



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:14 PM UTC

PDB ID : 5T9V / pdb_00005t9v
EMDB ID : EMD-8376
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

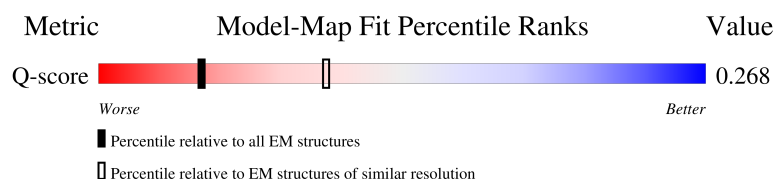
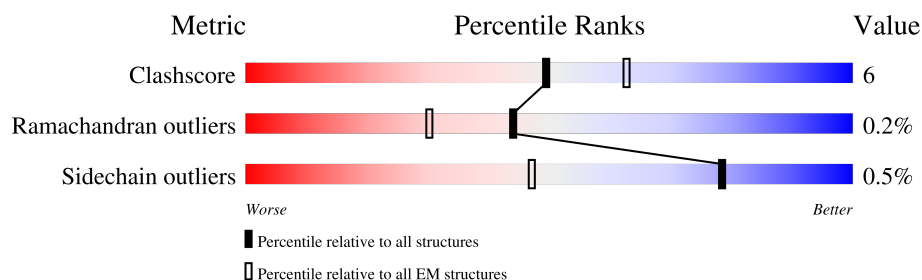
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	108	77% 80%19%.
1	F	108	77% 80%19%.
1	H	108	75% 80%19%.
1	J	108	75% 79%20%.

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

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

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

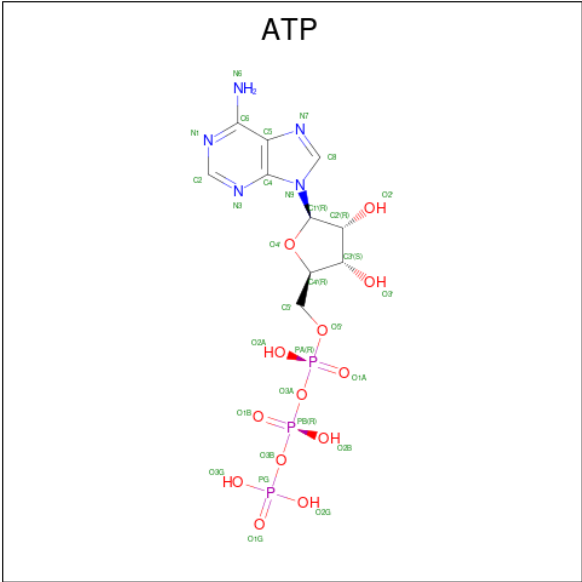
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

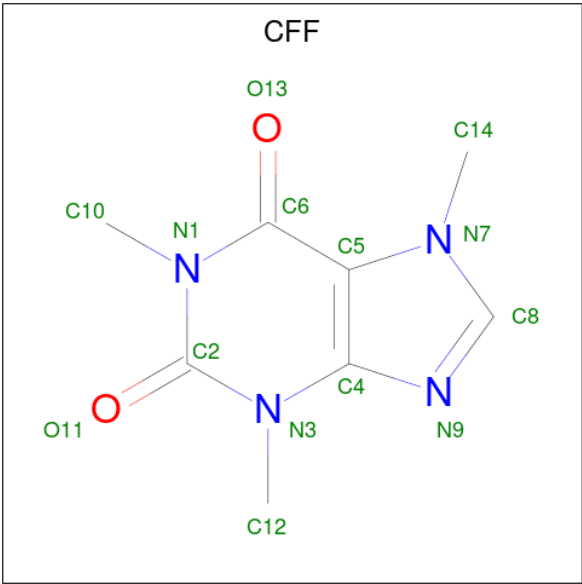
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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

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

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

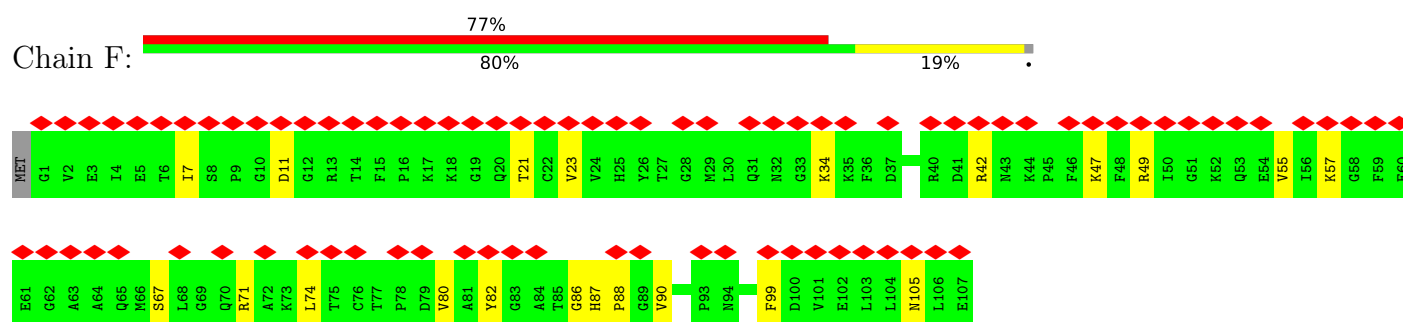
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

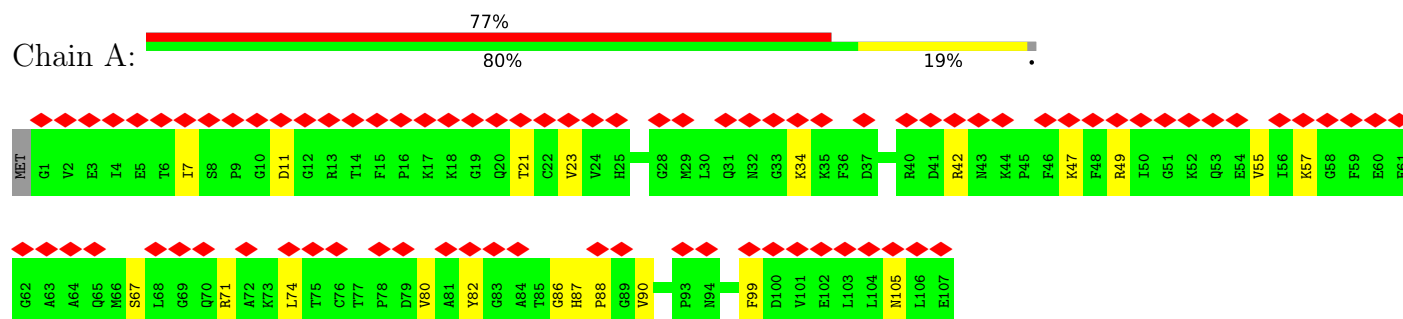
3 Residue-property plots [i](#)

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

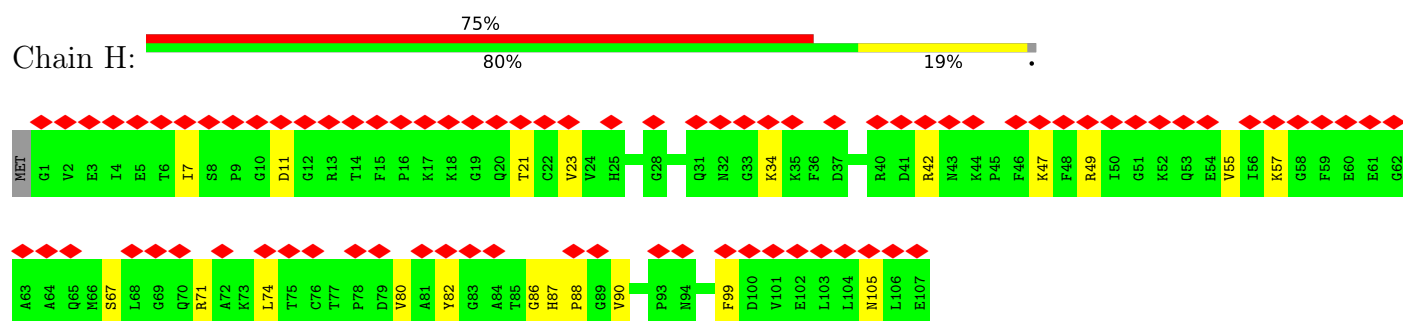
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



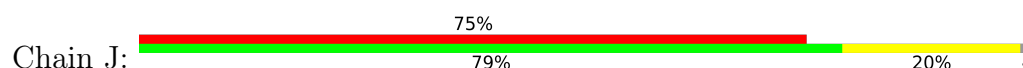
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

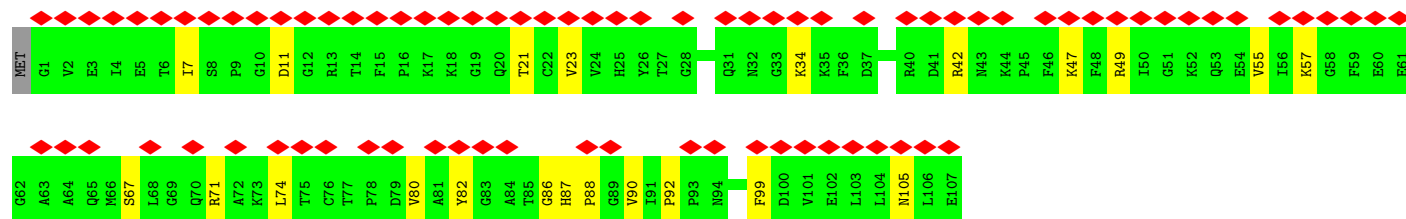


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

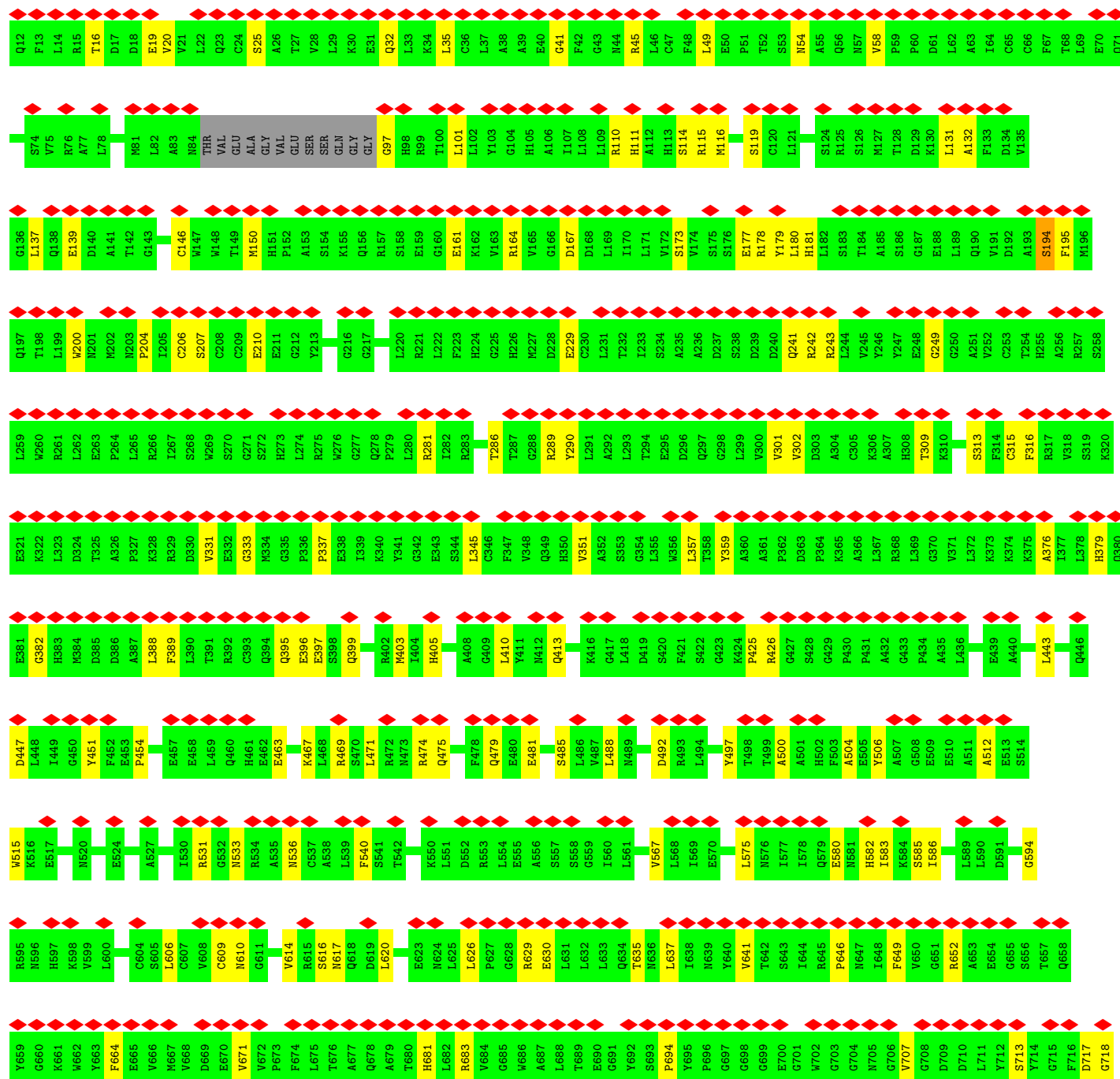
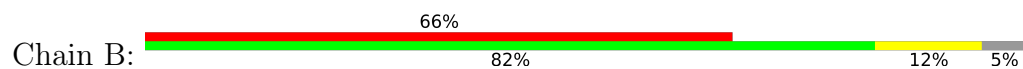


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



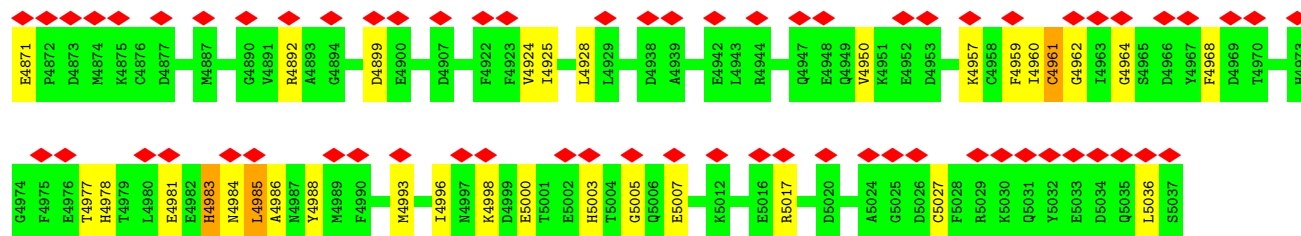


• Molecule 2: Ryanodine receptor 1

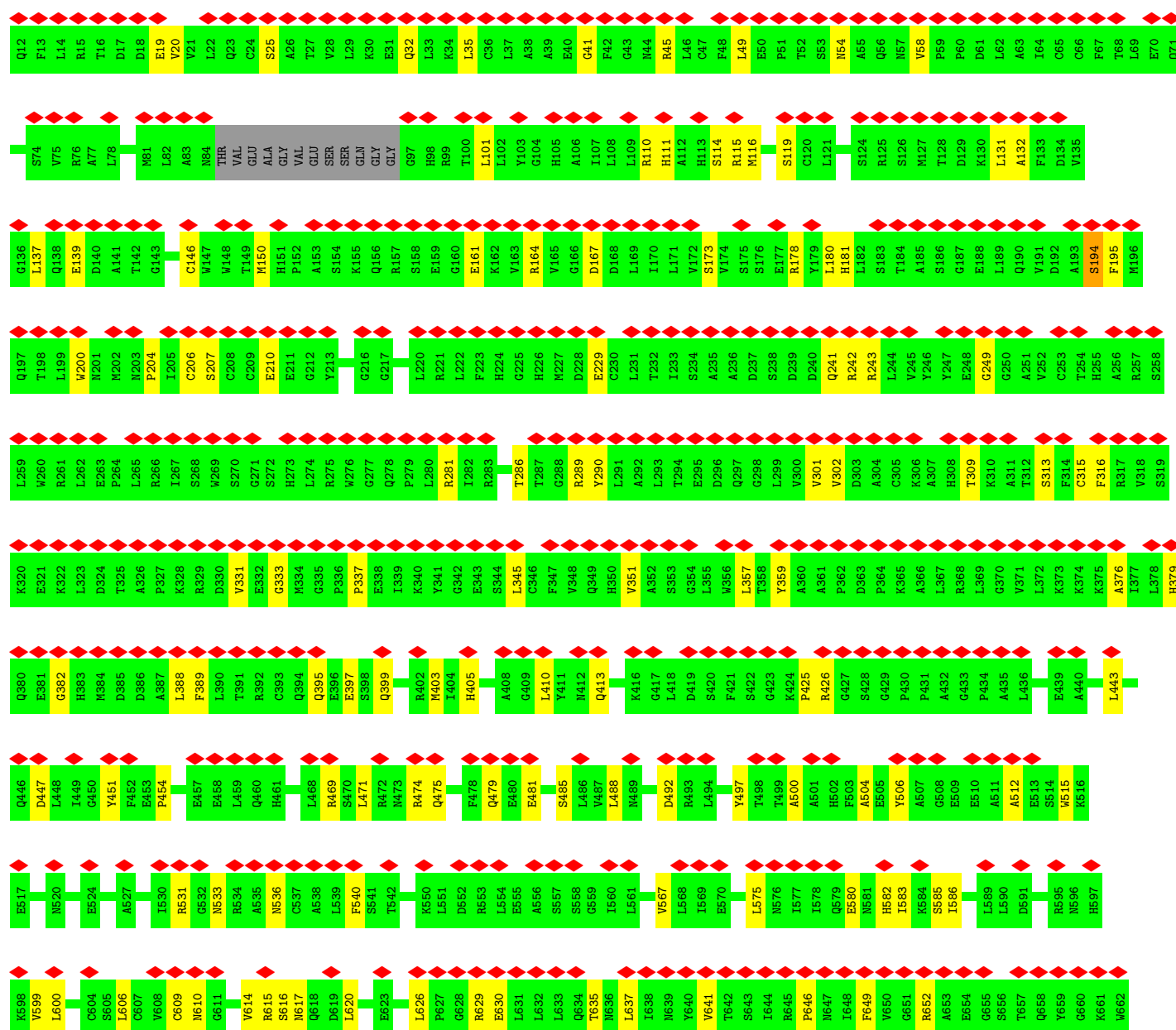
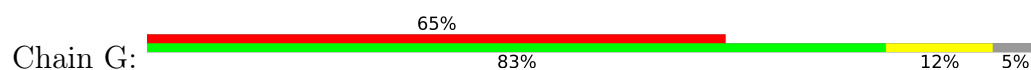


