



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:12 PM JST

PDB ID : 6JII
EMDB ID : EMD-9834
Title : Structure of RyR2 (F/A/C/L-Ca²⁺/apo-CaM-M dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-21
Resolution : 4.20 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

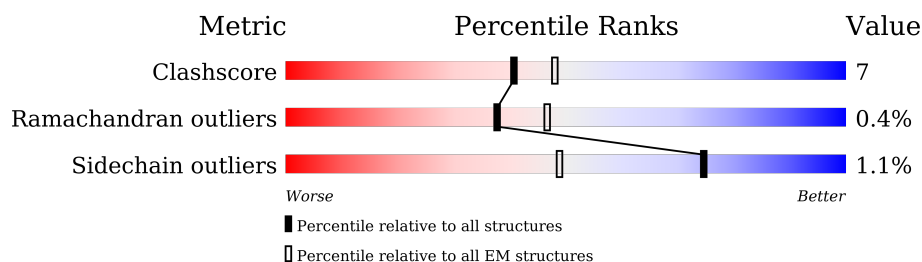
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	D	108	
1	G	108	
1	J	108	
2	B	4968	
2	E	4968	
2	H	4968	
2	K	4968	

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Mol	Chain	Length	Quality of chain
3	C	149	<div><div>32%</div><div><div></div><div>83%</div><div>9%</div><div>7%</div></div></div>
3	F	149	<div><div>32%</div><div><div></div><div>84%</div><div>8%</div><div>7%</div></div></div>
3	I	149	<div><div>32%</div><div><div></div><div>83%</div><div>9%</div><div>7%</div></div></div>
3	L	149	<div><div>32%</div><div><div></div><div>84%</div><div>8%</div><div>7%</div></div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 115028 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	A	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	J	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Ryr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	E	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	H	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	K	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	F	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	I	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	L	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

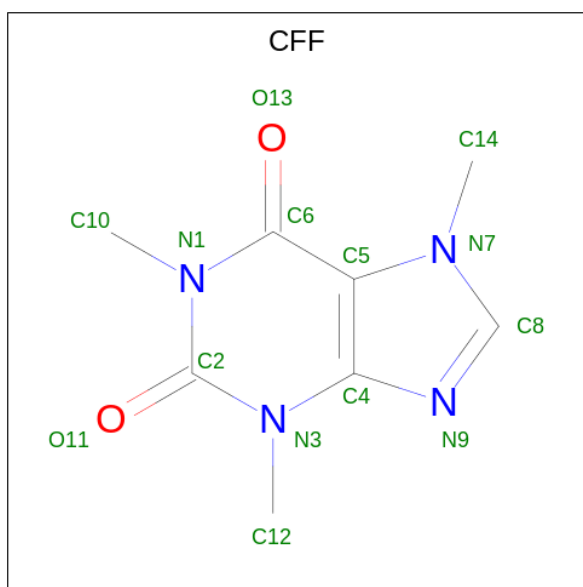
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Zn 1 1	0
4	E	1	Total Zn 1 1	0
4	H	1	Total Zn 1 1	0
4	K	1	Total Zn 1 1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

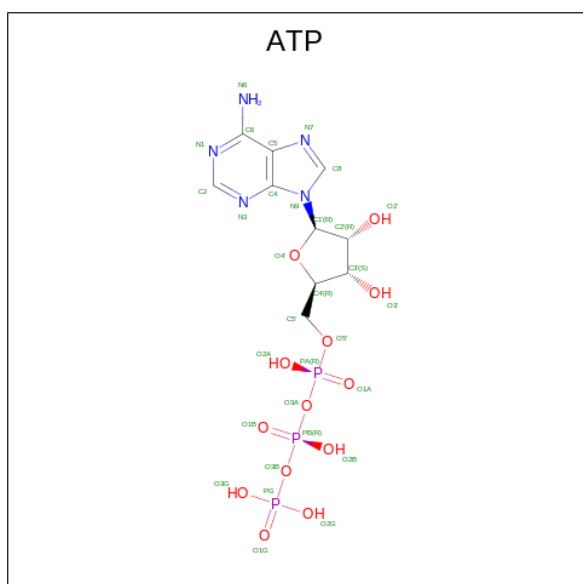
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Ca 1 1	0
5	E	1	Total Ca 1 1	0
5	H	1	Total Ca 1 1	0
5	K	1	Total Ca 1 1	0

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	H	1	Total	C	N	O	0
			14	8	4	2	
6	K	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).




Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total 31	C 10	N 5	O 13	P 3	0
7	E	1	Total 31	C 10	N 5	O 13	P 3	0
7	H	1	Total 31	C 10	N 5	O 13	P 3	0
7	K	1	Total 31	C 10	N 5	O 13	P 3	0

3 Residue-property plots


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

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

Chain A: 




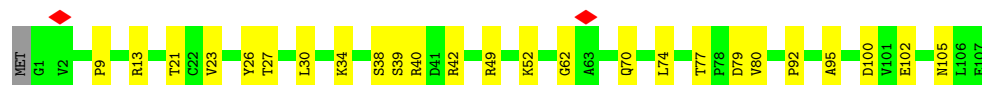
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D: 



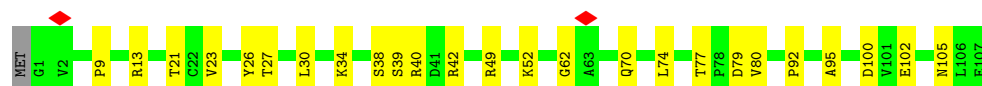
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



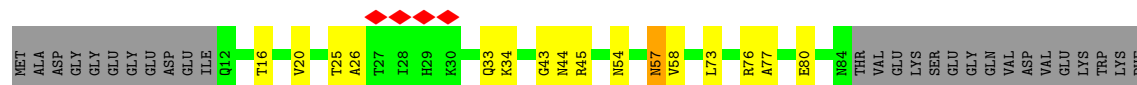
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



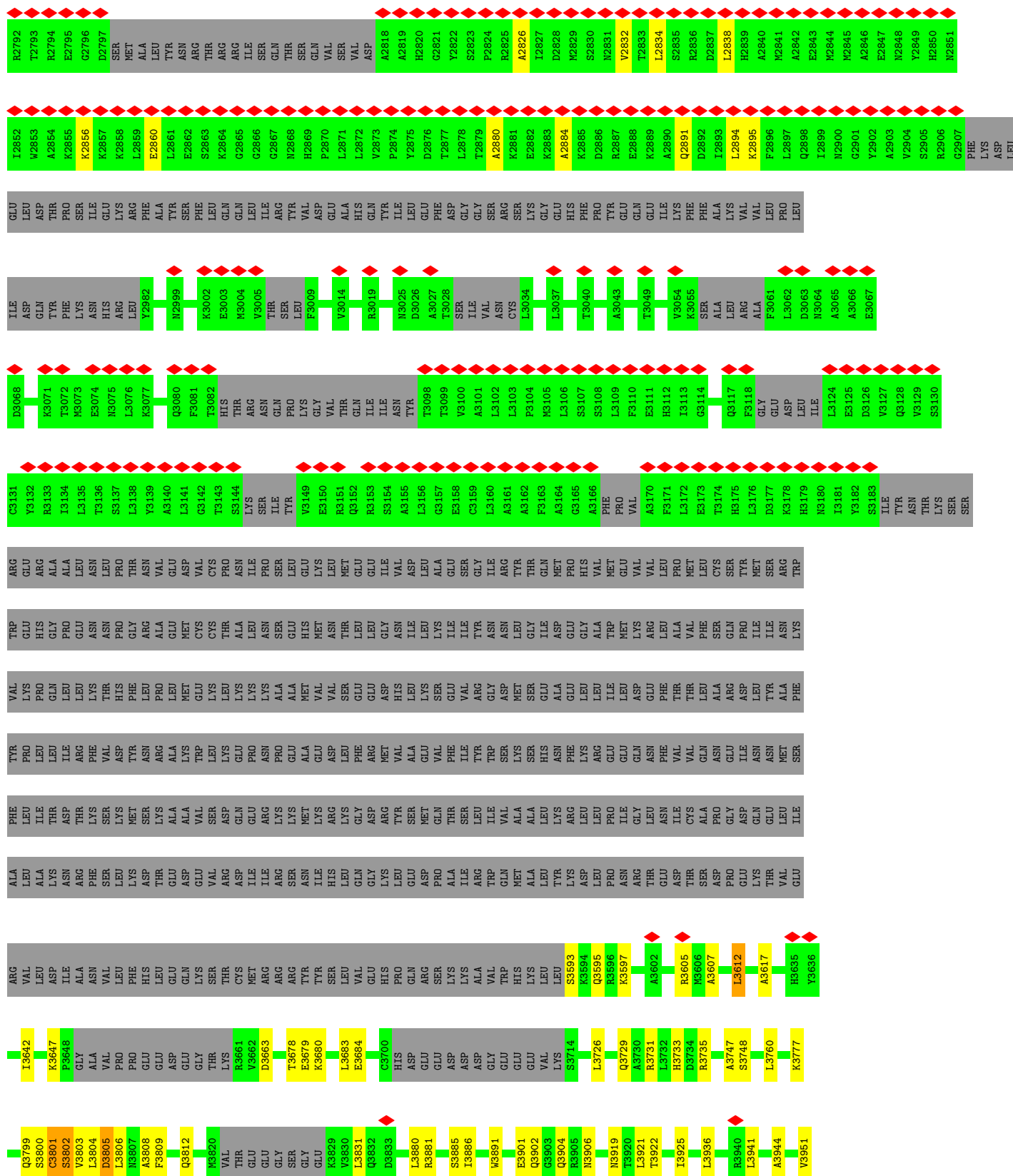
- Molecule 2: Ryr2

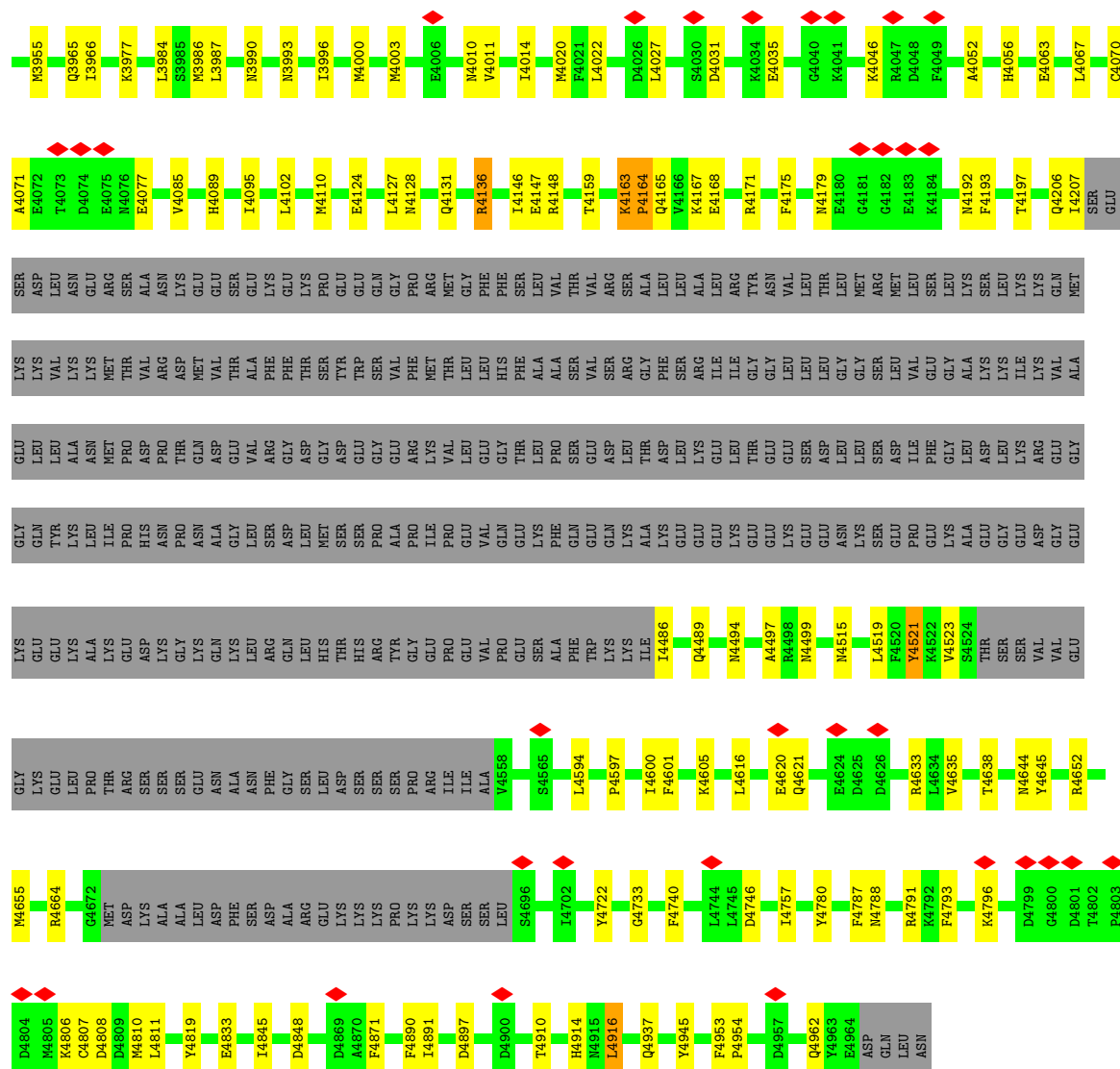
Chain B: 



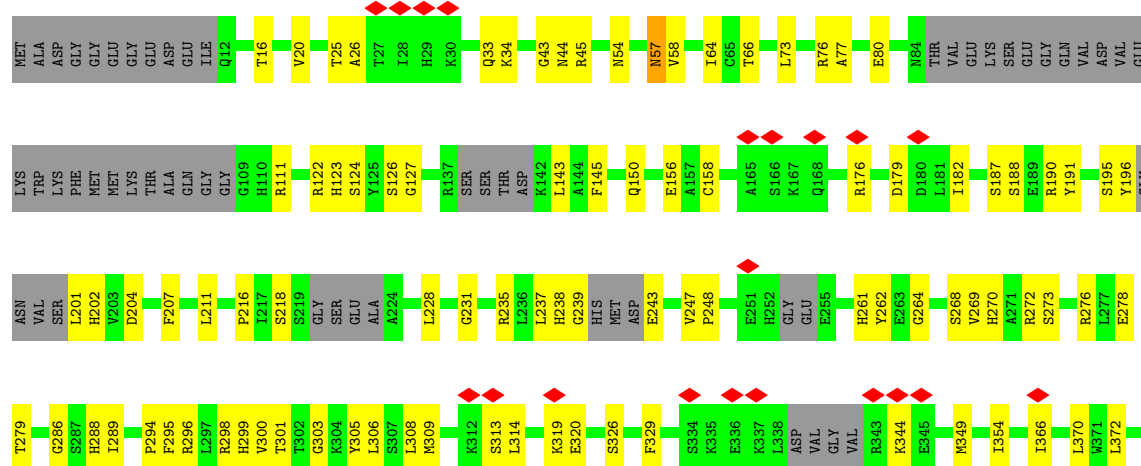








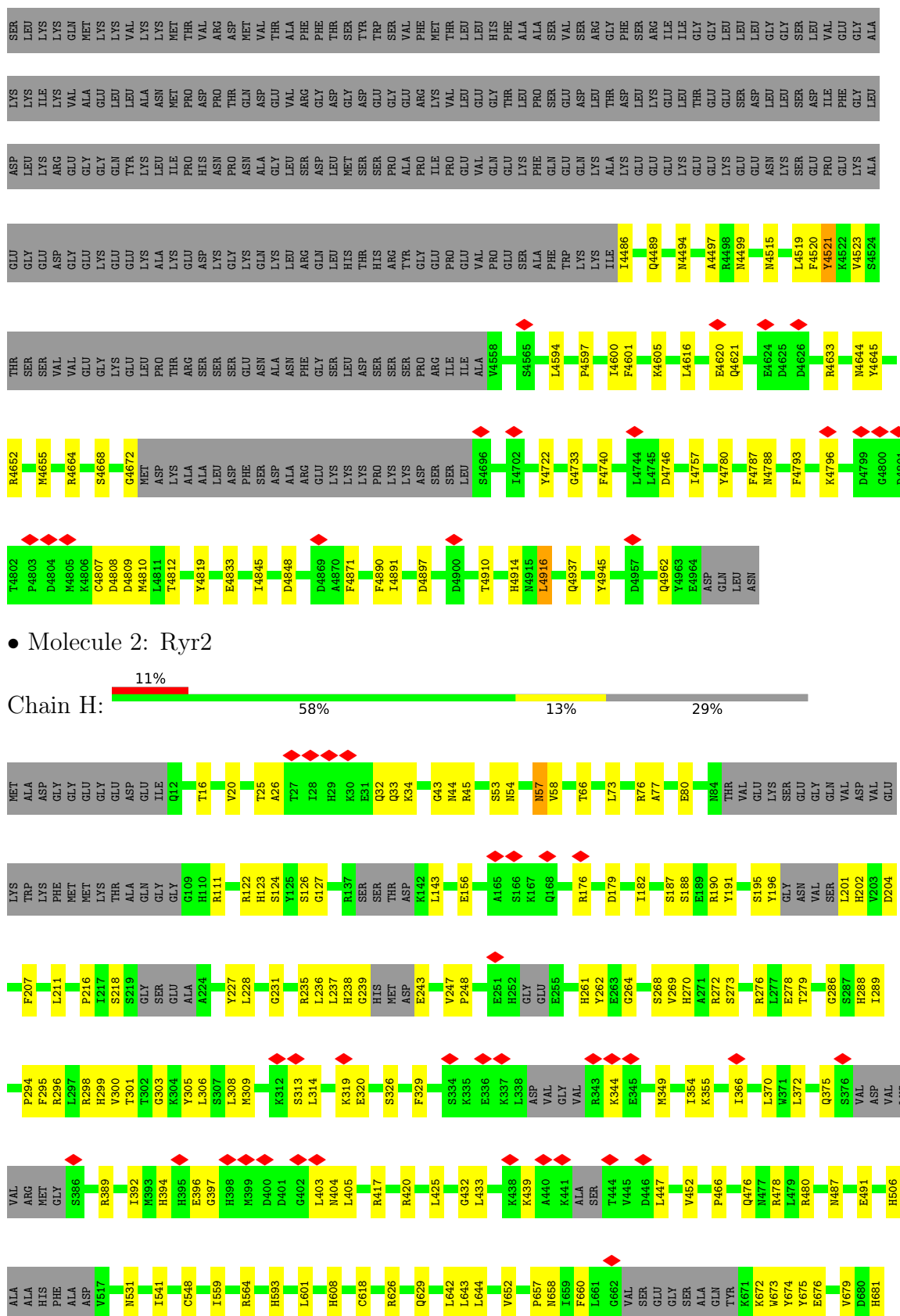
• Molecule 2: Ryr2





L1622	E1623	Q1626	P1627	M1628	S1629	H1631	Q1632	I1632	P1633	E1634	D1640	L1641	E1642	E1643	L1644	L1651	H1656	L1667	G1668	N1669	L1676	V1680	P1683	L1686	Y1687	H1688	I1689	Y1703	D1704	L1705	H1710	L1711	Y1714	I1726	T1733	K1734	L1738	F1739	P1740	L1748	G1752	L1753																	
S1754	T1755	S1756	L1757	R1758	P1759	R1760	M1761	Q1762	F1763	I1771	N1772	N1773	E1781	R1807	D1808	P1809	N1836	L1839	L1843	I1846	E1847	P1848	S1849	VAL	PHE	GLU	ALA	ALA	GLY	PRO	PRO	GLN	GLU	GLU	ILE	ASN	ASP	THR	LEU	LEU	ASN	PHE	LYS	ASP	ARG	GLU													
PRO	ALA	GLY	GLY	GLU	SER	LYS	GLY	GLY	LYS	PRO	LYS	GLU	G1893	L1894	Q1912	D1931	M1953	MET	SER	ALA	ALA	THR	SER	LYS	LYS	PHE	ARG	ALA	GLN	GLN	ILE	ASN	MET	LEU	LEU	ASN	PHE	LYS	ASP	LYS	GLU	LEU	GLY																
ASP	GLY	SER	LEU	ASP	GLY	ASN	ASP	L2024	L2024	R2029	S2032	Y2039	LEU	LYS	LYS	LYS	GLN	GLU	LYS	LEU	VAL	GLU	SER	THR	SER	GLY	T2058	Q2072	V2075	I2076	L2081	L2088	V2114	E2115	D2116	T2117	V2133	ARG	MET	GLY	LYS	E1986	C1989	D2013	V2155														
G2181	GLY	GLU	GLY	SER	LYS	GLY	ILE	THR	PHE	P2191	N2196	R2199	N2211	Q2212	K2213	L2241	N2252	E2253	L2254	L2275	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	TYR	PRO	ASP	THR	ILE	ASP	F2308	G2309	N2310	N2319	R2323	T2326	R2327	R2328																
P2329	E2330	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLY	ASN	G2343	E2349	L2352	K2353	L2354	ALA	GLU	ASP	PRO	SER	ARG	GLY	PRO	SER	GLY	SER	SER	PRO	PRO	THR	GLY	GLY	THR	ILE	HIS	MET	G2386	D2398	R2402	E2406																		
I2410	A2413	I2418	R2419	I2420	R2425	S2426	L2427	L2433	V2436	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	ALA	GLY	F2461	C2462	P2463	D2464	H2465	K2466	Y2477	GLY	ILE	GLU	V2481	L2488	I2489	VAL	G2492	L2503	ASP	THR											
ALA	ALA	LEU	SER	ALA	T2511	A2516	L2517	L2521	L2526	L2529	THR	ARG	CYS	ALA	PRO	LEU	PHE	A2537	V2553	TYR	ARG	LEU	SER	K2558	A2565	S2569	S2576	ILE	CYS	GLY	GLN	GLY	F2461	C2462	P2463	D2464	H2465	K2466	Y2477	GLY	ILE	GLU	V2481	L2488	I2489	VAL	G2492	L2503	ASP	THR									
A2634	S2635	L2653	SER	GLN	LYS	Y2658	K2664	L2665	A2666	C2669	V2673	A2674	G2675	P2678	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	TYR	SER	MET	MET	GLU	LYS	GLN	SER	SER	ASP	ASP	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717							
L2718	E2719	Y2720	F2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	D2731	K2732	N2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	Q2741	N2742	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	E2770	Y2771	Y2772	R2773	N2774	P2775	L2776	K2777		
E2778	S2779	L2780	K2781	T2782	M2783	L2784	A2785	W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	R2794	E2795	G2796	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ARG	ILE	ILE	GLN	THR	THR	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	I2827	D2828	M2829	S2830	N2831	Y2832	T2833	L2834	S2835	R2836	D2837						
L2838	H2839	A2840	M2841	A2842	E2843	M2844	M2845	E2846	E2847	N2848	Y2849	H2850	L2851	I2852	M2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	F2870	L2871	L2872	V2873	F2874	S2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	K2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897
Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	PHE	LYS	ASP	LEU	LEU	LEU	ASP	THR	PRO	SER	ILE	GLU	LYS	ARG	PHE	TYR	SER	PHE	LEU	GLN	LEU	ILE	ARG	TYR	VAL	ASP	GLU	ALA	HIS	GLN	TRP	ILE	LEU	GLU	PHE	ASP	GLY	SER	ARG	SER	LYS	GLY	HIS	PRO	TYR						

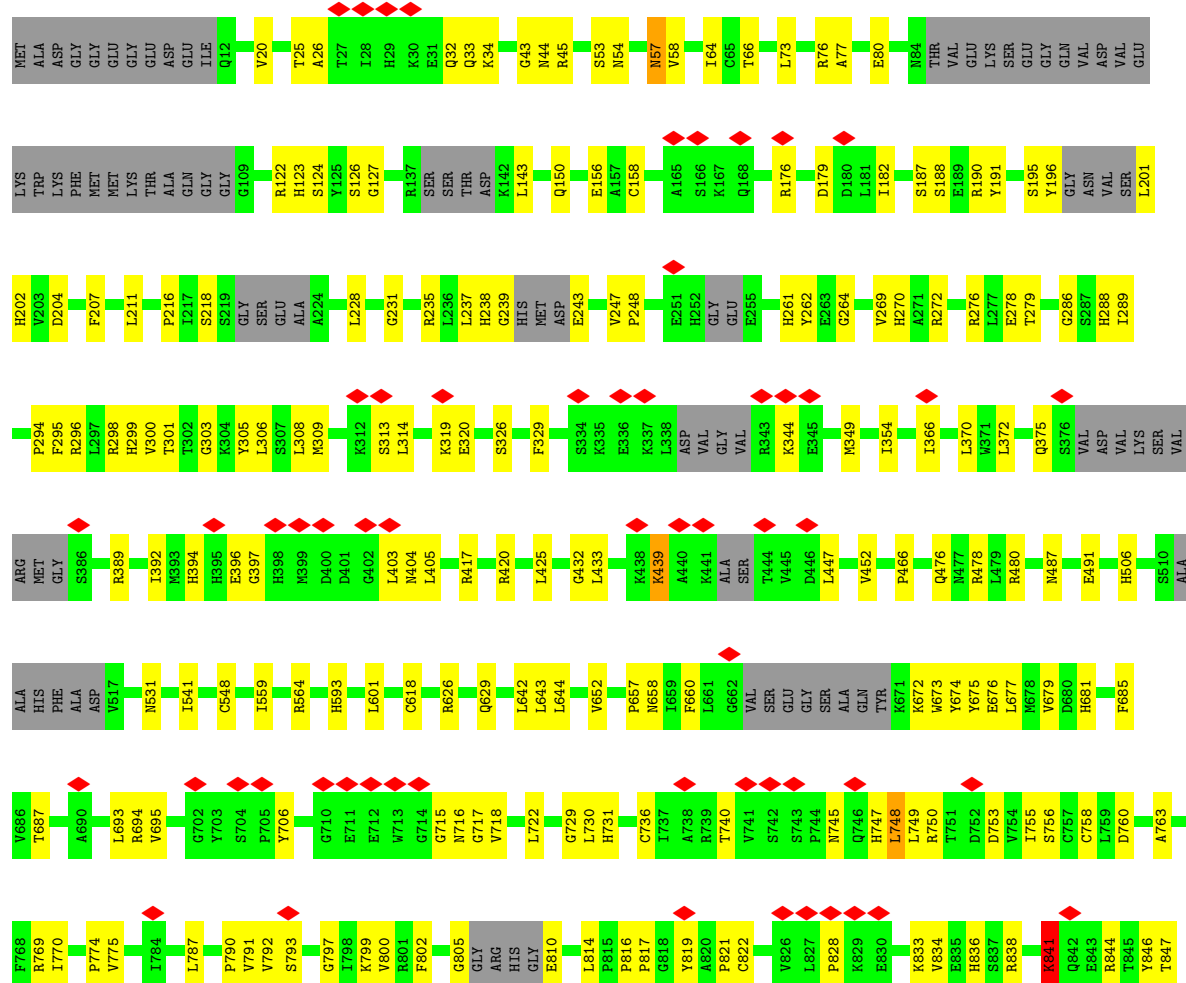






[illegible]

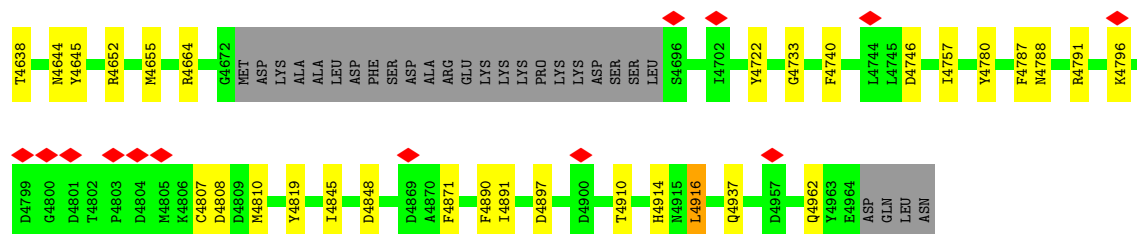




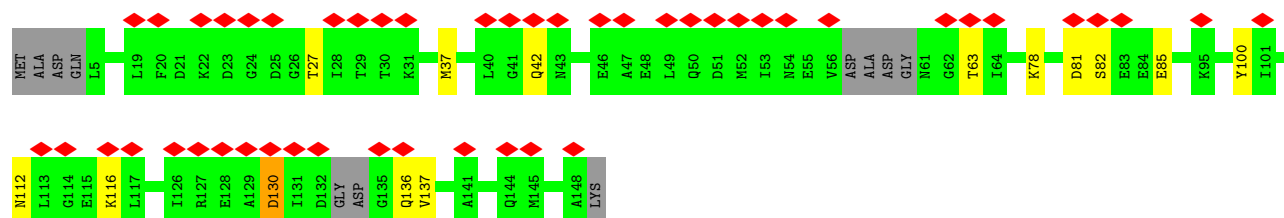
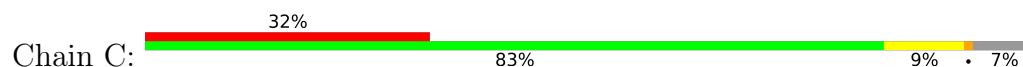


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GLY	GLY	GLY	ASP	LEU	LEU	ILE	ALA	L3124	L3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	TYR	V3149	E3150	R3151	Q3152	R3153	S3154	A3155	L3156	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	A3170	F3171	L3172	E3173	T3174	H3175	
THR	ALA	ALA	LEU	SER	ALA	T2511	A2516	L2517	L2521	L2526	L2529	THR	ARG	CYS	ALA	ALA	PRO	LEU	PHE	A2537	V2553	TYR	ARG	LEU	SER	ASN	VAL	VAL	GLU	PRO	SER	ASP	MET	ILE	S2569	S2576	ILE	CYS	GLY	GLN	LEU	R2582	V2601	GLU	HIS	ALA	K2605	T2612	Y2615	G2627	TRP	GLY	ASN	PHE	GLY						
ALA	A2634	S2635	L2653	GLN	LYS	Y2658	K2664	L2665	A2666	G2669	V2673	A2674	G2675	F2678	P2679	ASP	TYR	MET	GLU	SER	ASN	TYR	VAL	SER	MET	GLU	LYS	GLN	SER	ASP	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716													
K2717	L2718	E2719	Y2720	F2721	I2722	M2723	K2724	Y2725	A2726	E2727	H2728	S2729	D2731	K2732	M2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	N2742	I2743	Y2744	G2745	E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	I2771	Y2772	R2773	N2774	P2775	I2776				
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L2897	Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	LEU	THR	PRO	SER	ILE	GLU	LYS	ARG	PHE	ALA	TYR	SER	PHE	GLN	GLN	ARG	ILE	THR	VAL	ASP	GLU	ALA	HIS	THR	VAL	PHE	ASP	GLY	GLN	HIS	PHE	PRO														
TYR	GLU	GLN	GLY	ILE	LYS	PHE	PHE	ALA	LYS	VAL	VAL	PRO	LEU	LEU	LEU	ASP	GLN	TYR	PHE	LYS	ASN	HIS	ARG	LEU	Y2982	N2999	K3002	E3003	M3004	V3005	THR	SER	LEU	F3009	V3014	R3019	N3025	D3026	A3027	T3028	SER	ILE	VAL	ASN	CYS	L3034	L3037	T3040	A3043	T3049											
V3054	K3055	SR	ALA	LEU	ARG	ALA	F3061	L3062	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114				
Q3117	F3118	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114				
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN	TYR	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	E3111	H3112	T3113	G3114					
GLY	GLY	ASP	LEU	LEU	ILE	L3124	E3125	D3063	N3064	A3065	A3066	E3067	D3068	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3080	F3081	L3141	T3082	HIS	THR	ARG	ASN	GLN	ILE	PRO	LYS	GLY	VAL	THR	GLN	ILE	ILE	ASN																						

