1-C2	-3.36	120.20	125.66
3	B	5101	ATP	C4-C5-N7	-3.25	106.87	110.58
3	I	5101	ATP	C4-C5-N7	-3.25	106.87	110.58
3	G	5101	ATP	C4-C5-N7	-3.25	106.87	110.58
3	E	5101	ATP	C4-C5-N7	-3.22	106.90	110.58
4	G	5102	CFF	N3-C4-N9	3.10	131.15	126.27
4	B	5102	CFF	N3-C4-N9	3.08	131.11	126.27
4	I	5102	CFF	N3-C4-N9	3.05	131.07	126.27
4	E	5102	CFF	N3-C4-N9	3.05	131.06	126.27
4	G	5102	CFF	N7-C8-N9	-3.01	108.02	113.48
4	E	5102	CFF	N7-C8-N9	-2.99	108.06	113.48
4	B	5102	CFF	N7-C8-N9	-2.99	108.06	113.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	N7-C8-N9	-2.98	108.09	113.48
4	G	5102	CFF	O13-C6-C5	-2.86	120.52	126.38
4	E	5102	CFF	O13-C6-C5	-2.85	120.54	126.38
4	B	5102	CFF	O13-C6-C5	-2.85	120.55	126.38
4	I	5102	CFF	O13-C6-C5	-2.85	120.55	126.38
3	B	5101	ATP	C4-N9-C8	2.83	108.71	105.74
3	G	5101	ATP	C4-N9-C8	2.83	108.71	105.74
3	E	5101	ATP	C4-N9-C8	2.83	108.70	105.74
3	I	5101	ATP	C4-N9-C8	2.82	108.70	105.74
4	I	5102	CFF	C6-C5-C4	-2.60	119.64	122.92
4	G	5102	CFF	C6-C5-C4	-2.60	119.65	122.92
4	E	5102	CFF	C6-C5-C4	-2.59	119.66	122.92
4	B	5102	CFF	C6-C5-C4	-2.58	119.67	122.92
3	E	5101	ATP	C3'-C2'-C1'	2.48	106.15	101.46
3	B	5101	ATP	C3'-C2'-C1'	2.46	106.12	101.46
3	G	5101	ATP	C3'-C2'-C1'	2.45	106.11	101.46
3	B	5101	ATP	C5-N7-C8	2.45	107.31	103.45
3	G	5101	ATP	C5-N7-C8	2.45	107.31	103.45
3	I	5101	ATP	C3'-C2'-C1'	2.44	106.08	101.46
4	E	5102	CFF	C12-N3-C2	2.44	121.59	117.33
4	B	5102	CFF	C12-N3-C2	2.44	121.58	117.33
4	G	5102	CFF	C12-N3-C2	2.44	121.58	117.33
4	I	5102	CFF	C12-N3-C2	2.43	121.57	117.33
3	E	5101	ATP	C5-N7-C8	2.43	107.27	103.45
3	I	5101	ATP	C5-N7-C8	2.43	107.27	103.45
3	B	5101	ATP	N9-C8-N7	-2.09	110.97	113.94
3	G	5101	ATP	N9-C8-N7	-2.09	110.97	113.94
3	E	5101	ATP	N9-C8-N7	-2.07	110.99	113.94
3	I	5101	ATP	N9-C8-N7	-2.04	111.03	113.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	PB-O3A-PA-O5'
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	PB-O3A-PA-O5'
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	PB-O3A-PA-O5'
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

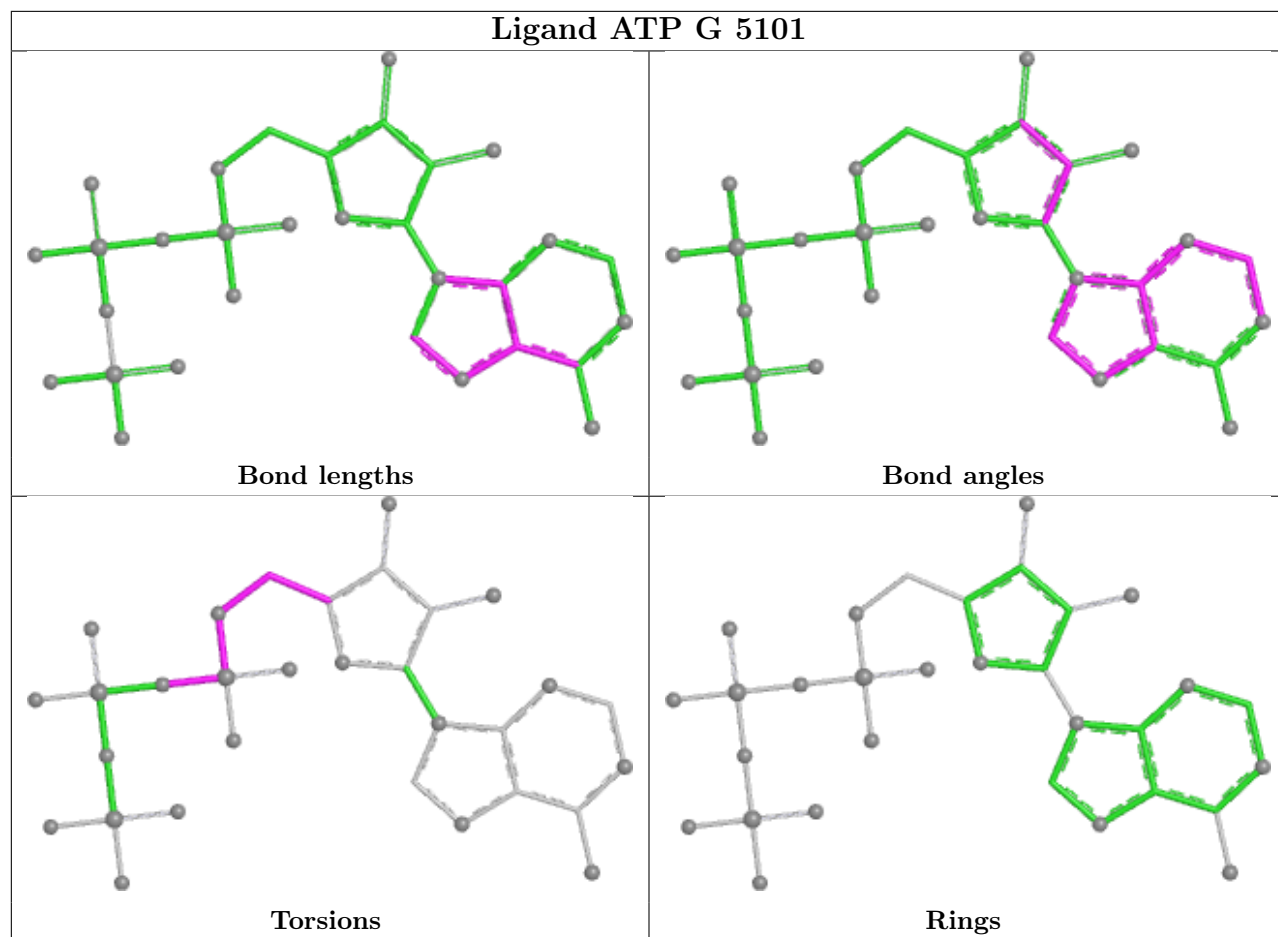
Mol	Chain	Res	Type	Atoms
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA