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X1557	X1558	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	L1581	S1582	E1583	R1584	K1585	N1586	P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	Q1598	M1599	L1600	S1604	W1605	R1606	R1607	M1608	L1613	Q1614	V1615	GLU	THR	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	H1702	L1703	Q1629	P1704	Q1631	D1632	P1633	L1634	T1635				
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X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1291	X1292	X1293	X1294	X1297	X1430	X1431	X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1468	X1469	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1484	X1485								
F1213	F1214	A1215	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	I1228	M1229	M1230	Q1231	R1232	P1233	T1234	T1235	T1236	W1237	K1240	P1243	Q1244	F1245	E1246	P1247	P1250	E1251	H1254	I1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	C1269	L1270	R1271	L1272	A1273	H1274	R1275	L1276	X1277	X1278	X1279	X1280							
V1149	G1150	C1151	M1152	T1153	D1154	L1155	T1156	E1157	N1158	T1159	I1160	I1161	F1162	T1163	L1164	M1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	T1182	E1183	I1184	G1185	D1186	G1187	F1188	C1192	S1193	L1194	Q1198	V1199	H1200	H1201	L1202	N1203	L1204	G1205	Q1206	D1207	V1208	S1209	L1210	L1211	R1212			
W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	W1102	G1103	W1104	R1105	L1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	V1122	V1123	F1124	N1125	G1126	H1127	R1128	R1131	W1132	H1133	L1134	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148		
L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	L1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	L1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	R1087		
G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	N991	G992	A997	R998	D999	R1000	V1001	A1002	Q1003	G1004	W1005	S1006	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026		
H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	H924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	N940	H941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	S952	T953	K954	L955	P956	K957	T958	Y959	N960	N961	S962	N963	
R844	C945	L846	S847	H848	T849	D850	H851	V852	P853	C854	P855	V856	D857	THR	VAL	GLN	I861	V862	L863	P864	H865	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	W882	A883	E884	T885	R886	K827	I887	E888	Q889	R830	H831	E832	G833	P834	R835	G836	P837	H838	L839	V840	P841	H842	S843
F783	S784	A785	H786	L787	K788	H789	R790	V791	S912	L913	P914	E915	P916	D857	E799	F800	H801	F802	L803	H804	P805	H806	G807	Y808	A809	P810	C811	H812	E813	A814	V815	F752	S754	I755	S756	F757	I759	N760	G761	C762	P763	V767	F768	E769	A770	F771	N772	L773	G775	L776	F777	F778	V779	H780	V781	S782				





• Molecule 2: Ryanodine receptor 1

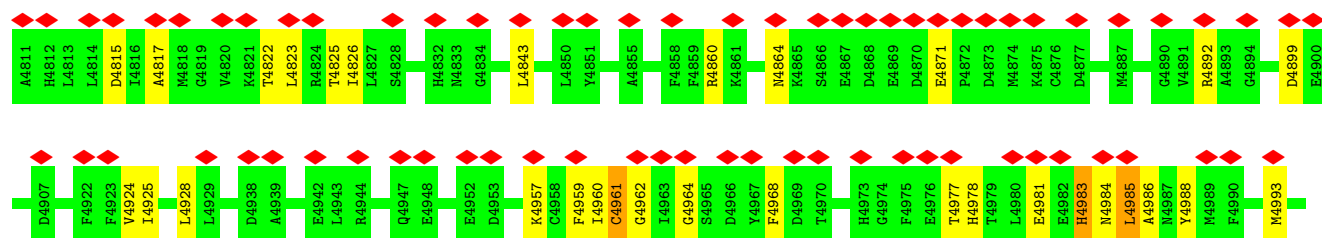


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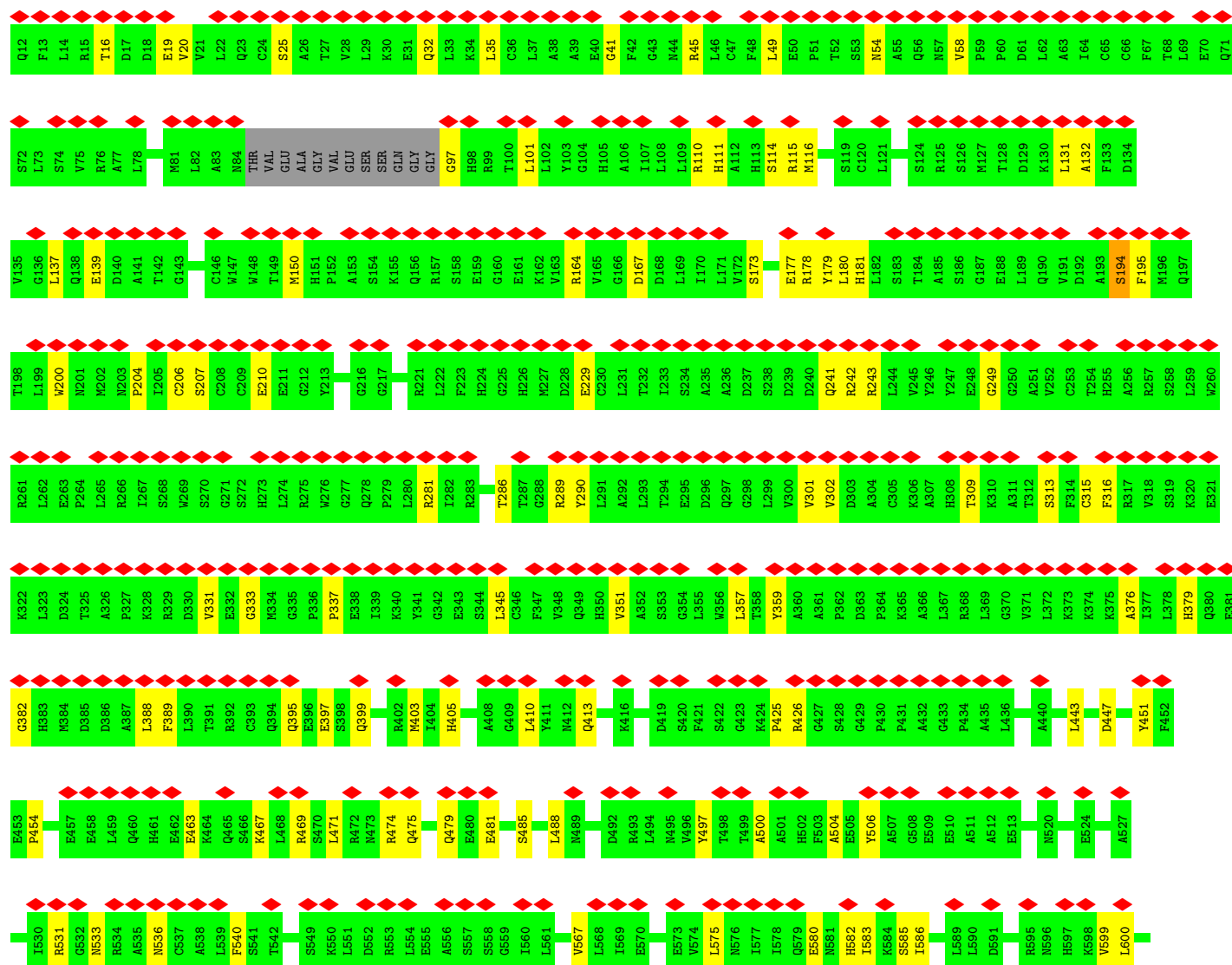
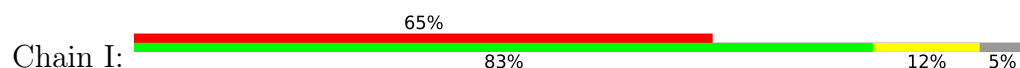
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D4696	P4760	GLU	Q4547	T4190	A4117	E4050	E4056	E3893	D3822	H3734	A3660	X3569
V4697	F4697	ASP	R4548	E4191	D4118	E4050	E4056	N3897	E3825	L3735	X3661	X3570
K4698	G4698	GLU	F4551	R4192	E4118	M4054	H3982	D3898	E3825	E3736	I3662	X3571
Q4699	E4699	GLU	F4551	E4196	E4119	V4055	S3983	D3898	E3825	E3737	L3663	X3572
Y4700	L4764	GLU	Y4554	E4199	E4121	M4055	E4056	Q3900	Q3830	G3738	T3664	X3573
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R4703	T4766	ASP	M4558	A4203	E4123	F4061	E4056	L3903	Q3833	E3741	X3577	X3575
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V4705	N4768	GLU	R4563	E4206	E4125	D4063	E4056	T3905	L3842	GLU	X3577	X3577
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F4711	L4771	T4636	F4571	Q4209	E4127	F4065	E4056	T3907	E3843	GLU	R3672	X3579
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W4715	Y4715	E4640	F4575	R4215	F4132	K4069	E4056	L3912	R3849	V3749	K3679	X3583
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F4809	A4810								G3871			X3607
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• Molecule 2: Ryanodine receptor 1

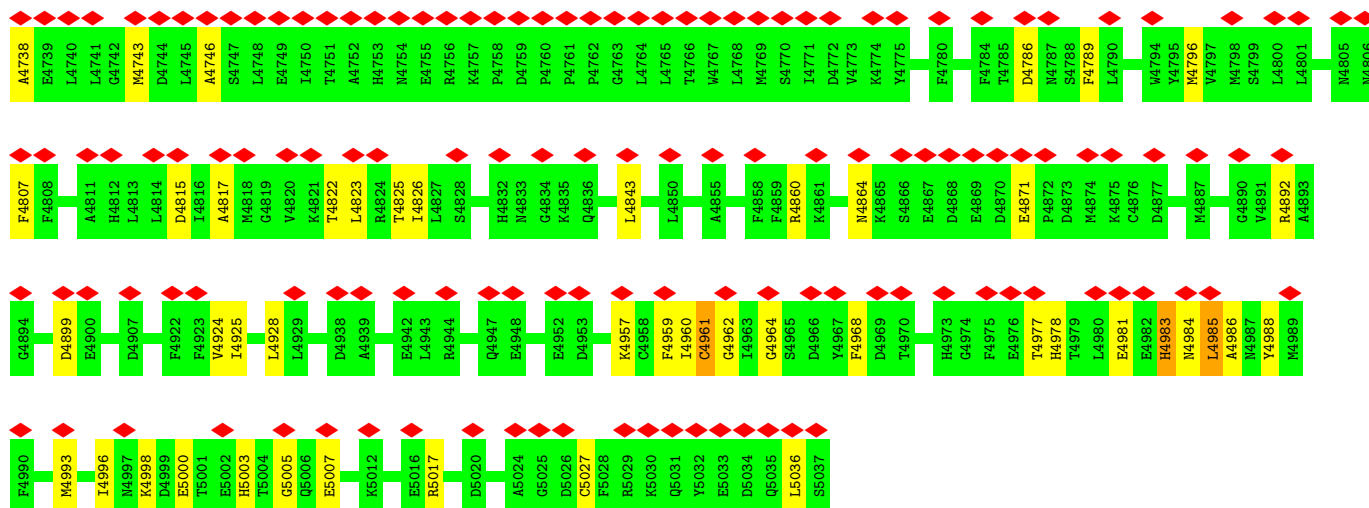


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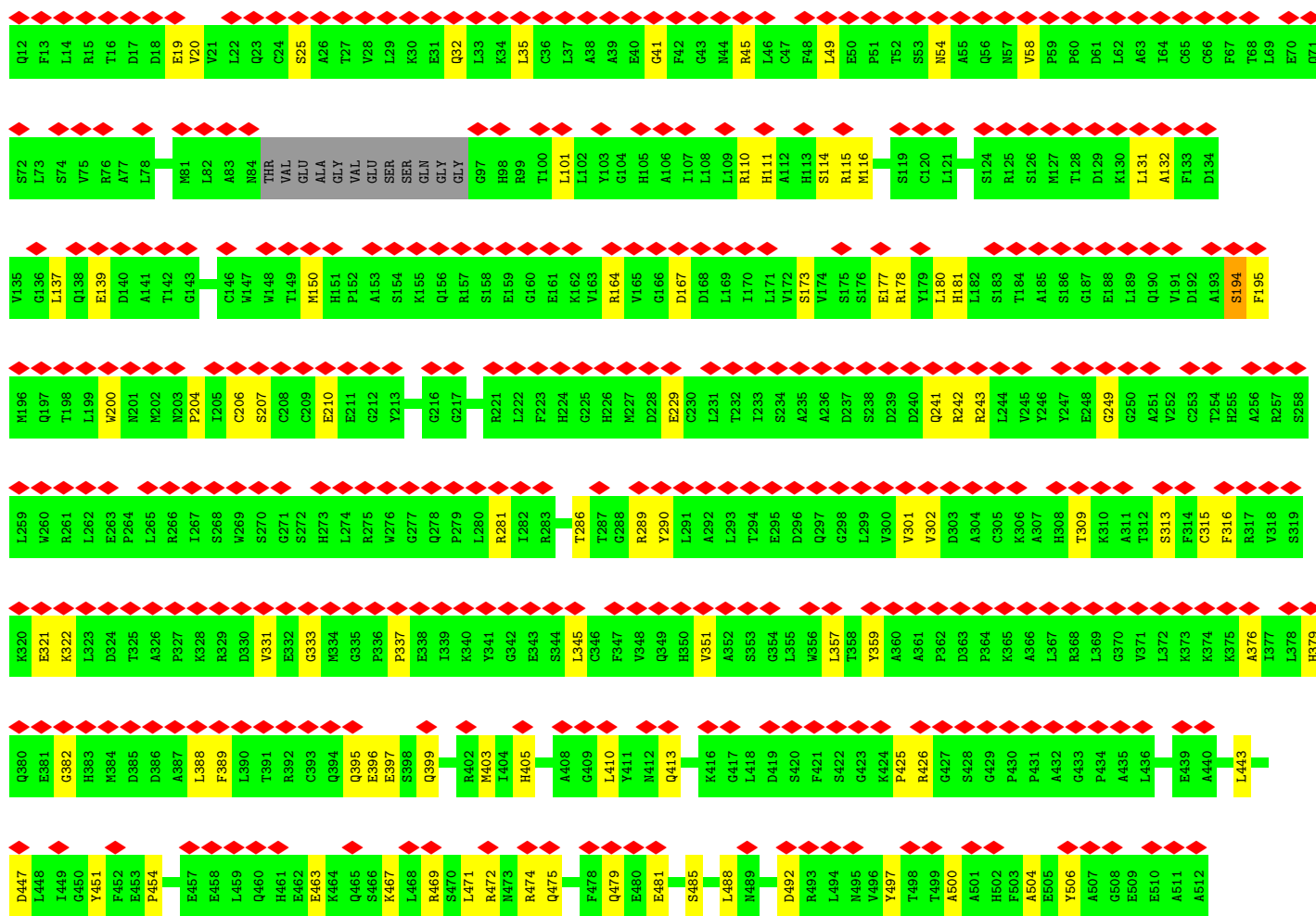
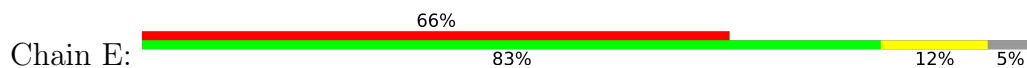