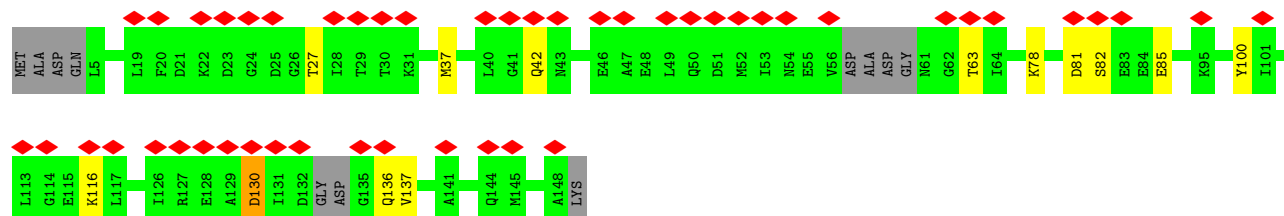
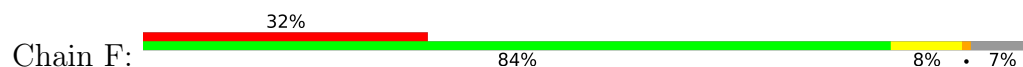




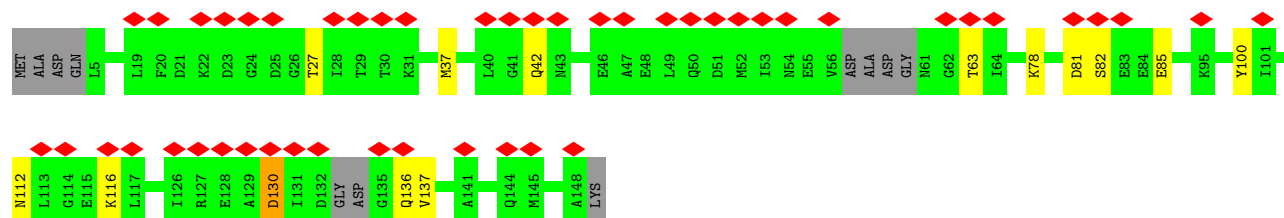
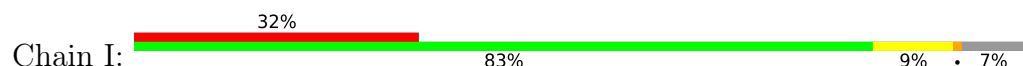
• Molecule 3: Calmodulin-1



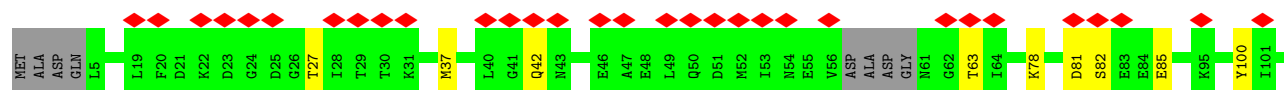
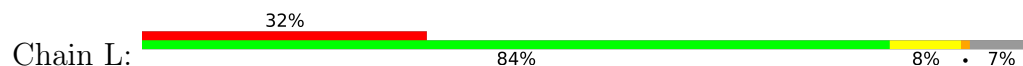
• Molecule 3: Calmodulin-1

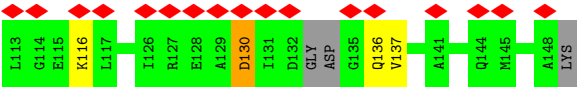


• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	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	0.096	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/835	0.56	0/1123
1	D	0.38	0/835	0.56	0/1123
1	G	0.38	0/835	0.56	0/1123
1	J	0.38	0/835	0.56	0/1123
2	B	0.41	0/27315	0.61	2/36936 (0.0%)
2	E	0.41	0/27315	0.61	2/36936 (0.0%)
2	H	0.41	0/27315	0.61	2/36936 (0.0%)
2	K	0.41	0/27315	0.61	2/36936 (0.0%)
3	C	0.33	0/1088	0.53	0/1459
3	F	0.33	0/1088	0.53	0/1459
3	I	0.33	0/1088	0.53	0/1459
3	L	0.33	0/1088	0.53	0/1459
All	All	0.41	0/116952	0.60	8/158072 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	24
2	E	0	24
2	H	0	24
2	K	0	24
All	All	0	96

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2517	LEU	CA-CB-CG	6.97	131.33	115.30
2	B	2517	LEU	CA-CB-CG	6.97	131.32	115.30
2	E	2517	LEU	CA-CB-CG	6.95	131.29	115.30
2	K	2517	LEU	CA-CB-CG	6.95	131.29	115.30
2	B	1738	LEU	CA-CB-CG	6.03	129.18	115.30
2	K	1738	LEU	CA-CB-CG	6.02	129.16	115.30
2	H	1738	LEU	CA-CB-CG	6.02	129.14	115.30
2	E	1738	LEU	CA-CB-CG	6.01	129.13	115.30

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1476	VAL	Peptide
2	B	1570	LEU	Peptide
2	B	1579	VAL	Peptide
2	B	1748	LEU	Peptide
2	B	1808	ASP	Peptide
2	B	1809	PRO	Peptide
2	B	1847	GLU	Peptide
2	B	2075	VAL	Peptide
2	B	2308	PHE	Peptide
2	B	3612	LEU	Peptide
2	B	3802	SER	Peptide
2	B	3805	ASP	Peptide
2	B	4070	CYS	Peptide
2	B	4163	LYS	Peptide
2	B	685	PHE	Peptide
2	B	729	GLY	Peptide
2	B	748	LEU	Peptide
2	B	791	VAL	Peptide
2	B	816	PRO	Peptide
2	B	817	PRO	Peptide
2	B	819	TYR	Peptide
2	B	838	ARG	Peptide
2	B	841	LYS	Peptide
2	B	854	THR	Peptide
2	E	1476	VAL	Peptide
2	E	1570	LEU	Peptide
2	E	1579	VAL	Peptide
2	E	1748	LEU	Peptide
2	E	1808	ASP	Peptide
2	E	1809	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	E	1847	GLU	Peptide
2	E	2075	VAL	Peptide
2	E	2308	PHE	Peptide
2	E	3612	LEU	Peptide
2	E	3802	SER	Peptide
2	E	3805	ASP	Peptide
2	E	4070	CYS	Peptide
2	E	4163	LYS	Peptide
2	E	685	PHE	Peptide
2	E	729	GLY	Peptide
2	E	748	LEU	Peptide
2	E	791	VAL	Peptide
2	E	816	PRO	Peptide
2	E	817	PRO	Peptide
2	E	819	TYR	Peptide
2	E	838	ARG	Peptide
2	E	841	LYS	Peptide
2	E	854	THR	Peptide
2	H	1476	VAL	Peptide
2	H	1570	LEU	Peptide
2	H	1579	VAL	Peptide
2	H	1748	LEU	Peptide
2	H	1808	ASP	Peptide
2	H	1809	PRO	Peptide
2	H	1847	GLU	Peptide
2	H	2075	VAL	Peptide
2	H	2308	PHE	Peptide
2	H	3612	LEU	Peptide
2	H	3802	SER	Peptide
2	H	3805	ASP	Peptide
2	H	4070	CYS	Peptide
2	H	4163	LYS	Peptide
2	H	685	PHE	Peptide
2	H	729	GLY	Peptide
2	H	748	LEU	Peptide
2	H	791	VAL	Peptide
2	H	816	PRO	Peptide
2	H	817	PRO	Peptide
2	H	819	TYR	Peptide
2	H	838	ARG	Peptide
2	H	841	LYS	Peptide
2	H	854	THR	Peptide

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Mol	Chain	Res	Type	Group
2	K	1476	VAL	Peptide
2	K	1570	LEU	Peptide
2	K	1579	VAL	Peptide
2	K	1748	LEU	Peptide
2	K	1808	ASP	Peptide
2	K	1809	PRO	Peptide
2	K	1847	GLU	Peptide
2	K	2075	VAL	Peptide
2	K	2308	PHE	Peptide
2	K	3612	LEU	Peptide
2	K	3802	SER	Peptide
2	K	3805	ASP	Peptide
2	K	4070	CYS	Peptide
2	K	4163	LYS	Peptide
2	K	685	PHE	Peptide
2	K	729	GLY	Peptide
2	K	748	LEU	Peptide
2	K	791	VAL	Peptide
2	K	816	PRO	Peptide
2	K	817	PRO	Peptide
2	K	819	TYR	Peptide
2	K	838	ARG	Peptide
2	K	841	LYS	Peptide
2	K	854	THR	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	819	0	824	13	0
1	D	819	0	824	13	0
1	G	819	0	824	14	0
1	J	819	0	824	14	0
2	B	26813	0	25339	450	0
2	E	26813	0	25339	437	0
2	H	26813	0	25339	441	0
2	K	26813	0	25339	439	0
3	C	1078	0	1032	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1078	0	1032	7	0
3	I	1078	0	1032	8	0
3	L	1078	0	1032	7	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	H	14	0	10	0	0
6	K	14	0	10	0	0
7	B	31	0	12	4	0
7	E	31	0	12	4	0
7	H	31	0	12	5	0
7	K	31	0	12	4	0
All	All	115028	0	108868	1669	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 7.