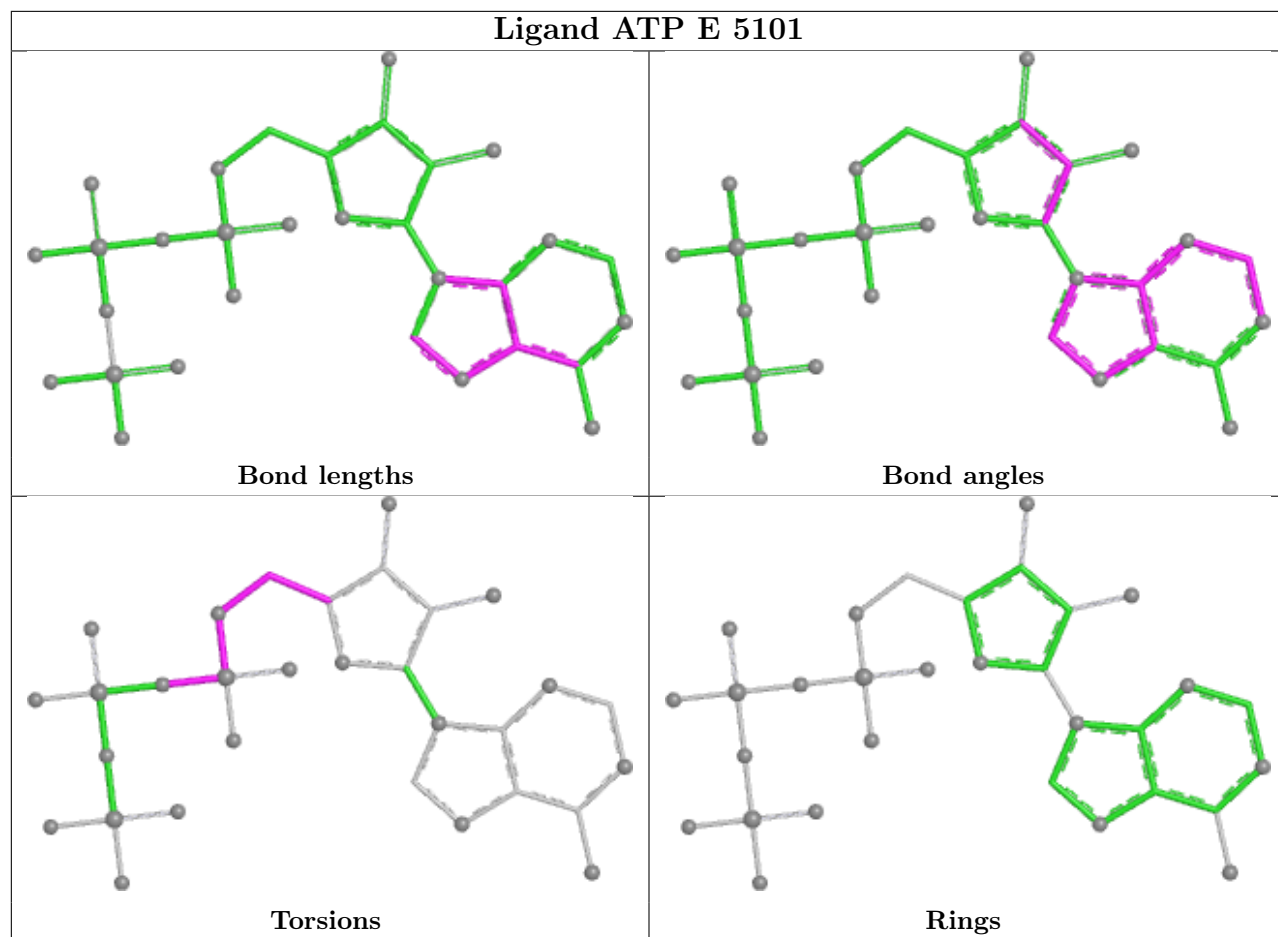
There are no ring outliers.

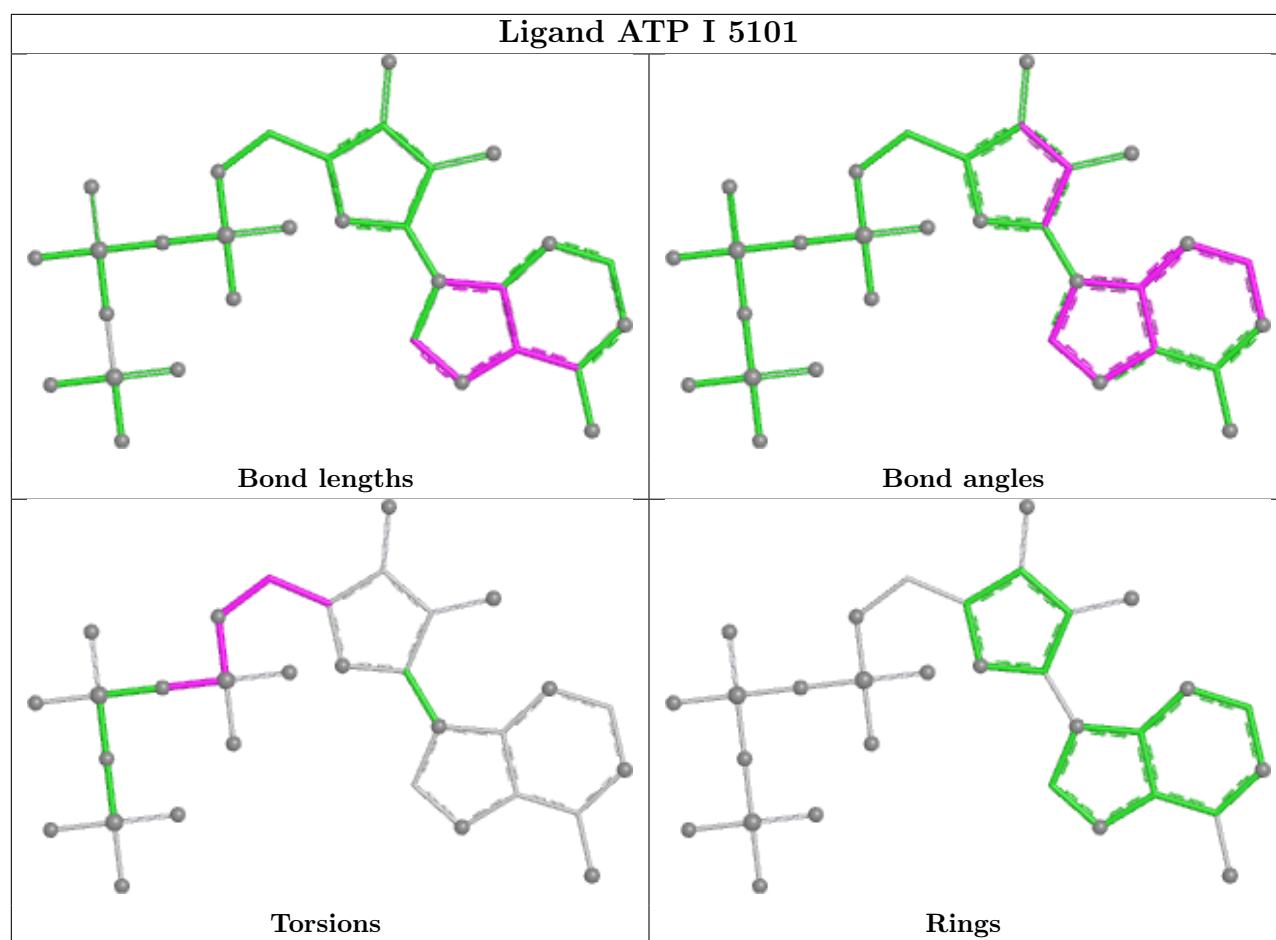
1 monomer is involved in 1 short contact:

