



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:41 AM UTC

PDB ID : 5TAN / pdb_00005tan
EMDB ID : EMD-8380
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 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:

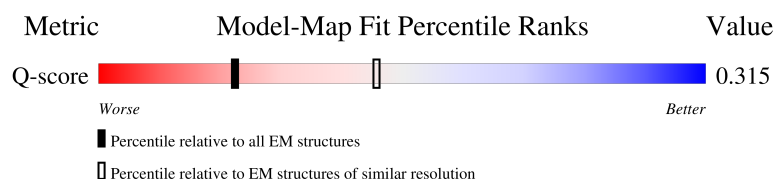
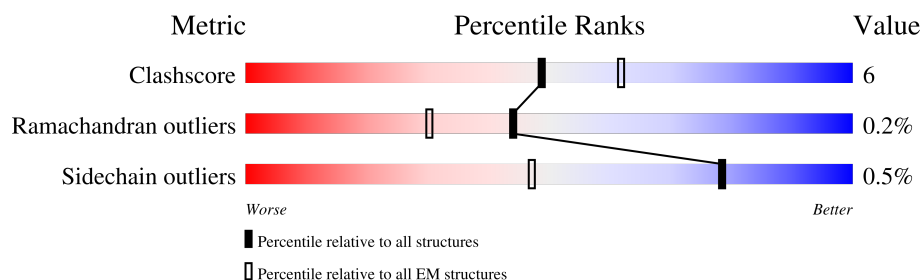
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.30 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.



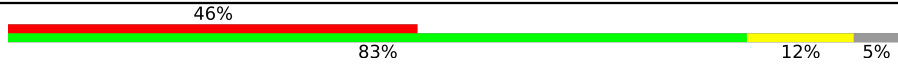
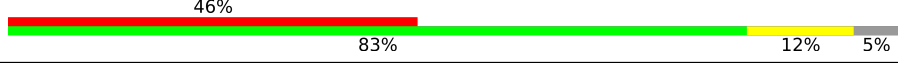
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	58% 79% 20% .
1	F	108	59% 79% 20% .
1	H	108	60% 79% 20% .
1	J	108	58% 79% 20% .

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

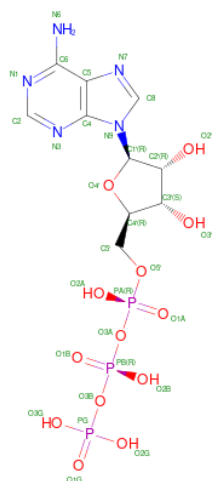
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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		

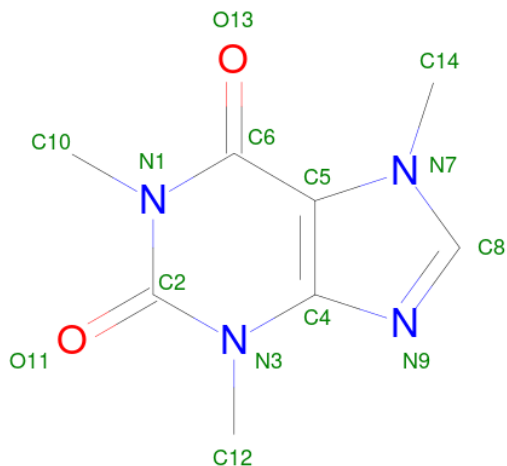
- Molecule 2 is a protein called Ryanodine receptor 1.

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).



- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



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	

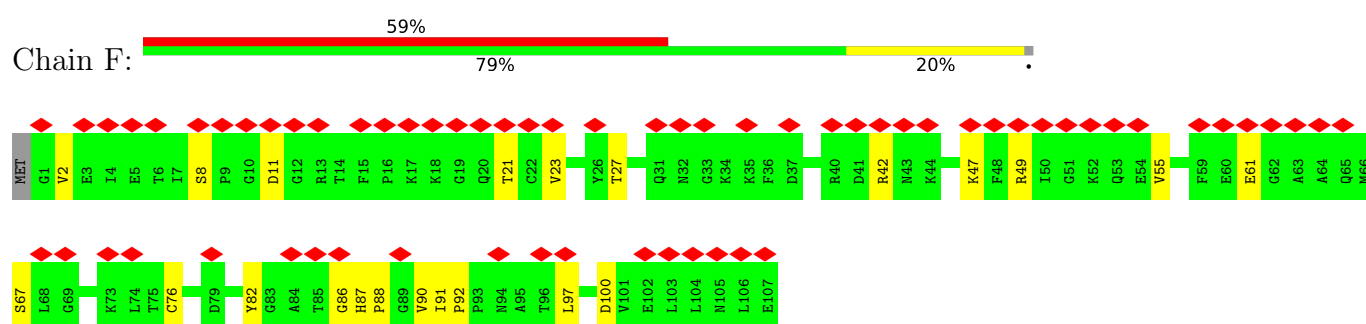
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	

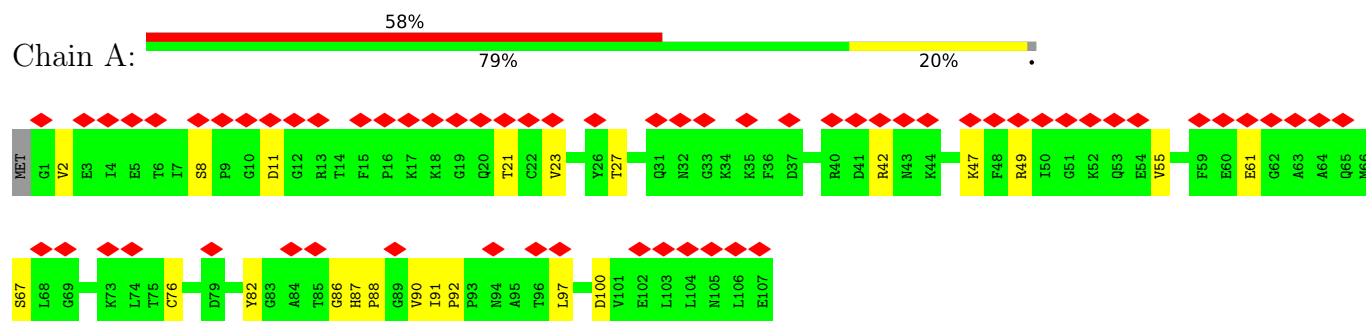
3 Residue-property plots [i](#)

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.

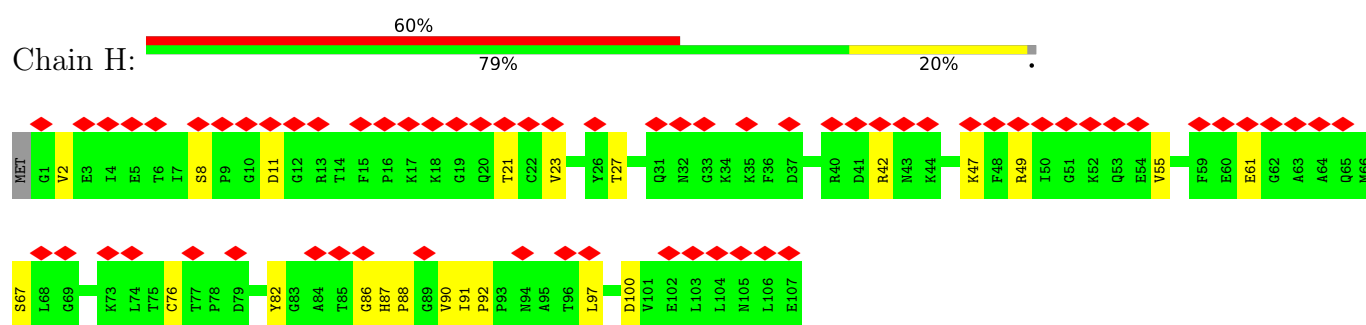
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



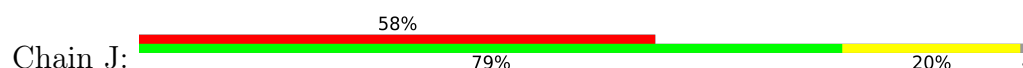
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

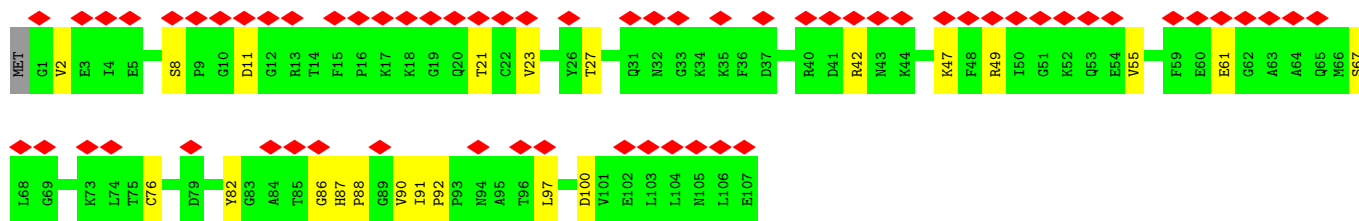


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

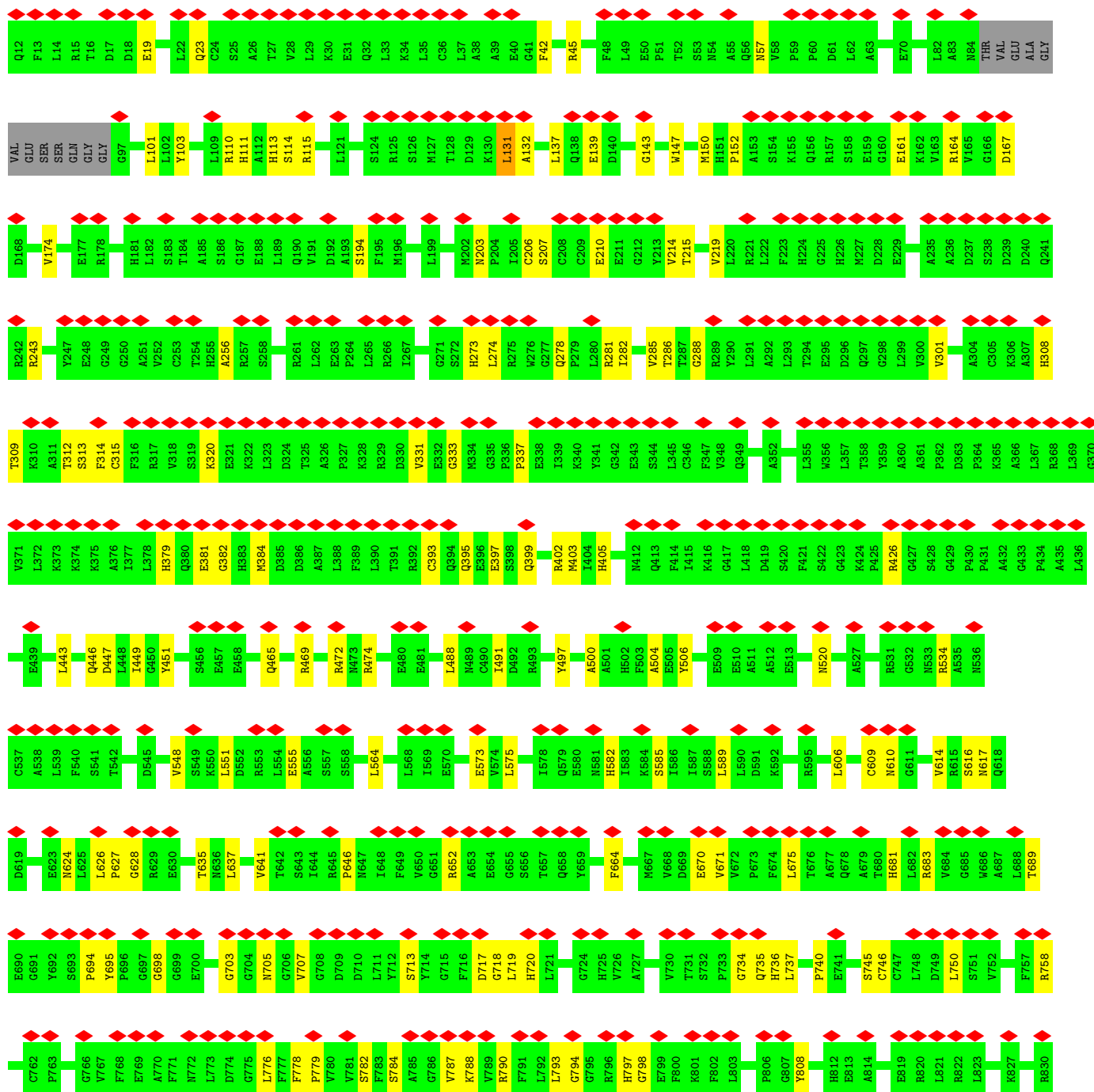
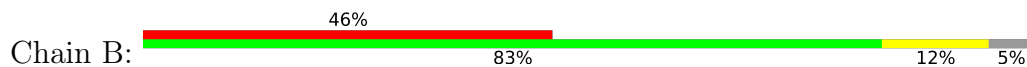