All (1669) 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:K:1986:GLU:N	2:K:1989:CYS:HG	1.54	1.05
2:B:1986:GLU:N	2:B:1989:CYS:HG	1.54	1.05
2:H:1986:GLU:N	2:H:1989:CYS:HG	1.55	1.03
2:B:4811:LEU:HD13	2:E:4519:LEU:HD21	1.39	1.03
2:E:1986:GLU:N	2:E:1989:CYS:HG	1.56	1.02
2:B:76:ARG:NH2	2:E:3806:LEU:HD11	1.77	1.00
2:E:76:ARG:NH2	2:H:3806:LEU:HD11	1.78	0.98
2:B:3806:LEU:HD11	2:K:76:ARG:NH2	1.77	0.98
2:H:76:ARG:NH2	2:K:3806:LEU:HD11	1.78	0.96
2:E:4848:ASP:CG	2:H:4819:TYR:HE1	1.67	0.96
2:B:207:PHE:CZ	2:E:2326:ILE:HG23	2.00	0.96
2:E:207:PHE:CZ	2:H:2326:ILE:HG23	2.00	0.96
2:B:4819:TYR:HE1	2:K:4848:ASP:CG	1.69	0.95
2:B:4848:ASP:CG	2:E:4819:TYR:HE1	1.68	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2326:ILE:HG23	2:K:207:PHE:CZ	2.01	0.95
2:H:4848:ASP:CG	2:K:4819:TYR:HE1	1.70	0.95
2:H:207:PHE:CZ	2:K:2326:ILE:HG23	2.01	0.93
2:B:1843:LEU:O	2:B:1847:GLU:HB2	1.71	0.91
2:E:76:ARG:HH21	2:H:3806:LEU:HD21	1.36	0.91
2:E:1843:LEU:O	2:E:1847:GLU:HB2	1.71	0.91
2:K:1843:LEU:O	2:K:1847:GLU:HB2	1.71	0.90
2:H:1843:LEU:O	2:H:1847:GLU:HB2	1.71	0.90
2:B:4796:LYS:NZ	2:B:4807:CYS:SG	2.45	0.90
2:H:143:LEU:HD11	2:K:2426:SER:O	1.72	0.90
2:E:143:LEU:HD11	2:H:2426:SER:O	1.72	0.89
2:H:76:ARG:HH21	2:K:3806:LEU:HD21	1.38	0.89
2:B:2426:SER:O	2:K:143:LEU:HD11	1.72	0.88
2:B:3806:LEU:HD21	2:K:76:ARG:HH21	1.38	0.88
2:B:76:ARG:HH21	2:E:3806:LEU:HD21	1.38	0.88
2:B:76:ARG:HH21	2:E:3806:LEU:HD11	1.36	0.87
2:B:143:LEU:HD11	2:E:2426:SER:O	1.73	0.86
2:E:76:ARG:HH21	2:H:3806:LEU:HD11	1.38	0.86
2:E:4848:ASP:CG	2:H:4819:TYR:CE1	2.48	0.86
2:B:4811:LEU:HD13	2:E:4519:LEU:CD2	2.04	0.85
2:B:4848:ASP:CG	2:E:4819:TYR:CE1	2.50	0.85
2:E:76:ARG:NH2	2:H:3806:LEU:HD21	1.91	0.84
2:H:76:ARG:NH2	2:K:3806:LEU:HD21	1.93	0.84
2:B:4819:TYR:CE1	2:K:4848:ASP:CG	2.50	0.84
2:H:4848:ASP:CG	2:K:4819:TYR:CE1	2.51	0.84
2:B:3806:LEU:HD21	2:K:76:ARG:NH2	1.92	0.84
2:B:3806:LEU:HD11	2:K:76:ARG:HH21	1.37	0.83
2:H:76:ARG:HH21	2:K:3806:LEU:HD11	1.37	0.83
2:B:76:ARG:NH2	2:E:3806:LEU:HD21	1.92	0.82
2:H:143:LEU:CD1	2:K:2426:SER:O	2.28	0.81
2:B:2426:SER:O	2:K:143:LEU:CD1	2.28	0.81
2:E:143:LEU:CD1	2:H:2426:SER:O	2.29	0.80
2:B:4848:ASP:OD2	2:E:4819:TYR:CE1	2.35	0.80
2:E:4848:ASP:OD2	2:H:4819:TYR:CE1	2.34	0.80
2:E:143:LEU:HD13	2:H:2426:SER:OG	1.81	0.80
2:B:4819:TYR:CE1	2:K:4848:ASP:OD2	2.35	0.80
2:B:143:LEU:CD1	2:E:2426:SER:O	2.29	0.80
2:H:4848:ASP:OD2	2:K:4819:TYR:CE1	2.36	0.79
2:H:143:LEU:HD13	2:K:2426:SER:OG	1.82	0.78
2:B:143:LEU:HD13	2:E:2426:SER:OG	1.84	0.78
2:B:2426:SER:OG	2:K:143:LEU:HD13	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4787:PHE:HD1	2:B:4808:ASP:O	1.66	0.78
2:K:123:HIS:HD2	2:K:126:SER:H	1.32	0.77
2:H:123:HIS:HD2	2:H:126:SER:H	1.32	0.77
2:B:2419:ARG:HD3	2:K:156:GLU:OE1	1.86	0.76
2:B:156:GLU:OE1	2:E:2419:ARG:HD3	1.85	0.75
2:H:156:GLU:OE1	2:K:2419:ARG:HD3	1.86	0.75
2:B:123:HIS:HD2	2:B:126:SER:H	1.32	0.74
2:B:143:LEU:CD1	2:E:2427:LEU:HD13	2.18	0.74
2:E:123:HIS:HD2	2:E:126:SER:H	1.32	0.74
2:E:156:GLU:OE1	2:H:2419:ARG:HD3	1.88	0.74
2:B:143:LEU:HD11	2:E:2427:LEU:HD13	1.69	0.74
2:B:2427:LEU:HD13	2:K:143:LEU:HD11	1.70	0.73
2:B:2427:LEU:HD13	2:K:143:LEU:CD1	2.19	0.73
2:H:143:LEU:CD1	2:K:2427:LEU:HD13	2.19	0.73
2:E:143:LEU:HD11	2:H:2427:LEU:HD13	1.71	0.72
2:H:143:LEU:HD11	2:K:2427:LEU:HD13	1.71	0.72
2:E:143:LEU:CD1	2:H:2427:LEU:HD13	2.20	0.72
2:B:4519:LEU:O	2:K:4810:MET:CB	2.39	0.71
2:E:207:PHE:CE2	2:H:2326:ILE:HG23	2.26	0.71
2:B:76:ARG:HH21	2:E:3806:LEU:CD1	2.04	0.70
3:F:100:TYR:HB3	3:F:136:GLN:HB3	1.72	0.70
2:H:4810:MET:CB	2:K:4519:LEU:O	2.38	0.70
2:B:207:PHE:CZ	2:E:2326:ILE:CG2	2.74	0.70
3:C:100:TYR:HB3	3:C:136:GLN:HB3	1.72	0.70
2:H:207:PHE:CZ	2:K:2326:ILE:CG2	2.75	0.70
2:E:207:PHE:CZ	2:H:2326:ILE:CG2	2.74	0.70
2:B:299:HIS:HE2	2:B:301:THR:HG1	1.40	0.69
2:H:1605:LYS:HD3	2:H:1606:VAL:HG23	1.74	0.69
3:L:100:TYR:HB3	3:L:136:GLN:HB3	1.72	0.69
2:E:299:HIS:HE2	2:E:301:THR:HG1	1.39	0.69
2:E:4848:ASP:CB	2:H:4819:TYR:HE1	2.04	0.69
3:I:100:TYR:HB3	3:I:136:GLN:HB3	1.72	0.69
2:B:2326:ILE:CG2	2:K:207:PHE:CZ	2.75	0.69
2:H:4046:LYS:H	2:H:4077:GLU:HB3	1.57	0.69
2:K:4046:LYS:H	2:K:4077:GLU:HB3	1.57	0.69
2:B:2326:ILE:HG23	2:K:207:PHE:CE2	2.27	0.69
2:B:207:PHE:CE2	2:E:2326:ILE:HG23	2.27	0.69
2:E:76:ARG:HH21	2:H:3806:LEU:CD1	2.06	0.69
2:E:76:ARG:HH21	2:H:3806:LEU:CD2	2.06	0.69
2:K:1605:LYS:HD3	2:K:1606:VAL:HG23	1.74	0.69
2:H:207:PHE:CE2	2:K:2326:ILE:HG23	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1089:ARG:HE	2:B:1600:PRO:HB3	1.59	0.68
2:B:3806:LEU:CD1	2:K:76:ARG:HH21	2.05	0.68
2:B:1605:LYS:HD3	2:B:1606:VAL:HG23	1.74	0.68
2:B:2327:ARG:HH21	2:K:191:TYR:HE2	1.42	0.68
2:E:4046:LYS:H	2:E:4077:GLU:HB3	1.57	0.68
2:B:3806:LEU:CD2	2:K:76:ARG:HH21	2.07	0.68
2:B:4046:LYS:H	2:B:4077:GLU:HB3	1.57	0.68
2:E:1089:ARG:HE	2:E:1600:PRO:HB3	1.59	0.68
2:E:1605:LYS:HD3	2:E:1606:VAL:HG23	1.74	0.68
2:E:4810:MET:CB	2:H:4519:LEU:O	2.42	0.68
2:H:191:TYR:HE2	2:K:2327:ARG:HH21	1.42	0.68
2:H:4848:ASP:CB	2:K:4819:TYR:HE1	2.06	0.68
2:K:657:PRO:HA	2:K:834:VAL:HA	1.76	0.67
2:B:4848:ASP:CB	2:E:4819:TYR:HE1	2.07	0.67
2:H:1089:ARG:HE	2:H:1600:PRO:HB3	1.59	0.67
2:K:1089:ARG:HE	2:K:1600:PRO:HB3	1.59	0.67
2:B:4819:TYR:HE1	2:K:4848:ASP:CB	2.07	0.67
2:B:850:LEU:HB3	2:B:1207:LEU:HD11	1.77	0.67
2:H:657:PRO:HA	2:H:834:VAL:HA	1.76	0.67
2:K:3951:VAL:O	2:K:3955:MET:HB2	1.95	0.67
2:E:191:TYR:HE2	2:H:2327:ARG:HH21	1.42	0.67
2:B:3951:VAL:O	2:B:3955:MET:HB2	1.95	0.66
2:E:758:CYS:HB3	2:E:767:SER:HB2	1.78	0.66
2:H:758:CYS:HB3	2:H:767:SER:HB2	1.78	0.66
2:E:3951:VAL:O	2:E:3955:MET:HB2	1.95	0.66
2:H:3951:VAL:O	2:H:3955:MET:HB2	1.96	0.66
2:E:657:PRO:HA	2:E:834:VAL:HA	1.76	0.66
2:H:76:ARG:HH21	2:K:3806:LEU:CD2	2.08	0.66
2:B:191:TYR:HE2	2:E:2327:ARG:HH21	1.42	0.66
2:H:76:ARG:HH21	2:K:3806:LEU:CD1	2.06	0.66
2:B:207:PHE:CE1	2:E:2326:ILE:CG2	2.79	0.66
2:E:850:LEU:HB3	2:E:1207:LEU:HD11	1.77	0.66
2:B:657:PRO:HA	2:B:834:VAL:HA	1.76	0.65
2:K:758:CYS:HB3	2:K:767:SER:HB2	1.78	0.65
2:B:758:CYS:HB3	2:B:767:SER:HB2	1.78	0.65
2:H:207:PHE:CE1	2:K:2326:ILE:CG2	2.80	0.65
2:K:850:LEU:HB3	2:K:1207:LEU:HD11	1.77	0.65
2:B:2326:ILE:CG2	2:K:207:PHE:CE1	2.79	0.65
2:E:207:PHE:CE1	2:H:2326:ILE:CG2	2.80	0.65
2:K:797:GLY:HA2	2:K:1622:LEU:HA	1.79	0.65
2:B:76:ARG:HH21	2:E:3806:LEU:CD2	2.07	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:LEU:HB2	2:B:1213:GLY:H	1.62	0.65
2:H:850:LEU:HB3	2:H:1207:LEU:HD11	1.77	0.65
2:H:299:HIS:HE2	2:H:301:THR:HG1	1.39	0.64
2:B:797:GLY:HA2	2:B:1622:LEU:HA	1.79	0.64
2:E:26:ALA:HB3	2:E:33:GLN:HB3	1.80	0.64
2:H:26:ALA:HB3	2:H:33:GLN:HB3	1.80	0.64
2:H:1303:ARG:HH12	2:H:1595:LEU:HB2	1.62	0.64
2:K:1303:ARG:HH12	2:K:1595:LEU:HB2	1.62	0.64
2:E:1303:ARG:HH12	2:E:1595:LEU:HB2	1.62	0.63
2:E:4796:LYS:NZ	2:E:4807:CYS:SG	2.71	0.63
2:K:26:ALA:HB3	2:K:33:GLN:HB3	1.80	0.63
2:E:850:LEU:HB2	2:E:1213:GLY:H	1.62	0.63
2:K:4796:LYS:NZ	2:K:4807:CYS:SG	2.71	0.63
2:B:26:ALA:HB3	2:B:33:GLN:HB3	1.80	0.63
2:H:797:GLY:HA2	2:H:1622:LEU:HA	1.79	0.63
2:H:4146:ILE:HD12	2:H:4962:GLN:HB2	1.81	0.63
2:H:4796:LYS:NZ	2:H:4807:CYS:SG	2.71	0.63
2:H:850:LEU:HB2	2:H:1213:GLY:H	1.62	0.63
2:K:850:LEU:HB2	2:K:1213:GLY:H	1.62	0.63
2:B:1303:ARG:HH12	2:B:1595:LEU:HB2	1.62	0.63
2:E:247:VAL:O	2:E:272:ARG:NH1	2.30	0.63
2:E:797:GLY:HA2	2:E:1622:LEU:HA	1.79	0.63
2:E:4146:ILE:HD12	2:E:4962:GLN:HB2	1.81	0.63
2:H:1299:ILE:HG12	2:H:1546:GLN:HG2	1.81	0.63
2:K:299:HIS:HE2	2:K:301:THR:HG1	1.40	0.63
2:B:1299:ILE:HG12	2:B:1546:GLN:HG2	1.81	0.62
2:K:4146:ILE:HD12	2:K:4962:GLN:HB2	1.81	0.62
2:B:3806:LEU:CD1	2:K:76:ARG:NH2	2.59	0.62
1:G:77:THR:HG22	1:G:79:ASP:H	1.63	0.62
2:K:476:GLN:HE22	2:K:3678:THR:HG22	1.65	0.62
2:B:247:VAL:O	2:B:272:ARG:NH1	2.30	0.62
2:B:80:GLU:HG3	2:E:3891:TRP:HZ3	1.63	0.62
2:B:4811:LEU:HD22	2:E:4520:PHE:CE1	2.35	0.62
1:J:77:THR:HG22	1:J:79:ASP:H	1.63	0.62
2:B:476:GLN:HE22	2:B:3678:THR:HG22	1.65	0.62
1:D:77:THR:HG22	1:D:79:ASP:H	1.63	0.62
2:B:143:LEU:HD12	2:E:2427:LEU:CD1	2.30	0.62
2:B:4146:ILE:HD12	2:B:4962:GLN:HB2	1.81	0.62
2:B:4808:ASP:OD2	2:E:4523:VAL:HG21	1.99	0.62
2:E:80:GLU:HG3	2:H:3891:TRP:HZ3	1.63	0.62
1:A:77:THR:HG22	1:A:79:ASP:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:476:GLN:HE22	2:E:3678:THR:HG22	1.65	0.62
2:H:76:ARG:NH2	2:K:3806:LEU:CD1	2.60	0.61
2:H:476:GLN:HE22	2:H:3678:THR:HG22	1.65	0.61
2:K:4020:MET:CE	2:K:4063:GLU:HB3	2.31	0.61
2:K:4031:ASP:HB3	2:K:4035:GLU:HB2	1.83	0.61
2:B:3891:TRP:HZ3	2:K:80:GLU:HG3	1.64	0.61
2:E:1299:ILE:HG12	2:E:1546:GLN:HG2	1.81	0.61
2:H:4031:ASP:HB3	2:H:4035:GLU:HB2	1.83	0.61
2:K:247:VAL:O	2:K:272:ARG:NH1	2.30	0.61
2:B:694:ARG:HB2	2:B:793:SER:HB2	1.83	0.61
2:B:1114:ARG:HB3	2:B:1128:LEU:HD22	1.83	0.61
2:B:4020:MET:CE	2:B:4063:GLU:HB3	2.30	0.61
2:K:195:SER:HB3	2:K:202:HIS:HB2	1.82	0.61
2:E:694:ARG:HB2	2:E:793:SER:HB2	1.83	0.61
2:E:4020:MET:CE	2:E:4063:GLU:HB3	2.30	0.61
2:K:930:ASN:HA	2:K:933:LEU:HB2	1.83	0.61
2:B:4810:MET:CB	2:E:4519:LEU:O	2.49	0.61
2:E:4022:LEU:HA	2:E:4089:HIS:HE1	1.66	0.61
2:H:195:SER:HB3	2:H:202:HIS:HB2	1.82	0.61
2:H:80:GLU:HG3	2:K:3891:TRP:HZ3	1.65	0.60
2:K:1114:ARG:HB3	2:K:1128:LEU:HD22	1.83	0.60
2:B:4022:LEU:HA	2:B:4089:HIS:HE1	1.66	0.60
2:B:4031:ASP:HB3	2:B:4035:GLU:HB2	1.83	0.60
2:K:1272:ARG:NH1	2:K:1587:HIS:O	2.34	0.60
2:E:4031:ASP:HB3	2:E:4035:GLU:HB2	1.83	0.60
2:H:694:ARG:HB2	2:H:793:SER:HB2	1.83	0.60
2:H:930:ASN:HA	2:H:933:LEU:HB2	1.83	0.60
2:B:195:SER:HB3	2:B:202:HIS:HB2	1.82	0.60
2:E:1114:ARG:HB3	2:E:1128:LEU:HD22	1.83	0.60
2:E:1272:ARG:NH1	2:E:1587:HIS:O	2.34	0.60
2:H:247:VAL:O	2:H:272:ARG:NH1	2.30	0.60
2:H:4020:MET:CE	2:H:4063:GLU:HB3	2.31	0.60
2:K:1299:ILE:HG12	2:K:1546:GLN:HG2	1.81	0.60
2:H:1272:ARG:NH1	2:H:1587:HIS:O	2.34	0.60
2:K:1249:MET:H	2:K:1603:PHE:HB2	1.67	0.60
2:B:2427:LEU:CD1	2:K:143:LEU:HD12	2.31	0.60
2:E:195:SER:HB3	2:E:202:HIS:HB2	1.82	0.60
2:E:3663:ASP:OD2	2:E:3735:ARG:NH2	2.35	0.60
2:H:1249:MET:H	2:H:1603:PHE:HB2	1.67	0.60
2:B:3663:ASP:OD2	2:B:3735:ARG:NH2	2.35	0.60
2:E:674:TYR:HB3	2:E:821:PRO:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3663:ASP:OD2	2:K:3735:ARG:NH2	2.35	0.60
2:H:3663:ASP:OD2	2:H:3735:ARG:NH2	2.35	0.60
2:K:4022:LEU:HA	2:K:4089:HIS:HE1	1.66	0.60
2:E:143:LEU:HD12	2:H:2427:LEU:CD1	2.32	0.60
2:H:191:TYR:CE2	2:K:2327:ARG:NH2	2.70	0.60
2:B:1272:ARG:NH1	2:B:1587:HIS:O	2.34	0.60
2:K:694:ARG:HB2	2:K:793:SER:HB2	1.83	0.60
2:B:930:ASN:HA	2:B:933:LEU:HB2	1.83	0.59
2:H:674:TYR:HB3	2:H:821:PRO:HA	1.84	0.59
2:E:1249:MET:H	2:E:1603:PHE:HB2	1.67	0.59
2:H:143:LEU:HD12	2:K:2427:LEU:CD1	2.32	0.59
2:H:1114:ARG:HB3	2:H:1128:LEU:HD22	1.83	0.59
2:H:4022:LEU:HA	2:H:4089:HIS:HE1	1.66	0.59
2:B:1171:HIS:ND1	2:B:1195:PHE:O	2.36	0.59
2:B:2327:ARG:NH2	2:K:191:TYR:CE2	2.70	0.59
2:E:191:TYR:CE2	2:H:2327:ARG:NH2	2.71	0.59
2:B:674:TYR:HB3	2:B:821:PRO:HA	1.84	0.59
2:B:1249:MET:H	2:B:1603:PHE:HB2	1.67	0.59
2:K:1090:ALA:HA	2:K:1249:MET:HG2	1.85	0.59
2:B:626:ARG:HD2	2:B:1669:ASN:HD21	1.68	0.59
2:B:1090:ALA:HA	2:B:1249:MET:HG2	1.85	0.59
2:E:930:ASN:HA	2:E:933:LEU:HB2	1.83	0.59
2:K:674:TYR:HB3	2:K:821:PRO:HA	1.84	0.59
2:K:3799:GLN:O	2:K:3881:ARG:NH1	2.35	0.59
2:B:76:ARG:NH2	2:E:3806:LEU:CD1	2.58	0.59
2:B:4791:ARG:HB3	2:B:4808:ASP:HB2	1.83	0.59
2:E:1090:ALA:HA	2:E:1249:MET:HG2	1.85	0.59
2:H:1754:SER:HB2	2:H:1758:ARG:HH12	1.68	0.58
2:B:3799:GLN:O	2:B:3881:ARG:NH1	2.35	0.58
2:E:76:ARG:NH2	2:H:3806:LEU:CD1	2.59	0.58
2:H:1090:ALA:HA	2:H:1249:MET:HG2	1.85	0.58
2:K:25:THR:HG22	2:K:34:LYS:HG2	1.85	0.58
2:B:25:THR:HG22	2:B:34:LYS:HG2	1.85	0.58
2:E:1154:ARG:HH21	2:E:1177:LEU:HD23	1.68	0.58
2:K:1171:HIS:ND1	2:K:1195:PHE:O	2.36	0.58
2:K:1754:SER:HB2	2:K:1758:ARG:HH12	1.69	0.58
2:K:2770:GLU:HA	2:K:2773:ARG:HB2	1.85	0.58
2:B:4124:GLU:HG3	2:B:4128:ASN:HD21	1.69	0.58
2:E:480:ARG:NH2	2:E:3679:GLU:OE2	2.36	0.58
2:H:25:THR:HG22	2:H:34:LYS:HG2	1.85	0.58
2:B:191:TYR:CE2	2:E:2327:ARG:NH2	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:THR:HG1	1:D:49:ARG:HH21	1.48	0.58
2:H:4124:GLU:HG3	2:H:4128:ASN:HD21	1.69	0.58
2:B:1754:SER:HB2	2:B:1758:ARG:HH12	1.69	0.58
2:E:1754:SER:HB2	2:E:1758:ARG:HH12	1.69	0.58
2:E:2770:GLU:HA	2:E:2773:ARG:HB2	1.85	0.58
2:H:2770:GLU:HA	2:H:2773:ARG:HB2	1.85	0.58
2:K:1154:ARG:HH21	2:K:1177:LEU:HD23	1.68	0.58
2:E:943:LEU:HB3	2:E:950:VAL:HG21	1.86	0.58
2:E:4124:GLU:HG3	2:E:4128:ASN:HD21	1.69	0.58
2:H:1154:ARG:HH21	2:H:1177:LEU:HD23	1.68	0.58
2:H:270:HIS:ND1	2:H:491:GLU:OE1	2.37	0.58
2:H:480:ARG:NH2	2:H:3679:GLU:OE2	2.36	0.58
2:K:480:ARG:NH2	2:K:3679:GLU:OE2	2.36	0.58
2:K:626:ARG:HD2	2:K:1669:ASN:HD21	1.68	0.58
2:E:626:ARG:HD2	2:E:1669:ASN:HD21	1.68	0.58
2:K:4124:GLU:HG3	2:K:4128:ASN:HD21	1.69	0.58
2:K:706:TYR:OH	2:K:1086:ARG:NH2	2.37	0.58
2:B:270:HIS:ND1	2:B:491:GLU:OE1	2.37	0.57
2:B:943:LEU:HB3	2:B:950:VAL:HG21	1.86	0.57
2:B:2275:LEU:H	2:B:2293:PRO:HD3	1.69	0.57
2:E:3799:GLN:O	2:E:3881:ARG:NH1	2.35	0.57
2:E:3805:ASP:OD2	2:E:3809:PHE:N	2.37	0.57
2:H:943:LEU:HB3	2:H:950:VAL:HG11	1.86	0.57
2:K:248:PRO:HD3	2:K:261:HIS:HD2	1.69	0.57
2:B:1146:HIS:HB2	2:B:1192:PHE:HE1	1.70	0.57
2:E:270:HIS:ND1	2:E:491:GLU:OE1	2.37	0.57
2:E:1171:HIS:ND1	2:E:1195:PHE:O	2.36	0.57
2:H:626:ARG:HD2	2:H:1669:ASN:HD21	1.68	0.57
2:K:300:VAL:O	2:K:420:ARG:NH2	2.37	0.57
2:B:2770:GLU:HA	2:B:2773:ARG:HB2	1.85	0.57
2:K:375:GLN:HE21	2:K:392:ILE:HD13	1.69	0.57
2:E:706:TYR:OH	2:E:1086:ARG:NH2	2.37	0.57
2:H:2436:VAL:O	2:H:2466:LYS:NZ	2.38	0.57
2:E:1628:MET:HB2	2:E:1687:TYR:HE2	1.70	0.57
2:H:300:VAL:O	2:H:420:ARG:NH2	2.37	0.57
2:B:300:VAL:O	2:B:420:ARG:NH2	2.37	0.57
2:B:375:GLN:HE21	2:B:392:ILE:HD13	1.69	0.57
2:E:248:PRO:HD3	2:E:261:HIS:HD2	1.69	0.57
2:E:375:GLN:HE21	2:E:392:ILE:HD13	1.69	0.57
2:E:2436:VAL:O	2:E:2466:LYS:NZ	2.38	0.57
2:B:2436:VAL:O	2:B:2466:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:867:VAL:O	2:E:1002:ASN:ND2	2.38	0.57
2:H:1171:HIS:ND1	2:H:1195:PHE:O	2.36	0.57
2:H:1628:MET:HB2	2:H:1687:TYR:HE2	1.70	0.57
2:H:3799:GLN:O	2:H:3881:ARG:NH1	2.35	0.57
2:K:1146:HIS:HB2	2:K:1192:PHE:HE1	1.70	0.57
2:B:248:PRO:HD3	2:B:261:HIS:HD2	1.69	0.57
2:E:25:THR:HG22	2:E:34:LYS:HG2	1.85	0.57
2:E:2275:LEU:H	2:E:2293:PRO:HD3	1.69	0.57
2:K:270:HIS:ND1	2:K:491:GLU:OE1	2.37	0.57
2:K:3805:ASP:OD2	2:K:3809:PHE:N	2.37	0.57
2:E:300:VAL:O	2:E:420:ARG:NH2	2.37	0.57
2:E:954:ASP:HB2	2:E:1061:GLY:HA3	1.87	0.57
2:H:706:TYR:OH	2:H:1086:ARG:NH2	2.37	0.57
2:K:4192:ASN:OD1	2:K:4605:LYS:NZ	2.29	0.57
2:K:4890:PHE:H	7:K:6003:ATP:HN61	1.53	0.57
2:B:278:GLU:HB2	2:B:296:ARG:HB2	1.87	0.56
2:B:480:ARG:NH2	2:B:3679:GLU:OE2	2.36	0.56
2:B:1154:ARG:HH21	2:B:1177:LEU:HD23	1.68	0.56
2:H:375:GLN:HE21	2:H:392:ILE:HD13	1.69	0.56
1:J:23:VAL:HB	1:J:105:ASN:H	1.70	0.56
2:B:867:VAL:O	2:B:1002:ASN:ND2	2.38	0.56
2:B:3901:GLU:OE1	2:B:3902:GLN:NE2	2.39	0.56
2:B:3919:ASN:O	2:B:3922:THR:OG1	2.23	0.56
2:H:3805:ASP:OD2	2:H:3809:PHE:N	2.37	0.56
2:K:1628:MET:HB2	2:K:1687:TYR:HE2	1.70	0.56
2:K:2275:LEU:H	2:K:2293:PRO:HD3	1.69	0.56
2:B:954:ASP:HB2	2:B:1061:GLY:HA3	1.87	0.56
2:B:3805:ASP:OD2	2:B:3809:PHE:N	2.37	0.56
2:E:1146:HIS:HB2	2:E:1192:PHE:HE1	1.70	0.56
2:E:2834:LEU:HD11	2:E:2894:LEU:HB3	1.88	0.56
2:E:4159:THR:O	2:E:4163:LYS:NZ	2.37	0.56
1:G:23:VAL:HB	1:G:105:ASN:H	1.70	0.56
2:H:248:PRO:HD3	2:H:261:HIS:HD2	1.69	0.56
2:H:867:VAL:O	2:H:1002:ASN:ND2	2.38	0.56
2:H:4890:PHE:H	7:H:6003:ATP:HN61	1.53	0.56
2:K:867:VAL:O	2:K:1002:ASN:ND2	2.38	0.56
2:K:3901:GLU:OE1	2:K:3902:GLN:NE2	2.39	0.56
2:B:2464:ASP:OD1	2:B:2464:ASP:N	2.36	0.56
2:E:2521:LEU:HD22	2:E:2565:ALA:HB2	1.88	0.56
2:E:2707:VAL:HG21	2:E:2786:TRP:HE1	1.71	0.56
2:H:954:ASP:HB2	2:H:1061:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3901:GLU:OE1	2:H:3902:GLN:NE2	2.39	0.56
2:H:4159:THR:O	2:H:4163:LYS:NZ	2.37	0.56
2:K:943:LEU:HB3	2:K:950:VAL:HG11	1.86	0.56
2:B:4791:ARG:CB	2:B:4808:ASP:CB	2.84	0.56
2:B:4890:PHE:H	7:B:6003:ATP:HN61	1.53	0.56
2:E:3901:GLU:OE1	2:E:3902:GLN:NE2	2.39	0.56
2:H:2275:LEU:H	2:H:2293:PRO:HD3	1.69	0.56
2:H:2707:VAL:HG21	2:H:2786:TRP:HE1	1.71	0.56
2:K:954:ASP:HB2	2:K:1061:GLY:HA3	1.87	0.56
1:D:23:VAL:HB	1:D:105:ASN:H	1.70	0.56
2:E:1144:ARG:NH2	2:E:1150:GLU:OE1	2.39	0.56
2:K:2436:VAL:O	2:K:2466:LYS:NZ	2.38	0.56
2:B:4168:GLU:HB2	2:B:4171:ARG:NH1	2.20	0.56
2:E:278:GLU:HB2	2:E:296:ARG:HB2	1.87	0.56
2:H:2521:LEU:HD22	2:H:2565:ALA:HB2	1.87	0.56
2:K:1144:ARG:NH2	2:K:1150:GLU:OE1	2.39	0.56
1:A:23:VAL:HB	1:A:105:ASN:H	1.70	0.56
2:B:1628:MET:HB2	2:B:1687:TYR:HE2	1.70	0.56
2:B:2834:LEU:HD11	2:B:2894:LEU:HB3	1.88	0.56
2:H:1303:ARG:HH22	2:H:1595:LEU:HD13	1.71	0.56
2:K:833:LYS:HA	2:K:1614:ARG:HH12	1.71	0.56
2:H:1144:ARG:NH2	2:H:1150:GLU:OE1	2.39	0.56
2:B:706:TYR:OH	2:B:1086:ARG:NH2	2.37	0.56
2:B:1303:ARG:HH22	2:B:1595:LEU:HD13	1.71	0.56
2:H:278:GLU:HB2	2:H:296:ARG:HB2	1.87	0.56
2:H:1146:HIS:HB2	2:H:1192:PHE:HE1	1.70	0.56
2:B:2426:SER:HG	2:K:143:LEU:HD13	1.70	0.55
2:K:278:GLU:HB2	2:K:296:ARG:HB2	1.87	0.55
2:K:4085:VAL:O	2:K:4089:HIS:N	2.40	0.55
2:B:1144:ARG:NH2	2:B:1150:GLU:OE1	2.39	0.55
2:B:2521:LEU:HD22	2:B:2565:ALA:HB2	1.87	0.55
2:E:4890:PHE:H	7:E:6003:ATP:HN61	1.54	0.55
2:K:417:ARG:HH11	2:K:420:ARG:HH11	1.55	0.55
2:B:289:ILE:HG22	2:B:354:ILE:HD12	1.88	0.55
2:B:417:ARG:HH11	2:B:420:ARG:HH11	1.54	0.55
2:H:2834:LEU:HD11	2:H:2894:LEU:HB3	1.88	0.55
2:H:289:ILE:HG22	2:H:354:ILE:HD12	1.88	0.55
2:H:298:ARG:HE	2:H:303:GLY:HA2	1.72	0.55
2:K:1303:ARG:HH22	2:K:1595:LEU:HD13	1.71	0.55
2:E:833:LYS:HA	2:E:1614:ARG:HH12	1.71	0.55
2:H:231:GLY:O	2:H:276:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:289:ILE:HG22	2:K:354:ILE:HD12	1.88	0.55
2:K:2521:LEU:HD22	2:K:2565:ALA:HB2	1.87	0.55
2:B:833:LYS:HA	2:B:1614:ARG:HH12	1.71	0.55
2:E:1303:ARG:HH22	2:E:1595:LEU:HD13	1.71	0.55
2:E:3919:ASN:O	2:E:3922:THR:OG1	2.23	0.55
2:B:2707:VAL:HG21	2:B:2786:TRP:HE1	1.71	0.54
2:E:289:ILE:HG22	2:E:354:ILE:HD12	1.88	0.54
2:H:833:LYS:HA	2:H:1614:ARG:HH12	1.71	0.54
2:K:231:GLY:O	2:K:276:ARG:NH1	2.40	0.54
2:K:298:ARG:HE	2:K:303:GLY:HA2	1.72	0.54
2:K:2834:LEU:HD11	2:K:2894:LEU:HB3	1.88	0.54
2:B:841:LYS:HB2	2:B:848:ARG:HD3	1.90	0.54
2:E:1572:LYS:HE2	2:E:1585:ARG:HB3	1.90	0.54
2:K:288:HIS:ND1	2:K:349:MET:O	2.40	0.54
2:K:841:LYS:HB2	2:K:848:ARG:HD3	1.90	0.54
2:B:1572:LYS:HE2	2:B:1585:ARG:HB3	1.90	0.54
2:H:1242:ASN:HB2	2:H:1807:ARG:HG2	1.90	0.54
2:K:2707:VAL:HG21	2:K:2786:TRP:HE1	1.71	0.54
2:H:1303:ARG:HB2	2:H:1593:HIS:HB2	1.90	0.54
2:B:288:HIS:ND1	2:B:349:MET:O	2.40	0.54
2:B:3800:SER:OG	2:B:3801:CYS:N	2.41	0.54
2:B:4791:ARG:HB2	2:B:4808:ASP:CB	2.38	0.54
2:E:231:GLY:O	2:E:276:ARG:NH1	2.40	0.54
2:B:626:ARG:NH2	2:B:1667:LEU:O	2.41	0.54
2:H:143:LEU:CD1	2:K:2427:LEU:CD1	2.86	0.54
2:H:841:LYS:HB2	2:H:848:ARG:HD3	1.90	0.54
2:K:626:ARG:NH2	2:K:1667:LEU:O	2.41	0.54
2:K:1242:ASN:HB2	2:K:1807:ARG:HG2	1.90	0.54
2:E:674:TYR:OH	2:E:676:GLU:OE2	2.21	0.54
2:H:288:HIS:ND1	2:H:349:MET:O	2.40	0.54
2:B:231:GLY:O	2:B:276:ARG:NH1	2.40	0.54
2:H:417:ARG:HH11	2:H:420:ARG:HH11	1.55	0.54
2:H:1272:ARG:HG3	2:H:1586:LEU:HD13	1.90	0.54
2:B:756:SER:HB3	2:B:769:ARG:H	1.73	0.54
2:B:2413:ALA:HB1	2:B:2418:ILE:HD11	1.90	0.54
2:E:841:LYS:HB2	2:E:848:ARG:HD3	1.90	0.54
2:E:4497:ALA:HB1	2:E:4594:LEU:HD13	1.90	0.54
2:H:626:ARG:NH2	2:H:1667:LEU:O	2.41	0.54
2:H:681:HIS:HB2	2:H:799:LYS:HG2	1.90	0.54
2:B:4085:VAL:O	2:B:4089:HIS:N	2.40	0.53
2:B:156:GLU:OE1	2:E:2419:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4159:THR:O	2:B:4163:LYS:NZ	2.37	0.53
2:E:417:ARG:HH11	2:E:420:ARG:HH11	1.55	0.53
2:E:844:ARG:HG2	2:E:846:TYR:H	1.74	0.53
2:H:207:PHE:CE1	2:K:2326:ILE:HG23	2.43	0.53
2:K:1572:LYS:HE2	2:K:1585:ARG:HB3	1.90	0.53
2:K:2464:ASP:OD1	2:K:2464:ASP:N	2.36	0.53
2:B:1429:SER:HA	2:B:1507:ILE:HG12	1.90	0.53
2:E:288:HIS:ND1	2:E:349:MET:O	2.40	0.53
2:K:309:MET:O	2:K:313:SER:N	2.42	0.53
2:E:298:ARG:HE	2:E:303:GLY:HA2	1.72	0.53
2:E:626:ARG:NH2	2:E:1667:LEU:O	2.41	0.53
2:E:2413:ALA:HB1	2:E:2418:ILE:HD11	1.91	0.53
2:E:1242:ASN:HB2	2:E:1807:ARG:HG2	1.90	0.53
2:E:1303:ARG:HB2	2:E:1593:HIS:HB2	1.90	0.53
2:H:1572:LYS:HE2	2:H:1585:ARG:HB3	1.90	0.53
2:K:1429:SER:HA	2:K:1507:ILE:HG12	1.91	0.53
2:B:681:HIS:HB2	2:B:799:LYS:HG2	1.90	0.53
2:E:1272:ARG:HG3	2:E:1586:LEU:HD13	1.90	0.53
2:K:1272:ARG:NH2	2:K:1590:PHE:O	2.42	0.53
2:B:1242:ASN:HB2	2:B:1807:ARG:HG2	1.90	0.53
2:B:4020:MET:CE	2:B:4067:LEU:HD13	2.39	0.53
2:B:4497:ALA:HB1	2:B:4594:LEU:HD13	1.90	0.53
2:E:66:THR:HG1	2:E:124:SER:HG	1.53	0.53
2:E:143:LEU:CD1	2:H:2427:LEU:CD1	2.86	0.53
2:H:309:MET:O	2:H:313:SER:N	2.42	0.53
2:H:756:SER:HB3	2:H:769:ARG:H	1.73	0.53
2:H:1272:ARG:NH2	2:H:1590:PHE:O	2.42	0.53
2:K:681:HIS:HB2	2:K:799:LYS:HG2	1.90	0.53
2:K:844:ARG:HG2	2:K:846:TYR:H	1.74	0.53
2:B:844:ARG:HG2	2:B:846:TYR:H	1.74	0.53
2:K:1272:ARG:HG3	2:K:1586:LEU:HD13	1.90	0.53
2:K:2413:ALA:HB1	2:K:2418:ILE:HD11	1.90	0.53
2:K:4020:MET:CE	2:K:4067:LEU:HD13	2.39	0.53
2:B:4787:PHE:CD1	2:B:4808:ASP:O	2.56	0.53
2:E:156:GLU:OE1	2:H:2419:ARG:NH1	2.42	0.53
2:E:681:HIS:HB2	2:E:799:LYS:HG2	1.90	0.53
2:K:674:TYR:OH	2:K:676:GLU:OE2	2.21	0.53
2:B:309:MET:O	2:B:313:SER:N	2.42	0.53
2:B:1303:ARG:HB2	2:B:1593:HIS:HB2	1.90	0.53
2:E:1429:SER:HA	2:E:1507:ILE:HG12	1.91	0.53
2:H:2413:ALA:HB1	2:H:2418:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:466:PRO:HB3	2:K:478:ARG:HD2	1.91	0.53
2:K:2406:GLU:O	2:K:2410:ILE:N	2.42	0.53
2:E:309:MET:O	2:E:313:SER:N	2.42	0.52
2:E:716:ASN:HA	2:E:722:LEU:HD13	1.91	0.52
2:E:4020:MET:CE	2:E:4067:LEU:HD13	2.39	0.52
2:E:4085:VAL:O	2:E:4089:HIS:N	2.40	0.52
2:E:4605:LYS:HG3	2:E:4645:TYR:HE1	1.73	0.52
2:H:466:PRO:HB3	2:H:478:ARG:HD2	1.91	0.52
2:H:1250:TRP:HB3	2:H:1600:PRO:HB2	1.91	0.52
2:H:4020:MET:CE	2:H:4067:LEU:HD13	2.39	0.52
2:K:2116:ASP:OD1	2:K:2153:ASN:ND2	2.43	0.52
2:K:4159:THR:O	2:K:4163:LYS:NZ	2.37	0.52
2:B:298:ARG:HE	2:B:303:GLY:HA2	1.72	0.52
2:B:1272:ARG:HG3	2:B:1586:LEU:HD13	1.90	0.52
2:B:4605:LYS:HG3	2:B:4645:TYR:HE1	1.73	0.52
2:E:756:SER:HB3	2:E:769:ARG:H	1.74	0.52
2:K:1250:TRP:HB3	2:K:1600:PRO:HB2	1.91	0.52
2:E:308:LEU:HD21	2:E:370:LEU:HD12	1.91	0.52
2:K:66:THR:OG1	2:K:124:SER:OG	2.25	0.52
2:K:756:SER:HB3	2:K:769:ARG:H	1.74	0.52
2:K:3800:SER:OG	2:K:3801:CYS:N	2.41	0.52
2:B:1272:ARG:NH2	2:B:1590:PHE:O	2.42	0.52
2:H:308:LEU:HD21	2:H:370:LEU:HD12	1.91	0.52
2:H:844:ARG:HG2	2:H:846:TYR:H	1.74	0.52
2:H:1114:ARG:NH1	2:H:1128:LEU:O	2.43	0.52
2:H:4085:VAL:O	2:H:4089:HIS:N	2.40	0.52
2:K:4605:LYS:HG3	2:K:4645:TYR:HE1	1.73	0.52
2:B:716:ASN:HA	2:B:722:LEU:HD13	1.91	0.52
2:B:2419:ARG:NH1	2:K:156:GLU:OE1	2.42	0.52
2:E:1250:TRP:HB3	2:E:1600:PRO:HB2	1.91	0.52
2:H:1429:SER:HA	2:H:1507:ILE:HG12	1.91	0.52
2:H:3919:ASN:O	2:H:3922:THR:OG1	2.23	0.52
2:K:3729:GLN:O	2:K:3733:HIS:ND1	2.43	0.52
2:H:716:ASN:HA	2:H:722:LEU:HD13	1.91	0.52
2:H:2116:ASP:OD1	2:H:2153:ASN:ND2	2.43	0.52
2:K:1114:ARG:NH1	2:K:1128:LEU:O	2.43	0.52
1:G:21:THR:HG1	1:G:49:ARG:HH21	1.54	0.52
2:H:4605:LYS:HG3	2:H:4645:TYR:HE1	1.73	0.52
2:K:644:LEU:HD22	2:K:1632:ILE:HG22	1.92	0.52
2:K:4497:ALA:HB1	2:K:4594:LEU:HD13	1.90	0.52
2:B:4192:ASN:OD1	2:B:4605:LYS:NZ	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3800:SER:OG	2:E:3801:CYS:N	2.41	0.52
2:H:687:THR:HG23	2:H:1626:GLN:HE21	1.75	0.52
2:K:1303:ARG:HB2	2:K:1593:HIS:HB2	1.90	0.52
2:B:1114:ARG:NH1	2:B:1128:LEU:O	2.43	0.51
2:B:2406:GLU:O	2:B:2410:ILE:N	2.42	0.51
2:E:466:PRO:HB3	2:E:478:ARG:HD2	1.91	0.51
2:E:1114:ARG:NH1	2:E:1128:LEU:O	2.43	0.51
2:E:2116:ASP:OD1	2:E:2153:ASN:ND2	2.43	0.51
2:E:2730:HIS:NE2	2:E:2759:LYS:O	2.43	0.51
2:K:1260:GLN:HG2	2:K:1591:LEU:HD13	1.92	0.51
2:B:1250:TRP:HB3	2:B:1600:PRO:HB2	1.92	0.51
2:B:2427:LEU:CD1	2:K:143:LEU:CD1	2.86	0.51
2:E:279:THR:O	2:E:296:ARG:NH2	2.43	0.51
2:E:805:GLY:HA2	2:E:810:GLU:HB2	1.92	0.51
2:E:1272:ARG:NH2	2:E:1590:PHE:O	2.42	0.51
2:E:2406:GLU:O	2:E:2410:ILE:N	2.42	0.51
2:H:4497:ALA:HB1	2:H:4594:LEU:HD13	1.90	0.51
2:B:279:THR:O	2:B:296:ARG:NH2	2.43	0.51
2:K:559:ILE:HD13	2:K:593:HIS:HB3	1.93	0.51
2:B:176:ARG:N	2:B:179:ASP:OD2	2.44	0.51
2:B:559:ILE:HD13	2:B:593:HIS:HB3	1.93	0.51
2:B:2730:HIS:NE2	2:B:2759:LYS:O	2.43	0.51
2:E:559:ILE:HD13	2:E:593:HIS:HB3	1.93	0.51
2:K:1209:VAL:N	2:K:1211:GLN:OE1	2.44	0.51
2:B:687:THR:HG23	2:B:1626:GLN:HE21	1.75	0.51
2:B:1209:VAL:N	2:B:1211:GLN:OE1	2.44	0.51
2:K:1111:GLY:HA3	2:K:1211:GLN:HE21	1.76	0.51
2:B:466:PRO:HB3	2:B:478:ARG:HD2	1.91	0.51
2:E:20:VAL:HG12	2:E:216:PRO:HA	1.93	0.51
2:E:644:LEU:HD22	2:E:1632:ILE:HG22	1.92	0.51
2:H:20:VAL:HG12	2:H:216:PRO:HA	1.93	0.51
2:H:182:ILE:HD11	2:H:211:LEU:HD23	1.92	0.51
2:H:279:THR:O	2:H:296:ARG:NH2	2.43	0.51
2:H:559:ILE:HD13	2:H:593:HIS:HB3	1.93	0.51
2:K:308:LEU:HD21	2:K:370:LEU:HD12	1.91	0.51
2:B:644:LEU:HD22	2:B:1632:ILE:HG22	1.92	0.51
2:B:2116:ASP:OD1	2:B:2153:ASN:ND2	2.43	0.51
1:D:27:THR:HA	1:D:38:SER:HA	1.93	0.51
2:K:176:ARG:N	2:K:179:ASP:OD2	2.44	0.51
2:B:308:LEU:HD21	2:B:370:LEU:HD12	1.91	0.51
2:B:760:ASP:HB2	2:B:763:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:TYR:HA	2:E:201:LEU:HD23	1.92	0.51
2:E:4192:ASN:OD1	2:E:4605:LYS:NZ	2.29	0.51
2:H:176:ARG:N	2:H:179:ASP:OD2	2.44	0.51
2:H:196:TYR:HA	2:H:201:LEU:HD23	1.92	0.51
1:J:9:PRO:HA	1:J:70:GLN:HG3	1.92	0.51
2:K:805:GLY:HA2	2:K:810:GLU:HB2	1.92	0.51
1:D:9:PRO:HA	1:D:70:GLN:HG3	1.92	0.51
2:E:1209:VAL:N	2:E:1211:GLN:OE1	2.44	0.51
2:H:1209:VAL:N	2:H:1211:GLN:OE1	2.44	0.51
2:K:687:THR:HG23	2:K:1626:GLN:HE21	1.75	0.51
2:K:2730:HIS:NE2	2:K:2759:LYS:O	2.43	0.51
2:B:3729:GLN:O	2:B:3733:HIS:ND1	2.43	0.51