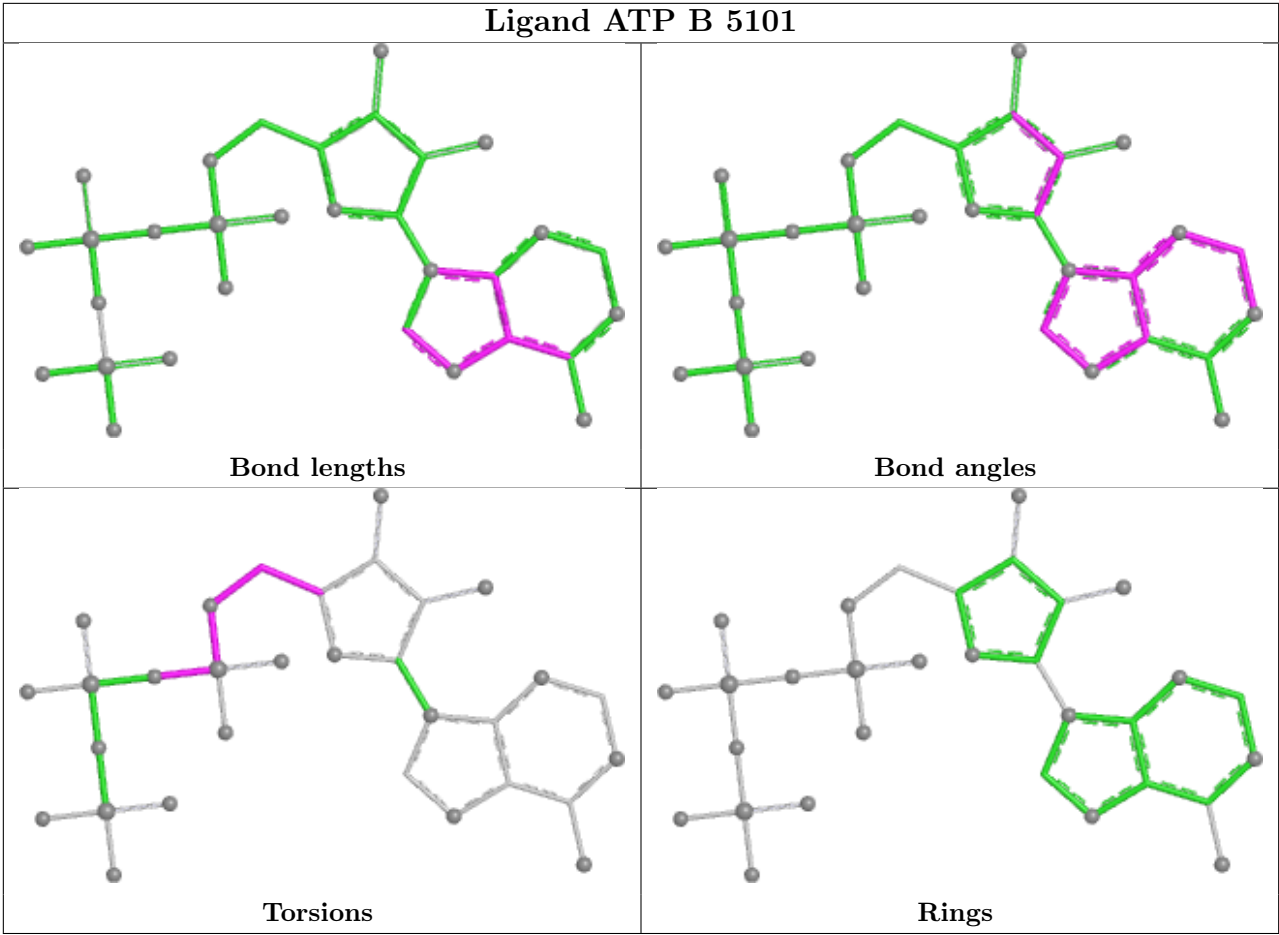
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5102	CFF	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63
1	E	3613:UNK	C	3639:THR	N	44.63
1	I	3613:UNK	C	3639:THR	N	44.63
1	G	3613:UNK	C	3639:THR	N	44.63
1	B	4253:GLU	C	4320:UNK	N	25.42
1	E	4253:GLU	C	4320:UNK	N	25.42
1	I	4253:GLU	C	4320:UNK	N	25.42
1	G	4253:GLU	C	4320:UNK	N	25.42
1	B	3163:UNK	C	3170:UNK	N	15.89
1	E	3163:UNK	C	3170:UNK	N	15.89
1	I	3163:UNK	C	3170:UNK	N	15.89
1	G	3163:UNK	C	3170:UNK	N	15.89
1	B	3063:UNK	C	3134:UNK	N	15.28
1	E	3063:UNK	C	3134:UNK	N	15.28
1	I	3063:UNK	C	3134:UNK	N	15.28
1	G	3063:UNK	C	3134:UNK	N	15.28
1	B	3468:UNK	C	3511:UNK	N	14.58
1	E	3468:UNK	C	3511:UNK	N	14.58
1	I	3468:UNK	C	3511:UNK	N	14.58
1	G	3468:UNK	C	3511:UNK	N	14.58
1	I	2703:UNK	C	2734:ASN	N	13.79
1	B	2703:UNK	C	2734:ASN	N	13.78
1	E	2703:UNK	C	2734:ASN	N	13.78
1	G	2703:UNK	C	2734:ASN	N	13.78
1	B	3236:UNK	C	3241:UNK	N	13.29
1	E	3236:UNK	C	3241:UNK	N	13.29
1	I	3236:UNK	C	3241:UNK	N	13.29
1	G	3236:UNK	C	3241:UNK	N	13.29
1	B	2976:UNK	C	2995:UNK	N	12.55
1	E	2976:UNK	C	2995:UNK	N	12.55
1	I	2976:UNK	C	2995:UNK	N	12.55
1	G	2976:UNK	C	2995:UNK	N	12.55
1	B	1564:UNK	C	1573:MET	N	12.52
1	E	1564:UNK	C	1573:MET	N	12.52
1	I	1564:UNK	C	1573:MET	N	12.52
1	G	1564:UNK	C	1573:MET	N	12.52
1	B	3254:UNK	C	3261:UNK	N	8.35
1	E	3254:UNK	C	3261:UNK	N	8.35
1	I	3254:UNK	C	3261:UNK	N	8.35
1	G	3254:UNK	C	3261:UNK	N	8.35

