



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 09:53 AM UTC

PDB ID : 9CGP / pdb_00009cgp
EMDB ID : EMD-45584
Title : RyR1 disease mutant Y523S with FKBP12.6, nanodisc and inhibitor dantrolene in the absence of calcium with refined P1 domain
Authors : Iyer, K.A.; Samso, M.
Deposited on : 2024-06-30
Resolution : 3.34 Å(reported)
Based on initial model : 7T64

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

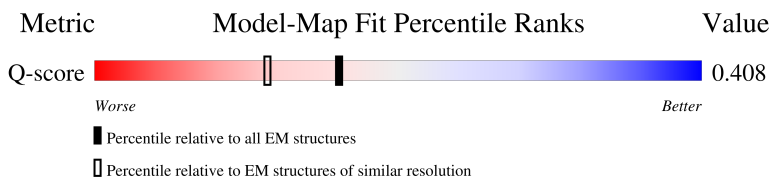
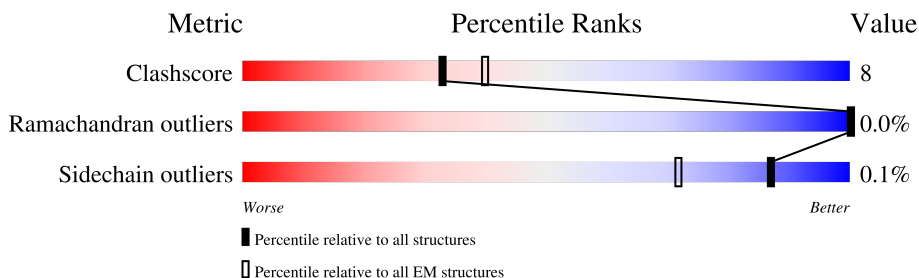
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14446 (2.84 - 3.84)

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	107	 70%30%
2	F	107	 75%25%
2	G	107	 71%29%
2	H	107	 70%30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	U1C	A	5103	-	X	-	-
5	U1C	B	5103	-	X	-	-
5	U1C	C	5103	-	X	-	-
5	U1C	D	5103	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 132860 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		
1	B	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		
1	C	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		
1	D	4258	Total	C	N	O	S	0	0
			32374	20609	5541	6025	199		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

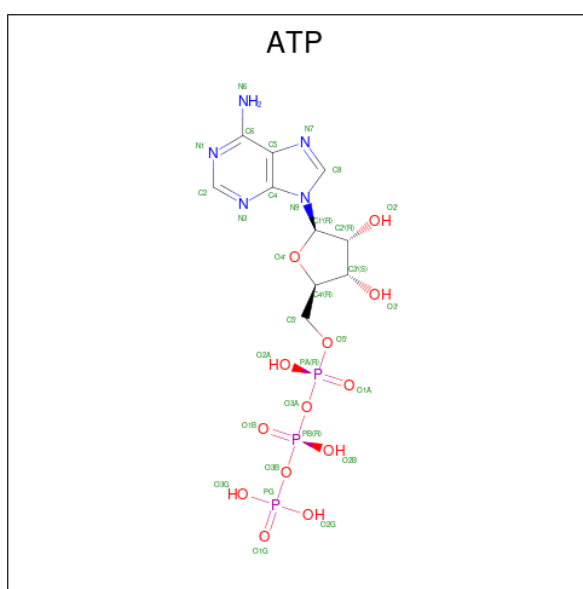
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			786	498	137	148	3		
2	F	107	Total	C	N	O	S	0	0
			786	498	137	148	3		
2	G	107	Total	C	N	O	S	0	0
			786	498	137	148	3		
2	H	107	Total	C	N	O	S	0	0
			786	498	137	148	3		

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

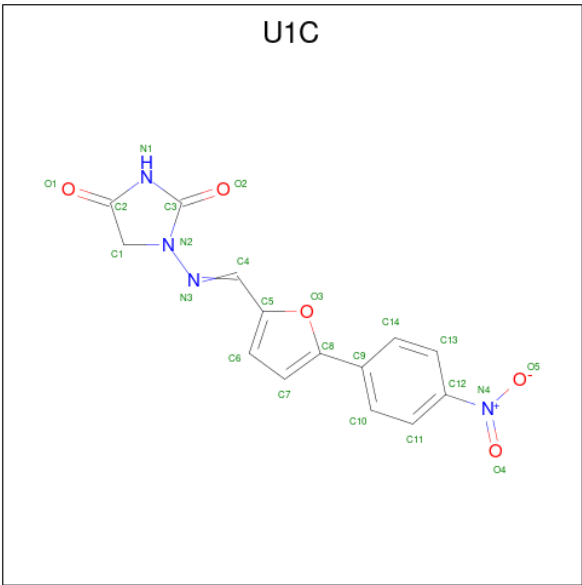
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is Dantrolene (CCD ID: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).

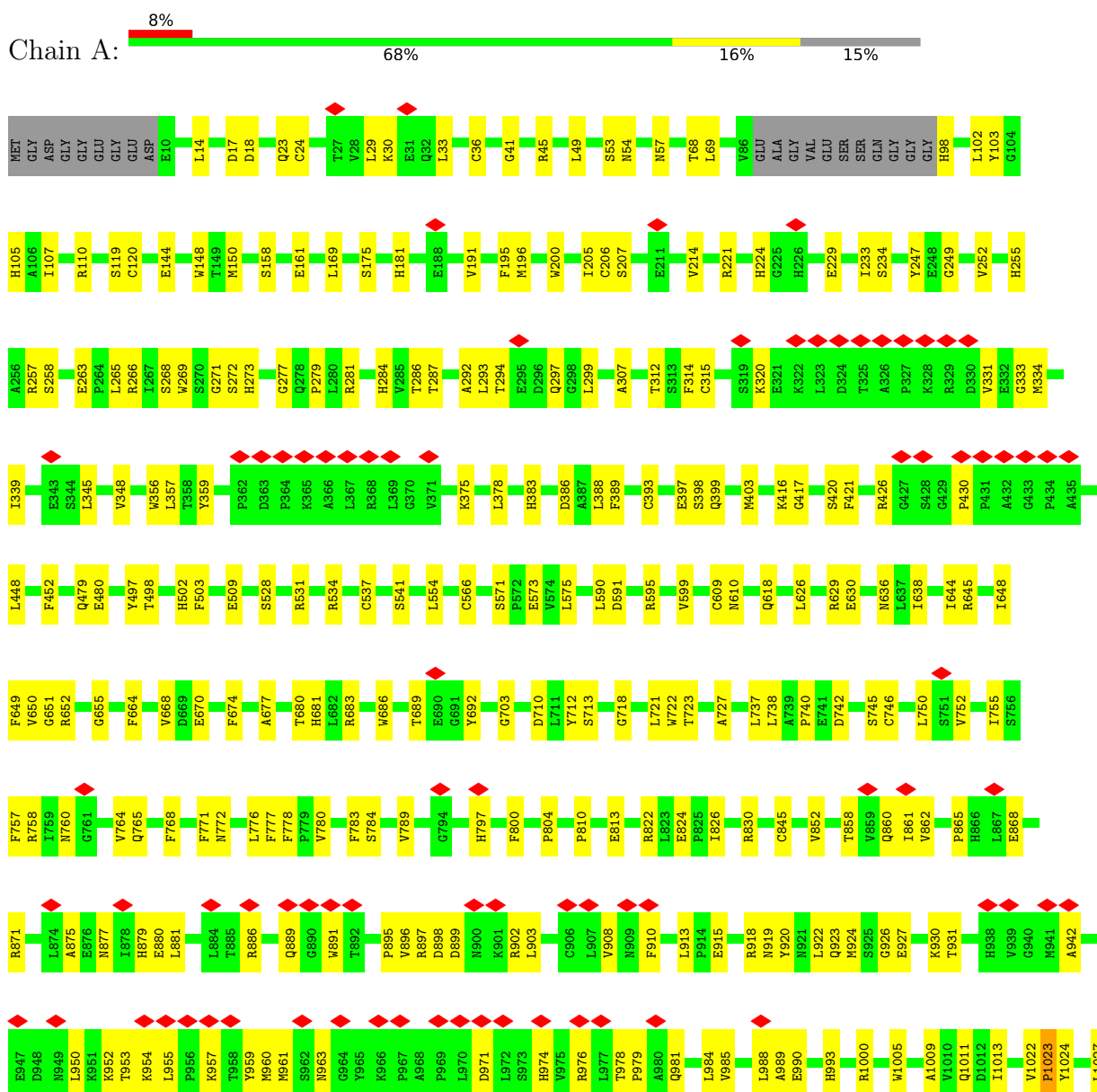


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			23	14	4	5	
5	B	1	Total	C	N	O	0
			23	14	4	5	
5	C	1	Total	C	N	O	0
			23	14	4	5	
5	D	1	Total	C	N	O	0
			23	14	4	5	

3 Residue-property plots

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

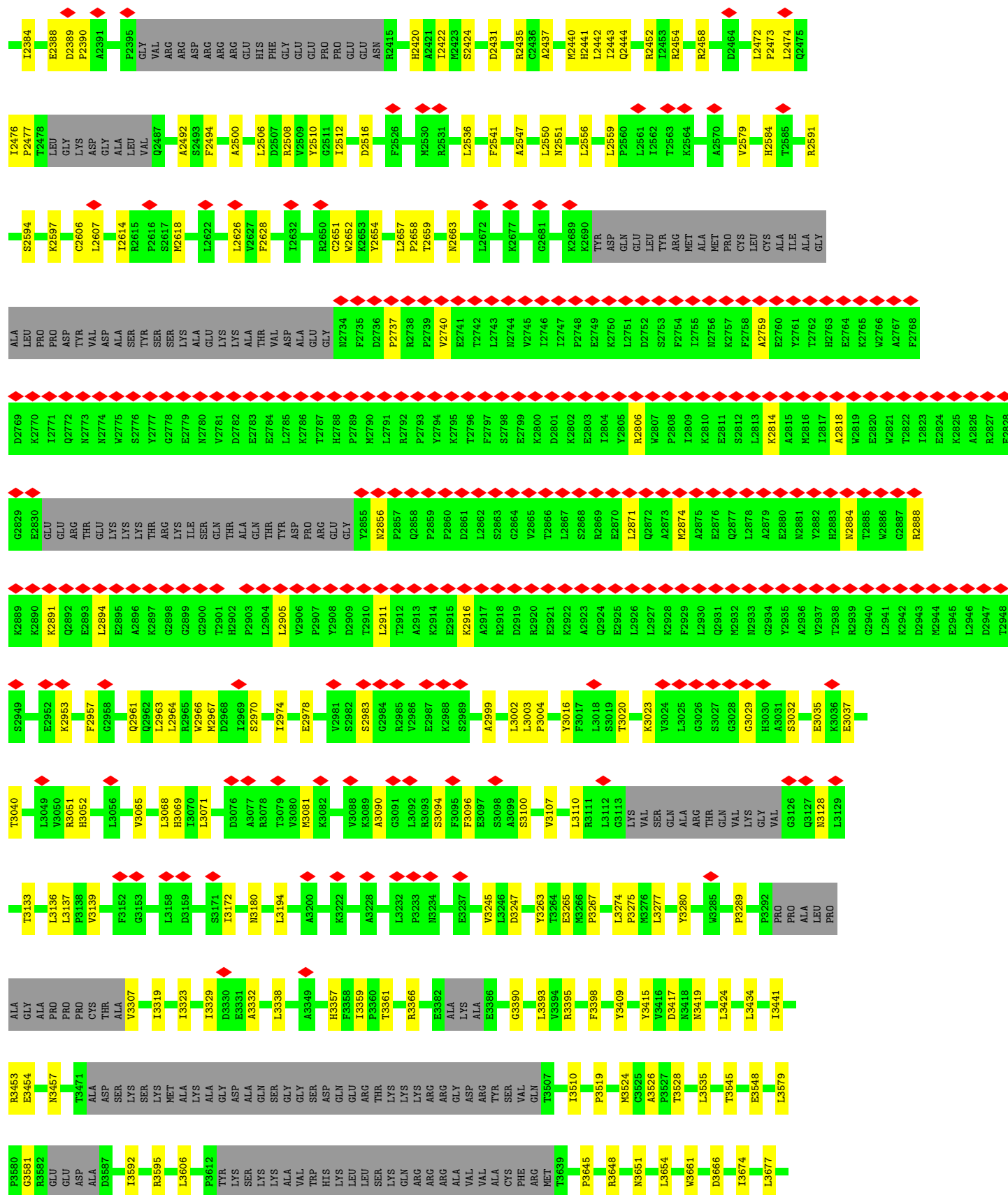
• Molecule 1: Ryanodine receptor 1



D1028	F1139	L1283	THR	PRO	M1527	R1656	GLU	K2013	V2098	D2282	H2420	D2516
K1032	G1140	V1284	ALA	HIS	T1530	L1657	GLU	D2017	V2102	N2283	A2421	H2520
N1035	V1148	F1288	LYS	ASP	T1530	D1658	GLU	E2018	R2103	L2286	M2422	V2524
R1036	G1151	L1289	GLY	VAL	E1535	N1678	GLU	C2021	E2108	S2309	S2424	L2527
L1039	M1152	Q1299	THR	PRO	S1536	D1700	GLU	P2022	R2118	C2310	D2431	M2530
R1044	T1153	HIS	PRO	ALA	N1537	L1703	GLU	L2023	L2124	P2311	R2435	R2531
L1047	D1154	PHE	THR	ARG	N1545	P1704	GLU	P2024	R2125	M2312	C2436	M2536
G1048	T1155	ARG	PRO	CYS	L1548	L1708	GLU	L2031	Q2127	L2313	A2437	L2536
N1052	I1160	CYS	GLN	THR	F1549	S1717	GLU	H2035	Q2127	Y2318	R2440	A2547
I1053	I1161	ALA	GLY	ALA	P1550	R1708	GLU	E2047	V2149	D2320	H2441	L2550
E1054	L1169	THR	VAL	ALA	A1551	A1708	GLU	GLY	E2150	I2321	I2442	N2551
PRO	M1170	ALA	GLU	ALA	V1554	S1717	GLU	GLU	S2153	P2325	Q2444	L2556
ASP	M1171	THR	GLN	ALA	L1555	E1721	GLU	GLU	S2154	S2345	R2452	L2561
GLN	D1172	LEU	PRO	VAL	H1558	T1742	GLU	GLU	R2159	R2355	I2453	I2562
GLU	F1179	ALA	ARG	ALA	V1561	K1753	GLU	GLU	F2191	R2369	R2454	K2563
ASN	R1180	PRO	ALA	ASN	I1562	V1767	GLU	PRO	M2188	R2374	R2458	K2564
GLN	E1181	LEU	GLY	ASN	Q1563	T1768	GLU	GLU	F2191	L2374	L2472	A2570
PRO	L1189	PRO	LYS	GLY	F1564	T1769	GLU	GLU	M2198	E2381	P2473	V2579
VAL	P1190	ALA	ASP	ASP	I1572	R1772	GLU	GLU	R2199	L2384	Q2475	H2584
ASN	H1201	ALA	THR	D1456	S1576	R1772	GLU	LEU	M2199	E2388	L2476	L2585
GLN	Q1206	ASP	THR	V1457	M1579	A1788	GLU	LEU	M2199	D2389	P2477	R2591
GLN	D1207	GLU	THR	Y1457	P1593	A1789	GLU	GLU	L2201	P2390	L2478	S2594
ARG	V1208	ARG	GLU	M1462	R1594	G1790	GLU	GLU	L2201	A2391	LEU	K2597
TRP	S1209	ALA	GLU	R1470	Q1598	V1791	GLU	GLU	V2212	P2395	GLY	C2606
D1070	S1210	ALA	GLU	A1471	E1793	A1792	GLU	VAL	V2213	GLY	L2607	L2607
A1077	L1211	PRO	GLY	G1477	V1603	E1805	GLU	ARG	V2214	VAL	M2608	M2608
E1078	C1217	ASP	PHE	D1478	V1615	R1808	ALA	ARG	G2218	VAL	L2614	L2614
K1079	G1218	PRO	LEU	M1482	R1618	L1815	GLU	LEU	L2223	ARG	A2491	R2615
S1080	L1219	ASP	PHE	S1486	R1618	L1815	GLY	VAL	M2228	ASP	A2492	P2616
R1087	Q1220	TYR	LYS	S1486	R1623	S1833	LYS	LYS	L2236	ARG	S2493	P2617
N1088	G1222	ASN	ALA	S1486	A1627	E1835	GLU	GLU	L2242	GLU	F2494	M2618
Y1089	F1223	LEU	LYS	L1634	L1634	F1836	GLU	GLU	R2244	GLU	D2497	L2622
E1093	M1230	ARG	ALA	H1640	I1641	V1845	GLU	GLU	Q2245	GLU	A2500	L2626
H1104	S1241	ARG	MET	T1641	P1642	T1847	GLU	LEU	N2250	PHE	L2506	L2627
P1107	P1253	GLY	THR	E1643	E1643	L1849	GLU	PRO	Y2256	GLY	L2507	V2628
R1110	H1254	GLY	GLN	E1644	N1645	V1850	GLU	GLU	L2257	GLU	R2508	R2650
D1112	T1263	GLY	PRO	E1644	C1647	M1851	GLU	GLU	L2258	GLU	Y2510	C2651
D1118	T1266	GLY	THR	N1645	M1648	P1868	GLU	GLU	V2275	GLU	G2511	M2652
M1125	L1270	GLY	PRO	C1647	M1648	T1872	GLU	ALA		ASN	I2512	Y2654
G1126	R1276	GLY	LEU	C1647	M1648	E1873	GLU	E2088				
T1276	T1276	GLU	PRO	C1647	M1648	A1988	GLU	L2094				
W1277	W1277	GLY	ARG	C1647	M1648	E1873	GLU					
			LEU	C1647	M1648	E1873	GLU					

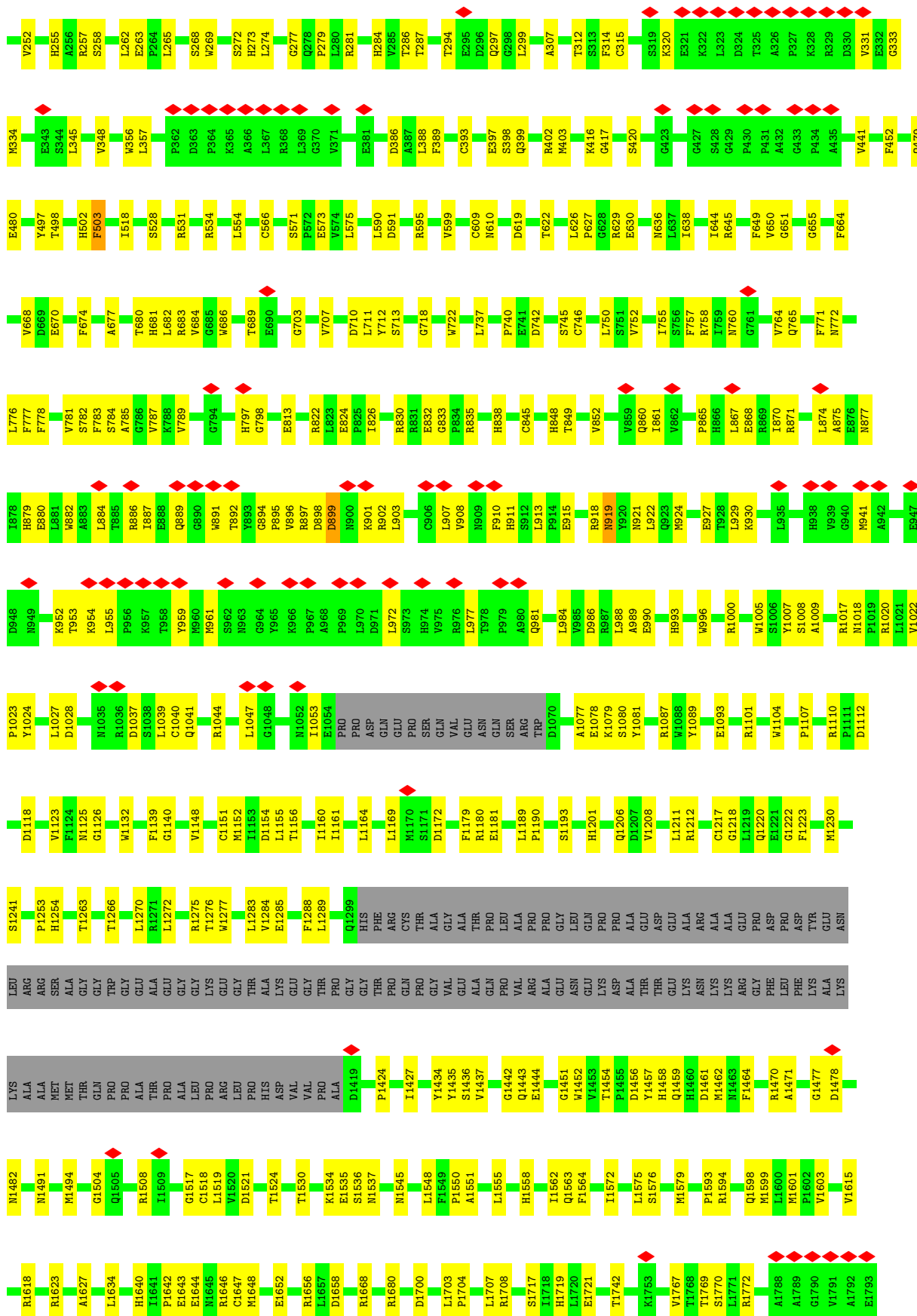
L3866	H3699	R3595	A3332	A3228	F3096	R2985	A2917	P2857	F2797	L2657
N3867	Q3700	P3612	T3353	L3232	E3097	V2986	R2918	Q2858	S2798	P2658
R3868	L3701	T3612	W3334	L3232	S3098	E2987	D2919	P2859	E2799	T2659
R3869	L3716	L3338	L3338	R3234	S3100	R2988	R2920	P2860	K2800	N2663
N3870	D3719	S3347	S3347	S3235	E3101	S2989	E2921	D2861	D2801	L2672
N3875	G3738	A3348	A3348	V3236	V3107	L3003	K2922	L2862	K2802	K2677
D3877	GLY	E3349	E3349	V3236	L3110	P3004	A2923	S2863	E2803	G2681
Q3889	GLY	T3359	T3359	V3245	L3110	Y3016	Q2924	Q2864	T2804	K2677
L3890	GLY	R3366	R3366	L3245	R3111	F3017	E2925	V2865	R2806	
Q3927	GLY	E3382	E3382	D3247	L3112	L3018	L2926	L2866	W2807	
E3928	ALA	E3382	E3382	R3248	G3113	S3019	L2927	L2867	P2808	
S3929	GLY	ALA	ALA	L3249	LYS	T3020	K2928	S2868	K2809	
L3965	GLY	LYS	LYS	I3253	VAL	K3023	F2929	E2870	T2809	
T3966	GLY	LYS	LYS	I3253	GLN	V3024	F2930	E2870	K2810	
E3967	GLY	E3386	E3386	Y3263	ALA	V3024	Q2931	L2871	E2811	
Y3968	GLY	G3390	G3390	T3264	ARG	L3025	M2932	Q2872	D2752	
L3969	VAL	G3390	G3390	E3265	THR	G3026	M2932	A2873	S2753	
Q3970	VAL	L3393	L3393	M3266	GLN	S3027	M2933	A2873	L2813	
G3971	TYR	V3394	V3394	P3267	VAL	S3027	Q2934	M2874	F2764	
F3972	ALA	R3395	R3395	I3270	LYS	G3028	Y2935	A2875	I2755	
C3973	CYS	F3398	F3398	F3271	GLY	G3029	A2936	E2876	K2756	
L3980	PHE	Y3409	Y3409	I3272	VAL	H3030	V2937	Q2877	N2757	
S3983	ARG	T3507	T3507	I3272	G3126	A3031	T2938	L2878	F2768	
R3984	GLY	S3508	S3508	I3274	Q3127	S3032	T2938	A2879	A2759	
L3985	GLY	L3509	L3509	L3277	N3128	E3035	R2939	E2880	E2760	
G3991	GLY	I3510	I3510	L3277	L3129	K3036	Q2940	E2881	Y2761	
V3995	GLY	Y3415	Y3415	Y3280	T3133	E3037	L2941	M2882	T2762	
M3999	GLY	V3416	V3416	Y3280	V3134	H3038	K2942	Y2882	H2763	
M4000	GLY	N3418	N3418	W3285	A3135	L3039	D2943	H2883	L2823	
L4003	GLY	N3419	N3419	P3289	L3136	S3041	M2944	N2884	E2824	
S4008	GLY	L3424	L3424	P3289	V3139	L3049	E2945	T2885	K2765	
Q4009	GLY	L3434	L3434	P3292	L3140	L2946	D2947	T2886	W2766	
L4012	GLY	V3438	V3438	P3292	T3141	D2947	T2948	G2887	A2767	
L4016	GLY	T3441	T3441	ALA	Q3145	H3052	T2948	R2888	F2768	
L4030	GLY	K3447	K3447	ALA	F3152	L3056	S2949	K2889	D2769	
E4032	GLY	R3453	R3453	PRO	G3153	L3070	I2951	K2890	K2770	
G4033	GLY	E3454	E3454	PRO	G3153	L3070	E2952	K2891	I2771	
M4034	GLY	N3457	N3457	PRO	L3156	L3070	R2953	Q2892	Q2772	
M4044	GLY	E3685	E3685	PRO	D3159	L3070	R2954	E2893	N2773	
V4049	GLY	GLY	GLY	PRO	S3171	L3070	G2958	L2894	N2774	
S4052	GLY	T3471	T3471	PRO	I3172	L3070	Q2961	E2895	W2775	
	GLY	ALA	ALA	PRO	L3175	L3070	Q2962	A2896	S2776	
	GLY	ASP	ASP	CYS	L3175	L3070	L2963	K2897	Y2777	
	GLY	SER	SER	THR	L3175	L3070	L2964	G2898	G2778	
	GLY	LYS	LYS	V3307	L3175	L3070	L2964	L2899	LYS	
	GLY	LYS	LYS	LYS	L3194	L3070	W2966	G2900	E2779	
	GLY	LYS	LYS	I3319	A3198	L3080	R2967	T2901	N2780	
	GLY	LYS	LYS	I3323	A3199	M3081	D2968	T2902	V2781	
	GLY	LYS	LYS	I3323	A3200	V3068	L2969	P2903	D2782	
	GLY	LYS	LYS	D3330	A3200	V3068	S2970	T2903	E2783	
	GLY	LYS	LYS	E3331	P3208	V3068	S2970	T2903	E2784	
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	GLY	LYS	LYS			V3068	S2970	T2903	K2786	
	GLY	LYS	LYS			V3068	S2970	T2903	T2787	
	GLY	LYS	LYS			V3068	S2970	T2903	H2788	
	GLY	LYS	LYS			V3068	S2970	T2903	P2789	
	GLY	LYS	LYS			V3068	S2970	T2903	M2790	
	GLY	LYS	LYS			V3068	S2970	T2903	L2791	
	GLY	LYS	LYS			V3068	S2970	T2903	R2792	
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	GLY	LYS	LYS			V3068	S2970	T2903	Y2794	
	GLY	LYS	LYS			V3068	S2970	T2903	K2795	
	GLY	LYS	LYS			V3068	S2970	T2903	T2796	







H106	A106	I107	R110	S119	C120	M127	E144	W148	M150	P162	V165	D168	L170	L171	S175	H181	E188	V191	M196	G197	T198	L199	W200	R201	M202	I205	C206	S207	E211	R221	H224	E229	I233	S234	Y247	F248	Z249								
Met	GLY	ASP	GLY	GLY	GLU	GLY	GLU	ASP	E10	V11	Q12	F13	L14	D18	Q23	C24	T27	K30	E31	Q32	L33	C36	G41	R45	L49	S53	N54	N57	T68	L69	V86	GLU	ALA	GLY	VAL	GLU	SER	SER	GLN	GLY	GLY	H98	L102	Y103	C108



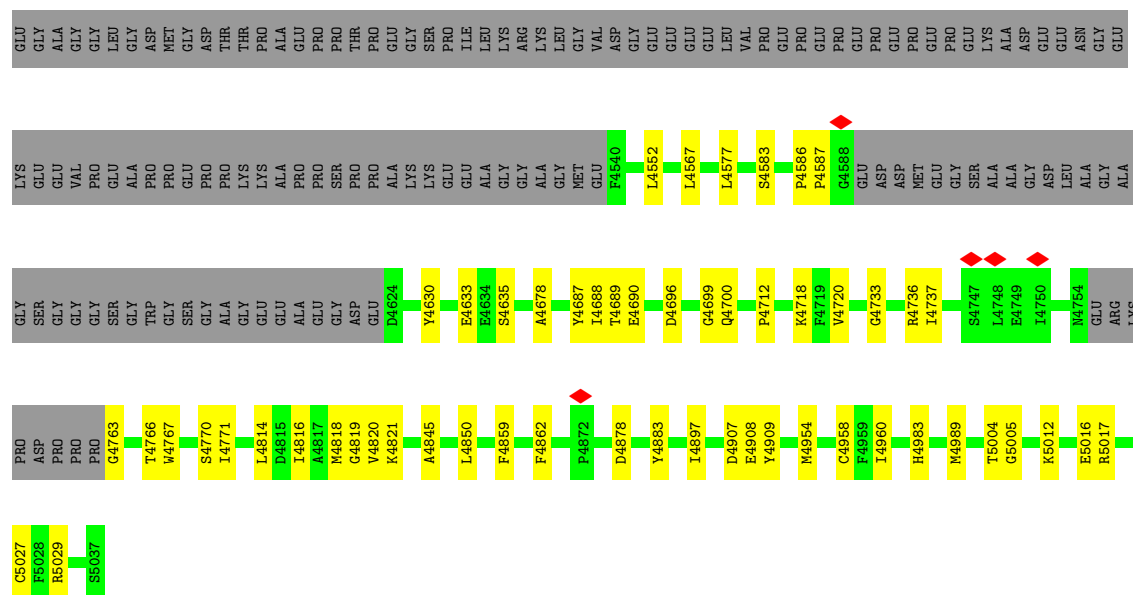






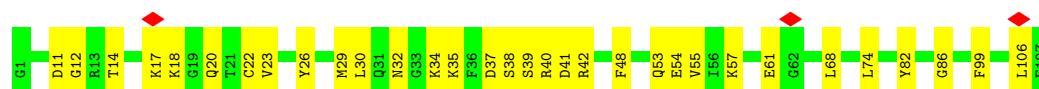
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I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	S2775	W2776	Y2777	Q2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	F2793	Y2794	K2795	D2796	L2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G2681	K2690	TYR	ASP	GLN	GLU	LEU	TYR	ARG	MET	ALA	PRO	CYS	LEU	CYS	ILE	GLY	ALA	LEU	PRO	ASP	TYR	VAL	ASP	ALA	SER	TYR	SER	THR	LYS	ALA	GLU	LYS	ALA	ASP	GLU	LYS	THR	VAL	ASP	GLU	GLY	ALA	GLU	GLY	ALA	THR	PRO	ALA	THR	PRO	ALA	THR	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
M2530	R2531	L2536	A2547	L2550	N2551	L2556	L2561	T2562	Y2563	K2564	A2570	V2579	H2584	T2585	R2591	S2594	K2597	C2606	L2607	M2608	T2614	R2615	P2616	S2617	M2618	L2622	L2626	V2627	F2628	R2650	C2651	M2652	V2653	Y2654	V2655	C2656	L2657	P2658	T2659	N2663	V2677																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
D2431	R2435	C2436	A2437	M2440	H2441	L2442	I2443	Q2444	R2452	L2453	R2454	R2458	D2464	L2472	P2473	L2474	Q2475	I2476	P2477	T2478	LEU	GLY	ASP	GLY	ALA	LEU	VAL	Q2487	A2492	S2493	F2494	A2500	L2506	D2507	R2508	Y2509	Y2510	G2511	I2512	D2516	H2520	V2524	G2525	F2526	N2527	S2424																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L2313	Y2318	P2319	D2320	P2325	H2326	S2345	R2355	R2359	K2360	L2368	R2369	Q2370	E2371	S2374	E2381	E2382	R2383	I2384	E2388	D2389	P2390	A2391	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	ALA	GLU	E2088	L2094	V2098	V2103	R2104	V2105																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A2106	Q2107	E2108	R2118	L2124	H2125	Q2127	M2153	S2154	L2159	I2179	M2186	N2187	N2188	F2191	Y2192	Q2193	H2194	M2198	R2199	A2200	L2201	V2212	M2213	V2214	G2218	I2223	M2228	F2235	I2242	S2243	R2244	Q2245	N2246	Y2256	D2282	N2283	L2286	C2310	F2311	M2312																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
M1986	S1987	A1988	A1989	D2017	H2035	E2047	GLY	GLU	GLU	GLU	PRO	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU





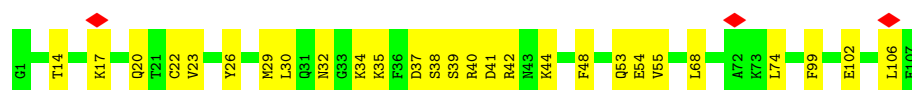
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 70% 30%



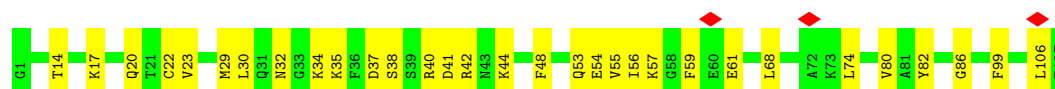
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 75% 25%



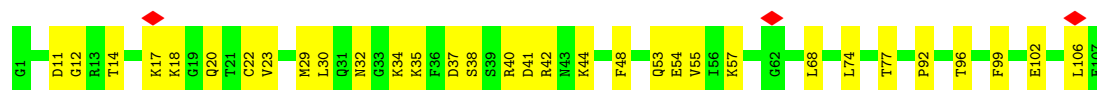
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 71% 29%



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 70% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249034	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.277	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.32	Depositor
Map size ($\text{\AA}$)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, U1C

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	0.11	0/33082	0.29	0/45015
1	B	0.10	0/33082	0.29	0/45015
1	C	0.11	0/33082	0.29	0/45015
1	D	0.11	0/33082	0.30	2/45015 (0.0%)
2	E	0.12	0/802	0.31	0/1086
2	F	0.14	0/802	0.36	0/1086
2	G	0.13	0/802	0.37	0/1086
2	H	0.13	0/802	0.32	0/1086
All	All	0.11	0/135536	0.29	2/184404 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	832	GLU	CB-CA-C	5.61	120.52	111.05
1	D	832	GLU	CB-CG-CD	5.13	121.33	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	LEU	Peptide
1	B	626	LEU	Peptide
1	C	626	LEU	Peptide
1	D	626	LEU	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	32374	0	30869	532	0
1	B	32374	0	30869	511	0
1	C	32374	0	30869	533	0
1	D	32374	0	30869	537	0
2	E	786	0	766	22	0
2	F	786	0	766	20	0
2	G	786	0	766	21	0
2	H	786	0	766	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	132860	0	126588	2178	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 8.