2:E:182:ILE:HD11	2:E:211:LEU:HD23	1.92	0.51
2:E:672:LYS:HA	2:E:760:ASP:HA	1.93	0.51
2:E:760:ASP:HB2	2:E:763:ALA:HB3	1.93	0.51
2:E:4020:MET:HE2	2:E:4063:GLU:HB3	1.93	0.51
2:H:1098:ALA:O	2:H:1101:TRP:NE1	2.38	0.51
2:H:1114:ARG:HB2	2:H:1206:SER:HB3	1.92	0.51
2:K:196:TYR:HA	2:K:201:LEU:HD23	1.92	0.51
2:K:672:LYS:HA	2:K:760:ASP:HA	1.93	0.51
2:K:716:ASN:HA	2:K:722:LEU:HD13	1.91	0.51
1:A:9:PRO:HA	1:A:70:GLN:HG3	1.92	0.50
2:B:143:LEU:CD1	2:E:2427:LEU:CD1	2.85	0.50
2:B:672:LYS:HA	2:B:760:ASP:HA	1.93	0.50
2:B:1114:ARG:HB2	2:B:1206:SER:HB3	1.92	0.50
3:C:27:THR:HA	3:C:63:THR:HB	1.94	0.50
2:E:1847:GLU:OE1	2:E:1849:SER:OG	2.25	0.50
2:E:4486:ILE:HG22	2:E:4489:GLN:H	1.77	0.50
2:H:156:GLU:OE1	2:K:2419:ARG:NH1	2.43	0.50
2:K:644:LEU:HB3	2:K:1630:LEU:HD12	1.94	0.50
2:K:1114:ARG:HB2	2:K:1206:SER:HB3	1.92	0.50
2:K:3919:ASN:O	2:K:3922:THR:OG1	2.23	0.50
2:B:196:TYR:HA	2:B:201:LEU:HD23	1.92	0.50
2:B:1038:LEU:HD12	2:B:1043:LYS:HE3	1.94	0.50
2:E:43:GLY:H	2:E:45:ARG:HH12	1.59	0.50
2:E:1038:LEU:HD12	2:E:1043:LYS:HE3	1.94	0.50
2:H:2114:VAL:O	2:H:2117:THR:OG1	2.28	0.50
2:K:4616:LEU:HA	2:K:4620:GLU:HB2	1.93	0.50
3:L:27:THR:HA	3:L:63:THR:HB	1.94	0.50
2:B:1303:ARG:O	2:B:1593:HIS:N	2.45	0.50
2:E:687:THR:HG23	2:E:1626:GLN:HE21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1771:ILE:HG22	2:E:1773:ASN:H	1.76	0.50
2:H:1111:GLY:HA3	2:H:1211:GLN:HE21	1.76	0.50
1:J:27:THR:HA	1:J:38:SER:HA	1.93	0.50
2:B:43:GLY:H	2:B:45:ARG:HH12	1.59	0.50
2:E:644:LEU:HB3	2:E:1630:LEU:HD12	1.94	0.50
2:E:1114:ARG:HB2	2:E:1206:SER:HB3	1.92	0.50
2:H:43:GLY:H	2:H:45:ARG:HH12	1.59	0.50
2:H:805:GLY:HA2	2:H:810:GLU:HB2	1.92	0.50
2:K:279:THR:O	2:K:296:ARG:NH2	2.43	0.50
2:B:295:PHE:N	2:B:329:PHE:O	2.44	0.50
2:B:1111:GLY:HA3	2:B:1211:GLN:HE21	1.76	0.50
2:E:1260:GLN:HG2	2:E:1591:LEU:HD13	1.92	0.50
2:E:4167:LYS:NZ	7:E:6003:ATP:O2B	2.44	0.50
1:G:27:THR:HA	1:G:38:SER:HA	1.93	0.50
2:H:644:LEU:HD22	2:H:1632:ILE:HG22	1.92	0.50
2:H:672:LYS:HA	2:H:760:ASP:HA	1.92	0.50
2:H:1303:ARG:O	2:H:1593:HIS:N	2.45	0.50
2:H:4486:ILE:HG22	2:H:4489:GLN:H	1.77	0.50
2:K:182:ILE:HD11	2:K:211:LEU:HD23	1.92	0.50
2:K:295:PHE:N	2:K:329:PHE:O	2.44	0.50
2:K:760:ASP:HB2	2:K:763:ALA:HB3	1.93	0.50
2:K:1303:ARG:O	2:K:1593:HIS:N	2.45	0.50
2:B:805:GLY:HA2	2:B:810:GLU:HB2	1.92	0.50
2:E:176:ARG:N	2:E:179:ASP:OD2	2.44	0.50
3:F:27:THR:HA	3:F:63:THR:HB	1.94	0.50
1:G:9:PRO:HA	1:G:70:GLN:HG3	1.92	0.50
2:H:1038:LEU:HD12	2:H:1043:LYS:HE3	1.94	0.50
2:H:4616:LEU:HA	2:H:4620:GLU:HB2	1.93	0.50
2:K:20:VAL:HG12	2:K:216:PRO:HA	1.93	0.50
2:H:1171:HIS:HE1	2:H:1197:VAL:H	1.60	0.50
2:B:20:VAL:HG12	2:B:216:PRO:HA	1.93	0.50
2:B:182:ILE:HD11	2:B:211:LEU:HD23	1.92	0.50
2:B:1260:GLN:HG2	2:B:1591:LEU:HD13	1.92	0.50
2:B:2832:VAL:O	2:B:2895:LYS:NZ	2.38	0.50
2:B:3803:VAL:HG22	2:B:3881:ARG:HH21	1.77	0.50
2:E:1611:ILE:HB	2:E:1620:GLN:HB3	1.94	0.50
2:E:4616:LEU:HA	2:E:4620:GLU:HB2	1.93	0.50
2:H:1304:LEU:HB3	2:H:1541:PRO:HG2	1.94	0.50
2:H:2730:HIS:NE2	2:H:2759:LYS:O	2.43	0.50
2:K:1171:HIS:HE1	2:K:1197:VAL:H	1.60	0.50
2:B:693:LEU:HD13	2:B:749:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1304:LEU:HB3	2:B:1541:PRO:HG2	1.94	0.50
2:E:1111:GLY:HA3	2:E:1211:GLN:HE21	1.76	0.50
2:H:1847:GLU:OE1	2:H:1849:SER:OG	2.25	0.50
3:I:27:THR:HA	3:I:63:THR:HB	1.94	0.50
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.30	0.49
2:B:1611:ILE:HB	2:B:1620:GLN:HB3	1.94	0.49
2:B:1771:ILE:HG22	2:B:1773:ASN:H	1.76	0.49
2:B:4486:ILE:HG22	2:B:4489:GLN:H	1.77	0.49
2:B:4521:TYR:HB3	2:K:4787:PHE:CZ	2.47	0.49
2:H:1771:ILE:HG22	2:H:1773:ASN:H	1.76	0.49
2:K:3803:VAL:HG22	2:K:3881:ARG:HH21	1.77	0.49
2:H:693:LEU:HD13	2:H:749:LEU:HD22	1.94	0.49
2:H:4787:PHE:CZ	2:K:4521:TYR:HB3	2.46	0.49
2:K:4486:ILE:HG22	2:K:4489:GLN:H	1.77	0.49
2:B:1154:ARG:NH2	2:B:1180:GLU:OE1	2.46	0.49
2:B:4616:LEU:HA	2:B:4620:GLU:HB2	1.93	0.49
2:H:295:PHE:N	2:H:329:PHE:O	2.44	0.49
2:H:1443:VAL:HB	2:H:1489:CYS:HB2	1.94	0.49
2:K:693:LEU:HD13	2:K:749:LEU:HD22	1.94	0.49
2:K:748:LEU:HD22	2:K:750:ARG:HE	1.78	0.49
2:K:1038:LEU:HD12	2:K:1043:LYS:HE3	1.94	0.49
2:K:1304:LEU:HB3	2:K:1541:PRO:HG2	1.94	0.49
2:B:644:LEU:HB3	2:B:1630:LEU:HD12	1.94	0.49
2:B:4168:GLU:CB	2:B:4171:ARG:NH1	2.75	0.49
2:B:4722:TYR:OH	2:B:4746:ASP:OD1	2.23	0.49
2:H:760:ASP:HB2	2:H:763:ALA:HB3	1.93	0.49
2:K:2114:VAL:O	2:K:2117:THR:OG1	2.28	0.49
2:B:4167:LYS:NZ	7:B:6003:ATP:O2B	2.44	0.49
2:H:991:SER:OG	2:H:1064:LEU:O	2.30	0.49
2:H:1260:GLN:HG2	2:H:1591:LEU:HD13	1.92	0.49
2:H:1611:ILE:HB	2:H:1620:GLN:HB3	1.94	0.49
2:K:1443:VAL:HB	2:K:1489:CYS:HB2	1.94	0.49
2:K:1611:ILE:HB	2:K:1620:GLN:HB3	1.94	0.49
2:K:1771:ILE:HG22	2:K:1773:ASN:H	1.76	0.49
2:B:748:LEU:HD22	2:B:750:ARG:HE	1.78	0.49
2:B:1171:HIS:HE1	2:B:1197:VAL:H	1.60	0.49
2:E:1304:LEU:HB3	2:E:1541:PRO:HG2	1.94	0.49
2:H:1154:ARG:NH2	2:H:1180:GLU:OE1	2.46	0.49
2:B:991:SER:OG	2:B:1064:LEU:O	2.30	0.49
2:B:1242:ASN:HD22	2:B:1807:ARG:HD2	1.78	0.49
2:B:4787:PHE:CZ	2:E:4521:TYR:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1184:ASP:N	2:E:1188:SER:O	2.45	0.49
2:H:3803:VAL:HG22	2:H:3881:ARG:HH21	1.77	0.49
2:K:1242:ASN:HD22	2:K:1807:ARG:HD2	1.78	0.49
2:K:1847:GLU:OE1	2:K:1849:SER:OG	2.25	0.49
1:A:27:THR:HA	1:A:38:SER:HA	1.93	0.49
2:E:3803:VAL:HG22	2:E:3881:ARG:HH21	1.77	0.49
2:E:4164:PRO:HB2	2:E:4165:GLN:HG3	1.95	0.49
2:E:4207:ILE:HD12	2:E:4494:ASN:HD22	1.78	0.49
2:E:295:PHE:N	2:E:329:PHE:O	2.44	0.49
2:E:991:SER:OG	2:E:1064:LEU:O	2.30	0.49
2:H:748:LEU:HD22	2:H:750:ARG:HE	1.77	0.49
2:H:2832:VAL:O	2:H:2895:LYS:NZ	2.38	0.49
2:H:4164:PRO:HB2	2:H:4165:GLN:HG3	1.95	0.49
2:B:76:ARG:NH2	2:E:3806:LEU:CD2	2.71	0.49
2:B:4207:ILE:HD12	2:B:4494:ASN:HD22	1.78	0.49
2:B:4910:THR:HG21	7:B:6003:ATP:C5	2.48	0.49
2:E:1154:ARG:NH2	2:E:1180:GLU:OE1	2.46	0.49
2:H:1589:GLN:NE2	2:H:1634:GLU:OE1	2.46	0.49
2:H:3977:LYS:HB2	2:H:4095:ILE:HG13	1.95	0.49
2:K:991:SER:OG	2:K:1064:LEU:O	2.30	0.49
2:B:1125:ASP:HA	2:B:1598:ARG:HH11	1.78	0.48
2:B:4791:ARG:HB2	2:B:4808:ASP:HB3	1.96	0.48
2:E:693:LEU:HD13	2:E:749:LEU:HD22	1.94	0.48
2:E:1171:HIS:HE1	2:E:1197:VAL:H	1.60	0.48
2:E:3729:GLN:O	2:E:3733:HIS:ND1	2.43	0.48
1:G:49:ARG:HB3	1:G:52:LYS:HE2	1.95	0.48
2:H:644:LEU:HB3	2:H:1630:LEU:HD12	1.94	0.48
2:H:1125:ASP:HA	2:H:1598:ARG:HH11	1.78	0.48
2:H:4207:ILE:HD12	2:H:4494:ASN:HD22	1.78	0.48
2:H:4655:MET:O	2:H:4664:ARG:NH1	2.46	0.48
2:K:43:GLY:H	2:K:45:ARG:HH12	1.59	0.48
2:K:2832:VAL:O	2:K:2895:LYS:NZ	2.38	0.48
1:A:49:ARG:HB3	1:A:52:LYS:HE2	1.95	0.48
2:B:674:TYR:OH	2:B:676:GLU:OE2	2.21	0.48
1:D:49:ARG:HB3	1:D:52:LYS:HE2	1.95	0.48
2:E:953:SER:OG	2:E:1061:GLY:O	2.32	0.48
2:E:1303:ARG:O	2:E:1593:HIS:N	2.45	0.48
2:E:3977:LYS:HB2	2:E:4095:ILE:HG13	1.95	0.48
2:H:4910:THR:HG21	7:H:6003:ATP:C5	2.48	0.48
1:J:49:ARG:HB3	1:J:52:LYS:HE2	1.95	0.48
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:GLY:O	2:B:243:GLU:N	2.46	0.48
2:B:1589:GLN:NE2	2:B:1634:GLU:OE1	2.46	0.48
2:B:4164:PRO:HB2	2:B:4165:GLN:HG3	1.95	0.48
2:E:1251:LEU:O	2:E:1601:ASN:N	2.47	0.48
2:H:1242:ASN:HD22	2:H:1807:ARG:HD2	1.78	0.48
2:K:218:SER:HB3	2:K:286:GLY:HA3	1.96	0.48
2:K:1733:THR:HG22	2:K:1755:THR:HB	1.96	0.48
2:K:3593:SER:O	2:K:3597:LYS:NZ	2.42	0.48
2:K:4207:ILE:HD12	2:K:4494:ASN:HD22	1.78	0.48
2:E:1443:VAL:HB	2:E:1489:CYS:HB2	1.94	0.48
2:E:4910:THR:HG21	7:E:6003:ATP:C5	2.48	0.48
2:H:58:VAL:HG22	2:H:320:GLU:HA	1.96	0.48
2:H:673:TRP:HE3	2:H:822:CYS:HA	1.78	0.48
3:I:37:MET:HB3	3:I:42:GLN:HB2	1.96	0.48
2:H:218:SER:HB3	2:H:286:GLY:HA3	1.96	0.48
2:K:1154:ARG:NH2	2:K:1180:GLU:OE1	2.46	0.48
2:B:718:VAL:HA	2:B:736:CYS:N	2.29	0.48
2:B:4891:ILE:HD13	2:B:4914:HIS:HB3	1.95	0.48
2:H:799:LYS:HB3	2:H:1620:GLN:HG3	1.95	0.48
2:K:673:TRP:HE3	2:K:822:CYS:HA	1.78	0.48
2:K:4891:ILE:HD13	2:K:4914:HIS:HB3	1.95	0.48
2:K:4910:THR:HG21	7:K:6003:ATP:C5	2.48	0.48
2:B:1733:THR:HG22	2:B:1755:THR:HB	1.96	0.48
2:E:673:TRP:HE3	2:E:822:CYS:HA	1.78	0.48
2:E:748:LEU:HD22	2:E:750:ARG:HE	1.78	0.48
2:H:674:TYR:OH	2:H:676:GLU:OE2	2.21	0.48
2:H:1733:THR:HG22	2:H:1755:THR:HB	1.96	0.48
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.96	0.48
2:K:239:GLY:O	2:K:243:GLU:N	2.47	0.48
2:E:1242:ASN:HD22	2:E:1807:ARG:HD2	1.78	0.48
2:E:1733:THR:HG22	2:E:1755:THR:HB	1.96	0.48
2:E:4022:LEU:HD12	2:E:4089:HIS:CE1	2.49	0.48
2:H:239:GLY:O	2:H:243:GLU:N	2.46	0.48
2:H:4891:ILE:HD13	2:H:4914:HIS:HB3	1.95	0.48
2:K:718:VAL:HA	2:K:736:CYS:N	2.29	0.48
2:K:1589:GLN:NE2	2:K:1634:GLU:OE1	2.46	0.48
2:K:4164:PRO:HB2	2:K:4165:GLN:HG3	1.95	0.48
2:B:58:VAL:HG22	2:B:320:GLU:HA	1.96	0.48
2:B:1443:VAL:HB	2:B:1489:CYS:HB2	1.94	0.48
2:E:218:SER:HB3	2:E:286:GLY:HA3	1.96	0.48
2:E:1589:GLN:NE2	2:E:1634:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:GLY:HA3	1:G:74:LEU:HD21	1.96	0.48
2:K:847:THR:OG1	2:K:1215:MET:O	2.32	0.48
2:K:3977:LYS:HB2	2:K:4095:ILE:HG13	1.95	0.48
2:B:1106:GLU:O	2:B:1214:ARG:N	2.47	0.48
2:B:4655:MET:O	2:B:4664:ARG:NH1	2.46	0.48
2:E:239:GLY:O	2:E:243:GLU:N	2.46	0.48
2:E:4722:TYR:OH	2:E:4746:ASP:OD1	2.23	0.48
2:K:799:LYS:HB3	2:K:1620:GLN:HG3	1.95	0.48
2:K:1445:TRP:H	2:K:1487:MET:HB2	1.79	0.48
2:K:4655:MET:O	2:K:4664:ARG:NH1	2.46	0.48
3:L:37:MET:HB3	3:L:42:GLN:HB2	1.96	0.48
2:B:799:LYS:HB3	2:B:1620:GLN:HG3	1.95	0.47
2:B:3977:LYS:HB2	2:B:4095:ILE:HG13	1.95	0.47
2:E:541:ILE:HG23	2:E:548:CYS:HB3	1.96	0.47
2:E:1106:GLU:O	2:E:1214:ARG:N	2.47	0.47
2:E:2114:VAL:O	2:E:2117:THR:OG1	2.28	0.47
3:F:37:MET:HB3	3:F:42:GLN:HB2	1.96	0.47
2:H:1251:LEU:O	2:H:1601:ASN:N	2.47	0.47
2:H:2464:ASP:OD1	2:H:2464:ASP:N	2.36	0.47
2:K:1106:GLU:O	2:K:1214:ARG:N	2.47	0.47
2:K:1143:GLN:HA	2:K:1151:HIS:HA	1.96	0.47
2:K:4167:LYS:NZ	7:K:6003:ATP:O2B	2.44	0.47
2:B:4791:ARG:HB3	2:B:4808:ASP:CB	2.43	0.47
1:D:62:GLY:HA3	1:D:74:LEU:HD21	1.96	0.47
2:E:4848:ASP:CB	2:H:4819:TYR:CE1	2.93	0.47
2:H:143:LEU:HD12	2:K:2427:LEU:HD13	1.93	0.47
2:H:1106:GLU:O	2:H:1214:ARG:N	2.47	0.47
2:H:1143:GLN:HA	2:H:1151:HIS:HA	1.96	0.47
2:H:1184:ASP:N	2:H:1188:SER:O	2.45	0.47
2:B:235:ARG:NH2	2:B:269:VAL:O	2.39	0.47
2:E:433:LEU:HD12	2:E:447:LEU:HD11	1.97	0.47
2:H:847:THR:OG1	2:H:1215:MET:O	2.32	0.47
2:H:2072:GLN:NE2	2:H:3647:LYS:O	2.47	0.47
2:H:4621:GLN:HE22	2:H:4633:ARG:HH12	1.62	0.47
2:K:58:VAL:HG22	2:K:320:GLU:HA	1.96	0.47
2:K:953:SER:OG	2:K:1061:GLY:O	2.32	0.47
2:K:3936:LEU:HD21	2:K:3941:LEU:HD22	1.96	0.47
2:K:4621:GLN:HE22	2:K:4633:ARG:HH12	1.62	0.47
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.96	0.47
2:B:953:SER:OG	2:B:1061:GLY:O	2.32	0.47
2:B:1445:TRP:H	2:B:1487:MET:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4655:MET:O	2:E:4664:ARG:NH1	2.46	0.47
2:E:4845:ILE:HG23	2:H:4819:TYR:HB2	1.97	0.47
2:H:2029:ARG:O	2:H:2032:SER:OG	2.28	0.47
2:K:1125:ASP:HA	2:K:1598:ARG:HH11	1.78	0.47
2:K:3904:GLN:NE2	2:K:3965:GLN:OE1	2.48	0.47
2:B:731:HIS:CG	2:B:740:THR:HA	2.50	0.47
2:B:1218:GLY:HA3	2:B:1240:ALA:H	1.79	0.47
2:E:1218:GLY:HA3	2:E:1240:ALA:H	1.78	0.47
2:E:2832:VAL:O	2:E:2895:LYS:NZ	2.38	0.47
2:E:4891:ILE:HD13	2:E:4914:HIS:HB3	1.95	0.47
2:H:143:LEU:HD13	2:K:2426:SER:O	2.13	0.47
2:H:1218:GLY:HA3	2:H:1240:ALA:H	1.78	0.47
2:H:1445:TRP:H	2:H:1487:MET:HB2	1.79	0.47
2:H:4020:MET:HE2	2:H:4063:GLU:HB3	1.96	0.47
2:H:4022:LEU:HD12	2:H:4089:HIS:CE1	2.49	0.47
2:B:433:LEU:HD12	2:B:447:LEU:HD11	1.97	0.47
2:B:673:TRP:HE3	2:B:822:CYS:HA	1.78	0.47
2:B:1143:GLN:HA	2:B:1151:HIS:HA	1.96	0.47
2:B:3904:GLN:NE2	2:B:3965:GLN:OE1	2.48	0.47
2:B:4621:GLN:HE22	2:B:4633:ARG:HH12	1.62	0.47
3:C:78:LYS:HA	3:C:81:ASP:HB2	1.97	0.47
2:E:188:SER:HB2	2:E:190:ARG:HH21	1.80	0.47
2:E:1125:ASP:HA	2:E:1598:ARG:HH11	1.78	0.47
2:E:1445:TRP:H	2:E:1487:MET:HB2	1.79	0.47
2:H:3729:GLN:O	2:H:3733:HIS:ND1	2.43	0.47
2:K:4010:ASN:OD1	2:K:4010:ASN:N	2.48	0.47
2:B:1184:ASP:N	2:B:1188:SER:O	2.45	0.47
2:B:1602:GLN:HE22	2:B:1642:LEU:HB3	1.80	0.47
2:B:2072:GLN:NE2	2:B:3647:LYS:O	2.47	0.47
2:B:4022:LEU:HD12	2:B:4089:HIS:CE1	2.49	0.47
3:C:37:MET:HB3	3:C:42:GLN:HB2	1.96	0.47
1:D:26:TYR:N	1:D:39:SER:OG	2.47	0.47
2:E:731:HIS:CG	2:E:740:THR:HA	2.50	0.47
2:E:1602:GLN:HE22	2:E:1642:LEU:HB3	1.80	0.47
2:E:4193:PHE:O	2:E:4197:THR:OG1	2.25	0.47
2:E:4787:PHE:CZ	2:H:4521:TYR:HB3	2.49	0.47
1:G:26:TYR:N	1:G:39:SER:OG	2.47	0.47
2:H:1602:GLN:HE22	2:H:1642:LEU:HB3	1.80	0.47
2:K:731:HIS:CG	2:K:740:THR:HA	2.50	0.47
2:K:2029:ARG:O	2:K:2032:SER:OG	2.28	0.47
2:K:2072:GLN:NE2	2:K:3647:LYS:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:GLU:HB2	2:B:187:SER:HB3	1.97	0.47
2:B:1847:GLU:OE1	2:B:1849:SER:OG	2.25	0.47
2:E:306:LEU:HD11	2:E:314:LEU:HG	1.97	0.47
2:E:3904:GLN:NE2	2:E:3965:GLN:OE1	2.48	0.47
2:H:953:SER:OG	2:H:1061:GLY:O	2.32	0.47
2:H:995:MET:HG2	2:H:998:LYS:HD2	1.97	0.47
2:K:541:ILE:HG23	2:K:548:CYS:HB3	1.96	0.47
2:K:995:MET:HG2	2:K:998:LYS:HD2	1.97	0.47
2:K:1167:ASP:OD2	2:K:1172:THR:OG1	2.32	0.47
2:B:2029:ARG:O	2:B:2032:SER:OG	2.27	0.47
2:B:3936:LEU:HD21	2:B:3941:LEU:HD22	1.96	0.47
2:E:4621:GLN:HE22	2:E:4633:ARG:HH12	1.62	0.47
2:H:262:TYR:HB2	2:H:389:ARG:HB3	1.96	0.47
2:H:433:LEU:HD12	2:H:447:LEU:HD11	1.97	0.47
2:H:541:ILE:HG23	2:H:548:CYS:HB3	1.96	0.47
2:K:4022:LEU:HD12	2:K:4089:HIS:CE1	2.49	0.47
2:B:4010:ASN:OD1	2:B:4010:ASN:N	2.48	0.47
1:G:40:ARG:NH2	1:G:102:GLU:OE1	2.48	0.47
2:H:306:LEU:HD11	2:H:314:LEU:HG	1.97	0.47
2:H:4010:ASN:OD1	2:H:4010:ASN:N	2.48	0.47
2:E:799:LYS:HB3	2:E:1620:GLN:HG3	1.95	0.46
2:E:2072:GLN:NE2	2:E:3647:LYS:O	2.47	0.46
2:H:731:HIS:CG	2:H:740:THR:HA	2.50	0.46
2:H:2406:GLU:O	2:H:2410:ILE:N	2.42	0.46
2:K:1218:GLY:HA3	2:K:1240:ALA:H	1.79	0.46
2:B:204:ASP:N	2:B:204:ASP:OD1	2.48	0.46
2:B:268:SER:O	2:B:273:SER:OG	2.31	0.46
2:B:541:ILE:HG23	2:B:548:CYS:HB3	1.96	0.46
2:B:995:MET:HG2	2:B:998:LYS:HD2	1.97	0.46
2:B:1132:GLU:HB3	2:B:1147:GLN:HE21	1.80	0.46
2:E:262:TYR:HB2	2:E:389:ARG:HB3	1.96	0.46
2:E:718:VAL:HA	2:E:736:CYS:N	2.29	0.46
2:E:836:HIS:CE1	2:E:1610:ARG:HD2	2.51	0.46
2:E:1608:VAL:HG12	2:E:1610:ARG:HB2	1.97	0.46
2:H:718:VAL:HA	2:H:736:CYS:N	2.29	0.46
2:K:188:SER:HB2	2:K:190:ARG:HH21	1.80	0.46
2:K:1602:GLN:HE22	2:K:1642:LEU:HB3	1.80	0.46
1:A:40:ARG:NH2	1:A:102:GLU:OE1	2.48	0.46
2:B:188:SER:HB2	2:B:190:ARG:HH21	1.80	0.46
2:E:204:ASP:OD1	2:E:204:ASP:N	2.48	0.46
2:E:1132:GLU:HB3	2:E:1147:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:78:LYS:HA	3:F:81:ASP:HB2	1.97	0.46
2:H:836:HIS:CE1	2:H:1610:ARG:HD2	2.51	0.46
1:A:26:TYR:N	1:A:39:SER:OG	2.47	0.46
2:B:1676:LEU:O	2:B:1680:VAL:N	2.47	0.46
2:E:58:VAL:HG22	2:E:320:GLU:HA	1.96	0.46
2:E:156:GLU:HB2	2:E:187:SER:HB3	1.97	0.46
1:G:92:PRO:HG2	1:G:95:ALA:HB2	1.98	0.46
2:H:679:VAL:HA	2:H:800:VAL:HG12	1.97	0.46
2:H:1676:LEU:O	2:H:1680:VAL:N	2.47	0.46
2:H:1912:GLN:HB2	2:H:2088:LEU:HD11	1.98	0.46
2:H:3680:LYS:NZ	2:H:3684:GLU:OE2	2.47	0.46
2:H:3904:GLN:NE2	2:H:3965:GLN:OE1	2.48	0.46
2:K:433:LEU:HD12	2:K:447:LEU:HD11	1.97	0.46
1:A:21:THR:HG1	1:A:49:ARG:HH21	1.59	0.46
1:D:92:PRO:HG2	1:D:95:ALA:HB2	1.98	0.46
2:E:1143:GLN:HA	2:E:1151:HIS:HA	1.96	0.46
2:E:2319:ASN:OD1	2:E:2323:ARG:NH2	2.49	0.46
2:E:3936:LEU:HD21	2:E:3941:LEU:HD22	1.96	0.46
2:H:1608:VAL:HG12	2:H:1610:ARG:HB2	1.97	0.46
2:H:3683:LEU:HD12	2:H:3748:SER:HB3	1.98	0.46
2:K:1184:ASP:OD2	2:K:1188:SER:OG	2.30	0.46
2:K:4000:MET:HA	2:K:4003:MET:HG2	1.98	0.46
2:K:4808:ASP:OD1	2:K:4808:ASP:N	2.47	0.46
3:L:78:LYS:HA	3:L:81:ASP:HB2	1.97	0.46
2:B:1608:VAL:HG12	2:B:1610:ARG:HB2	1.96	0.46
2:B:2114:VAL:O	2:B:2117:THR:OG1	2.28	0.46
2:B:3607:ALA:HB3	3:C:85:GLU:HG2	1.98	0.46
2:B:3808:ALA:O	2:B:3812:GLN:HB2	2.16	0.46
2:E:995:MET:HG2	2:E:998:LYS:HD2	1.97	0.46
2:E:3683:LEU:HD12	2:E:3748:SER:HB3	1.98	0.46
2:H:122:ARG:HH21	2:H:127:GLY:HA2	1.81	0.46
2:H:288:HIS:N	2:H:349:MET:O	2.47	0.46
2:H:1184:ASP:OD2	2:H:1188:SER:OG	2.30	0.46
2:H:4167:LYS:NZ	7:H:6003:ATP:O2B	2.44	0.46
1:J:92:PRO:HG2	1:J:95:ALA:HB2	1.98	0.46
2:K:306:LEU:HD11	2:K:314:LEU:HG	1.97	0.46
2:E:4757:ILE:HG23	2:E:4871:PHE:HZ	1.81	0.46
2:H:1470:GLY:HA2	2:H:1474:GLY:HA2	1.98	0.46
2:H:4000:MET:HA	2:H:4003:MET:HG2	1.98	0.46
2:H:4192:ASN:OD1	2:H:4605:LYS:NZ	2.29	0.46
2:K:3680:LYS:NZ	2:K:3684:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1912:GLN:HB2	2:B:2088:LEU:HD11	1.97	0.46
2:B:2319:ASN:OD1	2:B:2323:ARG:NH2	2.49	0.46
2:E:394:HIS:HD2	2:E:397:GLY:H	1.63	0.46
2:E:1098:ALA:O	2:E:1101:TRP:NE1	2.38	0.46
2:E:1756:SER:OG	2:E:1757:LEU:N	2.49	0.46
2:E:1912:GLN:HB2	2:E:2088:LEU:HD11	1.98	0.46
2:E:3607:ALA:HB3	3:F:85:GLU:HG2	1.98	0.46
2:H:156:GLU:HB2	2:H:187:SER:HB3	1.97	0.46
2:H:204:ASP:OD1	2:H:204:ASP:N	2.48	0.46
2:H:2117:THR:HG22	2:H:2155:VAL:HG11	1.98	0.46
2:H:3607:ALA:HB3	3:I:85:GLU:HG2	1.98	0.46
2:K:288:HIS:N	2:K:349:MET:O	2.47	0.46
2:K:836:HIS:CE1	2:K:1610:ARG:HD2	2.51	0.46
2:K:1132:GLU:HB3	2:K:1147:GLN:HE21	1.80	0.46
2:K:3683:LEU:HD12	2:K:3748:SER:HB3	1.98	0.46
1:A:92:PRO:HG2	1:A:95:ALA:HB2	1.98	0.46
2:B:122:ARG:HH21	2:B:127:GLY:HA2	1.81	0.46
2:B:836:HIS:CE1	2:B:1610:ARG:HD2	2.51	0.46
2:H:188:SER:HB2	2:H:190:ARG:HH21	1.80	0.46
2:H:2252:ASN:HD22	2:H:3595:GLN:HG3	1.81	0.46
2:H:3936:LEU:HD21	2:H:3941:LEU:HD22	1.96	0.46
2:K:262:TYR:HB2	2:K:389:ARG:HB3	1.96	0.46
2:K:1098:ALA:O	2:K:1101:TRP:NE1	2.38	0.46
2:K:2252:ASN:HD22	2:K:3595:GLN:HG3	1.81	0.46
2:B:262:TYR:HB2	2:B:389:ARG:HB3	1.96	0.46
2:B:306:LEU:HD11	2:B:314:LEU:HG	1.97	0.46
2:K:235:ARG:NH2	2:K:269:VAL:O	2.39	0.46
2:K:894:VAL:HG11	2:K:976:TYR:HD2	1.81	0.46
2:K:897:LYS:HE2	2:K:915:HIS:CG	2.51	0.46
2:K:1608:VAL:HG12	2:K:1610:ARG:HB2	1.96	0.46
2:K:1912:GLN:HB2	2:K:2088:LEU:HD11	1.98	0.46
2:K:3607:ALA:HB3	3:L:85:GLU:HG2	1.98	0.46
2:B:986:ILE:HB	2:B:1058:LEU:HB3	1.98	0.45
2:B:3806:LEU:CD2	2:K:76:ARG:NH2	2.72	0.45
2:E:2252:ASN:HD22	2:E:3595:GLN:HG3	1.81	0.45
2:E:2425:ARG:HH12	2:E:2477:TYR:HA	1.81	0.45
2:E:3993:ASN:HD22	2:E:4110:MET:HG3	1.81	0.45
2:H:894:VAL:HG11	2:H:976:TYR:HD2	1.81	0.45
2:H:1132:GLU:HB3	2:H:1147:GLN:HE21	1.80	0.45
1:J:26:TYR:N	1:J:39:SER:OG	2.47	0.45
2:K:3993:ASN:HD22	2:K:4110:MET:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4147:GLU:OE1	2:K:4937:GLN:NE2	2.49	0.45
2:B:894:VAL:HG11	2:B:976:TYR:HD2	1.81	0.45
2:B:2252:ASN:HD22	2:B:3595:GLN:HG3	1.81	0.45
2:E:288:HIS:N	2:E:349:MET:O	2.47	0.45
2:E:986:ILE:HB	2:E:1058:LEU:HB3	1.98	0.45
2:E:1511:VAL:HA	2:E:1517:LEU:H	1.81	0.45
2:E:2464:ASP:OD1	2:E:2464:ASP:N	2.36	0.45
2:H:1763:PHE:HB3	2:H:1781:GLU:HB3	1.98	0.45
3:I:78:LYS:HA	3:I:81:ASP:HB2	1.97	0.45
2:K:679:VAL:HA	2:K:800:VAL:HG12	1.97	0.45
2:K:769:ARG:HA	2:K:775:VAL:HG23	1.99	0.45
2:K:1251:LEU:O	2:K:1601:ASN:N	2.47	0.45
2:K:1763:PHE:HB3	2:K:1781:GLU:HB3	1.98	0.45
2:K:4757:ILE:HG23	2:K:4871:PHE:HZ	1.81	0.45
2:B:80:GLU:HG3	2:E:3891:TRP:CZ3	2.49	0.45
2:B:769:ARG:HA	2:B:775:VAL:HG23	1.99	0.45
2:B:4147:GLU:OE1	2:B:4937:GLN:NE2	2.49	0.45
2:E:76:ARG:HH21	2:H:3806:LEU:CG	2.29	0.45
2:E:897:LYS:HE2	2:E:915:HIS:CG	2.52	0.45
2:E:2117:THR:HG22	2:E:2155:VAL:HG11	1.98	0.45
2:E:3808:ALA:O	2:E:3812:GLN:HB2	2.16	0.45
2:H:66:THR:OG1	2:H:124:SER:OG	2.25	0.45
2:H:4722:TYR:OH	2:H:4746:ASP:OD1	2.23	0.45
2:H:4845:ILE:HG23	2:K:4819:TYR:HB2	1.99	0.45
2:K:156:GLU:HB2	2:K:187:SER:HB3	1.97	0.45
2:K:4722:TYR:OH	2:K:4746:ASP:OD1	2.23	0.45
2:K:4733:GLY:HA3	2:K:4740:PHE:HD1	1.82	0.45
2:B:394:HIS:HD2	2:B:397:GLY:H	1.63	0.45
2:B:4020:MET:HE2	2:B:4063:GLU:HB3	1.98	0.45
2:E:76:ARG:HH22	2:H:3806:LEU:HD11	1.75	0.45
2:E:268:SER:O	2:E:273:SER:OG	2.31	0.45
2:E:1763:PHE:HB3	2:E:1781:GLU:HB3	1.98	0.45
2:H:394:HIS:HD2	2:H:397:GLY:H	1.63	0.45
2:H:3984:LEU:HB2	2:H:4102:LEU:HD12	1.99	0.45
2:H:4147:GLU:OE1	2:H:4937:GLN:NE2	2.49	0.45
2:K:1710:HIS:HB2	2:K:1711:LEU:HD12	1.99	0.45
2:B:847:THR:OG1	2:B:1215:MET:O	2.32	0.45
2:B:1251:LEU:O	2:B:1601:ASN:N	2.47	0.45
2:B:1470:GLY:HA2	2:B:1474:GLY:HA2	1.98	0.45
2:B:1511:VAL:HA	2:B:1517:LEU:H	1.81	0.45
2:B:1726:ILE:HG13	2:B:1757:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1763:PHE:HB3	2:B:1781:GLU:HB3	1.98	0.45
2:B:2425:ARG:HH12	2:B:2477:TYR:HA	1.81	0.45
2:B:3993:ASN:HD22	2:B:4110:MET:HG3	1.81	0.45
2:E:770:ILE:HG12	2:E:775:VAL:HG21	1.99	0.45
2:E:847:THR:OG1	2:E:1215:MET:O	2.32	0.45
2:E:1710:HIS:HB2	2:E:1711:LEU:HD12	1.99	0.45
2:H:643:LEU:H	2:H:643:LEU:HG	1.60	0.45
2:K:3808:ALA:O	2:K:3812:GLN:HB2	2.16	0.45
2:B:897:LYS:HE2	2:B:915:HIS:CG	2.51	0.45
2:B:1710:HIS:HB2	2:B:1711:LEU:HD12	1.99	0.45
2:B:2117:THR:HG22	2:B:2155:VAL:HG11	1.98	0.45
2:B:2426:SER:O	2:K:143:LEU:HD13	2.13	0.45
2:B:3683:LEU:HD12	2:B:3748:SER:HB3	1.98	0.45
2:B:4819:TYR:CE1	2:K:4848:ASP:CB	2.95	0.45
2:E:1986:GLU:N	2:E:1989:CYS:SG	2.73	0.45
2:H:76:ARG:HH22	2:K:3806:LEU:HD11	1.76	0.45
2:H:1726:ILE:HG13	2:H:1757:LEU:HD23	1.98	0.45
2:H:3993:ASN:HD22	2:H:4110:MET:HG3	1.81	0.45
2:K:305:TYR:HE2	2:K:319:LYS:HG2	1.81	0.45
2:K:394:HIS:HD2	2:K:397:GLY:H	1.63	0.45
2:K:1470:GLY:HA2	2:K:1474:GLY:HA2	1.98	0.45
2:K:1756:SER:OG	2:K:1757:LEU:N	2.49	0.45
2:B:1756:SER:OG	2:B:1757:LEU:N	2.49	0.45
2:B:4897:ASP:N	2:B:4897:ASP:OD1	2.50	0.45
2:E:122:ARG:HH21	2:E:127:GLY:HA2	1.81	0.45
2:E:3844:LEU:HD23	2:E:3844:LEU:HA	1.79	0.45
2:H:1511:VAL:HA	2:H:1517:LEU:H	1.81	0.45
2:H:2425:ARG:HH12	2:H:2477:TYR:HA	1.81	0.45
2:H:4733:GLY:HA3	2:H:4740:PHE:HD1	1.82	0.45
2:K:308:LEU:N	2:K:326:SER:O	2.49	0.45
2:K:1184:ASP:N	2:K:1188:SER:O	2.45	0.45
2:K:1640:ASP:OD1	2:K:1640:ASP:N	2.44	0.45
2:K:4897:ASP:OD1	2:K:4897:ASP:N	2.50	0.45
2:B:16:THR:OG1	2:B:111:ARG:O	2.29	0.45
2:B:4000:MET:HA	2:B:4003:MET:HG2	1.98	0.45
2:B:4168:GLU:HA	2:B:4171:ARG:CZ	2.46	0.45
2:E:679:VAL:HA	2:E:800:VAL:HG12	1.97	0.45
2:E:769:ARG:HA	2:E:775:VAL:HG23	1.99	0.45
2:E:3984:LEU:HB2	2:E:4102:LEU:HD12	1.99	0.45
2:H:235:ARG:NH2	2:H:269:VAL:O	2.39	0.45
2:H:769:ARG:HA	2:H:775:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1756:SER:OG	2:H:1757:LEU:N	2.49	0.45
2:H:3808:ALA:O	2:H:3812:GLN:HB2	2.16	0.45
2:H:3921:LEU:HD23	2:H:3921:LEU:HA	1.73	0.45
2:K:204:ASP:OD1	2:K:204:ASP:N	2.48	0.45
2:K:986:ILE:HB	2:K:1058:LEU:HB3	1.98	0.45
2:K:2319:ASN:OD1	2:K:2323:ARG:NH2	2.49	0.45
2:B:76:ARG:HH21	2:E:3806:LEU:CG	2.30	0.45
2:B:770:ILE:HG12	2:B:775:VAL:HG21	1.99	0.45
2:B:3680:LYS:NZ	2:B:3684:GLU:OE2	2.47	0.45
2:B:4733:GLY:HA3	2:B:4740:PHE:HD1	1.82	0.45
2:B:4757:ILE:HG23	2:B:4871:PHE:HZ	1.81	0.45
2:E:1184:ASP:OD2	2:E:1188:SER:OG	2.30	0.45
2:E:4897:ASP:N	2:E:4897:ASP:OD1	2.50	0.45
2:H:305:TYR:HE2	2:H:319:LYS:HG2	1.81	0.45
2:H:4022:LEU:HA	2:H:4089:HIS:CE1	2.50	0.45
2:K:122:ARG:HH21	2:K:127:GLY:HA2	1.81	0.45
2:K:4022:LEU:HA	2:K:4089:HIS:CE1	2.50	0.45
2:B:660:PHE:HB3	2:B:787:LEU:HD22	1.99	0.45
2:B:679:VAL:HA	2:B:800:VAL:HG12	1.97	0.45
2:B:695:VAL:HA	2:B:792:VAL:HG22	1.99	0.45
2:E:80:GLU:HG3	2:H:3891:TRP:CZ3	2.49	0.45
2:E:3970:LYS:HB3	2:E:3970:LYS:HE2	1.82	0.45
2:E:4733:GLY:HA3	2:E:4740:PHE:HD1	1.82	0.45
2:K:54:ASN:HB3	2:K:57:ASN:HB3	1.99	0.45
2:K:394:HIS:CD2	2:K:396:GLU:H	2.35	0.45
3:L:130:ASP:O	3:L:137:VAL:HG22	2.17	0.45
2:B:1167:ASP:OD2	2:B:1172:THR:OG1	2.32	0.44
2:E:1470:GLY:HA2	2:E:1474:GLY:HA2	1.98	0.44
2:E:4000:MET:HA	2:E:4003:MET:HG2	1.98	0.44
2:E:4022:LEU:HA	2:E:4089:HIS:CE1	2.50	0.44
2:E:4147:GLU:OE1	2:E:4937:GLN:NE2	2.49	0.44
2:E:4808:ASP:OD1	2:E:4808:ASP:N	2.47	0.44
2:H:986:ILE:HB	2:H:1058:LEU:HB3	1.98	0.44
2:H:1710:HIS:HB2	2:H:1711:LEU:HD12	1.98	0.44
2:H:4897:ASP:OD1	2:H:4897:ASP:N	2.50	0.44
2:K:1726:ILE:HG13	2:K:1757:LEU:HD23	1.98	0.44
2:K:2117:THR:HG22	2:K:2155:VAL:HG11	1.98	0.44
2:B:54:ASN:HB3	2:B:57:ASN:HB3	1.99	0.44
2:B:143:LEU:HD12	2:E:2427:LEU:HD11	2.00	0.44
2:B:288:HIS:N	2:B:349:MET:O	2.47	0.44
2:B:643:LEU:H	2:B:643:LEU:HG	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:ALA:N	2:B:1211:GLN:OE1	2.50	0.44
2:B:4022:LEU:HA	2:B:4089:HIS:CE1	2.50	0.44
3:C:130:ASP:O	3:C:137:VAL:HG22	2.17	0.44
2:E:305:TYR:HE2	2:E:319:LYS:HG2	1.81	0.44
2:E:660:PHE:HB3	2:E:787:LEU:HD22	2.00	0.44
2:E:894:VAL:HG11	2:E:976:TYR:HD2	1.81	0.44
2:E:1726:ILE:HG13	2:E:1757:LEU:HD23	1.98	0.44
2:E:2891:GLN:HG2	2:E:2894:LEU:HD12	1.99	0.44
2:H:695:VAL:HA	2:H:792:VAL:HG22	1.99	0.44
2:H:748:LEU:HB2	2:H:750:ARG:HG3	1.99	0.44
2:H:2319:ASN:OD1	2:H:2323:ARG:NH2	2.48	0.44
2:K:1258:PHE:HB3	2:K:1303:ARG:NH1	2.33	0.44
2:K:3642:ILE:HG22	2:K:3731:ARG:HD3	1.99	0.44
2:K:3844:LEU:HD23	2:K:3844:LEU:HA	1.79	0.44
2:B:76:ARG:HH22	2:E:3806:LEU:HD11	1.74	0.44
2:B:394:HIS:CD2	2:B:396:GLU:H	2.35	0.44
2:B:2760:PRO:HD2	2:B:2763:LEU:HD12	1.99	0.44
2:E:750:ARG:N	2:E:753:ASP:OD2	2.46	0.44
2:E:4010:ASN:OD1	2:E:4010:ASN:N	2.48	0.44
3:F:130:ASP:O	3:F:137:VAL:HG22	2.17	0.44
2:H:191:TYR:OH	2:K:2327:ARG:CZ	2.66	0.44
2:H:2891:GLN:HG2	2:H:2894:LEU:HD12	1.99	0.44
3:I:130:ASP:O	3:I:137:VAL:HG22	2.17	0.44
2:K:1162:VAL:O	2:K:1176:THR:OG1	2.33	0.44
2:K:1511:VAL:HA	2:K:1517:LEU:H	1.81	0.44
2:K:2425:ARG:HH12	2:K:2477:TYR:HA	1.81	0.44
2:K:2760:PRO:HD2	2:K:2763:LEU:HD12	1.99	0.44
2:B:1640:ASP:OD1	2:B:1640:ASP:N	2.44	0.44
2:B:2891:GLN:HG2	2:B:2894:LEU:HD12	1.99	0.44
2:B:3806:LEU:HD11	2:K:76:ARG:HH22	1.75	0.44
2:B:4175:PHE:O	2:B:4179:ASN:ND2	2.51	0.44
2:E:294:PRO:HB3	2:E:366:ILE:HD11	1.99	0.44
2:E:3642:ILE:HG22	2:E:3731:ARG:HD3	1.99	0.44
2:H:308:LEU:N	2:H:326:SER:O	2.49	0.44
2:H:1601:ASN:ND2	2:H:1643:GLU:OE2	2.36	0.44
2:H:3760:LEU:HD23	2:H:3760:LEU:HA	1.81	0.44
2:H:4757:ILE:HG23	2:H:4871:PHE:HZ	1.81	0.44
2:K:3984:LEU:HB2	2:K:4102:LEU:HD12	1.99	0.44
2:B:674:TYR:HE2	2:B:814:LEU:HB2	1.83	0.44
2:B:2880:ALA:O	2:B:2884:ALA:N	2.49	0.44
2:E:394:HIS:CD2	2:E:396:GLU:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2398:ASP:OD1	2:E:2402:ARG:NH2	2.50	0.44