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	6.00
1	E	1297:UNK	C	1430:UNK	N	6.00
1	I	1297:UNK	C	1430:UNK	N	6.00
1	G	1297:UNK	C	1430:UNK	N	6.00
1	B	2939:ARG	C	2942:UNK	N	3.26
1	E	2939:ARG	C	2942:UNK	N	3.26
1	I	2939:ARG	C	2942:UNK	N	3.26
1	G	2939:ARG	C	2942:UNK	N	3.26
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24

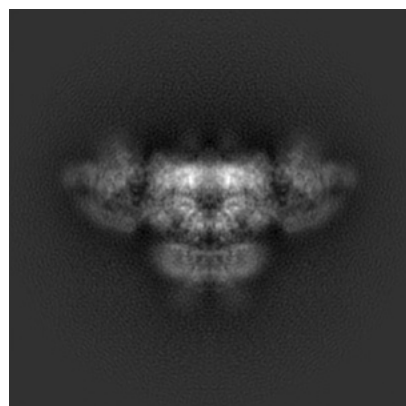
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8386. These allow visual inspection of the internal detail of the map and identification of artifacts.

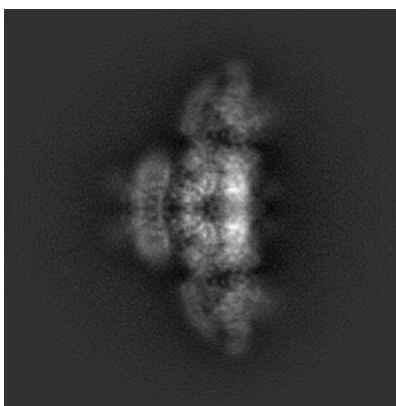
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

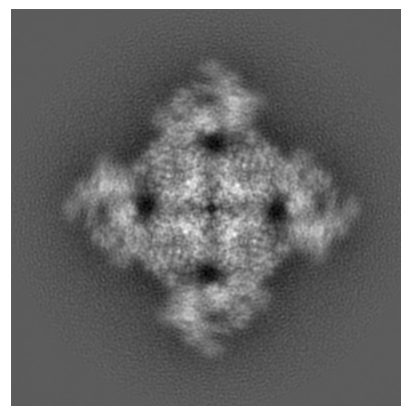
6.1.1 Primary map



X

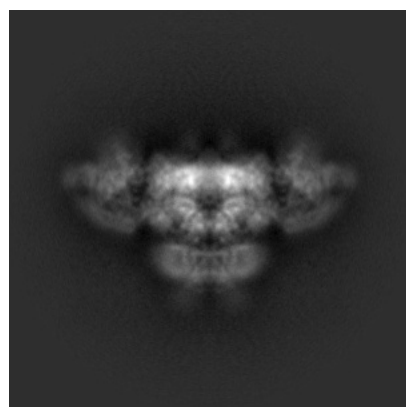


Y

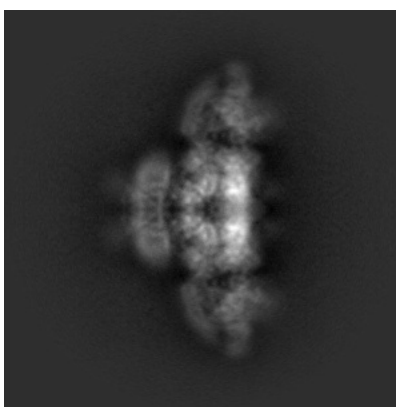


Z

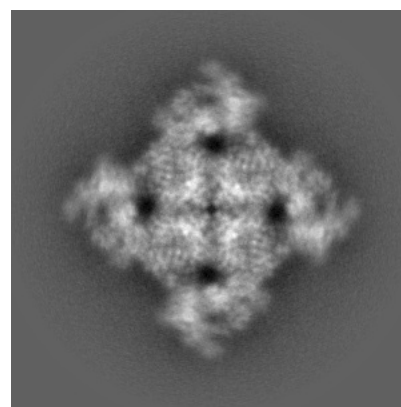
6.1.2 Raw map



X



Y



Z

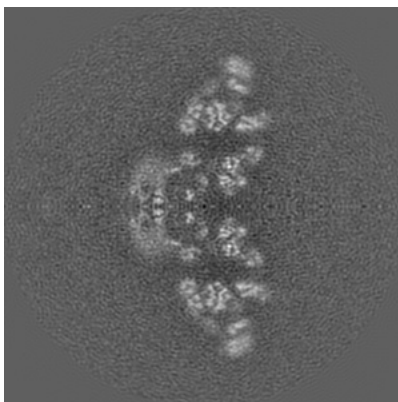
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

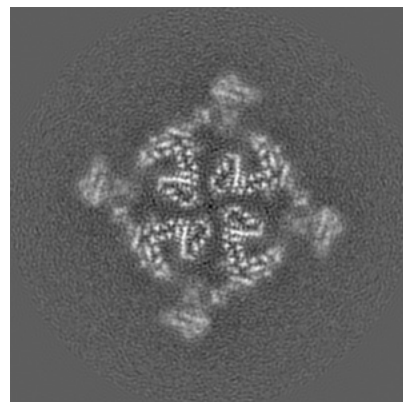
6.2.1 Primary map



X Index: 200

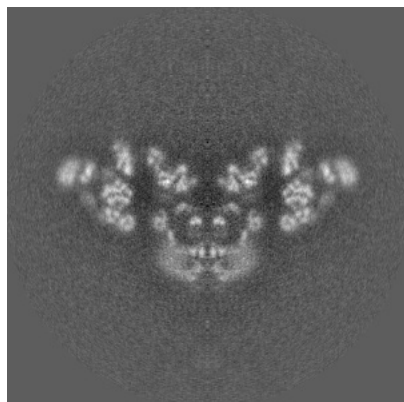


Y Index: 200

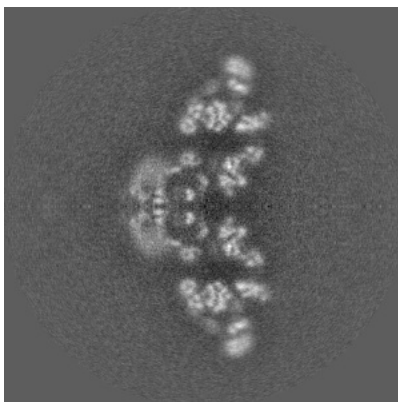


Z Index: 200

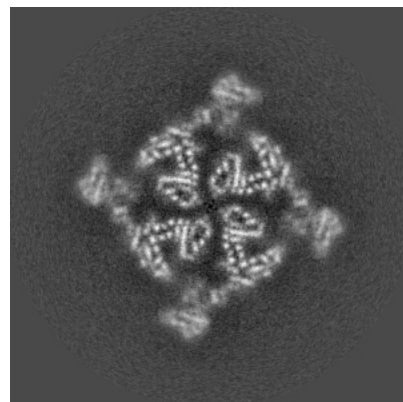
6.2.2 Raw map



X Index: 200



Y Index: 200

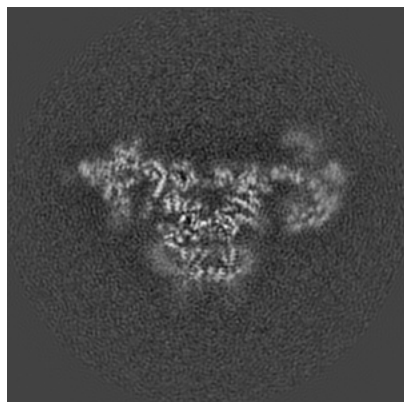


Z Index: 200

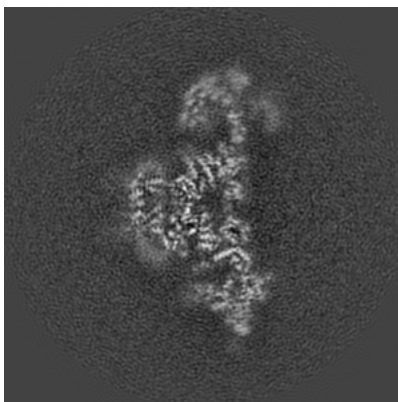
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