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





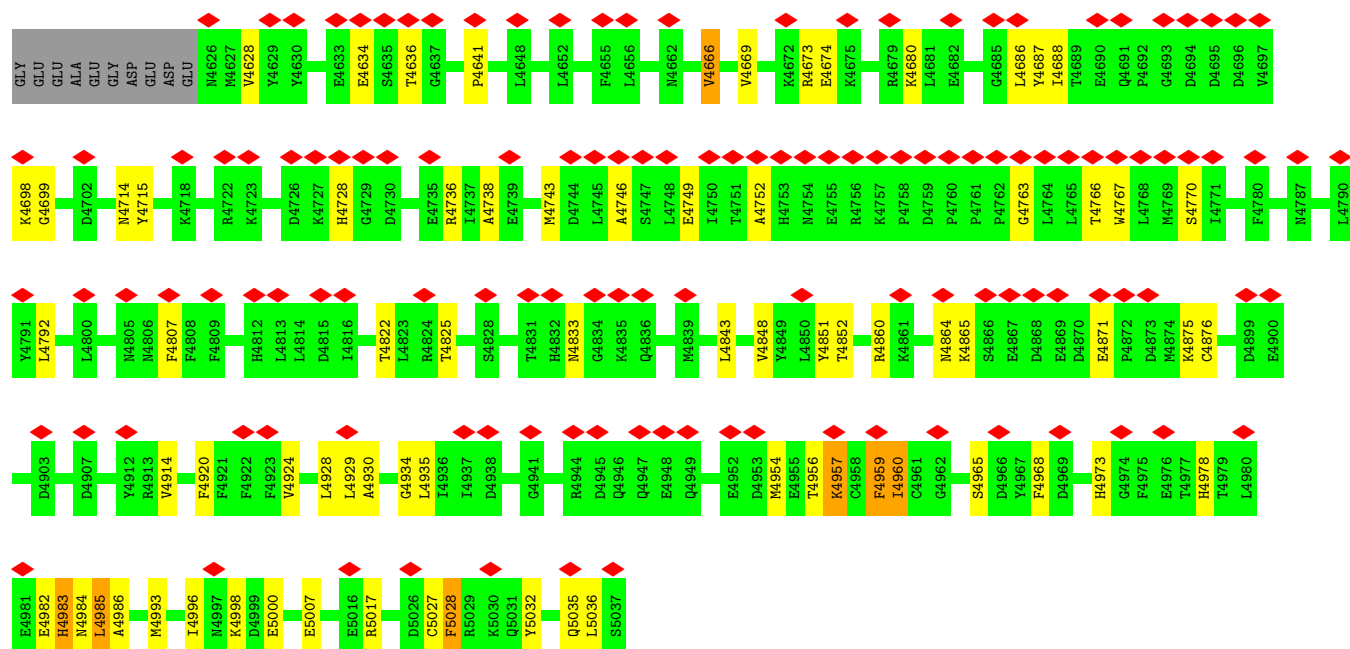
• Molecule 2: Ryanodine receptor 1



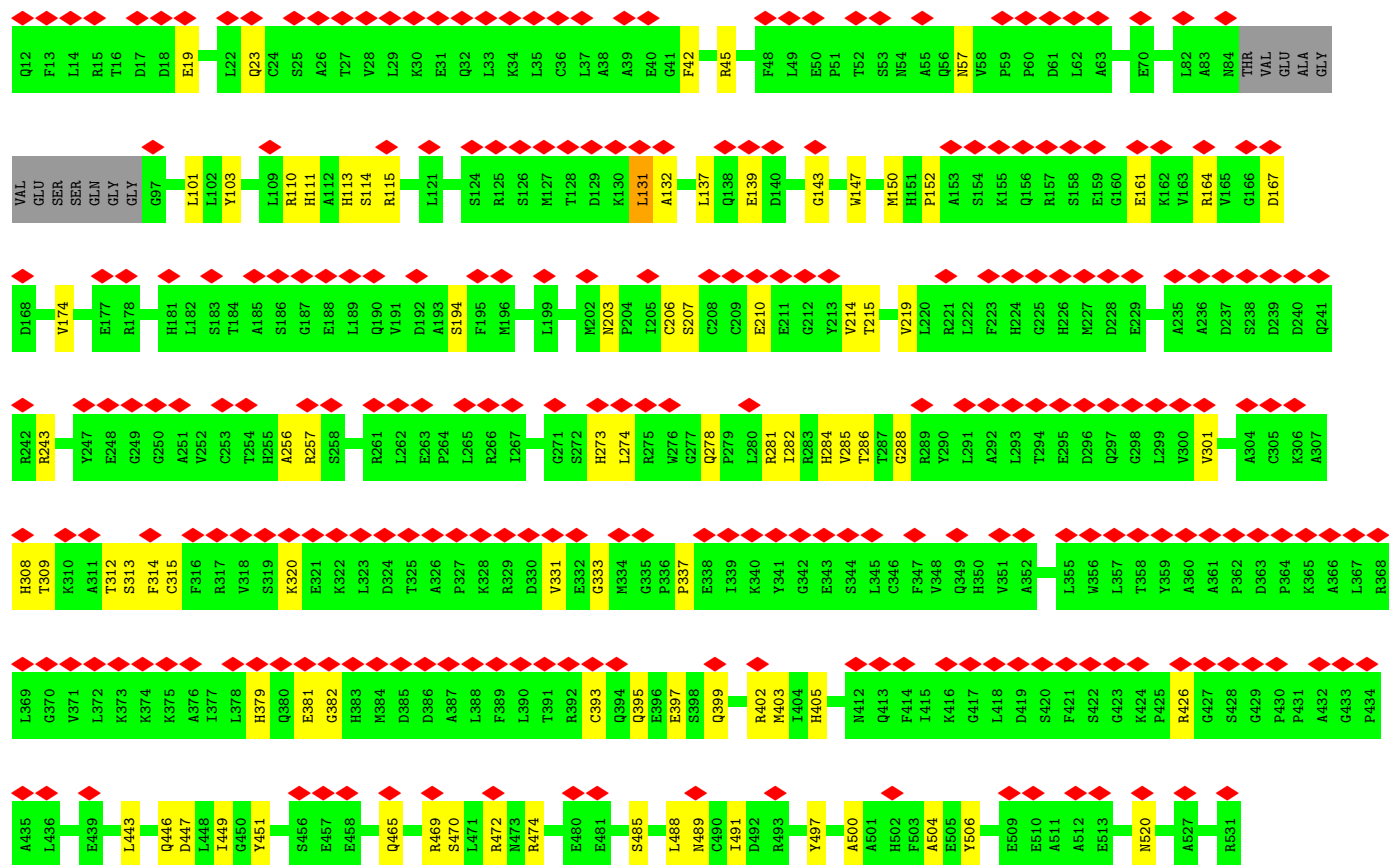
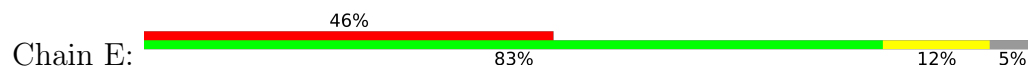








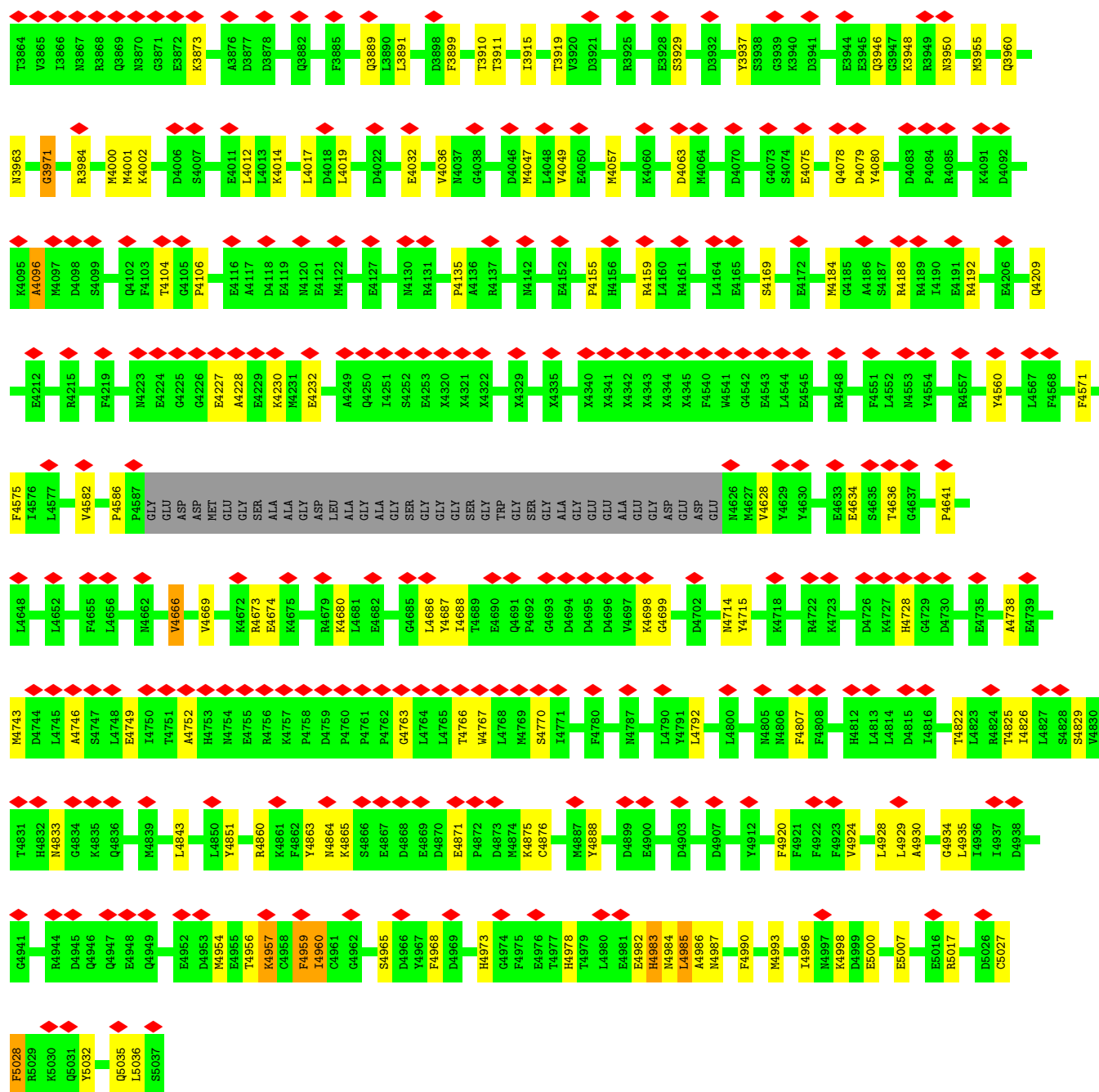
• Molecule 2: Ryanodine receptor 1



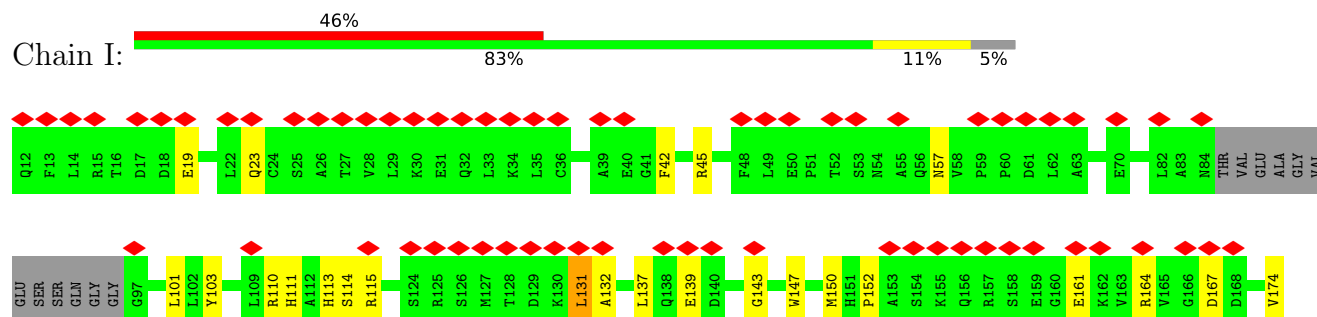








Chain I:

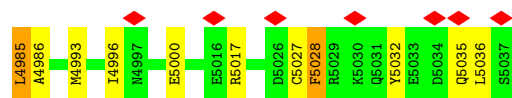




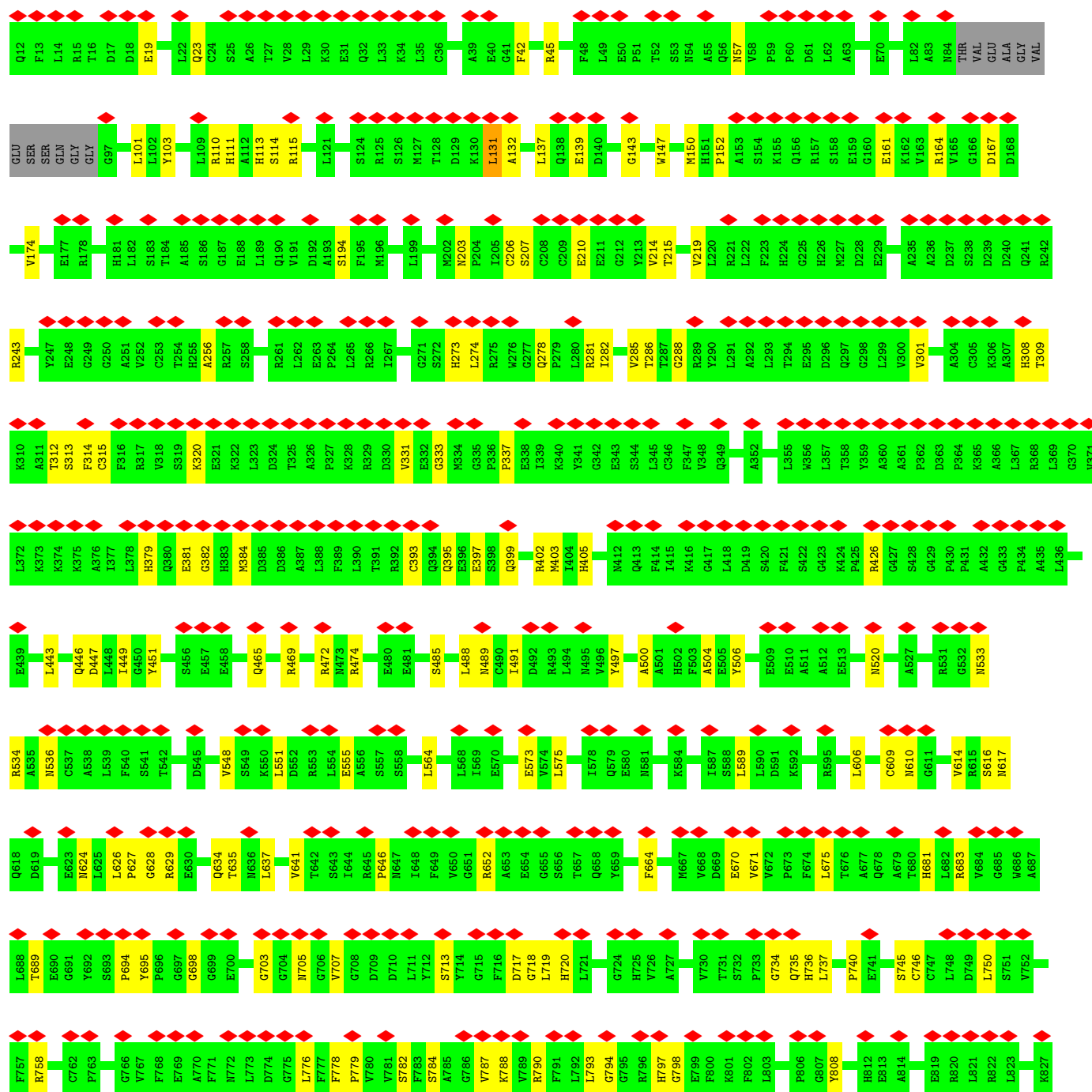
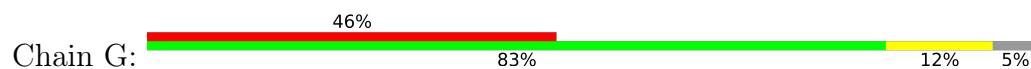


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X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3323	X3324	X3325	X3326	X3327	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355				
X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3225	X3226	X3227	X3228	X3229	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	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	
X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3182	X3183	X3184	X3185	X3186	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3200	X3201	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215				
X3004	X3005	X3006	X3011	X3014	X3015	X3016	X3018	X3019	X3020	X3021	X3022	X3023	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3143							
R2920	E2921	R2922	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	X2953	X2954	X2955	X2959	X2960	X2961	X2962	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X3000	X3003				
P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	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	K2914	E2915	N2916	A2917	R2918	D2919
R2415	V2416	H2417	L2418	G2419	H2420	F2425	Y2426	I2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	M2440	H2441	K2447	G2448	E2449	R2452	I2453	A2455	I2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	Q2476	P2477	T2478	L2479	X2488	X2489	X2490	X2493										
X2499	X2511	X2512	X2513	X2514	X2522	X2523	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2561	X2562	X2563	X2566	X2567	X2568	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2589	X2596	X2614	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630											
X2631	X2636	X2637	X2638	X2643	X2648	X2649	X2650	X2651	X2659	X2662	X2663	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	R2738	P2739							
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K2800	D2801	K2802	E2803	L2804	N2805	R2806	N2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	N2816	L2817	A2818	N2819	E2820	N2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	THR	ARG	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	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	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	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	K2914	E2915	N2916	A2917	R2918	D2919