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A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2940	X2941	Y2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	E2883	N2884	T2885	W2886	G2887	L2888	K2889	E2890	K2891	Q2892	E2893	L2894	E2895	X2896	X2897	X2898	X2899	X2900	X2901	X2902	X2903	X2904	X2905	X2906	X2907	X2908	X2909	X2910	X2911	X2912	X2913	X2914	X2915	X2916	X2917	X2918	X2919	X2920	X2921	X2922	X2923	X2924	X2925	X2926	X2927	X2928	X2929	X2930	X2931	X2932	X2933	X2934	X2935	X2936	X2937	X2938	X2939	X2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
E2803	I2804	Y2805	R2806	P2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	N2766	I2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	N2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	F2789	N2790	L2791	F2792	F2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	X2736	D2737	X2738	Y2739	X2740	X2741	X2742	X2743	X2744	X2745	X2746	X2747	X2748	X2749	X2750	X2751	X2752	X2753	X2754	X2755	X2756	X2757	X2758	X2759	X2760	X2761	X2762	X2763	X2764	X2765	X2766	X2767	X2768	X2769	X2770	X2771	X2772	X2773	X2774	X2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	F2789	N2790	L2791	F2792	F2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
X2592	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
X2517	X2518																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	</

SER	X3450	X3553	T3639	G3774	Q3869	D3941	L4028	F4093	R4161	I4251	SER	M4626	K4672
ALA	X3451	X3554	N3643	Q3781	N3870	V3942	S4029	Q4094	M4162	S4252	ALA	M4627	R4673
GLY	X3452	X3555	N3643	Q3781	G3871	I3943	L4030	K4095	F4163	E4253	GLY	M4628	E4674
ASP	X3453	X3556	P3645	L3783	E3872	E3944	L4031	M4096	L4164	X4320	ASP	M4629	E4675
LEU	X3454	X3557	P3645	S3784	E3873	E3945	E4032	M4097	E4165	X4321	LEU	M4630	
ALA	X3455	X3558	T3646	T3784	V3874	Q3946	E4033	D4098	L4166	X4322	ALA	E4634	
GLY	X3456	X3559	R3647	G3788	N3875	N3950	M4034	S4099	A4167	X4329	GLY	S4635	
GLY	X3457	X3560	R3648	E3789	A3876	N3950	V4035	Q4100	E4168	X4330	GLY	S4636	
SER	X3458	X3561	A3649	G3789	A3876	A3954	V4036	Q4101	S4169	X4331	SER	E4637	
GLY	X3459	X3562	C3650	S3803	D3877	A3954	M4037	Q4102	L4171	L4170	GLY	E4638	
GLY	X3460	X3563	N3651	L3804	D3878	K3959	D4038	F4103	E4172	X4332	GLY	E4639	
GLY		X3564	N3652	L3805	T3720	Q3960	M4039	T4104	F4173	X4333	GLY	D4694	
TRP		X3565	P3653	L3805	Y3722	N3963	A4041	G4105	F4174	X4336	TRP	D4695	
GLY		X3566	S3656	N3809	Y3722	N3963	R4042	P4106	R4180	X4340	GLY	D4696	
SER		X3567	S3657	A3810	K3723	E3967	D4046	Q4109	G4185	X4344	SER	M4697	
ALA		X3568	T3658	A3811	N3728	Y3968	M4047	F4110	G4186	X4345	ALA	M4698	
GLY		X3569	A3659	V3812	K3731	S3979	L4048	L4111	A4187	F4540	GLY	E4699	
GLY		X3570	A3660	Q3813	C3733	Q3889	V4049	L4112	S4188	W4541	GLY	Q4699	
ALA		X3573	W3661	K3814	S3732	L3890	E4050	S4113	R4188	G4542	ALA	Q4699	
GLY		X3574	L3663	K3815	H3734	L3891	S4053	E4116	R4189	E4543	GLY	D4699	
GLY		X3575	T3664	K3816	L3735	C3892	M4054	E4117	I4190	L4544	GLY	D4699	
ASP		X3576	E3665	K3817	L3736	E3893	V4055	D4118	E4191	E4545	ASP	D4699	
GLY		X3577	H3667	S3825	E3737	N3897	E4056	E4119	R4192	Q4547	GLY	D4699	
ASP		X3578	S3668	E3825	Q3738	D3898	E4056	E4120	E4196	R4548	ASP	K4698	
GLY		X3579	F3669	E3825	Q3739	F3899	L4059	M4121	E4199	F4551	GLY	D4699	
		X3580		Q3830	E3740	Q3900	K4060	M4122	T4200	Y4554		D4700	
		X3581		Q3830	N3741	N3901	F4061	I4123	A4203	Y4554		D4701	
		X3582		Q3833	GLY	V3902	F4062	F4125	E4206	R4557		D4702	
		X3583		M3836	GLY	L3903	D4063	M4126	E4206	L4562		D4703	
		X3584		L3842	ALA	T3905	D4063	E4127	Q4209	L4563		D4704	
		X3585		L3842	GLU	Q3906	M4064	E4127	E4212	F4571		D4705	
		X3586		D3843	GLU	T3907	F4065	E4127	E4212	L4573		D4706	
		X3587		E3747	E3747	Q3908	L4066	E4127	Q4209	L4573		F4711	
		X3588		E3748	E3748	N3909	K4067	E4128	E4212	L4573		S4713	
		X3589		V3749	V3749	N3909	L4068	E4129	E4212	L4573		S4714	
		X3590		E3750	E3750	N3911	K4069	E4130	E4215	F4571		E4640	
		X3591		E3751	E3751	T3912	D4070	E4131	E4215	A4572		P4641	
		X3592		S3752	S3752	T3913	L4071	E4132	E4219	A4573		E4642	
		X3593		F3753	F3753	N3914	V4072	E4133	F4219	I4574		E4643	
		X3594		E3754	E3754	K3852	Q4073	E4134	F4219	I4575		W4644	
		X3595		E3755	E3755	L3916	S4074	E4135	M4223	L4576		C4645	
		X3596		E3686	E3686	D3921	E4075	E4136	E4224	L4577		C4645	
		X3597		E3687	E3687	Q4005	A4076	E4137	E4224	Y4580		L4648	
		X3598		E3688	E3688	D4006	A4077	E4138	E4228	K4581		F4655	
		X3599		V3690	V3690	S4008	F4077	E4139	E4228	S4583		L4656	
		X3600		Q3761	Q3761	Q4009	Q4078	E4140	E4228	D4584		C4657	
		X3601		R3762	R3762	S3929	D4079	E4141	E4229	S4585		Y4658	
		X3602		L3763	L3763	Q3929	Y4080	E4142	E4230	P4586		I4659	
		X3603		Q3766	Q3766	D3932	Y4081	E4143	E4231	P4587		E4660	
		X3604		Q3767	Q3767	F3933	T4082	E4144	E4231	GLY		Y4661	
		X3605		S3768	S3768	Y3934	P4084	E4145	E4239	ASP		Y4662	
		X3606		R3769	R3769	Y3935	R4085	E4152	E4245	ASP			
		X3607		L3770	L3770	Y3936	R4086	E4153	E4245	GLY			
		X3608		R3771	R3771	S3938	L4087	E4154	E4249	GLY			
		X3609		T3772	T3772	G3939	K4091	E4155	Q4250				
		X3610		R3773	R3773	K3940	D4092	E4156					
		X3611						E4157					
		X3612						E4158					
		X3613						E4159					
								L4160					



• Molecule 2: Ryanodine receptor 1

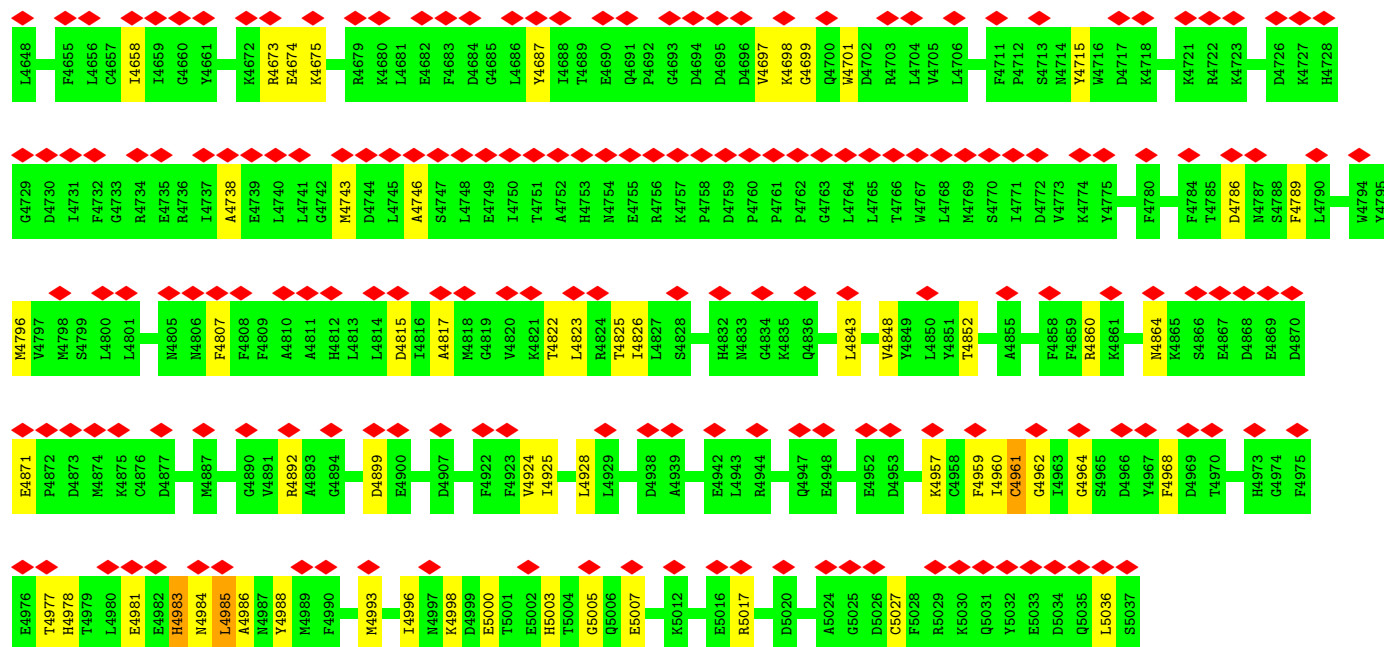


X1286	X1287	X1288	X1291	X1292	X1297	X1430	X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1468	X1469	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1484	X1485	X1486	X1487	X1488	X1492	X1493	X1494	X1495								
C1217	G1218	L1219	Q1220	E1221	G1222	F1223	I1228	N1229	M1230	Q1231	R1232	F1233	V1234	T1235	T1236	W1237	K1240	P1243	Q1244	F1245	E1246	P1247	P1250	E1251	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	C1269	L1270	R1271	L1272	A1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1285							
I1153	D1154	L1155	T1156	E1157	T1159	I1160	I1161	F1162	T1163	L1164	M1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	D1186	G1187	F1188	G1192	S1193	L1194	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216			
F1092	E1093	A1094	V1095	T1096	T1097	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	M1125	G1126	H1127	R1128	R1131	W1132	H1133	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	V1149	G1150	C1151	M1152			
T1031	K1032	S1033	S1034	M1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	M1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	
P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	Q983	L984	V985	D986	R987	L988	A989	E990	N991	G992	A997	R998	R999	R1000	V1001	A1002	Q1003	G1004	W1005	S1008	A1009	VAL	GLN	ASP	I1010	PRO	ALA	ARG	ASN	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030		
L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	G964	Y965	K966
S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	THR	VAL	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	L878	H879	E880	L881	V882	A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	
G786	W787	K788	W789	F791	L792	L793	G794	G795	R796	E799	F900	K901	F902	L903	P904	P905	P906	G907	Y908	A909	P910	C911	H912	E913	A914	V915	L916	P917	L918	E919	R920	L921	R922	L923	E924	P925	I926	K927	E928	Y929	R930	R931	E932	G933	P934	R935	G936	P937	H938	L939	V940	G941	P942	S943	R944	C945	L946		
W722	T723	G724	H725	V726	A727	R728	T729	V730	T731	S732	P733	Q734	Q735	H736	L737	L738	A739	P740	E741	S745	C746	G747	L748	H749	L750	L751	V752	P753	F754	I755	S756	F757	I758	I759	N760	G697	G698	G699	E700	G701	W702	G703	G704	N705	G706	V707	G708	D709	D710	L711	Y712	S713	F716	D717	G718	L719	H720	L721	
K661	V662	Y663	F664	E665	V666	M667	V668	D669	E670	V671	V672	P673	F674	L675	T676	A677	Q678	A679	T680	H681	L682	R683	V684	G685	W686	A687	L688	T689	E690	L692	G691	Y692	S693	P694	Y695	I696	G697	G698	G699	E700	G701	W702	G703	G704	N705	G706	V707	G708	D709	D710	L711	Y712	S713	F716	D717	G718	L719	H720	L721
N596	H597	K598	V599	L600	C604	S605	L606	C607	V608	C609	N610	G611	V614	R615	S616	N617	Q618	D619	L620	E623	L626	P627	L628	G628	R629	Y630	E630	L631	L632	L633	Q634	T635	N636	L637	I638	N639	Y640	V641	T642	S643	I644	R645	P646	N647	I648	E580	F649	V650	G651	R652	A653	E654	G655	Q658	Y659	G660			
E513	E517	N520	E524	A527	I530	R531	N533	R534	A535	N536	C537	A538	F540	S541	T542	K550	L551	D552	R553	L554	E555	A556	S557	S558	G559	I560	L561	V567	L568	I569	E570	L575	N576	I577	I578	Q579	N581	H582	I583	K584	S585	I586	L589	L590	D591	R595													



X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383																																																																												
X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323																																																																												
X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263																																																																						
X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3101	X3102	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3164	X3165	X3166	X3167	X3168	X3169	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193
R2918	D2919	R2920	E2921	R2922	A2923	Q2924	E2925	R2926	L2927	R2928	F2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	X2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997																																																								
Q2858	P2859	R2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	Q2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	L2914	E2915	K2916	A2917																																																																												
S2798	E2799	D2800	D2801	R2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	L2812	A2813	A2815	M2816	L2817	A2818	E2819	E2820	W2821	Y2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	Q2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857																																																																														
R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	T2755	N2756	K2757	F2758	A2759	E2760	V2761	T2762	H2763	E2764	K2765	V2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	V2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	V2794	K2795	T2796	F2797																																																																												
X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2704	F2705	D2706	P2707																																																																												
X2587	X2588	X2589	X2590	X2591	X2592	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2643	X2644	X2645	X2646	X2647																																																																													
G2434	R2435	C2436	A2437	P2438	E2439	N2440	H2441	L2442	A2445	G2446	R2447	E2448	E2449	A2450	L2451	R2452	L2453	R2454	A2455	L2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	L2470	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	T2478	L2479	K2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502																																																																														
X2511	X2512	X2513	X2514	X2514	X2517	X2518	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2549	X2550	X2555	X2556	X2557	X2558	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586																																																																																			





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.21	0/25428	0.52	2/34534 (0.0%)
2	E	0.21	0/25428	0.53	2/34534 (0.0%)
2	G	0.21	0/25428	0.53	4/34534 (0.0%)
2	I	0.21	0/25428	0.53	4/34534 (0.0%)
All	All	0.21	0/105048	0.52	12/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4639	MET	CA-C-N	5.24	134.57	121.80
2	B	4639	MET	C-N-CA	5.24	134.57	121.80
2	I	4639	MET	CA-C-N	5.24	134.57	121.80
2	I	4639	MET	C-N-CA	5.24	134.57	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4639	MET	CA-C-N	5.23	134.57	121.80
2	E	4639	MET	C-N-CA	5.23	134.57	121.80
2	G	4639	MET	CA-C-N	5.21	134.52	121.80
2	G	4639	MET	C-N-CA	5.21	134.52	121.80
2	G	1828	ASP	CA-C-N	5.01	125.00	119.89
2	G	1828	ASP	C-N-CA	5.01	125.00	119.89
2	I	1828	ASP	CA-C-N	5.00	125.00	119.89
2	I	1828	ASP	C-N-CA	5.00	125.00	119.89

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	14	0
1	F	818	0	824	14	0
1	H	818	0	824	13	0
1	J	818	0	824	16	0
2	B	29499	0	24748	320	0
2	E	29499	0	24748	308	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	29499	0	24748	310	0
2	I	29499	0	24748	314	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102376	1276	0