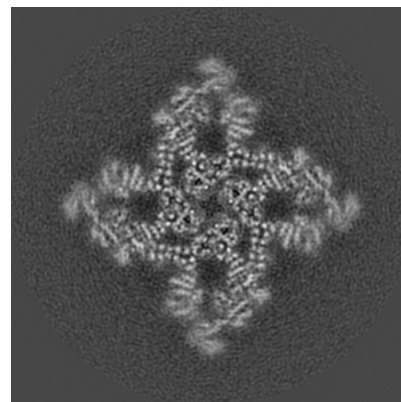
6.3.1 Primary map



X Index: 216

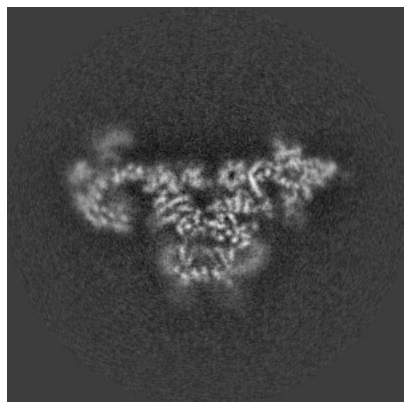


Y Index: 184

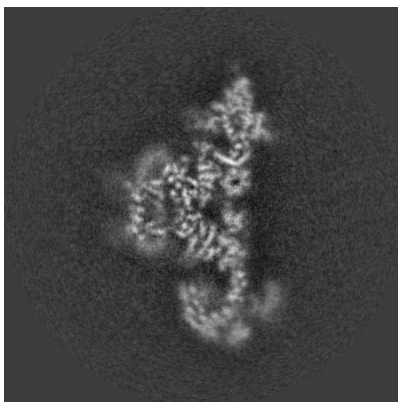


Z Index: 228

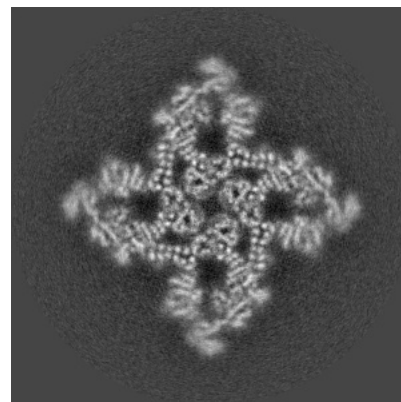
6.3.2 Raw map



X Index: 183



Y Index: 217

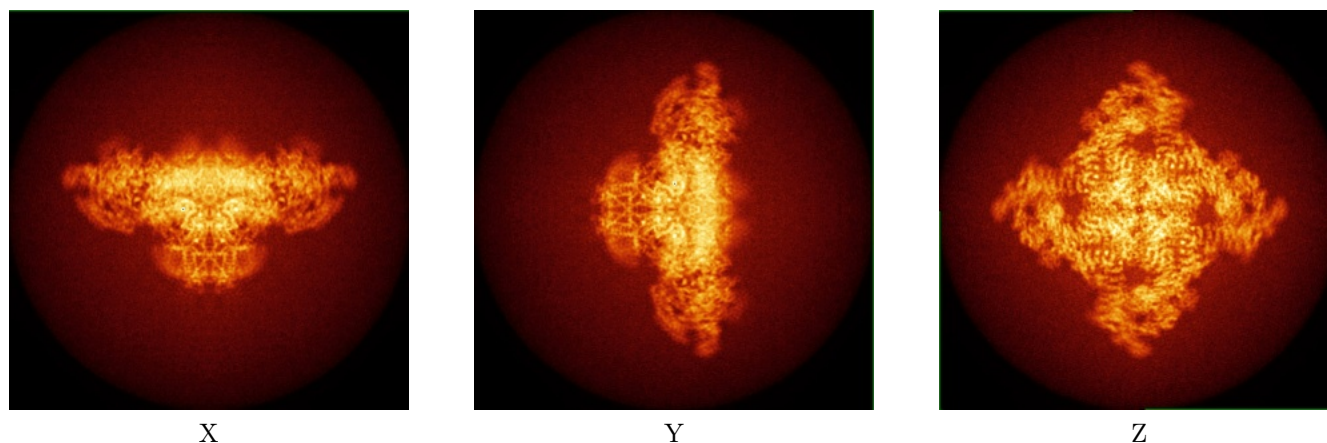


Z Index: 228

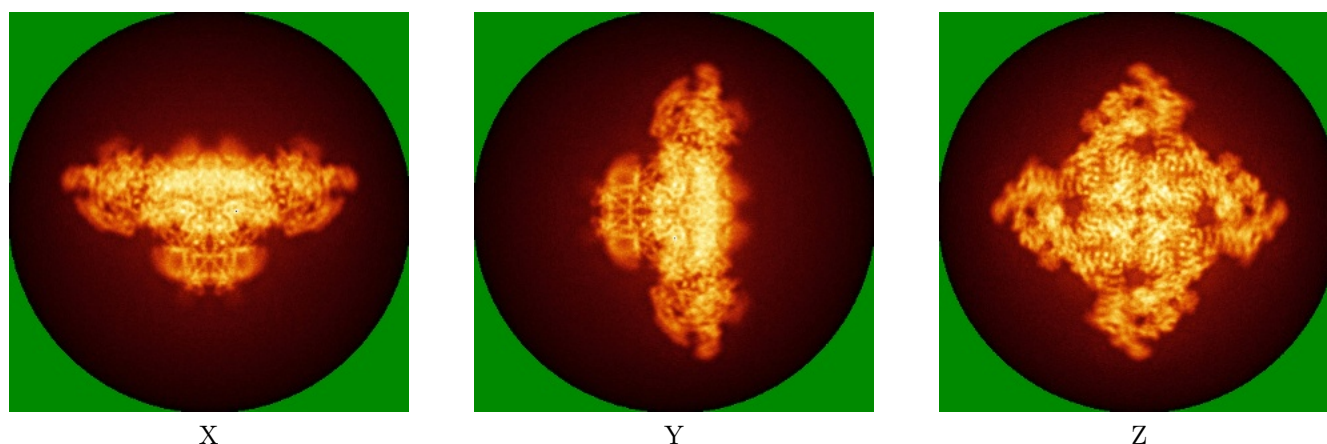
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