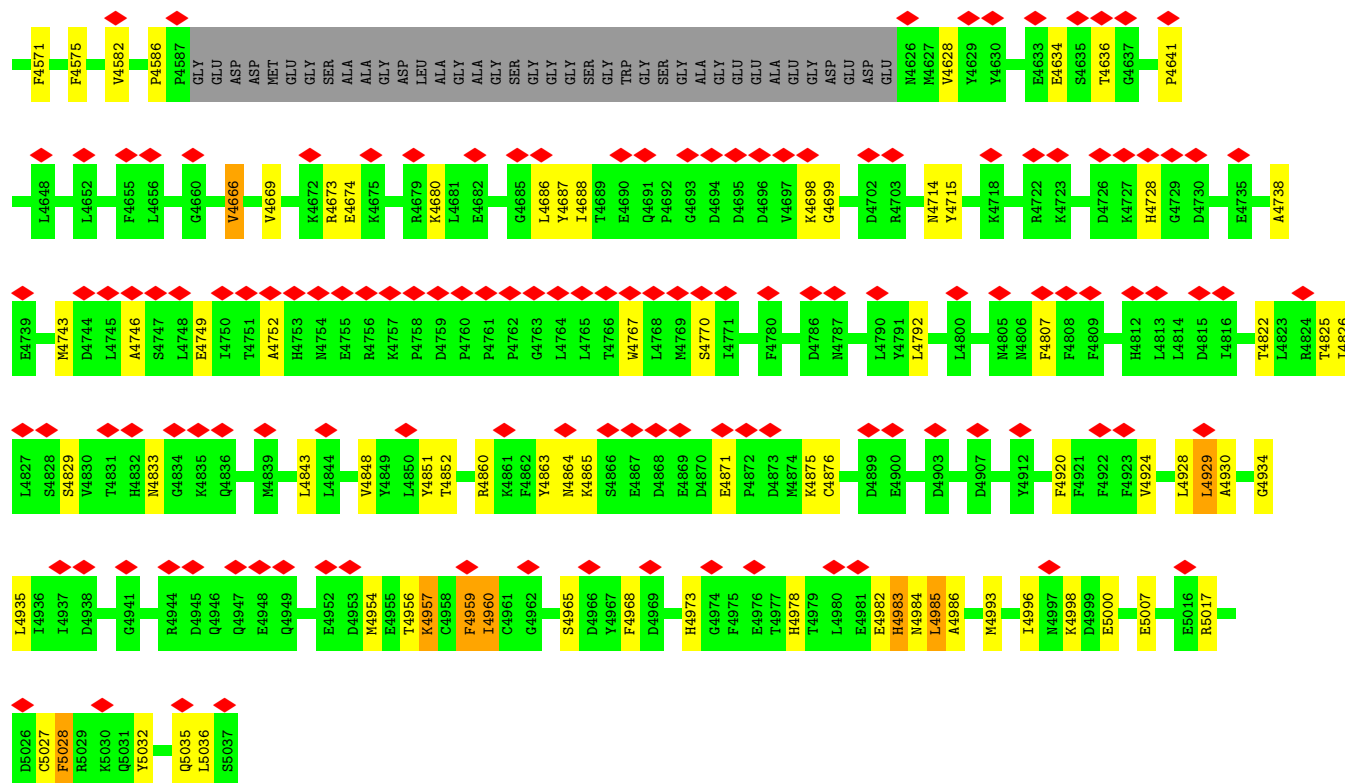
• Molecule 2: Ryanodine receptor 1





X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3003	X3004	X3005	X3006	X3011	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050				
T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	P2909	T2910	L2911	T2912	A2913	E2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2959	X2960	X2961	X2962	X2965		
LYS	ILE	SER	GLN	THR	ALA	GLN	THR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	A2872	N2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	T2884	T2885	W2886	Q2887	K2888	K2889	X2890	K2891	K2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	
V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	T2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2802	E2803	L2804	R2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG
X2596	X2605	X2614	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2636	X2643	X2648	X2649	X2650	X2651	X2658	X2659	X2662	X2663	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2686	X2687	X2688	X2689	X2690									
P2473	L2474	Q2475	L2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	X2493	X2499	X2506	X2511	X2512	X2513	X2514	X2518	X2522	X2523	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2561	X2562	X2563	X2566	X2567	X2568	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2589												
ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	R2415	V2416	H2417	L2418	G2419	H2420	F2425	Y2426	I2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	W2440	H2441	K2447	Q2448	E2449	R2452	I2453	R2454	A2455	L2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	T2469	X2470	S2471	L2472							
D2333	F2334	L2335	R2336	F2337	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	R2355	L2356	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	I2384	R2385	L2386	S2387	E2388	P2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ASP				
S2261	G2262	I2263	G2264	L2265	G2266	H2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2274	V2275	A2276	A2277	E2285	L2288	A2289	L2290	Q2291	E2292	C2293	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	L2307	Q2308	S2309	C2310	P2311	W2312	L2313	L2314	A2315	E2316	Q2317	Y2318	P2319	D2320	I2321	C2326	G2327	R2330	Y2331	L2332				
Q2003	E2004	Q2005	T2006	N2007	H2008	L2009	L2010	H2011	F2012	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	P2022	L2023	D2026	T2027	R2028	Q2029	D2030	L2031	Q2032	H2035	H2041	C2042	G2043	T2044	Q2045	L2046	E2047	G2048	GLU	GLU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	ARG	SER	LEU	GLU	GLU							
THR	VAL	ARG	LEU	VAL	VAL	LYS	LYS	LYS	GLU	GLU	GLU	GLU	LEU	PRO	ALA	GLU	K2089	K2090	P2091	Q2092	Q2095	R2104	Q2107	E2115	R2118	L2123	R2126	Q2127	L2131	L2138	P2139	R2140	A2141	Y2142	T2143	S2145	P2146	S2147	E2150	D2151	L2155	L2156	L2166															
Q2169	W2170	N2176	G2183	W2186	N2187	N2188	K2189	Y2192	Q2193	R2199	A2200	H2204	W2208	E2209	N2213	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	P2226	K2227	W2228	V2229	R2234	F2235	Y2238	F2239	I2242	S2246	Q2247	R2248	D2252	H2253	L2256	Y2257	N2260																





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	0.070	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	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: CA, ATP, ZN, CFF

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	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.48	0/1123
2	B	0.23	0/25428	0.53	3/34534 (0.0%)
2	E	0.23	0/25428	0.53	3/34534 (0.0%)
2	G	0.23	0/25428	0.53	4/34534 (0.0%)
2	I	0.23	0/25428	0.53	4/34534 (0.0%)
All	All	0.23	0/105048	0.53	14/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	137	LEU	CA-C-N	-5.93	114.43	121.90
2	G	137	LEU	C-N-CA	-5.93	114.43	121.90
2	B	137	LEU	CA-C-N	-5.93	114.43	121.90
2	B	137	LEU	C-N-CA	-5.93	114.43	121.90
2	E	137	LEU	CA-C-N	-5.93	114.43	121.90
2	E	137	LEU	C-N-CA	-5.93	114.43	121.90
2	I	137	LEU	CA-C-N	-5.93	114.43	121.90
2	I	137	LEU	C-N-CA	-5.93	114.43	121.90
2	I	131	LEU	CA-CB-CG	5.03	133.92	116.30
2	B	131	LEU	CA-CB-CG	5.03	133.90	116.30
2	E	131	LEU	CA-CB-CG	5.03	133.90	116.30
2	G	131	LEU	CA-CB-CG	5.03	133.90	116.30
2	I	1829	PRO	N-CA-C	5.01	119.08	111.11
2	G	1829	PRO	N-CA-C	5.00	119.07	111.11

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	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	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide

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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	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1795	PRO	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	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1795	PRO	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

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Mol	Chain	Res	Type	Group
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	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	13	0
1	F	818	0	824	13	0
1	H	818	0	824	13	0
1	J	818	0	824	13	0
2	B	29499	0	24753	315	0
2	E	29499	0	24753	325	0
2	G	29499	0	24753	319	0
2	I	29499	0	24753	309	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	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
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	1	0	0	0	0
All	All	121456	0	102396	1287	0

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

All (1287) 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:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.64	1.15
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.64	1.14
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.64	1.14
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.67	1.12
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.67	1.11
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.67	1.10
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.67	1.09
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.54	0.94
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.81	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.81	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	1.81	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.54	0.91
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.05	0.90
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.05	0.90
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.05	0.90
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.05	0.90
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	1.81	0.89
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.16	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.16	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.16	0.80
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.16	0.80
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	1.96	0.78
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	1.96	0.78
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	1.96	0.78
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4192:ARG:HH11	2:E:5028:PHE:HD2	1.36	0.74
2:B:4192:ARG:HH11	2:B:5028:PHE:HD2	1.36	0.73
2:G:4192:ARG:HH11	2:G:5028:PHE:HD2	1.36	0.73
2:I:4192:ARG:HH11	2:I:5028:PHE:HD2	1.36	0.72
2:B:111:HIS:HD2	2:B:114:SER:H	1.41	0.69
2:G:111:HIS:HD2	2:G:114:SER:H	1.41	0.68
2:E:111:HIS:HD2	2:E:114:SER:H	1.41	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.68
2:E:4957:LYS:NZ	2:E:4957:LYS:HB2	2.08	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:G:4957:LYS:HB2	2:G:4957:LYS:NZ	2.08	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:I:111:HIS:HD2	2:I:114:SER:H	1.41	0.68
2:B:4957:LYS:HB2	2:B:4957:LYS:NZ	2.08	0.67
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.39	0.67
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:I:4957:LYS:HB2	2:I:4957:LYS:NZ	2.08	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:4230:LYS:HG2	2:E:4959:PHE:HE1	1.60	0.66
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.78	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.65
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.78	0.65
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.15	0.65
2:B:4230:LYS:HG2	2:B:4959:PHE:HE1	1.60	0.65
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.78	0.65
2:I:4230:LYS:HG2	2:I:4959:PHE:HE1	1.60	0.65
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.62	0.65
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.62	0.64
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.15	0.64
2:I:4230:LYS:CD	2:I:4959:PHE:CE1	2.81	0.64
2:G:4230:LYS:HG2	2:G:4959:PHE:HE1	1.61	0.64
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.64
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.80	0.64
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.63	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.78	0.63
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.80	0.63
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.81	0.63
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.15	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:E:4230:LYS:CD	2:E:4959:PHE:CE1	2.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.80	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:G:4230:LYS:CD	2:G:4959:PHE:CE1	2.81	0.63
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.15	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.62
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.62
2:B:4228:ALA:HB2	2:E:4973:HIS:HE1	1.64	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.65	0.61
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.80	0.61
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.61
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.61
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.61
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.82	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.39	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.39	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.83	0.60
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.60
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.60
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.84	0.60
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.60
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.84	0.60
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.90	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.84	0.60
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.84	0.60
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.84	0.60
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.84	0.60
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.84	0.60
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.39	0.60
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.60
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.66	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.84	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.59
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.84	0.59
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.84	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.90	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.90	0.59
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.84	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.62	0.59
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.84	0.59
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
2:B:4973:HIS:HE1	2:I:4228:ALA:HB2	1.67	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.58
2:E:4228:ALA:HB2	2:G:4973:HIS:HE1	1.68	0.58
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.58
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.68	0.58
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.35	0.58
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.84	0.58
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.90	0.58
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.84	0.58
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.83	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.37	0.58
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.84	0.58
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.58
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.58
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.58
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.86	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.69	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.37	0.57
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.86	0.57
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:I:4973:HIS:HE1	2:G:4228:ALA:HB2	1.68	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.57
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.86	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.82	0.57
2:B:4001:MET:HG3	2:B:4057:MET:HE2	1.87	0.57
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.70	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:E:4001:MET:HG3	2:E:4057:MET:HE2	1.87	0.56
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.56
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.87	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.87	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.87	0.56
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.56
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.87	0.56
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.86	0.56
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.70	0.56
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.71	0.56
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.88	0.56
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.56
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.56
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.56
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.55
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.88	0.55
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.62	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.87	0.55
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.70	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.71	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.87	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.40	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.71	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.40	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.87	0.55
2:I:4001:MET:HG3	2:I:4057:MET:HE2	1.87	0.55
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.38	0.55
2:G:4001:MET:HG3	2:G:4057:MET:HE2	1.87	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.88	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.55
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.88	0.55
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.88	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.40	0.55
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.88	0.55
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.89	0.54
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.88	0.54
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.88	0.54
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.88	0.54
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.81	0.54
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.81	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.90	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.40	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.54
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.23	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.90	0.54
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.40	0.54
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.89	0.54
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.54
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.38	0.54
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.88	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.54
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.73	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.54
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.90	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.81	0.54
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.54
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	2.20	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.41	0.54
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.23	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.41	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.54
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.89	0.54
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.72	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.53
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.53
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.81	0.53
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.88	0.53
2:E:5028:PHE:CD1	2:E:5032:TYR:CD2	2.96	0.53
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.89	0.53
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.53
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.53
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.91	0.53
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.53
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.90	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.90	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.90	0.53
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.73	0.53
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.41	0.53
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.53
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.73	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.22	0.53
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.91	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.91	0.53
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.53
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.38	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.53
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	2.20	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.53
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.91	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.91	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.23	0.52
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.52
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.52
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.40	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:B:5028:PHE:CD1	2:B:5032:TYR:CD2	2.96	0.52
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.38	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.52
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.52
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.91	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.91	0.52
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:B:3760:LYS:NZ	2:B:5000:GLU:OE1	2.41	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.52
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.91	0.52
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.91	0.52
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.52
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.52
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.92	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.91	0.52
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.40	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.92	0.52
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.91	0.51
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.91	0.51
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.51
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.76	0.51
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.51
2:B:4957:LYS:HB2	2:B:4957:LYS:HZ1	1.75	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.51
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.51
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.51
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.51
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.51
2:G:5028:PHE:CD1	2:G:5032:TYR:CD2	2.95	0.51
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.93	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.51
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.91	0.51
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.92	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.93	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.51
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.91	0.51
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.92	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.51
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.76	0.51
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.76	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.76	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.77	0.51
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.51
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.28	0.50
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.77	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.93	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.76	0.50
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.50
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.77	0.50
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.92	0.50
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.77	0.50
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.93	0.50
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.92	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.50
2:B:4954:MET:HE3	3:B:5101:ATP:H1'	1.94	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.50
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.76	0.50
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.93	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.94	0.50
2:I:5028:PHE:CD1	2:I:5032:TYR:CD2	2.96	0.50
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.77	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.77	0.50
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.50
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.50
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.77	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.49
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.76	0.49
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.93	0.49
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.49
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.41	0.49
2:E:4954:MET:HE3	3:E:5101:ATP:H1'	1.94	0.49
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.94	0.49
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.93	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.94	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.93	0.49
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
2:B:320:LYS:NZ	2:B:381:GLU:O	2.42	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.76	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.95	0.49
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.95	0.49
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.95	0.49
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.95	0.49
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.94	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.49
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.95	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.46	0.49
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.49
2:I:4954:MET:HE3	3:I:5101:ATP:H1'	1.94	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.49
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.49
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.49
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.94	0.49
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.41	0.49
2:I:4822:THR:O	2:I:4825:THR:OG1	2.29	0.49
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.49
1:H:11:ASP:OD1	1:H:67:SER:OG	2.31	0.49
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.95	0.49
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.49
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.95	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.95	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.49
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.77	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.96	0.48
2:G:4954:MET:HE3	3:G:5101:ATP:HI'	1.94	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.48
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.39	0.48
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.46	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.95	0.48
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.95	0.48
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.95	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.94	0.48
2:E:4957:LYS:NZ	2:E:4957:LYS:CB	2.77	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.95	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.28	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.46	0.48
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.95	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.48
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.95	0.48
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.46	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.96	0.48
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.95	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.96	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.96	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.96	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.95	0.47
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.95	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.80	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.47	0.47
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.31	0.47
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.79	0.47
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	2.20	0.47
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.95	0.47
1:F:11:ASP:OD1	1:F:67:SER:OG	2.31	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.97	0.47
1:A:27:THR:HB	1:A:100:ASP:HB3	1.97	0.47
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.47
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	2.20	0.47
2:G:4957:LYS:NZ	2:G:4957:LYS:CB	2.77	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.47
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.39	0.47
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.79	0.47
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.28	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.39	0.47
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.96	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.47
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.47
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.47
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.47
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.47
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.80	0.47
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.80	0.47
2:G:320:LYS:NZ	2:G:381:GLU:O	2.42	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	1.96	0.47
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.41	0.47
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.95	0.47
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	1.96	0.47
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.47
2:E:243:ARG:NH1	2:E:301:VAL:O	2.43	0.47
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.47
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.48	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.48	0.47
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.48	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4047:MET:HE3	2:G:4047:MET:HB2	1.84	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:3915:ILE:O	2:B:3919:THR:N	2.47	0.47
2:I:320:LYS:NZ	2:I:381:GLU:O	2.42	0.47
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.46
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.97	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.33	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.48	0.46
1:J:11:ASP:OD1	1:J:67:SER:OG	2.31	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.46
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.46
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.31	0.46
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.46
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.48	0.46
2:B:215:THR:HG22	2:B:273:HIS:HA	1.97	0.46
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.97	0.46
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.96	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.48	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:4957:LYS:NZ	2:I:4957:LYS:CB	2.77	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.46
2:E:215:THR:HG22	2:E:273:HIS:HA	1.97	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.98	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.48	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.49	0.46
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.96	0.46
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.46
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	1.96	0.46
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.46
2:G:215:THR:HG22	2:G:273:HIS:HA	1.97	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:THR:HB	1:H:100:ASP:HB3	1.97	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.46
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.97	0.46
2:E:1991:THR:O	2:E:1995:THR:OG1	2.34	0.46
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	1.96	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.46
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.46
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.97	0.46
2:G:4930:ALA:O	2:G:4934:GLY:N	2.49	0.46
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.97	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.98	0.46
2:B:4957:LYS:NZ	2:B:4957:LYS:CB	2.77	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.98	0.46
2:I:4930:ALA:O	2:I:4934:GLY:N	2.49	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.46
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.98	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:G:1991:THR:O	2:G:1995:THR:OG1	2.34	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.46
2:G:3915:ILE:O	2:G:3919:THR:N	2.47	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.46
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.97	0.46
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.46
2:B:793:LEU:HB2	2:B:797:HIS:H	1.81	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.46
2:B:4930:ALA:O	2:B:4934:GLY:N	2.49	0.46
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.98	0.46
2:G:243:ARG:NH1	2:G:301:VAL:O	2.43	0.46
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.46
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.97	0.46
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.46
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.34	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.98	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.48	0.45
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.98	0.45
2:B:1936:LYS:O	2:B:1940:CYS:N	2.46	0.45
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.45
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.64	0.45
2:G:793:LEU:HB2	2:G:797:HIS:H	1.81	0.45
2:G:4957:LYS:HB2	2:G:4957:LYS:HZ1	1.80	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.33	0.45
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.98	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.98	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.97	0.45
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.98	0.45
2:G:4978:HIS:CD2	2:G:4982:GLU:HB2	2.52	0.45
1:A:11:ASP:OD1	1:A:67:SER:OG	2.31	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:I:793:LEU:HB2	2:I:797:HIS:H	1.81	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.99	0.45
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.31	0.45
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.99	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.89	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.97	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.98	0.45
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:940:GLY:O	2:B:1052:ASN:N	2.49	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.45
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.33	0.45
2:E:793:LEU:HB2	2:E:797:HIS:H	1.81	0.45
2:I:4978:HIS:CD2	2:I:4982:GLU:HB2	2.52	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.50	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.64	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.45
2:I:1991:THR:O	2:I:1995:THR:OG1	2.34	0.45
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1991:THR:O	2:B:1995:THR:OG1	2.34	0.45
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.82	0.45
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.99	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.89	0.45
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.64	0.45
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.98	0.45
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.99	0.45
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.45
2:E:4984:ASN:C	2:E:4986:ALA:H	2.23	0.45
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.99	0.45
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.45
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.44
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.50	0.44
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.99	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.44
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.82	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.44
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.82	0.44
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.50	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.44
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.82	0.44
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.44
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.82	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.48	0.44
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.44
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.39	0.44
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.64	0.44
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.44
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.44
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.44
2:B:4978:HIS:CD2	2:B:4982:GLU:HB2	2.52	0.44
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.83	0.44
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.44
2:B:1663:HIS:O	2:B:1667:LEU:N	2.51	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.44
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.99	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.44
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.50	0.44
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.50	0.44
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.00	0.44
2:E:5028:PHE:O	2:E:5028:PHE:CG	2.70	0.44
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.50	0.44
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.50	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.44
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.53	0.44
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.44
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.44
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.99	0.44
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.44
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.44
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.83	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.00	0.44
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.00	0.44
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.53	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.44
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.43
2:E:4047:MET:HE3	2:E:4047:MET:HB2	1.84	0.43
2:E:4978:HIS:CD2	2:E:4982:GLU:HB2	2.52	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.43
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.90	0.43
1:A:82:TYR:O	1:A:86:GLY:N	2.51	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.43
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.43
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.51	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.43
2:G:3722:TYR:CZ	2:G:3782:MET:HE3	2.53	0.43
2:G:4826:ILE:O	2:G:4829:SER:OG	2.34	0.43
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.34	0.43
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.43
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.83	0.43
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.00	0.43
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.43
2:G:5028:PHE:CG	2:G:5028:PHE:O	2.70	0.43
1:F:82:TYR:O	1:F:86:GLY:N	2.51	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:B:3722:TYR:CZ	2:B:3782:MET:HE3	2.54	0.43
2:E:167:ASP:HA	2:G:384:MET:HE1	2.00	0.43
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.83	0.43
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:I:446:GLN:HA	2:I:449:ILE:HD12	2.01	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.51	0.43
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.99	0.43
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.99	0.43
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.49	0.43
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.51	0.43
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.82	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.53	0.43
2:I:3722:TYR:CZ	2:I:3782:MET:HE3	2.53	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.00	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.82	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.43
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.52	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.43
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	2.00	0.43
2:G:446:GLN:HA	2:G:449:ILE:HD12	2.01	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.51	0.43
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.43
2:G:1936:LYS:O	2:G:1940:CYS:N	2.46	0.43
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.51	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:446:GLN:HA	2:E:449:ILE:HD12	2.01	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.43
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.43
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.43
2:E:3722:TYR:CZ	2:E:3782:MET:HE3	2.53	0.43
2:E:4957:LYS:HB2	2:E:4957:LYS:HZ1	1.83	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3915:ILE:O	2:I:3919:THR:N	2.47	0.43
2:B:446:GLN:HA	2:B:449:ILE:HD12	2.01	0.43
2:B:955:LEU:O	2:B:966:LYS:NZ	2.42	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.43
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.43
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.54	0.42
2:B:4984:ASN:C	2:B:4986:ALA:N	2.77	0.42
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.49	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.46	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.53	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.66	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.84	0.42
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.54	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.53	0.42
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.54	0.42
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.42
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.42
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.52	0.42
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:TYR:O	1:J:86:GLY:N	2.51	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.42
2:B:384:MET:HE1	2:I:167:ASP:HA	2.01	0.42
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.42
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.85	0.42
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.42
2:I:2138:LEU:HD11	2:I:3654:LEU:HD11	2.01	0.42
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.90	0.42
2:B:113:HIS:O	2:B:399:GLN:NE2	2.53	0.42
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	2.02	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.01	0.42
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.42
2:E:2138:LEU:HD11	2:E:3654:LEU:HD11	2.01	0.42
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.84	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	2.00	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.51	0.42
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.42
2:E:113:HIS:O	2:E:399:GLN:NE2	2.53	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:4984:ASN:C	2:E:4986:ALA:N	2.77	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.51	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.42
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:I:4984:ASN:C	2:I:4986:ALA:N	2.77	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:E:320:LYS:NZ	2:E:381:GLU:O	2.42	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.42
2:E:4000:MET:HE3	2:E:4017:LEU:HD21	2.02	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.77	0.42
2:I:1936:LYS:O	2:I:1940:CYS:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.01	0.42
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.53	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.02	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.42
2:B:4736:ARG:NH1	2:E:4079:ASP:OD1	2.53	0.42
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.01	0.42
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.55	0.42
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.83	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:G:4000:MET:HE3	2:G:4017:LEU:HD21	2.02	0.42
2:B:2138:LEU:HD11	2:B:3654:LEU:HD11	2.01	0.42
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.02	0.42
2:B:3677:LEU:O	2:B:3698:LEU:N	2.52	0.42
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.53	0.42
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	2.02	0.42
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.55	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	2.02	0.42
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.53	0.42
2:B:4000:MET:HE3	2:B:4017:LEU:HD21	2.02	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.84	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.02	0.42
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.42
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.50	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	2.02	0.42
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.84	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.90	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HB2	2.02	0.42
2:B:1124:PHE:HB2	2:B:1162:PHE:CE2	2.55	0.42
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.85	0.42
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.42
2:I:4000:MET:HE3	2:I:4017:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.42
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.55	0.42
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.77	0.42
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.01	0.42
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.50	0.42
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.01	0.41
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.41
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	2.02	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.01	0.41
2:E:3915:ILE:O	2:E:3919:THR:N	2.47	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.41
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.53	0.41
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.41
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.85	0.41
2:G:4984:ASN:C	2:G:4986:ALA:N	2.77	0.41
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.84	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.84	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:2138:LEU:HD11	2:G:3654:LEU:HD11	2.01	0.41
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.55	0.41
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.41
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.41
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.41
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.01	0.41
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.41
2:E:4826:ILE:O	2:E:4829:SER:OG	2.34	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.38	0.41
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.86	0.41
2:G:113:HIS:O	2:G:399:GLN:NE2	2.53	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.86	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.77	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.86	0.41
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.50	0.41
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.02	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.86	0.41
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.54	0.41
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.66	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.41
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.31	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.41
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.41
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.86	0.41
2:I:5027:CYS:SG	2:I:5027:CYS:O	2.79	0.41
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.41
2:I:113:HIS:O	2:I:399:GLN:NE2	2.53	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.02	0.41
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.41
2:I:4014:LYS:HE2	2:I:4135:PRO:HG3	2.03	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.53	0.41
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.02	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.53	0.41
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4014:LYS:HE2	2:E:4135:PRO:HG3	2.03	0.41
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.55	0.41
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.02	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.03	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.41
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.56	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.51	0.41
2:E:3706:SER:OG	2:E:3781:GLN:NE2	2.54	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.02	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.41
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.49	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.02	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.86	0.41
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.41
2:B:4014:LYS:HE2	2:B:4135:PRO:HG3	2.03	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.52	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.41
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.02	0.41
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.84	0.41
2:I:257:ARG:O	2:I:284:HIS:NE2	2.48	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.41
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.02	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.41
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.02	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.56	0.41
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.50	0.41
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.41
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.41
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.55	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HB2	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5027:CYS:O	2:G:5027:CYS:SG	2.79	0.41
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HB2	2.02	0.40
2:E:582:HIS:O	2:E:585:SER:OG	2.30	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.56	0.40
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.38	0.40
2:I:551:LEU:HD21	2:I:589:LEU:HB2	2.02	0.40
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.56	0.40
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.40
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.02	0.40
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	2.02	0.40
2:G:4929:LEU:HD13	2:G:4929:LEU:HA	1.92	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.40
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.87	0.40
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.40
2:B:3706:SER:OG	2:B:3781:GLN:NE2	2.54	0.40
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.55	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.87	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.87	0.40
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.84	0.40
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.02	0.40
2:B:3847:PHE:HE1	2:B:3950:ASN:HD22	1.70	0.40
2:B:5027:CYS:SG	2:B:5027:CYS:O	2.79	0.40
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.75	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.40
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.87	0.40
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.03	0.40
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.03	0.40
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.04	0.40
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.87	0.40
2:E:5028:PHE:CD1	2:E:5028:PHE:O	2.75	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.87	0.40
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.03	0.40
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.92	0.40
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.02	0.40
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.04	0.40
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1705:GLY:HA2	2:E:1709:ALA:HB3	2.04	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:5027:CYS:O	2:E:5027:CYS:SG	2.79	0.40
2:I:384:MET:HE1	2:G:167:ASP:HA	2.04	0.40
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.40
2:I:2298:VAL:HA	2:I:2301:TYR:HB2	2.03	0.40
2:I:3805:LEU:H	2:I:3805:LEU:HG	1.77	0.40
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.49	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.04	0.40
2:G:4014:LYS:HE2	2:G:4135:PRO:HG3	2.03	0.40
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.52	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.40
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.40
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.86	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.03	0.40
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.40
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.04	0.40
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.40
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.56	0.40
2:G:2298:VAL:HA	2:G:2301:TYR:HB2	2.03	0.40
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2890 (89%)	339 (10%)	6 (0%)	43	77
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	43	77
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	43	77
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	44	77