All (2178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:830:ARG:HD3	1:D:1612:PHE:CE2	1.70	1.26
1:D:1454:THR:CG2	1:D:1456:ASP:OD1	2.09	0.99
1:D:830:ARG:CD	1:D:1612:PHE:CE2	2.45	0.99
1:D:1454:THR:HG23	1:D:1456:ASP:OD1	1.63	0.97
1:B:4763:GLY:N	1:B:4766:THR:HG1	1.64	0.94
1:D:833:GLY:HA3	1:D:838:HIS:HD2	1.32	0.92
1:D:830:ARG:NH1	1:D:1612:PHE:CD2	2.39	0.91
1:C:4763:GLY:N	1:C:4766:THR:HG1	1.75	0.85
1:C:707:VAL:HG23	1:C:713:SER:OG	1.78	0.83
1:D:4763:GLY:N	1:D:4766:THR:HG1	1.76	0.83
1:D:3003:LEU:HD12	1:D:3004:PRO:HD3	1.60	0.83
1:D:897:ARG:HG2	1:D:898:ASP:H	1.44	0.82
1:C:911:HIS:ND1	1:C:911:HIS:O	2.12	0.82
1:B:3003:LEU:HD12	1:B:3004:PRO:HD3	1.61	0.81
1:B:1451:GLY:HA3	1:B:1494:MET:HB3	1.62	0.81
1:C:69:LEU:HD11	1:C:107:ILE:HD11	1.63	0.81
1:C:3003:LEU:HD12	1:C:3004:PRO:HD3	1.60	0.81
1:A:3003:LEU:HD12	1:A:3004:PRO:HD3	1.61	0.81
1:C:609:CYS:SG	1:C:610:ASN:N	2.53	0.81
1:B:707:VAL:HG23	1:B:713:SER:OG	1.81	0.80
1:D:609:CYS:SG	1:D:610:ASN:N	2.53	0.80
1:D:1454:THR:HG21	1:D:1456:ASP:OD1	1.81	0.79
1:D:830:ARG:NH1	1:D:1612:PHE:HD2	1.82	0.78
1:A:609:CYS:SG	1:A:610:ASN:N	2.53	0.78
1:C:1437:VAL:HG13	1:C:1562:ILE:HD11	1.66	0.77
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.67	0.76
1:D:3277:LEU:HA	1:D:3280:TYR:HB3	1.66	0.76
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.67	0.76
1:B:609:CYS:SG	1:B:610:ASN:N	2.53	0.76
1:D:833:GLY:HA3	1:D:838:HIS:CD2	2.20	0.76
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.66	0.76
1:B:3277:LEU:HA	1:B:3280:TYR:HB3	1.68	0.75
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.67	0.75
1:C:3277:LEU:HA	1:C:3280:TYR:HB3	1.68	0.75
1:A:3277:LEU:HA	1:A:3280:TYR:HB3	1.69	0.73
1:A:4763:GLY:N	1:A:4766:THR:HG1	1.85	0.73
1:B:205:ILE:HG22	1:B:206:CYS:H	1.54	0.72
1:C:3651:ASN:HA	1:C:3654:LEU:HD12	1.71	0.72
1:B:1018:ASN:HD21	1:B:1020:ARG:HG2	1.53	0.72
1:D:1130:GLN:NE2	1:D:1136:SER:OG	2.23	0.72
1:D:3651:ASN:HA	1:D:3654:LEU:HD12	1.72	0.72
1:B:897:ARG:HG2	1:B:898:ASP:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:ARG:HG2	1:C:898:ASP:H	1.56	0.71
1:A:897:ARG:HG2	1:A:898:ASP:H	1.56	0.71
1:A:3651:ASN:HA	1:A:3654:LEU:HD12	1.71	0.71
1:D:102:LEU:HB3	1:D:105:HIS:CD2	2.25	0.71
1:D:205:ILE:HG22	1:D:206:CYS:H	1.54	0.71
1:A:638:ILE:HG21	1:A:703:GLY:HA3	1.73	0.70
1:A:942:ALA:HB2	1:A:1052:ASN:HB3	1.73	0.70
1:A:2651:CYS:SG	1:A:2652:TRP:N	2.65	0.70
1:B:4766:THR:HA	1:B:4769:MET:HE1	1.73	0.70
1:C:961:MET:HE3	1:C:961:MET:H	1.56	0.70
1:D:794:GLY:O	1:D:812:HIS:ND1	2.25	0.69
1:D:2651:CYS:SG	1:D:2652:TRP:N	2.65	0.69
1:A:3438:VAL:HG11	1:A:3517:MET:HE3	1.74	0.69
1:B:2651:CYS:SG	1:B:2652:TRP:N	2.65	0.69
1:B:3651:ASN:HA	1:B:3654:LEU:HD12	1.72	0.69
1:A:4850:LEU:HD11	1:B:4814:LEU:HB2	1.74	0.69
1:B:2626:LEU:HG	1:B:2628:PHE:H	1.58	0.69
1:D:830:ARG:CD	1:D:1612:PHE:HE2	2.04	0.69
1:A:4814:LEU:HB2	1:D:4850:LEU:HD11	1.75	0.69
1:B:681:HIS:HB3	1:B:784:SER:HB3	1.73	0.69
1:A:2524:VAL:HA	1:A:2527:LEU:HD23	1.74	0.69
1:C:2651:CYS:SG	1:C:2652:TRP:N	2.64	0.69
1:B:1128:ARG:HB2	1:B:1130:GLN:HE21	1.58	0.69
1:C:941:MET:HA	1:C:941:MET:HE3	1.75	0.69
1:A:2626:LEU:HG	1:A:2628:PHE:H	1.58	0.68
1:B:4850:LEU:HD11	1:C:4814:LEU:HB2	1.74	0.68
1:C:2626:LEU:HG	1:C:2628:PHE:H	1.58	0.68
1:D:638:ILE:HG21	1:D:703:GLY:HA3	1.75	0.68
1:D:4820:VAL:HG23	1:D:4821:LYS:H	1.59	0.68
1:C:4850:LEU:HD11	1:D:4814:LEU:HB2	1.75	0.68
1:B:638:ILE:HG21	1:B:703:GLY:HA3	1.76	0.68
1:D:941:MET:HA	1:D:941:MET:HE3	1.75	0.68
1:A:4820:VAL:HG23	1:A:4821:LYS:H	1.59	0.68
1:C:629:ARG:O	1:C:630:GLU:HG3	1.93	0.68
1:C:861:ILE:HB	1:C:930:LYS:HZ2	1.58	0.68
1:B:4820:VAL:HG23	1:B:4821:LYS:H	1.59	0.68
1:C:3434:LEU:HG	1:C:3517:MET:HE1	1.75	0.68
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.76	0.68
1:B:941:MET:HA	1:B:941:MET:HE3	1.76	0.68
1:D:830:ARG:HD3	1:D:1612:PHE:CZ	2.26	0.67
1:B:2441:HIS:HA	1:B:2444:GLN:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD11	1:C:69:LEU:HD13	1.75	0.67
1:D:2626:LEU:HG	1:D:2628:PHE:H	1.58	0.67
1:D:3438:VAL:HG11	1:D:3517:MET:HE3	1.76	0.67
1:B:629:ARG:O	1:B:630:GLU:HG3	1.95	0.67
1:A:102:LEU:HB3	1:A:105:HIS:CD2	2.30	0.67
1:C:4820:VAL:HG23	1:C:4821:LYS:H	1.61	0.66
1:D:2579:VAL:HG22	1:D:2594:SER:HB2	1.78	0.66
1:A:590:LEU:HB2	1:A:599:VAL:HG11	1.78	0.66
1:C:638:ILE:HG21	1:C:703:GLY:HA3	1.77	0.66
1:D:23:GLN:NE2	1:D:36:CYS:SG	2.69	0.66
1:C:977:LEU:HB3	1:C:981:GLN:HB2	1.78	0.66
1:C:2579:VAL:HG22	1:C:2594:SER:HB2	1.77	0.66
1:D:102:LEU:HB3	1:D:105:HIS:HD2	1.61	0.66
1:D:3716:LEU:HD13	1:D:3793:MET:HG2	1.78	0.66
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.76	0.65
1:C:12:GLN:HE22	1:C:14:LEU:HD22	1.61	0.65
1:C:3697:PRO:O	1:C:3701:LEU:N	2.24	0.65
1:A:3716:LEU:HD13	1:A:3793:MET:HG2	1.78	0.65
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.76	0.65
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.77	0.65
1:B:772:ASN:HD22	1:B:1471:ALA:H	1.42	0.65
2:F:37:ASP:OD1	2:F:42:ARG:NH2	2.30	0.65
1:C:23:GLN:NE2	1:C:36:CYS:SG	2.69	0.65
1:D:590:LEU:HB2	1:D:599:VAL:HG11	1.79	0.65
1:D:2442:LEU:HG	1:D:2443:ILE:HG12	1.79	0.65
1:A:868:GLU:O	1:A:871:ARG:HG3	1.95	0.65
1:C:590:LEU:HB2	1:C:599:VAL:HG11	1.78	0.65
1:A:2579:VAL:HG22	1:A:2594:SER:HB2	1.77	0.65
1:A:3697:PRO:O	1:A:3701:LEU:N	2.26	0.64
1:B:2186:MET:HE1	1:B:2235:PHE:HA	1.80	0.64
1:B:2579:VAL:HG22	1:B:2594:SER:HB2	1.78	0.64
1:A:879:HIS:NE2	1:A:908:VAL:O	2.29	0.64
1:D:861:ILE:O	1:D:930:LYS:NZ	2.31	0.64
1:D:664:PHE:HB3	1:D:746:CYS:HB3	1.78	0.64
1:D:1804:LEU:HD12	1:D:1853:ILE:HG21	1.79	0.64
1:C:3052:HIS:NE2	1:C:3128:ASN:O	2.30	0.63
1:A:629:ARG:O	1:A:630:GLU:HG3	1.98	0.63
1:C:1459:GLN:HE22	1:C:1461:ASP:HB2	1.63	0.63
1:D:681:HIS:HB3	1:D:784:SER:HB3	1.80	0.63
1:D:1459:GLN:HE22	1:D:1461:ASP:HB2	1.63	0.63
1:A:23:GLN:NE2	1:A:36:CYS:SG	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2440:MET:HE2	1:A:2441:HIS:H	1.63	0.63
1:B:3319:ILE:HD11	1:B:3338:LEU:HD11	1.79	0.63
1:D:977:LEU:HB3	1:D:981:GLN:HB2	1.80	0.63
1:A:348:VAL:HG13	1:A:357:LEU:HD23	1.80	0.63
1:A:3999:MET:HE1	1:A:4003:LEU:HD22	1.80	0.63
1:B:348:VAL:HG13	1:B:357:LEU:HD23	1.81	0.63
2:G:23:VAL:HG21	2:G:106:LEU:HB2	1.80	0.63
2:E:37:ASP:OD1	2:E:42:ARG:NH2	2.32	0.63
1:A:2961:GLN:HA	1:A:2964:LEU:HB3	1.81	0.63
1:A:664:PHE:HB3	1:A:746:CYS:HB3	1.81	0.63
1:A:1457:TYR:HA	1:A:1491:ASN:HD22	1.63	0.63
1:C:879:HIS:NE2	1:C:908:VAL:O	2.31	0.63
1:A:722:TRP:CD1	1:A:727:ALA:HA	2.34	0.62
1:B:794:GLY:O	1:B:812:HIS:ND1	2.27	0.62
1:D:3697:PRO:O	1:D:3701:LEU:N	2.26	0.62
2:H:37:ASP:OD1	2:H:42:ARG:NH2	2.32	0.62
1:A:2441:HIS:HA	1:A:2444:GLN:HB3	1.81	0.62
1:B:1804:LEU:HD12	1:B:1853:ILE:HG21	1.80	0.62
1:C:2961:GLN:HA	1:C:2964:LEU:HB3	1.81	0.62
1:C:4166:LEU:HD23	1:C:4166:LEU:H	1.64	0.62
1:B:4088:ILE:HB	1:B:4092:ASP:HB2	1.81	0.62
2:F:23:VAL:HG21	2:F:106:LEU:HB2	1.80	0.62
2:H:23:VAL:HG21	2:H:106:LEU:HB2	1.79	0.62
1:A:1576:SER:HA	1:A:1579:MET:HB2	1.82	0.62
1:B:590:LEU:HB2	1:B:599:VAL:HG11	1.80	0.62
1:C:3592:ILE:HA	1:C:3595:ARG:HE	1.64	0.62
1:D:879:HIS:NE2	1:D:908:VAL:O	2.28	0.62
2:G:37:ASP:OD1	2:G:42:ARG:NH2	2.32	0.62
1:A:1289:LEU:HB2	1:A:1550:PRO:HD2	1.82	0.62
1:B:2440:MET:HE2	1:B:2441:HIS:H	1.64	0.62
1:B:4003:LEU:HG	1:B:4009:GLN:HG3	1.82	0.62
1:D:3592:ILE:HA	1:D:3595:ARG:HE	1.64	0.62
1:D:4088:ILE:HB	1:D:4092:ASP:HB2	1.82	0.62
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.82	0.62
1:A:1742:THR:HG22	1:A:1769:THR:HG21	1.82	0.61
1:A:205:ILE:HG22	1:A:206:CYS:H	1.65	0.61
1:A:988:LEU:HG	1:A:1039:LEU:HD12	1.81	0.61
1:B:1289:LEU:HB2	1:B:1550:PRO:HD2	1.81	0.61
1:B:3697:PRO:O	1:B:3701:LEU:N	2.30	0.61
1:C:1457:TYR:HA	1:C:1491:ASN:HD22	1.65	0.61
1:D:686:TRP:NE1	1:D:746:CYS:SG	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:HIS:HB3	1:A:784:SER:HB3	1.82	0.61
1:C:3016:TYR:HA	1:C:3029:GLY:HA2	1.82	0.61
1:A:737:LEU:HD23	1:A:738:LEU:H	1.65	0.61
1:D:348:VAL:HG13	1:D:357:LEU:HD23	1.81	0.61
1:D:677:ALA:HB1	2:H:40:ARG:HB3	1.82	0.61
1:D:1457:TYR:HA	1:D:1491:ASN:HD22	1.65	0.61
1:A:4088:ILE:HB	1:A:4092:ASP:HB2	1.83	0.61
1:D:1576:SER:HA	1:D:1579:MET:HB2	1.81	0.61
1:C:683:ARG:HH12	1:C:722:TRP:CG	2.19	0.61
2:G:74:LEU:HB2	2:G:99:PHE:HB2	1.83	0.61
1:A:2472:LEU:HD12	1:A:2473:PRO:HD2	1.83	0.61
1:A:4003:LEU:HG	1:A:4009:GLN:HG3	1.83	0.61
1:C:4003:LEU:HG	1:C:4009:GLN:HG3	1.82	0.61
1:A:895:PRO:HG2	1:A:896:VAL:HG23	1.83	0.61
1:B:645:ARG:HB3	1:B:826:ILE:HD11	1.83	0.61
1:D:299:LEU:HD11	1:D:314:PHE:HZ	1.66	0.61
1:B:765:GLN:NE2	1:B:1478:ASP:OD1	2.34	0.61
1:D:1742:THR:HG22	1:D:1769:THR:HG21	1.83	0.61
1:B:1576:SER:HA	1:B:1579:MET:HB2	1.82	0.60
1:C:645:ARG:HB3	1:C:826:ILE:HD11	1.83	0.60
1:B:1742:THR:HG22	1:B:1769:THR:HG21	1.83	0.60
1:C:1742:THR:HG22	1:C:1769:THR:HG21	1.83	0.60
1:D:737:LEU:HD23	1:D:738:LEU:H	1.65	0.60
1:D:4712:PRO:O	1:D:4718:LYS:NZ	2.34	0.60
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.83	0.60
1:B:892:THR:OG1	1:B:902:ARG:O	2.18	0.60
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.34	0.60
1:B:2472:LEU:HD12	1:B:2473:PRO:HD2	1.84	0.60
1:C:1545:ASN:OD1	2:G:32:ASN:ND2	2.33	0.60
1:D:765:GLN:NE2	1:D:1478:ASP:OD1	2.34	0.60
1:B:3016:TYR:HA	1:B:3029:GLY:HA2	1.84	0.60
1:C:1451:GLY:HA3	1:C:1494:MET:HB3	1.82	0.60
1:D:797:HIS:HB3	1:D:1623:ARG:HH21	1.66	0.60
1:A:2967:MET:HA	1:A:2970:SER:HB3	1.84	0.60
1:A:3592:ILE:HA	1:A:3595:ARG:HE	1.65	0.60
1:C:2591:ARG:O	1:C:2594:SER:OG	2.18	0.60
1:D:2659:THR:O	1:D:2663:ASN:ND2	2.35	0.60
1:D:3016:TYR:HA	1:D:3029:GLY:HA2	1.82	0.60
1:A:2474:LEU:HA	1:A:2494:PHE:HD2	1.67	0.60
1:B:879:HIS:NE2	1:B:908:VAL:O	2.31	0.60
1:C:986:ASP:N	1:C:986:ASP:OD1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4088:ILE:HB	1:C:4092:ASP:HB2	1.83	0.60
1:C:4158:PRO:O	1:C:4162:ASN:ND2	2.35	0.60
1:B:299:LEU:HD11	1:B:314:PHE:HZ	1.67	0.60
1:B:3052:HIS:NE2	1:B:3128:ASN:O	2.34	0.60
1:C:205:ILE:HG22	1:C:206:CYS:H	1.66	0.60
1:C:348:VAL:HG13	1:C:357:LEU:HD23	1.83	0.60
1:C:765:GLN:NE2	1:C:1478:ASP:OD1	2.35	0.60
1:D:421:PHE:HB3	1:D:426:ARG:HH21	1.67	0.60
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.84	0.60
1:B:659:TYR:HE1	1:B:1006:SER:HB3	1.66	0.60
1:C:1289:LEU:HB2	1:C:1550:PRO:HD2	1.83	0.60
1:D:2911:LEU:HB2	1:D:2916:LYS:HD3	1.84	0.60
1:B:1012:ASP:HB3	1:B:1017:ARG:HG3	1.84	0.60
1:A:645:ARG:HB3	1:A:826:ILE:HD11	1.84	0.59
1:C:2472:LEU:HD12	1:C:2473:PRO:HD2	1.83	0.59
1:C:4712:PRO:O	1:C:4718:LYS:NZ	2.33	0.59
1:D:1289:LEU:HB2	1:D:1550:PRO:HD2	1.83	0.59
1:D:2472:LEU:HD12	1:D:2473:PRO:HD2	1.84	0.59
2:G:53:GLN:HG2	2:G:54:GLU:H	1.66	0.59
1:A:3016:TYR:HA	1:A:3029:GLY:HA2	1.83	0.59
1:C:3040:THR:HG21	1:C:3080:VAL:HG21	1.85	0.59
1:D:649:PHE:HB3	1:D:776:LEU:HD22	1.84	0.59
1:D:3999:MET:HE1	1:D:4003:LEU:HD13	1.84	0.59
1:A:765:GLN:NE2	1:A:1478:ASP:OD1	2.34	0.59
1:A:4712:PRO:O	1:A:4718:LYS:NZ	2.34	0.59
1:B:630:GLU:HA	1:B:1642:PRO:HB2	1.84	0.59
1:B:668:VAL:HG22	1:B:789:VAL:HG12	1.85	0.59
1:B:686:TRP:NE1	1:B:746:CYS:SG	2.75	0.59
1:D:645:ARG:HD3	1:D:826:ILE:HG12	1.83	0.59
1:B:659:TYR:CE1	1:B:1006:SER:HB3	2.37	0.59
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.83	0.59
1:B:2961:GLN:HA	1:B:2964:LEU:HB3	1.82	0.59
1:C:1104:TRP:NE1	1:C:1151:CYS:SG	2.75	0.59
1:A:4158:PRO:O	1:A:4162:ASN:ND2	2.35	0.59
1:B:150:MET:HB3	1:B:169:LEU:HD13	1.84	0.59
1:B:649:PHE:HB3	1:B:776:LEU:HD22	1.85	0.59
1:B:1457:TYR:HA	1:B:1491:ASN:HD22	1.66	0.59
1:B:2967:MET:HA	1:B:2970:SER:HB3	1.84	0.59
1:D:265:LEU:HD23	1:D:279:PRO:HB2	1.85	0.59
1:D:1104:TRP:NE1	1:D:1151:CYS:SG	2.76	0.59
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:N	1:C:148:TRP:O	2.34	0.59
1:D:707:VAL:HG23	1:D:713:SER:HB2	1.85	0.59
1:D:957:LYS:HA	1:D:960:MET:HE3	1.84	0.59
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.36	0.59
1:A:797:HIS:HB3	1:A:1623:ARG:HH21	1.66	0.59
1:A:2191:PHE:HD1	1:A:2198:MET:HE3	1.68	0.59
1:A:813:GLU:OE1	1:A:813:GLU:N	2.36	0.59
1:A:2659:THR:O	1:A:2663:ASN:ND2	2.36	0.59
1:B:4712:PRO:O	1:B:4718:LYS:NZ	2.34	0.59
1:D:709:ASP:OD1	1:D:713:SER:OG	2.20	0.59
1:D:772:ASN:HD22	1:D:1471:ALA:H	1.49	0.59
1:A:2452:ARG:NH1	1:D:175:SER:O	2.36	0.59
1:A:2911:LEU:HB2	1:A:2916:LYS:HD3	1.84	0.59
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.35	0.59
1:D:168:ASP:HB3	1:D:199:LEU:HB3	1.84	0.59
1:D:331:VAL:HG22	1:D:333:GLY:H	1.68	0.59
2:E:11:ASP:OD1	2:E:12:GLY:N	2.36	0.59
1:A:421:PHE:HB3	1:A:426:ARG:HH21	1.68	0.58
1:A:3409:TYR:HE2	1:A:3510:ILE:HG23	1.68	0.58
1:B:4158:PRO:O	1:B:4162:ASN:ND2	2.36	0.58
1:C:265:LEU:HD23	1:C:279:PRO:HB2	1.85	0.58
1:C:331:VAL:HG22	1:C:333:GLY:H	1.68	0.58
1:A:331:VAL:HG22	1:A:333:GLY:H	1.67	0.58
1:A:2591:ARG:O	1:A:2594:SER:OG	2.19	0.58
1:B:797:HIS:HB3	1:B:1623:ARG:HH21	1.66	0.58
1:B:895:PRO:HG2	1:B:896:VAL:HG23	1.84	0.58
1:D:986:ASP:OD1	1:D:986:ASP:N	2.36	0.58
1:A:1545:ASN:OD1	2:E:32:ASN:ND2	2.34	0.58
1:B:3096:PHE:O	1:B:3100:SER:N	2.36	0.58
1:D:574:VAL:HA	1:D:577:ILE:HD12	1.85	0.58
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.85	0.58
1:C:813:GLU:N	1:C:813:GLU:OE1	2.36	0.58
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.36	0.58
2:E:23:VAL:HG21	2:E:106:LEU:HB2	1.85	0.58
1:A:195:PHE:C	1:A:196:MET:HE2	2.28	0.58
1:A:1451:GLY:HA3	1:A:1494:MET:HB3	1.84	0.58
1:C:686:TRP:NE1	1:C:746:CYS:SG	2.76	0.58
1:D:3052:HIS:NE2	1:D:3128:ASN:O	2.36	0.58
1:B:2659:THR:O	1:B:2663:ASN:ND2	2.36	0.58
1:C:1576:SER:HA	1:C:1579:MET:HB2	1.83	0.58
1:C:3409:TYR:HE2	1:C:3510:ILE:HG23	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4733:GLY:HA3	1:D:4736:ARG:HG3	1.85	0.58
2:E:53:GLN:HG2	2:E:54:GLU:H	1.67	0.58
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.84	0.58
1:D:1545:ASN:OD1	2:H:32:ASN:ND2	2.35	0.58
2:H:17:LYS:NZ	2:H:18:LYS:O	2.36	0.58
1:B:4733:GLY:HA3	1:B:4736:ARG:HG3	1.86	0.58
1:C:668:VAL:HG22	1:C:789:VAL:HG12	1.85	0.58
1:C:2911:LEU:HB2	1:C:2916:LYS:HD3	1.84	0.58
2:G:17:LYS:H	2:G:20:GLN:HE22	1.50	0.58
2:H:11:ASP:OD1	2:H:12:GLY:N	2.37	0.58
1:A:1000:ARG:HG3	1:A:1005:TRP:HB2	1.86	0.58
1:C:393:CYS:SG	1:C:398:SER:OG	2.62	0.58
1:D:19:GLU:HB2	1:D:205:ILE:HB	1.86	0.58
1:D:150:MET:HB3	1:D:169:LEU:HD13	1.86	0.58
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.85	0.58
1:A:534:ARG:NH2	1:A:573:GLU:OE2	2.37	0.57
1:A:4733:GLY:HA3	1:A:4736:ARG:HG3	1.86	0.57
1:C:534:ARG:NH2	1:C:573:GLU:OE2	2.37	0.57
1:C:649:PHE:HB3	1:C:776:LEU:HD22	1.85	0.57
1:C:4733:GLY:HA3	1:C:4736:ARG:HG3	1.85	0.57
1:D:534:ARG:NH2	1:D:573:GLU:OE2	2.36	0.57
1:A:668:VAL:HG22	1:A:789:VAL:HG12	1.86	0.57
1:B:175:SER:O	1:C:2452:ARG:NH1	2.37	0.57
1:C:636:ASN:HD21	2:G:35:LYS:HE3	1.69	0.57
1:C:2659:THR:O	1:C:2663:ASN:ND2	2.37	0.57
1:D:668:VAL:HG22	1:D:789:VAL:HG12	1.86	0.57
1:D:927:GLU:O	1:D:931:THR:HG23	2.04	0.57
2:E:14:THR:HG21	2:E:68:LEU:HD12	1.86	0.57
2:F:53:GLN:HG2	2:F:54:GLU:H	1.68	0.57
1:A:175:SER:O	1:B:2452:ARG:NH1	2.38	0.57
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.21	0.57
1:B:331:VAL:HG22	1:B:333:GLY:H	1.68	0.57
1:B:1104:TRP:NE1	1:B:1151:CYS:SG	2.76	0.57
1:C:1452:TRP:HE1	1:C:1518:CYS:HB3	1.70	0.57
1:A:1104:TRP:NE1	1:A:1151:CYS:SG	2.77	0.57
1:A:3980:LEU:HD23	1:A:3985:LEU:HD22	1.85	0.57
1:B:737:LEU:HD23	1:B:738:LEU:H	1.69	0.57
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.36	0.57
1:C:2967:MET:HA	1:C:2970:SER:HB3	1.86	0.57
1:C:3415:TYR:O	1:C:3419:ASN:ND2	2.37	0.57
1:D:2968:ASP:O	1:D:2971:GLN:NE2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3409:TYR:HE2	1:B:3510:ILE:HG23	1.70	0.57
1:C:3096:PHE:O	1:C:3100:SER:N	2.36	0.57
1:D:2961:GLN:HA	1:D:2964:LEU:HB3	1.87	0.57
1:B:651:GLY:HA3	1:B:776:LEU:HA	1.85	0.57
1:A:221:ARG:NH1	1:A:258:SER:OG	2.38	0.57
1:B:574:VAL:HA	1:B:577:ILE:HD12	1.85	0.57
1:B:2911:LEU:HB2	1:B:2916:LYS:HD3	1.86	0.57
1:C:221:ARG:NH1	1:C:258:SER:OG	2.37	0.57
1:C:865:PRO:HA	1:C:868:GLU:HB3	1.86	0.57
1:C:1164:LEU:HD23	1:C:1169:LEU:HB3	1.86	0.57
1:D:1241:SER:HA	1:D:1603:VAL:HG12	1.86	0.57
1:D:2524:VAL:HA	1:D:2527:LEU:HD23	1.85	0.57
1:D:4158:PRO:O	1:D:4162:ASN:ND2	2.37	0.57
1:A:651:GLY:HA3	1:A:776:LEU:HA	1.86	0.57
1:A:3666:ASP:OD1	1:A:3666:ASP:N	2.38	0.57
1:C:4567:LEU:HB2	1:C:4816:ILE:HG21	1.87	0.57
1:D:895:PRO:HD2	1:D:903:LEU:HD13	1.85	0.57
1:A:299:LEU:HD11	1:A:314:PHE:HZ	1.68	0.57
1:B:1140:GLY:HA3	1:B:1169:LEU:HD12	1.87	0.57
1:C:1462:MET:HE2	1:C:1462:MET:HA	1.87	0.57
1:D:3409:TYR:HE2	1:D:3510:ILE:HG23	1.70	0.57
1:A:393:CYS:SG	1:A:398:SER:OG	2.62	0.57
1:B:636:ASN:HD21	2:F:35:LYS:HE3	1.69	0.57
1:B:737:LEU:HD23	1:B:738:LEU:N	2.20	0.57
1:B:4696:ASP:O	1:B:4700:GLN:NE2	2.38	0.57
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.87	0.57
1:D:2967:MET:HA	1:D:2970:SER:HB3	1.87	0.57
1:D:3366:ARG:HA	1:D:3441:ILE:HD11	1.86	0.57
1:A:3052:HIS:NE2	1:A:3128:ASN:O	2.37	0.56
1:B:393:CYS:SG	1:B:398:SER:OG	2.63	0.56
1:B:753:PRO:HB2	1:B:771:PHE:CD2	2.40	0.56
1:D:860:GLN:OE1	1:D:860:GLN:N	2.38	0.56
1:A:636:ASN:HD21	2:E:35:LYS:HE3	1.70	0.56
1:A:2737:PRO:HG3	1:A:2888:ARG:HD2	1.87	0.56
1:B:265:LEU:HD23	1:B:279:PRO:HB2	1.87	0.56
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.37	0.56
1:C:14:LEU:HD12	1:C:18:ASP:HB3	1.86	0.56
1:D:3415:TYR:O	1:D:3419:ASN:ND2	2.38	0.56
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.38	0.56
1:A:644:ILE:HD11	1:A:1615:VAL:HG21	1.87	0.56
1:A:1140:GLY:HA3	1:A:1169:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ALA:HB1	2:F:40:ARG:HB3	1.87	0.56
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.85	0.56
1:C:3270:ILE:HA	1:C:3274:LEU:HD21	1.86	0.56
1:D:1089:TYR:HB2	1:D:1152:MET:HG2	1.87	0.56
1:D:1140:GLY:HA3	1:D:1169:LEU:HD12	1.87	0.56
2:H:53:GLN:HG2	2:H:54:GLU:H	1.69	0.56
1:A:416:LYS:HD3	1:A:416:LYS:C	2.30	0.56
1:A:3415:TYR:O	1:A:3419:ASN:ND2	2.38	0.56
1:C:3335:MET:HB3	1:C:3407:ALA:HB2	1.87	0.56
1:D:636:ASN:HD21	2:H:35:LYS:HE3	1.70	0.56
1:D:910:PHE:HA	1:D:913:LEU:HD11	1.87	0.56
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.39	0.56
1:B:1241:SER:HA	1:B:1603:VAL:HG12	1.86	0.56
1:B:3980:LEU:HD23	1:B:3985:LEU:HD22	1.87	0.56
1:D:689:THR:HB	1:D:778:PHE:CZ	2.40	0.56
1:D:1424:PRO:HA	1:D:1427:ILE:HG22	1.87	0.56
1:D:2118:ARG:NH2	1:D:3719:ASP:OD1	2.37	0.56
1:A:686:TRP:NE1	1:A:746:CYS:SG	2.77	0.56
1:B:977:LEU:HB3	1:B:981:GLN:HB2	1.88	0.56
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.87	0.56
1:C:860:GLN:N	1:C:860:GLN:OE1	2.38	0.56
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.87	0.56
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.87	0.56
1:B:860:GLN:OE1	1:B:860:GLN:N	2.39	0.56
1:C:664:PHE:HB3	1:C:746:CYS:HB3	1.88	0.56
1:D:221:ARG:NH1	1:D:258:SER:OG	2.38	0.56
1:A:150:MET:HB3	1:A:169:LEU:HD13	1.87	0.56
1:A:452:PHE:O	1:A:528:SER:OG	2.24	0.56
1:A:4567:LEU:HB2	1:A:4816:ILE:HG21	1.88	0.56
1:B:910:PHE:HA	1:B:913:LEU:HD11	1.86	0.56
1:C:651:GLY:HA3	1:C:776:LEU:HA	1.88	0.56
1:C:2884:ASN:OD1	1:C:2888:ARG:NH1	2.39	0.56
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.38	0.56
1:C:4766:THR:HA	1:C:4769:MET:HE1	1.88	0.56
1:C:4769:MET:N	1:C:4769:MET:SD	2.79	0.56
1:D:1452:TRP:HE1	1:D:1518:CYS:HB3	1.71	0.56
1:D:2512:ILE:HG22	1:D:2516:ASP:HB3	1.87	0.56
1:D:3980:LEU:HD23	1:D:3985:LEU:HD22	1.87	0.56
1:C:882:TRP:HZ3	1:C:921:ASN:HD21	1.53	0.56
1:C:895:PRO:HD2	1:C:903:LEU:HD13	1.86	0.56
1:C:3366:ARG:HA	1:C:3441:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:CYS:SG	1:D:398:SER:OG	2.63	0.56
1:D:1462:MET:HE2	1:D:1462:MET:HA	1.87	0.56
1:D:2737:PRO:HG3	1:D:2888:ARG:HD2	1.88	0.56
1:D:4567:LEU:HB2	1:D:4816:ILE:HG21	1.88	0.56
1:A:1112:ASP:OD1	1:A:1112:ASP:N	2.36	0.56
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.36	0.56
1:A:2118:ARG:NH2	1:A:3719:ASP:OD1	2.37	0.56
1:A:2740:VAL:HG21	1:A:2818:ALA:HB1	1.88	0.56
1:B:221:ARG:NH1	1:B:258:SER:OG	2.38	0.56
1:B:2891:LYS:HA	1:B:2894:LEU:HD12	1.88	0.56
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.39	0.56
1:C:830:ARG:NH2	1:C:832:GLU:OE2	2.36	0.56
1:C:3980:LEU:HD23	1:C:3985:LEU:HD22	1.87	0.56
1:A:2884:ASN:OD1	1:A:2888:ARG:NH1	2.39	0.55
1:B:4567:LEU:HB2	1:B:4816:ILE:HG21	1.88	0.55
1:C:2740:VAL:HG21	1:C:2818:ALA:HB1	1.88	0.55
1:D:81:MET:O	1:D:81:MET:HE3	2.05	0.55
1:D:864:PRO:HD2	1:D:867:LEU:HD12	1.87	0.55
1:D:1003:GLN:O	1:D:1016:ARG:NH2	2.39	0.55
1:D:3319:ILE:HD11	1:D:3338:LEU:HD11	1.87	0.55
1:D:5012:LYS:NZ	1:D:5016:GLU:OE2	2.39	0.55
1:A:107:ILE:N	1:A:148:TRP:O	2.38	0.55
1:A:4766:THR:HA	1:A:4769:MET:HE1	1.89	0.55
1:B:2512:ILE:HG22	1:B:2516:ASP:HB3	1.87	0.55
1:C:5012:LYS:NZ	1:C:5016:GLU:OE2	2.40	0.55
1:D:12:GLN:HG3	1:D:165:VAL:HA	1.88	0.55
1:D:4696:ASP:O	1:D:4700:GLN:NE2	2.40	0.55
1:A:229:GLU:HA	1:A:249:GLY:HA3	1.89	0.55
1:A:1241:SER:HA	1:A:1603:VAL:HG12	1.87	0.55
1:B:102:LEU:HB3	1:B:105:HIS:CD2	2.41	0.55
1:B:2740:VAL:HG21	1:B:2818:ALA:HB1	1.88	0.55
1:B:4087:LEU:HD22	1:B:4122:MET:HA	1.88	0.55
1:C:175:SER:O	1:D:2452:ARG:NH1	2.38	0.55
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.38	0.55
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.36	0.55
1:C:2737:PRO:HG3	1:C:2888:ARG:HD2	1.88	0.55
1:D:3666:ASP:OD1	1:D:3666:ASP:N	2.38	0.55
1:A:772:ASN:HD22	1:A:1471:ALA:H	1.54	0.55
1:B:2737:PRO:HG3	1:B:2888:ARG:HD2	1.87	0.55
1:B:3999:MET:HE1	1:B:4003:LEU:HD22	1.88	0.55
1:C:150:MET:HB3	1:C:169:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD11	1:C:314:PHE:HZ	1.71	0.55
1:C:452:PHE:O	1:C:528:SER:OG	2.24	0.55
1:C:755:ILE:HG13	1:C:771:PHE:CZ	2.42	0.55
1:A:677:ALA:HB1	2:E:40:ARG:HB3	1.88	0.55
1:A:4696:ASP:O	1:A:4700:GLN:NE2	2.40	0.55
1:B:1089:TYR:HB2	1:B:1152:MET:HG2	1.88	0.55
1:C:797:HIS:HB3	1:C:1623:ARG:HH21	1.70	0.55
1:C:2118:ARG:NH2	1:C:3719:ASP:OD1	2.38	0.55
1:C:4032:GLU:OE2	1:C:5004:THR:OG1	2.25	0.55
1:A:14:LEU:HD11	1:A:69:LEU:HD13	1.88	0.55
1:A:3270:ILE:HA	1:A:3274:LEU:HD21	1.88	0.55
1:B:2884:ASN:OD1	1:B:2888:ARG:NH1	2.39	0.55
1:B:5012:LYS:NZ	1:B:5016:GLU:OE2	2.39	0.55
1:C:689:THR:HB	1:C:778:PHE:CZ	2.42	0.55
1:C:2420:HIS:N	1:C:2492:ALA:O	2.40	0.55
1:D:107:ILE:N	1:D:148:TRP:O	2.38	0.55
1:D:4224:GLU:OE2	1:D:4224:GLU:N	2.40	0.55
1:A:399:GLN:O	1:A:403:MET:HG3	2.06	0.55
1:A:3366:ARG:HA	1:A:3441:ILE:HD11	1.88	0.55
1:A:5012:LYS:NZ	1:A:5016:GLU:OE2	2.39	0.55
1:B:2244:ARG:NH1	1:B:2283:ASN:OD1	2.40	0.55
1:B:3415:TYR:O	1:B:3419:ASN:ND2	2.40	0.55
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.89	0.55
1:D:2191:PHE:HD1	1:D:2198:MET:HE3	1.71	0.55
1:D:2244:ARG:NH1	1:D:2283:ASN:OD1	2.40	0.55
1:D:2884:ASN:OD1	1:D:2888:ARG:NH1	2.39	0.55
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.39	0.55
1:A:3417:ASP:OD1	1:A:3417:ASP:N	2.40	0.55
1:B:103:TYR:HE2	1:B:152:PRO:HA	1.71	0.55
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.20	0.55
1:D:1530:THR:HG22	1:D:1535:GLU:HA	1.89	0.55
1:D:3335:MET:HB3	1:D:3407:ALA:HB2	1.89	0.55
1:D:3678:SER:OG	1:D:3773:ARG:NH2	2.39	0.55
1:A:2512:ILE:HG22	1:A:2516:ASP:HB3	1.87	0.55
1:B:2654:TYR:HA	1:B:2657:LEU:HD23	1.89	0.55
1:B:4166:LEU:HD23	1:B:4166:LEU:H	1.70	0.55
1:C:1504:GLY:O	1:C:1508:ARG:NH1	2.40	0.55
1:C:2098:VAL:HG11	1:C:2127:GLN:HG3	1.88	0.55
1:C:4224:GLU:N	1:C:4224:GLU:OE1	2.40	0.55
1:D:3245:VAL:HG12	1:D:3247:ASP:H	1.72	0.55
1:A:649:PHE:HB3	1:A:776:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3319:ILE:HD11	1:A:3338:LEU:HD11	1.89	0.54
1:A:4818:MET:SD	1:A:4819:GLY:N	2.81	0.54
1:B:229:GLU:HA	1:B:249:GLY:HA3	1.89	0.54
1:B:284:HIS:ND1	1:B:287:THR:OG1	2.33	0.54
1:B:1018:ASN:ND2	1:B:1020:ARG:HG2	2.22	0.54
1:C:1028:ASP:OD1	1:C:1028:ASP:N	2.40	0.54
1:C:1140:GLY:HA3	1:C:1169:LEU:HD12	1.89	0.54
1:C:1530:THR:HG22	1:C:1535:GLU:HA	1.89	0.54
1:D:2654:TYR:HA	1:D:2657:LEU:HD23	1.89	0.54
1:A:4032:GLU:OE2	1:A:5004:THR:OG1	2.24	0.54
1:B:534:ARG:NH2	1:B:573:GLU:OE2	2.35	0.54
1:B:2098:VAL:HG11	1:B:2127:GLN:HG3	1.89	0.54
1:B:2191:PHE:HD1	1:B:2198:MET:HE3	1.72	0.54
1:B:4224:GLU:N	1:B:4224:GLU:OE2	2.40	0.54
1:D:580:GLU:HG3	1:D:620:LEU:HD21	1.89	0.54
1:D:867:LEU:HD22	1:D:929:LEU:HD11	1.88	0.54
1:A:910:PHE:HA	1:A:913:LEU:HD11	1.90	0.54
1:B:753:PRO:HB2	1:B:771:PHE:HD2	1.72	0.54
1:C:49:LEU:HD11	1:C:191:VAL:HG23	1.90	0.54
1:D:871:ARG:NH1	1:D:922:LEU:O	2.40	0.54
1:A:2891:LYS:HA	1:A:2894:LEU:HD12	1.90	0.54
1:A:3678:SER:OG	1:A:3773:ARG:NH2	2.41	0.54
1:B:4818:MET:SD	1:B:4819:GLY:N	2.81	0.54
1:C:3678:SER:OG	1:C:3773:ARG:NH2	2.41	0.54
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.40	0.54
1:A:144:GLU:O	1:A:175:SER:OG	2.25	0.54
1:D:2740:VAL:HG21	1:D:2818:ALA:HB1	1.89	0.54
1:D:4688:ILE:HD12	1:D:4737:ILE:HD12	1.90	0.54
1:A:54:ASN:HD22	1:A:57:ASN:HD21	1.54	0.54
1:A:1704:PRO:HG2	1:A:1707:LEU:HB2	1.90	0.54
1:A:3096:PHE:O	1:A:3100:SER:N	2.35	0.54
1:A:4688:ILE:HD12	1:A:4737:ILE:HD12	1.90	0.54
1:B:1152:MET:HB2	1:B:1161:ILE:O	2.08	0.54
1:B:1459:GLN:NE2	1:B:1470:ARG:HE	2.05	0.54
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.40	0.54
1:B:619:ASP:OD2	1:B:1680:ARG:NH2	2.37	0.54
1:D:4818:MET:SD	1:D:4819:GLY:N	2.81	0.54
1:B:1160:ILE:HB	1:B:1179:PHE:HD2	1.73	0.54
1:B:4768:LEU:HD12	1:B:4769:MET:SD	2.48	0.54
1:C:1089:TYR:HB2	1:C:1152:MET:HG2	1.89	0.54
1:C:3323:ILE:HD11	1:C:3338:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2891:LYS:HA	1:D:2894:LEU:HD12	1.89	0.54
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.38	0.54
1:A:1089:TYR:HB2	1:A:1152:MET:HG2	1.89	0.54
1:A:3673:MET:O	1:A:3677:LEU:HB2	2.08	0.54
1:A:4224:GLU:N	1:A:4224:GLU:OE2	2.40	0.54
1:C:2214:VAL:HG21	1:C:2228:MET:HE1	1.90	0.54
1:C:4087:LEU:HD22	1:C:4122:MET:HA	1.88	0.54
1:D:651:GLY:HA3	1:D:776:LEU:HA	1.88	0.54
1:A:1530:THR:HG22	1:A:1535:GLU:HA	1.90	0.54
1:A:2244:ARG:NH1	1:A:2283:ASN:OD1	2.40	0.54
1:B:659:TYR:OH	1:B:1017:ARG:HD3	2.07	0.54
1:B:1040:CYS:O	1:B:1044:ARG:HG2	2.07	0.54
1:B:2118:ARG:NH2	1:B:3719:ASP:OD1	2.37	0.54
1:C:2244:ARG:NH1	1:C:2283:ASN:OD1	2.40	0.54
1:C:2953:LYS:HA	1:C:2957:PHE:HB3	1.90	0.54
1:D:1704:PRO:HG2	1:D:1707:LEU:HB2	1.90	0.54
1:D:4032:GLU:OE2	1:D:5004:THR:OG1	2.25	0.54
1:A:1504:GLY:O	1:A:1508:ARG:NH1	2.41	0.53
1:A:2654:TYR:HA	1:A:2657:LEU:HD23	1.90	0.53
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.40	0.53
1:D:54:ASN:HD22	1:D:57:ASN:HD21	1.55	0.53
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.89	0.53
1:D:1443:GLN:NE2	1:D:1444:GLU:O	2.41	0.53
1:D:2420:HIS:N	1:D:2492:ALA:O	2.41	0.53
1:A:205:ILE:HG22	1:A:206:CYS:N	2.24	0.53
1:A:4162:ASN:HA	1:A:4165:GLU:HG2	1.89	0.53
1:B:644:ILE:HD11	1:B:1615:VAL:HG21	1.90	0.53
1:C:3319:ILE:HD11	1:C:3338:LEU:HD11	1.90	0.53
1:A:871:ARG:HH12	1:A:926:GLY:HA3	1.72	0.53
1:A:4769:MET:N	1:A:4769:MET:SD	2.81	0.53
1:B:813:GLU:HG3	1:B:1009:ALA:H	1.74	0.53
1:B:2420:HIS:CE1	1:B:2424:SER:HB3	2.43	0.53
1:B:2953:LYS:HA	1:B:2957:PHE:HB3	1.90	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.42	0.53
1:C:1241:SER:HA	1:C:1603:VAL:HG12	1.91	0.53
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.90	0.53
1:A:745:SER:HB3	1:A:758:ARG:HB2	1.91	0.53
1:B:1180:ARG:O	1:B:1181:GLU:HG2	2.09	0.53
1:B:4032:GLU:OE2	1:B:5004:THR:OG1	2.25	0.53
1:C:554:LEU:HD23	1:C:1593:PRO:HD3	1.90	0.53
1:C:681:HIS:HB3	1:C:784:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:LEU:HD22	1:C:1044:ARG:HB3	1.90	0.53
1:C:2441:HIS:HA	1:C:2444:GLN:HB3	1.90	0.53
1:D:229:GLU:HA	1:D:249:GLY:HA3	1.89	0.53
1:D:3133:THR:HA	1:D:3137:LEU:HD12	1.89	0.53
1:D:4003:LEU:HG	1:D:4009:GLN:HG3	1.90	0.53
1:B:1530:THR:HG22	1:B:1535:GLU:HA	1.91	0.53
1:C:54:ASN:HD22	1:C:57:ASN:HD21	1.56	0.53
1:C:4688:ILE:HD12	1:C:4737:ILE:HD12	1.91	0.53
1:D:24:CYS:HB2	1:D:200:TRP:HA	1.91	0.53
1:D:4055:VAL:HA	1:D:4058:ILE:HD12	1.90	0.53
2:H:17:LYS:H	2:H:20:GLN:HE22	1.56	0.53
1:B:3417:ASP:N	1:B:3417:ASP:OD1	2.42	0.53
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	1.90	0.53
1:C:3417:ASP:N	1:C:3417:ASP:OD1	2.39	0.53
2:H:17:LYS:HG3	2:H:18:LYS:H	1.73	0.53
1:B:1772:ARG:NH2	1:B:1952:GLN:OE1	2.42	0.53
1:B:3366:ARG:HA	1:B:3441:ILE:HD11	1.90	0.53
1:B:4688:ILE:HD12	1:B:4737:ILE:HD12	1.91	0.53
1:C:3037:GLU:O	1:C:3040:THR:OG1	2.26	0.53
1:C:3673:MET:O	1:C:3677:LEU:HB2	2.08	0.53
1:B:984:LEU:O	1:B:988:LEU:HG	2.09	0.53
1:C:745:SER:HB3	1:C:758:ARG:HB2	1.90	0.53
1:C:1180:ARG:O	1:C:1181:GLU:HG2	2.09	0.53
1:C:2654:TYR:HA	1:C:2657:LEU:HD23	1.91	0.53
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	1.90	0.53
1:A:5004:THR:OG1	1:A:5005:GLY:N	2.42	0.53
1:B:1461:ASP:HB3	1:B:1464:PHE:HB2	1.91	0.53
1:B:3245:VAL:HG12	1:B:3247:ASP:H	1.71	0.53
1:B:3794:VAL:HG21	1:B:3835:LEU:HD11	1.91	0.53
1:B:4767:TRP:O	1:B:4770:SER:OG	2.26	0.53
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.41	0.53
1:A:4087:LEU:HD22	1:A:4122:MET:HA	1.91	0.53
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	1.91	0.53
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.42	0.53
1:B:4820:VAL:HG23	1:B:4821:LYS:N	2.24	0.53
1:C:1704:PRO:HG2	1:C:1707:LEU:HB2	1.91	0.53
1:D:2420:HIS:CE1	1:D:2424:SER:HB3	2.44	0.53
1:A:692:TYR:CD1	1:A:713:SER:OG	2.59	0.52
1:A:871:ARG:HH21	1:A:922:LEU:HD23	1.74	0.52
1:C:205:ILE:HG22	1:C:206:CYS:N	2.24	0.52
1:C:1160:ILE:HB	1:C:1179:PHE:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1436:SER:HA	1:C:1517:GLY:HA2	1.90	0.52
1:C:3438:VAL:HG11	1:C:3517:MET:HE2	1.91	0.52
1:D:1180:ARG:O	1:D:1181:GLU:HG2	2.09	0.52
1:D:3438:VAL:HG11	1:D:3517:MET:CE	2.39	0.52
1:A:871:ARG:NH2	1:A:922:LEU:O	2.43	0.52
1:B:416:LYS:C	1:B:416:LYS:HD3	2.34	0.52
1:C:3545:THR:HG23	1:C:3548:GLU:H	1.73	0.52
1:C:4818:MET:SD	1:C:4819:GLY:N	2.82	0.52
1:C:5004:THR:OG1	1:C:5005:GLY:N	2.43	0.52
1:D:416:LYS:HD3	1:D:416:LYS:C	2.34	0.52
1:D:1079:LYS:HA	1:D:1189:LEU:HD11	1.91	0.52
1:D:1160:ILE:HB	1:D:1179:PHE:HD2	1.74	0.52
1:D:3673:MET:O	1:D:3677:LEU:HB2	2.09	0.52
1:A:265:LEU:HD11	1:A:281:ARG:HD3	1.91	0.52
1:A:750:LEU:C	1:A:752:VAL:H	2.16	0.52
1:B:1704:PRO:HG2	1:B:1707:LEU:HB2	1.91	0.52
1:D:119:SER:OG	1:D:120:CYS:N	2.43	0.52
1:D:981:GLN:O	1:D:985:VAL:HG23	2.10	0.52
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.74	0.52
1:B:452:PHE:O	1:B:528:SER:OG	2.22	0.52
1:B:1504:GLY:O	1:B:1508:ARG:NH1	2.40	0.52
1:C:229:GLU:HA	1:C:249:GLY:HA3	1.90	0.52
1:C:913:LEU:HB2	1:C:918:ARG:HG2	1.92	0.52
1:C:2891:LYS:HA	1:C:2894:LEU:HD12	1.90	0.52
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.41	0.52
1:A:981:GLN:O	1:A:985:VAL:HG23	2.10	0.52
1:A:3999:MET:HE2	1:A:4016:LEU:HD13	1.92	0.52
1:C:24:CYS:HB2	1:C:200:TRP:HA	1.91	0.52
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.73	0.52
1:A:49:LEU:HD11	1:A:191:VAL:HG23	1.91	0.52
1:B:882:TRP:HZ3	1:B:921:ASN:HD21	1.58	0.52
1:B:1443:GLN:NE2	1:B:1444:GLU:O	2.41	0.52
1:C:119:SER:OG	1:C:120:CYS:N	2.43	0.52
1:C:750:LEU:C	1:C:752:VAL:H	2.18	0.52
1:D:41:GLY:O	1:D:45:ARG:NH1	2.43	0.52
1:D:4087:LEU:HD22	1:D:4122:MET:HA	1.91	0.52
1:A:1079:LYS:HA	1:A:1189:LEU:HD11	1.92	0.52
1:A:3453:ARG:O	1:A:3457:ASN:ND2	2.43	0.52
1:B:498:THR:H	1:B:503:PHE:HE2	1.57	0.52
1:B:4055:VAL:HA	1:B:4058:ILE:HD12	1.92	0.52
1:C:910:PHE:HA	1:C:913:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1868:PRO:O	1:C:1872:THR:OG1	2.25	0.52
1:D:3579:LEU:HG	1:D:3581:GLY:H	1.75	0.52
1:B:772:ASN:ND2	1:B:1471:ALA:H	2.08	0.52
1:C:1079:LYS:HA	1:C:1189:LEU:HD11	1.92	0.52
1:C:1435:TYR:HB3	1:C:1575:LEU:HG	1.92	0.52
1:C:4633:GLU:HG2	1:C:4635:SER:H	1.75	0.52
1:D:554:LEU:HD23	1:D:1593:PRO:HD3	1.91	0.52
1:D:1152:MET:HB2	1:D:1161:ILE:O	2.09	0.52
1:D:3453:ARG:O	1:D:3457:ASN:ND2	2.43	0.52
1:A:1443:GLN:NE2	1:A:1444:GLU:O	2.41	0.52
1:A:2243:SER:OG	1:A:2245:GLN:OE1	2.28	0.52
1:A:2856:ASN:OD1	1:A:2856:ASN:N	2.43	0.52
1:B:49:LEU:HD11	1:B:191:VAL:HG23	1.92	0.52
1:B:2420:HIS:N	1:B:2492:ALA:O	2.42	0.52
1:D:674:PHE:N	1:D:680:THR:OG1	2.43	0.52
1:D:982:THR:HA	1:D:985:VAL:HG23	1.92	0.52
1:D:1772:ARG:NH2	1:D:1952:GLN:OE1	2.43	0.52
1:D:2214:VAL:HG21	1:D:2228:MET:HE1	1.92	0.52
1:D:4696:ASP:OD1	1:D:4696:ASP:N	2.37	0.52
1:A:1110:ARG:NH2	1:A:1112:ASP:OD2	2.43	0.52
1:A:1180:ARG:O	1:A:1181:GLU:HG2	2.10	0.52
1:A:3037:GLU:O	1:A:3040:THR:OG1	2.26	0.52
1:B:830:ARG:NH2	1:B:832:GLU:OE2	2.38	0.52
1:B:1208:VAL:HA	1:B:1211:LEU:HD12	1.91	0.52
1:B:3545:THR:HG23	1:B:3548:GLU:H	1.74	0.52
1:C:1152:MET:HB2	1:C:1161:ILE:O	2.09	0.52
1:C:1277:TRP:CD1	1:C:1277:TRP:O	2.63	0.52
1:D:644:ILE:HD11	1:D:1615:VAL:HG21	1.92	0.52
1:D:1110:ARG:NH2	1:D:1112:ASP:OD2	2.43	0.52
1:D:1172:ASP:OD1	1:D:1172:ASP:N	2.43	0.52
1:D:2345:SER:OG	1:D:2435:ARG:O	2.27	0.52
1:D:5004:THR:OG1	1:D:5005:GLY:N	2.42	0.52
1:A:4187:SER:OG	1:A:4191:GLU:OE2	2.28	0.51
1:A:4633:GLU:HG2	1:A:4635:SER:H	1.75	0.51
1:C:984:LEU:O	1:C:988:LEU:HG	2.09	0.51
1:C:4055:VAL:HA	1:C:4058:ILE:HD12	1.92	0.51
1:D:3417:ASP:OD1	1:D:3417:ASP:N	2.40	0.51
1:A:976:ARG:HA	1:A:1044:ARG:HH12	1.74	0.51
1:A:2420:HIS:CE1	1:A:2424:SER:HB3	2.45	0.51
1:B:961:MET:CE	1:B:963:ASN:H	2.23	0.51
1:D:284:HIS:ND1	1:D:287:THR:OG1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1208:VAL:HA	1:D:1211:LEU:HD12	1.93	0.51
1:D:1504:GLY:O	1:D:1508:ARG:NH1	2.40	0.51
1:A:3110:LEU:HD12	1:A:3175:LEU:HD11	1.92	0.51
1:C:871:ARG:NH2	1:C:922:LEU:HB2	2.24	0.51
1:C:1562:ILE:HD12	1:C:1563:GLN:H	1.74	0.51
1:C:2420:HIS:CE1	1:C:2424:SER:HB3	2.46	0.51
1:C:2440:MET:HE2	1:C:2441:HIS:H	1.75	0.51
1:D:3096:PHE:O	1:D:3100:SER:N	2.36	0.51
1:A:119:SER:OG	1:A:120:CYS:N	2.42	0.51
1:A:674:PHE:N	1:A:680:THR:OG1	2.42	0.51
1:A:1152:MET:HB2	1:A:1161:ILE:O	2.10	0.51
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.44	0.51
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.93	0.51
1:B:2154:SER:HB3	1:B:2188:ASN:HD21	1.75	0.51
1:B:3453:ARG:O	1:B:3457:ASN:ND2	2.43	0.51
1:C:1270:LEU:O	1:C:1564:PHE:N	2.36	0.51
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.78	0.51
1:D:1112:ASP:OD1	1:D:1112:ASP:N	2.36	0.51
1:D:4633:GLU:HG2	1:D:4635:SER:H	1.75	0.51
1:A:3065:VAL:O	1:A:3069:HIS:ND1	2.43	0.51
1:B:19:GLU:HB2	1:B:205:ILE:HB	1.91	0.51
1:B:1172:ASP:OD1	1:B:1172:ASP:N	2.44	0.51
1:B:4187:SER:OG	1:B:4191:GLU:OE2	2.27	0.51
1:C:989:ALA:HA	1:C:1039:LEU:HG	1.92	0.51
1:D:745:SER:HB3	1:D:758:ARG:HB2	1.91	0.51
1:A:860:GLN:OE1	1:A:860:GLN:N	2.44	0.51
1:A:886:ARG:NH2	1:A:889:GLN:OE1	2.44	0.51
1:A:1078:GLU:OE1	1:A:1080:SER:OG	2.29	0.51
1:B:119:SER:OG	1:B:120:CYS:N	2.43	0.51
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.20	0.51
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.40	0.51