2:H:394:HIS:CD2	2:H:396:GLU:H	2.35	0.44
2:H:660:PHE:HB3	2:H:787:LEU:HD22	1.99	0.44
2:H:3844:LEU:HD23	2:H:3844:LEU:HA	1.79	0.44
2:H:4175:PHE:O	2:H:4179:ASN:ND2	2.51	0.44
1:J:40:ARG:NH2	1:J:102:GLU:OE1	2.48	0.44
2:K:1121:GLY:O	2:K:1133:ARG:NH1	2.51	0.44
2:B:305:TYR:HE2	2:B:319:LYS:HG2	1.82	0.44
2:B:1258:PHE:HB3	2:B:1303:ARG:NH1	2.33	0.44
2:B:2327:ARG:CZ	2:K:191:TYR:OH	2.66	0.44
2:E:238:HIS:N	2:E:243:GLU:O	2.43	0.44
2:E:674:TYR:HE2	2:E:814:LEU:HB2	1.83	0.44
2:E:4136:ARG:HH21	2:E:4148:ARG:CZ	2.31	0.44
2:H:2770:GLU:O	2:H:2774:TRP:HB2	2.18	0.44
2:H:4136:ARG:HH21	2:H:4148:ARG:CZ	2.31	0.44
2:K:4601:PHE:HD1	2:K:4644:ASN:HB3	1.83	0.44
2:B:506:HIS:NE2	2:B:564:ARG:HG2	2.33	0.44
2:B:1121:GLY:O	2:B:1133:ARG:NH1	2.51	0.44
2:E:76:ARG:NH2	2:H:3806:LEU:CD2	2.70	0.44
2:E:1121:GLY:O	2:E:1133:ARG:NH1	2.51	0.44
2:E:1167:ASP:OD2	2:E:1172:THR:OG1	2.32	0.44
2:E:1258:PHE:HB3	2:E:1303:ARG:NH1	2.33	0.44
2:E:2880:ALA:O	2:E:2884:ALA:N	2.49	0.44
2:H:76:ARG:HH21	2:K:3806:LEU:CG	2.31	0.44
2:H:1305:SER:HB2	2:H:1591:LEU:HB2	2.00	0.44
2:K:32:GLN:O	2:K:53:SER:OG	2.28	0.44
2:K:4136:ARG:HH21	2:K:4148:ARG:CZ	2.31	0.44
2:K:4175:PHE:O	2:K:4179:ASN:ND2	2.51	0.44
2:B:308:LEU:N	2:B:326:SER:O	2.49	0.44
2:B:3806:LEU:CG	2:K:76:ARG:HH21	2.30	0.44
2:B:3984:LEU:HB2	2:B:4102:LEU:HD12	1.99	0.44
2:B:4791:ARG:CB	2:B:4808:ASP:HB3	2.47	0.44
1:D:30:LEU:HD12	1:D:34:LYS:HB2	2.00	0.44
1:D:40:ARG:NH2	1:D:102:GLU:OE1	2.48	0.44
2:H:294:PRO:HB3	2:H:366:ILE:HD11	2.00	0.44
2:H:770:ILE:HG12	2:H:775:VAL:HG21	1.99	0.44
2:H:897:LYS:HE2	2:H:915:HIS:CG	2.52	0.44
2:K:660:PHE:HB3	2:K:787:LEU:HD22	1.99	0.44
2:K:770:ILE:HG12	2:K:775:VAL:HG21	1.99	0.44
2:K:3921:LEU:HD23	2:K:3921:LEU:HA	1.73	0.44
2:K:4020:MET:HE2	2:K:4063:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:TYR:OH	2:E:2327:ARG:CZ	2.65	0.44
2:B:1274:ASP:HB2	2:B:1286:THR:HA	2.00	0.44
2:E:54:ASN:HB3	2:E:57:ASN:HB3	1.99	0.44
2:E:695:VAL:HA	2:E:792:VAL:HG22	1.99	0.44
2:E:3680:LYS:NZ	2:E:3684:GLU:OE2	2.47	0.44
2:H:3642:ILE:HG22	2:H:3731:ARG:HD3	1.99	0.44
2:H:4601:PHE:HD1	2:H:4644:ASN:HB3	1.83	0.44
2:K:748:LEU:HB2	2:K:750:ARG:HG3	1.99	0.44
2:K:2891:GLN:HG2	2:K:2894:LEU:HD12	1.99	0.44
2:E:228:LEU:HD11	2:E:405:LEU:HD13	2.00	0.43
2:E:769:ARG:HG2	2:E:774:PRO:HA	2.00	0.43
2:E:2856:LYS:O	2:E:2860:GLU:HB2	2.18	0.43
2:H:694:ARG:HG2	2:H:716:ASN:HB3	2.00	0.43
2:H:750:ARG:N	2:H:753:ASP:OD2	2.46	0.43
2:H:769:ARG:HG2	2:H:774:PRO:HA	2.00	0.43
2:K:1305:SER:HB2	2:K:1591:LEU:HB2	2.00	0.43
2:K:2770:GLU:O	2:K:2774:TRP:HB2	2.18	0.43
2:K:3880:LEU:HD23	2:K:3944:ALA:HB2	2.00	0.43
2:B:694:ARG:HG2	2:B:716:ASN:HB3	2.00	0.43
2:B:3593:SER:O	2:B:3597:LYS:NZ	2.42	0.43
2:B:4020:MET:HE1	2:B:4063:GLU:HB3	2.00	0.43
2:B:4819:TYR:HB2	2:K:4845:ILE:HG23	2.00	0.43
2:E:506:HIS:NE2	2:E:564:ARG:HG2	2.33	0.43
2:E:748:LEU:HB2	2:E:750:ARG:HG3	1.99	0.43
1:J:30:LEU:HD12	1:J:34:LYS:HB2	2.00	0.43
2:K:1757:LEU:HD13	2:K:1757:LEU:HA	1.88	0.43
2:B:2241:LEU:HD12	2:B:2298:ARG:HG3	2.01	0.43
2:B:4845:ILE:HG23	2:E:4819:TYR:HB2	2.00	0.43
2:E:143:LEU:HD13	2:H:2426:SER:O	2.14	0.43
2:E:898:ILE:HD13	2:E:973:THR:HG22	2.00	0.43
2:H:2241:LEU:HD12	2:H:2298:ARG:HG3	2.00	0.43
2:H:2856:LYS:O	2:H:2860:GLU:HB2	2.18	0.43
2:K:694:ARG:HG2	2:K:716:ASN:HB3	2.00	0.43
2:K:2856:LYS:O	2:K:2860:GLU:HB2	2.18	0.43
2:B:769:ARG:HG2	2:B:774:PRO:HA	2.00	0.43
2:B:4601:PHE:HD1	2:B:4644:ASN:HB3	1.83	0.43
2:E:2241:LEU:HD12	2:E:2298:ARG:HG3	2.01	0.43
2:H:54:ASN:HB3	2:H:57:ASN:HB3	1.99	0.43
2:H:718:VAL:HA	2:H:736:CYS:H	1.83	0.43
2:H:1057:LEU:O	2:H:1062:TYR:N	2.51	0.43
2:H:1121:GLY:O	2:H:1133:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1258:PHE:HB3	2:H:1303:ARG:NH1	2.33	0.43
2:K:674:TYR:HE2	2:K:814:LEU:HB2	1.83	0.43
2:K:695:VAL:HA	2:K:792:VAL:HG22	1.99	0.43
2:B:1098:ALA:O	2:B:1101:TRP:NE1	2.38	0.43
2:E:4011:VAL:HA	2:E:4014:ILE:HG12	2.00	0.43
2:H:674:TYR:HE2	2:H:814:LEU:HB2	1.83	0.43
2:H:1734:LYS:HE2	2:H:1931:ASP:HB3	2.00	0.43
2:H:2397:ILE:HD12	2:H:2397:ILE:HA	1.94	0.43
2:H:2760:PRO:HD2	2:H:2763:LEU:HD12	1.99	0.43
2:H:2880:ALA:O	2:H:2884:ALA:N	2.49	0.43
2:H:3800:SER:OG	2:H:3801:CYS:N	2.41	0.43
2:H:4848:ASP:CB	2:K:4819:TYR:CE1	2.95	0.43
2:K:718:VAL:HA	2:K:736:CYS:H	1.83	0.43
2:K:2241:LEU:HD12	2:K:2298:ARG:HG3	2.00	0.43
2:K:2463:PRO:HB3	2:K:2516:ALA:HB2	2.01	0.43
2:B:4523:VAL:HG21	2:K:4791:ARG:HD2	2.00	0.43
2:B:4780:TYR:OH	2:E:4515:ASN:HB3	2.19	0.43
2:E:2760:PRO:HD2	2:E:2763:LEU:HD12	1.99	0.43
2:E:4175:PHE:O	2:E:4179:ASN:ND2	2.51	0.43
2:E:4601:PHE:HD1	2:E:4644:ASN:HB3	1.83	0.43
1:G:30:LEU:HD12	1:G:34:LYS:HB2	2.00	0.43
2:H:1274:ASP:HB2	2:H:1286:THR:HA	2.00	0.43
2:H:2252:ASN:HB2	2:H:2310:ASN:HD21	1.84	0.43
2:K:769:ARG:HG2	2:K:774:PRO:HA	2.00	0.43
2:K:1305:SER:HA	2:K:1593:HIS:HD2	1.84	0.43
2:K:2398:ASP:OD1	2:K:2402:ARG:NH2	2.50	0.43
2:K:2731:ASP:HB3	2:K:2826:ALA:HB2	2.01	0.43
2:K:4020:MET:HE1	2:K:4063:GLU:HB3	2.01	0.43
2:B:294:PRO:HB3	2:B:366:ILE:HD11	1.99	0.43
2:B:601:LEU:HG	2:B:642:LEU:HD23	2.01	0.43
2:B:1734:LYS:HE2	2:B:1931:ASP:HB3	2.00	0.43
2:B:3921:LEU:HD23	2:B:3921:LEU:HA	1.73	0.43
2:E:601:LEU:HG	2:E:642:LEU:HD23	2.01	0.43
2:E:1057:LEU:O	2:E:1062:TYR:N	2.51	0.43
2:E:1305:SER:HA	2:E:1593:HIS:HD2	1.84	0.43
2:E:2252:ASN:HB2	2:E:2310:ASN:HD21	1.84	0.43
2:H:425:LEU:HD21	2:H:452:VAL:HG13	2.01	0.43
2:H:1228:THR:HA	2:H:1232:LEU:HD12	2.01	0.43
2:H:1785:ASP:OD1	2:H:1788:LYS:NZ	2.51	0.43
2:H:1986:GLU:N	2:H:1989:CYS:SG	2.73	0.43
2:K:652:VAL:HG11	2:K:715:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1310:CYS:HB2	2:K:1536:SER:HA	2.01	0.43
2:K:1785:ASP:OD1	2:K:1788:LYS:NZ	2.50	0.43
2:B:228:LEU:HD11	2:B:405:LEU:HD13	2.00	0.43
2:B:1714:TYR:CD1	2:B:1761:MET:HB3	2.54	0.43
2:B:2463:PRO:HB3	2:B:2516:ALA:HB2	2.01	0.43
2:B:3642:ILE:HG22	2:B:3731:ARG:HD3	1.99	0.43
2:B:4136:ARG:HH21	2:B:4148:ARG:CZ	2.31	0.43
2:E:308:LEU:N	2:E:326:SER:O	2.49	0.43
2:E:1601:ASN:ND2	2:E:1643:GLU:OE2	2.36	0.43
2:H:2759:LYS:HA	2:H:2760:PRO:HD3	1.92	0.43
2:H:3986:MET:HG2	2:H:3996:ILE:HD11	2.01	0.43
2:K:898:ILE:HD13	2:K:973:THR:HG22	2.00	0.43
2:K:1676:LEU:O	2:K:1680:VAL:N	2.47	0.43
2:K:4787:PHE:HD1	2:K:4808:ASP:O	2.02	0.43
2:B:898:ILE:HD13	2:B:973:THR:HG22	2.00	0.43
2:B:2770:GLU:O	2:B:2774:TRP:HB2	2.18	0.43
2:B:3891:TRP:CZ3	2:K:80:GLU:HG3	2.50	0.43
2:E:3612:LEU:HD23	2:E:3617:ALA:HB2	2.01	0.43
2:H:228:LEU:HD11	2:H:405:LEU:HD13	2.00	0.43
2:H:506:HIS:NE2	2:H:564:ARG:HG2	2.33	0.43
2:H:898:ILE:HD13	2:H:973:THR:HG22	2.00	0.43
2:K:506:HIS:NE2	2:K:564:ARG:HG2	2.33	0.43
2:K:1274:ASP:HB2	2:K:1286:THR:HA	2.00	0.43
2:K:3612:LEU:HD23	2:K:3617:ALA:HB2	2.01	0.43
2:B:718:VAL:HA	2:B:736:CYS:H	1.83	0.43
2:B:1305:SER:HB2	2:B:1591:LEU:HB2	2.00	0.43
2:B:2252:ASN:HB2	2:B:2310:ASN:HD21	1.84	0.43
2:B:2427:LEU:HD11	2:K:143:LEU:HD12	2.01	0.43
2:B:3760:LEU:HD23	2:B:3760:LEU:HA	1.81	0.43
2:E:425:LEU:HD21	2:E:452:VAL:HG13	2.01	0.43
2:E:940:LEU:HD23	2:E:940:LEU:HA	1.89	0.43
2:E:1274:ASP:HB2	2:E:1286:THR:HA	2.00	0.43
2:E:2770:GLU:O	2:E:2774:TRP:HB2	2.18	0.43
2:H:601:LEU:HG	2:H:642:LEU:HD23	2.01	0.43
2:H:1305:SER:HA	2:H:1593:HIS:HD2	1.84	0.43
2:H:1310:CYS:HB2	2:H:1536:SER:HA	2.01	0.43
2:H:1836:ASN:HA	2:H:1839:LEU:HB2	2.01	0.43
2:H:2076:ILE:HG21	2:H:2081:LEU:HD22	2.00	0.43
2:H:2731:ASP:HB3	2:H:2826:ALA:HB2	2.01	0.43
2:K:601:LEU:HG	2:K:642:LEU:HD23	2.01	0.43
2:K:1601:ASN:ND2	2:K:1643:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD12	1:A:34:LYS:HB2	2.00	0.42
2:B:243:GLU:HA	2:B:264:GLY:HA2	2.01	0.42
2:B:4011:VAL:HA	2:B:4014:ILE:HG12	2.00	0.42
2:B:4515:ASN:HB3	2:K:4780:TYR:OH	2.19	0.42
1:D:9:PRO:HD2	2:E:748:LEU:HD11	2.01	0.42
2:E:64:ILE:H	2:E:64:ILE:HG13	1.74	0.42
2:E:191:TYR:OH	2:H:2327:ARG:CZ	2.67	0.42
2:E:235:ARG:NH2	2:E:269:VAL:O	2.39	0.42
2:E:243:GLU:HA	2:E:264:GLY:HA2	2.00	0.42
2:E:1228:THR:HA	2:E:1232:LEU:HD12	2.01	0.42
2:E:1310:CYS:HB2	2:E:1536:SER:HA	2.01	0.42
2:E:1714:TYR:CD1	2:E:1761:MET:HB3	2.54	0.42
2:E:2076:ILE:HG21	2:E:2081:LEU:HD22	2.01	0.42
2:E:2716:GLU:HA	2:E:2719:GLU:HB2	2.01	0.42
2:E:2731:ASP:HB3	2:E:2826:ALA:HB2	2.01	0.42
2:E:3880:LEU:HD23	2:E:3944:ALA:HB2	2.00	0.42
2:E:4787:PHE:HD1	2:E:4808:ASP:O	2.02	0.42
2:H:1466:THR:HG22	2:H:1482:ARG:HG2	2.01	0.42
2:H:3777:LYS:HE3	2:H:3777:LYS:HB2	1.87	0.42
2:H:3871:ILE:O	2:H:3874:SER:OG	2.26	0.42
2:K:238:HIS:N	2:K:243:GLU:O	2.43	0.42
2:K:1210:ALA:N	2:K:1211:GLN:OE1	2.50	0.42
2:K:1836:ASN:HA	2:K:1839:LEU:HB2	2.01	0.42
2:K:4635:VAL:O	2:K:4638:THR:OG1	2.33	0.42
2:B:1057:LEU:O	2:B:1062:TYR:N	2.51	0.42
2:B:1305:SER:HA	2:B:1593:HIS:HD2	1.84	0.42
2:B:1310:CYS:HB2	2:B:1536:SER:HA	2.01	0.42
2:B:2759:LYS:HA	2:B:2760:PRO:HD3	1.92	0.42
2:B:4168:GLU:HB2	2:B:4171:ARG:HH12	1.84	0.42
2:B:4193:PHE:O	2:B:4197:THR:OG1	2.25	0.42
1:D:77:THR:HB	1:D:80:VAL:HG23	2.01	0.42
2:E:694:ARG:HG2	2:E:716:ASN:HB3	2.00	0.42
2:E:2834:LEU:HD13	2:E:2838:LEU:HB3	2.01	0.42
2:H:243:GLU:HA	2:H:264:GLY:HA2	2.01	0.42
2:H:3605:ARG:HH12	3:I:82:SER:HB3	1.85	0.42
2:H:3612:LEU:HD23	2:H:3617:ALA:HB2	2.01	0.42
2:H:4787:PHE:HD1	2:H:4808:ASP:O	2.02	0.42
2:H:4890:PHE:H	7:H:6003:ATP:N6	2.17	0.42
2:K:243:GLU:HA	2:K:264:GLY:HA2	2.01	0.42
2:K:425:LEU:HD21	2:K:452:VAL:HG13	2.01	0.42
2:K:1714:TYR:CD1	2:K:1761:MET:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2252:ASN:HB2	2:K:2310:ASN:HD21	1.84	0.42
2:K:2834:LEU:HD13	2:K:2838:LEU:HB3	2.01	0.42
2:K:4011:VAL:HA	2:K:4014:ILE:HG12	2.00	0.42
2:B:143:LEU:HD13	2:E:2426:SER:O	2.13	0.42
2:B:237:LEU:HB2	2:B:404:ASN:HB3	2.02	0.42
2:B:675:TYR:CE1	2:B:790:PRO:HB3	2.54	0.42
2:B:676:GLU:HG3	2:B:814:LEU:HB3	2.01	0.42
2:B:748:LEU:HB2	2:B:750:ARG:HG3	1.99	0.42
2:B:2731:ASP:HB3	2:B:2826:ALA:HB2	2.01	0.42
2:B:2856:LYS:O	2:B:2860:GLU:HB2	2.18	0.42
2:B:3612:LEU:HD23	2:B:3617:ALA:HB2	2.01	0.42
2:E:2433:LEU:HD22	2:E:2488:LEU:HD22	2.01	0.42
2:E:4597:PRO:HA	2:E:4600:ILE:HG22	2.01	0.42
1:G:77:THR:HB	1:G:80:VAL:HG23	2.01	0.42
2:H:652:VAL:HG11	2:H:715:GLY:HA2	2.01	0.42
2:H:1092:LYS:H	2:H:1250:TRP:HZ3	1.67	0.42
2:H:2463:PRO:HB3	2:H:2516:ALA:HB2	2.00	0.42
1:J:21:THR:HG1	1:J:49:ARG:HH21	1.59	0.42
2:K:1730:THR:O	2:K:1733:THR:OG1	2.28	0.42
2:K:1734:LYS:HE2	2:K:1931:ASP:HB3	2.00	0.42
2:K:3986:MET:HG2	2:K:3996:ILE:HD11	2.01	0.42
2:B:294:PRO:HD3	2:B:344:LYS:HE3	2.02	0.42
2:B:1228:THR:HA	2:B:1232:LEU:HD12	2.01	0.42
2:B:3605:ARG:HH12	3:C:82:SER:HB3	1.85	0.42
2:E:143:LEU:HD12	2:H:2427:LEU:HD11	2.01	0.42
2:E:294:PRO:HD3	2:E:344:LYS:HE3	2.02	0.42
2:E:652:VAL:HG11	2:E:715:GLY:HA2	2.01	0.42
2:E:1734:LYS:HE2	2:E:1931:ASP:HB3	2.00	0.42
2:E:3987:LEU:HG	2:E:3990:ASN:HD21	1.85	0.42
2:H:1167:ASP:OD2	2:H:1172:THR:OG1	2.32	0.42
2:K:294:PRO:HB3	2:K:366:ILE:HD11	1.99	0.42
2:K:675:TYR:CE1	2:K:790:PRO:HB3	2.54	0.42
2:K:4020:MET:HE2	2:K:4067:LEU:HD13	2.01	0.42
2:B:394:HIS:CD2	2:B:397:GLY:H	2.38	0.42
2:B:745:ASN:HB3	2:B:747:HIS:HB2	2.02	0.42
2:B:2076:ILE:HG21	2:B:2081:LEU:HD22	2.00	0.42
2:B:2433:LEU:HD22	2:B:2488:LEU:HD22	2.01	0.42
2:B:2716:GLU:HA	2:B:2719:GLU:HB2	2.01	0.42
2:B:3986:MET:HG2	2:B:3996:ILE:HD11	2.01	0.42
2:E:439:LYS:HE3	2:E:439:LYS:HB3	1.91	0.42
2:E:618:CYS:SG	2:E:629:GLN:NE2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:718:VAL:HA	2:E:736:CYS:H	1.83	0.42
2:E:745:ASN:HB3	2:E:747:HIS:HB2	2.02	0.42
2:E:755:ILE:HA	2:E:770:ILE:HD13	2.02	0.42
2:E:1305:SER:HB2	2:E:1591:LEU:HB2	2.00	0.42
2:H:3880:LEU:HD23	2:H:3944:ALA:HB2	2.00	0.42
2:H:4791:ARG:HD2	2:K:4523:VAL:HG21	2.00	0.42
2:K:618:CYS:SG	2:K:629:GLN:NE2	2.93	0.42
2:K:1092:LYS:H	2:K:1250:TRP:HZ3	1.67	0.42
2:K:3605:ARG:HH12	3:L:82:SER:HB3	1.85	0.42
2:B:1836:ASN:HA	2:B:1839:LEU:HB2	2.01	0.42
2:B:1986:GLU:N	2:B:1989:CYS:SG	2.73	0.42
2:B:3880:LEU:HD23	2:B:3944:ALA:HB2	2.00	0.42
2:B:4635:VAL:O	2:B:4638:THR:OG1	2.33	0.42
2:E:3921:LEU:HD23	2:E:3921:LEU:HA	1.73	0.42
2:H:32:GLN:O	2:H:53:SER:OG	2.28	0.42
2:H:268:SER:O	2:H:273:SER:OG	2.31	0.42
2:H:676:GLU:HG3	2:H:814:LEU:HB3	2.01	0.42
2:H:1124:PRO:HG2	2:H:1598:ARG:HG3	2.01	0.42
2:H:2433:LEU:HD22	2:H:2488:LEU:HD22	2.01	0.42
2:H:3987:LEU:HG	2:H:3990:ASN:HD21	1.85	0.42
2:K:228:LEU:HD11	2:K:405:LEU:HD13	2.00	0.42
2:K:1466:THR:HG22	2:K:1482:ARG:HG2	2.01	0.42
2:K:1732:GLU:O	2:K:1735:SER:OG	2.32	0.42
2:B:73:LEU:HB3	2:B:77:ALA:HB3	2.02	0.42
2:B:675:TYR:CZ	2:B:790:PRO:HB3	2.55	0.42
2:B:983:LEU:HD23	2:B:1056:THR:HA	2.02	0.42
2:B:1124:PRO:HG2	2:B:1598:ARG:HG3	2.01	0.42
2:B:2834:LEU:HD13	2:B:2838:LEU:HB3	2.01	0.42
2:B:4020:MET:HE2	2:B:4067:LEU:HD13	2.01	0.42
2:E:16:THR:OG1	2:E:111:ARG:O	2.29	0.42
2:E:675:TYR:CE1	2:E:790:PRO:HB3	2.54	0.42
2:E:1676:LEU:O	2:E:1680:VAL:N	2.47	0.42
2:E:2463:PRO:HB3	2:E:2516:ALA:HB2	2.01	0.42
2:H:618:CYS:SG	2:H:629:GLN:NE2	2.93	0.42
2:H:675:TYR:CE1	2:H:790:PRO:HB3	2.54	0.42
2:H:1210:ALA:N	2:H:1211:GLN:OE1	2.51	0.42
2:H:1676:LEU:HD23	2:H:1676:LEU:HA	1.89	0.42
2:K:237:LEU:HB2	2:K:404:ASN:HB3	2.02	0.42
2:K:294:PRO:HD3	2:K:344:LYS:HE3	2.02	0.42
2:K:394:HIS:CD2	2:K:397:GLY:H	2.38	0.42
2:K:676:GLU:HG3	2:K:814:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:745:ASN:HB3	2:K:747:HIS:HB2	2.02	0.42
2:K:755:ILE:HA	2:K:770:ILE:HD13	2.02	0.42
2:K:2076:ILE:HG21	2:K:2081:LEU:HD22	2.01	0.42
2:B:652:VAL:HG11	2:B:715:GLY:HA2	2.01	0.42
2:B:4597:PRO:HA	2:B:4600:ILE:HG22	2.01	0.42
2:E:3986:MET:HG2	2:E:3996:ILE:HD11	2.01	0.42
2:H:294:PRO:HD3	2:H:344:LYS:HE3	2.02	0.42
2:H:2398:ASP:OD1	2:H:2402:ARG:NH2	2.50	0.42
1:J:9:PRO:HD2	2:K:748:LEU:HD11	2.01	0.42
2:K:372:LEU:HD23	2:K:403:LEU:HD11	2.02	0.42
2:K:2716:GLU:HA	2:K:2719:GLU:HB2	2.01	0.42
2:B:3777:LYS:HB2	2:B:3777:LYS:HE3	1.87	0.42
2:B:3804:LEU:HB3	2:B:3885:SER:OG	2.20	0.42
2:E:237:LEU:HB2	2:E:404:ASN:HB3	2.02	0.42
2:E:675:TYR:CZ	2:E:790:PRO:HB3	2.55	0.42
2:E:676:GLU:HG3	2:E:814:LEU:HB3	2.01	0.42
2:E:3683:LEU:HD11	2:E:3747:ALA:HB3	2.02	0.42
2:H:675:TYR:CZ	2:H:790:PRO:HB3	2.55	0.42
2:H:940:LEU:HD23	2:H:940:LEU:HA	1.89	0.42
2:H:1714:TYR:CD1	2:H:1761:MET:HB3	2.54	0.42
2:H:4597:PRO:HA	2:H:4600:ILE:HG22	2.01	0.42
2:K:2880:ALA:O	2:K:2884:ALA:N	2.49	0.42
2:K:3925:ILE:HD11	2:K:3936:LEU:HD13	2.02	0.42
1:A:77:THR:HB	1:A:80:VAL:HG23	2.01	0.42
2:B:1846:ILE:HG23	2:B:1894:LEU:HB3	2.02	0.42
2:E:195:SER:OG	2:E:196:TYR:N	2.53	0.42
2:E:881:ILE:O	2:E:885:LEU:HB2	2.20	0.42
2:E:1210:ALA:N	2:E:1211:GLN:OE1	2.51	0.42
2:E:1466:THR:HG22	2:E:1482:ARG:HG2	2.01	0.42
2:E:2029:ARG:O	2:E:2032:SER:OG	2.28	0.42
2:E:3605:ARG:HH12	3:F:82:SER:HB3	1.85	0.42
2:H:372:LEU:HD23	2:H:403:LEU:HD11	2.02	0.42
2:H:2213:LYS:HA	2:H:2254:LEU:HD21	2.02	0.42
2:H:2716:GLU:HA	2:H:2719:GLU:HB2	2.01	0.42
2:K:73:LEU:HB3	2:K:77:ALA:HB3	2.02	0.42
2:K:675:TYR:CZ	2:K:790:PRO:HB3	2.55	0.42
2:K:1118:SER:HB2	2:K:1122:CYS:SG	2.60	0.42
1:A:9:PRO:HD2	2:B:748:LEU:HD11	2.01	0.41
2:B:76:ARG:CZ	2:E:3806:LEU:HD21	2.50	0.41
2:B:425:LEU:HD21	2:B:452:VAL:HG13	2.01	0.41
2:B:755:ILE:HA	2:B:770:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4521:TYR:HD1	2:B:4521:TYR:HA	1.72	0.41
2:E:394:HIS:CD2	2:E:397:GLY:H	2.38	0.41
2:E:4027:LEU:HD22	2:E:4056:HIS:HB3	2.02	0.41
2:H:73:LEU:HB3	2:H:77:ALA:HB3	2.02	0.41
2:H:195:SER:OG	2:H:196:TYR:N	2.53	0.41
2:H:1446:ILE:O	2:H:1540:PHE:N	2.42	0.41
2:H:4011:VAL:HA	2:H:4014:ILE:HG12	2.00	0.41
2:K:195:SER:OG	2:K:196:TYR:N	2.53	0.41
2:K:1683:PRO:HA	2:K:1686:LEU:HD12	2.02	0.41
2:K:1846:ILE:HG23	2:K:1894:LEU:HB3	2.02	0.41
2:K:3804:LEU:HB3	2:K:3885:SER:OG	2.20	0.41
2:K:3987:LEU:HG	2:K:3990:ASN:HD21	1.85	0.41
2:B:2773:ARG:HD3	2:B:2777:LYS:HE3	2.02	0.41
2:H:1683:PRO:HA	2:H:1686:LEU:HD12	2.02	0.41
2:H:3804:LEU:HB3	2:H:3885:SER:OG	2.20	0.41
2:H:3925:ILE:HD11	2:H:3936:LEU:HD13	2.02	0.41
2:H:4780:TYR:OH	2:K:4515:ASN:HB3	2.19	0.41
2:K:2433:LEU:HD22	2:K:2488:LEU:HD22	2.01	0.41
2:B:1683:PRO:HA	2:B:1686:LEU:HD12	2.02	0.41
2:E:983:LEU:HD23	2:E:1056:THR:HA	2.02	0.41
2:E:1705:LEU:HD23	2:E:1705:LEU:HA	1.90	0.41
2:E:1836:ASN:HA	2:E:1839:LEU:HB2	2.01	0.41
2:E:2213:LYS:HA	2:E:2254:LEU:HD21	2.02	0.41
2:E:2773:ARG:HD3	2:E:2777:LYS:HE3	2.03	0.41
2:E:3683:LEU:HD23	2:E:3683:LEU:HA	1.92	0.41
2:E:3804:LEU:HB3	2:E:3885:SER:OG	2.20	0.41
2:H:394:HIS:CD2	2:H:397:GLY:H	2.38	0.41
2:H:745:ASN:HB3	2:H:747:HIS:HB2	2.02	0.41
2:H:3804:LEU:HD22	2:H:3886:ILE:HD13	2.02	0.41
2:K:1057:LEU:O	2:K:1062:TYR:N	2.51	0.41
2:K:1228:THR:HA	2:K:1232:LEU:HD12	2.01	0.41
2:K:4027:LEU:HD22	2:K:4056:HIS:HB3	2.02	0.41
2:B:195:SER:OG	2:B:196:TYR:N	2.53	0.41
2:B:881:ILE:O	2:B:885:LEU:HB2	2.20	0.41
2:B:1268:ILE:HD11	2:B:1300:MET:HG3	2.01	0.41
2:B:3831:LEU:HD13	2:B:3831:LEU:HA	1.97	0.41
2:E:1739:PHE:HA	2:E:1740:PRO:HD3	1.91	0.41
1:G:9:PRO:HD2	2:H:748:LEU:HD11	2.01	0.41
2:H:16:THR:OG1	2:H:111:ARG:O	2.29	0.41
2:H:1118:SER:HB2	2:H:1122:CYS:SG	2.60	0.41
2:K:750:ARG:N	2:K:753:ASP:OD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1092:LYS:H	2:B:1250:TRP:HZ3	1.67	0.41
2:B:1466:THR:HG22	2:B:1482:ARG:HG2	2.02	0.41
2:B:1689:ILE:HA	2:B:1703:TYR:CE1	2.56	0.41
2:B:1730:THR:O	2:B:1733:THR:OG1	2.28	0.41
2:E:73:LEU:HB3	2:E:77:ALA:HB3	2.02	0.41
2:E:717:GLY:H	2:E:722:LEU:HB3	1.85	0.41
2:E:4891:ILE:HD11	2:E:4916:LEU:HD13	2.03	0.41
2:H:143:LEU:HD13	2:K:2426:SER:HG	1.83	0.41
2:H:237:LEU:HB2	2:H:404:ASN:HB3	2.02	0.41
2:H:1510:VAL:HG12	2:H:1511:VAL:HG23	2.03	0.41
2:H:1689:ILE:HA	2:H:1703:TYR:CE1	2.56	0.41
2:H:2349:GLU:HA	2:H:2352:ILE:HD11	2.03	0.41
1:J:77:THR:HB	1:J:80:VAL:HG23	2.01	0.41
2:K:1091:GLU:HB3	2:K:1094:TYR:HD2	1.86	0.41
2:K:1268:ILE:HD11	2:K:1300:MET:HG3	2.02	0.41
2:K:3677:LEU:HD23	2:K:3677:LEU:HA	1.90	0.41
2:B:1118:SER:HB2	2:B:1122:CYS:SG	2.60	0.41
2:B:3683:LEU:HD11	2:B:3747:ALA:HB3	2.02	0.41
2:B:4910:THR:HG21	7:B:6003:ATP:C4	2.55	0.41
2:E:1124:PRO:HG2	2:E:1598:ARG:HG3	2.01	0.41
2:E:1640:ASP:OD1	2:E:1640:ASP:N	2.44	0.41
2:E:1683:PRO:HA	2:E:1686:LEU:HD12	2.02	0.41
2:E:1689:ILE:HA	2:E:1703:TYR:CE1	2.56	0.41
2:E:3925:ILE:HD11	2:E:3936:LEU:HD13	2.02	0.41
2:E:4052:ALA:O	2:E:4056:HIS:ND1	2.54	0.41
2:H:432:GLY:HA3	2:H:447:LEU:HG	2.03	0.41
2:H:755:ILE:HA	2:H:770:ILE:HD13	2.02	0.41
2:H:2834:LEU:HD13	2:H:2838:LEU:HB3	2.01	0.41
2:H:4020:MET:HE2	2:H:4067:LEU:HD13	2.02	0.41
2:K:123:HIS:CD2	2:K:126:SER:H	2.23	0.41
2:K:983:LEU:HD23	2:K:1056:THR:HA	2.02	0.41
2:K:4597:PRO:HA	2:K:4600:ILE:HG22	2.01	0.41
2:B:1733:THR:HA	2:B:1755:THR:HG21	2.03	0.41
2:B:1757:LEU:HD13	2:B:1757:LEU:HA	1.88	0.41
2:B:3804:LEU:HD22	2:B:3886:ILE:HD13	2.02	0.41
2:B:4891:ILE:HD11	2:B:4916:LEU:HD13	2.03	0.41
2:E:150:GLN:NE2	2:E:158:CYS:SG	2.85	0.41
2:E:1091:GLU:HB3	2:E:1094:TYR:HD2	1.86	0.41
2:K:677:LEU:HD23	2:K:802:PHE:HA	2.03	0.41
2:K:1510:VAL:HG12	2:K:1511:VAL:HG23	2.03	0.41
2:B:372:LEU:HD23	2:B:403:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1601:ASN:ND2	2:B:1643:GLU:OE2	2.36	0.41
2:B:4848:ASP:CB	2:E:4819:TYR:CE1	2.95	0.41
2:E:1092:LYS:H	2:E:1250:TRP:HZ3	1.66	0.41
2:E:1306:MET:HB2	2:E:1575:HIS:HE2	1.86	0.41
2:E:1733:THR:HA	2:E:1755:THR:HG21	2.03	0.41
2:E:4793:PHE:HD1	2:E:4833:GLU:HB2	1.86	0.41
2:H:2416:GLU:HB3	2:H:2419:ARG:HH21	1.85	0.41
2:H:3911:ILE:HD13	2:H:3911:ILE:HA	1.94	0.41
2:K:643:LEU:H	2:K:643:LEU:HG	1.60	0.41
2:K:1124:PRO:HG2	2:K:1598:ARG:HG3	2.01	0.41
2:K:2213:LYS:HA	2:K:2254:LEU:HD21	2.02	0.41
2:K:4052:ALA:O	2:K:4056:HIS:ND1	2.54	0.41
2:K:4910:THR:HG21	7:K:6003:ATP:C4	2.56	0.41
2:B:227:TYR:HE1	2:B:355:LYS:HG2	1.86	0.41
2:B:750:ARG:N	2:B:753:ASP:OD2	2.46	0.41
2:B:2213:LYS:HA	2:B:2254:LEU:HD21	2.02	0.41
2:B:3806:LEU:HD21	2:K:76:ARG:CZ	2.50	0.41
2:B:3925:ILE:HD11	2:B:3936:LEU:HD13	2.02	0.41
2:B:3966:ILE:H	2:B:3966:ILE:HG13	1.70	0.41
2:B:3987:LEU:HG	2:B:3990:ASN:HD21	1.85	0.41
2:B:4806:LYS:O	2:B:4807:CYS:SG	2.73	0.41
2:B:4953:PHE:HA	2:B:4954:PRO:HD3	1.94	0.41
2:E:372:LEU:HD23	2:E:403:LEU:HD11	2.02	0.41
2:E:432:GLY:HA3	2:E:447:LEU:HG	2.03	0.41
2:E:530:LEU:HD23	2:E:530:LEU:HA	1.91	0.41
2:E:1268:ILE:HD11	2:E:1300:MET:HG3	2.01	0.41
2:E:1846:ILE:HG23	2:E:1894:LEU:HB3	2.02	0.41
2:E:3677:LEU:HD23	2:E:3677:LEU:HA	1.91	0.41
2:E:4809:ASP:HB2	2:E:4812:THR:CG2	2.51	0.41
2:H:80:GLU:HG3	2:K:3891:TRP:CZ3	2.51	0.41
2:H:143:LEU:HD12	2:K:2427:LEU:HD11	2.01	0.41
2:H:238:HIS:N	2:H:243:GLU:O	2.43	0.41
2:H:506:HIS:CE1	2:H:564:ARG:HG2	2.56	0.41
2:H:657:PRO:HB3	2:H:834:VAL:HG22	2.03	0.41
2:H:1733:THR:HA	2:H:1755:THR:HG21	2.03	0.41
2:H:4027:LEU:HD22	2:H:4056:HIS:HB3	2.02	0.41
2:H:4100:ALA:O	2:H:4104:THR:OG1	2.33	0.41
2:H:4910:THR:HG21	7:H:6003:ATP:C4	2.55	0.41
2:K:506:HIS:CE1	2:K:564:ARG:HG2	2.56	0.41
2:K:717:GLY:H	2:K:722:LEU:HB3	1.85	0.41
2:K:881:ILE:O	2:K:885:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1689:ILE:HA	2:K:1703:TYR:CE1	2.56	0.41
2:K:1986:GLU:N	2:K:1989:CYS:SG	2.73	0.41
2:K:2349:GLU:HA	2:K:2352:ILE:HD11	2.03	0.41
2:K:3804:LEU:HD22	2:K:3886:ILE:HD13	2.02	0.41
2:K:4891:ILE:HD11	2:K:4916:LEU:HD13	2.03	0.41
2:B:618:CYS:SG	2:B:629:GLN:NE2	2.93	0.41
2:B:717:GLY:H	2:B:722:LEU:HB3	1.85	0.41
2:B:1306:MET:HB2	2:B:1575:HIS:HE2	1.85	0.41
2:B:4027:LEU:HD22	2:B:4056:HIS:HB3	2.02	0.41
2:B:4127:LEU:O	2:B:4131:GLN:N	2.54	0.41
2:E:1118:SER:HB2	2:E:1122:CYS:SG	2.60	0.41
1:G:27:THR:HG23	1:G:100:ASP:HB3	2.03	0.41
2:H:717:GLY:H	2:H:722:LEU:HB3	1.85	0.41
2:H:881:ILE:O	2:H:885:LEU:HB2	2.20	0.41
2:H:1846:ILE:HG23	2:H:1894:LEU:HB3	2.02	0.41
2:K:1057:LEU:HB3	2:K:1062:TYR:HB2	2.03	0.41
2:K:4127:LEU:O	2:K:4131:GLN:N	2.54	0.41
2:B:432:GLY:HA3	2:B:447:LEU:HG	2.03	0.40
2:E:1644:LEU:HD21	2:E:1651:LEU:HA	2.03	0.40
2:E:3804:LEU:HD22	2:E:3886:ILE:HD13	2.02	0.40
2:E:3831:LEU:HD23	2:E:3906:ASN:HD21	1.86	0.40
2:H:227:TYR:HE1	2:H:355:LYS:HG2	1.86	0.40
2:H:983:LEU:HD23	2:H:1056:THR:HA	2.02	0.40
2:H:2201:LEU:HD23	2:H:2201:LEU:HA	1.92	0.40
2:H:2773:ARG:HD3	2:H:2777:LYS:HE3	2.02	0.40
2:H:3683:LEU:HD11	2:H:3747:ALA:HB3	2.02	0.40
2:H:4809:ASP:HB2	2:H:4812:THR:CG2	2.51	0.40
2:K:150:GLN:NE2	2:K:158:CYS:SG	2.85	0.40
2:K:228:LEU:HB3	2:K:289:ILE:HB	2.04	0.40
2:K:432:GLY:HA3	2:K:447:LEU:HG	2.03	0.40
2:K:1177:LEU:N	2:K:1180:GLU:O	2.55	0.40
2:K:1644:LEU:HD21	2:K:1651:LEU:HA	2.04	0.40
2:K:1733:THR:HA	2:K:1755:THR:HG21	2.03	0.40
2:K:2416:GLU:HB3	2:K:2419:ARG:HH21	1.85	0.40
2:K:2759:LYS:HA	2:K:2760:PRO:HD3	1.92	0.40
2:K:3683:LEU:HD11	2:K:3747:ALA:HB3	2.02	0.40
2:K:3777:LYS:HE3	2:K:3777:LYS:HB2	1.87	0.40
2:B:1091:GLU:HB3	2:B:1094:TYR:HD2	1.86	0.40
2:B:1785:ASP:OD1	2:B:1788:LYS:NZ	2.50	0.40
2:B:2398:ASP:OD1	2:B:2402:ARG:NH2	2.50	0.40
2:B:4793:PHE:HD1	2:B:4833:GLU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:145:PHE:HD1	2:E:145:PHE:HA	1.76	0.40
2:E:506:HIS:CE1	2:E:564:ARG:HG2	2.56	0.40
2:E:1057:LEU:HB3	2:E:1062:TYR:HB2	2.03	0.40
2:E:1445:TRP:N	2:E:1487:MET:HB2	2.36	0.40
2:E:4020:MET:HE2	2:E:4067:LEU:HD13	2.03	0.40
2:H:228:LEU:HB3	2:H:289:ILE:HB	2.04	0.40
2:H:608:HIS:HB2	2:H:1656:HIS:CD2	2.57	0.40
2:H:1177:LEU:N	2:H:1180:GLU:O	2.55	0.40
2:H:1268:ILE:HD11	2:H:1300:MET:HG3	2.01	0.40
2:H:4582:VAL:O	2:H:4586:PHE:HB2	2.21	0.40
2:H:4793:PHE:HD1	2:H:4833:GLU:HB2	1.86	0.40
2:K:1445:TRP:N	2:K:1487:MET:HB2	2.36	0.40
2:B:1177:LEU:N	2:B:1180:GLU:O	2.55	0.40
2:B:1510:VAL:HG12	2:B:1511:VAL:HG23	2.03	0.40
2:B:4168:GLU:HG3	2:B:4171:ARG:HH11	1.85	0.40
2:E:1162:VAL:O	2:E:1176:THR:OG1	2.33	0.40
2:H:236:LEU:HD12	2:H:236:LEU:HA	1.92	0.40
2:H:1445:TRP:N	2:H:1487:MET:HB2	2.36	0.40
2:H:1644:LEU:HD21	2:H:1651:LEU:HA	2.04	0.40
2:H:4052:ALA:O	2:H:4056:HIS:ND1	2.54	0.40
2:H:4891:ILE:HD11	2:H:4916:LEU:HD13	2.03	0.40
1:J:27:THR:HG23	1:J:100:ASP:HB3	2.03	0.40
2:K:1306:MET:HB2	2:K:1575:HIS:HE2	1.85	0.40
2:K:1446:ILE:O	2:K:1540:PHE:N	2.42	0.40
2:K:2168:MET:H	2:K:2168:MET:HG3	1.74	0.40
2:K:2773:ARG:HD3	2:K:2777:LYS:HE3	2.02	0.40
2:B:163:HIS:HA	2:B:164:PRO:HD3	1.93	0.40
2:B:227:TYR:CE1	2:B:355:LYS:HG2	2.57	0.40
2:B:1014:GLN:HA	2:B:1029:ASN:HB2	2.03	0.40
2:B:2103:LEU:HD23	2:B:2103:LEU:HA	1.92	0.40
2:B:4052:ALA:O	2:B:4056:HIS:ND1	2.54	0.40
2:E:643:LEU:H	2:E:643:LEU:HG	1.60	0.40
2:E:1014:GLN:HA	2:E:1029:ASN:HB2	2.03	0.40
2:E:4780:TYR:OH	2:H:4515:ASN:HB3	2.22	0.40
2:E:4910:THR:HG21	7:E:6003:ATP:C4	2.55	0.40
2:E:4945:TYR:OH	6:E:6002:CFF:H81	2.22	0.40
2:H:76:ARG:CZ	2:K:3806:LEU:HD21	2.51	0.40
2:H:123:HIS:CD2	2:H:126:SER:H	2.23	0.40
2:H:227:TYR:CE1	2:H:355:LYS:HG2	2.57	0.40
2:B:228:LEU:HB3	2:B:289:ILE:HB	2.04	0.40
2:B:657:PRO:HB3	2:B:834:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1809:PRO:O	2:B:1812:GLY:N	2.55	0.40
2:B:1993:ILE:HG23	3:C:112:ASN:HA	2.03	0.40
2:B:4945:TYR:OH	6:B:6002:CFF:H81	2.22	0.40
2:E:228:LEU:HB3	2:E:289:ILE:HB	2.04	0.40
2:E:608:HIS:HB2	2:E:1656:HIS:CD2	2.57	0.40
2:E:2088:LEU:HD23	2:E:2088:LEU:HA	1.89	0.40
2:E:2349:GLU:HA	2:E:2352:ILE:HD11	2.03	0.40
2:E:4668:SER:O	2:E:4672:GLY:N	2.54	0.40
2:H:1446:ILE:HB	2:H:1540:PHE:HB2	2.04	0.40
2:H:1993:ILE:HG23	3:I:112:ASN:HA	2.03	0.40
2:H:3804:LEU:HD13	2:H:3910:ALA:HB2	2.04	0.40
2:H:3831:LEU:HD23	2:H:3906:ASN:HD21	1.86	0.40
2:H:4923:LEU:HD12	2:H:4923:LEU:HA	1.93	0.40
2:K:64:ILE:H	2:K:64:ILE:HG13	1.74	0.40
2:K:439:LYS:HE3	2:K:439:LYS:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	G	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3386/4968 (68%)	2990 (88%)	383 (11%)	13 (0%)	34	72
2	E	3386/4968 (68%)	2986 (88%)	387 (11%)	13 (0%)	34	72
2	H	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	34	72
2	K	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
3	F	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
3	I	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
3	L	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
All	All	14492/20900 (69%)	12806 (88%)	1630 (11%)	56 (0%)	38	72