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

All (1276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.43	1.01
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.43	1.00
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.43	1.00
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.43	0.99
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.82	0.78
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.82	0.78
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	2.02	0.78
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	2.02	0.77
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.82	0.77
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	2.02	0.76
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.51	0.75
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.51	0.75
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.75
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.72	0.72
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.72	0.71
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.73	0.71
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.72	0.71
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.73	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.76	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.68
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.76	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.76	0.67
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.43	0.66
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.60	0.66
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.28	0.66
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.28	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.60	0.66
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.28	0.65
2:B:379:HIS:HD2	2:B:382:GLY:H	1.43	0.65
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.43	0.65
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.79	0.65
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.16	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.16	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.16	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.43	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.80	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.81	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.81	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.81	0.63
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.60	0.63
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.81	0.62
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.16	0.62
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.33	0.62
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.81	0.62
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.82	0.62
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.82	0.62
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.62
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.81	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:G:626:LEU:HD23	2:G:630:GLU:H	1.65	0.61
2:I:626:LEU:HD23	2:I:630:GLU:H	1.65	0.61
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.61
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.61
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.82	0.61
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.82	0.61
2:E:626:LEU:HD23	2:E:630:GLU:H	1.65	0.61
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.82	0.61
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.81	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.81	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.82	0.61
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.61
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.82	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.61
2:B:626:LEU:HD23	2:B:630:GLU:H	1.65	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.61
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.82	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.48	0.61
2:I:4978:HIS:CE1	2:I:5027:CYS:SG	2.94	0.61
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.33	0.61
2:B:4978:HIS:CE1	2:B:5027:CYS:SG	2.94	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.61
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.81	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.61
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.60
2:G:4978:HIS:CE1	2:G:5027:CYS:SG	2.94	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4978:HIS:CE1	2:E:5027:CYS:SG	2.94	0.60
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.82	0.60
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.82	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.60
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.60
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.82	0.60
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.66	0.60
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.60
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.60
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.60
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.60
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.67	0.60
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.60
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.67	0.60
2:I:359:TYR:HA	2:I:376:ALA:HA	1.84	0.60
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.67	0.60
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.67	0.59
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.59
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.59
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.85	0.59
2:B:359:TYR:HA	2:B:376:ALA:HA	1.84	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.59
2:G:359:TYR:HA	2:G:376:ALA:HA	1.84	0.59
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.85	0.59
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.59
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.85	0.59
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.84	0.59
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.33	0.59
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.85	0.59
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.59
2:B:4957:LYS:HG2	2:B:4964:GLY:CA	2.33	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.84	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.59
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.84	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.84	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.58
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.67	0.58
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.68	0.58
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.85	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.58
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.85	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.84	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.67	0.58
2:E:4977:THR:HG23	2:E:4981:GLU:HG3	1.85	0.58
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.67	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.58
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.85	0.58
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.33	0.58
2:G:4977:THR:HG23	2:G:4981:GLU:HG3	1.85	0.58
2:I:313:SER:HB3	2:I:351:VAL:HB	1.86	0.58
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.85	0.58
2:B:4977:THR:HG23	2:B:4981:GLU:HG3	1.85	0.58
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.85	0.58
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.85	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.85	0.58
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.86	0.58
2:E:313:SER:HB3	2:E:351:VAL:HB	1.86	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.86	0.58
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.84	0.58
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.86	0.57
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.86	0.57
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.68	0.57
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.67	0.57
2:G:313:SER:HB3	2:G:351:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.57
2:G:4957:LYS:HG2	2:G:4964:GLY:CA	2.33	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.85	0.57
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.85	0.57
2:I:4957:LYS:HG2	2:I:4964:GLY:CA	2.33	0.57
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.70	0.57
2:G:173:SER:HB3	2:G:178:ARG:H	1.70	0.57
2:I:4977:THR:HG23	2:I:4981:GLU:HG3	1.85	0.57
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.87	0.57
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.86	0.57
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.86	0.57
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.57
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.57
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.70	0.57
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.86	0.57
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.86	0.57
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.87	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.86	0.57
2:I:173:SER:HB3	2:I:178:ARG:H	1.70	0.57
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.86	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
2:B:313:SER:HB3	2:B:351:VAL:HB	1.86	0.57
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.86	0.57
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.68	0.57
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.85	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.57
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.87	0.57
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.57
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.28	0.57
2:E:173:SER:HB3	2:E:178:ARG:H	1.70	0.57
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.70	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.86	0.56
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.87	0.56
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.86	0.56
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	1.86	0.56
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.68	0.56
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.86	0.56
2:B:173:SER:HB3	2:B:178:ARG:H	1.70	0.56
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.86	0.56
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.79	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.79	0.56
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.79	0.56
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.86	0.56
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.28	0.56
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.71	0.56
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.56
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.86	0.56
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.38	0.56
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.28	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.87	0.56
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.38	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.71	0.56
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.71	0.56
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.71	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.79	0.56
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.56
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.56
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.38	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.56
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.87	0.56
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.56
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.56
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.71	0.56
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.56
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.88	0.56
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.71	0.56
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.70	0.55
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.38	0.55
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.87	0.55
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.88	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.55
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.72	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.87	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.88	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.71	0.55
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.72	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.55
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.89	0.54
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.54
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.89	0.54
2:G:395:GLN:HG3	2:G:397:GLU:H	1.72	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.54
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.41	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.54
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.41	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.73	0.54
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.38	0.54
2:E:1032:LYS:O	2:E:1036:ARG:N	2.40	0.54
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.41	0.54
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.54
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.41	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.54
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.72	0.54
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.54
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.90	0.54
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.41	0.54
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.39	0.54
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.41	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.53
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.72	0.53
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.41	0.53
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.90	0.53
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.90	0.53
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.89	0.53
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.90	0.53
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.90	0.53
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.90	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.42	0.53
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.56	0.53
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.89	0.53
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.53
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.90	0.53
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.90	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.73	0.53
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.41	0.53
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.53
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.91	0.53
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.53
2:I:395:GLN:HG3	2:I:397:GLU:H	1.73	0.53
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.90	0.53
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.41	0.53
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.90	0.53
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.41	0.53
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.42	0.53
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.41	0.53
2:I:180:LEU:O	2:I:200:TRP:NE1	2.37	0.53
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.74	0.53
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.41	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.53
2:B:25:SER:O	2:B:32:GLN:NE2	2.42	0.53
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.74	0.53
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.42	0.53
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.42	0.53
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.53
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.41	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.42	0.53
2:G:180:LEU:O	2:G:200:TRP:NE1	2.37	0.52
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.73	0.52
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.90	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.52
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.73	0.52
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.56	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.52
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.92	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:G:25:SER:O	2:G:32:GLN:NE2	2.42	0.52
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.92	0.52
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.41	0.52
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.73	0.52
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.90	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:180:LEU:O	2:B:200:TRP:NE1	2.37	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.52
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.91	0.52
1:J:21:THR:HA	1:J:49:ARG:HA	1.92	0.52
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.91	0.52
2:I:25:SER:O	2:I:32:GLN:NE2	2.42	0.52
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.52
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.42	0.52
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.52
2:G:793:LEU:HD11	2:G:1626:TRP:HE1	1.75	0.52
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.91	0.52
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.43	0.52
2:I:793:LEU:HD11	2:I:1626:TRP:HE1	1.75	0.52
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.90	0.52
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.38	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.92	0.52
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.92	0.52
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.73	0.52
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.91	0.52
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.92	0.52
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.38	0.52
2:E:25:SER:O	2:E:32:GLN:NE2	2.42	0.52
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.52
2:B:1032:LYS:O	2:B:1036:ARG:N	2.40	0.52
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.92	0.52
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.42	0.52
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.43	0.52
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.91	0.51
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.92	0.51
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.43	0.51
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.74	0.51
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.92	0.51
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.51
2:I:4983:HIS:H	2:I:4983:HIS:HD2	1.56	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.92	0.51
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.91	0.51
1:H:21:THR:HA	1:H:49:ARG:HA	1.92	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.51
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.92	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.91	0.51
2:E:2479:LEU:O	2:E:2487:UNK:N	2.44	0.51
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.91	0.51
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.90	0.51
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.43	0.51
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.43	0.51
2:G:1032:LYS:O	2:G:1036:ARG:N	2.40	0.51
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.43	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51
2:E:793:LEU:HD11	2:E:1626:TRP:HE1	1.75	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.43	0.51
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.51
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.74	0.51
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.42	0.51
1:F:21:THR:HA	1:F:49:ARG:HA	1.92	0.51
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.44	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.76	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.42	0.51
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.92	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.51
2:I:1032:LYS:O	2:I:1036:ARG:N	2.40	0.51
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.44	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.76	0.51
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.92	0.51
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.43	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.76	0.51
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.44	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.44	0.51
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.92	0.51
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.51
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.92	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.93	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.51
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.51
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.51
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.92	0.51
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.43	0.51
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.93	0.51
2:B:793:LEU:HD11	2:B:1626:TRP:HE1	1.75	0.51
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.93	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:G:911:HIS:O	2:G:918:ARG:NH2	2.44	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.51
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.51
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.92	0.51
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.50
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.77	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.91	0.50
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.91	0.50
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.93	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.92	0.50
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.50
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.93	0.50
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.94	0.50
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.94	0.50
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.44	0.50
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.50
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.94	0.50
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.44	0.50
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.93	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.45	0.50
2:I:2159:LEU:HA	2:I:2162:ILE:HD12	1.94	0.50
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.77	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.50
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.93	0.50
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.93	0.50
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.93	0.50
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.50
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.94	0.50
2:E:206:CYS:SG	2:E:207:SER:N	2.84	0.50
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.44	0.50
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.92	0.50
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.76	0.50
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.76	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.93	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.92	0.50
2:B:290:TYR:O	2:B:302:VAL:N	2.45	0.50
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.50
2:B:2159:LEU:HA	2:B:2162:ILE:HD12	1.94	0.50
2:I:1771:LEU:HD12	2:I:2153:MET:HE3	1.94	0.50
2:I:2479:LEU:O	2:I:2487:UNK:N	2.44	0.50
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.94	0.50
2:B:1771:LEU:HD12	2:B:2153:MET:HE3	1.93	0.50
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.47	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.77	0.50
1:H:82:TYR:O	1:H:86:GLY:N	2.44	0.50
2:G:2479:LEU:O	2:G:2487:UNK:N	2.44	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.44	0.50
2:B:2479:LEU:O	2:B:2487:UNK:N	2.44	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.49
2:G:206:CYS:SG	2:G:207:SER:N	2.84	0.49
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.49
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.45	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.49
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.45	0.49
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.76	0.49
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.93	0.49
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.94	0.49
2:G:880:GLU:OE1	2:G:968:ALA:N	2.43	0.49
2:I:866:HIS:O	2:I:1051:TYR:OH	2.29	0.49
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.49
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.94	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.94	0.49
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.93	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.46	0.49
2:I:290:TYR:O	2:I:302:VAL:N	2.45	0.49
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.49
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.94	0.49
2:E:290:TYR:O	2:E:302:VAL:N	2.45	0.49
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.44	0.49
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.45	0.49
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.47	0.49
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.49
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.46	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.95	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.93	0.49
2:E:1771:LEU:HD12	2:E:2153:MET:HE3	1.94	0.49
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.49
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.76	0.49
2:B:206:CYS:SG	2:B:207:SER:N	2.84	0.49
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.49
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.49
2:G:1771:LEU:HD12	2:G:2153:MET:HE3	1.93	0.49
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.49
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.39	0.49
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.49
2:E:2159:LEU:HA	2:E:2162:ILE:HD12	1.94	0.49
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.94	0.49
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.95	0.49
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.49
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.93	0.49
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.94	0.49
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.47	0.49
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.93	0.49
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.49
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.93	0.49
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.95	0.49
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.46	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.93	0.49
2:G:290:TYR:O	2:G:302:VAL:N	2.45	0.49
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.77	0.49
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.39	0.49
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.76	0.49
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.95	0.49
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.94	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.95	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.95	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.95	0.49
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.39	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.48
2:E:4822:THR:O	2:E:4825:THR:OG1	2.31	0.48
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.48
2:G:866:HIS:O	2:G:1051:TYR:OH	2.29	0.48
2:E:41:GLY:O	2:E:45:ARG:NH1	2.47	0.48
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.48
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.95	0.48
2:G:2159:LEU:HA	2:G:2162:ILE:HD12	1.94	0.48
2:G:4822:THR:O	2:G:4825:THR:OG1	2.31	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.95	0.48
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.95	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.45	0.48
2:E:880:GLU:OE1	2:E:968:ALA:N	2.43	0.48
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.93	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.48
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.95	0.48
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.46	0.48
2:E:180:LEU:O	2:E:200:TRP:NE1	2.37	0.48
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.95	0.48
2:B:41:GLY:O	2:B:45:ARG:NH1	2.47	0.48
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.95	0.48
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.44	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.42	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.48
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.48
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.95	0.48
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.48
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.95	0.48
2:I:41:GLY:O	2:I:45:ARG:NH1	2.47	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.82	0.48
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.94	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.95	0.48
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.82	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.46	0.48
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.95	0.48
2:I:164:ARG:N	2:I:167:ASP:OD2	2.43	0.48
2:I:4817:ALA:HA	2:I:4823:LEU:HD22	1.96	0.48
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:G:41:GLY:O	2:G:45:ARG:NH1	2.47	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.96	0.48
1:A:11:ASP:OD1	1:A:67:SER:OG	2.32	0.47
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.47
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.47
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.96	0.47