1:C:299:LEU:HD22	1:C:357:LEU:HD11	1.92	0.51
1:C:645:ARG:HD3	1:C:826:ILE:HG13	1.91	0.51
1:C:674:PHE:N	1:C:680:THR:OG1	2.36	0.51
1:C:772:ASN:HD22	1:C:1471:ALA:H	1.59	0.51
1:C:2512:ILE:HG22	1:C:2516:ASP:HB3	1.91	0.51
1:C:3263:TYR:O	1:C:3267:PRO:HD2	2.11	0.51
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.43	0.51
1:D:452:PHE:O	1:D:528:SER:OG	2.24	0.51
1:D:1078:GLU:OE1	1:D:1080:SER:OG	2.29	0.51
1:D:4162:ASN:HA	1:D:4165:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:LYS:HG3	2:E:18:LYS:H	1.74	0.51
2:E:17:LYS:H	2:E:20:GLN:HE22	1.57	0.51
1:A:3842:LEU:O	1:A:3929:SER:OG	2.28	0.51
1:B:24:CYS:HB2	1:B:200:TRP:HA	1.92	0.51
1:B:181:HIS:CG	1:B:196:MET:HB2	2.46	0.51
1:B:1078:GLU:OE1	1:B:1080:SER:OG	2.29	0.51
1:B:2243:SER:OG	1:B:2245:GLN:OE1	2.29	0.51
1:B:5004:THR:OG1	1:B:5005:GLY:N	2.42	0.51
1:C:3453:ARG:O	1:C:3457:ASN:ND2	2.42	0.51
1:D:961:MET:CE	1:D:963:ASN:H	2.24	0.51
1:D:2243:SER:OG	1:D:2245:GLN:OE1	2.29	0.51
1:A:645:ARG:HD3	1:A:826:ILE:HG13	1.93	0.51
1:A:895:PRO:HD2	1:A:903:LEU:HD23	1.93	0.51
1:A:957:LYS:HA	1:A:960:MET:HE3	1.93	0.51
1:A:2420:HIS:N	1:A:2492:ALA:O	2.43	0.51
1:A:3696:ASP:CG	1:A:3697:PRO:HD3	2.35	0.51
1:B:1545:ASN:ND2	2:F:32:ASN:HD22	2.09	0.51
1:B:4633:GLU:HG2	1:B:4635:SER:H	1.76	0.51
1:C:320:LYS:HB3	1:C:356:TRP:NE1	2.26	0.51
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.41	0.51
1:A:554:LEU:HD23	1:A:1593:PRO:HD3	1.92	0.51
1:A:3969:ILE:HD13	1:A:4030:LEU:HD13	1.92	0.51
1:B:960:MET:SD	1:B:966:LYS:NZ	2.83	0.51
1:B:1110:ARG:NH2	1:B:1112:ASP:OD2	2.43	0.51
1:B:2214:VAL:HG21	1:B:2228:MET:HE1	1.92	0.51
1:B:3666:ASP:OD1	1:B:3666:ASP:N	2.37	0.51
1:C:1139:PHE:CE1	1:C:1169:LEU:HD11	2.45	0.51
1:C:3337:ARG:HG2	1:C:3341:PHE:HE2	1.75	0.51
1:C:3842:LEU:O	1:C:3929:SER:OG	2.28	0.51
1:C:3965:LEU:HD22	1:C:3980:LEU:HD21	1.93	0.51
1:D:181:HIS:CG	1:D:196:MET:HB2	2.46	0.51
1:A:498:THR:H	1:A:503:PHE:HE2	1.57	0.51
1:A:4055:VAL:HA	1:A:4058:ILE:HD12	1.92	0.51
1:B:689:THR:HB	1:B:778:PHE:CZ	2.45	0.51
1:C:3395:ARG:HG2	1:C:3453:ARG:HH22	1.75	0.51
1:C:3579:LEU:HG	1:C:3581:GLY:H	1.76	0.51
1:D:4218:ILE:HD13	1:D:4954:MET:HE2	1.93	0.51
2:G:48:PHE:CE1	2:G:55:VAL:HG21	2.46	0.51
1:A:3579:LEU:HG	1:A:3581:GLY:H	1.76	0.50
1:A:3965:LEU:HD22	1:A:3980:LEU:HD21	1.92	0.50
1:B:41:GLY:O	1:B:45:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:GLU:OE1	1:B:813:GLU:N	2.43	0.50
1:C:1284:VAL:HG22	1:C:1555:LEU:HD13	1.94	0.50
1:D:3037:GLU:O	1:D:3040:THR:OG1	2.25	0.50
1:A:668:VAL:HB	1:A:742:ASP:OD1	2.12	0.50
1:A:1717:SER:HA	1:A:1721:GLU:HB2	1.92	0.50
1:B:107:ILE:N	1:B:148:TRP:O	2.40	0.50
1:B:986:ASP:OD1	1:B:986:ASP:N	2.42	0.50
1:B:3674:ILE:HG13	1:B:3732:SER:HB2	1.92	0.50
1:C:990:GLU:HG2	1:C:1024:TYR:CE2	2.46	0.50
1:C:1717:SER:HA	1:C:1721:GLU:HB2	1.93	0.50
1:D:2186:MET:HE1	1:D:2235:PHE:HA	1.92	0.50
1:A:681:HIS:O	1:A:783:PHE:HA	2.10	0.50
1:A:989:ALA:HA	1:A:1039:LEU:HG	1.93	0.50
1:B:1452:TRP:HE1	1:B:1518:CYS:HB3	1.76	0.50
1:C:4000:MET:HE1	1:C:4058:ILE:HG23	1.93	0.50
1:D:3842:LEU:O	1:D:3929:SER:OG	2.30	0.50
1:A:320:LYS:HB3	1:A:356:TRP:NE1	2.27	0.50
1:A:1160:ILE:HB	1:A:1179:PHE:HD2	1.75	0.50
1:A:2104:ARG:NH1	1:A:2108:GLU:OE2	2.43	0.50
1:A:2474:LEU:HA	1:A:2494:PHE:CD2	2.46	0.50
1:A:4000:MET:HE1	1:A:4058:ILE:HG23	1.93	0.50
1:B:645:ARG:HD3	1:B:826:ILE:HG13	1.93	0.50
1:C:416:LYS:C	1:C:416:LYS:HD3	2.37	0.50
1:C:1263:THR:N	1:C:1266:THR:O	2.38	0.50
1:C:4958:CYS:SG	1:C:4983:HIS:HD2	2.34	0.50
1:D:1263:THR:N	1:D:1266:THR:O	2.38	0.50
1:A:3645:PRO:HG2	1:A:3648:ARG:HH11	1.77	0.50
1:B:1289:LEU:HD12	1:B:1550:PRO:HG2	1.94	0.50
1:B:3927:GLN:HE21	1:B:3991:GLY:HA3	1.76	0.50
1:C:1288:PHE:HE1	1:C:1598:GLN:HB2	1.77	0.50
1:C:3927:GLN:HE21	1:C:3991:GLY:HA3	1.77	0.50
1:C:4008:SER:OG	1:C:4009:GLN:OE1	2.26	0.50
1:D:718:GLY:HA3	1:D:737:LEU:HA	1.93	0.50
1:D:1717:SER:HA	1:D:1721:GLU:HB2	1.93	0.50
1:D:3065:VAL:O	1:D:3069:HIS:ND1	2.45	0.50
1:A:41:GLY:O	1:A:45:ARG:NH1	2.44	0.50
1:A:284:HIS:ND1	1:A:287:THR:OG1	2.34	0.50
1:A:4003:LEU:HD21	1:A:4012:LEU:HB3	1.93	0.50
1:C:1078:GLU:OE1	1:C:1080:SER:OG	2.29	0.50
1:C:1110:ARG:NH2	1:C:1112:ASP:OD2	2.43	0.50
1:C:4820:VAL:HG23	1:C:4821:LYS:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4820:VAL:HG23	1:D:4821:LYS:N	2.24	0.50
2:E:48:PHE:CE1	2:E:55:VAL:HG21	2.47	0.50
1:A:1289:LEU:HD12	1:A:1550:PRO:HG2	1.94	0.50
1:A:2440:MET:SD	1:A:2442:LEU:N	2.84	0.50
1:A:3263:TYR:O	1:A:3267:PRO:HD2	2.12	0.50
1:B:307:ALA:HB1	1:B:312:THR:HG21	1.94	0.50
1:B:1263:THR:HG22	1:B:1266:THR:HB	1.94	0.50
1:B:1717:SER:HA	1:B:1721:GLU:HB2	1.93	0.50
1:C:884:LEU:HG	1:C:959:TYR:HE2	1.77	0.50
1:C:2243:SER:OG	1:C:2245:GLN:OE1	2.29	0.50
1:C:4218:ILE:HD13	1:C:4954:MET:HE2	1.94	0.50
1:D:299:LEU:HD22	1:D:357:LEU:HD11	1.94	0.50
1:D:498:THR:H	1:D:503:PHE:HE2	1.59	0.50
1:D:4908:GLU:O	1:D:4908:GLU:HG2	2.12	0.50
2:H:30:LEU:HD21	2:H:92:PRO:HD2	1.93	0.50
1:A:3927:GLN:HE21	1:A:3991:GLY:HA3	1.77	0.50
1:B:4003:LEU:HD21	1:B:4012:LEU:HB3	1.93	0.50
1:C:1172:ASP:OD1	1:C:1172:ASP:N	2.44	0.50
1:C:2963:LEU:HA	1:C:2966:TRP:HB2	1.93	0.50
1:D:320:LYS:HB3	1:D:356:TRP:NE1	2.27	0.50
1:D:2154:SER:HB3	1:D:2188:ASN:HD21	1.76	0.50
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.45	0.50
1:D:4187:SER:OG	1:D:4191:GLU:OE2	2.28	0.50
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.30	0.50
1:A:1155:LEU:H	1:A:1155:LEU:HD12	1.77	0.50
1:B:72:SER:O	1:B:105:HIS:ND1	2.45	0.50
1:B:2104:ARG:NH1	1:B:2108:GLU:OE2	2.44	0.50
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.38	0.50
1:C:1208:VAL:HA	1:C:1211:LEU:HD12	1.94	0.50
1:C:1644:GLU:OE1	1:C:1646:ARG:NE	2.43	0.50
1:C:3969:ILE:HD13	1:C:4030:LEU:HD13	1.92	0.50
1:D:3965:LEU:HD22	1:D:3980:LEU:HD21	1.94	0.50
2:F:14:THR:OG1	2:F:68:LEU:N	2.45	0.50
1:A:502:HIS:CE1	1:A:1263:THR:HA	2.47	0.49
1:A:4820:VAL:HG23	1:A:4821:LYS:N	2.25	0.49
1:B:895:PRO:HD2	1:B:903:LEU:HD23	1.94	0.49
1:B:4218:ILE:HD13	1:B:4954:MET:HE2	1.94	0.49
1:C:3645:PRO:HG2	1:C:3648:ARG:HH11	1.77	0.49
1:D:2104:ARG:NH1	1:D:2108:GLU:OE2	2.43	0.49
1:B:1288:PHE:HE1	1:B:1598:GLN:HB2	1.77	0.49
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3677:LEU:HD22	1:B:3697:PRO:HG3	1.95	0.49
1:B:3842:LEU:O	1:B:3929:SER:OG	2.30	0.49
1:C:1289:LEU:HD12	1:C:1550:PRO:HG2	1.94	0.49
1:C:2187:ASN:OD1	1:C:2187:ASN:N	2.44	0.49
1:C:3390:GLY:HA2	1:C:3393:LEU:HD12	1.95	0.49
1:D:2591:ARG:O	1:D:2594:SER:OG	2.30	0.49
1:A:1703:LEU:HD23	1:A:1704:PRO:HD2	1.93	0.49
1:B:4696:ASP:OD1	1:B:4696:ASP:N	2.39	0.49
1:C:181:HIS:CG	1:C:196:MET:HB2	2.47	0.49
1:C:2104:ARG:NH1	1:C:2108:GLU:OE2	2.45	0.49
1:D:822:ARG:NH2	1:D:824:GLU:OE1	2.46	0.49
1:D:3927:GLN:HE21	1:D:3991:GLY:HA3	1.77	0.49
1:A:4908:GLU:O	1:A:4908:GLU:HG2	2.12	0.49
1:B:1277:TRP:O	1:B:1277:TRP:CD1	2.65	0.49
1:B:4000:MET:HE1	1:B:4058:ILE:HG23	1.94	0.49
1:C:1155:LEU:H	1:C:1155:LEU:HD12	1.77	0.49
1:D:3695:PRO:HD2	1:D:3699:HIS:HB2	1.94	0.49
1:A:4878:ASP:OD1	1:A:4878:ASP:N	2.44	0.49
1:B:649:PHE:HE2	1:B:845:CYS:HB2	1.76	0.49
1:B:1703:LEU:HD23	1:B:1704:PRO:HD2	1.94	0.49
1:B:2474:LEU:HA	1:B:2494:PHE:HD2	1.76	0.49
1:C:252:VAL:HB	1:C:257:ARG:HH12	1.78	0.49
1:C:2556:LEU:HD21	1:C:2597:LYS:HA	1.95	0.49
1:D:224:HIS:HE2	1:D:386:ASP:HA	1.78	0.49
1:A:1087:ARG:NE	1:A:1222:GLY:O	2.46	0.49
1:A:1208:VAL:HA	1:A:1211:LEU:HD12	1.94	0.49
1:A:2214:VAL:HG21	1:A:2228:MET:HE1	1.94	0.49
1:A:3136:LEU:HA	1:A:3139:VAL:HG22	1.94	0.49
1:A:3535:LEU:HD23	1:A:3535:LEU:H	1.77	0.49
1:A:3677:LEU:HG	1:A:3697:PRO:HG2	1.94	0.49
1:B:4878:ASP:OD1	1:B:4878:ASP:N	2.44	0.49
1:C:668:VAL:HB	1:C:742:ASP:OD1	2.13	0.49
1:D:4000:MET:HE1	1:D:4058:ILE:HG23	1.95	0.49
1:D:4958:CYS:SG	1:D:4983:HIS:HD2	2.35	0.49
1:A:877:ASN:O	1:A:880:GLU:HG3	2.12	0.49
1:A:1270:LEU:O	1:A:1564:PHE:N	2.41	0.49
1:A:2431:ASP:OD1	1:A:2435:ARG:NE	2.46	0.49
1:B:320:LYS:HB3	1:B:356:TRP:NE1	2.27	0.49
1:B:684:VAL:HG12	1:B:781:VAL:HG12	1.95	0.49
1:B:990:GLU:HG2	1:B:1024:TYR:CZ	2.47	0.49
1:B:1112:ASP:OD1	1:B:1112:ASP:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3535:LEU:HD23	1:B:3535:LEU:H	1.77	0.49
1:A:2098:VAL:HG11	1:A:2127:GLN:HG3	1.95	0.49
1:B:3698:LEU:HD12	1:B:3773:ARG:HG3	1.95	0.49
1:B:3965:LEU:HD22	1:B:3980:LEU:HD21	1.94	0.49
1:C:41:GLY:O	1:C:45:ARG:NH1	2.46	0.49
1:C:2191:PHE:HD1	1:C:2198:MET:HE3	1.76	0.49
1:C:2871:LEU:HD23	1:C:2874:MET:HE2	1.94	0.49
1:A:307:ALA:HB1	1:A:312:THR:HG21	1.94	0.49
1:A:3395:ARG:HG2	1:A:3453:ARG:HH22	1.78	0.49
1:B:810:PRO:HD2	1:B:813:GLU:OE1	2.13	0.49
1:C:144:GLU:O	1:C:175:SER:OG	2.26	0.49
1:C:2657:LEU:N	1:C:2658:PRO:HD2	2.28	0.49
1:C:3081:MET:HE2	1:C:3081:MET:HA	1.95	0.49
1:D:3395:ARG:HG2	1:D:3453:ARG:HH22	1.78	0.49
1:A:822:ARG:NH2	1:A:824:GLU:OE1	2.45	0.49
1:B:2325:PRO:HB3	1:B:2422:ILE:HA	1.94	0.49
1:B:3695:PRO:HD2	1:B:3699:HIS:HB2	1.95	0.49
1:C:644:ILE:HD11	1:C:1615:VAL:HG21	1.95	0.49
1:C:2474:LEU:HA	1:C:2494:PHE:HD2	1.78	0.49
1:D:668:VAL:HB	1:D:742:ASP:OD1	2.13	0.49
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.31	0.49
1:D:1459:GLN:NE2	1:D:1461:ASP:HB2	2.27	0.49
1:D:2950:SER:HB3	1:D:2954:ARG:HH21	1.78	0.49
1:D:4115:SER:OG	1:D:4116:GLU:N	2.46	0.49
1:A:649:PHE:HE2	1:A:845:CYS:HB2	1.78	0.48
1:A:3081:MET:HE2	1:A:3081:MET:HA	1.95	0.48
1:A:4218:ILE:HD13	1:A:4954:MET:HE2	1.93	0.48
1:B:252:VAL:HB	1:B:257:ARG:HH12	1.78	0.48
1:B:822:ARG:NH2	1:B:824:GLU:OE1	2.46	0.48
1:B:971:ASP:O	1:B:974:HIS:NE2	2.46	0.48
1:B:2431:ASP:O	1:B:2435:ARG:HG2	2.13	0.48
1:B:2657:LEU:N	1:B:2658:PRO:HD2	2.28	0.48
1:C:1047:LEU:HD12	1:C:1053:ILE:HD12	1.95	0.48
1:C:3427:PRO:HG2	1:C:3579:LEU:HD12	1.95	0.48
1:D:1703:LEU:HD23	1:D:1704:PRO:HD2	1.93	0.48
1:D:2282:ASP:OD1	1:D:2282:ASP:N	2.46	0.48
1:D:2440:MET:HG3	1:D:2441:HIS:H	1.78	0.48
1:D:3390:GLY:HA2	1:D:3393:LEU:HD12	1.95	0.48
2:F:14:THR:HG21	2:F:68:LEU:HB2	1.95	0.48
1:A:689:THR:HB	1:A:778:PHE:CZ	2.48	0.48
1:A:993:HIS:ND1	1:A:1023:PRO:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1930:LYS:HE3	1:B:1930:LYS:HB3	1.69	0.48
1:B:3409:TYR:CE2	1:B:3510:ILE:HG23	2.48	0.48
1:C:1459:GLN:NE2	1:C:1461:ASP:HB2	2.27	0.48
1:D:307:ALA:HB1	1:D:312:THR:HG21	1.94	0.48
1:D:2953:LYS:HA	1:D:2957:PHE:HB3	1.94	0.48
1:A:813:GLU:HG3	1:A:1009:ALA:H	1.77	0.48
1:A:2282:ASP:OD1	1:A:2282:ASP:N	2.46	0.48
1:B:668:VAL:HB	1:B:742:ASP:OD1	2.14	0.48
1:B:977:LEU:HG	1:B:1044:ARG:HH11	1.77	0.48
1:B:3133:THR:HA	1:B:3137:LEU:HD12	1.94	0.48
1:C:294:THR:HG23	1:C:297:GLN:H	1.78	0.48
1:C:1112:ASP:OD1	1:C:1112:ASP:N	2.37	0.48
1:C:2154:SER:HB3	1:C:2188:ASN:HD21	1.78	0.48
1:C:2186:MET:HE1	1:C:2235:PHE:HA	1.95	0.48
1:D:689:THR:OG1	1:D:689:THR:O	2.30	0.48
1:D:1087:ARG:NE	1:D:1222:GLY:O	2.45	0.48
1:D:3081:MET:HE2	1:D:3081:MET:HA	1.96	0.48
1:D:3263:TYR:O	1:D:3267:PRO:HD2	2.13	0.48
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.31	0.48
1:B:3645:PRO:HG2	1:B:3648:ARG:HH11	1.77	0.48
1:D:753:PRO:HB2	1:D:771:PHE:CD2	2.49	0.48
1:D:1277:TRP:O	1:D:1277:TRP:CD1	2.66	0.48
1:A:978:THR:HG22	1:A:979:PRO:HD2	1.95	0.48
1:A:2657:LEU:N	1:A:2658:PRO:HD2	2.28	0.48
1:B:653:ALA:HB2	1:B:848:HIS:HD2	1.79	0.48
1:B:4115:SER:OG	1:B:4116:GLU:N	2.46	0.48
1:C:875:ALA:HB1	1:C:910:PHE:CZ	2.48	0.48
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.31	0.48
1:C:2814:LYS:HD3	1:C:2814:LYS:HA	1.66	0.48
1:C:3245:VAL:HG12	1:C:3247:ASP:H	1.77	0.48
1:D:252:VAL:HB	1:D:257:ARG:HH12	1.78	0.48
1:D:920:TYR:HD1	1:D:923:GLN:HE21	1.62	0.48
1:D:3068:LEU:HA	1:D:3071:LEU:HB2	1.95	0.48
1:D:3794:VAL:HG21	1:D:3835:LEU:HD11	1.96	0.48
2:E:53:GLN:HG2	2:E:54:GLU:N	2.29	0.48
2:F:38:SER:OG	2:F:41:ASP:OD2	2.31	0.48
2:H:38:SER:OG	2:H:41:ASP:OD2	2.30	0.48
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.96	0.48
1:B:3068:LEU:HA	1:B:3071:LEU:HB2	1.96	0.48
1:C:677:ALA:HB1	2:G:40:ARG:HB3	1.96	0.48
1:C:1521:ASP:OD1	1:C:1524:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2384:ILE:O	1:C:2388:GLU:HG2	2.14	0.48
1:D:2384:ILE:O	1:D:2388:GLU:HG2	2.13	0.48
2:E:30:LEU:N	2:E:34:LYS:O	2.46	0.48
1:A:718:GLY:HA3	1:A:737:LEU:HA	1.95	0.48
1:A:1772:ARG:NH2	1:A:1952:GLN:OE1	2.46	0.48
1:A:2506:LEU:HD12	1:A:2510:TYR:HB2	1.96	0.48
1:A:3794:VAL:HG21	1:A:3835:LEU:HD11	1.96	0.48
1:A:4166:LEU:HD23	1:A:4166:LEU:H	1.78	0.48
1:B:1087:ARG:NE	1:B:1222:GLY:O	2.46	0.48
1:B:3081:MET:HE2	1:B:3081:MET:HA	1.95	0.48
1:C:102:LEU:HB3	1:C:105:HIS:CD2	2.49	0.48
1:D:49:LEU:HD11	1:D:191:VAL:HG23	1.95	0.48
1:D:1284:VAL:HG22	1:D:1555:LEU:HD13	1.95	0.48
1:D:1868:PRO:O	1:D:1872:THR:OG1	2.24	0.48
1:D:3535:LEU:HD23	1:D:3535:LEU:H	1.79	0.48
2:F:17:LYS:H	2:F:20:GLN:HE22	1.60	0.48
1:A:1435:TYR:HE1	1:A:1452:TRP:CZ2	2.32	0.48
1:B:1093:GLU:HG2	1:B:1148:VAL:HG12	1.96	0.48
1:B:1833:SER:OG	1:B:1834:VAL:N	2.47	0.48
1:B:3065:VAL:O	1:B:3069:HIS:ND1	2.47	0.48
1:C:1220:GLN:NE2	1:D:3519:PRO:O	2.45	0.48
1:D:919:ASN:O	1:D:923:GLN:HG2	2.13	0.48
1:D:2355:ARG:HB3	1:D:2359:ARG:HH21	1.79	0.48
1:D:3645:PRO:HG2	1:D:3648:ARG:HH11	1.77	0.48
1:A:1217:CYS:SG	1:A:1218:GLY:N	2.86	0.48
1:A:1700:ASP:HB3	1:A:1703:LEU:HD12	1.96	0.48
1:A:1833:SER:OG	1:A:1834:VAL:N	2.47	0.48
1:A:3032:SER:N	1:A:3035:GLU:OE1	2.45	0.48
1:A:3319:ILE:HG13	1:A:3338:LEU:HD21	1.95	0.48
1:A:4059:LEU:HD21	1:A:4143:VAL:HG11	1.95	0.48
1:B:54:ASN:HD22	1:B:57:ASN:HD21	1.60	0.48
1:B:868:GLU:HA	1:B:871:ARG:HG3	1.95	0.48
1:B:2193:GLN:HB3	1:B:2194:HIS:HD1	1.79	0.48
1:B:4059:LEU:HD21	1:B:4143:VAL:HG11	1.96	0.48
1:B:4958:CYS:SG	1:B:4983:HIS:HD2	2.37	0.48
1:C:822:ARG:NH2	1:C:824:GLU:OE1	2.46	0.48
1:C:4003:LEU:HD21	1:C:4012:LEU:HB3	1.95	0.48
1:C:4115:SER:OG	1:C:4116:GLU:N	2.46	0.48
1:C:4878:ASP:OD1	1:C:4878:ASP:N	2.44	0.48
1:D:1018:ASN:OD1	1:D:1020:ARG:NE	2.46	0.48
1:D:1087:ARG:HB3	1:D:1223:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2098:VAL:HG11	1:D:2127:GLN:HG3	1.96	0.48
1:D:2193:GLN:HB3	1:D:2194:HIS:HD1	1.78	0.48
1:D:2506:LEU:HD12	1:D:2510:TYR:HB2	1.95	0.48
1:D:2657:LEU:N	1:D:2658:PRO:HD2	2.28	0.48
1:A:252:VAL:HB	1:A:257:ARG:HH12	1.78	0.48
1:B:1520:VAL:HG12	1:B:1527:MET:HG2	1.96	0.48
1:B:2282:ASP:N	1:B:2282:ASP:OD1	2.46	0.48
1:B:2506:LEU:HD12	1:B:2510:TYR:HB2	1.95	0.48
1:B:4908:GLU:HG2	1:B:4908:GLU:O	2.12	0.48
1:C:1443:GLN:NE2	1:C:1444:GLU:O	2.44	0.48
1:C:1833:SER:OG	1:C:1834:VAL:N	2.47	0.48
1:C:3051:ARG:HG3	1:C:3052:HIS:H	1.79	0.48
1:D:571:SER:O	1:D:571:SER:OG	2.32	0.48
1:D:1833:SER:OG	1:D:1834:VAL:N	2.47	0.48
1:D:3696:ASP:CG	1:D:3697:PRO:HD3	2.39	0.48
1:A:3198:ALA:HB1	1:A:3280:TYR:HB2	1.95	0.47
1:A:4115:SER:OG	1:A:4116:GLU:N	2.46	0.47
1:A:4696:ASP:OD1	1:A:4696:ASP:N	2.38	0.47
1:B:277:GLY:HA2	1:B:315:CYS:SG	2.54	0.47
1:C:399:GLN:O	1:C:403:MET:HG3	2.14	0.47
1:C:2974:ILE:O	1:C:2978:GLU:N	2.43	0.47
1:C:3359:ILE:HD11	1:C:3434:LEU:HB2	1.96	0.47
1:D:892:THR:OG1	1:D:902:ARG:O	2.25	0.47
1:D:1289:LEU:HD12	1:D:1550:PRO:HG2	1.95	0.47
1:D:4059:LEU:HD21	1:D:4143:VAL:HG11	1.96	0.47
2:G:14:THR:HG21	2:G:68:LEU:HB2	1.95	0.47
1:B:224:HIS:HE2	1:B:386:ASP:HA	1.79	0.47
1:B:3395:ARG:HG2	1:B:3453:ARG:HH22	1.79	0.47
1:C:681:HIS:O	1:C:783:PHE:HA	2.14	0.47
1:C:861:ILE:O	1:C:930:LYS:NZ	2.44	0.47
1:C:1452:TRP:HE3	1:C:1548:LEU:HB3	1.79	0.47
1:C:2431:ASP:O	1:C:2435:ARG:HG2	2.14	0.47
1:D:689:THR:HB	1:D:778:PHE:HZ	1.79	0.47
1:D:1288:PHE:HE1	1:D:1598:GLN:HB2	1.79	0.47
1:A:299:LEU:HD22	1:A:357:LEU:HD11	1.95	0.47
1:A:359:TYR:HB2	1:A:383:HIS:HE1	1.78	0.47
1:A:2355:ARG:HB3	1:A:2359:ARG:HH21	1.79	0.47
1:A:3409:TYR:CE2	1:A:3510:ILE:HG23	2.48	0.47
1:B:3592:ILE:HA	1:B:3595:ARG:HE	1.79	0.47
1:C:571:SER:O	1:C:571:SER:OG	2.32	0.47
1:C:848:HIS:CE1	1:C:849:THR:HG23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1040:CYS:O	1:C:1044:ARG:HG2	2.13	0.47
1:C:1125:ASN:HB2	1:C:1132:TRP:HD1	1.79	0.47
1:D:3032:SER:N	1:D:3035:GLU:OE1	2.46	0.47
1:A:1644:GLU:OE1	1:A:1646:ARG:NE	2.43	0.47
1:A:2013:LYS:HE3	1:A:2031:LEU:HD23	1.95	0.47
1:B:1457:TYR:CZ	1:B:1459:GLN:HB2	2.48	0.47
1:B:2814:LYS:HD3	1:B:2814:LYS:HA	1.66	0.47
1:C:497:TYR:HA	1:C:503:PHE:CE2	2.50	0.47
1:C:877:ASN:O	1:C:880:GLU:HG3	2.14	0.47
1:C:1087:ARG:HB3	1:C:1223:PHE:CD1	2.49	0.47
1:C:2242:ILE:HG23	1:C:2246:ASN:HD22	1.80	0.47
1:C:2506:LEU:HD12	1:C:2510:TYR:HB2	1.95	0.47
1:C:3768:SER:HA	1:C:3771:HIS:ND1	2.30	0.47
2:F:53:GLN:HG2	2:F:54:GLU:N	2.29	0.47
2:H:53:GLN:HG2	2:H:54:GLU:N	2.28	0.47
1:A:2556:LEU:HD21	1:A:2597:LYS:HA	1.96	0.47
1:A:2963:LEU:HA	1:A:2966:TRP:HB2	1.96	0.47
1:B:595:ARG:NH2	1:B:1643:GLU:OE1	2.46	0.47
1:B:898:ASP:O	1:B:901:LYS:N	2.43	0.47
2:G:53:GLN:HG2	2:G:54:GLU:N	2.29	0.47
1:A:24:CYS:HB2	1:A:200:TRP:HA	1.96	0.47
1:A:1087:ARG:HB3	1:A:1223:PHE:CD1	2.49	0.47
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.96	0.47
1:B:1155:LEU:HD12	1:B:1155:LEU:H	1.80	0.47
1:B:2094:LEU:O	1:B:2098:VAL:HG12	2.14	0.47
1:B:2983:SER:O	1:B:2983:SER:OG	2.30	0.47
1:C:630:GLU:HA	1:C:1642:PRO:HB2	1.96	0.47
1:C:3068:LEU:HA	1:C:3071:LEU:HB2	1.97	0.47
1:D:772:ASN:ND2	1:D:1471:ALA:H	2.10	0.47
1:D:1700:ASP:HB3	1:D:1703:LEU:HD12	1.96	0.47
1:D:2242:ILE:HG23	1:D:2246:ASN:HD22	1.80	0.47
1:A:224:HIS:HE2	1:A:386:ASP:HA	1.79	0.47
1:A:1011:GLN:NE2	1:A:1013:ILE:HG12	2.29	0.47
1:A:1277:TRP:CD1	1:A:1277:TRP:O	2.67	0.47
1:A:2257:LEU:HD21	1:A:2275:VAL:HG13	1.96	0.47
1:A:2310:CYS:HB3	1:A:2313:LEU:HD23	1.97	0.47
1:B:913:LEU:HB2	1:B:918:ARG:HG2	1.96	0.47
1:B:1217:CYS:SG	1:B:1218:GLY:N	2.87	0.47
1:B:2013:LYS:HE3	1:B:2031:LEU:HD23	1.96	0.47
1:B:2384:ILE:O	1:B:2388:GLU:HG2	2.13	0.47
1:B:2389:ASP:N	1:B:2390:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2871:LEU:HD23	1:B:2874:MET:HE2	1.96	0.47
1:B:3003:LEU:HD12	1:B:3004:PRO:CD	2.40	0.47
1:B:3037:GLU:O	1:B:3040:THR:OG1	2.27	0.47
1:B:3136:LEU:HA	1:B:3139:VAL:HG22	1.97	0.47
1:B:3263:TYR:O	1:B:3267:PRO:HD2	2.13	0.47
1:C:205:ILE:CG2	1:C:206:CYS:H	2.27	0.47
1:C:1000:ARG:HB3	1:C:1005:TRP:HB2	1.95	0.47
1:D:277:GLY:HA2	1:D:315:CYS:SG	2.55	0.47
1:D:877:ASN:O	1:D:880:GLU:HG3	2.15	0.47
1:D:1708:ARG:NH1	1:D:1836:PHE:O	2.47	0.47
1:D:2389:ASP:N	1:D:2390:PRO:HD3	2.30	0.47
2:H:22:CYS:O	2:H:48:PHE:N	2.48	0.47
1:A:1452:TRP:HE1	1:A:1518:CYS:HB3	1.79	0.47
1:B:2310:CYS:HB3	1:B:2313:LEU:HD23	1.97	0.47
1:B:3768:SER:HA	1:B:3771:HIS:ND1	2.29	0.47
1:C:1018:ASN:OD1	1:C:1020:ARG:NH1	2.48	0.47
1:D:893:TYR:H	1:D:961:MET:HE3	1.80	0.47
1:D:2431:ASP:O	1:D:2435:ARG:HG2	2.15	0.47
1:D:3768:SER:HA	1:D:3771:HIS:ND1	2.29	0.47
1:D:4159:ARG:HA	1:D:4162:ASN:HD21	1.80	0.47
1:A:772:ASN:ND2	1:A:1471:ALA:H	2.13	0.47
1:A:2431:ASP:O	1:A:2435:ARG:HG2	2.15	0.47
1:A:2500:ALA:HB1	1:A:2550:LEU:HD22	1.97	0.47
1:A:3359:ILE:HD11	1:A:3434:LEU:HB2	1.97	0.47
1:A:4034:ASN:HD21	1:A:4153:HIS:CE1	2.33	0.47
1:B:399:GLN:O	1:B:403:MET:HG3	2.15	0.47
1:B:2440:MET:SD	1:B:2442:LEU:N	2.88	0.47
1:B:2963:LEU:HA	1:B:2966:TRP:HB2	1.97	0.47
1:C:895:PRO:HG2	1:C:896:VAL:HG23	1.96	0.47
1:C:1703:LEU:HD23	1:C:1704:PRO:HD2	1.95	0.47
1:C:4908:GLU:HG2	1:C:4908:GLU:O	2.14	0.47
1:D:2102:VAL:HG11	1:D:2124:LEU:HB2	1.97	0.47
2:E:38:SER:OG	2:E:41:ASP:OD2	2.32	0.47
1:B:1700:ASP:HB3	1:B:1703:LEU:HD12	1.97	0.47
1:C:813:GLU:HG3	1:C:1009:ALA:H	1.80	0.47
1:C:2389:ASP:N	1:C:2390:PRO:HD3	2.29	0.47
1:D:1125:ASN:HB2	1:D:1132:TRP:HD1	1.79	0.47
1:D:2310:CYS:HB3	1:D:2313:LEU:HD23	1.97	0.47
2:F:30:LEU:N	2:F:34:LYS:O	2.48	0.47
2:H:57:LYS:HB3	2:H:57:LYS:HE2	1.75	0.47
1:A:1462:MET:HE2	1:A:1462:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.15	0.46
1:A:4958:CYS:SG	1:A:4983:HIS:HD2	2.37	0.46
1:B:1087:ARG:HB3	1:B:1223:PHE:CD1	2.50	0.46
1:B:3390:GLY:HA2	1:B:3393:LEU:HD12	1.96	0.46
1:C:224:HIS:HE2	1:C:386:ASP:HA	1.80	0.46
1:C:307:ALA:HB1	1:C:312:THR:HG21	1.96	0.46
1:C:498:THR:H	1:C:503:PHE:HE2	1.62	0.46
1:C:1708:ARG:NH1	1:C:1836:PHE:O	2.48	0.46
1:C:2968:ASP:O	1:C:2971:GLN:NE2	2.32	0.46
1:C:4059:LEU:HD21	1:C:4143:VAL:HG11	1.96	0.46
1:A:630:GLU:HA	1:A:1642:PRO:HB2	1.98	0.46
1:A:915:GLU:HA	1:A:918:ARG:HB2	1.97	0.46
1:B:144:GLU:O	1:B:175:SER:OG	2.26	0.46
1:B:664:PHE:HB3	1:B:746:CYS:HB3	1.96	0.46
1:B:1270:LEU:O	1:B:1564:PHE:N	2.42	0.46
1:B:1521:ASP:OD1	1:B:1524:THR:OG1	2.33	0.46
1:C:1277:TRP:O	1:C:1277:TRP:HD1	1.98	0.46
1:D:2441:HIS:HA	1:D:2444:GLN:HB3	1.96	0.46
1:D:3051:ARG:HD2	1:D:3051:ARG:HA	1.74	0.46
1:D:3409:TYR:CE2	1:D:3510:ILE:HG23	2.48	0.46
1:A:861:ILE:HB	1:A:930:LYS:NZ	2.30	0.46
1:A:1930:LYS:HE3	1:A:1930:LYS:HB3	1.70	0.46
1:A:3133:THR:HG23	1:A:3134:VAL:HG13	1.96	0.46
1:A:3141:THR:O	1:A:3145:GLN:HG2	2.14	0.46
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.32	0.46
1:B:571:SER:O	1:B:571:SER:OG	2.32	0.46
1:C:3032:SER:N	1:C:3035:GLU:OE1	2.46	0.46
1:C:3409:TYR:CE2	1:C:3510:ILE:HG23	2.48	0.46
1:D:595:ARG:NH2	1:D:1643:GLU:OE1	2.48	0.46
1:D:884:LEU:HG	1:D:959:TYR:HE2	1.81	0.46
1:D:4034:ASN:HD21	1:D:4153:HIS:CE1	2.34	0.46
1:D:4878:ASP:OD1	1:D:4878:ASP:N	2.44	0.46
1:A:755:ILE:HG13	1:A:771:PHE:CZ	2.50	0.46
1:B:977:LEU:HG	1:B:1044:ARG:NH1	2.30	0.46
1:B:3107:VAL:HA	1:B:3110:LEU:HB2	1.97	0.46
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.14	0.46
1:D:18:ASP:OD1	1:D:19:GLU:N	2.49	0.46
1:D:502:HIS:CE1	1:D:1263:THR:HA	2.50	0.46
1:D:2614:ILE:O	1:D:2618:MET:N	2.49	0.46
1:A:1288:PHE:HE1	1:A:1598:GLN:HB2	1.79	0.46
1:A:1452:TRP:HE3	1:A:1548:LEU:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2983:SER:O	1:A:2983:SER:OG	2.29	0.46
1:B:292:ALA:O	1:B:299:LEU:HD12	2.16	0.46
1:B:299:LEU:HD22	1:B:357:LEU:HD11	1.96	0.46
1:B:861:ILE:O	1:B:930:LYS:NZ	2.48	0.46
1:C:861:ILE:HB	1:C:930:LYS:NZ	2.29	0.46
1:C:924:MET:HA	1:C:927:GLU:OE2	2.15	0.46
1:C:977:LEU:HG	1:C:1044:ARG:HH21	1.81	0.46
1:C:1087:ARG:NE	1:C:1222:GLY:O	2.47	0.46
1:D:1077:ALA:HB3	1:D:1190:PRO:HD2	1.98	0.46
2:G:22:CYS:SG	2:G:48:PHE:HB3	2.55	0.46
2:H:30:LEU:N	2:H:34:LYS:O	2.47	0.46
1:A:181:HIS:CG	1:A:196:MET:HB2	2.50	0.46
1:A:205:ILE:CG2	1:A:206:CYS:H	2.27	0.46
1:A:1470:ARG:HD3	1:A:1470:ARG:HA	1.70	0.46
1:C:3065:VAL:O	1:C:3069:HIS:ND1	2.48	0.46
1:D:441:VAL:HG13	1:D:518:ILE:HD11	1.97	0.46
1:D:913:LEU:HB2	1:D:918:ARG:HG2	1.98	0.46
1:D:996:TRP:C	1:D:996:TRP:CD1	2.93	0.46
1:A:2389:ASP:N	1:A:2390:PRO:HD3	2.31	0.46
1:B:284:HIS:CE1	1:B:286:THR:HB	2.50	0.46
1:C:591:ASP:OD1	1:C:1594:ARG:NH1	2.48	0.46
1:C:1470:ARG:HD3	1:C:1470:ARG:HA	1.71	0.46
1:C:2098:VAL:HG23	1:C:2101:MET:HE2	1.98	0.46
1:C:2282:ASP:OD1	1:C:2282:ASP:N	2.47	0.46
1:D:830:ARG:NE	1:D:1612:PHE:HE2	2.13	0.46
1:D:886:ARG:NH2	1:D:889:GLN:OE1	2.44	0.46
1:D:2906:VAL:HG11	1:D:2911:LEU:HA	1.97	0.46
2:H:44:LYS:HD2	2:H:44:LYS:HA	1.80	0.46
1:A:3768:SER:HA	1:A:3771:HIS:ND1	2.30	0.46
1:A:4159:ARG:HA	1:A:4162:ASN:HD21	1.81	0.46
1:B:830:ARG:HH12	1:B:832:GLU:HG3	1.81	0.46
1:B:2242:ILE:HG23	1:B:2246:ASN:HD22	1.80	0.46
1:C:772:ASN:ND2	1:C:1471:ALA:H	2.13	0.46
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.96	0.46
1:C:1452:TRP:CE3	1:C:1548:LEU:HB3	2.51	0.46
1:C:1772:ARG:NH2	1:C:1952:GLN:OE1	2.48	0.46
1:C:2310:CYS:HB3	1:C:2313:LEU:HD23	1.98	0.46
1:C:3845:ASN:N	1:C:3845:ASN:OD1	2.49	0.46
1:C:4109:GLN:HA	1:C:4112:LEU:HD12	1.97	0.46
1:D:1155:LEU:H	1:D:1155:LEU:HD12	1.80	0.46
1:D:1217:CYS:SG	1:D:1218:GLY:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.16	0.46
1:D:2431:ASP:OD1	1:D:2435:ARG:NE	2.46	0.46
1:A:2150:GLU:HA	1:A:2153:MET:HB2	1.98	0.46
1:A:3068:LEU:HA	1:A:3071:LEU:HB2	1.98	0.46
1:A:3390:GLY:HA2	1:A:3393:LEU:HD12	1.98	0.46
1:B:2556:LEU:HD21	1:B:2597:LYS:HA	1.97	0.46
1:B:4034:ASN:HD21	1:B:4153:HIS:CE1	2.34	0.46
1:C:284:HIS:ND1	1:C:287:THR:OG1	2.33	0.46
1:C:718:GLY:HA3	1:C:737:LEU:HA	1.96	0.46
1:C:2193:GLN:HB3	1:C:2194:HIS:HD1	1.81	0.46
1:D:924:MET:HA	1:D:927:GLU:OE2	2.15	0.46
1:D:1093:GLU:HG2	1:D:1148:VAL:HG12	1.98	0.46
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.97	0.46
1:D:1454:THR:OG1	1:D:1455:PRO:HD2	2.15	0.46
1:D:2556:LEU:HD21	1:D:2597:LYS:HA	1.97	0.46
2:H:14:THR:HG21	2:H:68:LEU:HB2	1.98	0.46
1:A:359:TYR:HB2	1:A:383:HIS:CE1	2.51	0.46
1:A:595:ARG:NH2	1:A:1643:GLU:OE1	2.49	0.46
1:A:954:LYS:HA	1:A:954:LYS:HD2	1.79	0.46
1:A:2950:SER:HB3	1:A:2954:ARG:HH21	1.80	0.46
1:B:630:GLU:HA	1:B:1642:PRO:CB	2.45	0.46
1:B:3329:ILE:HG12	1:B:3332:ALA:HB2	1.97	0.46
1:B:3999:MET:HE2	1:B:4016:LEU:HD13	1.97	0.46
1:C:168:ASP:HB3	1:C:199:LEU:HB3	1.97	0.46
1:C:284:HIS:CE1	1:C:286:THR:HB	2.51	0.46
1:C:886:ARG:NH2	1:C:889:GLN:OE1	2.47	0.46
1:C:4187:SER:OG	1:C:4191:GLU:OE2	2.28	0.46
1:D:630:GLU:HA	1:D:1642:PRO:HB2	1.98	0.46
1:D:1767:VAL:HG12	1:D:1767:VAL:O	2.16	0.46
1:D:3133:THR:HG23	1:D:3134:VAL:HG13	1.98	0.46
1:A:871:ARG:NH2	1:A:922:LEU:HD23	2.31	0.45
1:A:1220:GLN:NE2	1:B:3519:PRO:O	2.47	0.45
1:A:2154:SER:HB3	1:A:2188:ASN:HD21	1.81	0.45
1:A:2242:ILE:HG23	1:A:2246:ASN:HD22	1.81	0.45
1:B:755:ILE:HG13	1:B:771:PHE:CZ	2.51	0.45
1:B:1534:LYS:HA	1:B:1534:LYS:HD2	1.82	0.45
1:B:1708:ARG:NH1	1:B:1836:PHE:O	2.48	0.45
1:B:2591:ARG:O	1:B:2594:SER:OG	2.30	0.45
1:B:3032:SER:N	1:B:3035:GLU:OE1	2.45	0.45
1:B:3845:ASN:OD1	1:B:3845:ASN:N	2.49	0.45
1:B:4162:ASN:HA	1:B:4165:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4586:PRO:HB3	1:B:4628:VAL:HG21	1.98	0.45
1:C:24:CYS:SG	1:C:198:THR:OG1	2.74	0.45
1:C:502:HIS:CE1	1:C:1263:THR:HA	2.51	0.45
1:C:3526:ALA:HB2	1:C:3595:ARG:HH12	1.81	0.45
1:C:3573:MET:HA	1:C:3573:MET:HE2	1.97	0.45
2:F:22:CYS:SG	2:F:48:PHE:HB3	2.55	0.45
1:A:1022:VAL:HG23	1:A:1027:LEU:HG	1.98	0.45
1:A:1494:MET:HB3	1:A:1494:MET:HE2	1.74	0.45
1:A:3323:ILE:HD11	1:A:3338:LEU:HD22	1.99	0.45
1:B:263:GLU:HB3	1:B:281:ARG:HB2	1.99	0.45
1:B:961:MET:HE1	1:B:963:ASN:H	1.80	0.45
1:B:1077:ALA:HB3	1:B:1190:PRO:HD2	1.98	0.45
1:B:1868:PRO:O	1:B:1872:THR:OG1	2.25	0.45
1:C:531:ARG:HA	1:C:566:CYS:SG	2.56	0.45
1:C:2474:LEU:HA	1:C:2494:PHE:CD2	2.52	0.45
1:C:3971:GLY:O	1:C:3973:CYS:N	2.49	0.45
1:D:961:MET:HE1	1:D:963:ASN:H	1.81	0.45
1:D:1008:SER:HB3	1:D:1017:ARG:HB3	1.98	0.45
1:A:102:LEU:HD12	1:A:161:GLU:O	2.16	0.45
1:A:1077:ALA:HB3	1:A:1190:PRO:HD2	1.98	0.45
1:A:1708:ARG:NH1	1:A:1836:PHE:O	2.48	0.45
1:A:1868:PRO:O	1:A:1872:THR:OG1	2.25	0.45
1:A:2384:ILE:O	1:A:2388:GLU:HG2	2.17	0.45
1:B:899:ASP:HB2	1:B:902:ARG:CZ	2.46	0.45
1:B:4181:ILE:HG22	1:B:4182:GLU:H	1.81	0.45
1:C:2500:ALA:HB1	1:C:2550:LEU:HD22	1.97	0.45
1:D:68:THR:HG23	1:D:110:ARG:HB2	1.99	0.45
1:D:399:GLN:O	1:D:403:MET:HG3	2.15	0.45
1:D:1270:LEU:O	1:D:1564:PHE:N	2.37	0.45
1:A:531:ARG:HA	1:A:566:CYS:SG	2.56	0.45
1:A:591:ASP:OD1	1:A:1594:ARG:NH1	2.49	0.45
1:A:2906:VAL:HG11	1:A:2911:LEU:HA	1.99	0.45
1:A:3208:PRO:HD2	1:A:3245:VAL:HG22	1.98	0.45
1:A:3245:VAL:HG12	1:A:3247:ASP:H	1.81	0.45
1:A:3804:ILE:HD12	1:A:3804:ILE:HA	1.87	0.45
1:B:996:TRP:CD1	1:B:996:TRP:C	2.94	0.45
1:B:1767:VAL:O	1:B:1767:VAL:HG12	2.17	0.45
1:C:1077:ALA:HB3	1:C:1190:PRO:HD2	1.99	0.45
1:C:1275:ARG:HG3	1:C:1276:THR:HG23	1.97	0.45
1:D:684:VAL:HG12	1:D:781:VAL:HG12	1.99	0.45
1:D:755:ILE:HG13	1:D:771:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2871:LEU:HD23	1:D:2874:MET:HE2	1.98	0.45
2:H:48:PHE:CE1	2:H:55:VAL:HG21	2.51	0.45
1:A:269:TRP:CD1	1:A:272:SER:HB2	2.52	0.45
1:A:284:HIS:CE1	1:A:286:THR:HB	2.52	0.45
1:A:1521:ASP:OD1	1:A:1524:THR:OG1	2.31	0.45
1:B:168:ASP:HB3	1:B:199:LEU:HB3	1.99	0.45
1:B:893:TYR:H	1:B:961:MET:HE3	1.82	0.45
1:B:1462:MET:HE2	1:B:1462:MET:HA	1.97	0.45
1:B:2614:ILE:O	1:B:2618:MET:N	2.49	0.45
1:C:269:TRP:NE1	1:C:333:GLY:O	2.50	0.45
1:C:441:VAL:HG13	1:C:518:ILE:HD11	1.97	0.45
1:C:1435:TYR:HE1	1:C:1452:TRP:CZ2	2.34	0.45
1:C:3107:VAL:HA	1:C:3110:LEU:HB2	1.97	0.45
1:D:2474:LEU:HA	1:D:2494:PHE:HD2	1.82	0.45
2:E:22:CYS:SG	2:E:48:PHE:HB3	2.57	0.45
1:A:430:PRO:HB2	1:A:509:GLU:HB2	1.99	0.45
1:A:899:ASP:HB2	1:A:902:ARG:CZ	2.47	0.45
1:A:1520:VAL:HG12	1:A:1527:MET:HG2	1.97	0.45
1:A:2871:LEU:HA	1:A:2874:MET:HE2	1.99	0.45
1:B:2974:ILE:O	1:B:2978:GLU:N	2.46	0.45
1:B:3068:LEU:H	1:B:3068:LEU:HD12	1.82	0.45
1:C:1562:ILE:HD12	1:C:1563:GLN:N	2.32	0.45
1:C:2983:SER:O	1:C:2983:SER:OG	2.29	0.45
1:C:3003:LEU:HD12	1:C:3004:PRO:CD	2.40	0.45
1:D:830:ARG:HD2	1:D:1608:MET:HE3	1.99	0.45
1:D:4181:ILE:HG22	1:D:4182:GLU:H	1.82	0.45
1:A:2345:SER:OG	1:A:2435:ARG:O	2.27	0.45
1:A:2442:LEU:HG	1:A:2443:ILE:HG12	1.98	0.45
1:A:3526:ALA:HB2	1:A:3595:ARG:HH12	1.82	0.45
1:B:875:ALA:HB1	1:B:910:PHE:CZ	2.51	0.45
1:B:959:TYR:HB3	1:B:967:PRO:HD2	1.98	0.45
1:B:1263:THR:N	1:B:1266:THR:O	2.47	0.45
1:C:263:GLU:HB3	1:C:281:ARG:HB2	1.98	0.45
1:C:977:LEU:CG	1:C:1044:ARG:HH21	2.30	0.45
1:D:871:ARG:HH22	1:D:922:LEU:HD13	1.80	0.45
1:D:894:GLY:HA3	1:D:903:LEU:HD22	1.98	0.45
1:D:986:ASP:HB3	1:D:1036:ARG:NH1	2.32	0.45
1:D:1008:SER:HB2	1:D:1017:ARG:NH2	2.32	0.45
1:D:2608:MET:HE2	1:D:2608:MET:HB2	1.84	0.45
1:D:3319:ILE:HG13	1:D:3338:LEU:HD21	1.97	0.45
1:D:3524:MET:H	1:D:3524:MET:HG2	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:80:VAL:HG23	2:G:80:VAL:O	2.16	0.45
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.17	0.45
1:A:4181:ILE:HG22	1:A:4182:GLU:H	1.81	0.45
1:B:269:TRP:NE1	1:B:333:GLY:O	2.49	0.45
1:B:1545:ASN:O	1:B:1545:ASN:CG	2.60	0.45
1:C:479:GLN:O	1:C:479:GLN:NE2	2.50	0.45
1:C:1434:TYR:HA	1:C:1519:LEU:HD23	1.98	0.45
1:C:2442:LEU:HG	1:C:2443:ILE:HG12	1.99	0.45
1:C:3794:VAL:HG21	1:C:3835:LEU:HD11	1.99	0.45
1:C:4181:ILE:HG22	1:C:4182:GLU:H	1.82	0.45
1:D:430:PRO:HB2	1:D:509:GLU:HB2	1.98	0.45
1:D:531:ARG:HA	1:D:566:CYS:SG	2.56	0.45
2:F:48:PHE:CE1	2:F:55:VAL:HG21	2.51	0.45
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.84	0.45
1:A:681:HIS:NE2	1:A:683:ARG:HD2	2.32	0.45
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.97	0.45
1:A:3347:SER:O	1:A:3347:SER:OG	2.29	0.45
1:B:915:GLU:HA	1:B:918:ARG:HB2	1.98	0.45
1:B:924:MET:HA	1:B:927:GLU:OE2	2.16	0.45
1:B:1000:ARG:HB3	1:B:1005:TRP:HB2	1.98	0.45
1:C:2013:LYS:HE3	1:C:2031:LEU:HD23	1.97	0.45
1:A:103:TYR:HB2	1:A:161:GLU:O	2.17	0.45
1:A:292:ALA:O	1:A:299:LEU:HD12	2.17	0.45
1:A:1172:ASP:OD1	1:A:1172:ASP:N	2.44	0.45
1:A:1767:VAL:O	1:A:1767:VAL:HG12	2.17	0.45
1:A:4044:MET:HE3	1:A:4044:MET:HB2	1.74	0.45
1:B:2474:LEU:HA	1:B:2494:PHE:CD2	2.50	0.45
1:B:4958:CYS:C	1:B:4960:ILE:H	2.25	0.45
1:C:1093:GLU:HG2	1:C:1148:VAL:HG12	1.99	0.45
1:C:1217:CYS:SG	1:C:1218:GLY:N	2.90	0.45
1:C:1767:VAL:O	1:C:1767:VAL:HG12	2.17	0.45
1:D:266:ARG:NH2	1:D:331:VAL:O	2.37	0.45
1:D:1037:ASP:O	1:D:1041:GLN:HG2	2.16	0.45
1:D:1769:THR:O	1:D:1769:THR:OG1	2.34	0.45
1:D:3398:PHE:HB3	1:D:3454:GLU:HG2	1.99	0.45
1:D:3434:LEU:O	1:D:3438:VAL:HG12	2.17	0.45
2:E:17:LYS:NZ	2:E:18:LYS:O	2.46	0.45
1:A:417:GLY:O	1:A:420:SER:OG	2.35	0.44
1:A:721:LEU:HD21	1:A:768:PHE:CZ	2.53	0.44
1:A:3845:ASN:OD1	1:A:3845:ASN:N	2.49	0.44
1:B:925:SER:O	1:B:928:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2187:ASN:OD1	1:B:2187:ASN:N	2.43	0.44
1:B:2759:ALA:HB2	1:B:2806:ARG:HH22	1.83	0.44
1:B:3526:ALA:O	1:B:3528:THR:N	2.50	0.44
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.32	0.44
1:C:24:CYS:HB3	1:C:200:TRP:CE3	2.53	0.44
1:C:710:ASP:O	1:C:712:TYR:N	2.50	0.44
1:D:15:ARG:O	1:D:98:HIS:ND1	2.39	0.44
1:D:269:TRP:CD1	1:D:272:SER:HB2	2.53	0.44
1:D:649:PHE:HE2	1:D:845:CYS:HB2	1.82	0.44
1:D:2187:ASN:OD1	1:D:2187:ASN:N	2.44	0.44
2:G:57:LYS:HB3	2:G:57:LYS:HE2	1.78	0.44
1:A:2491:SER:O	1:A:2491:SER:OG	2.31	0.44
1:A:3971:GLY:O	1:A:3973:CYS:N	2.50	0.44
1:B:1685:LEU:HD23	1:B:1718:ILE:HD11	1.99	0.44
1:C:277:GLY:HA2	1:C:315:CYS:SG	2.57	0.44
1:C:3398:PHE:HB3	1:C:3454:GLU:HG2	1.98	0.44
1:D:292:ALA:O	1:D:299:LEU:HD12	2.17	0.44
1:D:757:PHE:HB2	1:D:764:VAL:HG11	1.99	0.44
1:D:2325:PRO:HB3	1:D:2422:ILE:HA	2.00	0.44
1:D:3526:ALA:O	1:D:3528:THR:N	2.50	0.44
1:D:4109:GLN:HA	1:D:4112:LEU:HD12	2.00	0.44
1:A:830:ARG:HE	1:A:830:ARG:HB3	1.58	0.44
1:A:886:ARG:HB3	1:A:891:TRP:CD1	2.53	0.44
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.83	0.44
1:A:1452:TRP:CE3	1:A:1548:LEU:HB3	2.52	0.44
1:A:4189:ARG:NE	1:A:5032:TYR:OH	2.29	0.44
1:A:4958:CYS:C	1:A:4960:ILE:H	2.25	0.44
1:B:269:TRP:CD1	1:B:272:SER:HB2	2.52	0.44
1:B:531:ARG:HA	1:B:566:CYS:SG	2.56	0.44
1:B:2355:ARG:HB3	1:B:2359:ARG:HH21	1.82	0.44
1:B:2500:ALA:HB1	1:B:2550:LEU:HD22	1.99	0.44
1:C:3110:LEU:HD23	1:C:3110:LEU:HA	1.85	0.44
1:C:3695:PRO:HD2	1:C:3699:HIS:HB2	1.98	0.44
1:D:24:CYS:HB3	1:D:200:TRP:CE3	2.53	0.44
1:D:2474:LEU:HA	1:D:2494:PHE:CD2	2.52	0.44
1:B:760:ASN:N	1:B:760:ASN:OD1	2.49	0.44
1:C:2614:ILE:O	1:C:2618:MET:N	2.50	0.44
1:C:2858:GLN:H	1:C:2858:GLN:HG3	1.67	0.44
1:C:3999:MET:HE2	1:C:4016:LEU:HD13	1.99	0.44
1:C:4034:ASN:HD21	1:C:4153:HIS:CE1	2.35	0.44
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ASP:O	1:B:712:TYR:N	2.50	0.44
1:B:1128:ARG:HD3	1:B:1130:GLN:NE2	2.33	0.44
1:B:4159:ARG:HA	1:B:4162:ASN:HD21	1.82	0.44
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.29	0.44
1:C:757:PHE:HB2	1:C:764:VAL:HG11	1.99	0.44
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.99	0.44
1:C:2325:PRO:HB3	1:C:2422:ILE:HA	2.00	0.44
1:C:3172:ILE:HG21	1:C:3194:LEU:HD21	1.99	0.44
1:D:477:LEU:HD12	1:D:477:LEU:HA	1.90	0.44
1:D:497:TYR:HA	1:D:503:PHE:CE2	2.52	0.44
1:D:1206:GLN:NE2	1:D:1230:MET:O	2.51	0.44
1:D:2500:ALA:HB1	1:D:2550:LEU:HD22	2.00	0.44
1:D:2974:ILE:O	1:D:2978:GLU:N	2.44	0.44
1:D:4003:LEU:HD21	1:D:4012:LEU:HB3	1.98	0.44
1:D:4008:SER:OG	1:D:4009:GLN:OE1	2.27	0.44
1:A:263:GLU:HB3	1:A:281:ARG:HB2	1.99	0.44
1:A:479:GLN:O	1:A:479:GLN:NE2	2.51	0.44
1:A:497:TYR:HA	1:A:503:PHE:CE2	2.53	0.44
1:A:760:ASN:N	1:A:760:ASN:OD1	2.49	0.44
1:A:1000:ARG:HD2	1:A:1005:TRP:CG	2.52	0.44
1:A:2536:LEU:HA	1:A:2584:HIS:CE1	2.53	0.44
1:B:24:CYS:HB3	1:B:200:TRP:CE3	2.53	0.44
1:B:3579:LEU:HG	1:B:3581:GLY:H	1.82	0.44
1:C:1700:ASP:HB3	1:C:1703:LEU:HD12	1.99	0.44
1:C:1770:SER:OG	1:C:1956:GLU:OE2	2.27	0.44
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.30	0.44
1:D:760:ASN:N	1:D:760:ASN:OD1	2.49	0.44
1:D:1454:THR:HG22	1:D:1491:ASN:HA	1.99	0.44
2:G:30:LEU:N	2:G:34:LYS:O	2.48	0.44
2:H:77:THR:HA	2:H:96:THR:HG22	2.00	0.44
1:A:1125:ASN:HB2	1:A:1132:TRP:HD1	1.83	0.44
1:A:1263:THR:N	1:A:1266:THR:O	2.41	0.44
1:A:4583:SER:HB3	1:A:4630:TYR:HE2	1.83	0.44
1:B:68:THR:HG23	1:B:110:ARG:HB2	2.00	0.44
1:B:772:ASN:CG	1:B:1470:ARG:HH11	2.25	0.44
1:B:3274:LEU:HG	1:B:3275:PRO:HD3	1.99	0.44
1:B:4109:GLN:HA	1:B:4112:LEU:HD12	2.00	0.44
1:B:4769:MET:SD	1:B:4769:MET:N	2.90	0.44
1:B:4907:ASP:C	1:B:4909:TYR:H	2.26	0.44
1:C:269:TRP:CD1	1:C:272:SER:HB2	2.52	0.44