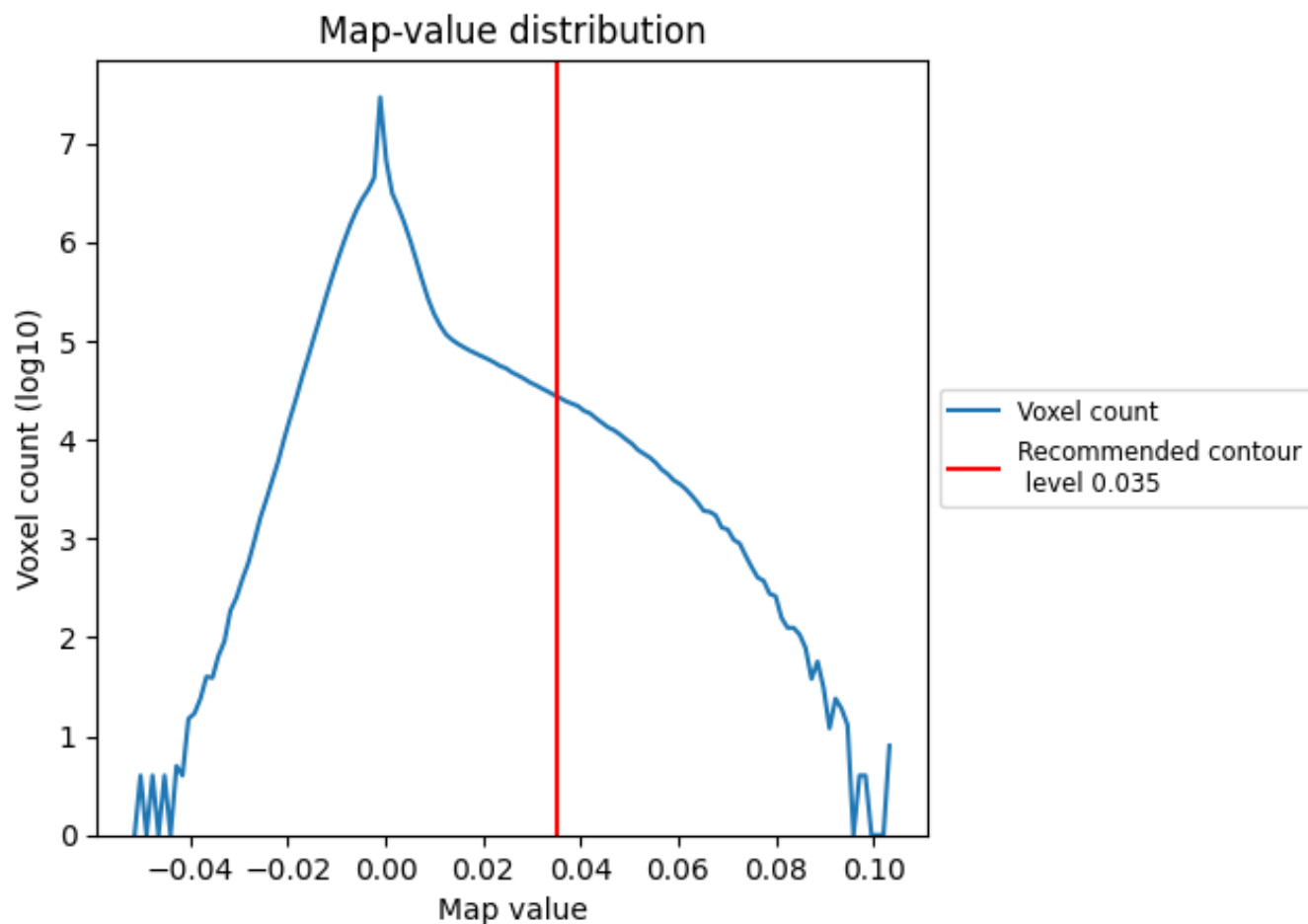
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

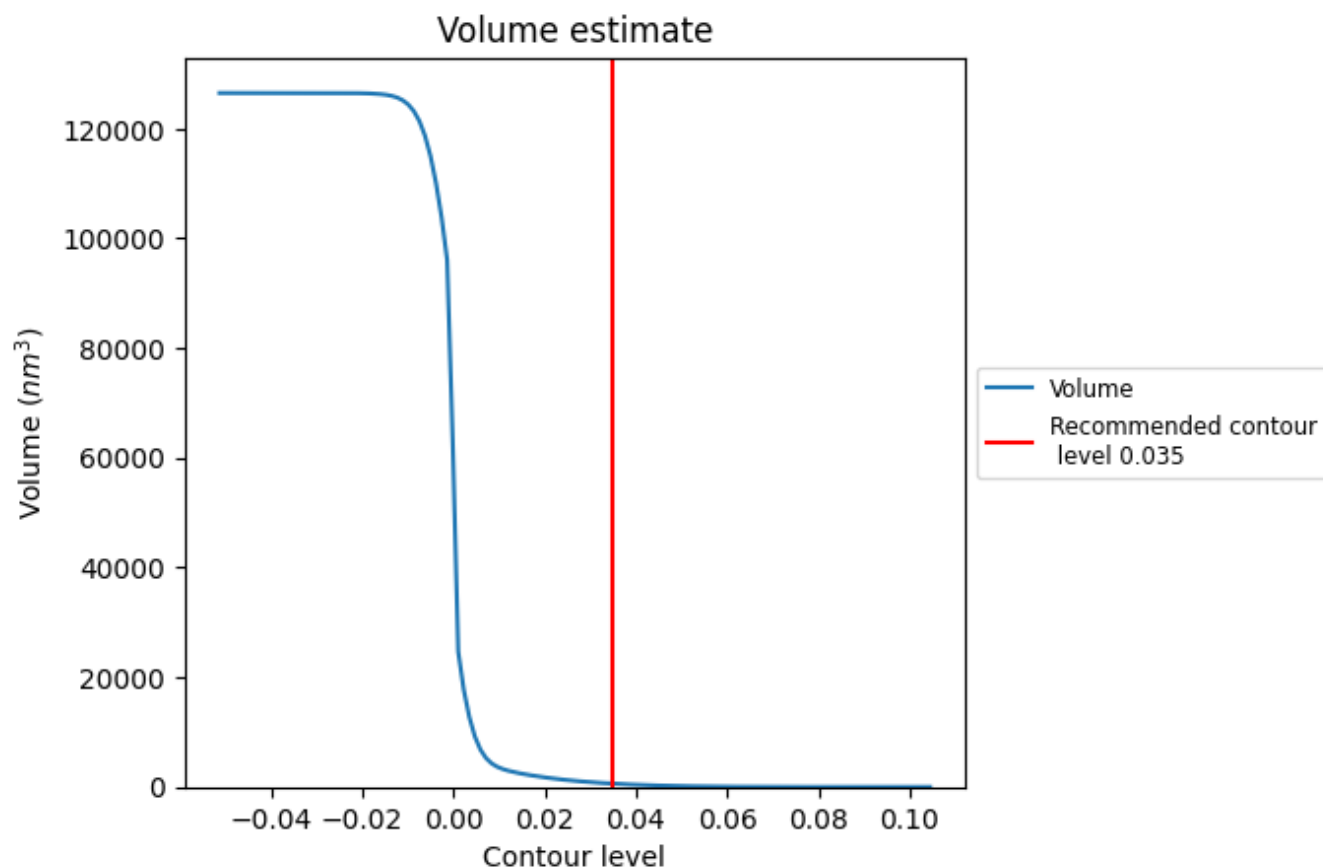
This section contains the results of statistical analysis of the map.