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.47	0.47
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.82	0.47
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.47
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.95	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.47
2:E:4817:ALA:HA	2:E:4823:LEU:HD22	1.96	0.47
2:B:54:ASN:O	2:B:58:VAL:N	2.44	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.95	0.47
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.39	0.47
2:G:4817:ALA:HA	2:G:4823:LEU:HD22	1.96	0.47
2:I:500:ALA:HB1	2:I:504:ALA:HB2	1.96	0.47
2:E:1516:UNK:N	2:E:1529:UNK:O	2.48	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.47	0.47
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.97	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:G:500:ALA:HB1	2:G:504:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.47
2:I:1516:UNK:N	2:I:1529:UNK:O	2.48	0.47
2:B:4066:LEU:HD12	2:B:4169:SER:HB2	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.48	0.47
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.47
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.47
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.96	0.47
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.97	0.47
2:B:4817:ALA:HA	2:B:4823:LEU:HD22	1.96	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.97	0.47
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.97	0.47
2:E:500:ALA:HB1	2:E:504:ALA:HB2	1.97	0.47
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.41	0.47
2:B:500:ALA:HB1	2:B:504:ALA:HB2	1.96	0.47
2:B:1516:UNK:N	2:B:1529:UNK:O	2.48	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.47	0.47
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.97	0.47
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.47
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.81	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.97	0.47
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.81	0.47
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.47
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.97	0.47
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.47
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.39	0.47
2:E:4066:LEU:HD12	2:E:4169:SER:HB2	1.97	0.47
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.97	0.47
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.97	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.80	0.47
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.47
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.97	0.47
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.80	0.47
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	1.97	0.47
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.13	0.47
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.97	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.47
2:B:866:HIS:O	2:B:1051:TYR:OH	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.47
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.13	0.47
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	1.97	0.47
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.47	0.47
2:I:206:CYS:SG	2:I:207:SER:N	2.84	0.47
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.47
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.96	0.47
2:B:614:VAL:HG22	2:B:616:SER:H	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.97	0.47
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.47
2:I:2347:GLU:O	2:I:2351:ASN:N	2.48	0.47
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	1.97	0.47
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.96	0.47
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.46
2:B:4823:LEU:HA	2:B:4826:ILE:HD12	1.97	0.46
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.46
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.48	0.46
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.97	0.46
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.98	0.46
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.80	0.46
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.46
2:E:866:HIS:O	2:E:1051:TYR:OH	2.29	0.46
2:E:4823:LEU:HA	2:E:4826:ILE:HD12	1.97	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.48	0.46
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.48	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:B:2347:GLU:O	2:B:2351:ASN:N	2.48	0.46
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.97	0.46
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.82	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.80	0.46
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.46	0.46
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.95	0.46
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.46
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.46
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.46
2:I:4066:LEU:HD12	2:I:4169:SER:HB2	1.96	0.46
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.46	0.46
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.48	0.46
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.48	0.46
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.46
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.51	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.49	0.46
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.49	0.46
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.97	0.46
2:G:1077:ALA:HB1	2:G:1234:VAL:HG11	1.98	0.46
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.98	0.46
2:G:2868:SER:O	2:G:2872:GLN:N	2.49	0.46
2:I:4822:THR:O	2:I:4825:THR:OG1	2.31	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.49	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.97	0.46
2:E:2868:SER:O	2:E:2872:GLN:N	2.49	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.49	0.46
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.49	0.46
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.97	0.46
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.48	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.46
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.49	0.46
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.51	0.46
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.49	0.46
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.81	0.46
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.98	0.46
2:G:4066:LEU:HD12	2:G:4169:SER:HB2	1.96	0.46
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.98	0.46
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.51	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.46
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.46
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.98	0.46
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.46	0.46
2:G:54:ASN:O	2:G:58:VAL:N	2.44	0.46
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.98	0.46
2:I:1077:ALA:HB1	2:I:1234:VAL:HG11	1.98	0.46
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.98	0.46
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.98	0.46
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.46
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.51	0.46
2:B:911:HIS:O	2:B:918:ARG:NH2	2.44	0.46
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.39	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.49	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.49	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.45
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.98	0.45
2:B:1077:ALA:HB1	2:B:1234:VAL:HG11	1.98	0.45
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.48	0.45
2:G:471:LEU:O	2:G:475:GLN:N	2.47	0.45
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.45
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.97	0.45
2:I:3361:UNK:O	2:I:3365:UNK:N	2.49	0.45
2:E:614:VAL:HG22	2:E:616:SER:H	1.80	0.45
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.98	0.45
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.98	0.45
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.45
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.98	0.45
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.45
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.97	0.45
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.45
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.45
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.45
2:B:3361:UNK:O	2:B:3365:UNK:N	2.49	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:2347:GLU:O	2:G:2351:ASN:N	2.48	0.45
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.49	0.45
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4823:LEU:HA	2:I:4826:ILE:HD12	1.97	0.45
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.99	0.45
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.80	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.49	0.45
2:I:911:HIS:O	2:I:918:ARG:NH2	2.44	0.45
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.98	0.45
2:E:1077:ALA:HB1	2:E:1234:VAL:HG11	1.98	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.48	0.45
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.45
2:B:4826:ILE:O	2:B:4829:SER:OG	2.32	0.45
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.98	0.45
2:G:614:VAL:HG22	2:G:616:SER:H	1.80	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.35	0.45
2:G:4823:LEU:HA	2:G:4826:ILE:HD12	1.97	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.35	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.13	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.45
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	1.99	0.45
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.98	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.45
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.97	0.45
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.48	0.45
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.99	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.49	0.45
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.45
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.99	0.45
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	1.99	0.45
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.45
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.82	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.45
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.70	0.45
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.45
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.43	0.45
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.99	0.45
2:E:3361:UNK:O	2:E:3365:UNK:N	2.49	0.45
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.45
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.99	0.45
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.98	0.45
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.98	0.45
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.45
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.45
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.45
2:E:471:LEU:O	2:E:475:GLN:N	2.47	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.99	0.45
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.45
2:E:4984:ASN:C	2:E:4986:ALA:H	2.23	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.99	0.44
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.98	0.44
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.49	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.70	0.44
2:I:54:ASN:O	2:I:58:VAL:N	2.44	0.44
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.82	0.44
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.98	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.99	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.49	0.44
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.98	0.44
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.44
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.98	0.44
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.82	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
1:A:7:ILE:N	1:A:71:ARG:O	2.47	0.44
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.00	0.44
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.53	0.44
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.00	0.44
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	1.99	0.44
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ASP:OD1	1:H:67:SER:OG	2.32	0.44
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.88	0.44
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.41	0.44
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.35	0.44
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.00	0.44
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.00	0.44
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.44
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	1.99	0.44
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.53	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.13	0.44
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.00	0.44
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.70	0.44
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.00	0.44
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.44
2:G:485:SER:HA	2:G:488:LEU:HB2	1.99	0.44
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.39	0.44
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.98	0.44
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.88	0.44
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.99	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.00	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.33	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.44
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.00	0.44
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.41	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.99	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.99	0.44
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.00	0.44
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.00	0.44
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.51	0.44
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.44
2:B:4822:THR:O	2:B:4825:THR:OG1	2.31	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.44
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.70	0.44
1:F:11:ASP:OD1	1:F:67:SER:OG	2.32	0.44
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	2.00	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.44
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.00	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.44
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.51	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.99	0.44
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.51	0.44
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.44
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.53	0.44
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.53	0.43
2:G:488:LEU:O	2:G:492:ASP:N	2.48	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.43
2:E:286:THR:HA	2:E:405:HIS:HB2	2.00	0.43
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.39	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.99	0.43
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.83	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.70	0.43
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.82	0.43
2:I:357:LEU:HD12	2:I:388:LEU:HD11	2.00	0.43
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.00	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.43
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.43
2:E:485:SER:HA	2:E:488:LEU:HB2	1.99	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.48	0.43
2:B:451:TYR:O	2:B:474:ARG:NH1	2.49	0.43
2:I:475:GLN:NE2	2:I:531:ARG:O	2.42	0.43
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.43
2:E:425:PRO:HA	2:E:506:TYR:HD1	1.83	0.43
2:E:4959:PHE:O	2:E:4959:PHE:CD1	2.70	0.43
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.53	0.43
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.00	0.43
2:G:924:MET:O	2:G:928:THR:OG1	2.34	0.43
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	2.01	0.43
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.00	0.43
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.53	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:876:GLU:O	2:I:880:GLU:N	2.50	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.43
2:E:488:LEU:O	2:E:492:ASP:N	2.48	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.00	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.84	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.51	0.43
2:B:5000:GLU:HA	2:B:5003:HIS:CD2	2.53	0.43
2:G:286:THR:HA	2:G:405:HIS:HB2	2.00	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.99	0.43
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	2.00	0.43
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.81	0.43
2:I:5000:GLU:HA	2:I:5003:HIS:CD2	2.53	0.43
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	2.01	0.43
2:B:425:PRO:HA	2:B:506:TYR:HD1	1.83	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:G:161:GLU:HA	2:I:3984:ARG:HH22	1.83	0.43
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.00	0.43
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.43
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.48	0.43
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.43
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.48	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.43
2:B:485:SER:HA	2:B:488:LEU:HB2	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.43
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	2.00	0.43
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.54	0.43
2:I:582:HIS:O	2:I:585:SER:OG	2.30	0.43
2:I:4984:ASN:C	2:I:4986:ALA:N	2.77	0.43
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.46	0.43
1:J:23:VAL:H	1:J:105:ASN:HB3	1.84	0.43
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.88	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	2.01	0.43
2:G:425:PRO:HA	2:G:506:TYR:HD1	1.83	0.43
2:G:2107:GLN:NE2	2:G:3680:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.54	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.43
2:B:286:THR:HA	2:B:405:HIS:HB2	2.00	0.42
2:B:582:HIS:O	2:B:585:SER:OG	2.29	0.42
2:B:2107:GLN:NE2	2:B:3680:ALA:O	2.52	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.01	0.42
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.42
2:I:2107:GLN:NE2	2:I:3680:ALA:O	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.48	0.42
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.42
2:E:4984:ASN:C	2:E:4986:ALA:N	2.77	0.42
2:B:4984:ASN:C	2:B:4986:ALA:N	2.77	0.42
2:I:425:PRO:HA	2:I:506:TYR:HD1	1.83	0.42
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.84	0.42
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	2.00	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.54	0.42
2:B:488:LEU:O	2:B:492:ASP:N	2.48	0.42
2:B:756:SER:HB3	2:B:767:VAL:HG22	2.00	0.42
2:B:1817:GLU:O	2:B:1821:ASP:N	2.49	0.42
2:B:4658:ILE:HD11	2:B:4796:MET:HG3	2.01	0.42
2:G:4658:ILE:HD11	2:G:4796:MET:HG3	2.00	0.42
2:I:1817:GLU:O	2:I:1821:ASP:N	2.49	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.42
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.52	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.02	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.54	0.42
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.01	0.42
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	2.01	0.42
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.00	0.42
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.01	0.42
1:F:23:VAL:H	1:F:105:ASN:HB3	1.85	0.42
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.85	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.84	0.42
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.42
2:G:4892:ARG:NH2	2:E:4899:ASP:OD1	2.52	0.42
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.42
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.48	0.42
1:A:23:VAL:H	1:A:105:ASN:HB3	1.84	0.42
1:J:34:LYS:HE3	2:I:634:GLN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:THR:O	2:B:987:ARG:N	2.52	0.42
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.53	0.42
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.53	0.42
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	2.02	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.02	0.42
2:E:475:GLN:NE2	2:E:531:ARG:O	2.42	0.42
2:E:2107:GLN:NE2	2:E:3680:ALA:O	2.52	0.42
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.02	0.42
2:B:4017:LEU:HD22	2:B:4139:ILE:HG12	2.02	0.42
2:G:475:GLN:NE2	2:G:531:ARG:O	2.42	0.42
2:G:792:LEU:HD22	2:G:799:GLU:H	1.83	0.42
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.85	0.42
2:I:286:THR:HA	2:I:405:HIS:HB2	2.00	0.42
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.42
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.53	0.42
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42
2:E:1078:GLU:HB2	2:E:1235:THR:HG22	2.02	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:E:4017:LEU:HD22	2:E:4139:ILE:HG12	2.02	0.42
1:H:23:VAL:H	1:H:105:ASN:HB3	1.85	0.42
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:B:471:LEU:O	2:B:475:GLN:N	2.47	0.42
2:B:540:PHE:HD2	2:B:567:VAL:HG11	1.85	0.42
2:B:792:LEU:HD22	2:B:799:GLU:H	1.83	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.42
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.84	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.52	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	2.02	0.42
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.02	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.88	0.42
1:J:11:ASP:OD1	1:J:67:SER:OG	2.32	0.42
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.42
2:G:4017:LEU:HD22	2:G:4139:ILE:HG12	2.02	0.42
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	2.00	0.42
2:I:540:PHE:HD2	2:I:567:VAL:HG11	1.85	0.42
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.53	0.42
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.85	0.42
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.85	0.42
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.84	0.42
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.01	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.02	0.42
2:G:730:VAL:O	2:G:735:GLN:NE2	2.53	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:I:924:MET:O	2:I:928:THR:OG1	2.34	0.42
2:I:1747:LEU:HD13	2:I:1760:HIS:CE1	2.55	0.42
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.02	0.42
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.48	0.42
2:E:54:ASN:O	2:E:58:VAL:N	2.44	0.42
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.85	0.42
2:E:792:LEU:HD22	2:E:799:GLU:H	1.83	0.42
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	2.01	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.42
2:B:730:VAL:O	2:B:735:GLN:NE2	2.53	0.41
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.85	0.41
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.52	0.41
2:E:730:VAL:O	2:E:735:GLN:NE2	2.53	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.86	0.41
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.02	0.41
2:B:1747:LEU:HD13	2:B:1760:HIS:CE1	2.55	0.41
2:G:1817:GLU:O	2:G:1821:ASP:N	2.49	0.41
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	2.02	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.02	0.41
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.85	0.41
2:I:3677:LEU:O	2:I:3698:LEU:N	2.51	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.03	0.41
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.52	0.41
2:G:540:PHE:HD2	2:G:567:VAL:HG11	1.85	0.41
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.49	0.41
2:G:2297:LYS:O	2:G:2300:SER:OG	2.35	0.41
2:G:4984:ASN:C	2:G:4986:ALA:N	2.77	0.41
2:I:792:LEU:HD22	2:I:799:GLU:H	1.83	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.49	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41
2:E:4658:ILE:HD11	2:E:4796:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:GLN:NE2	2:B:531:ARG:O	2.42	0.41
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.02	0.41
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	2.01	0.41
2:G:4899:ASP:OD1	2:I:4892:ARG:NH2	2.52	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.03	0.41
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	2.02	0.41
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.86	0.41
2:E:3847:PHE:HD1	2:E:3850:GLN:HE21	1.69	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.47	0.41
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.33	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.41
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.48	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.02	0.41
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.03	0.41
2:G:3847:PHE:HD1	2:G:3850:GLN:HE21	1.69	0.41
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.41
2:I:3847:PHE:HD1	2:I:3850:GLN:HE21	1.69	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:E:1747:LEU:HD13	2:E:1760:HIS:CE1	2.55	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.41
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.95	0.41
2:G:1078:GLU:HB2	2:G:1235:THR:HG22	2.02	0.41
2:G:1747:LEU:HD13	2:G:1760:HIS:CE1	2.55	0.41
2:I:1078:GLU:HB2	2:I:1235:THR:HG22	2.02	0.41
2:I:4658:ILE:HD11	2:I:4796:MET:HG3	2.01	0.41
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.41
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.28	0.41
2:E:4928:LEU:HD13	2:E:4928:LEU:HA	1.90	0.41
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	2.02	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.29	0.41
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.85	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.52	0.41
2:I:4017:LEU:HD22	2:I:4139:ILE:HG12	2.02	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.03	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.47	0.41
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.41
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.03	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4222:VAL:HG23	2:B:4950:VAL:HG12	2.02	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.03	0.41
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	2.03	0.41
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.86	0.41
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.54	0.41
2:I:730:VAL:O	2:I:735:GLN:NE2	2.53	0.41
2:I:1716:ILE:HG23	2:I:1720:LEU:HD13	2.03	0.41
2:I:3771:HIS:O	2:I:3774:GLY:N	2.48	0.41
2:E:540:PHE:HD2	2:E:567:VAL:HG11	1.85	0.41
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.03	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.02	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.54	0.41
2:B:3847:PHE:HD1	2:B:3850:GLN:HE21	1.69	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.03	0.41
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	2.02	0.41
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.54	0.41
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.49	0.41
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.44	0.41
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	2.03	0.41
2:E:3677:LEU:O	2:E:3698:LEU:N	2.51	0.41
2:B:16:THR:OG1	2:B:97:GLY:O	2.39	0.40
2:B:512:ALA:HA	2:B:515:TRP:HB2	2.03	0.40
2:B:1657:LEU:HD13	2:B:1657:LEU:HA	1.95	0.40
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.41	0.40
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.40
2:I:16:THR:OG1	2:I:97:GLY:O	2.39	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.85	0.40
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.92	0.40
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.02	0.40
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.86	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.02	0.40
2:B:2029:GLN:O	2:B:2033:ASP:N	2.50	0.40
2:B:4697:VAL:O	2:B:4701:TRP:N	2.50	0.40
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.04	0.40
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.04	0.40
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.40
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.03	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.50	0.40
2:I:3722:TYR:CZ	2:I:3782:MET:HE3	2.57	0.40
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	2.03	0.40
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.86	0.40
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.95	0.40
2:B:4710:SER:HB3	2:B:4713:SER:HB3	2.03	0.40
2:G:983:THR:O	2:G:987:ARG:N	2.52	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.47	0.40
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	2.03	0.40
2:E:924:MET:O	2:E:928:THR:OG1	2.34	0.40
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.04	0.40
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.86	0.40
2:G:512:ALA:HA	2:G:515:TRP:HB2	2.03	0.40
2:G:1592:PRO:HA	2:G:1593:PRO:HD3	1.98	0.40
2:G:1716:ILE:HG23	2:G:1720:LEU:HD13	2.03	0.40
2:G:3989:VAL:HG13	2:G:4023:MET:HE2	2.04	0.40
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.86	0.40
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.40
2:I:983:THR:O	2:I:987:ARG:N	2.52	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.04	0.40
2:B:119:SER:HA	2:B:146:CYS:HA	2.03	0.40
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.87	0.40
2:B:907:LEU:O	2:B:963:ASN:ND2	2.40	0.40
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.03	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	2.03	0.40
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.03	0.40
2:E:321:GLU:HB3	2:E:322:LYS:H	1.76	0.40
2:E:472:ARG:HA	2:E:475:GLN:HB2	2.03	0.40
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.40
2:E:2029:GLN:O	2:E:2033:ASP:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	43	77
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	43	77
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	43	77
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	43	77
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	44	77