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1477	HIS
2	E	1477	HIS
2	H	1477	HIS
2	K	1477	HIS
2	B	1580	PRO
2	B	4916	LEU
3	C	130	ASP
2	E	1580	PRO
2	E	4916	LEU
3	F	130	ASP
2	H	1580	PRO
2	H	4916	LEU
3	I	130	ASP
2	K	1580	PRO
2	K	4916	LEU
3	L	130	ASP
2	B	730	LEU
2	B	1581	GLN
2	B	4071	ALA
2	E	730	LEU
2	E	1581	GLN
2	E	4071	ALA
2	H	730	LEU
2	H	1581	GLN
2	H	4071	ALA
2	K	730	LEU
2	K	1581	GLN
2	K	4071	ALA
2	B	3802	SER
2	E	3802	SER
2	H	3802	SER
2	K	3802	SER

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Mol	Chain	Res	Type
2	B	853	PRO
2	E	853	PRO
2	H	853	PRO
2	K	853	PRO
2	B	3801	CYS
2	B	4164	PRO
2	E	3801	CYS
2	E	4164	PRO
2	H	3801	CYS
2	H	4164	PRO
2	K	3801	CYS
2	K	4164	PRO
2	B	1535	PRO
2	E	1535	PRO
2	H	1535	PRO
2	K	1535	PRO
2	B	828	PRO
2	B	1848	PRO
2	E	828	PRO
2	E	1848	PRO
2	H	828	PRO
2	H	1848	PRO
2	K	828	PRO
2	K	1848	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%)	86 (98%)	2 (2%)	50	70
1	D	88/89 (99%)	86 (98%)	2 (2%)	50	70
1	G	88/89 (99%)	86 (98%)	2 (2%)	50	70
1	J	88/89 (99%)	86 (98%)	2 (2%)	50	70
2	B	2698/4355 (62%)	2670 (99%)	28 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	2698/4355 (62%)	2670 (99%)	28 (1%)	76	86
2	H	2699/4355 (62%)	2670 (99%)	29 (1%)	73	84
2	K	2699/4355 (62%)	2670 (99%)	29 (1%)	73	84
3	C	115/123 (94%)	114 (99%)	1 (1%)	78	87
3	F	115/123 (94%)	114 (99%)	1 (1%)	78	87
3	I	115/123 (94%)	114 (99%)	1 (1%)	78	87
3	L	115/123 (94%)	114 (99%)	1 (1%)	78	87
All	All	11606/18268 (64%)	11480 (99%)	126 (1%)	74	84