All (24) 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	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	B	4641	PRO
2	B	4985	LEU
2	E	1932	PRO
2	E	4641	PRO
2	E	4985	LEU
2	I	1932	PRO
2	I	4641	PRO
2	I	4985	LEU
2	G	1932	PRO
2	G	4641	PRO
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	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%)	2481 (100%)	12 (0%)	81	81
2	E	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	G	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	I	2493/3022 (82%)	2480 (100%)	13 (0%)	81	81
All	All	10324/12444 (83%)	10275 (100%)	49 (0%)	78	81

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	3663	LEU
2	B	3805	LEU
2	B	4792	LEU
2	B	4929	LEU
2	B	4957	LYS
2	B	4959	PHE
2	B	4960	ILE
2	B	4983	HIS
2	E	131	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4792	LEU

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Mol	Chain	Res	Type
2	E	4929	LEU
2	E	4957	LYS
2	E	4959	PHE
2	E	4960	ILE
2	E	4983	HIS
2	I	131	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1676	LEU
2	I	2339	VAL
2	I	3663	LEU
2	I	3805	LEU
2	I	4792	LEU
2	I	4929	LEU
2	I	4957	LYS
2	I	4959	PHE
2	I	4960	ILE
2	I	4983	HIS
2	G	131	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	3663	LEU
2	G	3805	LEU
2	G	4792	LEU
2	G	4929	LEU
2	G	4957	LYS
2	G	4959	PHE
2	G	4960	ILE
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (248) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	HIS
1	F	87	HIS
1	A	25	HIS
1	A	87	HIS
1	H	25	HIS
1	H	87	HIS
1	J	25	HIS
1	J	87	HIS

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	151	HIS
2	B	156	GLN
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	399	GLN
2	B	405	HIS
2	B	413	GLN
2	B	582	HIS
2	B	725	HIS
2	B	797	HIS
2	B	838	HIS
2	B	877	ASN
2	B	1133	HIS
2	B	1220	GLN
2	B	1598	GLN
2	B	1678	ASN
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	2005	GLN
2	B	2007	ASN
2	B	2260	ASN
2	B	2772	GLN
2	B	2773	ASN
2	B	3647	HIS
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3850	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN

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Mol	Chain	Res	Type
2	B	3994	HIS
2	B	4034	ASN
2	B	4037	ASN
2	B	4054	ASN
2	B	4109	GLN
2	B	4142	ASN
2	B	4201	ASN
2	B	4209	GLN
2	B	4246	GLN
2	B	4553	ASN
2	B	4691	GLN
2	B	4707	ASN
2	B	4728	HIS
2	B	4776	GLN
2	B	4806	ASN
2	B	4933	GLN
2	B	4987	ASN
2	B	5003	HIS
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	151	HIS
2	E	156	GLN
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	399	GLN
2	E	405	HIS
2	E	413	GLN
2	E	582	HIS
2	E	725	HIS
2	E	797	HIS
2	E	838	HIS
2	E	866	HIS
2	E	877	ASN
2	E	1220	GLN
2	E	1598	GLN
2	E	1678	ASN
2	E	1679	ASN
2	E	1691	GLN
2	E	1693	GLN

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Mol	Chain	Res	Type
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	2005	GLN
2	E	2007	ASN
2	E	2260	ASN
2	E	2772	GLN
2	E	2773	ASN
2	E	2780	ASN
2	E	3647	HIS
2	E	3781	GLN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3850	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4109	GLN
2	E	4142	ASN
2	E	4201	ASN
2	E	4209	GLN
2	E	4246	GLN
2	E	4553	ASN
2	E	4691	GLN
2	E	4707	ASN
2	E	4728	HIS
2	E	4776	GLN
2	E	4806	ASN
2	E	4933	GLN
2	E	4987	ASN
2	E	5003	HIS
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	151	HIS
2	I	156	GLN

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Mol	Chain	Res	Type
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	399	GLN
2	I	405	HIS
2	I	413	GLN
2	I	520	ASN
2	I	582	HIS
2	I	725	HIS
2	I	797	HIS
2	I	838	HIS
2	I	866	HIS
2	I	877	ASN
2	I	1220	GLN
2	I	1598	GLN
2	I	1678	ASN
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	2005	GLN
2	I	2007	ASN
2	I	2260	ASN
2	I	2772	GLN
2	I	2773	ASN
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3850	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3994	HIS
2	I	4034	ASN
2	I	4037	ASN
2	I	4054	ASN
2	I	4109	GLN

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Mol	Chain	Res	Type
2	I	4142	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4728	HIS
2	I	4776	GLN
2	I	4806	ASN
2	I	4933	GLN
2	I	4987	ASN
2	I	5003	HIS
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	399	GLN
2	G	405	HIS
2	G	413	GLN
2	G	520	ASN
2	G	582	HIS
2	G	725	HIS
2	G	797	HIS
2	G	838	HIS
2	G	877	ASN
2	G	1220	GLN
2	G	1598	GLN
2	G	1678	ASN
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	2005	GLN
2	G	2007	ASN
2	G	2260	ASN
2	G	2772	GLN

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Mol	Chain	Res	Type
2	G	2773	ASN
2	G	3647	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3850	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3994	HIS
2	G	4034	ASN
2	G	4037	ASN
2	G	4054	ASN
2	G	4109	GLN
2	G	4142	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4553	ASN
2	G	4691	GLN
2	G	4707	ASN
2	G	4728	HIS
2	G	4776	GLN
2	G	4806	ASN
2	G	4933	GLN
2	G	4987	ASN
2	G	5003	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	B	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.75	10 (20%)
3	ATP	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.75	10 (20%)
4	CFF	B	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.75	11 (47%)
4	CFF	G	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.75	11 (47%)
3	ATP	G	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.76	10 (20%)
3	ATP	I	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	10 (20%)
4	CFF	E	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.74	11 (47%)
4	CFF	I	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.74	11 (47%)