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.

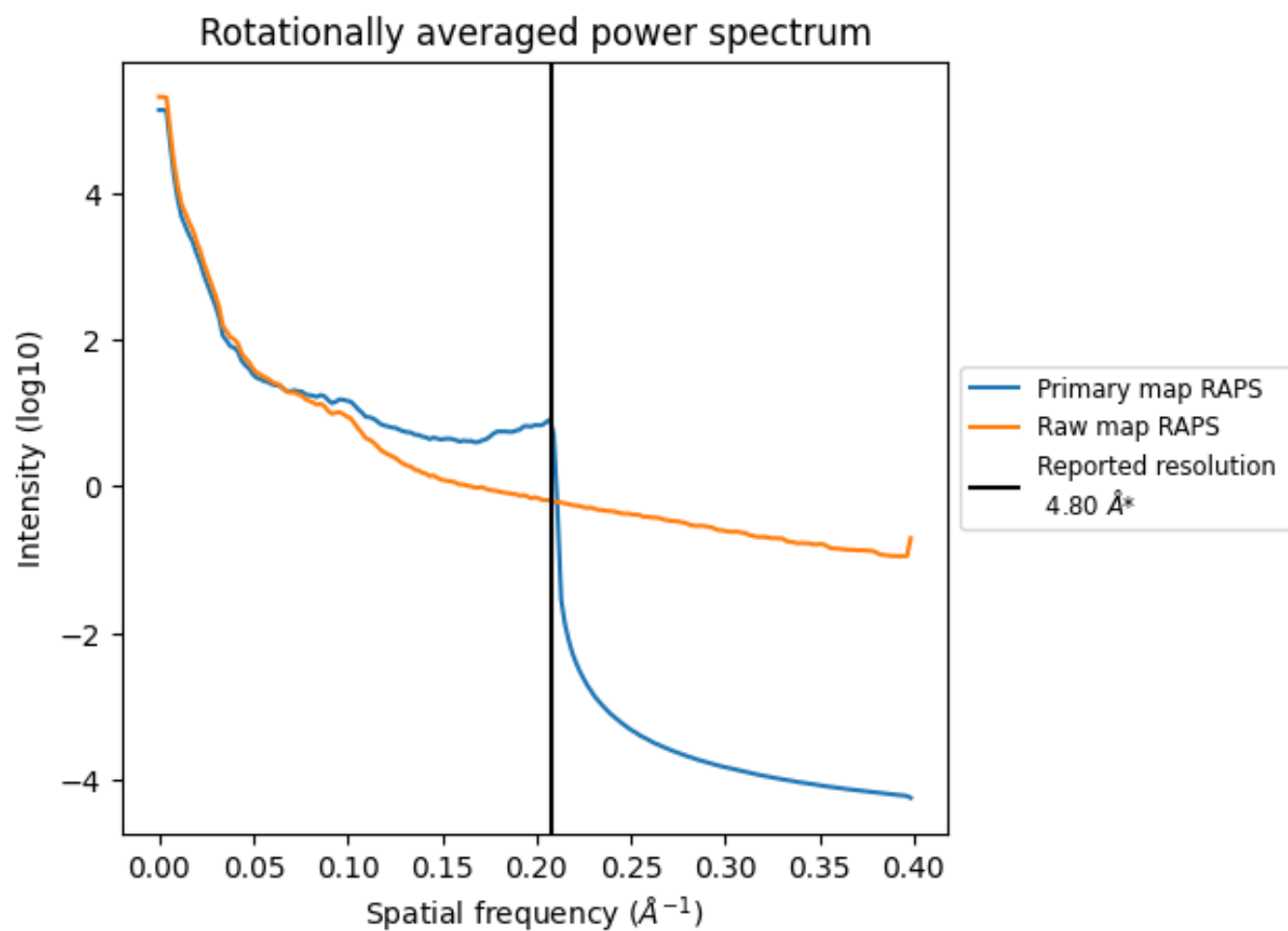
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 605 nm³; this corresponds to an approximate mass of 547 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 ⓘ