1:C:3535:LEU:HD23	1:C:3535:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:HD12	1:D:161:GLU:O	2.17	0.44
1:D:830:ARG:NE	1:D:1612:PHE:CE2	2.83	0.44
1:D:954:LYS:HA	1:D:954:LYS:HD2	1.80	0.44
1:D:1644:GLU:OE1	1:D:1646:ARG:NE	2.42	0.44
1:D:3971:GLY:O	1:D:3973:CYS:N	2.50	0.44
2:G:38:SER:OG	2:G:41:ASP:OD2	2.35	0.44
1:A:158:SER:N	1:A:161:GLU:OE1	2.49	0.44
1:A:269:TRP:HZ2	1:A:334:MET:HE2	1.82	0.44
1:A:2614:ILE:O	1:A:2618:MET:N	2.51	0.44
1:A:4008:SER:OG	1:A:4009:GLN:OE1	2.24	0.44
1:C:68:THR:HG23	1:C:110:ARG:HB2	1.99	0.44
1:C:3999:MET:HE1	1:C:4003:LEU:HD22	1.99	0.44
1:C:4958:CYS:C	1:C:4960:ILE:H	2.25	0.44
1:D:1040:CYS:O	1:D:1044:ARG:HG2	2.18	0.44
1:D:3526:ALA:HB2	1:D:3595:ARG:HH12	1.82	0.44
1:D:3845:ASN:OD1	1:D:3845:ASN:N	2.49	0.44
2:G:14:THR:OG1	2:G:68:LEU:N	2.51	0.44
1:A:1435:TYR:CZ	1:A:1550:PRO:HB3	2.53	0.44
1:A:4586:PRO:HB3	1:A:4628:VAL:HG21	1.98	0.44
1:B:30:LYS:HA	1:B:30:LYS:HD3	1.84	0.44
1:B:2368:LEU:HA	1:B:2374:SER:HB2	2.00	0.44
1:B:3875:MET:C	1:B:3877:ASP:H	2.26	0.44
1:C:3289:PRO:HG2	1:C:3307:VAL:HG22	1.99	0.44
1:D:619:ASP:OD2	1:D:1680:ARG:NH2	2.50	0.44
1:D:2983:SER:O	1:D:2983:SER:OG	2.29	0.44
1:D:3359:ILE:HD11	1:D:3434:LEU:HB2	2.00	0.44
2:F:17:LYS:HD3	2:F:17:LYS:N	2.33	0.44
1:A:68:THR:HG23	1:A:110:ARG:HB2	2.00	0.43
1:A:277:GLY:HA2	1:A:315:CYS:SG	2.57	0.43
1:A:279:PRO:HA	1:A:314:PHE:O	2.18	0.43
1:A:757:PHE:HB2	1:A:764:VAL:HG11	1.99	0.43
1:A:1486:SER:O	1:A:1486:SER:OG	2.29	0.43
1:A:2258:LEU:HD12	1:A:2258:LEU:HA	1.87	0.43
1:B:2431:ASP:OD1	1:B:2435:ARG:NE	2.47	0.43
1:C:798:GLY:HA2	1:C:1623:ARG:HD3	1.99	0.43
1:C:1125:ASN:OD1	1:C:1126:GLY:N	2.51	0.43
1:C:2159:LEU:HD22	1:C:2201:LEU:HD21	2.00	0.43
1:D:269:TRP:NE1	1:D:333:GLY:O	2.51	0.43
1:D:448:LEU:HD23	1:D:448:LEU:HA	1.84	0.43
1:D:1805:GLU:OE2	1:D:1808:ARG:NH2	2.51	0.43
1:D:3940:LYS:HE2	1:D:3940:LYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LYS:HB2	1:A:375:LYS:HE3	1.81	0.43
1:A:652:ARG:HG2	1:A:750:LEU:HD13	2.00	0.43
1:A:3249:LEU:O	1:A:3253:ILE:HG12	2.18	0.43
1:A:3526:ALA:O	1:A:3528:THR:N	2.51	0.43
1:B:1018:ASN:HA	1:B:1019:PRO:HD3	1.78	0.43
1:B:3289:PRO:HG2	1:B:3307:VAL:HG22	2.00	0.43
1:C:651:GLY:H	1:C:776:LEU:HD23	1.83	0.43
1:C:1283:LEU:HD12	1:C:1283:LEU:HA	1.84	0.43
1:C:1652:GLU:OE1	1:C:1656:ARG:NH2	2.51	0.43
1:C:3327:LEU:HD12	1:C:3327:LEU:HA	1.82	0.43
1:D:263:GLU:HB3	1:D:281:ARG:HB2	1.99	0.43
1:D:1139:PHE:CE1	1:D:1169:LEU:HD11	2.53	0.43
1:D:4958:CYS:C	1:D:4960:ILE:H	2.25	0.43
2:H:22:CYS:SG	2:H:23:VAL:N	2.91	0.43
1:A:865:PRO:HA	1:A:868:GLU:HB2	2.00	0.43
1:A:1079:LYS:HG3	1:A:1107:PRO:HB3	2.00	0.43
1:A:1634:LEU:HD12	1:A:1634:LEU:HA	1.79	0.43
1:A:1805:GLU:OE2	1:A:1808:ARG:NH2	2.52	0.43
1:A:2440:MET:HE2	1:A:2441:HIS:N	2.31	0.43
1:A:3424:LEU:HD23	1:A:3424:LEU:HA	1.86	0.43
1:A:3695:PRO:HD2	1:A:3699:HIS:HB2	1.99	0.43
1:A:4763:GLY:N	1:A:4766:THR:OG1	2.49	0.43
1:B:268:SER:OG	1:B:269:TRP:N	2.51	0.43
1:B:689:THR:HB	1:B:778:PHE:HZ	1.83	0.43
1:C:760:ASN:OD1	1:C:760:ASN:N	2.50	0.43
1:C:1442:GLY:HA3	1:C:1558:HIS:CD2	2.53	0.43
1:C:1461:ASP:HB3	1:C:1464:PHE:HB2	2.01	0.43
1:C:2536:LEU:HA	1:C:2584:HIS:CE1	2.53	0.43
1:C:2606:CYS:SG	1:C:2607:LEU:N	2.91	0.43
1:C:3051:ARG:HA	1:C:3051:ARG:HD2	1.73	0.43
1:D:919:ASN:O	1:D:922:LEU:HD12	2.18	0.43
1:D:1815:LEU:HD12	1:D:1815:LEU:HA	1.90	0.43
1:D:2368:LEU:HA	1:D:2374:SER:HB2	2.01	0.43
1:D:3875:MET:C	1:D:3877:ASP:H	2.26	0.43
1:D:4583:SER:HB3	1:D:4630:TYR:HE2	1.83	0.43
1:A:2325:PRO:HB3	1:A:2422:ILE:HA	2.00	0.43
1:A:2476:ILE:HD12	1:A:2477:PRO:HD2	2.01	0.43
1:A:3232:LEU:HD12	1:A:3233:PRO:HD2	1.99	0.43
1:B:417:GLY:O	1:B:420:SER:OG	2.35	0.43
1:B:757:PHE:HB2	1:B:764:VAL:HG11	1.99	0.43
1:B:960:MET:HG3	1:B:966:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:ASP:HB3	1:B:1036:ARG:HE	1.82	0.43
1:B:1000:ARG:HD2	1:B:1005:TRP:CG	2.53	0.43
1:B:1125:ASN:OD1	1:B:1126:GLY:N	2.51	0.43
1:B:1436:SER:HA	1:B:1517:GLY:HA2	1.99	0.43
1:B:1457:TYR:O	1:B:1458:HIS:ND1	2.51	0.43
1:C:830:ARG:HH12	1:C:832:GLU:HG3	1.83	0.43
1:C:3677:LEU:HG	1:C:3697:PRO:HG2	2.00	0.43
1:C:4162:ASN:HA	1:C:4165:GLU:HG2	2.00	0.43
1:C:4798:MET:HE2	1:C:4798:MET:HB2	1.87	0.43
1:D:681:HIS:O	1:D:783:PHE:HA	2.19	0.43
1:D:1842:LEU:HD23	1:D:1842:LEU:HA	1.89	0.43
1:D:2556:LEU:HD11	1:D:2597:LYS:HA	2.01	0.43
1:D:4845:ALA:O	1:D:4883:TYR:OH	2.34	0.43
1:A:1206:GLN:NE2	1:A:1230:MET:O	2.52	0.43
1:A:3524:MET:HE2	1:A:3524:MET:HB3	1.93	0.43
1:A:3875:MET:C	1:A:3877:ASP:H	2.26	0.43
1:B:591:ASP:OD1	1:B:1594:ARG:NH1	2.51	0.43
1:B:718:GLY:HA3	1:B:737:LEU:HA	2.00	0.43
1:B:1141:ARG:NH2	1:B:1167:GLU:OE2	2.51	0.43
1:B:1805:GLU:OE2	1:B:1808:ARG:NH2	2.52	0.43
1:B:2159:LEU:HD22	1:B:2201:LEU:HD21	2.00	0.43
1:B:4189:ARG:NE	1:B:5032:TYR:OH	2.29	0.43
1:B:4583:SER:HB3	1:B:4630:TYR:HE2	1.83	0.43
1:B:4951:LYS:HE2	1:B:4951:LYS:HB2	1.88	0.43
1:C:103:TYR:HE1	1:C:152:PRO:HA	1.83	0.43
1:C:269:TRP:HZ2	1:C:334:MET:HE2	1.84	0.43
1:C:1125:ASN:HB2	1:C:1132:TRP:CD1	2.53	0.43
1:C:1494:MET:HB3	1:C:1494:MET:HE2	1.73	0.43
1:C:2759:ALA:HB2	1:C:2806:ARG:HH22	1.84	0.43
1:C:3103:ILE:HD11	1:C:3168:THR:HG22	2.00	0.43
1:C:3875:MET:C	1:C:3877:ASP:H	2.26	0.43
1:C:4583:SER:HB3	1:C:4630:TYR:HE2	1.83	0.43
1:C:4907:ASP:C	1:C:4909:TYR:H	2.24	0.43
1:D:575:LEU:HD22	1:D:609:CYS:HB2	2.00	0.43
1:D:4044:MET:HE3	1:D:4044:MET:HB2	1.73	0.43
1:A:268:SER:OG	1:A:269:TRP:N	2.52	0.43
1:A:294:THR:HG23	1:A:297:GLN:H	1.83	0.43
1:A:1125:ASN:OD1	1:A:1126:GLY:N	2.51	0.43
1:A:2520:HIS:O	1:A:2524:VAL:HG23	2.19	0.43
1:B:224:HIS:HB2	1:B:388:LEU:HG	2.01	0.43
1:B:561:LEU:HD11	1:B:589:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:ARG:HB3	1:B:891:TRP:CD1	2.53	0.43
1:B:2313:LEU:HB3	1:B:2318:TYR:HD2	1.84	0.43
1:B:3524:MET:H	1:B:3524:MET:HG2	1.65	0.43
1:B:3971:GLY:O	1:B:3973:CYS:N	2.50	0.43
1:C:996:TRP:CD1	1:C:996:TRP:C	2.96	0.43
1:C:1805:GLU:OE2	1:C:1808:ARG:NH2	2.51	0.43
1:C:1947:CYS:HB3	1:C:2126:ARG:HH21	1.84	0.43
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.32	0.43
1:D:591:ASP:OD1	1:D:1594:ARG:NH1	2.52	0.43
1:D:977:LEU:H	1:D:1044:ARG:NH2	2.16	0.43
1:D:1442:GLY:HA3	1:D:1558:HIS:CD2	2.54	0.43
1:D:3524:MET:HE2	1:D:3524:MET:HB3	1.92	0.43
2:G:56:ILE:HG22	2:G:59:PHE:H	1.83	0.43
2:H:68:LEU:HD23	2:H:68:LEU:HA	1.80	0.43
1:A:871:ARG:HH12	1:A:926:GLY:CA	2.32	0.43
1:A:2212:VAL:HG22	1:A:2256:TYR:CZ	2.54	0.43
1:A:4798:MET:HE2	1:A:4798:MET:HB2	1.87	0.43
1:A:4907:ASP:C	1:A:4909:TYR:H	2.26	0.43
1:A:5027:CYS:C	1:A:5029:ARG:H	2.27	0.43
1:B:479:GLN:O	1:B:479:GLN:NE2	2.50	0.43
1:B:955:LEU:HD13	1:B:959:TYR:CG	2.53	0.43
1:B:1442:GLY:HA3	1:B:1558:HIS:CD2	2.54	0.43
1:B:2476:ILE:HD12	1:B:2477:PRO:HD2	2.01	0.43
1:B:4989:MET:HE3	1:B:4989:MET:HB3	1.95	0.43
1:C:649:PHE:HE2	1:C:845:CYS:HB2	1.83	0.43
1:D:294:THR:HG23	1:D:297:GLN:H	1.84	0.43
1:D:858:THR:OG1	1:D:930:LYS:HG3	2.18	0.43
1:D:881:LEU:HD12	1:D:881:LEU:HA	1.84	0.43
1:D:1006:SER:O	1:D:1017:ARG:NH1	2.51	0.43
2:H:17:LYS:O	2:H:18:LYS:HG2	2.19	0.43
1:A:269:TRP:NE1	1:A:333:GLY:O	2.52	0.43
1:A:2228:MET:HE3	1:A:2228:MET:HB3	1.77	0.43
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.34	0.43
1:B:359:TYR:HB2	1:B:383:HIS:CE1	2.54	0.43
1:B:2556:LEU:HD11	1:B:2597:LYS:HA	2.01	0.43
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.18	0.43
1:C:3232:LEU:HD12	1:C:3233:PRO:HD2	1.99	0.43
1:D:915:GLU:HA	1:D:918:ARG:HB2	2.00	0.43
1:D:1770:SER:OG	1:D:1956:GLU:OE2	2.28	0.43
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.86	0.43
1:D:2159:LEU:HD22	1:D:2201:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3447:LYS:HA	1:D:3447:LYS:HD2	1.75	0.43
1:D:4907:ASP:O	1:D:4908:GLU:HB3	2.19	0.43
1:A:858:THR:OG1	1:A:930:LYS:HG3	2.19	0.43
1:A:913:LEU:HB2	1:A:918:ARG:HG2	1.99	0.43
1:A:1277:TRP:O	1:A:1277:TRP:HD1	2.02	0.43
1:A:1648:MET:HE2	1:A:1648:MET:HB3	1.85	0.43
1:A:2310:CYS:O	1:A:2312:MET:N	2.52	0.43
1:A:2556:LEU:HD11	1:A:2597:LYS:HA	2.01	0.43
1:A:3235:SER:O	1:A:3235:SER:OG	2.35	0.43
1:B:2199:ARG:HG3	1:B:2246:ASN:OD1	2.19	0.43
1:B:2536:LEU:HA	1:B:2584:HIS:CE1	2.53	0.43
1:B:2856:ASN:OD1	1:B:2856:ASN:N	2.52	0.43
1:B:3398:PHE:HB3	1:B:3454:GLU:HG2	2.00	0.43
1:C:684:VAL:HG12	1:C:781:VAL:HG12	2.00	0.43
1:C:977:LEU:HB3	1:C:981:GLN:CB	2.48	0.43
1:C:1022:VAL:HG23	1:C:1027:LEU:HG	2.01	0.43
1:C:1288:PHE:HA	1:C:1551:ALA:HA	2.01	0.43
1:C:1648:MET:HE2	1:C:1648:MET:HB3	1.86	0.43
1:C:2021:CYS:SG	1:C:2023:LEU:HB3	2.59	0.43
1:D:402:ARG:HA	1:D:402:ARG:HD2	1.85	0.43
1:D:1634:LEU:HD12	1:D:1634:LEU:HA	1.79	0.43
1:D:1652:GLU:OE1	1:D:1656:ARG:NH2	2.52	0.43
1:D:3141:THR:O	1:D:3145:GLN:HG2	2.19	0.43
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.83	0.43
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.26	0.43
1:A:990:GLU:HG2	1:A:1024:TYR:CE2	2.53	0.43
1:A:3509:LEU:HD12	1:A:3509:LEU:HA	1.84	0.43
1:A:4109:GLN:HA	1:A:4112:LEU:HD12	2.00	0.43
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.52	0.43
1:B:961:MET:HE2	1:B:962:SER:N	2.34	0.43
1:B:2283:ASN:HB3	1:B:2286:LEU:H	1.84	0.43
1:B:3172:ILE:HG21	1:B:3194:LEU:HD21	2.01	0.43
1:B:3263:TYR:O	1:B:3265:GLU:N	2.52	0.43
1:C:919:ASN:O	1:C:922:LEU:HD12	2.18	0.43
1:C:1272:LEU:HD11	1:C:1285:GLU:OE1	2.18	0.43
1:C:2556:LEU:HD11	1:C:2597:LYS:HA	2.01	0.43
1:C:2916:LYS:HA	1:C:2916:LYS:HD2	1.80	0.43
1:D:359:TYR:HB2	1:D:383:HIS:CE1	2.54	0.43
1:D:1028:ASP:O	1:D:1032:LYS:HG3	2.19	0.43
1:D:3274:LEU:HG	1:D:3275:PRO:HD3	2.01	0.43
1:D:3994:HIS:O	1:D:3998:HIS:ND1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5027:CYS:C	1:D:5029:ARG:H	2.27	0.43
1:A:971:ASP:O	1:A:974:HIS:NE2	2.51	0.42
1:A:981:GLN:HA	1:A:984:LEU:HD23	2.01	0.42
1:A:3519:PRO:O	1:D:1220:GLN:NE2	2.50	0.42
1:B:294:THR:HG23	1:B:297:GLN:H	1.84	0.42
1:B:2310:CYS:O	1:B:2312:MET:N	2.52	0.42
1:B:3359:ILE:HD11	1:B:3434:LEU:HB2	2.01	0.42
1:C:670:GLU:HA	1:C:740:PRO:HB3	2.01	0.42
1:C:2310:CYS:O	1:C:2312:MET:N	2.52	0.42
1:C:2355:ARG:HB3	1:C:2359:ARG:HH21	1.84	0.42
1:C:2454:ARG:HG2	1:C:2458:ARG:HH12	1.84	0.42
1:C:2476:ILE:HD12	1:C:2477:PRO:HD2	2.00	0.42
1:C:3447:LYS:HD2	1:C:3447:LYS:HA	1.74	0.42
1:C:3771:HIS:HD2	1:C:3815:LYS:HD2	1.84	0.42
1:D:29:LEU:HD12	1:D:30:LYS:N	2.34	0.42
1:D:479:GLN:O	1:D:479:GLN:NE2	2.50	0.42
1:D:1436:SER:HA	1:D:1517:GLY:HA2	2.01	0.42
1:D:1771:LEU:HD22	1:D:2153:MET:HE1	2.01	0.42
1:D:2283:ASN:HB3	1:D:2286:LEU:H	1.84	0.42
1:D:2606:CYS:SG	1:D:2607:LEU:N	2.92	0.42
1:D:3677:LEU:HG	1:D:3697:PRO:HG2	2.01	0.42
1:A:14:LEU:HD12	1:A:18:ASP:HB3	2.01	0.42
1:A:266:ARG:NH2	1:A:331:VAL:O	2.35	0.42
1:A:571:SER:O	1:A:571:SER:OG	2.32	0.42
1:A:881:LEU:HD12	1:A:881:LEU:HA	1.78	0.42
1:A:1283:LEU:HD12	1:A:1283:LEU:HA	1.84	0.42
1:A:1442:GLY:HA3	1:A:1558:HIS:CD2	2.54	0.42
1:A:2035:HIS:CE1	1:A:3661:TRP:HB3	2.54	0.42
1:A:2149:VAL:O	1:A:2153:MET:N	2.49	0.42
1:A:2967:MET:H	1:A:2967:MET:HG2	1.60	0.42
1:A:3398:PHE:HB3	1:A:3454:GLU:HG2	2.00	0.42
1:B:497:TYR:HA	1:B:503:PHE:CE2	2.54	0.42
1:B:1079:LYS:HG3	1:B:1107:PRO:HB3	2.01	0.42
1:B:1459:GLN:HA	1:B:1459:GLN:OE1	2.19	0.42
1:B:1771:LEU:HD22	1:B:2153:MET:HE1	2.01	0.42
1:B:4198:SER:HB3	1:B:4201:ASN:ND2	2.34	0.42
1:C:345:LEU:HD22	1:C:389:PHE:HB3	2.01	0.42
1:C:595:ARG:NH2	1:C:1643:GLU:OE1	2.50	0.42
1:C:655:GLY:HA3	1:C:852:VAL:HG12	2.01	0.42
1:C:1206:GLN:NE2	1:C:1230:MET:O	2.51	0.42
1:C:2283:ASN:HB3	1:C:2286:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2431:ASP:OD1	1:C:2435:ARG:NE	2.49	0.42
1:C:2999:ALA:HA	1:C:3002:LEU:HG	2.00	0.42
1:C:4198:SER:HB3	1:C:4201:ASN:ND2	2.34	0.42
1:C:4897:ILE:HD12	1:C:4897:ILE:HA	1.89	0.42
1:D:269:TRP:HZ2	1:D:334:MET:HE2	1.84	0.42
1:D:2199:ARG:HG3	1:D:2246:ASN:OD1	2.19	0.42
1:D:2656:CYS:O	1:D:2659:THR:OG1	2.37	0.42
1:D:4049:VAL:O	1:D:4052:SER:OG	2.35	0.42
1:D:4198:SER:HB3	1:D:4201:ASN:ND2	2.35	0.42
1:A:902:ARG:O	1:A:903:LEU:HD12	2.19	0.42
1:A:993:HIS:NE2	1:A:1027:LEU:HD11	2.34	0.42
1:A:2454:ARG:HG2	1:A:2458:ARG:HH12	1.85	0.42
1:A:3289:PRO:HG2	1:A:3307:VAL:HG22	2.00	0.42
1:A:3332:ALA:HB1	1:A:3334:TRP:CD1	2.54	0.42
1:B:12:GLN:HE21	1:B:14:LEU:HD11	1.84	0.42
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.18	0.42
1:B:1125:ASN:HB2	1:B:1132:TRP:HD1	1.84	0.42
1:C:273:HIS:HE1	1:C:334:MET:HG3	1.84	0.42
1:C:882:TRP:HZ3	1:C:921:ASN:ND2	2.17	0.42
1:C:899:ASP:HB2	1:C:902:ARG:CZ	2.49	0.42
1:C:1634:LEU:HD12	1:C:1634:LEU:HA	1.79	0.42
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.52	0.42
1:D:1434:TYR:HA	1:D:1519:LEU:HD23	2.01	0.42
1:D:2476:ILE:HD12	1:D:2477:PRO:HD2	2.00	0.42
1:D:3804:ILE:HD12	1:D:3804:ILE:HA	1.87	0.42
1:D:4184:MET:HB2	1:D:4190:ILE:HD13	2.02	0.42
1:A:345:LEU:HD22	1:A:389:PHE:HB3	2.00	0.42
1:A:710:ASP:O	1:A:712:TYR:N	2.52	0.42
1:A:961:MET:CE	1:A:963:ASN:H	2.33	0.42
1:A:1253:PRO:HB2	1:A:1254:HIS:CE1	2.54	0.42
1:A:3756:LYS:HE2	1:A:3756:LYS:HB3	1.86	0.42
1:B:725:HIS:O	1:B:725:HIS:ND1	2.52	0.42
1:B:3936:TYR:O	1:B:3940:LYS:NZ	2.40	0.42
1:C:887:ILE:HG13	1:C:891:TRP:O	2.20	0.42
1:C:1640:HIS:HA	1:C:1647:CYS:HA	2.01	0.42
1:C:2547:ALA:O	1:C:2551:ASN:ND2	2.52	0.42
1:C:2608:MET:HE2	1:C:2608:MET:HB2	1.83	0.42
1:C:3208:PRO:HD2	1:C:3245:VAL:HG22	2.02	0.42
1:D:268:SER:OG	1:D:269:TRP:N	2.52	0.42
1:D:871:ARG:HH11	1:D:926:GLY:HA3	1.83	0.42
1:D:1125:ASN:OD1	1:D:1126:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1253:PRO:HB2	1:D:1254:HIS:CE1	2.54	0.42
1:D:1451:GLY:HA3	1:D:1494:MET:HG2	2.02	0.42
2:E:29:MET:HA	2:E:35:LYS:HA	2.01	0.42
1:A:670:GLU:HA	1:A:740:PRO:HB3	2.00	0.42
1:A:886:ARG:HB3	1:A:891:TRP:HD1	1.85	0.42
1:A:2103:VAL:HG13	1:A:3696:ASP:OD2	2.19	0.42
1:A:3806:ASN:HA	1:A:3890:LEU:HD21	2.01	0.42
1:A:4184:MET:HB2	1:A:4190:ILE:HD13	2.02	0.42
1:B:273:HIS:HE1	1:B:334:MET:HG3	1.84	0.42
1:B:345:LEU:HD22	1:B:389:PHE:HB3	2.01	0.42
1:B:954:LYS:HD2	1:B:954:LYS:HA	1.83	0.42
1:B:1263:THR:HG23	1:B:1265:ASP:H	1.85	0.42
1:B:1434:TYR:O	1:B:1435:TYR:C	2.63	0.42
1:B:1618:ARG:HG2	1:B:1627:ALA:HB3	2.01	0.42
1:B:1652:GLU:OE1	1:B:1656:ARG:NH2	2.53	0.42
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.85	0.42
1:C:2199:ARG:HG3	1:C:2246:ASN:OD1	2.19	0.42
1:C:4951:LYS:HE2	1:C:4951:LYS:HB2	1.88	0.42
1:D:710:ASP:O	1:D:712:TYR:N	2.52	0.42
1:D:887:ILE:HG13	1:D:891:TRP:O	2.19	0.42
1:D:977:LEU:HD12	1:D:1044:ARG:HH21	1.83	0.42
1:D:2858:GLN:H	1:D:2858:GLN:HG3	1.67	0.42
1:D:3263:TYR:O	1:D:3265:GLU:N	2.53	0.42
1:A:924:MET:HA	1:A:927:GLU:OE2	2.18	0.42
1:A:2313:LEU:HB3	1:A:2318:TYR:HD2	1.84	0.42
1:A:3107:VAL:HA	1:A:3110:LEU:HB2	2.02	0.42
1:B:266:ARG:NH2	1:B:331:VAL:O	2.37	0.42
1:B:2035:HIS:CE1	1:B:3661:TRP:HB3	2.55	0.42
1:B:2442:LEU:HG	1:B:2443:ILE:HG12	2.01	0.42
1:C:417:GLY:O	1:C:420:SER:OG	2.35	0.42
1:C:1719:HIS:CE1	1:C:1800:PRO:HB2	2.55	0.42
1:C:2035:HIS:CE1	1:C:3661:TRP:HB3	2.55	0.42
1:C:3526:ALA:O	1:C:3528:THR:N	2.52	0.42
1:D:950:LEU:HD23	1:D:950:LEU:HA	1.84	0.42
1:D:3289:PRO:HG2	1:D:3307:VAL:HG22	2.00	0.42
1:D:3771:HIS:HD2	1:D:3815:LYS:HD2	1.84	0.42
2:G:29:MET:HA	2:G:35:LYS:HA	2.02	0.42
1:A:255:HIS:ND1	1:A:480:GLU:OE2	2.52	0.42
1:A:575:LEU:HD22	1:A:609:CYS:HB2	2.02	0.42
1:A:1436:SER:HA	1:A:1517:GLY:HA2	2.01	0.42
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2974:ILE:O	1:A:2978:GLU:N	2.44	0.42
1:A:3771:HIS:HD2	1:A:3815:LYS:HD2	1.84	0.42
1:A:4907:ASP:O	1:A:4908:GLU:HB3	2.19	0.42
1:B:1288:PHE:CE1	1:B:1598:GLN:HB2	2.54	0.42
1:B:2021:CYS:SG	1:B:2023:LEU:HB3	2.60	0.42
1:B:2606:CYS:SG	1:B:2607:LEU:N	2.92	0.42
1:B:5027:CYS:C	1:B:5029:ARG:H	2.27	0.42
1:C:233:ILE:HG22	1:C:234:SER:N	2.35	0.42
1:C:268:SER:OG	1:C:269:TRP:N	2.51	0.42
1:C:575:LEU:HD22	1:C:609:CYS:HB2	2.02	0.42
1:C:907:LEU:HD13	1:C:961:MET:HE2	2.02	0.42
1:C:952:LYS:HG2	1:C:953:THR:H	1.84	0.42
1:C:993:HIS:NE2	1:C:1027:LEU:HD11	2.35	0.42
1:C:1079:LYS:HG3	1:C:1107:PRO:HB3	2.00	0.42
1:C:1101:ARG:HB3	1:C:1123:VAL:HG21	2.00	0.42
1:C:1618:ARG:HG2	1:C:1627:ALA:HB3	2.01	0.42
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.84	0.42
1:C:3396:ASP:OD1	1:C:3397:GLU:N	2.53	0.42
1:C:4159:ARG:HA	1:C:4162:ASN:HD21	1.84	0.42
1:D:981:GLN:O	1:D:984:LEU:HG	2.19	0.42
1:D:990:GLU:HG2	1:D:1024:TYR:CZ	2.55	0.42
1:D:2212:VAL:HG22	1:D:2256:TYR:CZ	2.55	0.42
1:D:3068:LEU:H	1:D:3068:LEU:HD12	1.84	0.42
1:D:3136:LEU:HA	1:D:3139:VAL:HG22	2.01	0.42
1:D:4586:PRO:HA	1:D:4587:PRO:HD3	1.91	0.42
1:A:875:ALA:HB1	1:A:910:PHE:CZ	2.55	0.42
1:A:1275:ARG:HG3	1:A:1276:THR:HG23	2.01	0.42
1:A:2159:LEU:HD22	1:A:2201:LEU:HD21	2.02	0.42
1:A:2236:LEU:HD22	1:A:2250:MET:SD	2.60	0.42
1:A:2759:ALA:HB2	1:A:2806:ARG:HH22	1.84	0.42
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.85	0.42
1:A:3447:LYS:HA	1:A:3447:LYS:HD2	1.75	0.42
1:B:575:LEU:HD22	1:B:609:CYS:HB2	2.01	0.42
1:B:1470:ARG:HA	1:B:1470:ARG:HD3	1.70	0.42
1:B:4845:ALA:O	1:B:4883:TYR:OH	2.36	0.42
1:C:33:LEU:HG	1:C:53:SER:OG	2.20	0.42
1:C:2212:VAL:HG22	1:C:2256:TYR:CZ	2.55	0.42
1:C:3272:ILE:HG13	1:C:3273:THR:HG22	2.02	0.42
1:C:3509:LEU:HD12	1:C:3509:LEU:HA	1.84	0.42
1:D:829:TYR:HE2	1:D:1608:MET:HG2	1.85	0.42
1:D:875:ALA:HB1	1:D:910:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1275:ARG:HG3	1:D:1276:THR:HG23	2.01	0.42
1:D:2035:HIS:CE1	1:D:3661:TRP:HB3	2.55	0.42
1:D:2360:LYS:HE3	1:D:2360:LYS:HB2	1.95	0.42
1:D:4907:ASP:C	1:D:4909:TYR:H	2.26	0.42
2:E:57:LYS:HB3	2:E:57:LYS:HE2	1.76	0.42
2:H:29:MET:HA	2:H:35:LYS:HA	2.02	0.42
1:A:17:ASP:HB2	1:A:98:HIS:HE1	1.84	0.42
1:A:723:THR:HG21	1:A:768:PHE:HE2	1.85	0.42
1:A:1618:ARG:HG2	1:A:1627:ALA:HB3	2.01	0.42
1:A:2199:ARG:HG3	1:A:2246:ASN:OD1	2.20	0.42
1:A:2283:ASN:HB3	1:A:2286:LEU:H	1.84	0.42
1:A:2420:HIS:ND1	1:A:2423:MET:HE2	2.35	0.42
1:A:4989:MET:HE3	1:A:4989:MET:HB3	1.95	0.42
1:B:233:ILE:HG22	1:B:234:SER:N	2.35	0.42
1:B:681:HIS:O	1:B:783:PHE:HA	2.20	0.42
1:B:3323:ILE:HD11	1:B:3338:LEU:HD22	2.01	0.42
1:B:4008:SER:OG	1:B:4009:GLN:OE1	2.27	0.42
1:C:892:THR:OG1	1:C:902:ARG:O	2.28	0.42
1:C:1000:ARG:HD2	1:C:1000:ARG:HA	1.81	0.42
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.42
1:C:2313:LEU:HB3	1:C:2318:TYR:HD2	1.84	0.42
1:C:3674:ILE:HG13	1:C:3732:SER:HB2	2.02	0.42
1:C:4049:VAL:O	1:C:4052:SER:OG	2.32	0.42
1:D:299:LEU:HD12	1:D:299:LEU:HA	1.81	0.42
1:D:1947:CYS:HB3	1:D:2126:ARG:HH21	1.84	0.42
1:D:2741:GLU:HB3	1:D:2744:ASN:HB2	2.01	0.42
1:D:2963:LEU:HA	1:D:2966:TRP:HB2	2.01	0.42
1:D:3323:ILE:HD11	1:D:3338:LEU:HD22	2.01	0.42
1:D:3347:SER:O	1:D:3347:SER:OG	2.29	0.42
1:D:3714:SER:O	1:D:3714:SER:OG	2.37	0.42
1:A:33:LEU:HG	1:A:53:SER:OG	2.20	0.42
1:A:233:ILE:HG22	1:A:234:SER:N	2.35	0.42
1:A:1288:PHE:HA	1:A:1551:ALA:HA	2.02	0.42
1:A:1947:CYS:HB3	1:A:2126:ARG:HH21	1.85	0.42
1:A:2021:CYS:SG	1:A:2023:LEU:HB3	2.60	0.42
1:A:3777:GLU:H	1:A:3777:GLU:HG2	1.64	0.42
1:B:913:LEU:H	1:B:913:LEU:HD12	1.85	0.42
1:B:1275:ARG:HG3	1:B:1276:THR:HG23	2.01	0.42
1:B:2440:MET:HE2	1:B:2441:HIS:N	2.31	0.42
1:B:2454:ARG:HG2	1:B:2458:ARG:HH12	1.84	0.42
1:B:3771:HIS:HD2	1:B:3815:LYS:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:HG22	1:C:148:TRP:HB2	2.01	0.42
1:C:224:HIS:HB2	1:C:388:LEU:HG	2.02	0.42
1:C:915:GLU:HA	1:C:918:ARG:HB2	2.01	0.42
1:C:2930:LEU:HB2	1:C:2935:TYR:HB3	2.02	0.42
1:C:3940:LYS:HB2	1:C:3940:LYS:HE2	1.83	0.42
1:D:22:LEU:HB3	1:D:200:TRP:CE3	2.55	0.42
1:D:33:LEU:HG	1:D:53:SER:OG	2.20	0.42
1:D:1008:SER:HB2	1:D:1017:ARG:CZ	2.50	0.42
1:D:1079:LYS:HG3	1:D:1107:PRO:HB3	2.01	0.42
1:D:1536:SER:OG	1:D:1537:ASN:N	2.53	0.42
1:D:2310:CYS:O	1:D:2312:MET:N	2.52	0.42
1:D:4767:TRP:O	1:D:4770:SER:OG	2.35	0.42
1:A:920:TYR:HD1	1:A:923:GLN:HE21	1.68	0.41
1:A:2858:GLN:H	1:A:2858:GLN:HG3	1.67	0.41
1:A:3172:ILE:HG21	1:A:3194:LEU:HD21	2.01	0.41
1:B:880:GLU:HG3	1:B:968:ALA:H	1.84	0.41
1:B:1220:GLN:HG3	1:C:3519:PRO:HB3	2.02	0.41
1:B:1644:GLU:OE1	1:B:1646:ARG:NE	2.42	0.41
1:B:4170:ILE:HD13	1:B:4170:ILE:HA	1.94	0.41
1:C:867:LEU:O	1:C:870:ILE:HG22	2.19	0.41
1:C:1435:TYR:CZ	1:C:1550:PRO:HB3	2.55	0.41
1:C:2179:ILE:HD11	1:C:2228:MET:HG2	2.02	0.41
1:C:3677:LEU:HG	1:C:3697:PRO:CG	2.50	0.41
1:C:4845:ALA:O	1:C:4883:TYR:OH	2.35	0.41
1:D:72:SER:H	1:D:99:ARG:HH12	1.68	0.41
1:D:2905:LEU:HD23	1:D:2905:LEU:H	1.83	0.41
2:E:48:PHE:HE1	2:E:55:VAL:HG21	1.84	0.41
1:A:24:CYS:HB3	1:A:200:TRP:CE3	2.54	0.41
1:A:655:GLY:HA3	1:A:852:VAL:HG12	2.01	0.41
1:A:952:LYS:HG2	1:A:953:THR:H	1.85	0.41
1:A:1028:ASP:O	1:A:1032:LYS:HG3	2.20	0.41
1:A:1640:HIS:HA	1:A:1647:CYS:HA	2.02	0.41
1:A:1652:GLU:OE1	1:A:1656:ARG:NH2	2.53	0.41
1:A:1849:LEU:HD23	1:A:1849:LEU:HA	1.87	0.41
1:A:2179:ILE:HD11	1:A:2228:MET:HG2	2.02	0.41
1:A:3983:SER:OG	1:A:3984:ARG:N	2.54	0.41
1:B:1253:PRO:HB2	1:B:1254:HIS:CE1	2.54	0.41
1:B:3051:ARG:HD2	1:B:3051:ARG:HA	1.62	0.41
1:B:3806:ASN:HA	1:B:3890:LEU:HD21	2.01	0.41
1:B:4907:ASP:O	1:B:4908:GLU:HB3	2.19	0.41
1:B:4957:LYS:HB3	1:B:4957:LYS:HE2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:833:GLY:HA3	1:C:838:HIS:ND1	2.35	0.41
1:C:1037:ASP:O	1:C:1041:GLN:HG2	2.20	0.41
1:C:1927:LEU:HD22	1:C:2097:LEU:HD11	2.02	0.41
1:C:3994:HIS:O	1:C:3998:HIS:ND1	2.49	0.41
1:D:833:GLY:N	1:D:836:GLY:O	2.52	0.41
1:D:955:LEU:HD13	1:D:959:TYR:CG	2.55	0.41
1:D:987:ARG:O	1:D:991:ASN:ND2	2.43	0.41
1:D:2520:HIS:O	1:D:2524:VAL:HG23	2.20	0.41
1:D:3103:ILE:HD11	1:D:3168:THR:HG22	2.02	0.41
1:D:3416:VAL:HG21	1:D:3517:MET:SD	2.60	0.41
2:G:44:LYS:HA	2:G:44:LYS:HD2	1.81	0.41
1:A:955:LEU:HD13	1:A:959:TYR:CG	2.54	0.41
1:A:1139:PHE:CE1	1:A:1169:LEU:HD11	2.55	0.41
1:A:2236:LEU:HD23	1:A:2236:LEU:HA	1.90	0.41
1:A:3038:MET:O	1:A:3041:SER:OG	2.33	0.41
1:A:4951:LYS:HE2	1:A:4951:LYS:HB2	1.88	0.41
1:B:255:HIS:ND1	1:B:480:GLU:OE2	2.54	0.41
1:B:774:ASP:O	1:B:848:HIS:ND1	2.52	0.41
1:B:1634:LEU:HD12	1:B:1634:LEU:HA	1.79	0.41
1:B:3793:MET:HA	1:B:3793:MET:HE2	2.02	0.41
1:C:619:ASP:OD2	1:C:1680:ARG:NH2	2.48	0.41
1:C:682:LEU:HD12	1:C:787:VAL:HG12	2.00	0.41
1:C:2906:VAL:HG11	1:C:2911:LEU:HA	2.03	0.41
1:C:3777:GLU:H	1:C:3777:GLU:HG2	1.64	0.41
1:C:3793:MET:HE3	1:C:3793:MET:HB3	1.91	0.41
1:D:393:CYS:HB2	1:D:397:GLU:HG3	2.03	0.41
1:D:881:LEU:HD23	1:D:1041:GLN:HG3	2.02	0.41
1:D:913:LEU:H	1:D:913:LEU:HD12	1.84	0.41
1:D:1521:ASP:OD1	1:D:1524:THR:OG1	2.32	0.41
1:D:3989:VAL:HG21	1:D:4047:MET:HE2	2.01	0.41
1:A:778:PHE:HB2	1:A:780:VAL:HG13	2.01	0.41
1:A:2309:SER:OG	1:A:2321:ILE:O	2.32	0.41
1:B:1636:MET:HE2	1:B:1636:MET:HB3	1.94	0.41
1:B:2541:PHE:HD1	1:B:2541:PHE:HA	1.81	0.41
1:B:3940:LYS:HB2	1:B:3940:LYS:HE2	1.83	0.41
1:C:12:GLN:HB2	1:C:165:VAL:HG13	2.03	0.41
1:C:255:HIS:ND1	1:C:480:GLU:OE2	2.54	0.41
1:C:711:LEU:HD12	1:C:1470:ARG:HB3	2.02	0.41
1:C:2524:VAL:HA	1:C:2527:LEU:HD23	2.02	0.41
1:D:284:HIS:CE1	1:D:286:THR:HB	2.55	0.41
1:D:884:LEU:O	1:D:887:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1288:PHE:HA	1:D:1551:ALA:HA	2.03	0.41
1:D:2420:HIS:ND1	1:D:2423:MET:HE2	2.35	0.41
1:D:3110:LEU:HD12	1:D:3175:LEU:HD11	2.02	0.41
1:D:3592:ILE:HA	1:D:3595:ARG:NE	2.34	0.41
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.53	0.41
1:A:537:CYS:O	1:A:541:SER:OG	2.39	0.41
1:A:1284:VAL:HG22	1:A:1555:LEU:HD13	2.02	0.41
1:A:1434:TYR:HB2	1:A:1572:ILE:HG21	2.02	0.41
1:A:2458:ARG:NH2	1:A:2509:VAL:O	2.54	0.41
1:A:2608:MET:HE2	1:A:2608:MET:HB2	1.83	0.41
1:A:3416:VAL:HG21	1:A:3517:MET:SD	2.60	0.41
1:B:393:CYS:HB2	1:B:397:GLU:HG3	2.03	0.41
1:B:830:ARG:HE	1:B:830:ARG:HB3	1.67	0.41
1:B:987:ARG:O	1:B:991:ASN:ND2	2.46	0.41
1:B:1139:PHE:CE1	1:B:1169:LEU:HD11	2.55	0.41
1:B:1206:GLN:NE2	1:B:1230:MET:O	2.52	0.41
1:C:689:THR:HB	1:C:778:PHE:HZ	1.84	0.41
1:C:874:LEU:HD13	1:C:929:LEU:HD21	2.02	0.41
1:D:224:HIS:HB2	1:D:388:LEU:HG	2.02	0.41
1:D:3040:THR:HG21	1:D:3080:VAL:HG21	2.01	0.41
1:D:3509:LEU:HD12	1:D:3509:LEU:HA	1.85	0.41
1:D:3832:ILE:HD13	1:D:3832:ILE:HA	1.97	0.41
1:A:4897:ILE:HD12	1:A:4897:ILE:HA	1.91	0.41
1:B:72:SER:H	1:B:99:ARG:HH12	1.69	0.41
1:B:902:ARG:O	1:B:903:LEU:HD12	2.20	0.41
1:B:2547:ALA:O	1:B:2551:ASN:ND2	2.54	0.41
1:B:3714:SER:O	1:B:3714:SER:OG	2.36	0.41
1:B:3891:LEU:HD22	1:B:3899:PHE:CE2	2.56	0.41
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.53	0.41
1:C:402:ARG:HA	1:C:402:ARG:HD2	1.85	0.41
1:C:913:LEU:H	1:C:913:LEU:HD12	1.85	0.41
1:C:3068:LEU:HD12	1:C:3068:LEU:H	1.85	0.41
1:C:3430:ASN:OD1	1:C:3430:ASN:N	2.54	0.41
1:D:345:LEU:HD22	1:D:389:PHE:HB3	2.01	0.41
1:D:1851:MET:HB2	1:D:1853:ILE:HG13	2.03	0.41
1:D:2454:ARG:HG2	1:D:2458:ARG:HH12	1.85	0.41
1:D:3107:VAL:HA	1:D:3110:LEU:HB2	2.03	0.41
1:D:3327:LEU:HA	1:D:3327:LEU:HD12	1.84	0.41
1:D:3359:ILE:HD13	1:D:3359:ILE:HA	1.93	0.41
1:A:206:CYS:N	1:A:271:GLY:HA3	2.36	0.41
1:A:247:TYR:OH	1:A:388:LEU:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:VAL:HG12	1:A:777:PHE:HB2	2.02	0.41
1:A:800:PHE:HD2	1:A:804:PRO:HG3	1.86	0.41
1:A:2741:GLU:HB3	1:A:2744:ASN:HB2	2.02	0.41
1:B:1288:PHE:HA	1:B:1551:ALA:HA	2.03	0.41
1:B:2179:ILE:HD11	1:B:2228:MET:HG2	2.02	0.41
1:B:2964:LEU:HA	1:B:2967:MET:HE2	2.03	0.41
1:B:2999:ALA:HA	1:B:3002:LEU:HG	2.03	0.41
1:B:4686:LEU:HD23	1:B:4687:TYR:CE1	2.55	0.41
1:C:630:GLU:HA	1:C:1642:PRO:CB	2.51	0.41
1:C:955:LEU:HD13	1:C:959:TYR:CG	2.55	0.41
1:D:839:LEU:O	1:D:1200:GLY:N	2.46	0.41
1:D:1434:TYR:O	1:D:1435:TYR:C	2.63	0.41
1:D:2536:LEU:HA	1:D:2584:HIS:CE1	2.55	0.41
1:D:2547:ALA:O	1:D:2551:ASN:ND2	2.54	0.41
1:D:3606:LEU:HD12	1:D:3606:LEU:HA	1.93	0.41
1:A:293:LEU:HD22	1:A:378:LEU:HD13	2.02	0.41
1:A:927:GLU:O	1:A:931:THR:HG23	2.21	0.41
1:A:1207:ASP:O	1:A:1210:SER:N	2.52	0.41
1:A:2102:VAL:HG11	1:A:2124:LEU:HB2	2.03	0.41
1:A:2606:CYS:SG	1:A:2607:LEU:N	2.91	0.41
1:A:4182:GLU:OE2	1:A:4192:ARG:NH1	2.54	0.41
1:B:12:GLN:HB2	1:B:165:VAL:HG13	2.03	0.41
1:B:29:LEU:HD12	1:B:30:LYS:N	2.36	0.41
1:B:205:ILE:HG22	1:B:206:CYS:N	2.30	0.41
1:B:269:TRP:HZ2	1:B:334:MET:HE2	1.85	0.41
1:B:2191:PHE:HA	1:B:2198:MET:HE3	2.03	0.41
1:B:4859:PHE:HB3	1:B:4862:PHE:HD2	1.86	0.41
1:C:622:THR:O	1:C:627:PRO:HD3	2.21	0.41
1:C:1253:PRO:HB2	1:C:1254:HIS:CE1	2.55	0.41
1:C:1536:SER:OG	1:C:1537:ASN:N	2.53	0.41
1:C:5027:CYS:C	1:C:5029:ARG:H	2.27	0.41
1:D:959:TYR:HB3	1:D:967:PRO:HD2	2.03	0.41
1:D:1618:ARG:HG2	1:D:1627:ALA:HB3	2.02	0.41
1:D:2191:PHE:HA	1:D:2198:MET:HE3	2.03	0.41
1:D:2313:LEU:HB3	1:D:2318:TYR:HD2	1.84	0.41
1:D:2759:ALA:HB2	1:D:2806:ARG:HH22	1.85	0.41
1:D:3891:LEU:HG	1:D:3899:PHE:CE2	2.55	0.41
1:D:4859:PHE:HB3	1:D:4862:PHE:HD2	1.86	0.41
2:G:82:TYR:HB3	2:G:86:GLY:HA2	2.03	0.41
1:A:29:LEU:HD12	1:A:30:LYS:N	2.35	0.41
1:A:320:LYS:HB3	1:A:356:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:TYR:O	1:A:1435:TYR:C	2.64	0.41
1:A:2023:LEU:HG	1:A:2024:PRO:HD2	2.02	0.41
1:A:3263:TYR:O	1:A:3265:GLU:N	2.54	0.41
1:A:3272:ILE:HG13	1:A:3273:THR:HG22	2.03	0.41
1:A:4790:LEU:HD23	1:A:4790:LEU:HA	1.92	0.41
1:A:4801:LEU:HD12	1:A:4801:LEU:HA	1.94	0.41
1:B:707:VAL:HG12	1:B:782:SER:HB3	2.02	0.41
1:B:1434:TYR:HA	1:B:1519:LEU:HD23	2.01	0.41
1:B:3606:LEU:HD12	1:B:3606:LEU:HA	1.93	0.41
1:B:4184:MET:HB2	1:B:4190:ILE:HD13	2.02	0.41
1:C:393:CYS:HB2	1:C:397:GLU:HG3	2.03	0.41
1:C:772:ASN:ND2	1:C:1470:ARG:HA	2.35	0.41
1:C:784:SER:OG	1:C:785:ALA:N	2.53	0.41
1:C:1041:GLN:O	1:C:1044:ARG:HB2	2.21	0.41
1:C:1599:MET:HE3	1:C:1601:MET:HE2	2.03	0.41
1:C:1668:ARG:HE	1:C:1668:ARG:HB2	1.58	0.41
1:C:1847:THR:O	1:C:1851:MET:HG3	2.21	0.41
1:C:2368:LEU:HA	1:C:2374:SER:HB2	2.02	0.41
1:C:3592:ILE:HA	1:C:3595:ARG:NE	2.34	0.41
1:C:3989:VAL:HG21	1:C:4047:MET:HE2	2.03	0.41
1:D:866:HIS:HA	1:D:869:ARG:HD3	2.03	0.41
1:D:952:LYS:HG2	1:D:953:THR:H	1.85	0.41
1:D:2106:ALA:HB3	1:D:3696:ASP:OD1	2.21	0.41
1:D:2179:ILE:HD11	1:D:2228:MET:HG2	2.02	0.41
1:D:2789:PRO:O	1:D:2792:ARG:NH1	2.53	0.41
1:D:4897:ILE:HD12	1:D:4897:ILE:HA	1.92	0.41
2:E:26:TYR:CE1	2:E:39:SER:HB3	2.55	0.41
2:F:29:MET:HA	2:F:35:LYS:HA	2.02	0.41
1:A:206:CYS:SG	1:A:207:SER:N	2.94	0.41
1:A:1536:SER:OG	1:A:1537:ASN:N	2.53	0.41
1:A:4049:VAL:O	1:A:4052:SER:OG	2.34	0.41
1:B:375:LYS:HE3	1:B:375:LYS:HB2	1.81	0.41
1:B:674:PHE:N	1:B:680:THR:OG1	2.54	0.41
1:B:886:ARG:HB3	1:B:891:TRP:HD1	1.86	0.41
1:C:206:CYS:SG	1:C:207:SER:N	2.93	0.41
1:C:247:TYR:OH	1:C:388:LEU:HD11	2.20	0.41
1:C:860:GLN:HG2	1:C:860:GLN:O	2.21	0.41
1:C:1101:ARG:HB2	1:C:1193:SER:HB3	2.03	0.41
1:C:2283:ASN:C	1:C:2285:GLU:H	2.29	0.41
1:D:49:LEU:HD21	1:D:191:VAL:HG23	2.03	0.41
1:D:255:HIS:ND1	1:D:480:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:655:GLY:HA3	1:D:852:VAL:HG12	2.03	0.41
1:D:1277:TRP:O	1:D:1277:TRP:HD1	2.04	0.41
1:D:4577:LEU:HD23	1:D:4577:LEU:HA	1.95	0.41
1:D:4989:MET:HE3	1:D:4989:MET:HB3	1.95	0.41
1:A:273:HIS:HE1	1:A:334:MET:HG3	1.85	0.40
1:A:1477:GLY:HA2	1:A:1482:ASN:O	2.21	0.40
1:A:1847:THR:O	1:A:1851:MET:HG3	2.21	0.40
1:A:2098:VAL:CG1	1:A:2127:GLN:HG3	2.51	0.40
1:B:299:LEU:HD12	1:B:299:LEU:HA	1.81	0.40
1:B:650:VAL:HG12	1:B:777:PHE:HB2	2.03	0.40
1:B:1815:LEU:HD12	1:B:1815:LEU:HA	1.89	0.40
1:B:3424:LEU:HA	1:B:3424:LEU:HD23	1.87	0.40
1:C:171:LEU:HD11	1:C:202:MET:HE2	2.02	0.40
1:C:835:ARG:HH12	1:C:1212:ARG:HG3	1.87	0.40
1:C:952:LYS:HE2	1:C:952:LYS:HB3	1.97	0.40
1:C:1457:TYR:O	1:C:1458:HIS:ND1	2.54	0.40
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	2.04	0.40
1:C:3832:ILE:HD13	1:C:3832:ILE:HA	1.97	0.40
1:C:4859:PHE:HB3	1:C:4862:PHE:HD2	1.86	0.40
1:D:17:ASP:HB2	1:D:98:HIS:HE1	1.86	0.40
1:D:320:LYS:HB3	1:D:356:TRP:CD1	2.56	0.40
1:A:4859:PHE:HB3	1:A:4862:PHE:HD2	1.85	0.40
1:B:1640:HIS:HA	1:B:1647:CYS:HA	2.04	0.40
1:B:2905:LEU:H	1:B:2905:LEU:HD23	1.86	0.40
1:B:4763:GLY:N	1:B:4766:THR:OG1	2.40	0.40
1:C:262:LEU:HD13	1:C:274:LEU:HD22	2.04	0.40
1:C:901:LYS:HE3	1:C:903:LEU:HD12	2.03	0.40
1:C:954:LYS:HA	1:C:954:LYS:HD2	1.85	0.40
1:C:1434:TYR:HB2	1:C:1572:ILE:HG21	2.02	0.40
1:C:3507:THR:HB	1:C:3508:SER:H	1.74	0.40
1:D:3103:ILE:H	1:D:3103:ILE:HG12	1.76	0.40
1:D:4170:ILE:HD13	1:D:4170:ILE:HA	1.94	0.40
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.34	0.40
2:E:82:TYR:HB3	2:E:86:GLY:HA2	2.04	0.40
1:A:810:PRO:HD2	1:A:813:GLU:OE1	2.21	0.40
1:B:670:GLU:HA	1:B:740:PRO:HB3	2.02	0.40
1:B:1536:SER:OG	1:B:1537:ASN:N	2.53	0.40
1:B:2360:LYS:HE3	1:B:2360:LYS:HB2	1.93	0.40
1:C:650:VAL:HG12	1:C:777:PHE:HB2	2.04	0.40
1:C:1519:LEU:HD23	1:C:1519:LEU:HA	1.95	0.40
1:C:1534:LYS:HD2	1:C:1534:LYS:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2191:PHE:HA	1:C:2198:MET:HE3	2.03	0.40
1:D:830:ARG:CZ	1:D:1612:PHE:CE2	3.04	0.40
1:D:918:ARG:O	1:D:922:LEU:HG	2.22	0.40
1:A:214:VAL:HG11	1:A:339:ILE:HG13	2.04	0.40
1:A:961:MET:HE1	1:A:963:ASN:HB2	2.02	0.40
1:A:2359:ARG:HE	1:A:2359:ARG:HB2	1.77	0.40
1:A:2497:ASP:HA	1:A:2547:ALA:HB2	2.03	0.40
1:A:2547:ALA:O	1:A:2551:ASN:ND2	2.54	0.40
1:A:2905:LEU:H	1:A:2905:LEU:HD23	1.87	0.40
1:B:784:SER:OG	1:B:785:ALA:N	2.54	0.40
1:B:863:LEU:H	1:B:863:LEU:HD23	1.87	0.40
1:B:887:ILE:HG13	1:B:891:TRP:O	2.21	0.40
1:B:1152:MET:HE2	1:B:1152:MET:HB3	2.00	0.40
1:B:2102:VAL:HG11	1:B:2124:LEU:HB2	2.03	0.40
1:B:2309:SER:OG	1:B:2321:ILE:O	2.32	0.40
1:B:3090:ALA:O	1:B:3094:SER:N	2.46	0.40
1:B:3180:ASN:OD1	1:B:3180:ASN:N	2.54	0.40
1:C:1008:SER:HB2	1:C:1017:ARG:CZ	2.51	0.40
1:D:682:LEU:HD12	1:D:787:VAL:HG12	2.04	0.40
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.87	0.40
1:D:4771:ILE:HD13	1:D:4771:ILE:HA	1.90	0.40
2:F:44:LYS:HA	2:F:44:LYS:HD2	1.79	0.40
1:A:393:CYS:HB2	1:A:397:GLU:HG3	2.04	0.40
1:A:648:ILE:HG12	1:A:648:ILE:O	2.21	0.40
1:A:1093:GLU:HG2	1:A:1148:VAL:HG12	2.02	0.40
1:A:2368:LEU:HA	1:A:2374:SER:HB2	2.04	0.40
1:B:33:LEU:HG	1:B:53:SER:OG	2.20	0.40
1:B:1847:THR:O	1:B:1851:MET:HG3	2.22	0.40
1:B:1947:CYS:HB3	1:B:2126:ARG:HH21	1.86	0.40
1:B:2023:LEU:HG	1:B:2024:PRO:HD2	2.03	0.40
1:B:2212:VAL:HG22	1:B:2256:TYR:CZ	2.56	0.40
1:B:2228:MET:HE3	1:B:2228:MET:HB3	1.77	0.40
1:B:2440:MET:SD	1:B:2442:LEU:HB3	2.61	0.40
1:C:707:VAL:HG12	1:C:782:SER:HB3	2.03	0.40
1:C:1081:TYR:CD1	1:C:1230:MET:HE1	2.57	0.40
1:C:1180:ARG:NE	1:C:1180:ARG:HA	2.36	0.40
1:C:1477:GLY:HA2	1:C:1482:ASN:O	2.22	0.40
1:C:2420:HIS:ND1	1:C:2423:MET:HE2	2.37	0.40
1:C:3804:ILE:HD12	1:C:3804:ILE:HA	1.87	0.40
1:D:158:SER:N	1:D:161:GLU:OE1	2.54	0.40
1:D:359:TYR:HB2	1:D:383:HIS:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:972:LEU:HD22	1:D:1044:ARG:HB3	2.03	0.40
1:D:1562:ILE:HD13	1:D:1562:ILE:HA	1.94	0.40
1:D:4055:VAL:HG11	1:D:4163:PHE:HZ	1.87	0.40
2:F:26:TYR:CE1	2:F:39:SER:HB3	2.56	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	4214/5037 (84%)	3883 (92%)	329 (8%)	2 (0%)	100	100
1	B	4214/5037 (84%)	3873 (92%)	340 (8%)	1 (0%)	100	100
1	C	4214/5037 (84%)	3878 (92%)	334 (8%)	2 (0%)	100	100
1	D	4214/5037 (84%)	3886 (92%)	327 (8%)	1 (0%)	100	100
2	E	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
2	F	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	G	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	H	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
All	All	17276/20576 (84%)	15878 (92%)	1392 (8%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	862	VAL
1	C	899	ASP
1	A	1023	PRO
1	C	1023	PRO
1	D	1023	PRO
1	B	1023	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	3334/4276 (78%)	3333 (100%)	1 (0%)	100	100
1	B	3334/4276 (78%)	3328 (100%)	6 (0%)	87	87
1	C	3334/4276 (78%)	3329 (100%)	5 (0%)	88	89
1	D	3334/4276 (78%)	3330 (100%)	4 (0%)	88	89
2	E	80/88 (91%)	79 (99%)	1 (1%)	61	73
2	F	80/88 (91%)	80 (100%)	0	100	100
2	G	80/88 (91%)	79 (99%)	1 (1%)	61	73
2	H	80/88 (91%)	80 (100%)	0	100	100
All	All	13656/17456 (78%)	13638 (100%)	18 (0%)	87	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	919	ASN
1	B	919	ASN
1	B	983	THR
1	B	1435	TYR
1	B	1553	PHE
1	B	2559	LEU
1	B	4044	MET
1	C	503	PHE
1	C	919	ASN
1	C	2382	GLU
1	C	3444	TYR
1	C	4706	LEU
1	D	919	ASN
1	D	1435	TYR
1	D	2382	GLU
1	D	4552	LEU
2	E	61	GLU
2	G	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (170) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	181	HIS
1	A	772	ASN
1	A	1011	GLN
1	A	1130	GLN
1	A	1203	ASN
1	A	1254	HIS
1	A	1480	GLN
1	A	1505	GLN
1	A	1563	GLN
1	A	1631	GLN
1	A	1973	GLN
1	A	2005	GLN
1	A	2029	GLN
1	A	2112	GLN
1	A	2125	HIS
1	A	2176	ASN
1	A	2188	ASN
1	A	2246	ASN
1	A	2247	GLN
1	A	2291	GLN
1	A	2599	GLN
1	A	2663	ASN
1	A	2788	HIS
1	A	3007	ASN
1	A	3013	HIS
1	A	3109	ASN
1	A	3572	GLN
1	A	3771	HIS
1	A	3809	ASN
1	A	3837	GLN
1	A	3850	GLN
1	A	3882	GLN
1	A	3977	GLN
1	A	4034	ASN
1	A	4162	ASN
1	A	4201	ASN
1	A	4650	HIS
1	A	4700	GLN
1	A	4707	ASN
1	B	181	HIS