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	42	ARG
2	B	44	ASN
2	B	57	ASN
2	B	439	LYS
2	B	487	ASN
2	B	531	ASN
2	B	658	ASN
2	B	841	LYS
2	B	881	ILE
2	B	925	PRO
2	B	990	PRO
2	B	1042	THR
2	B	1054	VAL
2	B	1089	ARG
2	B	1760	ARG
2	B	1761	MET
2	B	2196	ASN
2	B	2199	ARG
2	B	2211	ASN
2	B	2328	ARG
2	B	2420	ILE
2	B	3726	LEU
2	B	3906	ASN
2	B	4136	ARG
2	B	4206	GLN
2	B	4499	ASN
2	B	4521	TYR

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Mol	Chain	Res	Type
2	B	4652	ARG
2	B	4788	ASN
3	C	116	LYS
1	D	13	ARG
1	D	42	ARG
2	E	44	ASN
2	E	57	ASN
2	E	439	LYS
2	E	487	ASN
2	E	531	ASN
2	E	658	ASN
2	E	841	LYS
2	E	881	ILE
2	E	925	PRO
2	E	990	PRO
2	E	1042	THR
2	E	1054	VAL
2	E	1089	ARG
2	E	1760	ARG
2	E	1761	MET
2	E	2196	ASN
2	E	2199	ARG
2	E	2211	ASN
2	E	2328	ARG
2	E	2420	ILE
2	E	3726	LEU
2	E	3906	ASN
2	E	4136	ARG
2	E	4206	GLN
2	E	4499	ASN
2	E	4521	TYR
2	E	4652	ARG
2	E	4788	ASN
3	F	116	LYS
1	G	13	ARG
1	G	42	ARG
2	H	44	ASN
2	H	57	ASN
2	H	439	LYS
2	H	487	ASN
2	H	531	ASN
2	H	658	ASN

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Mol	Chain	Res	Type
2	H	841	LYS
2	H	881	ILE
2	H	925	PRO
2	H	950	VAL
2	H	990	PRO
2	H	1042	THR
2	H	1054	VAL
2	H	1089	ARG
2	H	1760	ARG
2	H	1761	MET
2	H	2196	ASN
2	H	2199	ARG
2	H	2211	ASN
2	H	2328	ARG
2	H	2420	ILE
2	H	3726	LEU
2	H	3906	ASN
2	H	4136	ARG
2	H	4206	GLN
2	H	4499	ASN
2	H	4521	TYR
2	H	4652	ARG
2	H	4788	ASN
3	I	116	LYS
1	J	13	ARG
1	J	42	ARG
2	K	44	ASN
2	K	57	ASN
2	K	439	LYS
2	K	487	ASN
2	K	531	ASN
2	K	658	ASN
2	K	841	LYS
2	K	881	ILE
2	K	925	PRO
2	K	950	VAL
2	K	990	PRO
2	K	1042	THR
2	K	1054	VAL
2	K	1089	ARG
2	K	1760	ARG
2	K	1761	MET

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Mol	Chain	Res	Type
2	K	2196	ASN
2	K	2199	ARG
2	K	2211	ASN
2	K	2328	ARG
2	K	2420	ILE
2	K	3726	LEU
2	K	3906	ASN
2	K	4136	ARG
2	K	4206	GLN
2	K	4499	ASN
2	K	4521	TYR
2	K	4652	ARG
2	K	4788	ASN
3	L	116	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	44	ASN
2	B	57	ASN
2	B	123	HIS
2	B	252	HIS
2	B	261	HIS
2	B	293	GLN
2	B	375	GLN
2	B	394	HIS
2	B	476	GLN
2	B	486	GLN
2	B	487	ASN
2	B	531	ASN
2	B	544	ASN
2	B	621	HIS
2	B	635	ASN
2	B	776	GLN
2	B	1146	HIS
2	B	1147	GLN
2	B	1149	ASN
2	B	1242	ASN
2	B	1265	HIS
2	B	1587	HIS
2	B	1656	HIS
2	B	1669	ASN

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Mol	Chain	Res	Type
2	B	1722	ASN
2	B	1746	HIS
2	B	2090	HIS
2	B	2211	ASN
2	B	2212	GLN
2	B	2251	ASN
2	B	2310	ASN
2	B	2711	ASN
2	B	2820	HIS
2	B	3666	HIS
2	B	3902	GLN
2	B	3904	GLN
2	B	3954	HIS
2	B	3965	GLN
2	B	3976	GLN
2	B	3993	ASN
2	B	4089	HIS
2	B	4128	ASN
2	B	4494	ASN
2	B	4499	ASN
2	B	4621	GLN
2	E	44	ASN
2	E	57	ASN
2	E	123	HIS
2	E	150	GLN
2	E	252	HIS
2	E	261	HIS
2	E	293	GLN
2	E	375	GLN
2	E	394	HIS
2	E	476	GLN
2	E	486	GLN
2	E	487	ASN
2	E	531	ASN
2	E	544	ASN
2	E	621	HIS
2	E	635	ASN
2	E	776	GLN
2	E	1146	HIS
2	E	1147	GLN
2	E	1149	ASN
2	E	1242	ASN

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Mol	Chain	Res	Type
2	E	1265	HIS
2	E	1587	HIS
2	E	1656	HIS
2	E	1669	ASN
2	E	1722	ASN
2	E	1746	HIS
2	E	2090	HIS
2	E	2211	ASN
2	E	2212	GLN
2	E	2251	ASN
2	E	2310	ASN
2	E	2711	ASN
2	E	2820	HIS
2	E	3666	HIS
2	E	3902	GLN
2	E	3904	GLN
2	E	3954	HIS
2	E	3965	GLN
2	E	3976	GLN
2	E	3993	ASN
2	E	4089	HIS
2	E	4128	ASN
2	E	4494	ASN
2	E	4499	ASN
2	E	4559	HIS
2	E	4621	GLN
3	F	136	GLN
2	H	44	ASN
2	H	57	ASN
2	H	123	HIS
2	H	150	GLN
2	H	252	HIS
2	H	261	HIS
2	H	293	GLN
2	H	375	GLN
2	H	394	HIS
2	H	476	GLN
2	H	486	GLN
2	H	487	ASN
2	H	531	ASN
2	H	544	ASN
2	H	621	HIS

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Mol	Chain	Res	Type
2	H	635	ASN
2	H	1146	HIS
2	H	1147	GLN
2	H	1149	ASN
2	H	1242	ASN
2	H	1265	HIS
2	H	1587	HIS
2	H	1656	HIS
2	H	1669	ASN
2	H	1722	ASN
2	H	1746	HIS
2	H	2090	HIS
2	H	2211	ASN
2	H	2212	GLN
2	H	2251	ASN
2	H	2310	ASN
2	H	2711	ASN
2	H	2820	HIS
2	H	3666	HIS
2	H	3902	GLN
2	H	3904	GLN
2	H	3954	HIS
2	H	3965	GLN
2	H	3976	GLN
2	H	3993	ASN
2	H	4089	HIS
2	H	4128	ASN
2	H	4494	ASN
2	H	4499	ASN
2	H	4621	GLN
2	K	44	ASN
2	K	57	ASN
2	K	123	HIS
2	K	150	GLN
2	K	252	HIS
2	K	261	HIS
2	K	293	GLN
2	K	375	GLN
2	K	394	HIS
2	K	476	GLN
2	K	486	GLN
2	K	487	ASN

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Mol	Chain	Res	Type
2	K	531	ASN
2	K	544	ASN
2	K	621	HIS
2	K	635	ASN
2	K	1146	HIS
2	K	1147	GLN
2	K	1149	ASN
2	K	1242	ASN
2	K	1265	HIS
2	K	1587	HIS
2	K	1656	HIS
2	K	1669	ASN
2	K	1722	ASN
2	K	1746	HIS
2	K	2090	HIS
2	K	2211	ASN
2	K	2212	GLN
2	K	2251	ASN
2	K	2310	ASN
2	K	2711	ASN
2	K	2820	HIS
2	K	2891	GLN
2	K	3666	HIS
2	K	3902	GLN
2	K	3904	GLN
2	K	3954	HIS
2	K	3965	GLN
2	K	3976	GLN
2	K	3993	ASN
2	K	4089	HIS
2	K	4128	ASN
2	K	4494	ASN
2	K	4499	ASN
2	K	4621	GLN

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 monosaccharides 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
6	CFF	K	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.27	1 (12%)
6	CFF	B	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.28	1 (12%)
7	ATP	E	6003	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	4 (12%)
7	ATP	H	6003	-	26,33,33	0.90	1 (3%)	31,52,52	1.55	4 (12%)
7	ATP	K	6003	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	4 (12%)
6	CFF	H	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.28	1 (12%)
6	CFF	E	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.28	1 (12%)
7	ATP	B	6003	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	4 (12%)

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
6	CFF	K	6002	-	-	-	0/2/2/2
7	ATP	E	6003	-	-	7/18/38/38	0/3/3/3
6	CFF	B	6002	-	-	-	0/2/2/2
7	ATP	H	6003	-	-	7/18/38/38	0/3/3/3
7	ATP	K	6003	-	-	7/18/38/38	0/3/3/3
6	CFF	H	6002	-	-	-	0/2/2/2
6	CFF	E	6002	-	-	-	0/2/2/2
7	ATP	B	6003	-	-	7/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6002	CFF	C5-C4	-4.92	1.32	1.39
6	E	6002	CFF	C5-C4	-4.91	1.32	1.39
6	H	6002	CFF	C5-C4	-4.91	1.32	1.39
6	K	6002	CFF	C5-C4	-4.91	1.32	1.39
6	E	6002	CFF	C6-N1	-4.82	1.31	1.38
6	B	6002	CFF	C6-N1	-4.79	1.31	1.38
6	H	6002	CFF	C6-N1	-4.79	1.31	1.38
6	K	6002	CFF	C6-N1	-4.79	1.31	1.38
6	B	6002	CFF	O13-C6	-2.33	1.18	1.24
6	E	6002	CFF	O13-C6	-2.33	1.18	1.24
6	H	6002	CFF	O13-C6	-2.33	1.18	1.24
6	K	6002	CFF	O13-C6	-2.33	1.18	1.24
6	K	6002	CFF	C5-C6	-2.19	1.37	1.41
6	B	6002	CFF	C5-C6	-2.16	1.37	1.41
6	H	6002	CFF	C5-C6	-2.16	1.37	1.41
6	E	6002	CFF	C5-C6	-2.13	1.37	1.41
7	B	6003	ATP	C5-C4	2.02	1.46	1.40
7	E	6003	ATP	C5-C4	2.02	1.46	1.40
7	H	6003	ATP	C5-C4	2.02	1.46	1.40
7	K	6003	ATP	C5-C4	2.02	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	6003	ATP	PA-O3A-PB	-3.41	121.14	132.83
7	H	6003	ATP	PA-O3A-PB	-3.41	121.14	132.83
7	E	6003	ATP	PA-O3A-PB	-3.40	121.14	132.83
7	K	6003	ATP	PA-O3A-PB	-3.40	121.16	132.83
7	B	6003	ATP	N3-C2-N1	-3.39	123.38	128.68
7	H	6003	ATP	N3-C2-N1	-3.38	123.39	128.68
7	E	6003	ATP	N3-C2-N1	-3.38	123.39	128.68
7	K	6003	ATP	N3-C2-N1	-3.38	123.40	128.68
7	B	6003	ATP	C3'-C2'-C1'	3.24	105.85	100.98
7	K	6003	ATP	C3'-C2'-C1'	3.24	105.85	100.98
7	H	6003	ATP	C3'-C2'-C1'	3.23	105.84	100.98
7	E	6003	ATP	C3'-C2'-C1'	3.22	105.82	100.98
6	B	6002	CFF	C14-N7-C8	-2.79	112.01	125.43
6	H	6002	CFF	C14-N7-C8	-2.79	112.01	125.43
6	E	6002	CFF	C14-N7-C8	-2.78	112.04	125.43
6	K	6002	CFF	C14-N7-C8	-2.78	112.04	125.43
7	K	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83
7	H	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83
7	E	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	6003	ATP	PB-O3B-PG-O2G
7	B	6003	ATP	PB-O3B-PG-O3G
7	B	6003	ATP	C5'-O5'-PA-O1A
7	B	6003	ATP	C5'-O5'-PA-O2A
7	E	6003	ATP	PB-O3B-PG-O2G
7	E	6003	ATP	PB-O3B-PG-O3G
7	E	6003	ATP	C5'-O5'-PA-O1A
7	E	6003	ATP	C5'-O5'-PA-O2A
7	H	6003	ATP	PB-O3B-PG-O2G
7	H	6003	ATP	PB-O3B-PG-O3G
7	H	6003	ATP	C5'-O5'-PA-O1A
7	H	6003	ATP	C5'-O5'-PA-O2A
7	K	6003	ATP	PB-O3B-PG-O2G
7	K	6003	ATP	PB-O3B-PG-O3G
7	K	6003	ATP	C5'-O5'-PA-O1A
7	K	6003	ATP	C5'-O5'-PA-O2A
7	B	6003	ATP	O4'-C4'-C5'-O5'
7	E	6003	ATP	O4'-C4'-C5'-O5'
7	H	6003	ATP	O4'-C4'-C5'-O5'
7	K	6003	ATP	O4'-C4'-C5'-O5'
7	B	6003	ATP	PB-O3A-PA-O1A
7	E	6003	ATP	PB-O3A-PA-O1A
7	H	6003	ATP	PB-O3A-PA-O1A
7	K	6003	ATP	PB-O3A-PA-O1A
7	B	6003	ATP	C5'-O5'-PA-O3A
7	E	6003	ATP	C5'-O5'-PA-O3A
7	H	6003	ATP	C5'-O5'-PA-O3A
7	K	6003	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 19 short contacts:

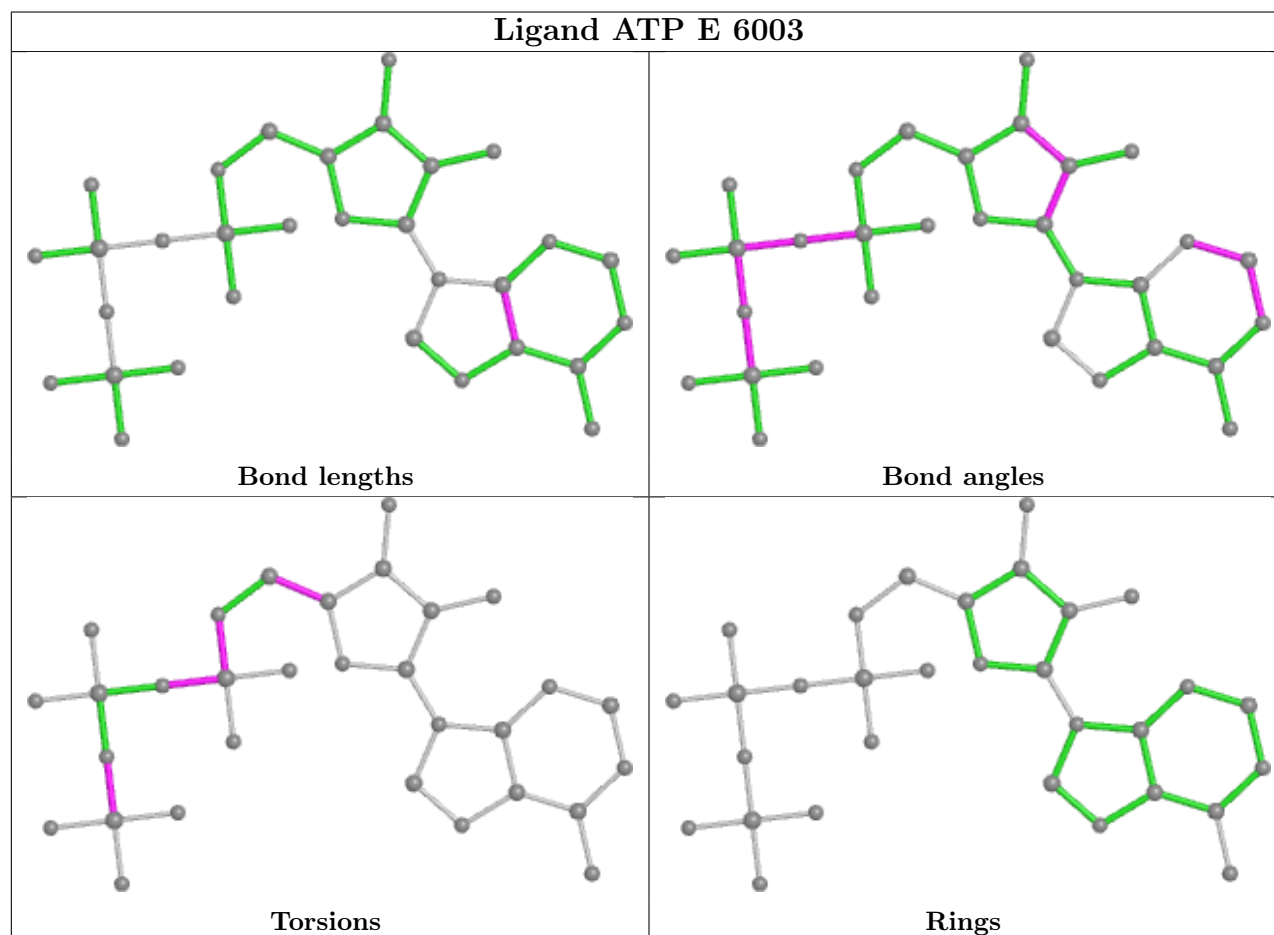
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	6002	CFF	1	0

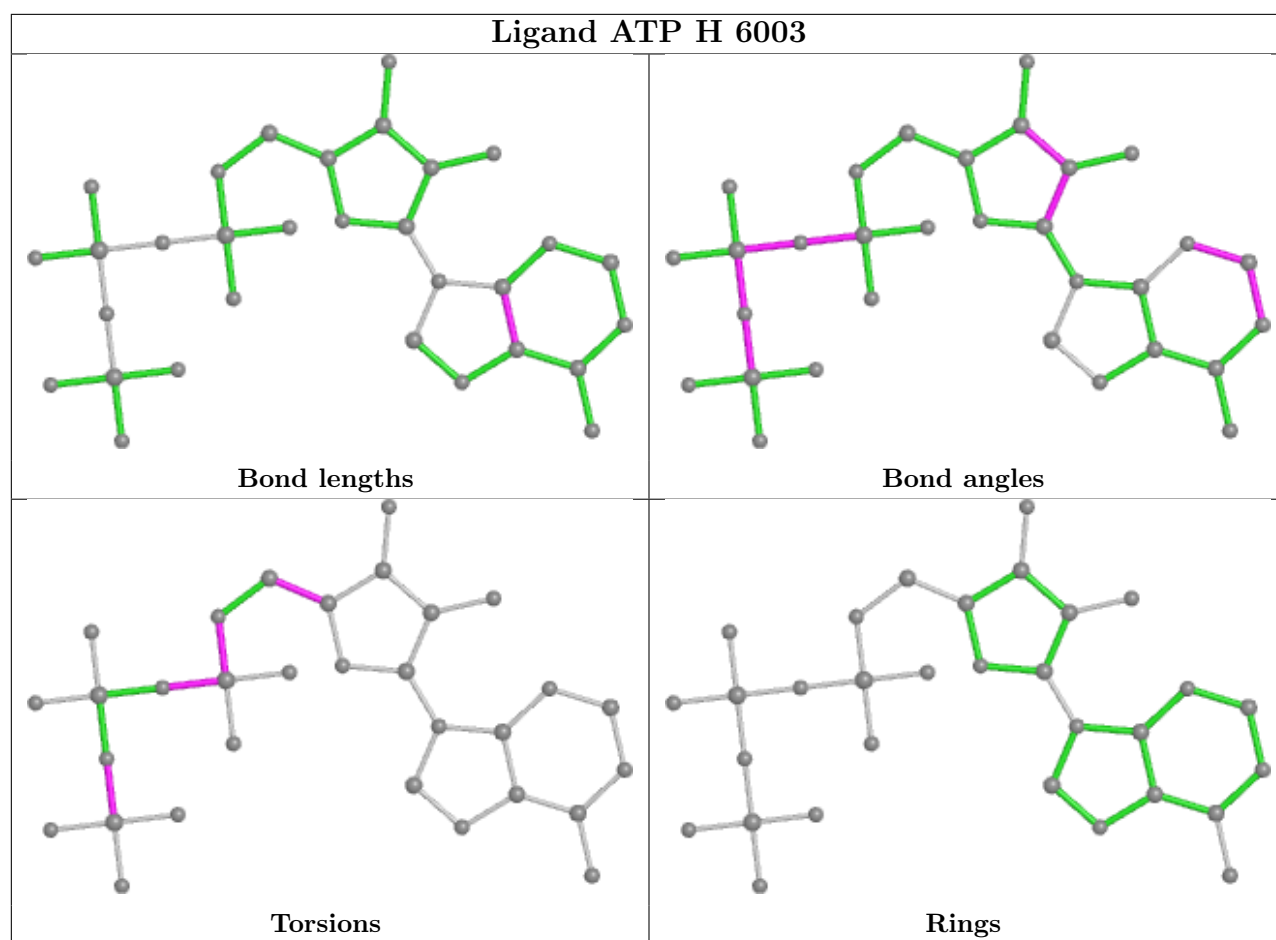
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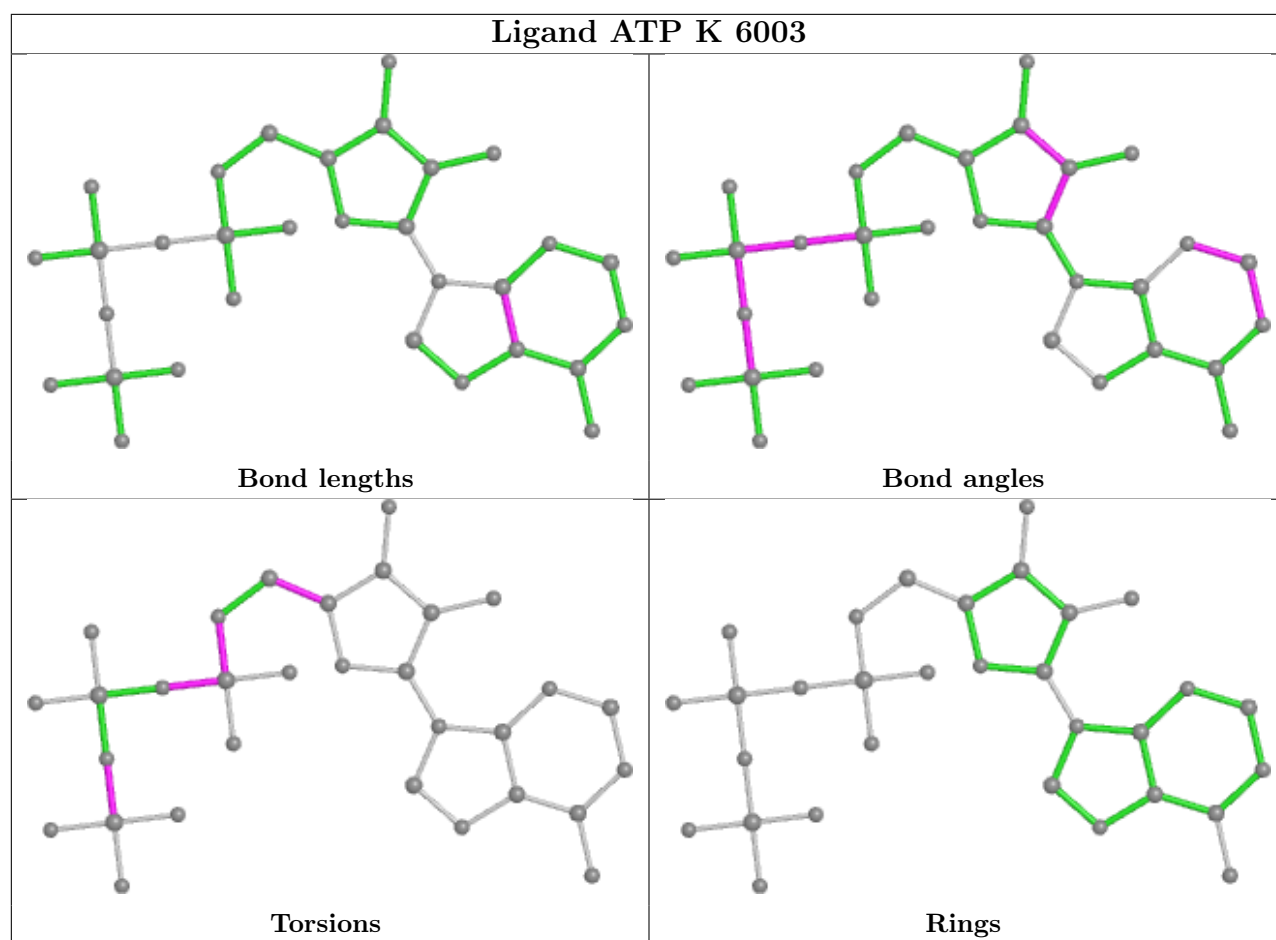
Continued from previous page...

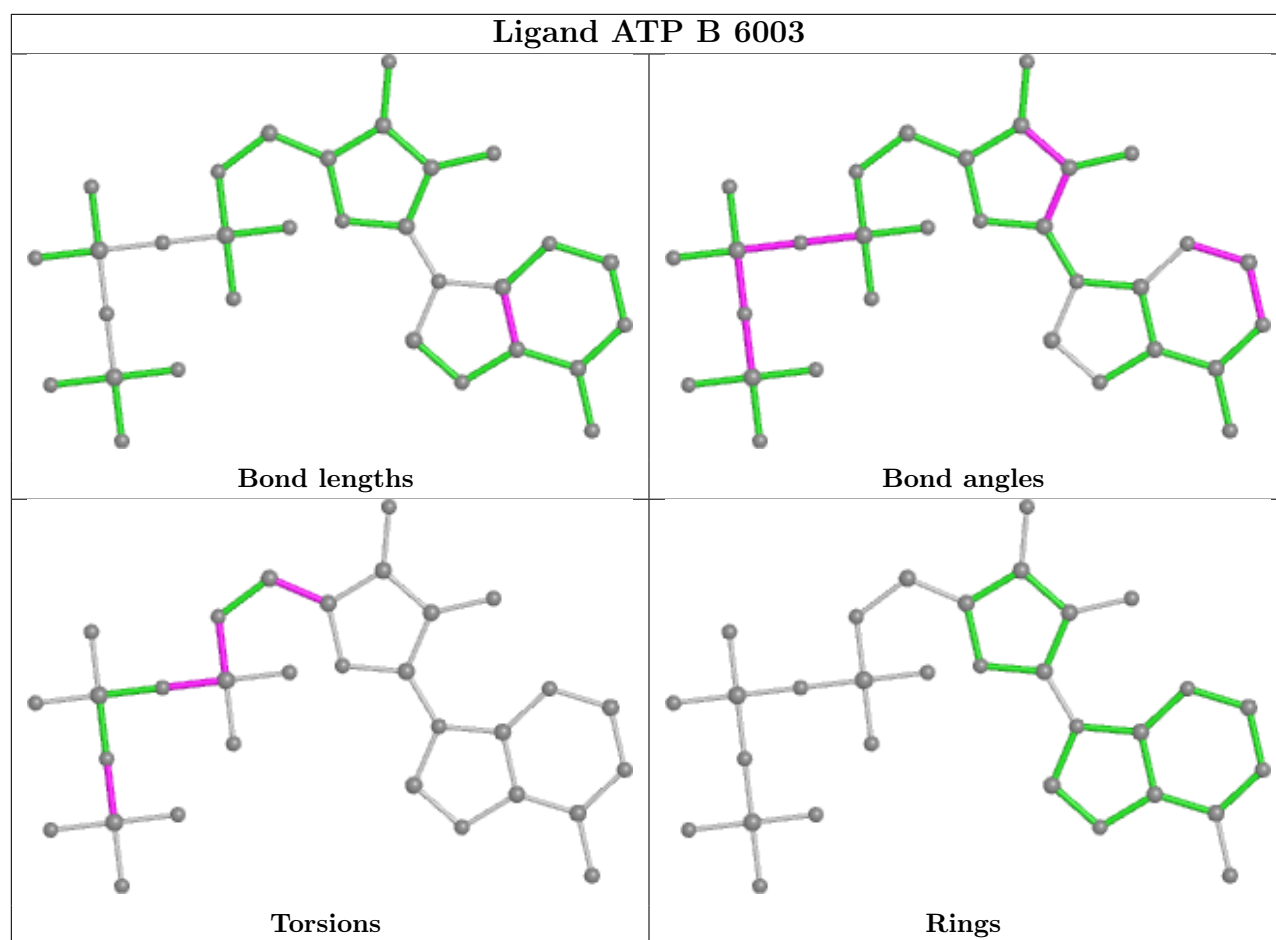
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	6003	ATP	4	0
7	H	6003	ATP	5	0
7	K	6003	ATP	4	0
6	E	6002	CFF	1	0
7	B	6003	ATP	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

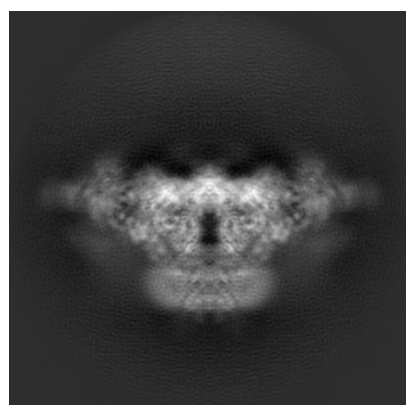
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9834. These allow visual inspection of the internal detail of the map and identification of artifacts.