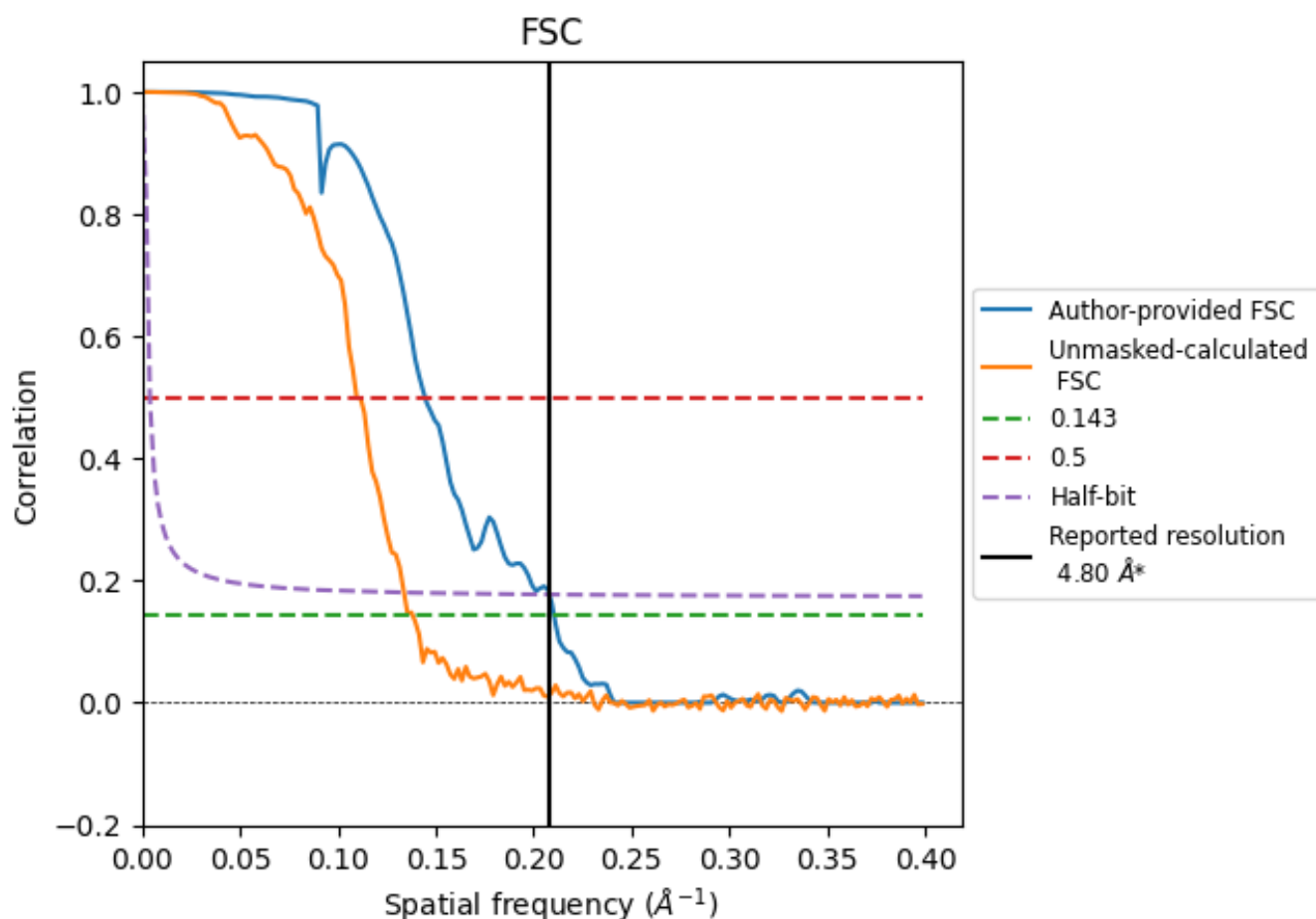


*Reported resolution corresponds to spatial frequency of 0.208 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.76	6.92	4.81
Unmasked-calculated*	7.24	9.13	7.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.24 differs from the reported value 4.8 by more than 10 %

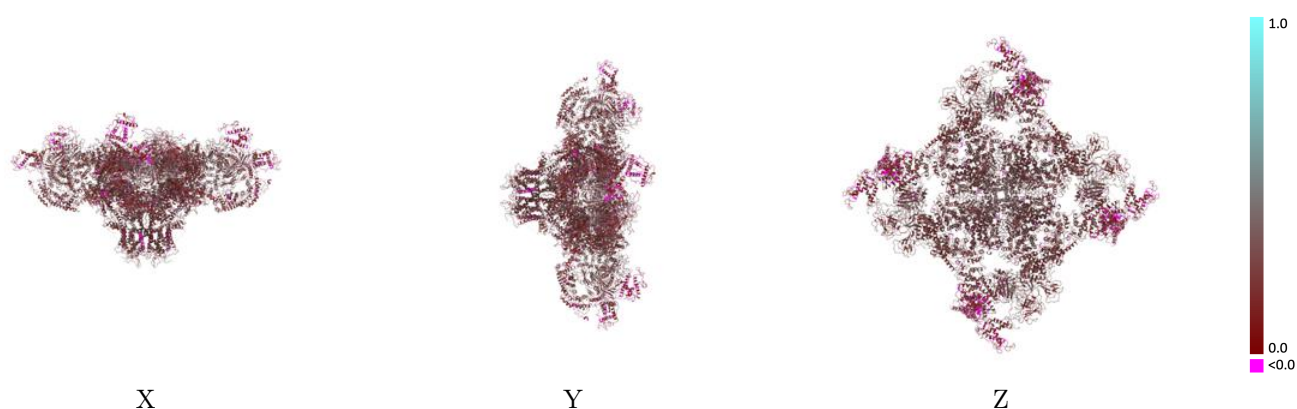
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8386 and PDB model 5TAV. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

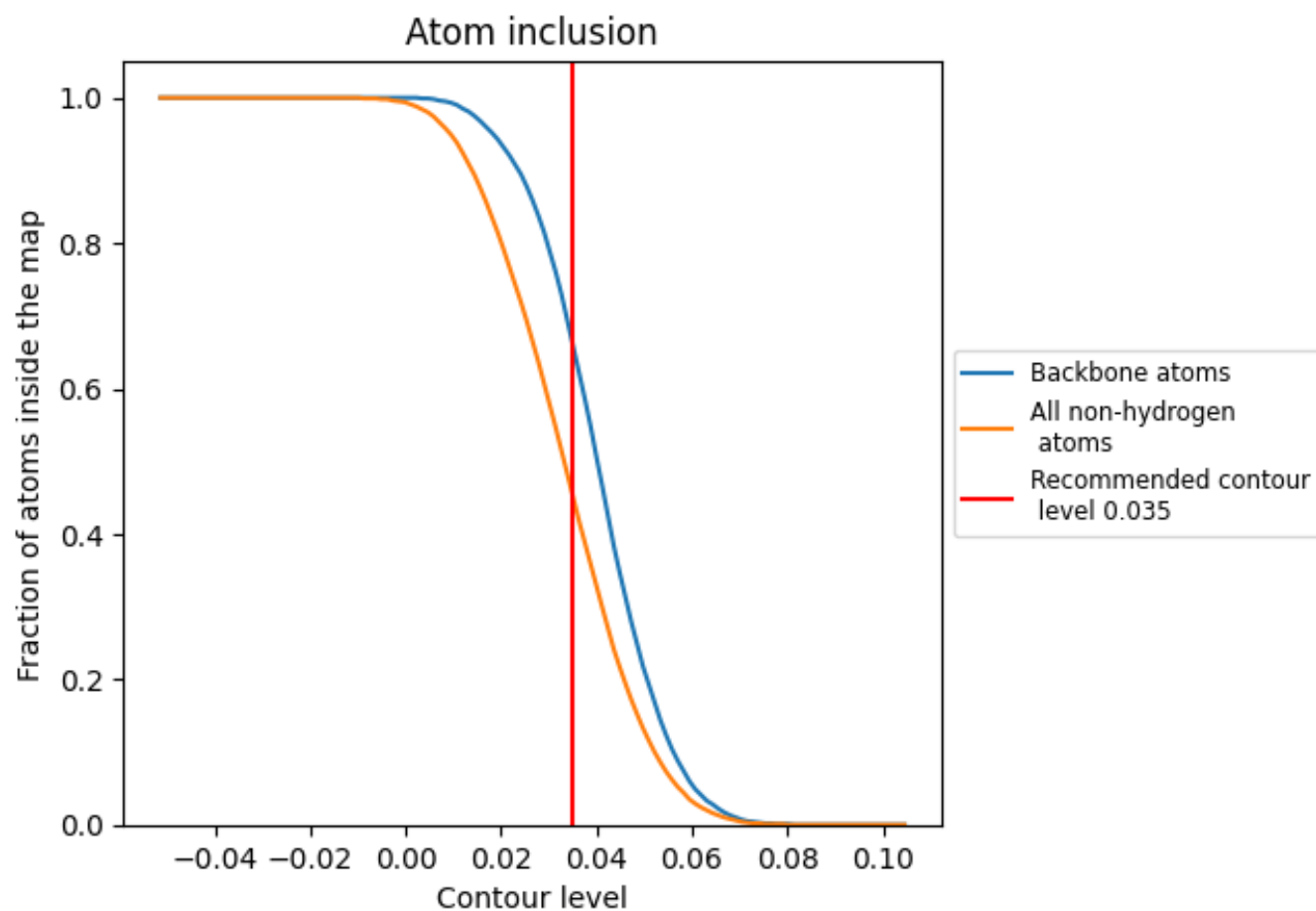


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4530	0.2520
A	0.4630	0.2710
B	0.4530	0.2520
E	0.4520	0.2520
F	0.4650	0.2720
G	0.4520	0.2510
H	0.4620	0.2720
I	0.4530	0.2520
J	0.4620	0.2720

1.0

0.0

<0.0