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Mol	Chain	Res	Type
1	B	394	GLN
1	B	399	GLN
1	B	617	ASN
1	B	772	ASN
1	B	938	HIS
1	B	1052	ASN
1	B	1130	GLN
1	B	1133	HIS
1	B	1203	ASN
1	B	1254	HIS
1	B	1480	GLN
1	B	1563	GLN
1	B	1631	GLN
1	B	1973	GLN
1	B	2005	GLN
1	B	2029	GLN
1	B	2112	GLN
1	B	2125	HIS
1	B	2176	ASN
1	B	2188	ASN
1	B	2246	ASN
1	B	2247	GLN
1	B	2291	GLN
1	B	2420	HIS
1	B	2663	ASN
1	B	2772	GLN
1	B	2788	HIS
1	B	2962	GLN
1	B	3109	ASN
1	B	3268	HIS
1	B	3572	GLN
1	B	3771	HIS
1	B	3809	ASN
1	B	3837	GLN
1	B	3850	GLN
1	B	3882	GLN
1	B	4034	ASN
1	B	4162	ASN
1	B	4650	HIS
1	B	4700	GLN
1	B	4707	ASN
1	B	4714	ASN

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Mol	Chain	Res	Type
1	B	4754	ASN
1	B	4983	HIS
1	C	12	GLN
1	C	23	GLN
1	C	617	ASN
1	C	681	HIS
1	C	772	ASN
1	C	921	ASN
1	C	938	HIS
1	C	1041	GLN
1	C	1130	GLN
1	C	1203	ASN
1	C	1254	HIS
1	C	1480	GLN
1	C	1505	GLN
1	C	1545	ASN
1	C	1590	GLN
1	C	1631	GLN
1	C	1973	GLN
1	C	2005	GLN
1	C	2029	GLN
1	C	2112	GLN
1	C	2125	HIS
1	C	2176	ASN
1	C	2188	ASN
1	C	2246	ASN
1	C	2247	GLN
1	C	2260	ASN
1	C	2599	GLN
1	C	2663	ASN
1	C	2788	HIS
1	C	3013	HIS
1	C	3109	ASN
1	C	3572	GLN
1	C	3771	HIS
1	C	3837	GLN
1	C	3850	GLN
1	C	3882	GLN
1	C	3977	GLN
1	C	4162	ASN
1	C	4201	ASN
1	C	4626	ASN