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

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5101	ATP	C5-C4	4.25	1.46	1.39
3	B	5101	ATP	C5-C4	4.23	1.46	1.39
3	G	5101	ATP	C5-C4	4.23	1.46	1.39
3	I	5101	ATP	C5-C4	4.20	1.46	1.39
4	E	5102	CFF	C6-N1	-3.81	1.32	1.40
4	B	5102	CFF	C6-N1	-3.80	1.32	1.40
4	G	5102	CFF	C6-N1	-3.78	1.32	1.40
4	I	5102	CFF	C6-N1	-3.76	1.32	1.40
4	I	5102	CFF	C4-N3	-2.87	1.33	1.38
4	B	5102	CFF	C4-N3	-2.83	1.33	1.38
4	E	5102	CFF	C4-N3	-2.79	1.33	1.38
4	G	5102	CFF	C4-N3	-2.78	1.33	1.38
3	G	5101	ATP	C5-N7	-2.52	1.34	1.39
3	B	5101	ATP	C5-N7	-2.50	1.34	1.39
3	I	5101	ATP	C5-N7	-2.50	1.34	1.39
4	E	5102	CFF	C5-N7	-2.49	1.34	1.38
3	E	5101	ATP	C5-N7	-2.49	1.34	1.39
4	B	5102	CFF	C5-N7	-2.48	1.34	1.38
4	G	5102	CFF	C5-N7	-2.45	1.34	1.38
4	I	5102	CFF	C5-N7	-2.43	1.34	1.38
3	E	5101	ATP	C8-N7	2.28	1.36	1.31
3	G	5101	ATP	C4-N9	-2.26	1.33	1.37
3	G	5101	ATP	C5-C6	2.25	1.47	1.41
3	I	5101	ATP	C8-N7	2.25	1.36	1.31
3	B	5101	ATP	C8-N7	2.24	1.36	1.31
3	B	5101	ATP	C5-C6	2.23	1.47	1.41
3	I	5101	ATP	C5-C6	2.23	1.47	1.41
4	G	5102	CFF	C2-N3	-2.23	1.34	1.39
3	B	5101	ATP	C4-N9	-2.22	1.33	1.37
3	E	5101	ATP	C5-C6	2.22	1.47	1.41
3	G	5101	ATP	C8-N7	2.21	1.35	1.31
4	B	5102	CFF	C2-N3	-2.21	1.34	1.39
4	E	5102	CFF	C2-N3	-2.21	1.34	1.39
4	I	5102	CFF	C2-N3	-2.21	1.34	1.39
3	I	5101	ATP	C4-N9	-2.20	1.33	1.37
3	E	5101	ATP	C4-N9	-2.19	1.33	1.37
4	E	5102	CFF	O11-C2	-2.11	1.18	1.22
4	E	5102	CFF	O13-C6	-2.11	1.18	1.23
4	B	5102	CFF	O13-C6	-2.11	1.18	1.23
4	I	5102	CFF	O13-C6	-2.11	1.18	1.23
4	G	5102	CFF	O13-C6	-2.11	1.18	1.23
4	I	5102	CFF	O11-C2	-2.10	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	O11-C2	-2.08	1.18	1.22
4	G	5102	CFF	O11-C2	-2.06	1.18	1.22
4	E	5102	CFF	C2-N1	-2.05	1.35	1.39
4	B	5102	CFF	C2-N1	-2.05	1.35	1.39
4	I	5102	CFF	C2-N1	-2.05	1.35	1.39
4	G	5102	CFF	C2-N1	-2.05	1.35	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	C14-N7-C8	-7.71	111.86	126.28
4	B	5102	CFF	C14-N7-C8	-7.70	111.88	126.28
4	I	5102	CFF	C14-N7-C8	-7.68	111.91	126.28
4	G	5102	CFF	C14-N7-C8	-7.68	111.91	126.28
3	B	5101	ATP	C5-C4-N3	-5.17	119.60	126.72
3	G	5101	ATP	C5-C4-N3	-5.17	119.60	126.72
3	I	5101	ATP	C5-C4-N3	-5.13	119.66	126.72
3	E	5101	ATP	C5-C4-N3	-5.12	119.66	126.72
4	E	5102	CFF	C14-N7-C5	5.11	139.93	127.77
4	B	5102	CFF	C14-N7-C5	5.10	139.90	127.77
4	I	5102	CFF	C14-N7-C5	5.09	139.89	127.77
4	G	5102	CFF	C14-N7-C5	5.08	139.85	127.77
3	G	5101	ATP	N3-C4-N9	4.55	134.90	127.17
3	B	5101	ATP	N3-C4-N9	4.52	134.85	127.17
3	E	5101	ATP	N3-C4-N9	4.48	134.79	127.17
3	I	5101	ATP	N3-C4-N9	4.48	134.78	127.17
4	G	5102	CFF	C5-C6-N1	4.17	119.70	112.06
4	B	5102	CFF	C5-C6-N1	4.15	119.66	112.06
4	I	5102	CFF	C5-C6-N1	4.13	119.63	112.06
4	E	5102	CFF	C5-C6-N1	4.12	119.61	112.06
3	G	5101	ATP	C4-N9-C8	3.67	109.59	105.74
3	B	5101	ATP	C4-N9-C8	3.62	109.54	105.74
3	E	5101	ATP	C4-N9-C8	3.61	109.53	105.74
3	I	5101	ATP	C4-N9-C8	3.59	109.50	105.74
3	G	5101	ATP	N3-C2-N1	-3.53	123.24	128.58
3	B	5101	ATP	N3-C2-N1	-3.52	123.26	128.58
3	I	5101	ATP	N3-C2-N1	-3.52	123.26	128.58
3	E	5101	ATP	N3-C2-N1	-3.51	123.26	128.58
3	G	5101	ATP	C2-N3-C4	3.51	120.40	111.83
3	B	5101	ATP	C2-N3-C4	3.50	120.39	111.83
3	I	5101	ATP	C2-N3-C4	3.49	120.35	111.83
3	E	5101	ATP	C2-N3-C4	3.48	120.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C6-N1-C2	-3.39	120.15	125.66
4	I	5102	CFF	C6-N1-C2	-3.37	120.19	125.66
4	B	5102	CFF	C6-N1-C2	-3.35	120.21	125.66
4	E	5102	CFF	C6-N1-C2	-3.32	120.27	125.66
3	B	5101	ATP	C4-C5-N7	-2.94	107.22	110.58
3	E	5101	ATP	C4-C5-N7	-2.93	107.24	110.58
3	I	5101	ATP	C4-C5-N7	-2.92	107.24	110.58
3	G	5101	ATP	C4-C5-N7	-2.92	107.25	110.58
4	E	5102	CFF	N7-C8-N9	-2.87	108.28	113.48
4	B	5102	CFF	N7-C8-N9	-2.86	108.31	113.48
4	I	5102	CFF	N7-C8-N9	-2.84	108.34	113.48
4	G	5102	CFF	N7-C8-N9	-2.84	108.34	113.48
4	E	5102	CFF	O13-C6-C5	-2.84	120.57	126.38
4	B	5102	CFF	O13-C6-C5	-2.83	120.58	126.38
4	G	5102	CFF	O13-C6-C5	-2.82	120.60	126.38
4	I	5102	CFF	N3-C4-N9	2.81	130.68	126.27
4	I	5102	CFF	O13-C6-C5	-2.80	120.64	126.38
4	B	5102	CFF	N3-C4-N9	2.78	130.65	126.27
4	G	5102	CFF	N3-C4-N9	2.77	130.63	126.27
4	E	5102	CFF	N3-C4-N9	2.76	130.61	126.27
4	B	5102	CFF	C6-C5-C4	-2.63	119.61	122.92
4	G	5102	CFF	C6-C5-C4	-2.61	119.63	122.92
4	E	5102	CFF	C6-C5-C4	-2.59	119.65	122.92
4	I	5102	CFF	C6-C5-C4	-2.58	119.67	122.92
3	G	5101	ATP	N9-C8-N7	-2.52	110.36	113.94
3	B	5101	ATP	N9-C8-N7	-2.50	110.39	113.94
3	E	5101	ATP	N9-C8-N7	-2.50	110.39	113.94
3	I	5101	ATP	N9-C8-N7	-2.48	110.41	113.94
3	G	5101	ATP	C5-N7-C8	2.45	107.30	103.45
3	B	5101	ATP	C5-N7-C8	2.45	107.30	103.45
3	E	5101	ATP	C5-N7-C8	2.44	107.29	103.45
3	I	5101	ATP	C5-N7-C8	2.43	107.28	103.45
4	G	5102	CFF	C10-N1-C6	2.32	121.24	117.64
4	B	5102	CFF	C10-N1-C6	2.32	121.23	117.64
4	I	5102	CFF	C10-N1-C6	2.30	121.20	117.64
4	E	5102	CFF	C10-N1-C6	2.29	121.18	117.64
4	G	5102	CFF	N3-C2-N1	2.18	119.86	117.14
3	G	5101	ATP	C2-N1-C6	2.15	122.26	118.73
3	E	5101	ATP	C2-N1-C6	2.14	122.24	118.73
4	B	5102	CFF	N3-C2-N1	2.13	119.81	117.14
4	I	5102	CFF	N3-C2-N1	2.13	119.81	117.14
3	B	5101	ATP	C2-N1-C6	2.13	122.23	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	C2-N1-C6	2.13	122.23	118.73
4	G	5102	CFF	C12-N3-C2	2.10	121.00	117.33
4	E	5102	CFF	N3-C2-N1	2.10	119.76	117.14
3	E	5101	ATP	C6-C5-N7	2.07	136.09	132.09
4	E	5102	CFF	C12-N3-C2	2.07	120.94	117.33
4	B	5102	CFF	C12-N3-C2	2.07	120.94	117.33
3	B	5101	ATP	C6-C5-N7	2.06	136.06	132.09
3	I	5101	ATP	C6-C5-N7	2.06	136.06	132.09
3	G	5101	ATP	C6-C5-N7	2.05	136.04	132.09
4	I	5102	CFF	C12-N3-C2	2.05	120.90	117.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

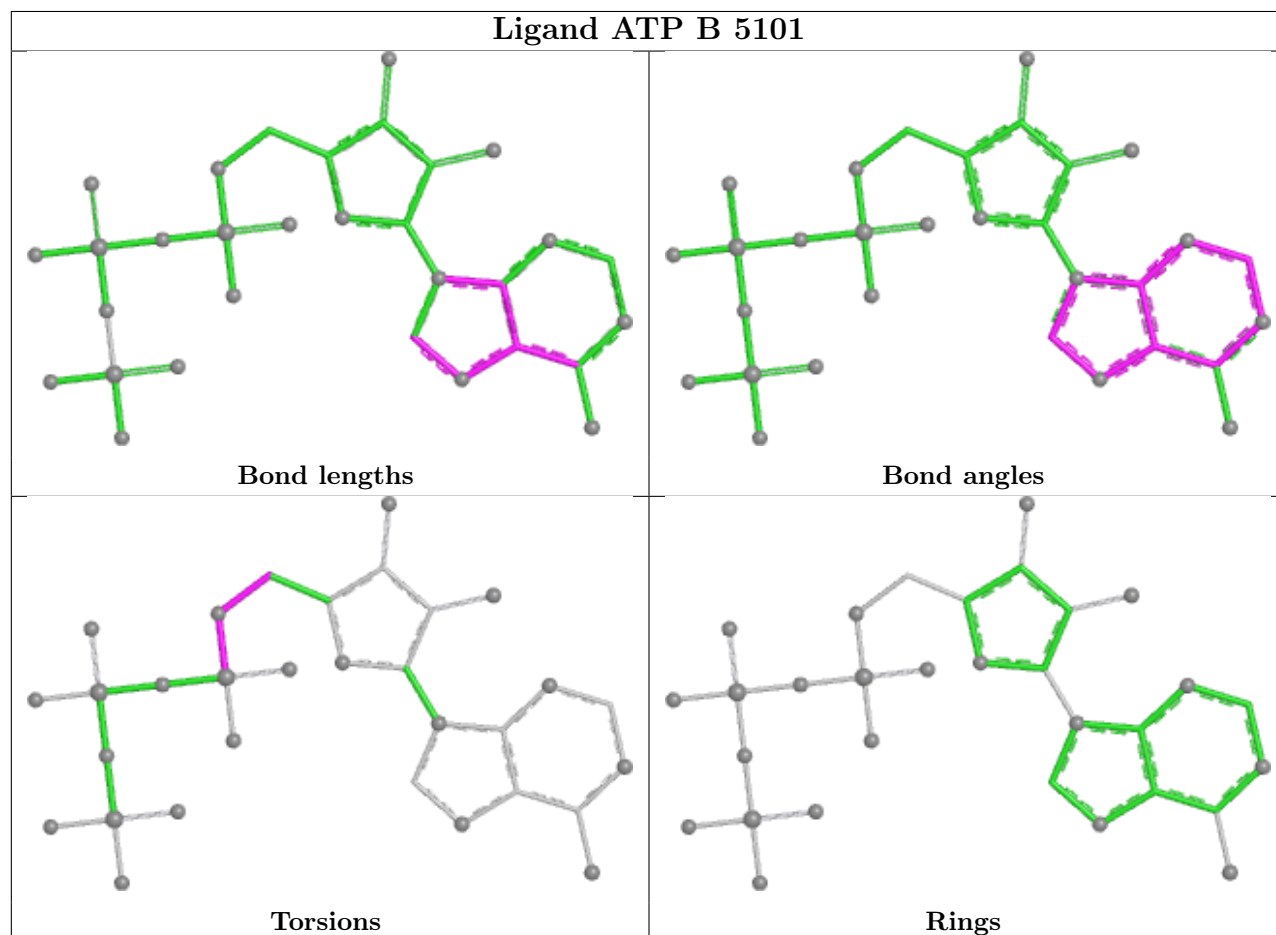
There are no ring outliers.

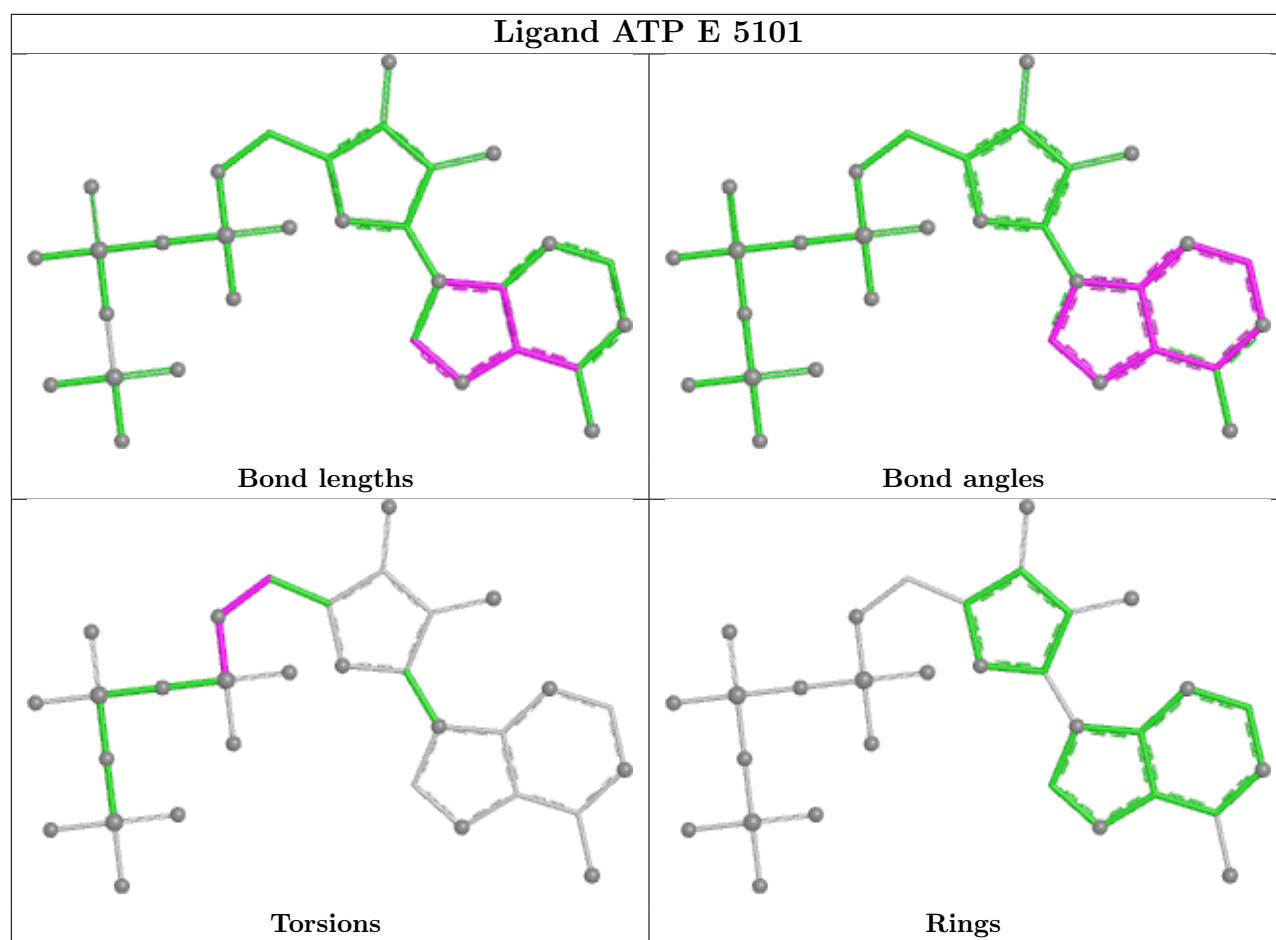
4 monomers are involved in 8 short contacts:

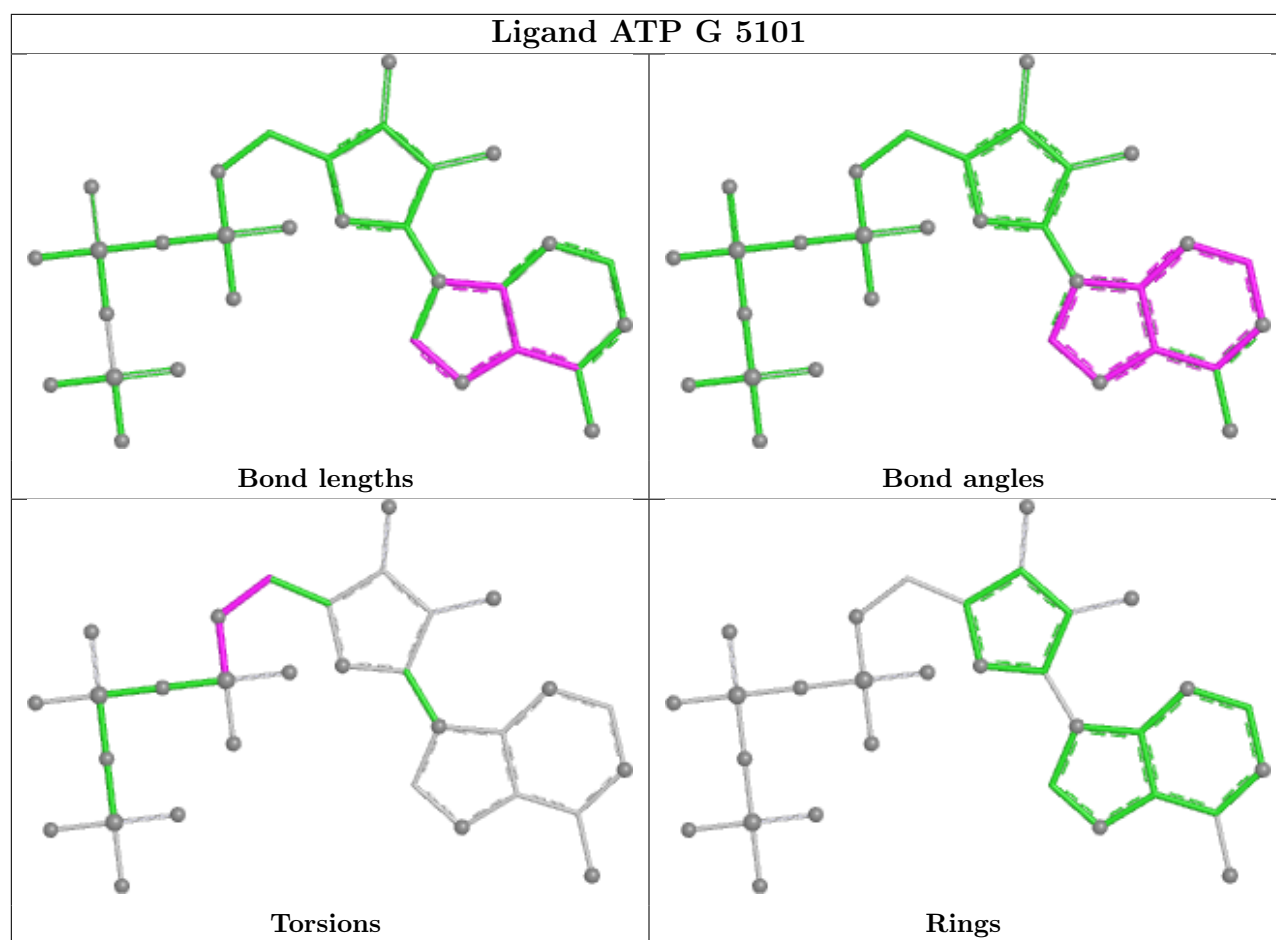
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	0

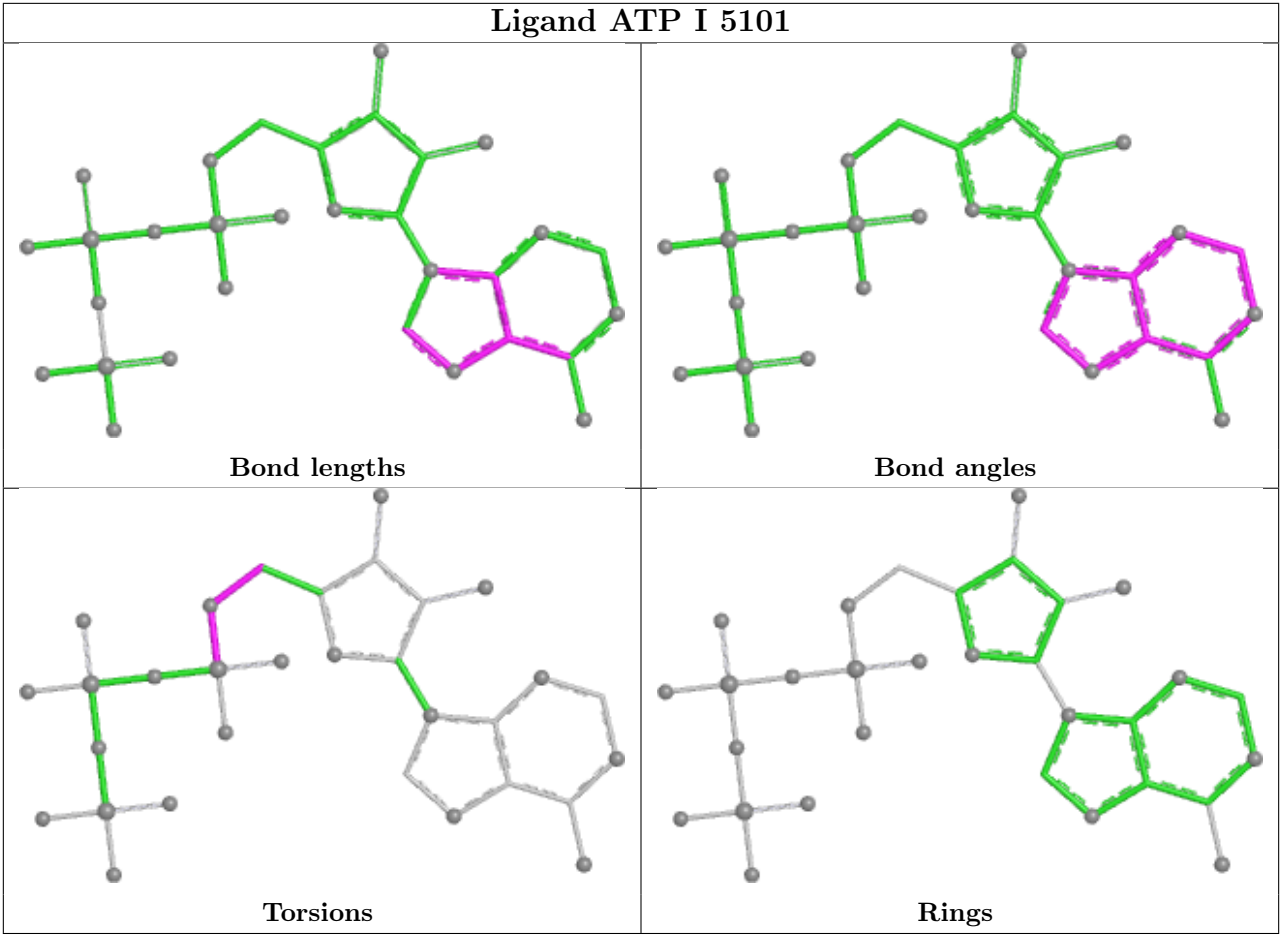
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93
1	E	3613:UNK	C	3639:THR	N	42.93
1	I	3613:UNK	C	3639:THR	N	42.93
1	G	3613:UNK	C	3639:THR	N	42.93
1	B	4253:GLU	C	4320:UNK	N	27.35
1	E	4253:GLU	C	4320:UNK	N	27.35
1	I	4253:GLU	C	4320:UNK	N	27.35
1	G	4253:GLU	C	4320:UNK	N	27.35
1	B	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.81
1	E	3063:UNK	C	3134:UNK	N	14.81
1	I	3063:UNK	C	3134:UNK	N	14.81
1	G	3063:UNK	C	3134:UNK	N	14.81
1	B	2703:UNK	C	2734:ASN	N	14.74
1	E	2703:UNK	C	2734:ASN	N	14.74
1	I	2703:UNK	C	2734:ASN	N	14.74
1	G	2703:UNK	C	2734:ASN	N	14.74
1	B	3468:UNK	C	3511:UNK	N	14.16
1	E	3468:UNK	C	3511:UNK	N	14.16
1	I	3468:UNK	C	3511:UNK	N	14.16
1	G	3468:UNK	C	3511:UNK	N	14.16
1	B	3236:UNK	C	3241:UNK	N	13.24
1	E	3236:UNK	C	3241:UNK	N	13.24
1	I	3236:UNK	C	3241:UNK	N	13.24
1	G	3236:UNK	C	3241:UNK	N	13.24
1	B	2976:UNK	C	2995:UNK	N	12.70
1	E	2976:UNK	C	2995:UNK	N	12.70
1	I	2976:UNK	C	2995:UNK	N	12.70
1	G	2976:UNK	C	2995:UNK	N	12.70
1	B	1564:UNK	C	1573:MET	N	12.34
1	E	1564:UNK	C	1573:MET	N	12.34
1	I	1564:UNK	C	1573:MET	N	12.34
1	G	1564:UNK	C	1573:MET	N	12.34
1	B	3254:UNK	C	3261:UNK	N	8.53
1	E	3254:UNK	C	3261:UNK	N	8.53
1	I	3254:UNK	C	3261:UNK	N	8.53
1	G	3254:UNK	C	3261:UNK	N	8.53

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	6.12
1	E	1297:UNK	C	1430:UNK	N	6.12
1	I	1297:UNK	C	1430:UNK	N	6.12
1	G	1297:UNK	C	1430:UNK	N	6.12
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
1	B	2939:ARG	C	2942:UNK	N	3.23
1	E	2939:ARG	C	2942:UNK	N	3.23
1	G	2939:ARG	C	2942:UNK	N	3.23
1	I	2939:ARG	C	2942:UNK	N	3.22

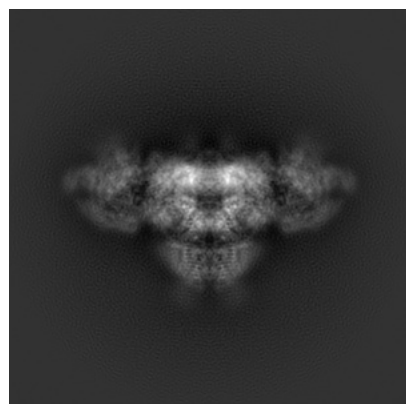
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8380. These allow visual inspection of the internal detail of the map and identification of artifacts.

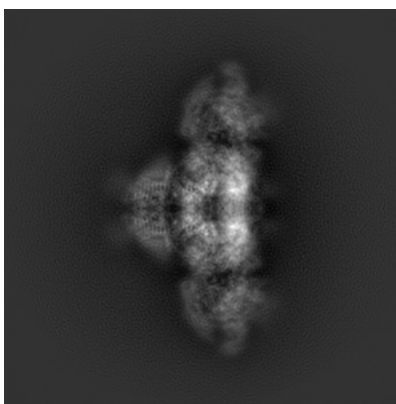
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

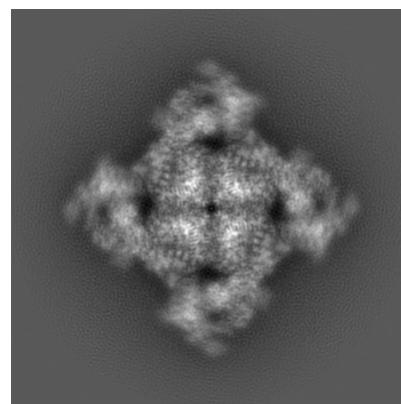
6.1.1 Primary map



X

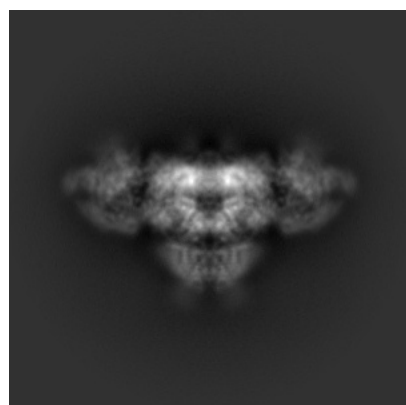


Y

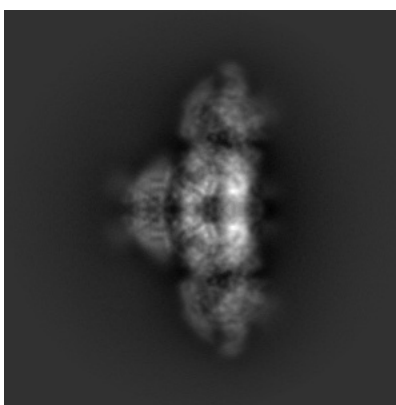


Z

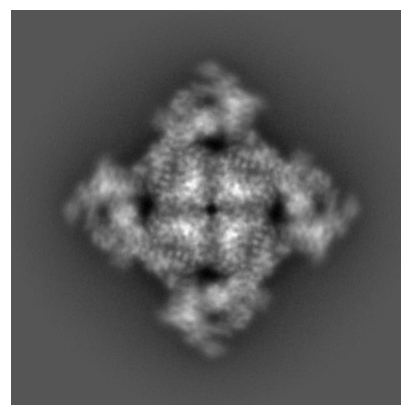
6.1.2 Raw map



X



Y

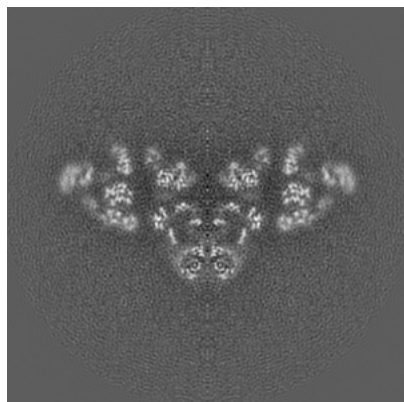


Z

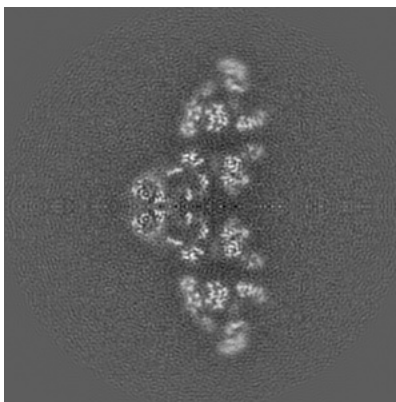
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

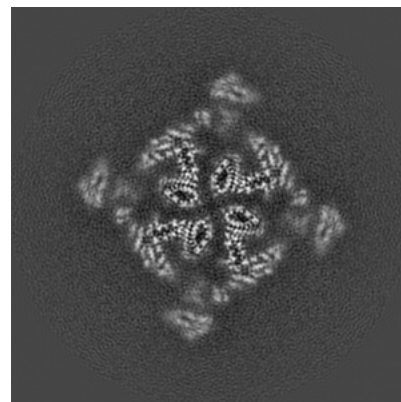
6.2.1 Primary map



X Index: 200

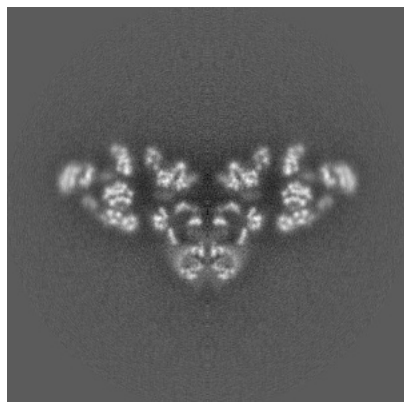


Y Index: 200

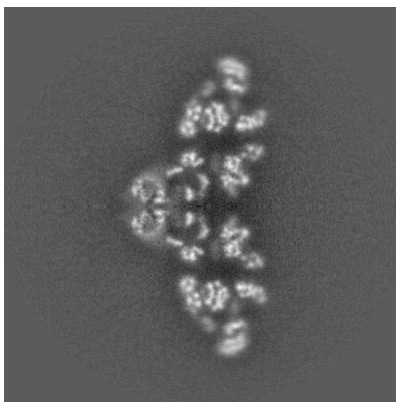


Z Index: 200

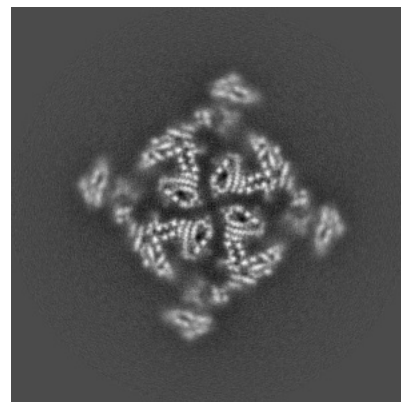
6.2.2 Raw map



X Index: 200



Y Index: 200

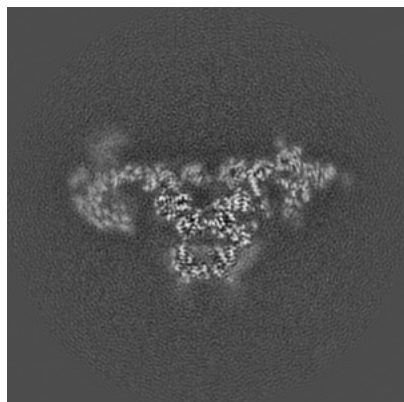


Z Index: 200

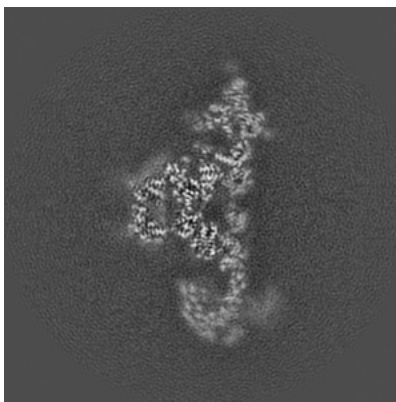
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