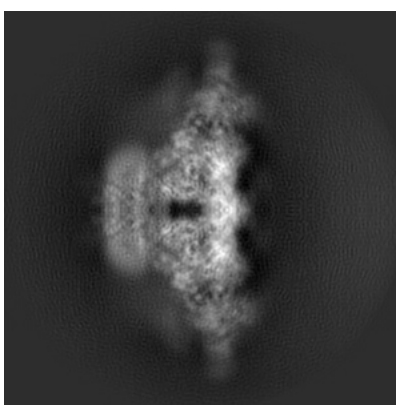
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

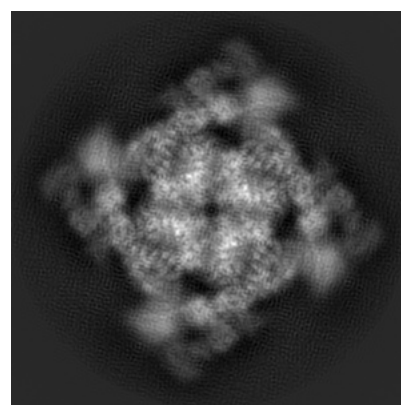
6.1.1 Primary map



X



Y

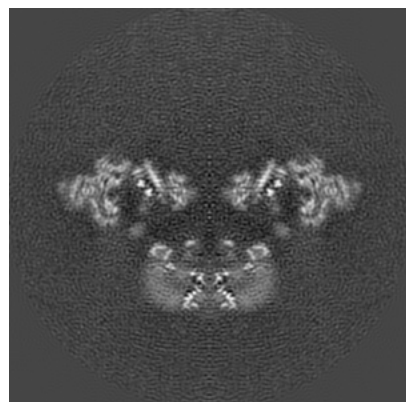


Z

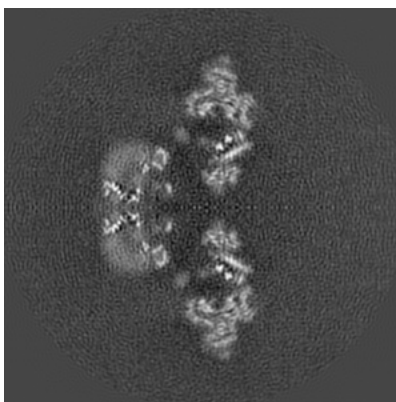
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

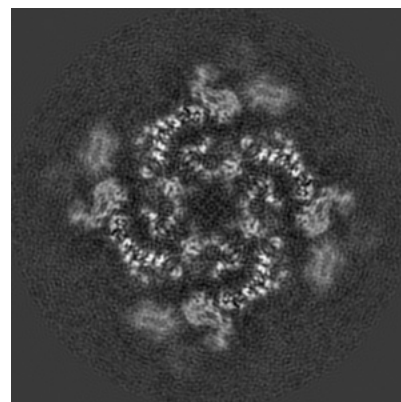
6.2.1 Primary map



X Index: 200



Y Index: 200

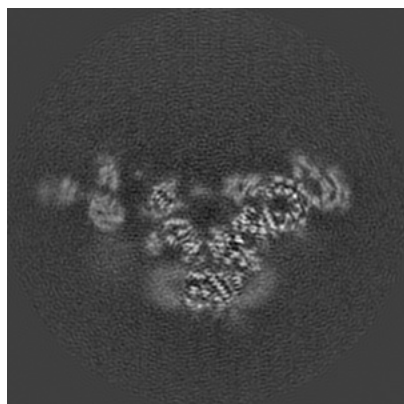


Z Index: 200

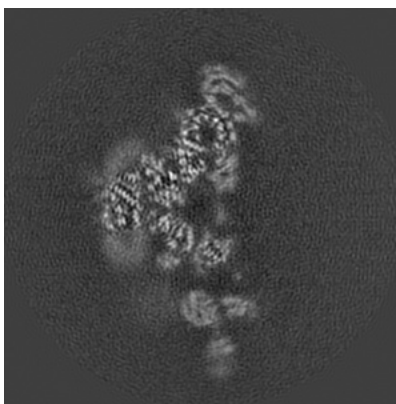
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

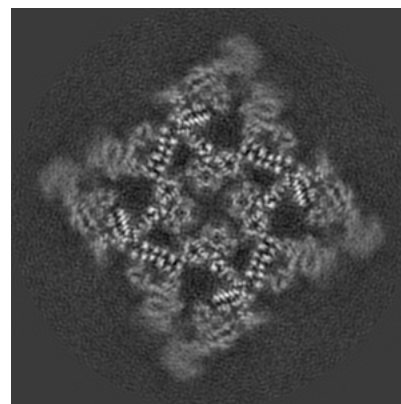
6.3.1 Primary map



X Index: 185



Y Index: 215



Z Index: 212

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

6.4 Orthogonal surface views [i](#)

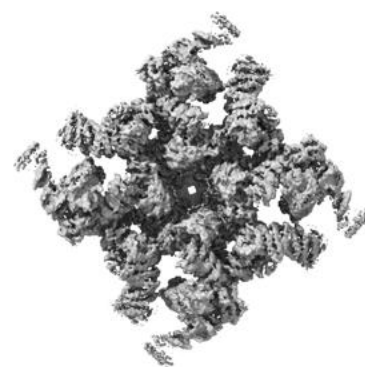
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

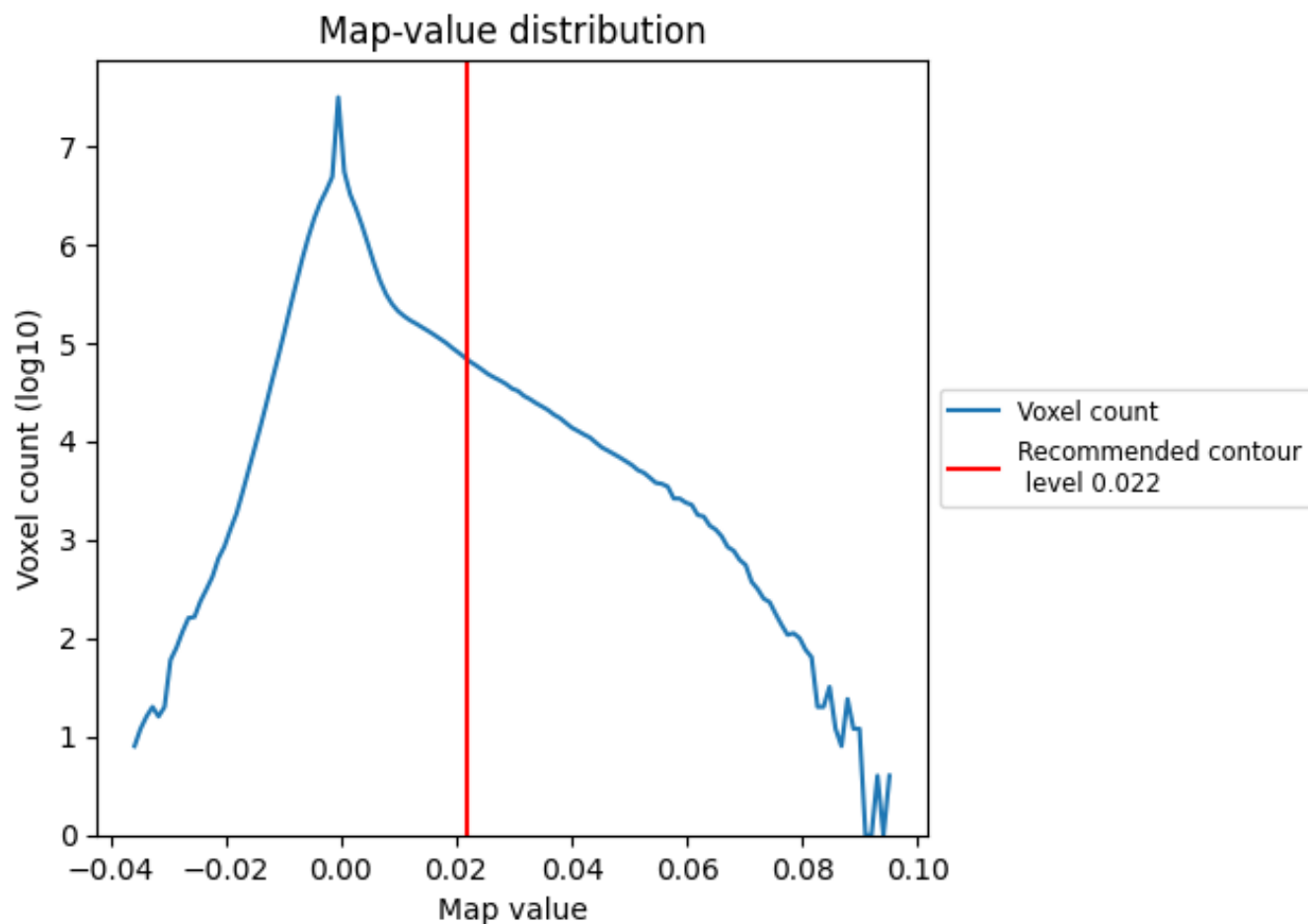
6.5 Mask visualisation

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

7 Map analysis [i](#)

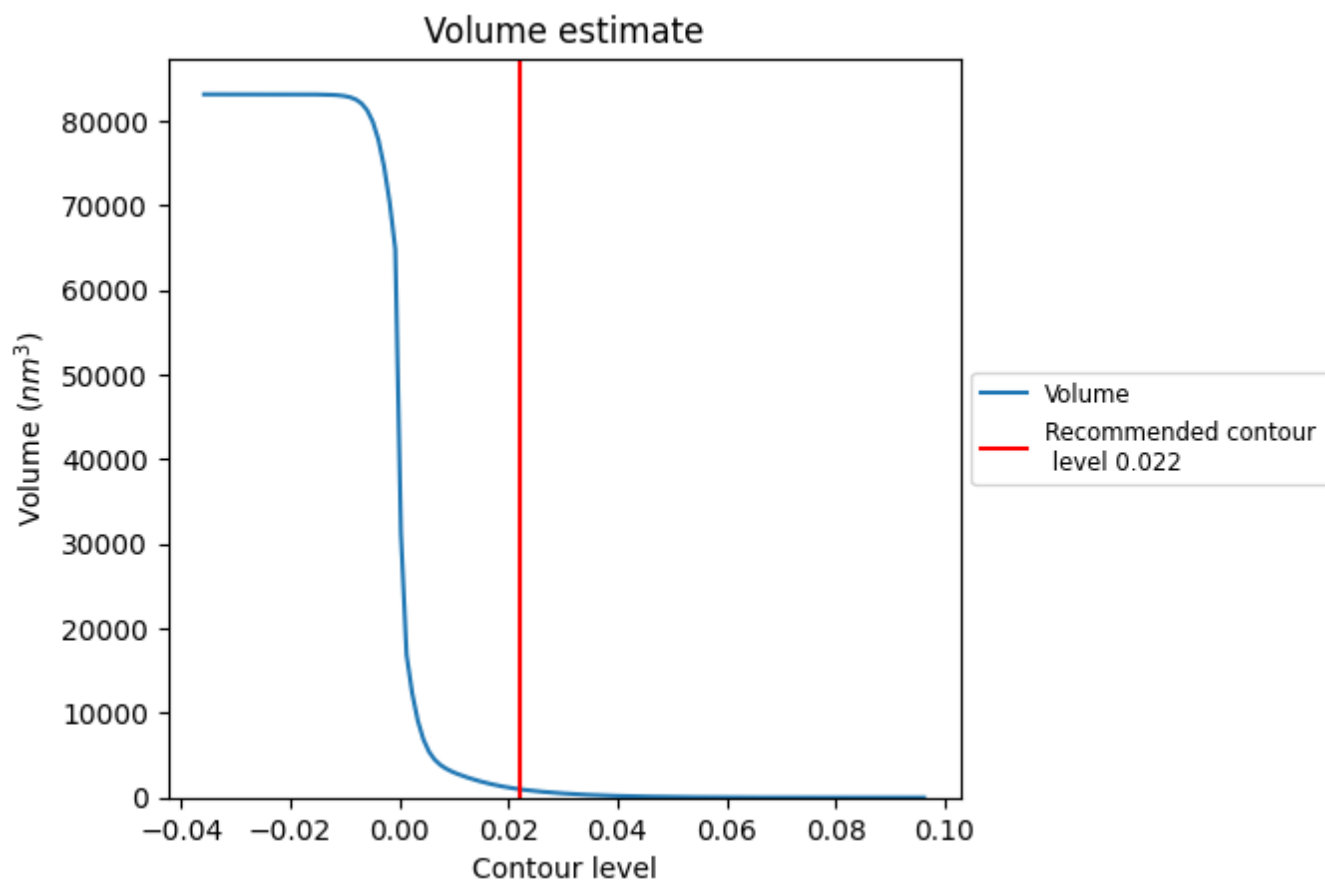
This section contains the results of statistical analysis of the map.

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.

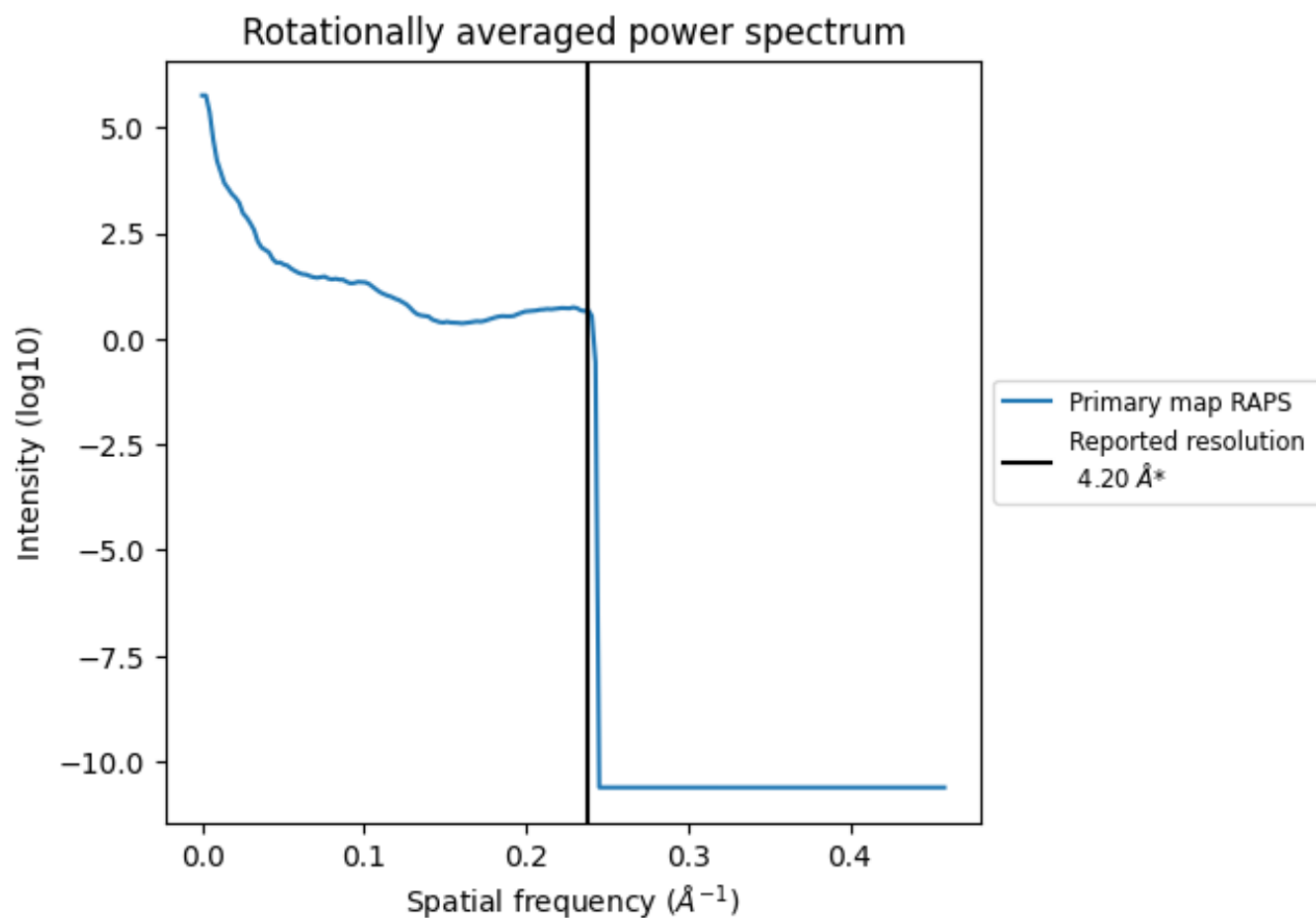
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 992 nm^3 ; this corresponds to an approximate mass of 896 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 ⓘ

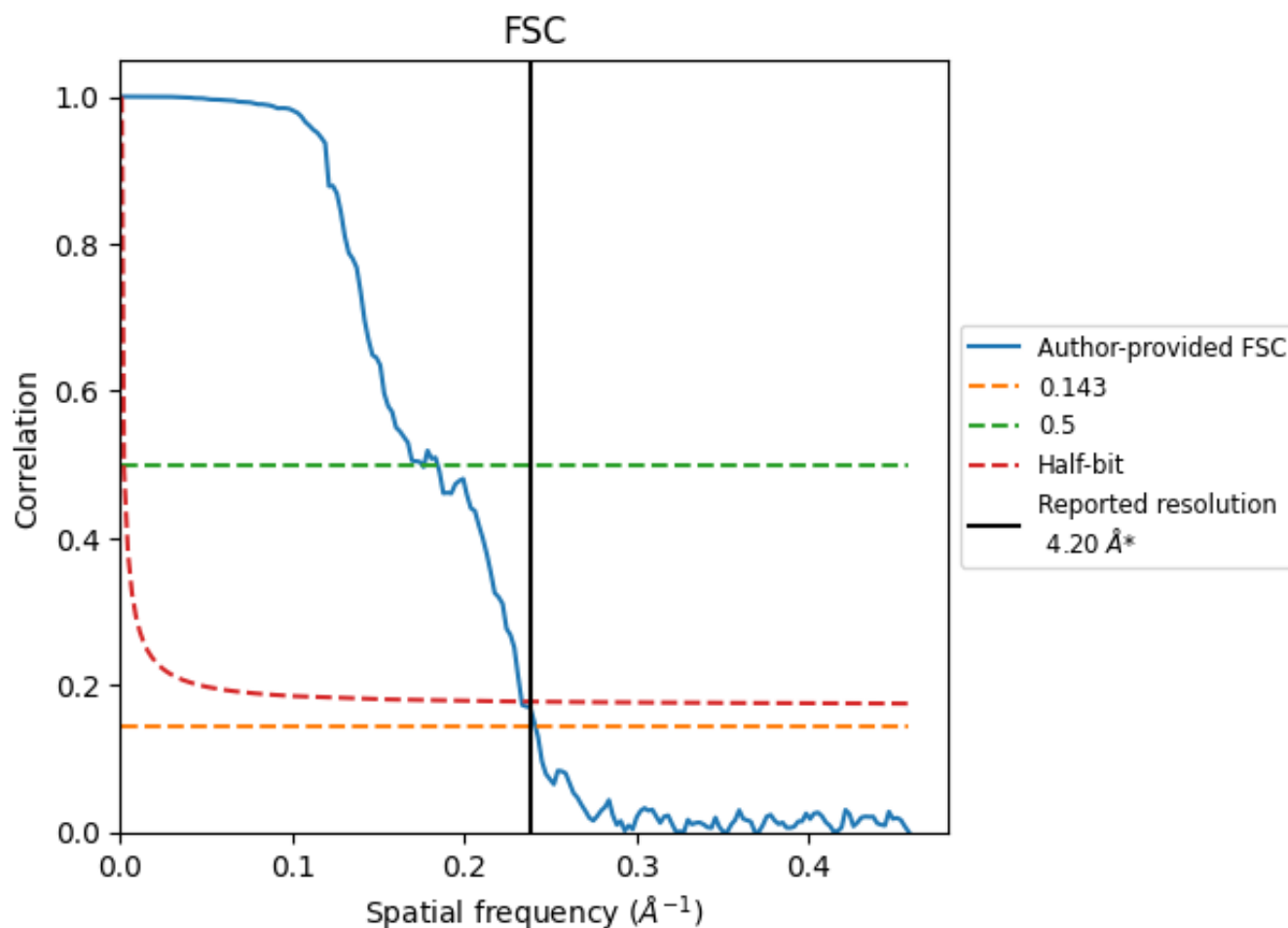


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

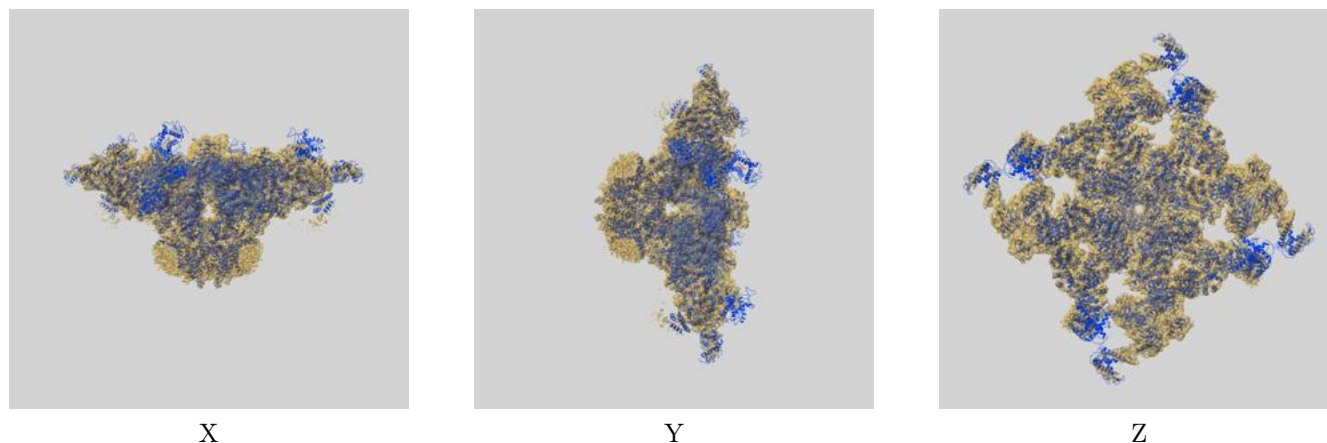
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.14	5.71	4.28
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

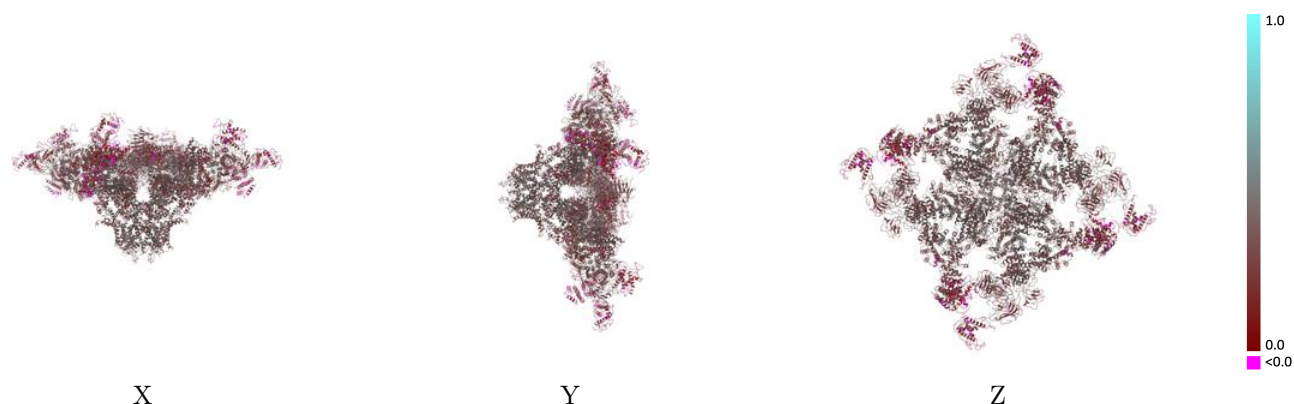
This section contains information regarding the fit between EMDB map EMD-9834 and PDB model 6JII. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



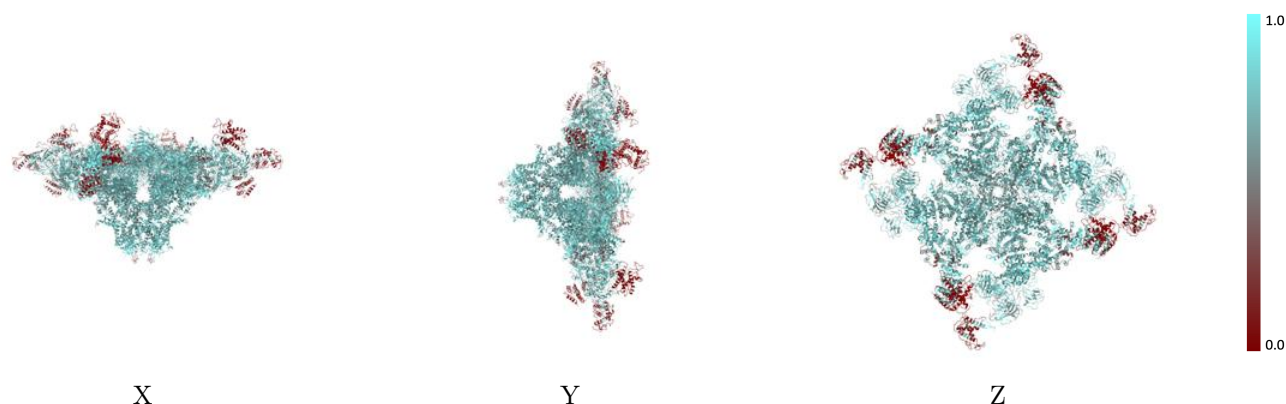
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



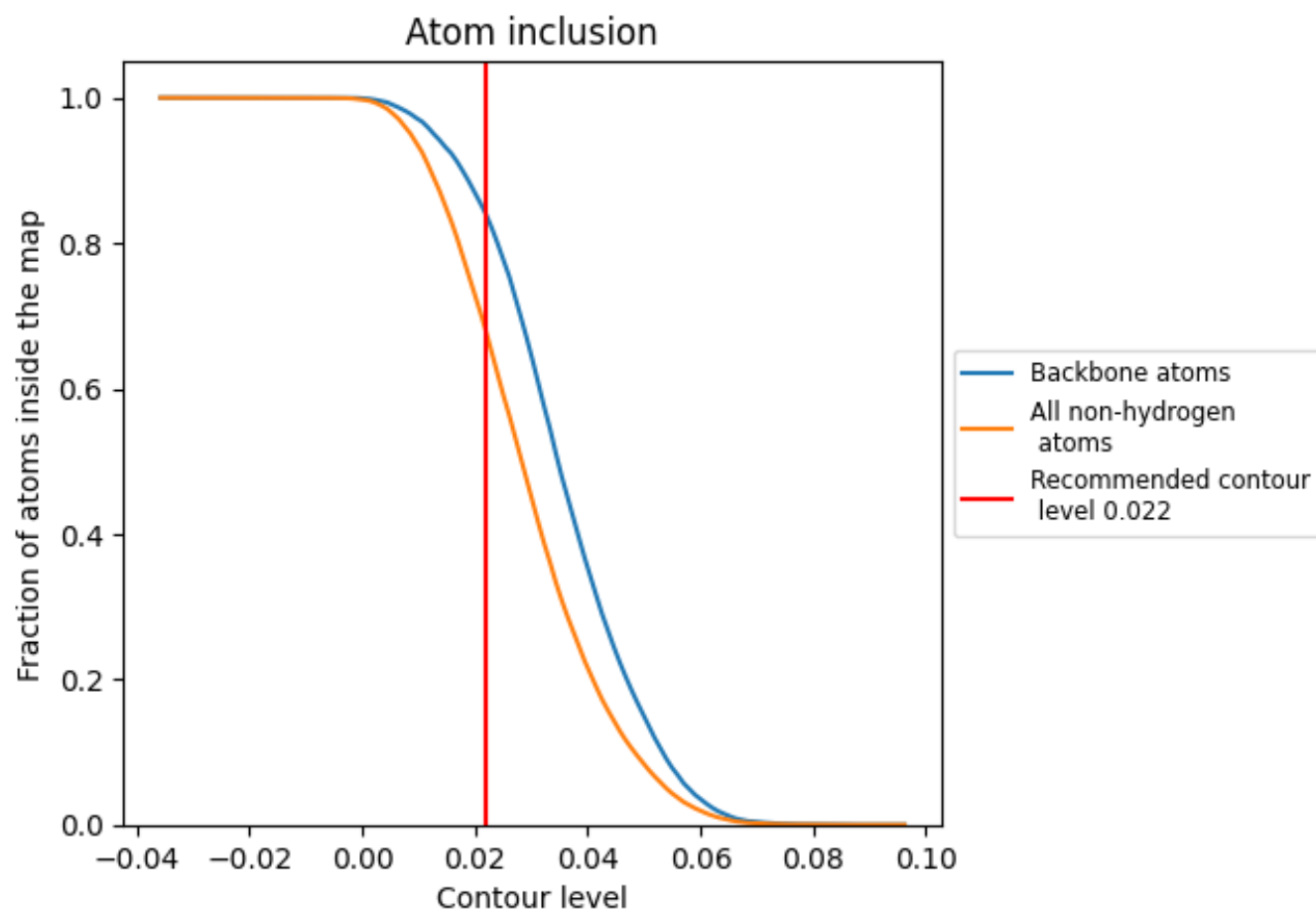
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 68% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6773	<div></div> 0.3190
A	<div></div> 0.7088	<div></div> 0.3340
B	<div></div> 0.6838	<div></div> 0.3210
C	<div></div> 0.4915	<div></div> 0.2490
D	<div></div> 0.7100	<div></div> 0.3380
E	<div></div> 0.6837	<div></div> 0.3220
F	<div></div> 0.4915	<div></div> 0.2470
G	<div></div> 0.7113	<div></div> 0.3370
H	<div></div> 0.6840	<div></div> 0.3220
I	<div></div> 0.4906	<div></div> 0.2480
J	<div></div> 0.7100	<div></div> 0.3360
K	<div></div> 0.6839	<div></div> 0.3210
L	<div></div> 0.4915	<div></div> 0.2490