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Mol	Chain	Res	Type
1	C	4650	HIS
1	C	4707	ASN
1	C	4714	ASN
1	D	23	GLN
1	D	394	GLN
1	D	617	ASN
1	D	772	ASN
1	D	838	HIS
1	D	1130	GLN
1	D	1203	ASN
1	D	1254	HIS
1	D	1480	GLN
1	D	1505	GLN
1	D	1631	GLN
1	D	1973	GLN
1	D	2005	GLN
1	D	2029	GLN
1	D	2112	GLN
1	D	2125	HIS
1	D	2176	ASN
1	D	2188	ASN
1	D	2246	ASN
1	D	2247	GLN
1	D	2599	GLN
1	D	2663	ASN
1	D	2788	HIS
1	D	3007	ASN
1	D	3013	HIS
1	D	3109	ASN
1	D	3572	GLN
1	D	3809	ASN
1	D	3837	GLN
1	D	3850	GLN
1	D	3882	GLN
1	D	4162	ASN
1	D	4626	ASN
1	D	4650	HIS
1	D	4700	GLN
1	D	4707	ASN
2	E	94	ASN
2	F	32	ASN
2	F	94	ASN

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Mol	Chain	Res	Type
2	G	32	ASN
2	G	94	ASN
2	H	94	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	C	5102	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	D	5102	-	32,33,33	0.26	0	48,52,52	0.27	0
5	U1C	B	5103	-	25,25,25	6.18	16 (64%)	33,35,35	3.39	15 (45%)
5	U1C	D	5103	-	25,25,25	6.18	16 (64%)	33,35,35	3.38	15 (45%)
5	U1C	C	5103	-	25,25,25	6.19	16 (64%)	33,35,35	3.38	15 (45%)
4	ATP	B	5102	-	32,33,33	0.27	0	48,52,52	0.27	0
4	ATP	A	5102	-	32,33,33	0.26	0	48,52,52	0.27	0
5	U1C	A	5103	-	25,25,25	6.19	16 (64%)	33,35,35	3.39	15 (45%)