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	4962	GLY
2	B	4985	LEU
2	G	4641	PRO
2	G	4962	GLY
2	G	4985	LEU
2	I	4641	PRO
2	I	4962	GLY
2	I	4985	LEU
2	E	4962	GLY
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	I	1840	PRO
2	E	1840	PRO
2	E	4641	PRO
2	B	2291	GLN
2	G	2291	GLN
2	I	2291	GLN
2	E	2291	GLN

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Mol	Chain	Res	Type
2	B	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	E	1932	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	E	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	G	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	I	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
All	All	10324/12444 (83%)	10268 (100%)	56 (0%)	78	81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	2144	ILE
2	B	3663	LEU
2	B	3805	LEU
2	B	4081	VAL
2	B	4154	VAL

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Mol	Chain	Res	Type
2	B	4166	LEU
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	2144	ILE
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4154	VAL
2	G	4166	LEU
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1657	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	2144	ILE
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4154	VAL
2	I	4166	LEU
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	2144	ILE
2	E	3663	LEU
2	E	3805	LEU
2	E	4081	VAL
2	E	4154	VAL

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Mol	Chain	Res	Type
2	E	4166	LEU
2	E	4961	CYS
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (211) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	201	ASN
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	520	ASN
2	B	725	HIS
2	B	765	GLN
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1611	HIS
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	2194	HIS
2	B	2260	ASN
2	B	2772	GLN
2	B	2773	ASN

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Mol	Chain	Res	Type
2	B	3781	GLN
2	B	3809	ASN
2	B	3814	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3900	GLN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4037	ASN
2	B	4109	GLN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4776	GLN
2	B	4806	ASN
2	B	4833	ASN
2	B	4978	HIS
2	B	4983	HIS
2	B	4987	ASN
2	B	5003	HIS
2	B	5031	GLN
2	G	57	ASN
2	G	201	ASN
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	520	ASN
2	G	725	HIS
2	G	765	GLN
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1611	HIS
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1760	HIS

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Mol	Chain	Res	Type
2	G	1775	HIS
2	G	1861	GLN
2	G	2005	GLN
2	G	2041	HIS
2	G	2127	GLN
2	G	2260	ASN
2	G	2772	GLN
2	G	2773	ASN
2	G	2884	ASN
2	G	3781	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3900	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4037	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4776	GLN
2	G	4806	ASN
2	G	4833	ASN
2	G	4978	HIS
2	G	4983	HIS
2	G	4987	ASN
2	G	5003	HIS
2	G	5031	GLN
2	I	201	ASN
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	520	ASN
2	I	725	HIS

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Mol	Chain	Res	Type
2	I	765	GLN
2	I	797	HIS
2	I	838	HIS
2	I	1220	GLN
2	I	1598	GLN
2	I	1611	HIS
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	2005	GLN
2	I	2127	GLN
2	I	2194	HIS
2	I	2260	ASN
2	I	2772	GLN
2	I	2773	ASN
2	I	3781	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3900	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4037	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4776	GLN
2	I	4806	ASN
2	I	4833	ASN
2	I	4978	HIS
2	I	4983	HIS
2	I	4987	ASN
2	I	5003	HIS
2	I	5031	GLN

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Mol	Chain	Res	Type
2	E	57	ASN
2	E	201	ASN
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	725	HIS
2	E	797	HIS
2	E	838	HIS
2	E	1220	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	2005	GLN
2	E	2041	HIS
2	E	2127	GLN
2	E	2194	HIS
2	E	2260	ASN
2	E	2772	GLN
2	E	2773	ASN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3900	GLN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4037	ASN
2	E	4109	GLN
2	E	4120	ASN
2	E	4142	ASN
2	E	4246	GLN

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Mol	Chain	Res	Type
2	E	4776	GLN
2	E	4806	ASN
2	E	4833	ASN
2	E	4978	HIS
2	E	4983	HIS
2	E	4987	ASN
2	E	5003	HIS
2	E	5031	GLN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CFF	I	5102	-	15,15,15	1.93	7 (46%)	23,23,23	2.72	10 (43%)
3	ATP	B	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.77	10 (20%)
3	ATP	E	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.77	10 (20%)
4	CFF	B	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.73	10 (43%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.77	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	G	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.73	10 (43%)
4	CFF	E	5102	-	15,15,15	1.93	8 (53%)	23,23,23	2.72	9 (39%)
3	ATP	G	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.76	10 (20%)

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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	4.54	1.47	1.39
3	B	5101	ATP	C5-C4	4.53	1.47	1.39
3	E	5101	ATP	C5-C4	4.53	1.47	1.39
3	G	5101	ATP	C5-C4	4.51	1.47	1.39
4	G	5102	CFF	C6-N1	-3.96	1.32	1.40
4	B	5102	CFF	C6-N1	-3.94	1.32	1.40
4	E	5102	CFF	C6-N1	-3.94	1.32	1.40
4	I	5102	CFF	C6-N1	-3.94	1.32	1.40
3	G	5101	ATP	C5-C6	2.74	1.48	1.41
3	B	5101	ATP	C5-C6	2.73	1.48	1.41
3	I	5101	ATP	C5-C6	2.72	1.48	1.41
3	E	5101	ATP	C5-C6	2.71	1.48	1.41
4	E	5102	CFF	C4-N3	-2.51	1.34	1.38
4	B	5102	CFF	C4-N3	-2.51	1.34	1.38
4	I	5102	CFF	C4-N3	-2.51	1.34	1.38
4	G	5102	CFF	C4-N3	-2.49	1.34	1.38
3	G	5101	ATP	C5-N7	-2.37	1.34	1.39
3	B	5101	ATP	C5-N7	-2.35	1.34	1.39
3	G	5101	ATP	C8-N7	2.33	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-N7	-2.32	1.34	1.39
3	E	5101	ATP	C5-N7	-2.32	1.34	1.39
4	B	5102	CFF	C5-N7	-2.31	1.34	1.38
3	B	5101	ATP	C8-N7	2.30	1.36	1.31
4	I	5102	CFF	C5-N7	-2.30	1.34	1.38
4	E	5102	CFF	C5-N7	-2.30	1.34	1.38
4	G	5102	CFF	C5-N7	-2.30	1.34	1.38
3	I	5101	ATP	C8-N7	2.27	1.36	1.31
3	E	5101	ATP	C8-N7	2.27	1.36	1.31
4	G	5102	CFF	C2-N3	-2.21	1.34	1.39
4	B	5102	CFF	C2-N3	-2.21	1.34	1.39
4	I	5102	CFF	C2-N3	-2.20	1.34	1.39
4	E	5102	CFF	C2-N3	-2.18	1.34	1.39
4	I	5102	CFF	O13-C6	-2.18	1.18	1.23
4	G	5102	CFF	O11-C2	-2.16	1.18	1.22
4	B	5102	CFF	O13-C6	-2.15	1.18	1.23
4	G	5102	CFF	O13-C6	-2.14	1.18	1.23
4	B	5102	CFF	O11-C2	-2.14	1.18	1.22
4	I	5102	CFF	O11-C2	-2.14	1.18	1.22
4	E	5102	CFF	C2-N1	-2.14	1.34	1.39
4	E	5102	CFF	O13-C6	-2.13	1.18	1.23
4	E	5102	CFF	O11-C2	-2.10	1.18	1.22
4	G	5102	CFF	C2-N1	-2.09	1.34	1.39
3	B	5101	ATP	C4-N9	-2.09	1.33	1.37
4	B	5102	CFF	C2-N1	-2.09	1.34	1.39
3	G	5101	ATP	C4-N9	-2.09	1.33	1.37
3	I	5101	ATP	C4-N9	-2.09	1.33	1.37
4	I	5102	CFF	C2-N1	-2.07	1.35	1.39
3	E	5101	ATP	C4-N9	-2.05	1.33	1.37
4	E	5102	CFF	C5-C6	-2.01	1.38	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	C14-N7-C8	-7.66	111.94	126.28
4	B	5102	CFF	C14-N7-C8	-7.65	111.96	126.28
4	G	5102	CFF	C14-N7-C8	-7.64	111.98	126.28
4	I	5102	CFF	C14-N7-C8	-7.64	111.99	126.28
3	I	5101	ATP	C5-C4-N3	-5.82	118.71	126.72
3	E	5101	ATP	C5-C4-N3	-5.80	118.73	126.72
3	B	5101	ATP	C5-C4-N3	-5.80	118.73	126.72
3	G	5101	ATP	C5-C4-N3	-5.79	118.75	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	C14-N7-C5	5.20	140.14	127.77
4	G	5102	CFF	C14-N7-C5	5.18	140.10	127.77
4	B	5102	CFF	C14-N7-C5	5.18	140.09	127.77
4	I	5102	CFF	C14-N7-C5	5.18	140.09	127.77
3	I	5101	ATP	N3-C4-N9	4.33	134.53	127.17
3	E	5101	ATP	N3-C4-N9	4.32	134.51	127.17
3	B	5101	ATP	N3-C4-N9	4.31	134.50	127.17
3	G	5101	ATP	N3-C4-N9	4.30	134.48	127.17
4	G	5102	CFF	C5-C6-N1	4.18	119.72	112.06
4	B	5102	CFF	C5-C6-N1	4.17	119.71	112.06
4	I	5102	CFF	C5-C6-N1	4.16	119.69	112.06
4	E	5102	CFF	C5-C6-N1	4.16	119.67	112.06
3	E	5101	ATP	C4-C5-N7	-3.83	106.20	110.58
3	I	5101	ATP	C4-C5-N7	-3.83	106.21	110.58
3	B	5101	ATP	C4-C5-N7	-3.80	106.24	110.58
3	G	5101	ATP	C4-C5-N7	-3.79	106.25	110.58
3	E	5101	ATP	C2-N3-C4	3.61	120.65	111.83
3	I	5101	ATP	C2-N3-C4	3.60	120.64	111.83
3	B	5101	ATP	C2-N3-C4	3.60	120.63	111.83
3	G	5101	ATP	C2-N3-C4	3.60	120.61	111.83
4	I	5102	CFF	C6-N1-C2	-3.13	120.57	125.66
4	B	5102	CFF	C6-N1-C2	-3.13	120.57	125.66
4	E	5102	CFF	C6-N1-C2	-3.11	120.60	125.66
4	G	5102	CFF	C6-N1-C2	-3.11	120.60	125.66
4	G	5102	CFF	N3-C4-N9	3.09	131.12	126.27
4	I	5102	CFF	N3-C4-N9	3.07	131.09	126.27
4	B	5102	CFF	N3-C4-N9	3.06	131.08	126.27
4	E	5102	CFF	N3-C4-N9	3.04	131.05	126.27
3	E	5101	ATP	N3-C2-N1	-2.89	124.20	128.58
3	B	5101	ATP	N3-C2-N1	-2.87	124.23	128.58
3	G	5101	ATP	N3-C2-N1	-2.86	124.25	128.58
3	I	5101	ATP	N3-C2-N1	-2.86	124.26	128.58
4	E	5102	CFF	N7-C8-N9	-2.84	108.34	113.48
4	G	5102	CFF	N7-C8-N9	-2.82	108.38	113.48
4	B	5102	CFF	N7-C8-N9	-2.81	108.39	113.48
4	G	5102	CFF	C6-C5-C4	-2.81	119.38	122.92
4	B	5102	CFF	C6-C5-C4	-2.81	119.38	122.92
4	I	5102	CFF	N7-C8-N9	-2.79	108.42	113.48
4	I	5102	CFF	C6-C5-C4	-2.78	119.41	122.92
4	G	5102	CFF	O13-C6-C5	-2.78	120.69	126.38
4	E	5102	CFF	C6-C5-C4	-2.77	119.43	122.92
4	B	5102	CFF	O13-C6-C5	-2.76	120.73	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	O13-C6-C5	-2.75	120.74	126.38
4	E	5102	CFF	O13-C6-C5	-2.75	120.75	126.38
3	E	5101	ATP	C5-N7-C8	2.65	107.62	103.45
3	I	5101	ATP	C5-N7-C8	2.65	107.61	103.45
3	B	5101	ATP	C5-N7-C8	2.62	107.58	103.45
3	G	5101	ATP	C5-N7-C8	2.61	107.56	103.45
3	I	5101	ATP	C3'-C2'-C1'	2.57	106.33	101.46
3	E	5101	ATP	C3'-C2'-C1'	2.57	106.32	101.46
3	B	5101	ATP	C3'-C2'-C1'	2.57	106.32	101.46
3	G	5101	ATP	C3'-C2'-C1'	2.55	106.28	101.46
3	I	5101	ATP	C4-N9-C8	2.49	108.35	105.74
3	B	5101	ATP	C4-N9-C8	2.47	108.33	105.74
3	E	5101	ATP	C4-N9-C8	2.46	108.33	105.74
3	G	5101	ATP	C4-N9-C8	2.46	108.32	105.74
3	E	5101	ATP	C6-C5-N7	2.43	136.78	132.09
3	G	5101	ATP	C6-C5-N7	2.42	136.76	132.09
3	B	5101	ATP	C6-C5-N7	2.42	136.76	132.09
3	I	5101	ATP	C6-C5-N7	2.41	136.74	132.09
4	B	5102	CFF	N3-C2-N1	2.11	119.77	117.14
4	E	5102	CFF	N3-C2-N1	2.10	119.76	117.14
4	I	5102	CFF	N3-C2-N1	2.09	119.75	117.14
4	G	5102	CFF	N3-C2-N1	2.07	119.72	117.14
3	I	5101	ATP	N9-C8-N7	-2.02	111.07	113.94
4	G	5102	CFF	C10-N1-C6	2.01	120.75	117.64
3	B	5101	ATP	N9-C8-N7	-2.01	111.09	113.94
4	I	5102	CFF	C10-N1-C6	2.01	120.75	117.64
3	G	5101	ATP	N9-C8-N7	-2.00	111.09	113.94
3	E	5101	ATP	N9-C8-N7	-2.00	111.09	113.94
4	B	5102	CFF	C10-N1-C6	2.00	120.74	117.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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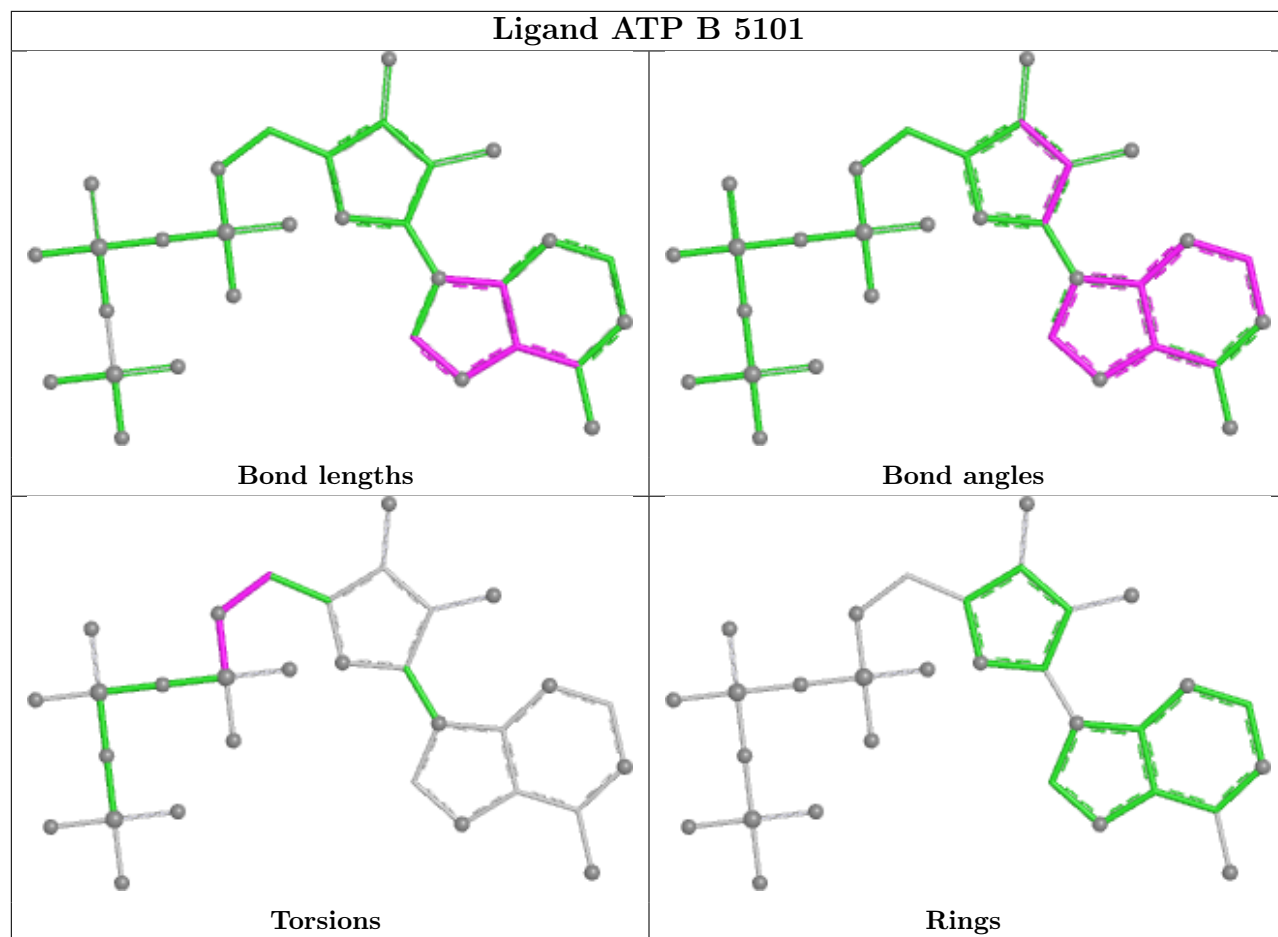
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A