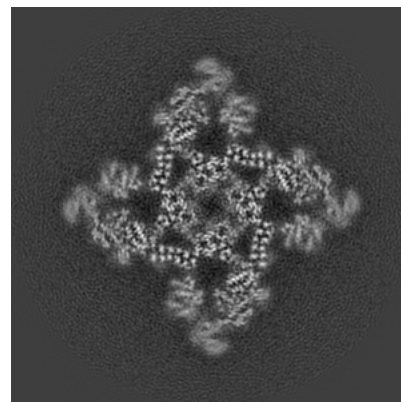
6.3.1 Primary map



X Index: 183

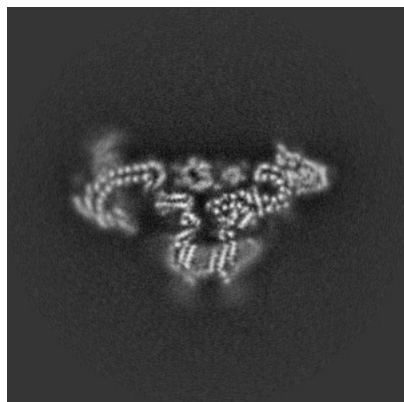


Y Index: 217

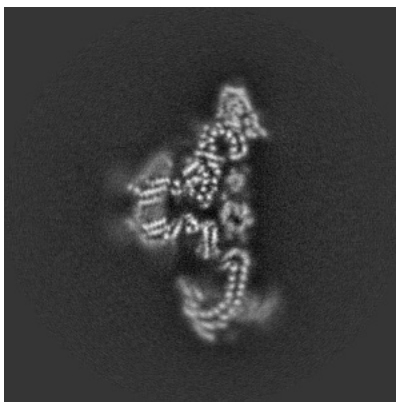


Z Index: 226

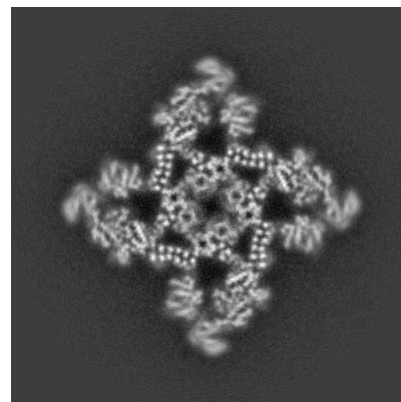
6.3.2 Raw map



X Index: 176



Y Index: 224

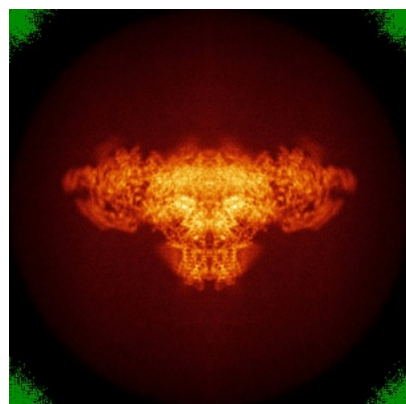


Z Index: 226

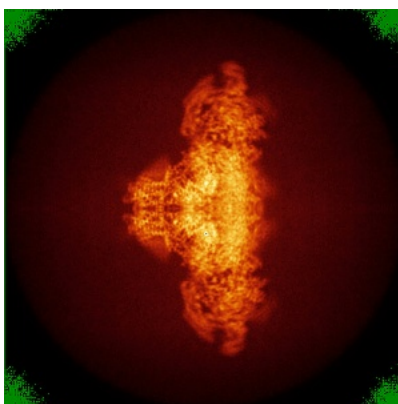
The images above show the largest variance slices of the map in three orthogonal directions.

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

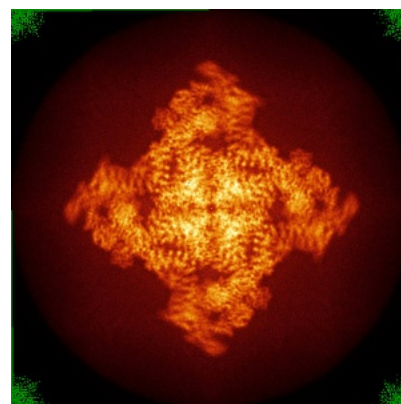
6.4.1 Primary map



X

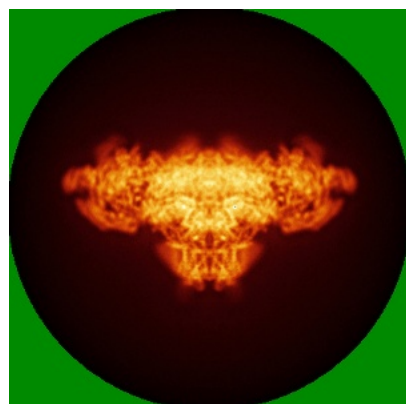


Y

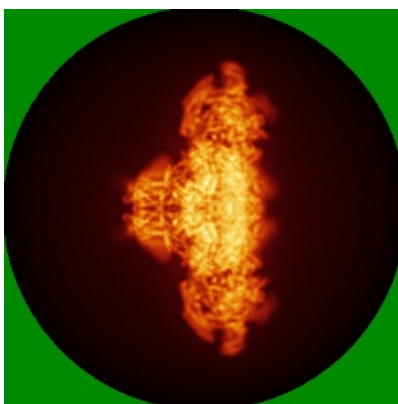


Z

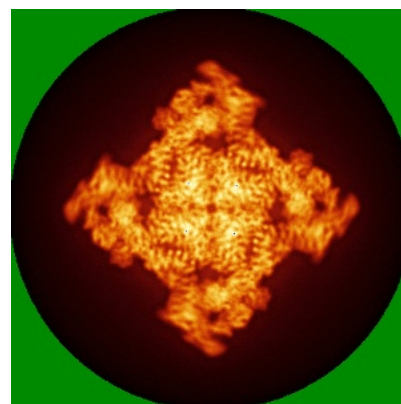
6.4.2 Raw map



X



Y

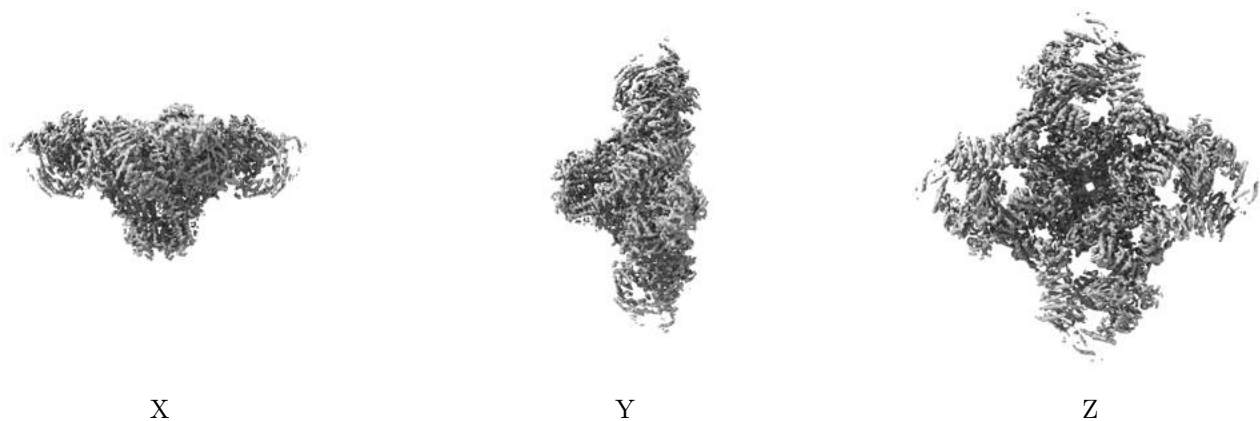


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

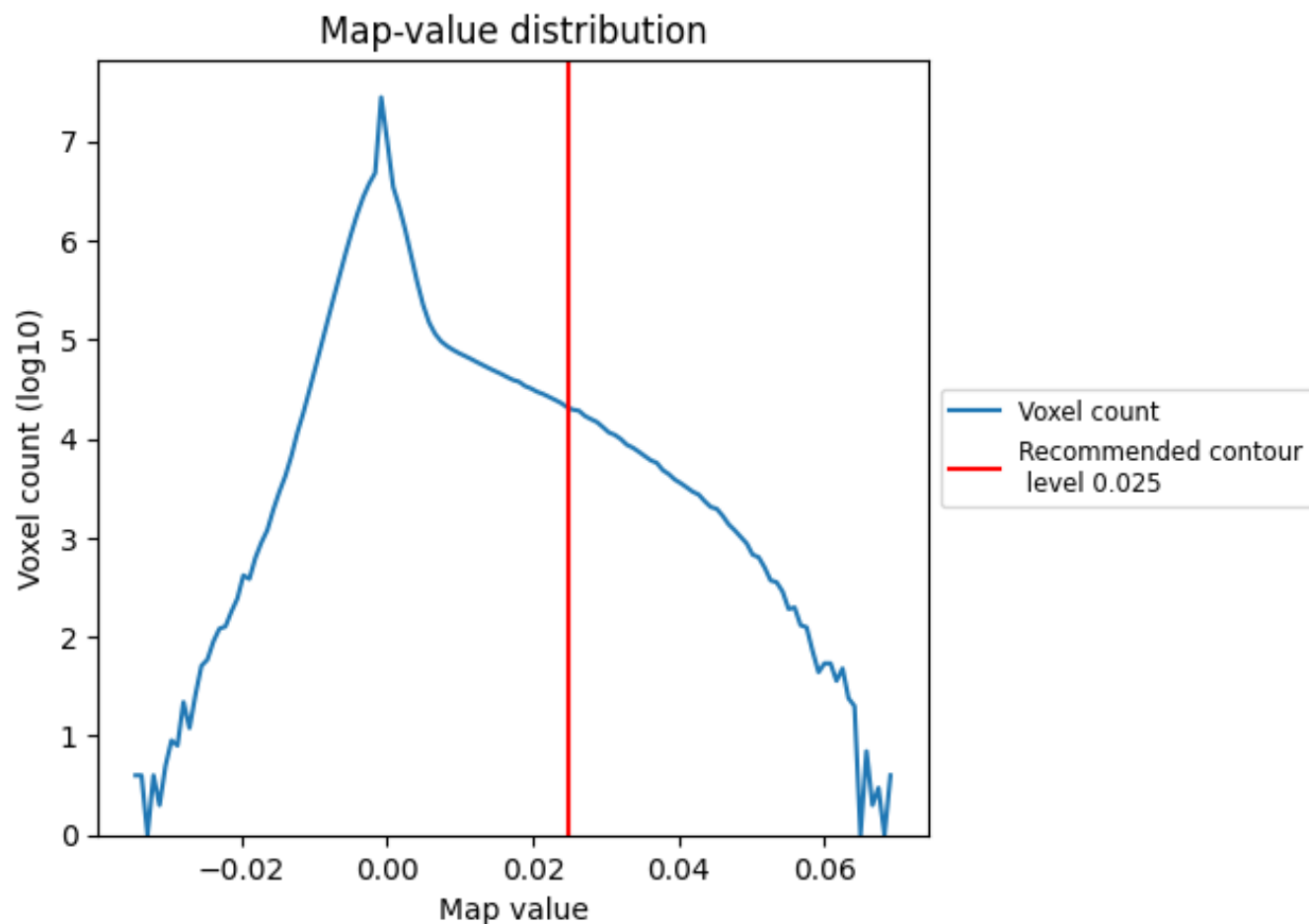
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

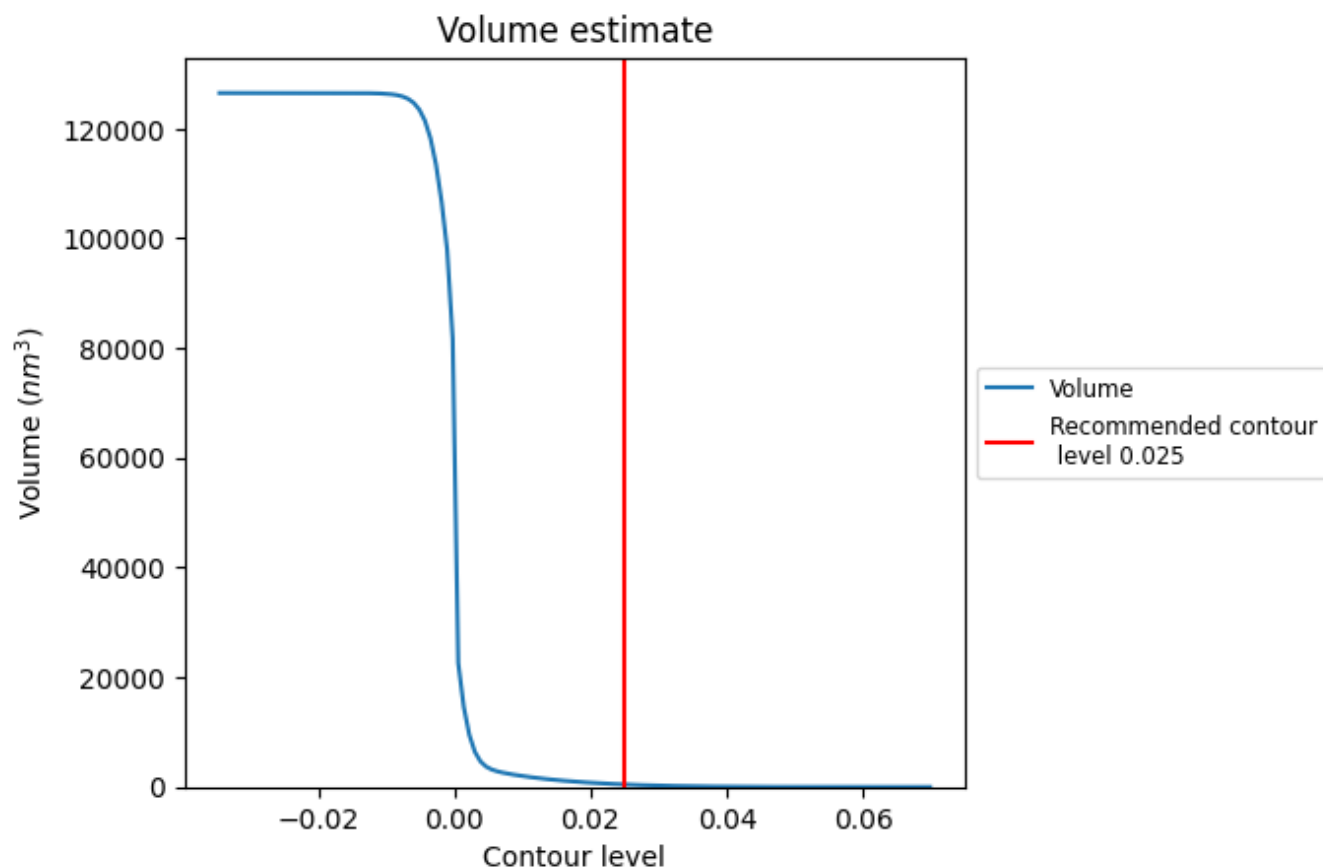
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