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
4	ATP	C	5102	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5102	-	-	9/22/38/38	0/3/3/3
5	U1C	B	5103	-	-	7/11/25/25	0/3/3/3
5	U1C	D	5103	-	-	7/11/25/25	0/3/3/3
5	U1C	C	5103	-	-	7/11/25/25	0/3/3/3
4	ATP	B	5102	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5102	-	-	9/22/38/38	0/3/3/3
5	U1C	A	5103	-	-	7/11/25/25	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	U1C	C1-N2	-18.77	1.32	1.45
5	A	5103	U1C	C1-N2	-18.76	1.32	1.45
5	D	5103	U1C	C1-N2	-18.64	1.32	1.45
5	B	5103	U1C	C1-N2	-18.59	1.32	1.45
5	B	5103	U1C	C1-C2	-10.54	1.39	1.51
5	D	5103	U1C	C1-C2	-10.54	1.39	1.51
5	C	5103	U1C	C1-C2	-10.51	1.39	1.51
5	A	5103	U1C	C1-C2	-10.49	1.39	1.51
5	B	5103	U1C	O4-N4	10.46	1.40	1.22
5	A	5103	U1C	O4-N4	10.42	1.40	1.22
5	C	5103	U1C	O4-N4	10.41	1.40	1.22
5	D	5103	U1C	O4-N4	10.41	1.40	1.22
5	A	5103	U1C	O2-C3	9.84	1.40	1.23
5	B	5103	U1C	O2-C3	9.81	1.40	1.23
5	C	5103	U1C	O2-C3	9.81	1.40	1.23
5	D	5103	U1C	O2-C3	9.80	1.40	1.23
5	A	5103	U1C	O1-C2	8.68	1.40	1.23
5	B	5103	U1C	O1-C2	8.67	1.40	1.23
5	D	5103	U1C	O1-C2	8.67	1.40	1.23
5	C	5103	U1C	O1-C2	8.61	1.40	1.23
5	B	5103	U1C	C4-N3	8.25	1.45	1.28
5	C	5103	U1C	C4-N3	8.25	1.45	1.28
5	D	5103	U1C	C4-N3	8.25	1.45	1.28
5	A	5103	U1C	C4-N3	8.25	1.45	1.28
5	B	5103	U1C	C4-C5	5.61	1.53	1.44
5	A	5103	U1C	C4-C5	5.60	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5103	U1C	C4-C5	5.56	1.53	1.44
5	C	5103	U1C	C4-C5	5.52	1.53	1.44
5	D	5103	U1C	C3-N2	-5.27	1.32	1.37
5	B	5103	U1C	C3-N2	-5.24	1.32	1.37
5	C	5103	U1C	C3-N2	-5.23	1.32	1.37
5	A	5103	U1C	C3-N2	-5.22	1.32	1.37
5	B	5103	U1C	O3-C5	-4.39	1.30	1.38
5	D	5103	U1C	O3-C5	-4.39	1.30	1.38
5	C	5103	U1C	O3-C5	-4.35	1.30	1.38
5	A	5103	U1C	O3-C5	-4.32	1.30	1.38
5	C	5103	U1C	O3-C8	-4.31	1.30	1.38
5	B	5103	U1C	O3-C8	-4.28	1.30	1.38
5	D	5103	U1C	O3-C8	-4.28	1.30	1.38
5	A	5103	U1C	O3-C8	-4.28	1.30	1.38
5	D	5103	U1C	N2-N3	3.86	1.41	1.37
5	C	5103	U1C	N2-N3	3.81	1.41	1.37
5	A	5103	U1C	N2-N3	3.79	1.41	1.37
5	B	5103	U1C	N2-N3	3.77	1.41	1.37
5	A	5103	U1C	C3-N1	-3.29	1.32	1.38
5	C	5103	U1C	C3-N1	-3.25	1.32	1.38
5	B	5103	U1C	C3-N1	-3.22	1.32	1.38
5	D	5103	U1C	C3-N1	-3.22	1.32	1.38
5	A	5103	U1C	C2-N1	-2.94	1.32	1.37
5	B	5103	U1C	C2-N1	-2.90	1.32	1.37
5	D	5103	U1C	C2-N1	-2.90	1.32	1.37
5	C	5103	U1C	C2-N1	-2.85	1.32	1.37
5	D	5103	U1C	C7-C8	2.62	1.40	1.35
5	A	5103	U1C	C7-C8	2.61	1.40	1.35
5	B	5103	U1C	C7-C8	2.60	1.40	1.35
5	C	5103	U1C	C7-C8	2.58	1.40	1.35
5	A	5103	U1C	C9-C8	2.33	1.53	1.48
5	C	5103	U1C	C9-C8	2.32	1.53	1.48
5	B	5103	U1C	C9-C8	2.30	1.53	1.48
5	D	5103	U1C	C9-C8	2.29	1.53	1.48
5	C	5103	U1C	C6-C5	2.08	1.40	1.35
5	B	5103	U1C	C6-C5	2.07	1.40	1.35
5	A	5103	U1C	C6-C5	2.05	1.40	1.35
5	D	5103	U1C	C6-C5	2.04	1.40	1.35

All (60) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	U1C	C2-C1-N2	8.41	106.93	101.45
5	B	5103	U1C	C2-C1-N2	8.40	106.92	101.45
5	A	5103	U1C	C2-C1-N2	8.38	106.91	101.45
5	D	5103	U1C	C2-C1-N2	8.37	106.90	101.45
5	B	5103	U1C	O3-C8-C9	7.50	125.61	116.73
5	D	5103	U1C	O3-C8-C9	7.47	125.58	116.73
5	C	5103	U1C	O3-C8-C9	7.46	125.57	116.73
5	A	5103	U1C	O3-C8-C9	7.40	125.49	116.73
5	B	5103	U1C	C1-N2-C3	-7.36	108.27	112.31
5	A	5103	U1C	C1-N2-C3	-7.32	108.29	112.31
5	D	5103	U1C	C1-N2-C3	-7.29	108.31	112.31
5	A	5103	U1C	C3-N2-N3	7.24	125.89	119.83
5	C	5103	U1C	C1-N2-C3	-7.24	108.33	112.31
5	B	5103	U1C	C3-N2-N3	7.17	125.83	119.83
5	D	5103	U1C	C3-N2-N3	7.15	125.80	119.83
5	C	5103	U1C	C3-N2-N3	7.13	125.79	119.83
5	B	5103	U1C	C2-N1-C3	-4.84	108.22	112.47
5	D	5103	U1C	C2-N1-C3	-4.84	108.22	112.47
5	C	5103	U1C	C2-N1-C3	-4.81	108.25	112.47
5	A	5103	U1C	C5-C4-N3	-4.76	110.43	120.22
5	A	5103	U1C	C2-N1-C3	-4.75	108.30	112.47
5	C	5103	U1C	C5-C4-N3	-4.72	110.52	120.22
5	D	5103	U1C	C5-C4-N3	-4.71	110.52	120.22
5	B	5103	U1C	C5-C4-N3	-4.71	110.52	120.22
5	C	5103	U1C	O3-C5-C4	4.22	125.67	117.55
5	A	5103	U1C	O3-C5-C4	4.22	125.66	117.55
5	D	5103	U1C	O3-C5-C4	4.20	125.63	117.55
5	B	5103	U1C	O3-C5-C4	4.19	125.62	117.55
5	C	5103	U1C	C8-O3-C5	3.96	112.23	107.04
5	B	5103	U1C	C8-O3-C5	3.94	112.20	107.04
5	D	5103	U1C	C8-O3-C5	3.94	112.20	107.04
5	A	5103	U1C	C8-O3-C5	3.90	112.16	107.04
5	B	5103	U1C	N1-C3-N2	3.65	109.63	106.12
5	D	5103	U1C	N1-C3-N2	3.63	109.61	106.12
5	A	5103	U1C	N1-C3-N2	3.62	109.59	106.12
5	C	5103	U1C	N1-C3-N2	3.61	109.58	106.12
5	A	5103	U1C	C6-C7-C8	-3.21	104.97	107.04
5	D	5103	U1C	C6-C7-C8	-3.17	105.00	107.04
5	C	5103	U1C	C6-C7-C8	-3.13	105.02	107.04
5	A	5103	U1C	C4-N3-N2	3.12	119.84	116.60
5	D	5103	U1C	C4-N3-N2	3.11	119.84	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	U1C	C4-N3-N2	3.11	119.84	116.60
5	B	5103	U1C	C4-N3-N2	3.11	119.83	116.60
5	B	5103	U1C	C6-C7-C8	-3.05	105.07	107.04
5	A	5103	U1C	O2-C3-N2	-2.69	125.13	127.67
5	B	5103	U1C	O2-C3-N2	-2.64	125.18	127.67
5	C	5103	U1C	O2-C3-N2	-2.60	125.22	127.67
5	D	5103	U1C	O2-C3-N2	-2.60	125.22	127.67
5	C	5103	U1C	C9-C8-C7	-2.58	125.57	132.99
5	D	5103	U1C	C9-C8-C7	-2.57	125.57	132.99
5	B	5103	U1C	C9-C8-C7	-2.57	125.58	132.99
5	A	5103	U1C	C9-C8-C7	-2.57	125.59	132.99
5	A	5103	U1C	C1-N2-N3	-2.54	125.82	127.64
5	A	5103	U1C	C6-C5-C4	-2.51	125.63	131.75
5	D	5103	U1C	C6-C5-C4	-2.50	125.65	131.75
5	B	5103	U1C	C6-C5-C4	-2.49	125.68	131.75
5	C	5103	U1C	C6-C5-C4	-2.48	125.71	131.75
5	C	5103	U1C	C1-N2-N3	-2.46	125.88	127.64
5	D	5103	U1C	C1-N2-N3	-2.45	125.89	127.64
5	B	5103	U1C	C1-N2-N3	-2.43	125.90	127.64

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5102	ATP	C5'-O5'-PA-O1A
4	A	5102	ATP	C5'-O5'-PA-O2A
4	A	5102	ATP	C5'-O5'-PA-O3A
4	A	5102	ATP	O4'-C4'-C5'-O5'
4	B	5102	ATP	C5'-O5'-PA-O1A
4	B	5102	ATP	C5'-O5'-PA-O2A
4	B	5102	ATP	C5'-O5'-PA-O3A
4	B	5102	ATP	O4'-C4'-C5'-O5'
4	C	5102	ATP	C5'-O5'-PA-O1A
4	C	5102	ATP	C5'-O5'-PA-O2A
4	C	5102	ATP	C5'-O5'-PA-O3A
4	C	5102	ATP	O4'-C4'-C5'-O5'
4	D	5102	ATP	C5'-O5'-PA-O1A
4	D	5102	ATP	C5'-O5'-PA-O2A
4	D	5102	ATP	C5'-O5'-PA-O3A
4	D	5102	ATP	O4'-C4'-C5'-O5'
5	A	5103	U1C	C5-C4-N3-N2
5	B	5103	U1C	C5-C4-N3-N2

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Mol	Chain	Res	Type	Atoms
5	C	5103	U1C	C5-C4-N3-N2
5	D	5103	U1C	C5-C4-N3-N2
5	A	5103	U1C	C7-C8-C9-C10
5	A	5103	U1C	C7-C8-C9-C14
5	B	5103	U1C	N3-C4-C5-O3
5	C	5103	U1C	N3-C4-C5-O3
5	D	5103	U1C	N3-C4-C5-O3
5	A	5103	U1C	O3-C8-C9-C10
5	A	5103	U1C	O3-C8-C9-C14
4	A	5102	ATP	C3'-C4'-C5'-O5'
4	B	5102	ATP	C3'-C4'-C5'-O5'
4	C	5102	ATP	C3'-C4'-C5'-O5'
4	D	5102	ATP	C3'-C4'-C5'-O5'
5	B	5103	U1C	O3-C8-C9-C10
5	B	5103	U1C	O3-C8-C9-C14
5	C	5103	U1C	O3-C8-C9-C10
5	C	5103	U1C	O3-C8-C9-C14
5	D	5103	U1C	O3-C8-C9-C10
5	D	5103	U1C	O3-C8-C9-C14
5	A	5103	U1C	N3-C4-C5-O3
5	C	5103	U1C	C7-C8-C9-C14
5	B	5103	U1C	C7-C8-C9-C14
5	D	5103	U1C	C7-C8-C9-C14
5	B	5103	U1C	C7-C8-C9-C10
5	C	5103	U1C	C7-C8-C9-C10
5	D	5103	U1C	C7-C8-C9-C10
5	A	5103	U1C	N3-C4-C5-C6
5	B	5103	U1C	N3-C4-C5-C6
5	C	5103	U1C	N3-C4-C5-C6
5	D	5103	U1C	N3-C4-C5-C6
4	A	5102	ATP	PB-O3A-PA-O2A
4	B	5102	ATP	PB-O3A-PA-O2A
4	C	5102	ATP	PB-O3A-PA-O2A
4	D	5102	ATP	PB-O3A-PA-O2A
4	A	5102	ATP	C4'-C5'-O5'-PA
4	B	5102	ATP	C4'-C5'-O5'-PA
4	C	5102	ATP	C4'-C5'-O5'-PA
4	D	5102	ATP	C4'-C5'-O5'-PA
4	A	5102	ATP	PG-O3B-PB-O2B
4	B	5102	ATP	PG-O3B-PB-O2B
4	C	5102	ATP	PG-O3B-PB-O2B
4	D	5102	ATP	PG-O3B-PB-O2B

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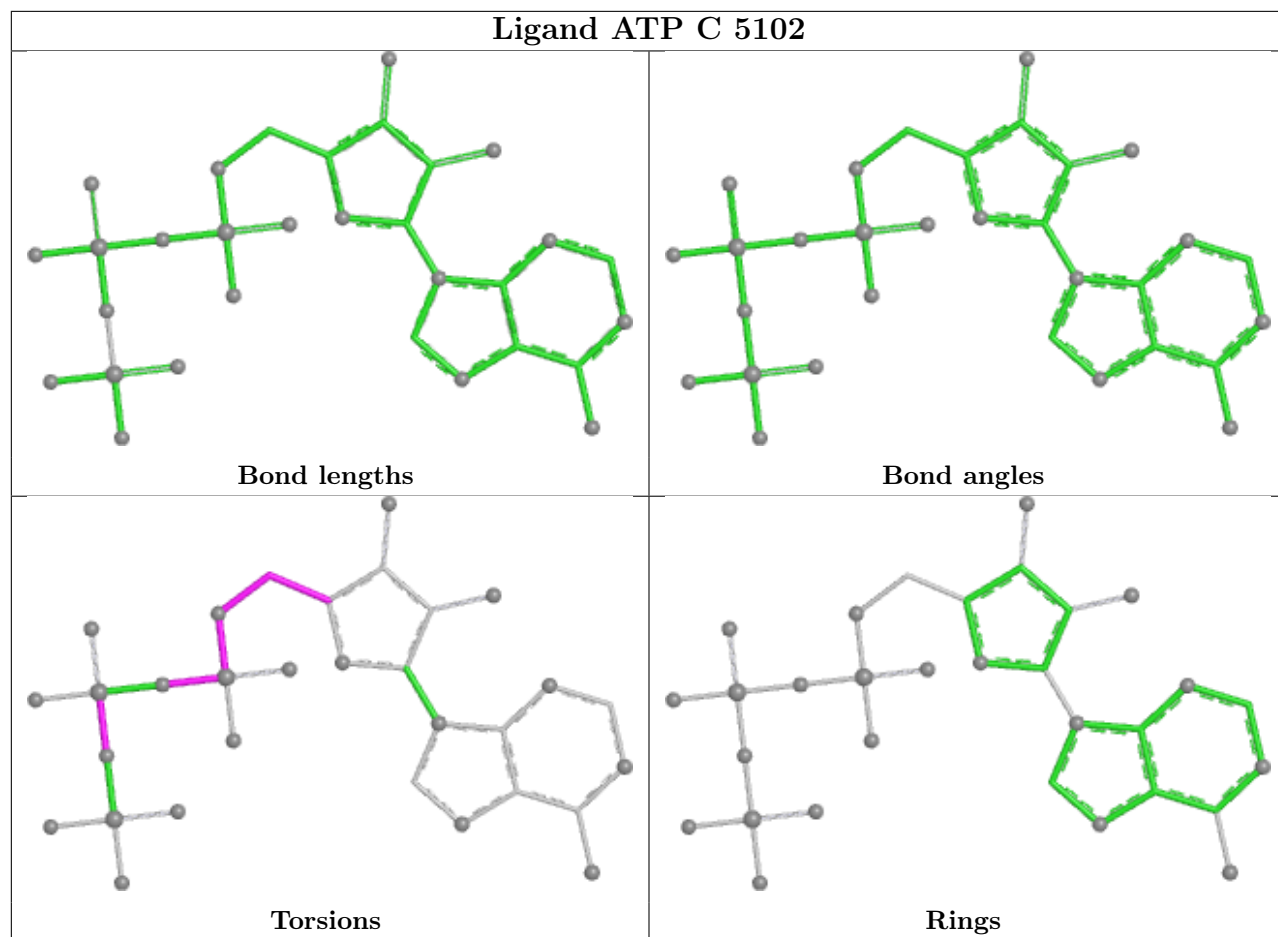
Continued from previous page...

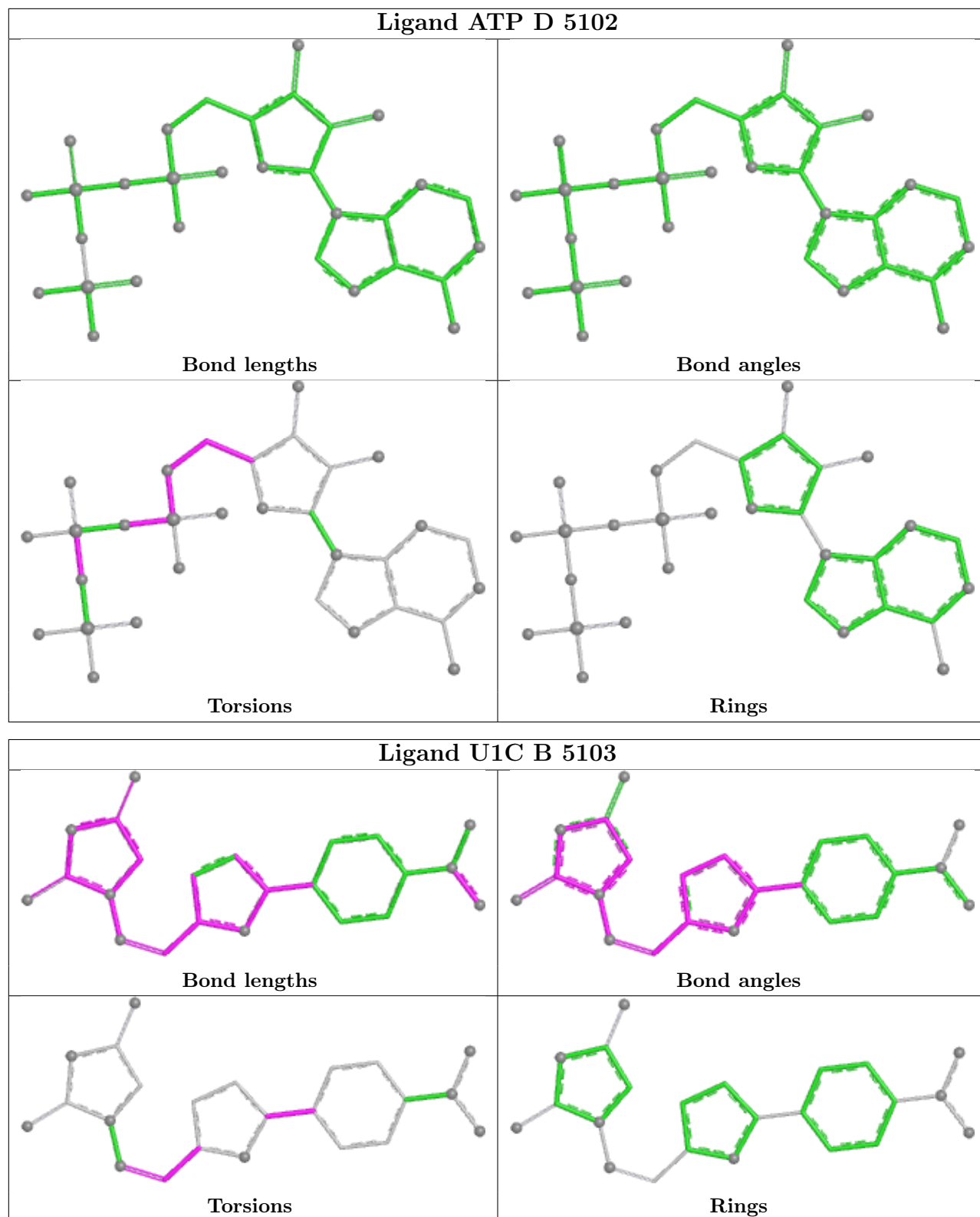
Mol	Chain	Res	Type	Atoms
4	A	5102	ATP	PB-O3A-PA-O1A
4	B	5102	ATP	PB-O3A-PA-O1A
4	C	5102	ATP	PB-O3A-PA-O1A
4	D	5102	ATP	PB-O3A-PA-O1A

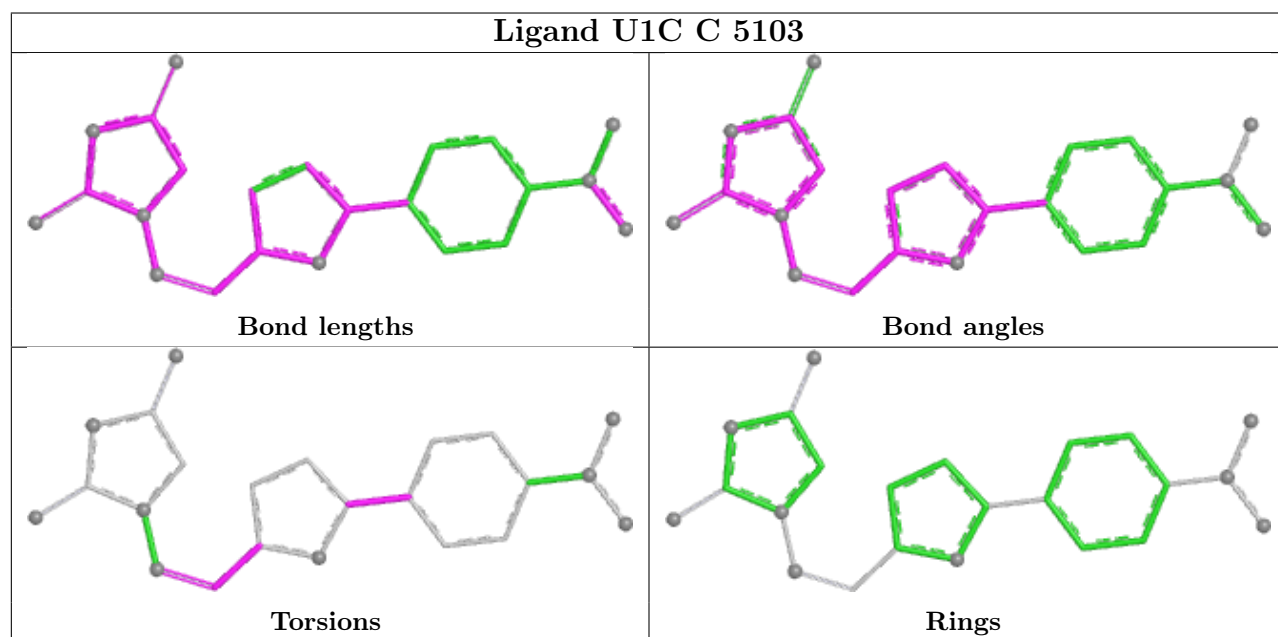
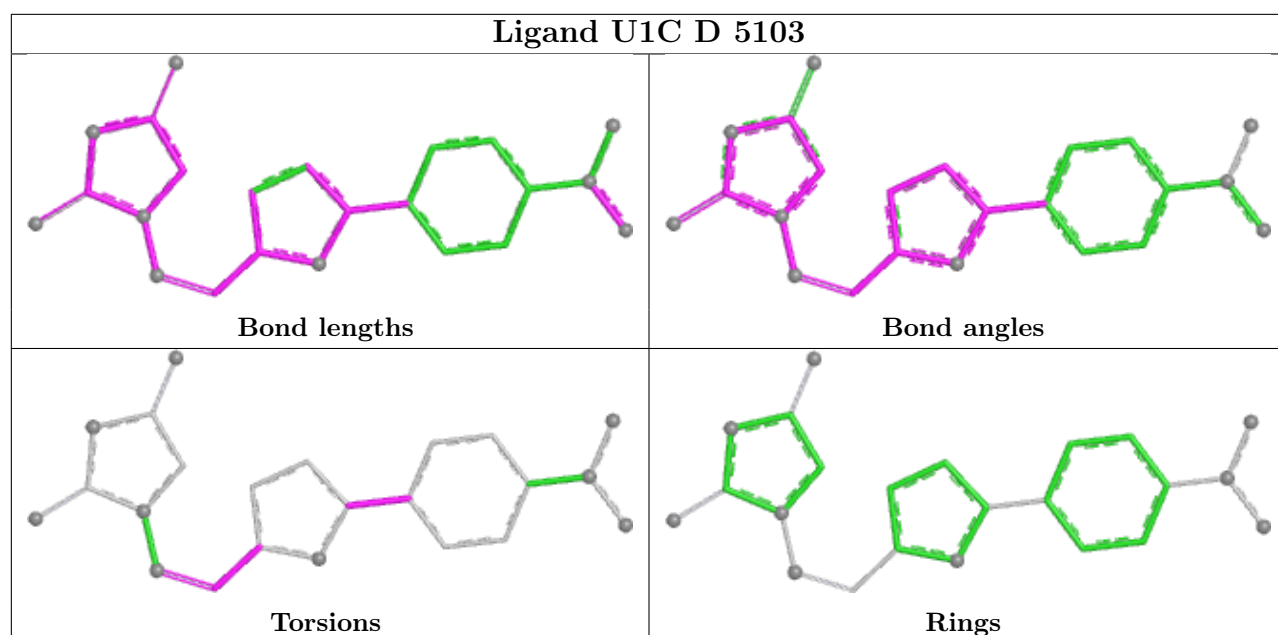
There are no ring outliers.