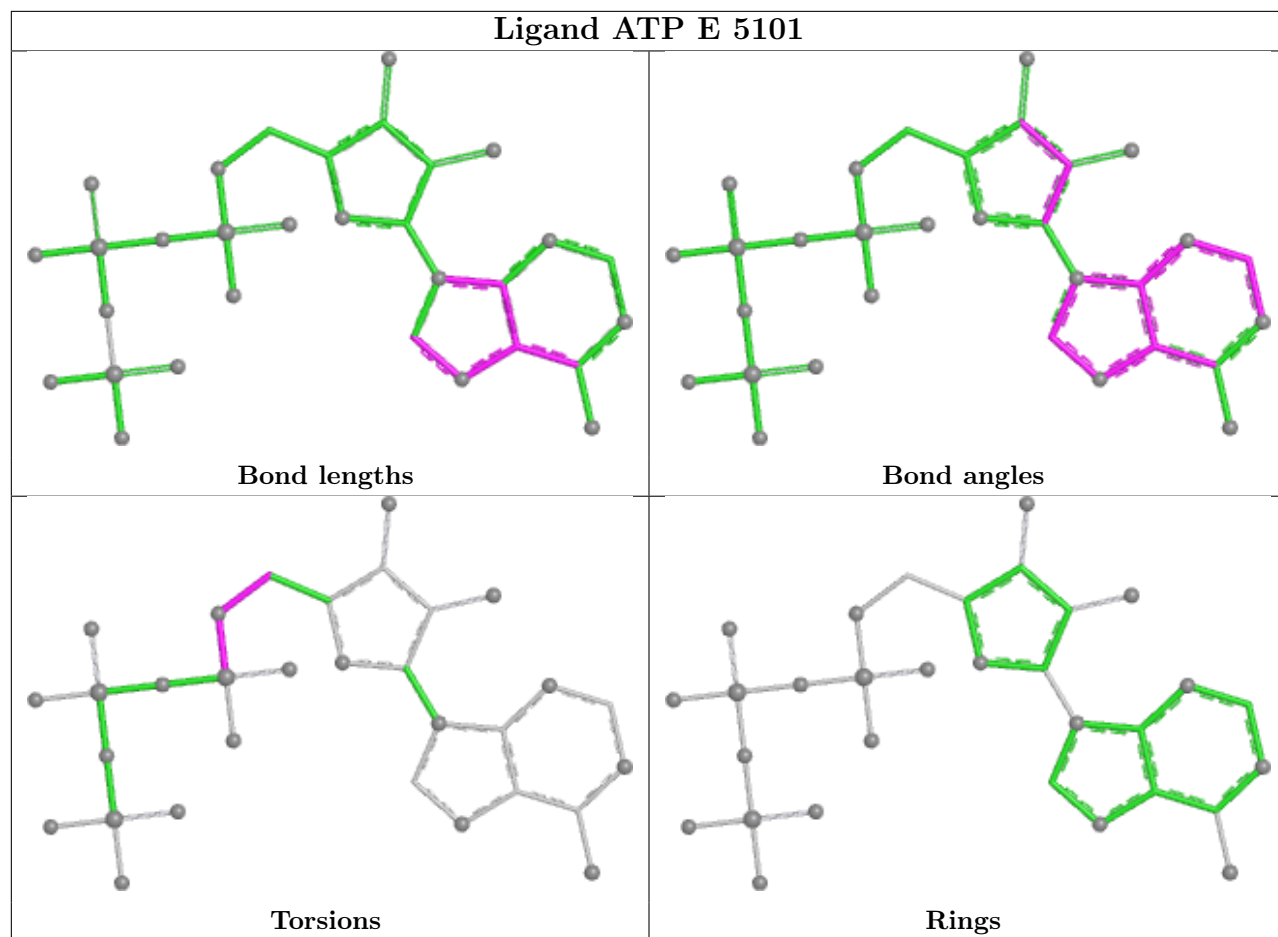
There are no ring outliers.

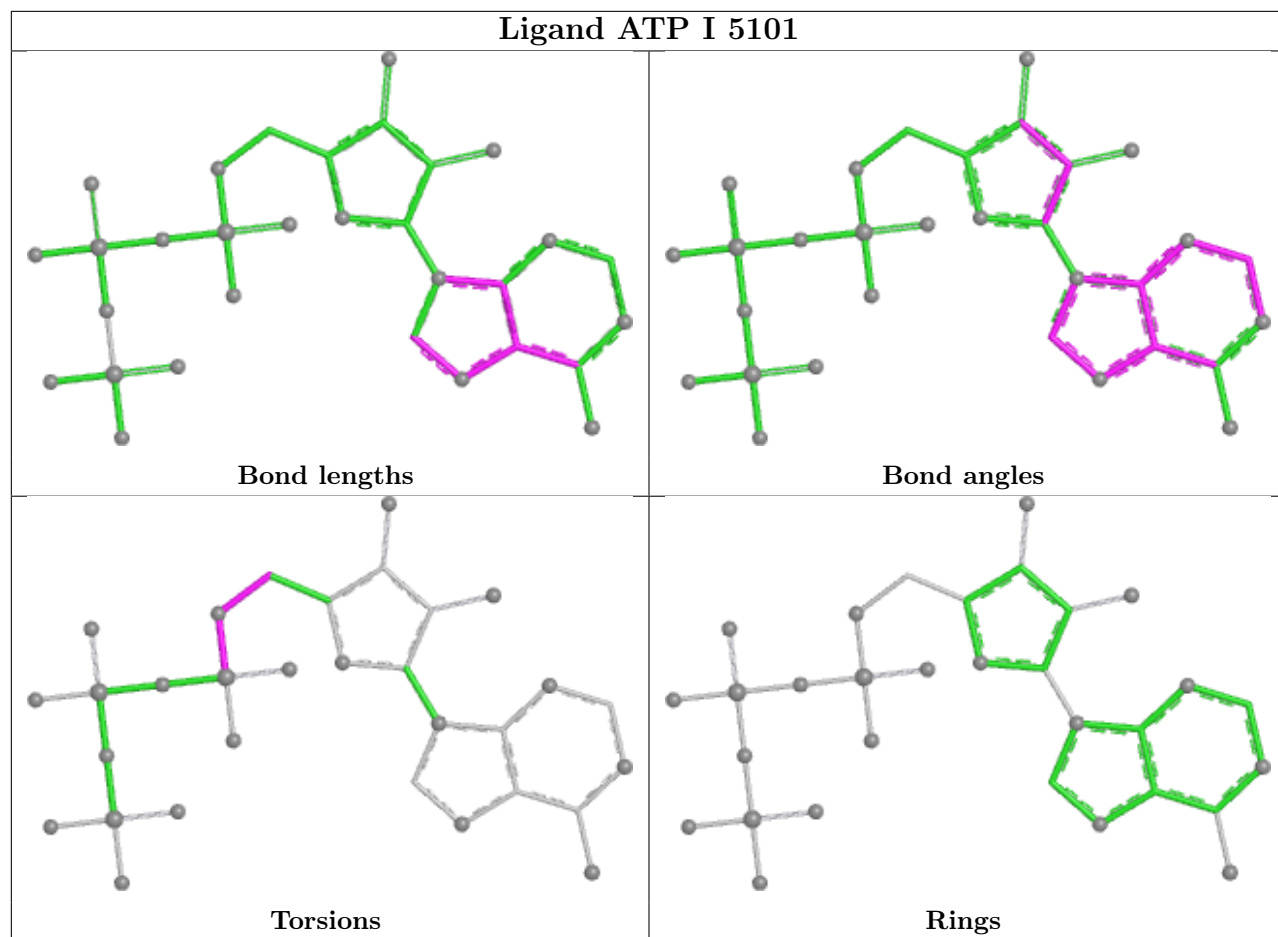
4 monomers are involved in 4 short contacts:

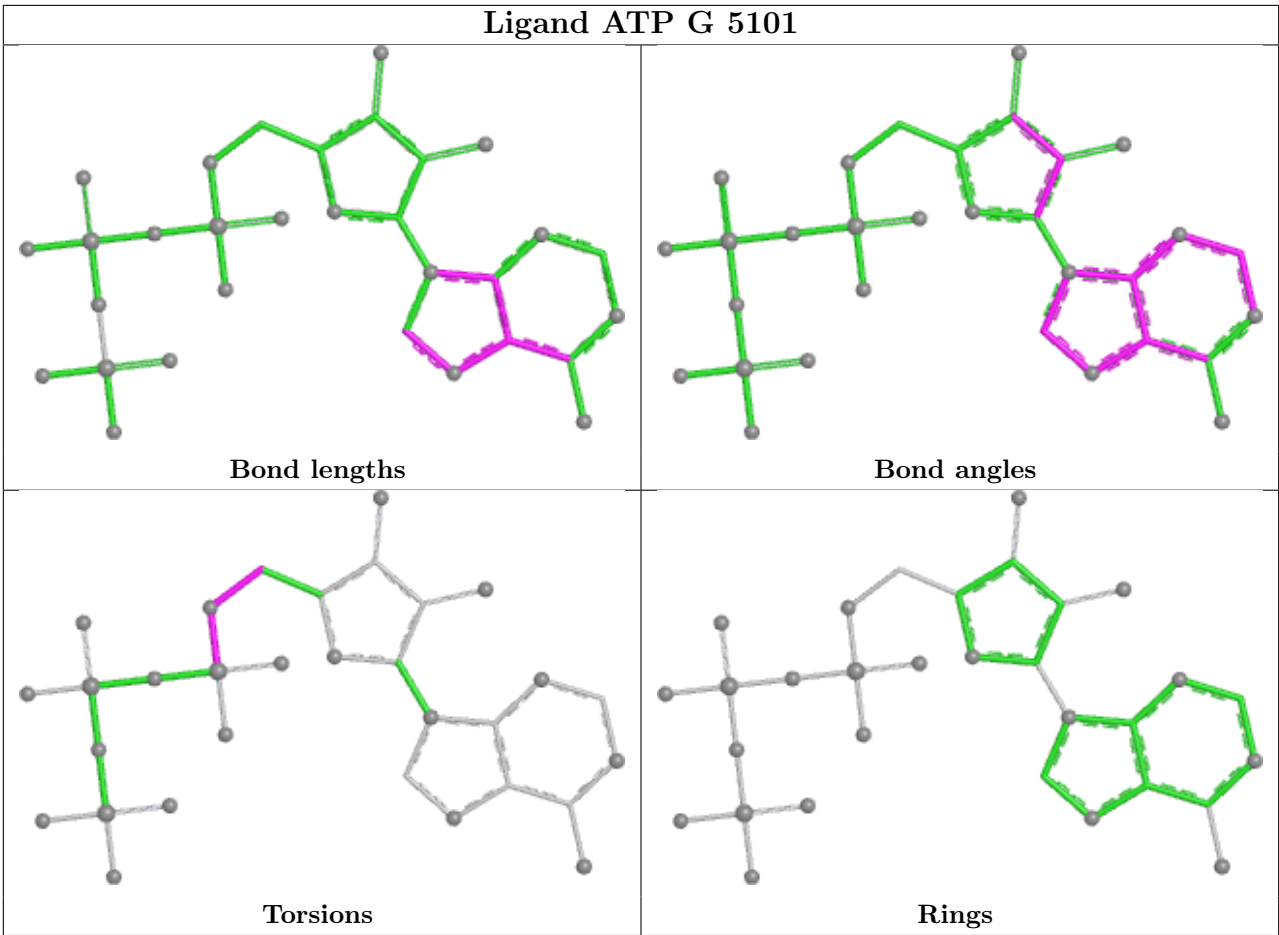
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	E	5101	ATP	1	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62
1	G	3613:UNK	C	3639:THR	N	45.62
1	I	3613:UNK	C	3639:THR	N	45.62
1	E	3613:UNK	C	3639:THR	N	45.62
1	B	4253:GLU	C	4320:UNK	N	27.90
1	G	4253:GLU	C	4320:UNK	N	27.90
1	I	4253:GLU	C	4320:UNK	N	27.90
1	E	4253:GLU	C	4320:UNK	N	27.90
1	B	3163:UNK	C	3170:UNK	N	15.83
1	G	3163:UNK	C	3170:UNK	N	15.83
1	I	3163:UNK	C	3170:UNK	N	15.83
1	E	3163:UNK	C	3170:UNK	N	15.83
1	B	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.87
1	I	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	B	3468:UNK	C	3511:UNK	N	14.52
1	G	3468:UNK	C	3511:UNK	N	14.52
1	I	3468:UNK	C	3511:UNK	N	14.52
1	E	3468:UNK	C	3511:UNK	N	14.52
1	B	2703:UNK	C	2734:ASN	N	13.45
1	G	2703:UNK	C	2734:ASN	N	13.45
1	I	2703:UNK	C	2734:ASN	N	13.45
1	E	2703:UNK	C	2734:ASN	N	13.45
1	B	3236:UNK	C	3241:UNK	N	12.87
1	G	3236:UNK	C	3241:UNK	N	12.87
1	I	3236:UNK	C	3241:UNK	N	12.87
1	E	3236:UNK	C	3241:UNK	N	12.87
1	B	1564:UNK	C	1573:MET	N	12.40
1	G	1564:UNK	C	1573:MET	N	12.40
1	I	1564:UNK	C	1573:MET	N	12.40
1	E	1564:UNK	C	1573:MET	N	12.40
1	B	2976:UNK	C	2995:UNK	N	12.24
1	G	2976:UNK	C	2995:UNK	N	12.24
1	I	2976:UNK	C	2995:UNK	N	12.24
1	E	2976:UNK	C	2995:UNK	N	12.24
1	B	3254:UNK	C	3261:UNK	N	8.57
1	G	3254:UNK	C	3261:UNK	N	8.57
1	I	3254:UNK	C	3261:UNK	N	8.57
1	E	3254:UNK	C	3261:UNK	N	8.57

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	B	2939:ARG	C	2942:UNK	N	3.33
1	G	2939:ARG	C	2942:UNK	N	3.33
1	I	2939:ARG	C	2942:UNK	N	3.33
1	E	2939:ARG	C	2942:UNK	N	3.33
1	B	2479:LEU	C	2487:UNK	N	3.30
1	G	2479:LEU	C	2487:UNK	N	3.30
1	I	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30

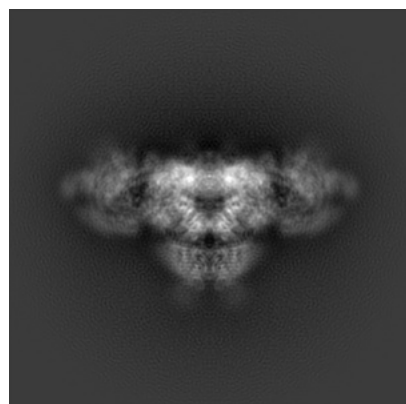
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8376. These allow visual inspection of the internal detail of the map and identification of artifacts.