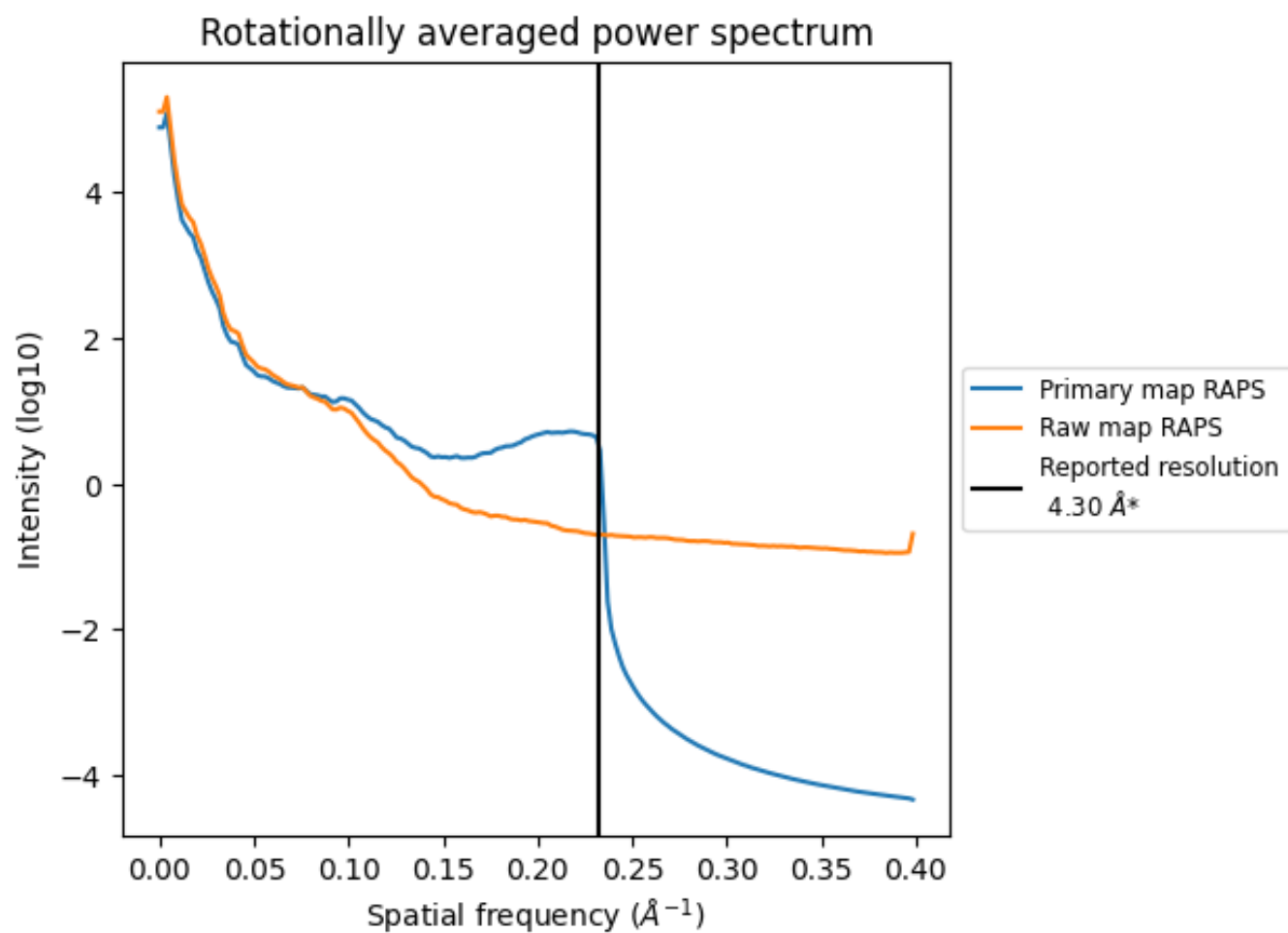
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

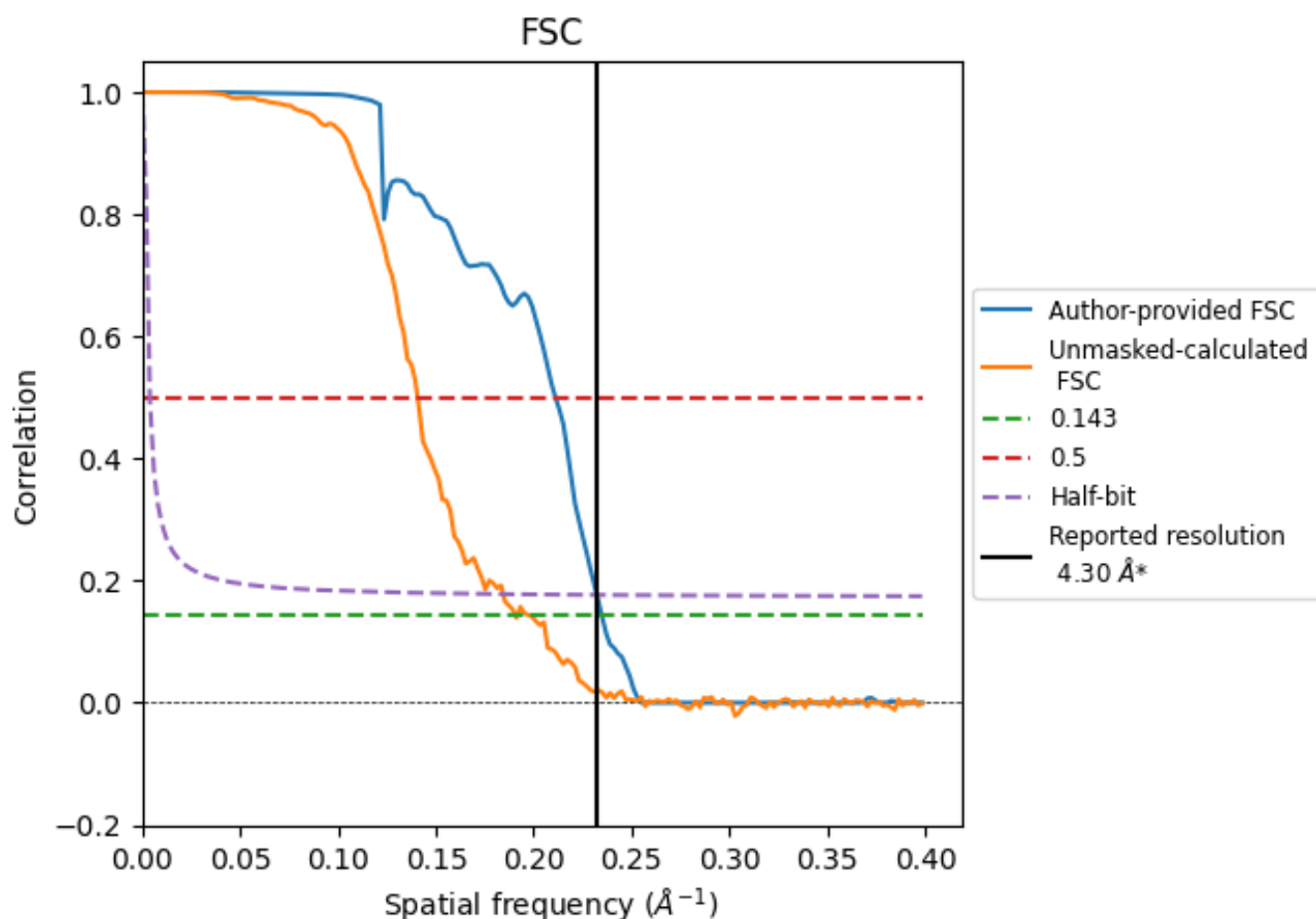


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

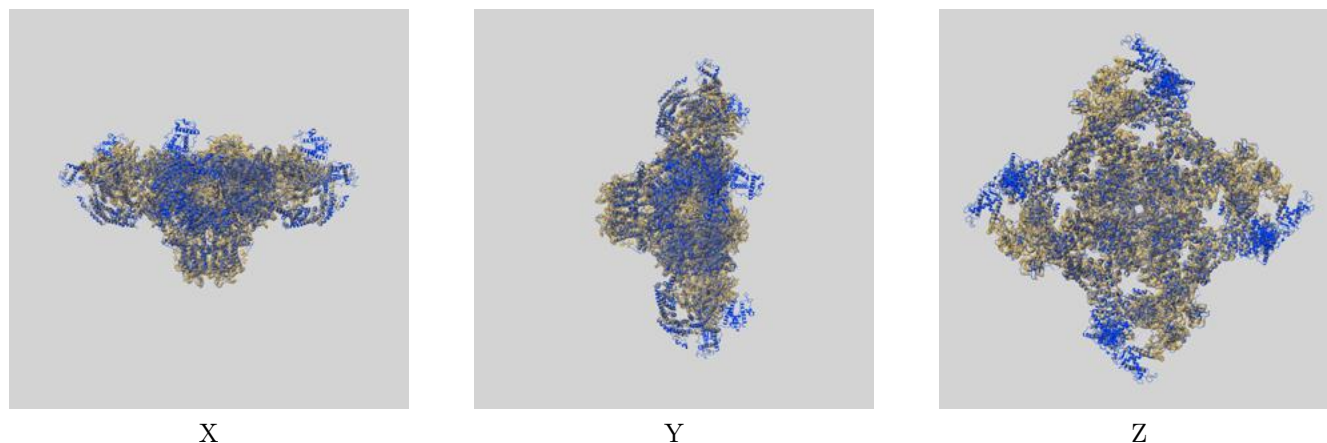
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	4.74	4.31
Unmasked-calculated*	5.24	7.11	5.43

*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 5.24 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

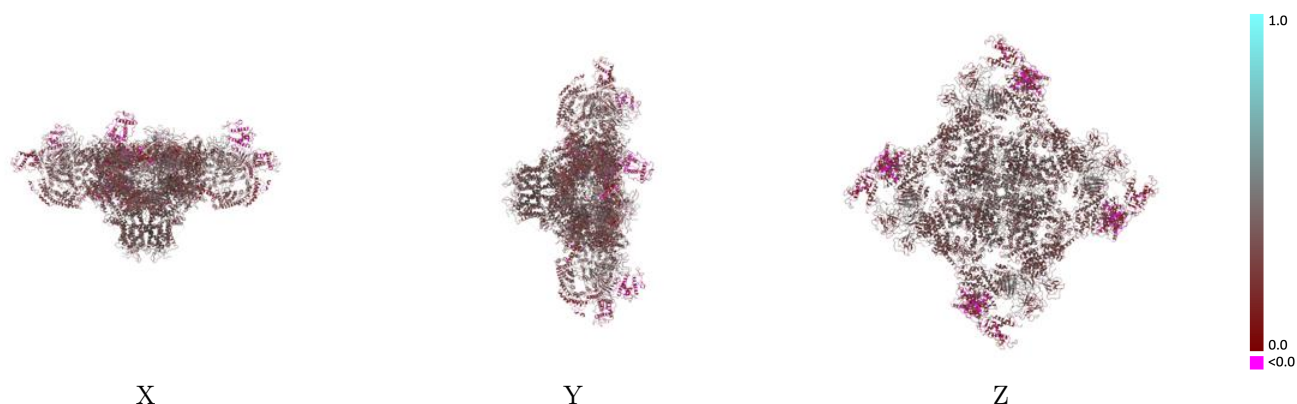
This section contains information regarding the fit between EMDB map EMD-8380 and PDB model 5TAN. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



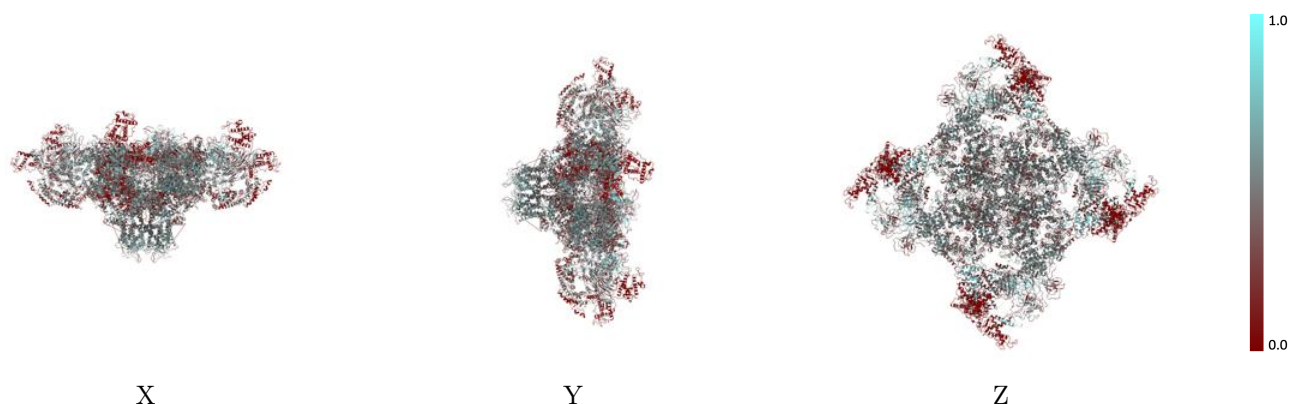
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



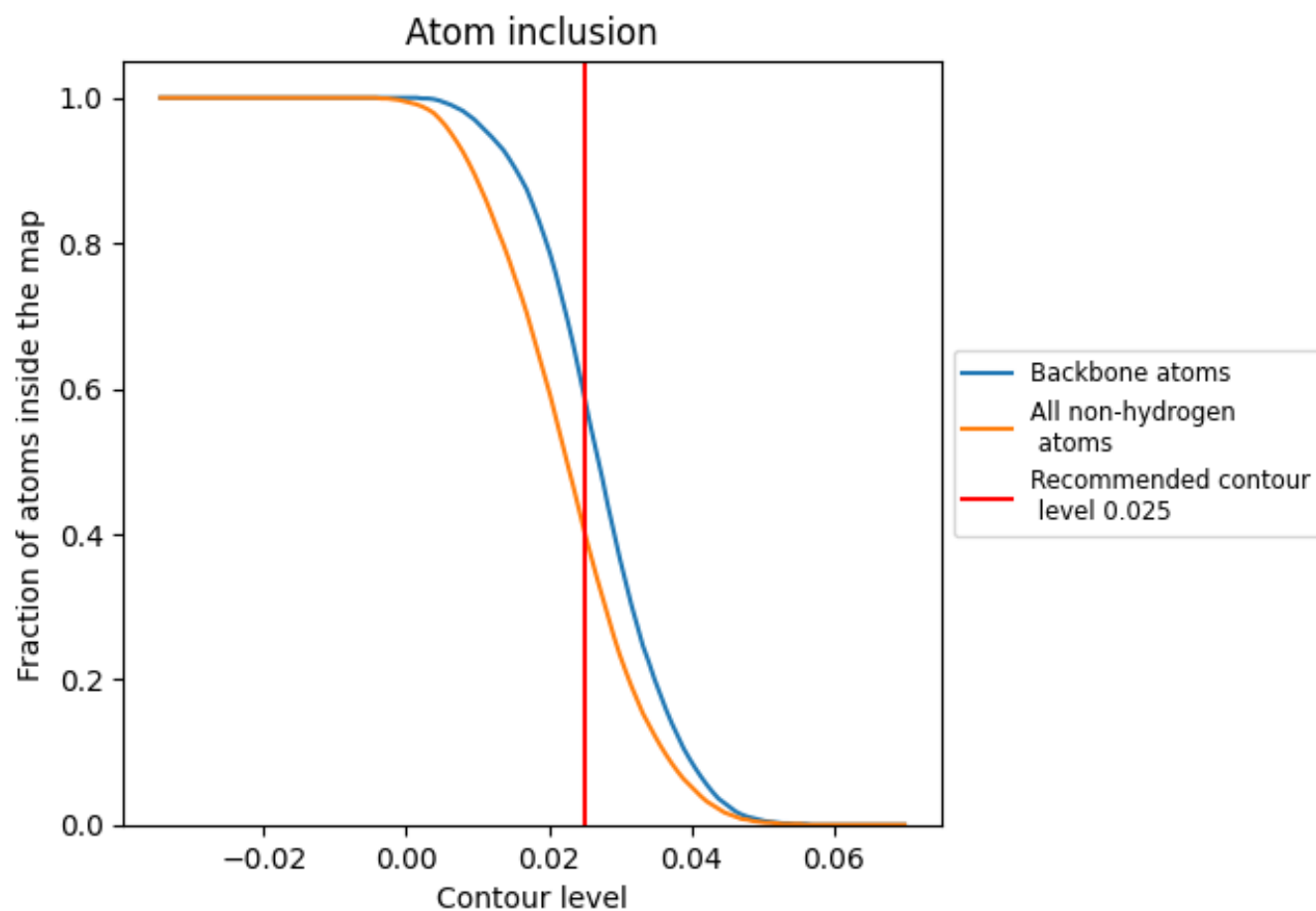
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 40% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4020	0.3150
A	0.3500	0.3180
B	0.4040	0.3140
E	0.4030	0.3140
F	0.3450	0.3230
G	0.4030	0.3140
H	0.3470	0.3230
I	0.4040	0.3140
J	0.3500	0.3190

1.0

0.0

<0.0