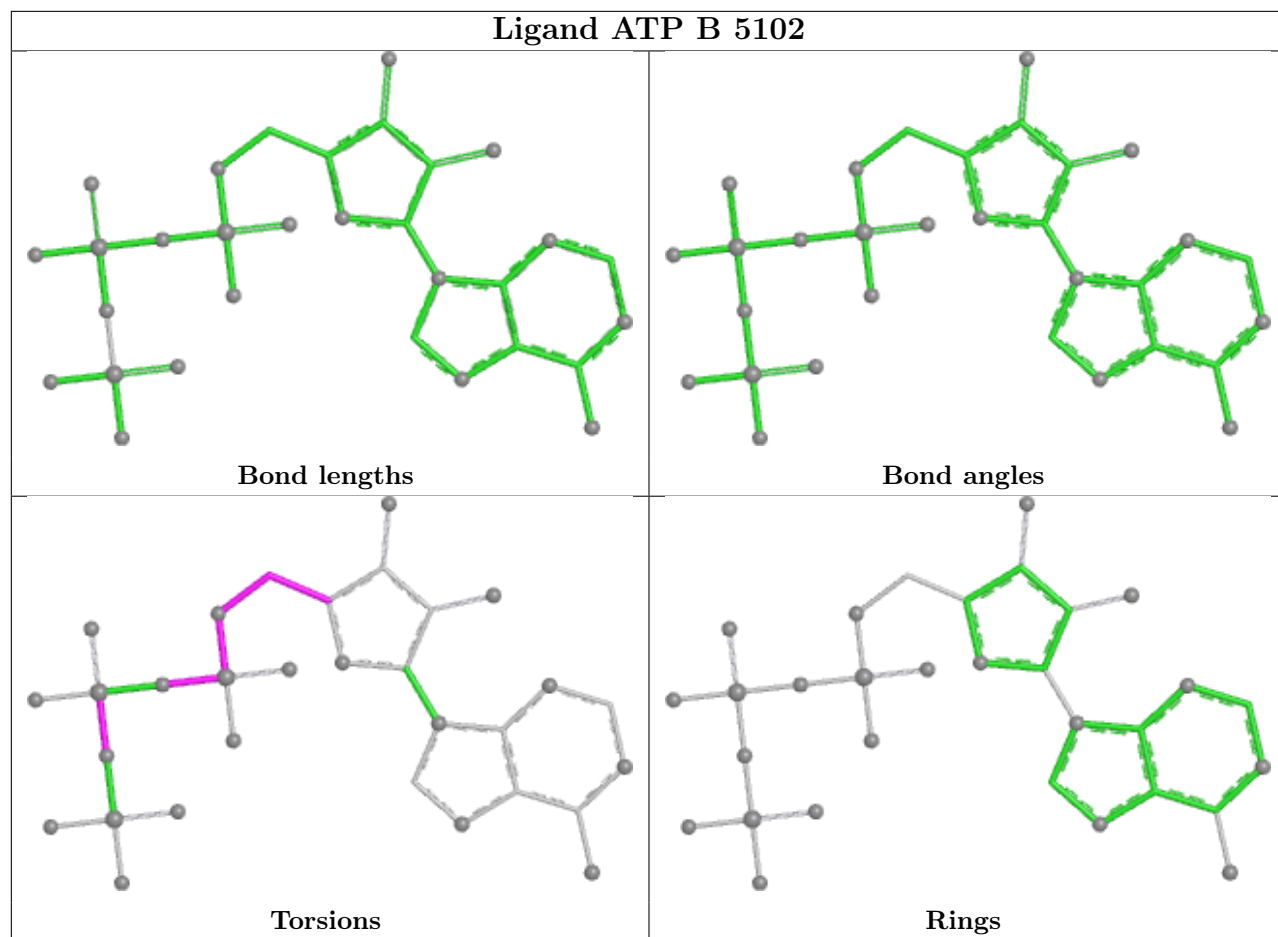
No monomer is involved in short contacts.

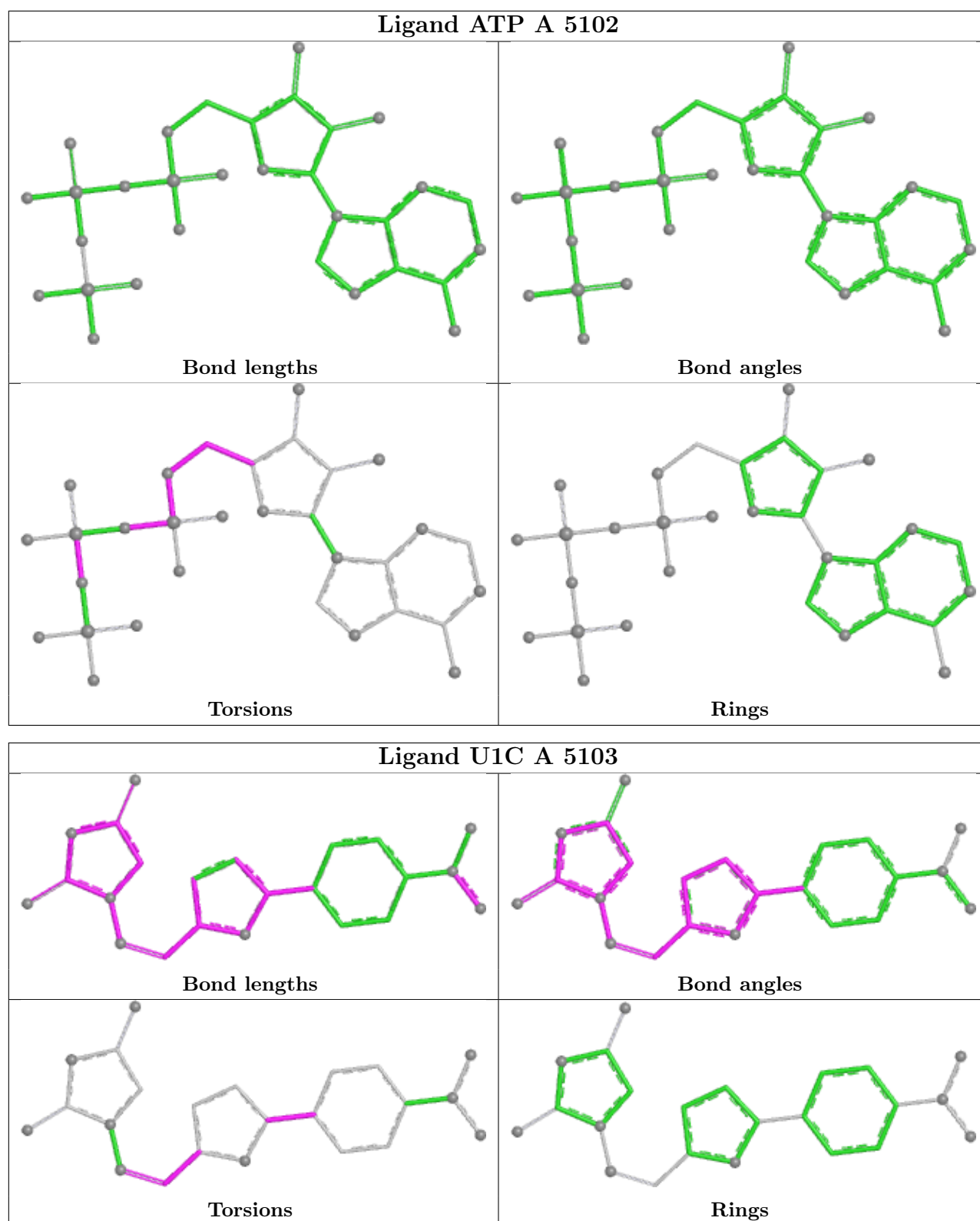
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no chain breaks in this entry.

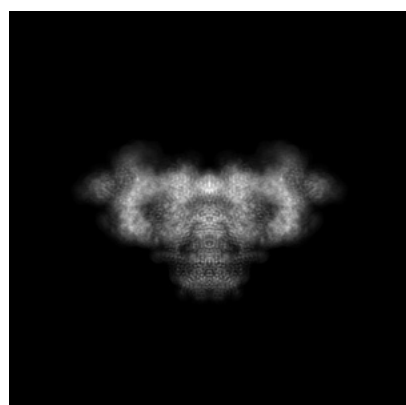
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45584. These allow visual inspection of the internal detail of the map and identification of artifacts.

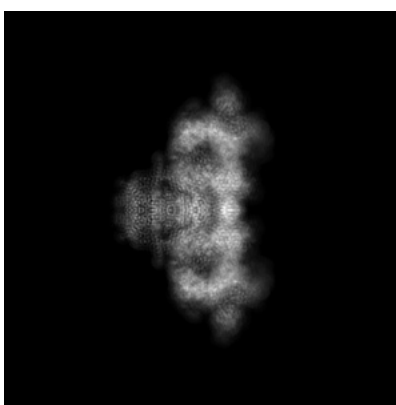
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

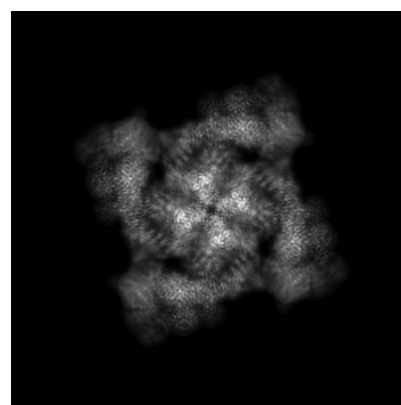
6.1.1 Primary map



X



Y

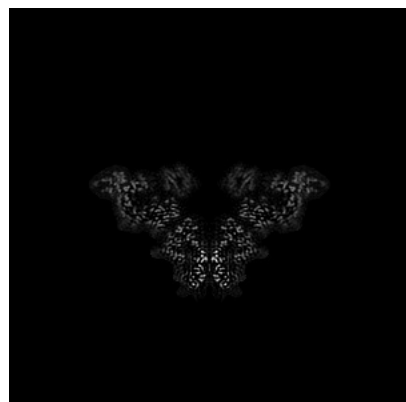


Z

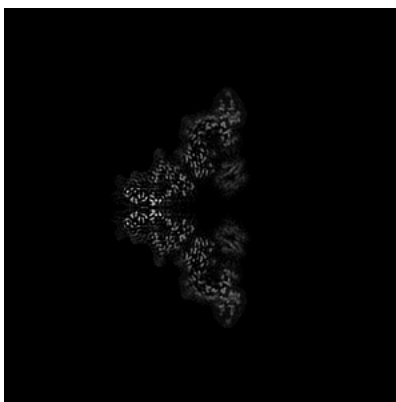
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

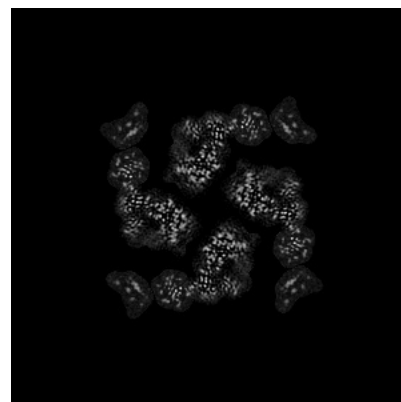
6.2.1 Primary map



X Index: 232



Y Index: 232

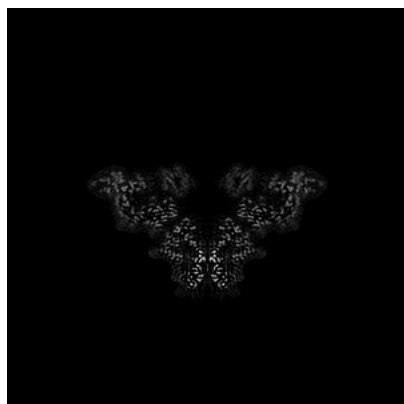


Z Index: 232

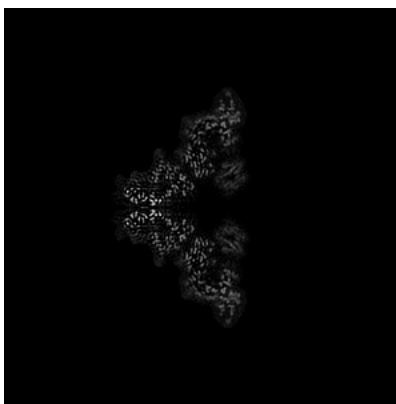
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

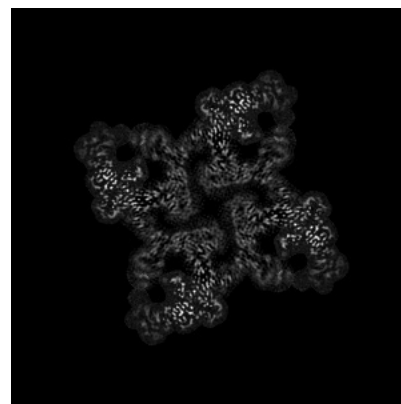
6.3.1 Primary map



X Index: 232



Y Index: 232

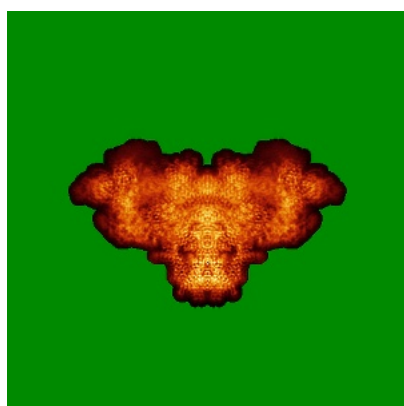


Z Index: 261

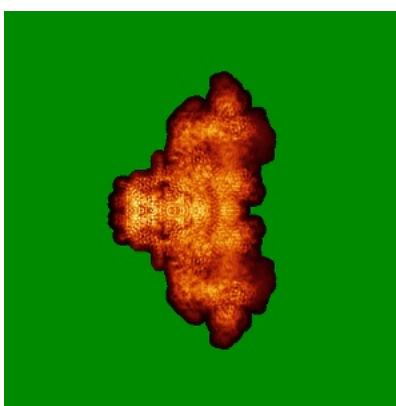
The images above show the largest variance slices of the map in three orthogonal directions.

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

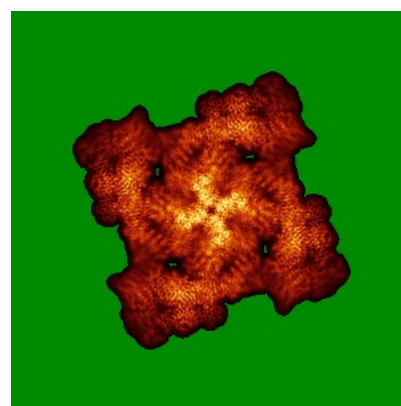
6.4.1 Primary map



X



Y

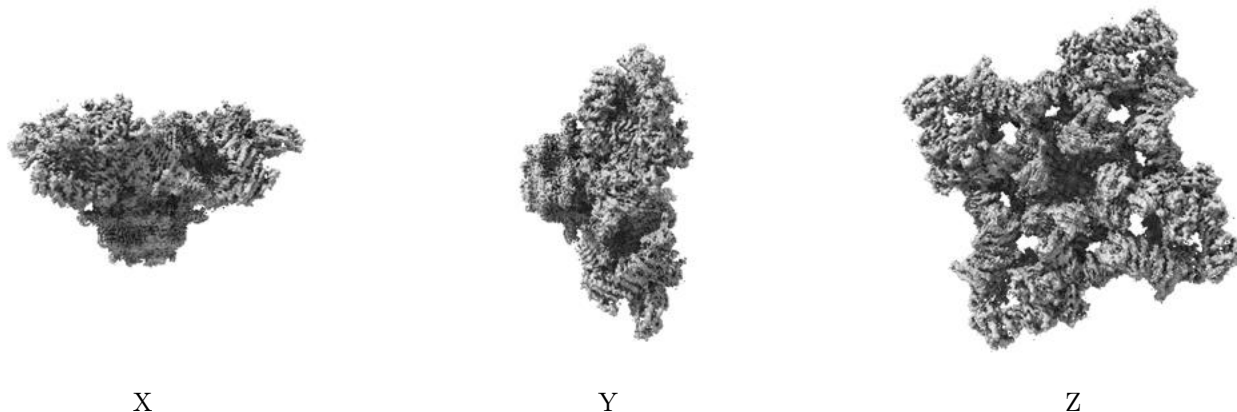


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

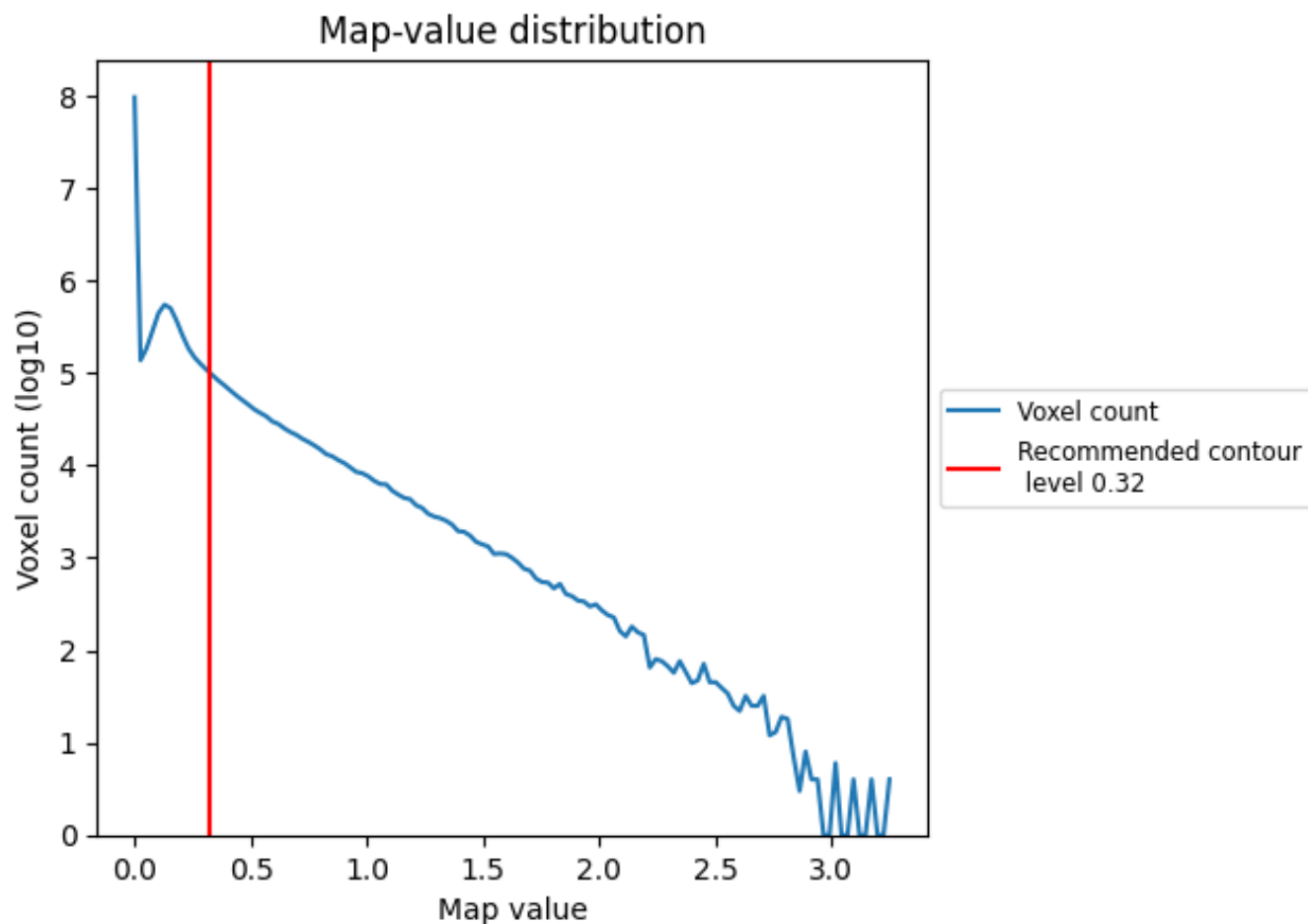
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

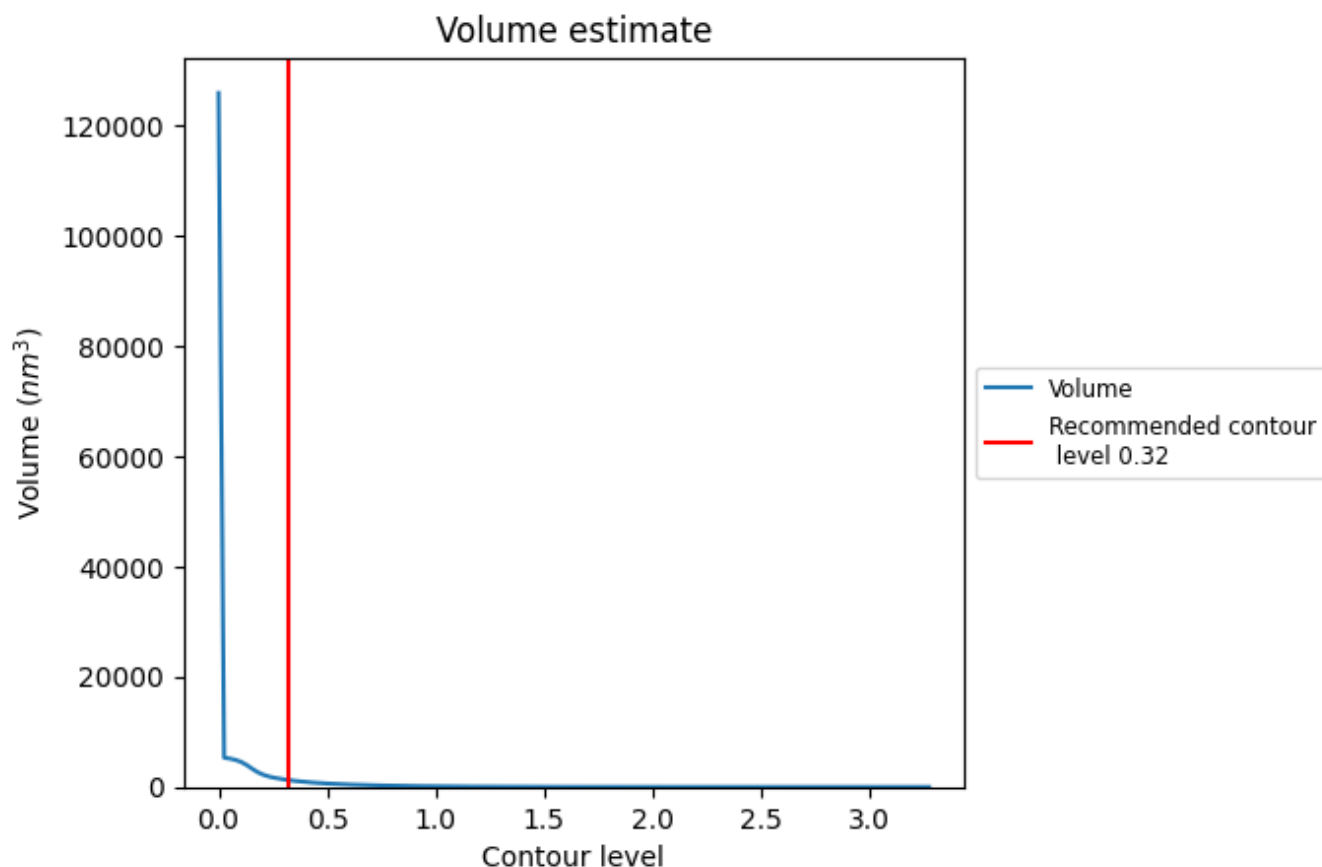
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

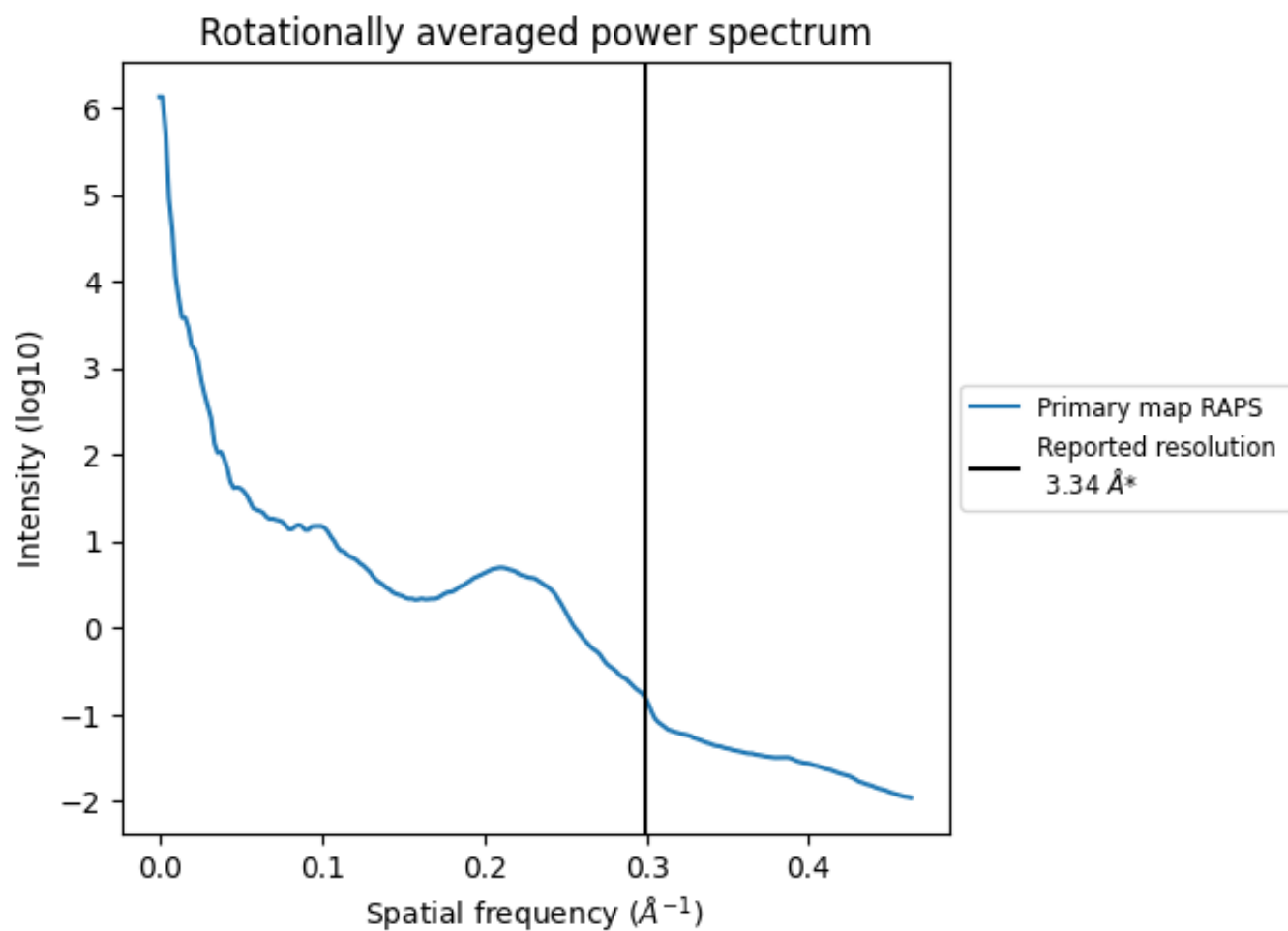
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1262 nm³; this corresponds to an approximate mass of 1140 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 0.299 $\text{\AA}^{-1}$

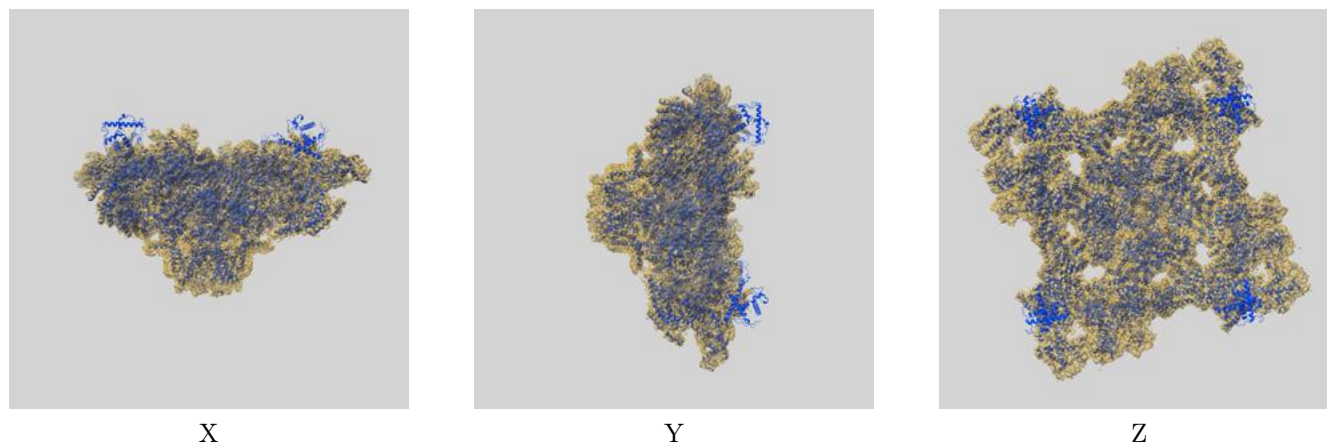
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

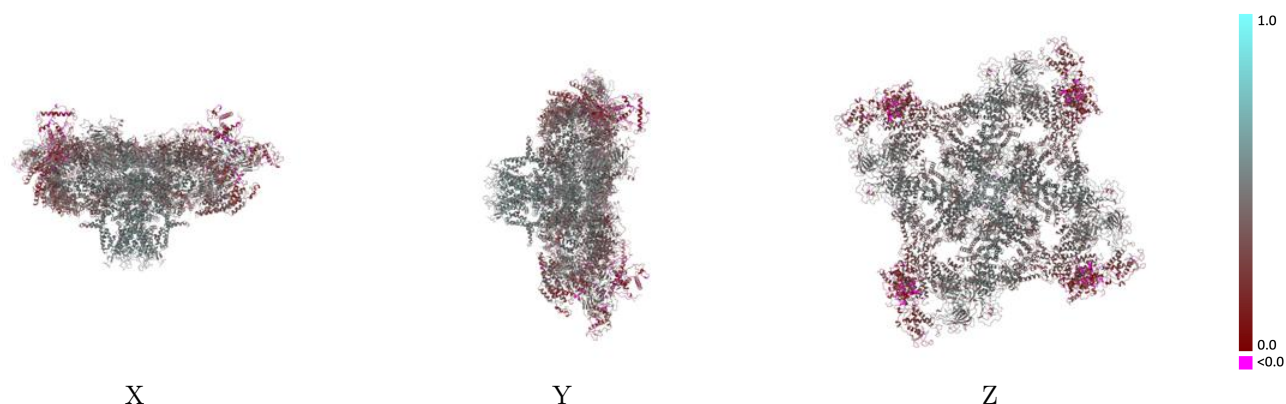
This section contains information regarding the fit between EMDB map EMD-45584 and PDB model 9CGP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



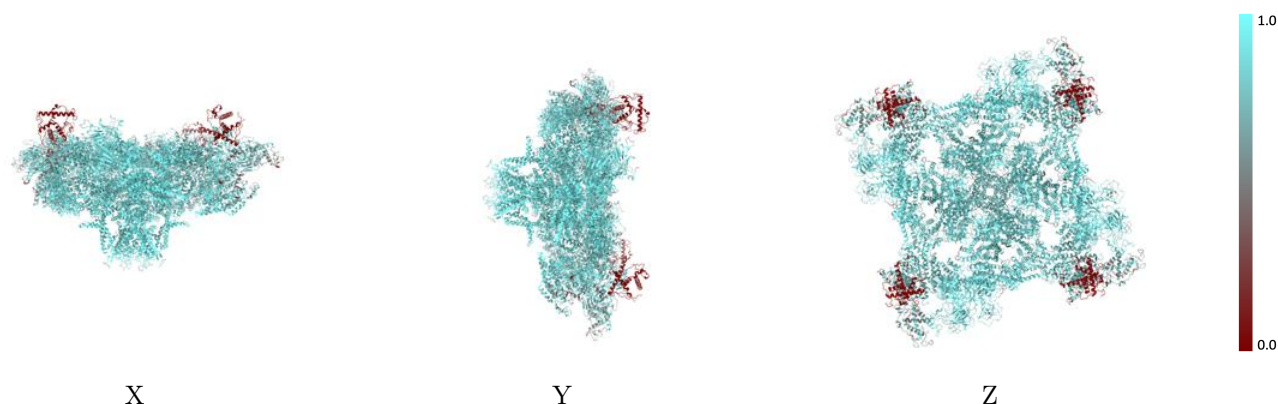
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



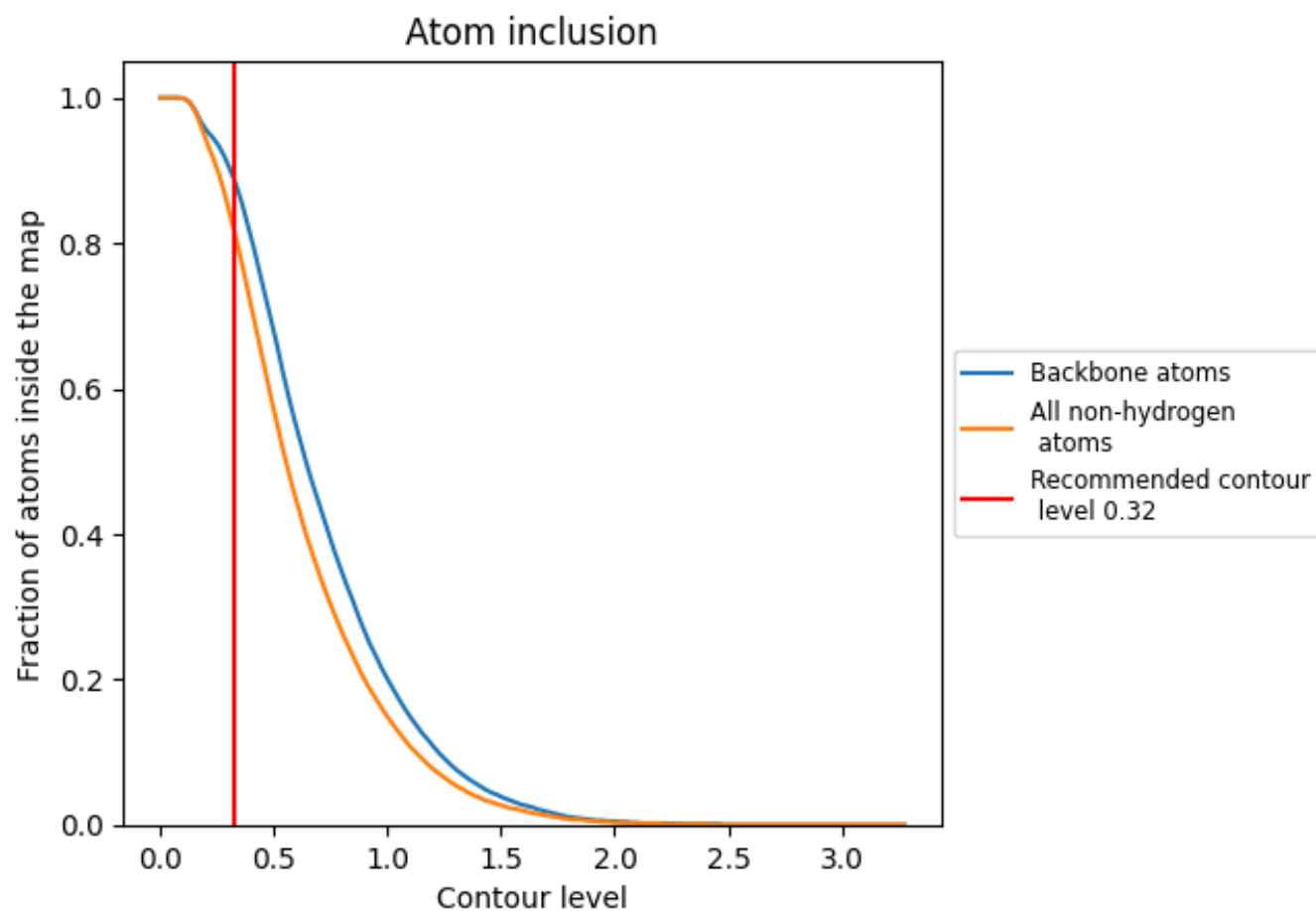
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.4080
A	0.8210	0.4070
B	0.8220	0.4080
C	0.8210	0.4070
D	0.8230	0.4080
E	0.8530	0.4190
F	0.8480	0.4210
G	0.8490	0.4200
H	0.8490	0.4230