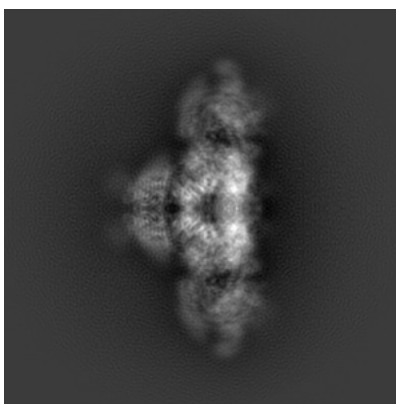
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

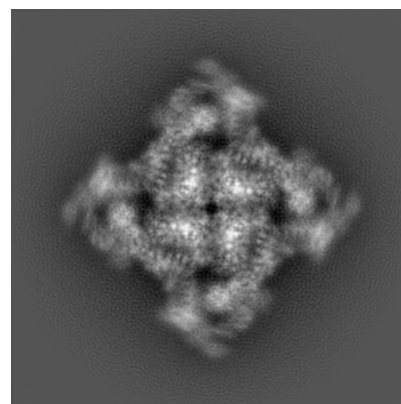
6.1.1 Primary map



X

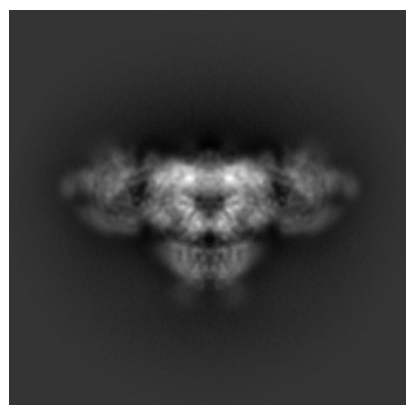


Y

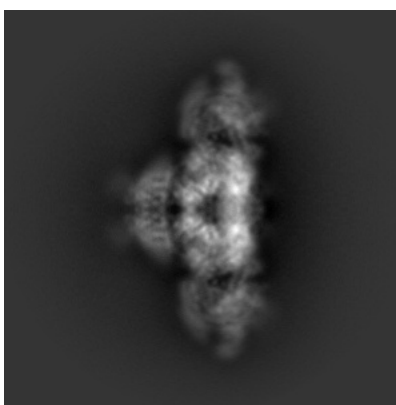


Z

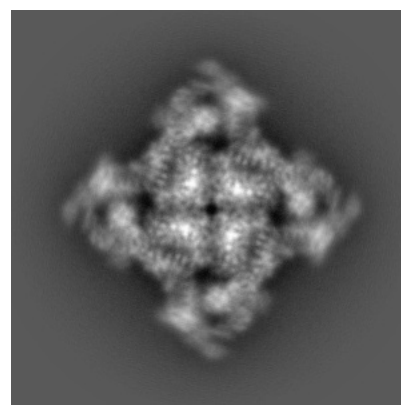
6.1.2 Raw map



X



Y

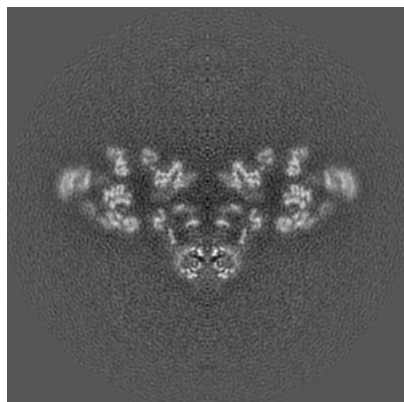


Z

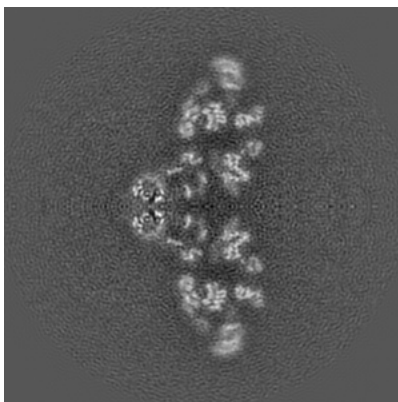
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

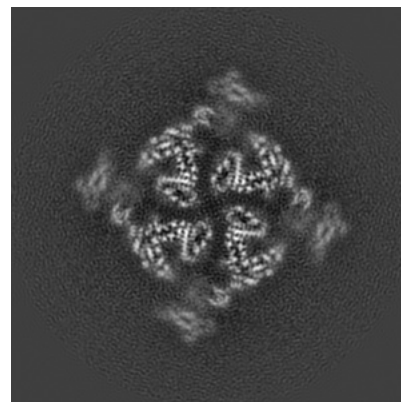
6.2.1 Primary map



X Index: 200

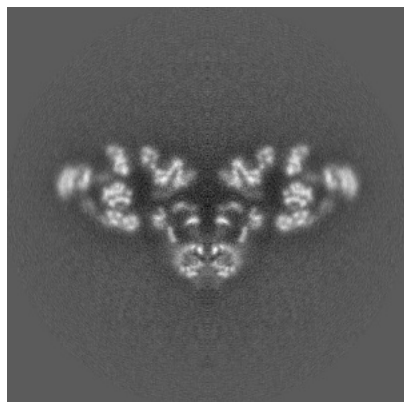


Y Index: 200

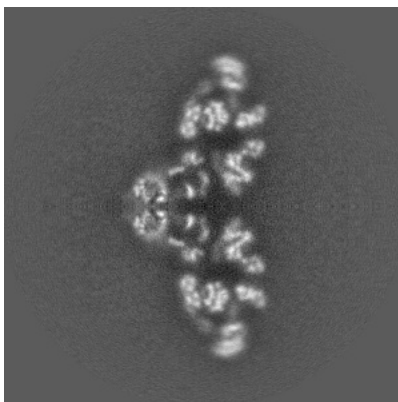


Z Index: 200

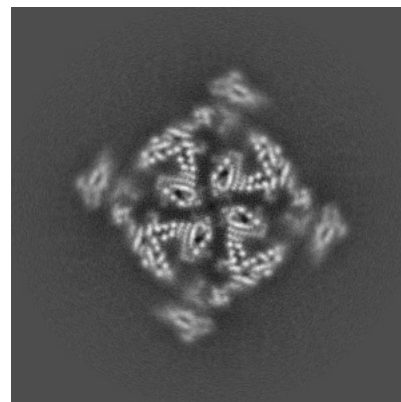
6.2.2 Raw map



X Index: 200



Y Index: 200

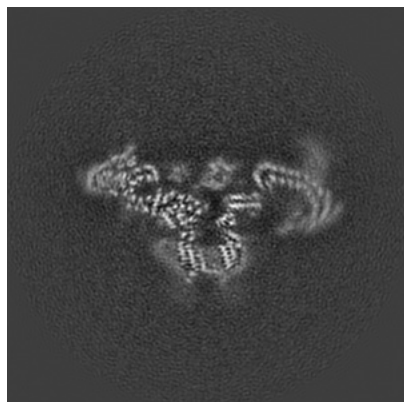


Z Index: 200

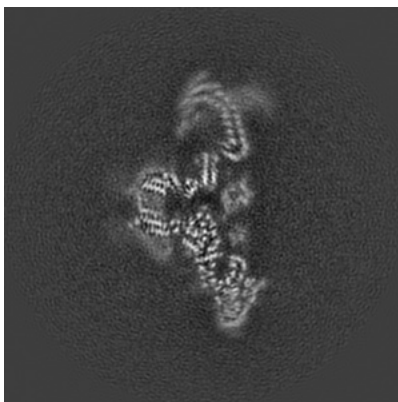
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

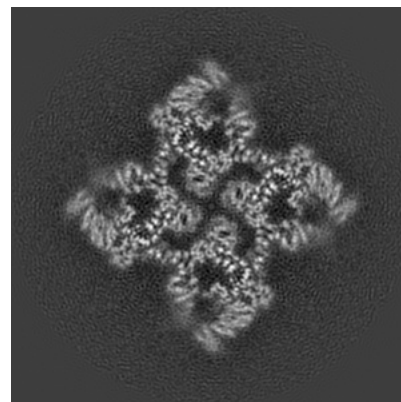
6.3.1 Primary map



X Index: 225

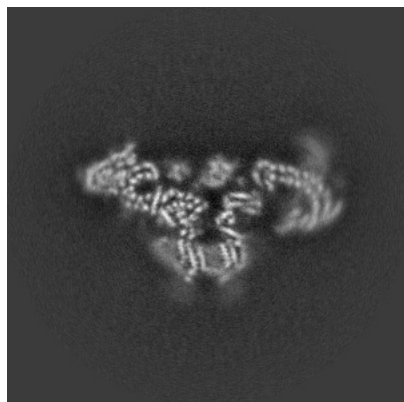


Y Index: 175

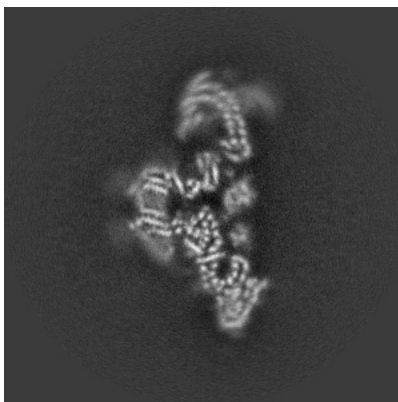


Z Index: 232

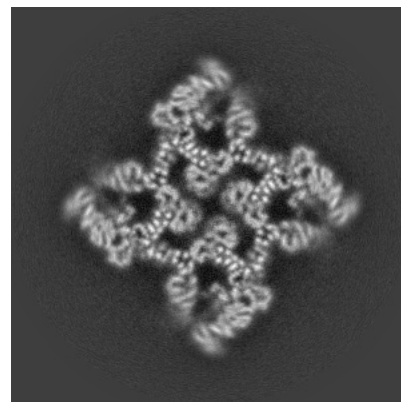
6.3.2 Raw map



X Index: 224



Y Index: 176

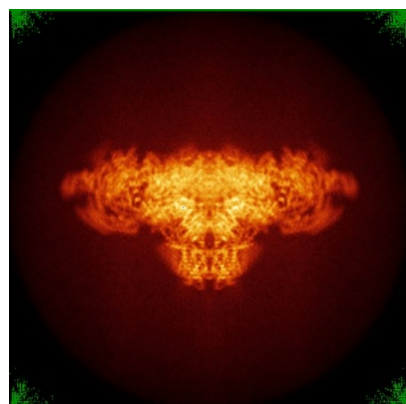


Z Index: 232

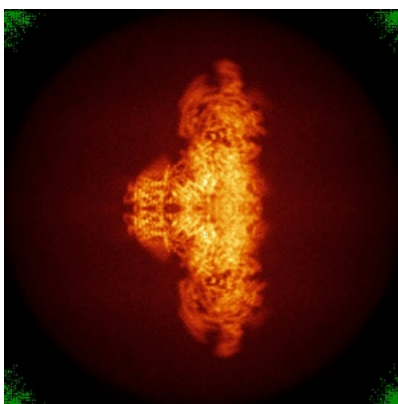
The images above show the largest variance slices of the map in three orthogonal directions.

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

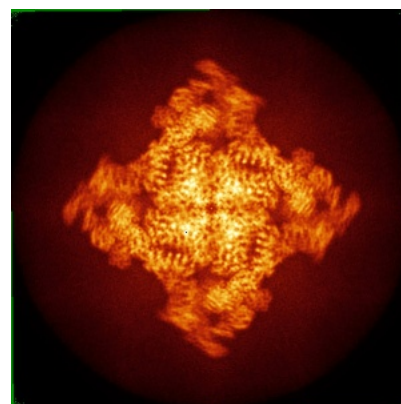
6.4.1 Primary map



X

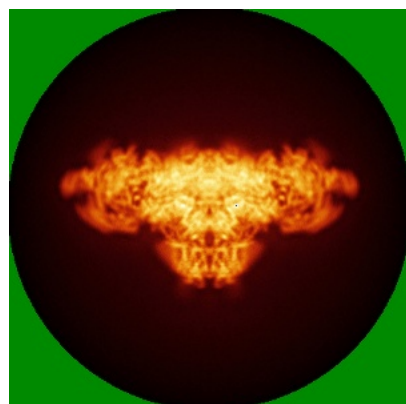


Y

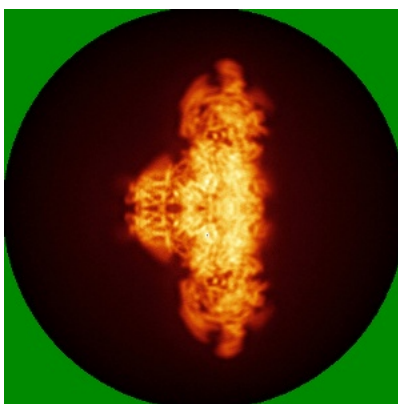


Z

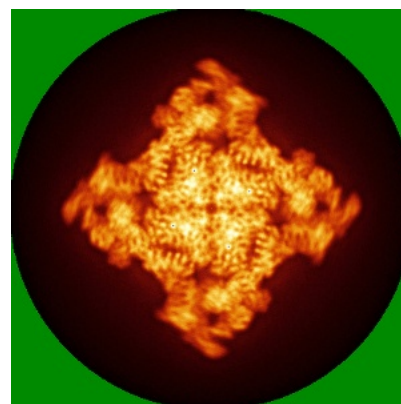
6.4.2 Raw map



X



Y

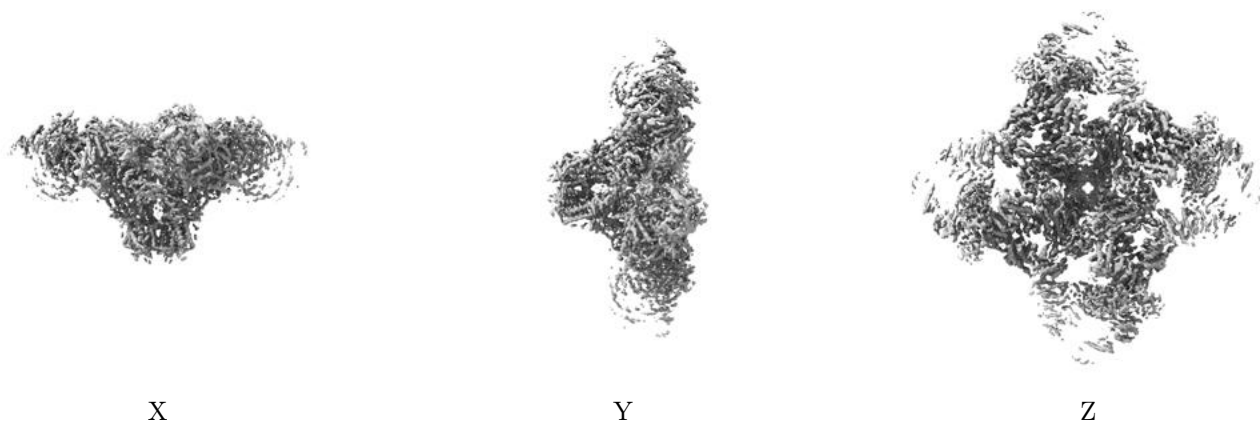


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

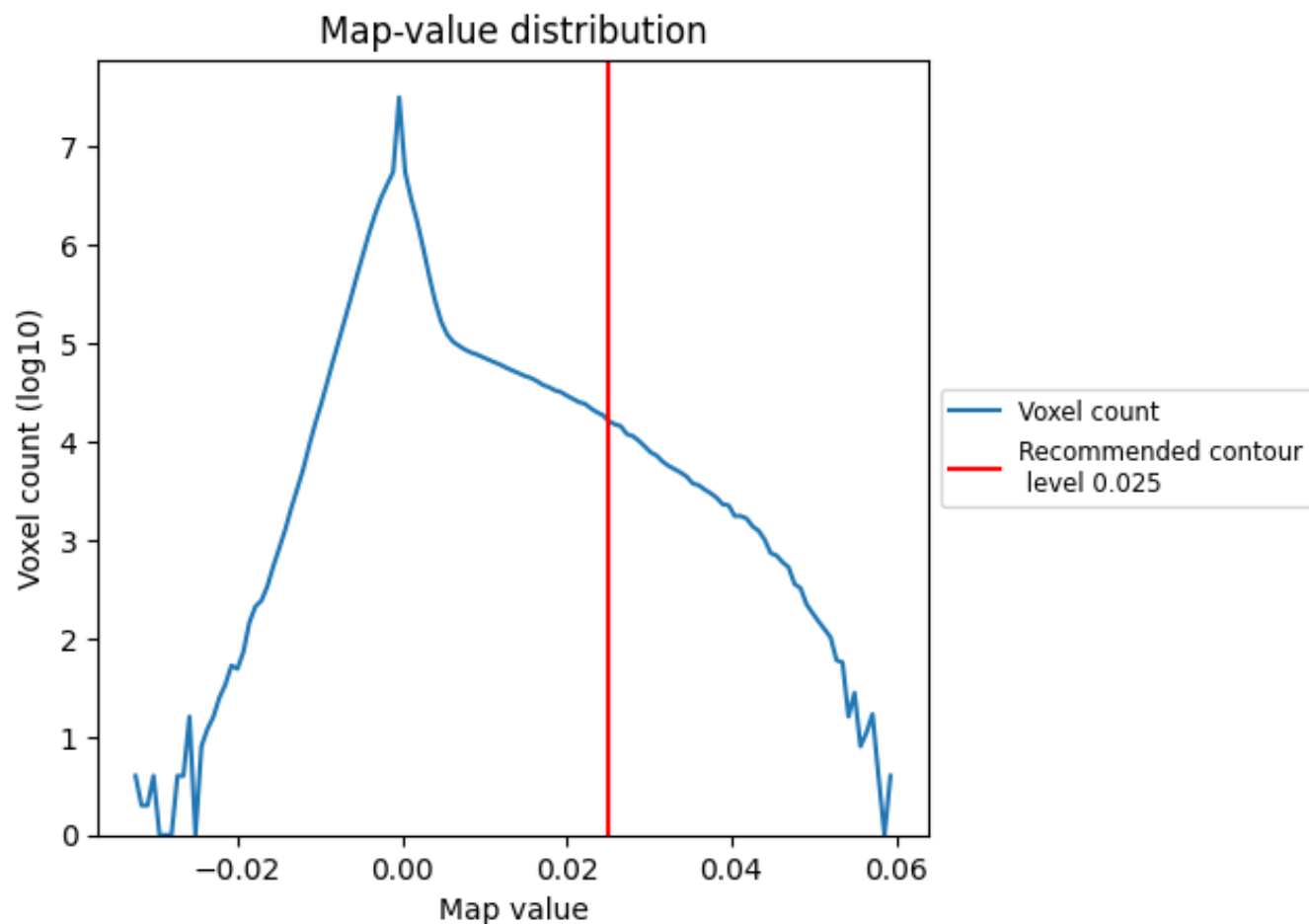
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

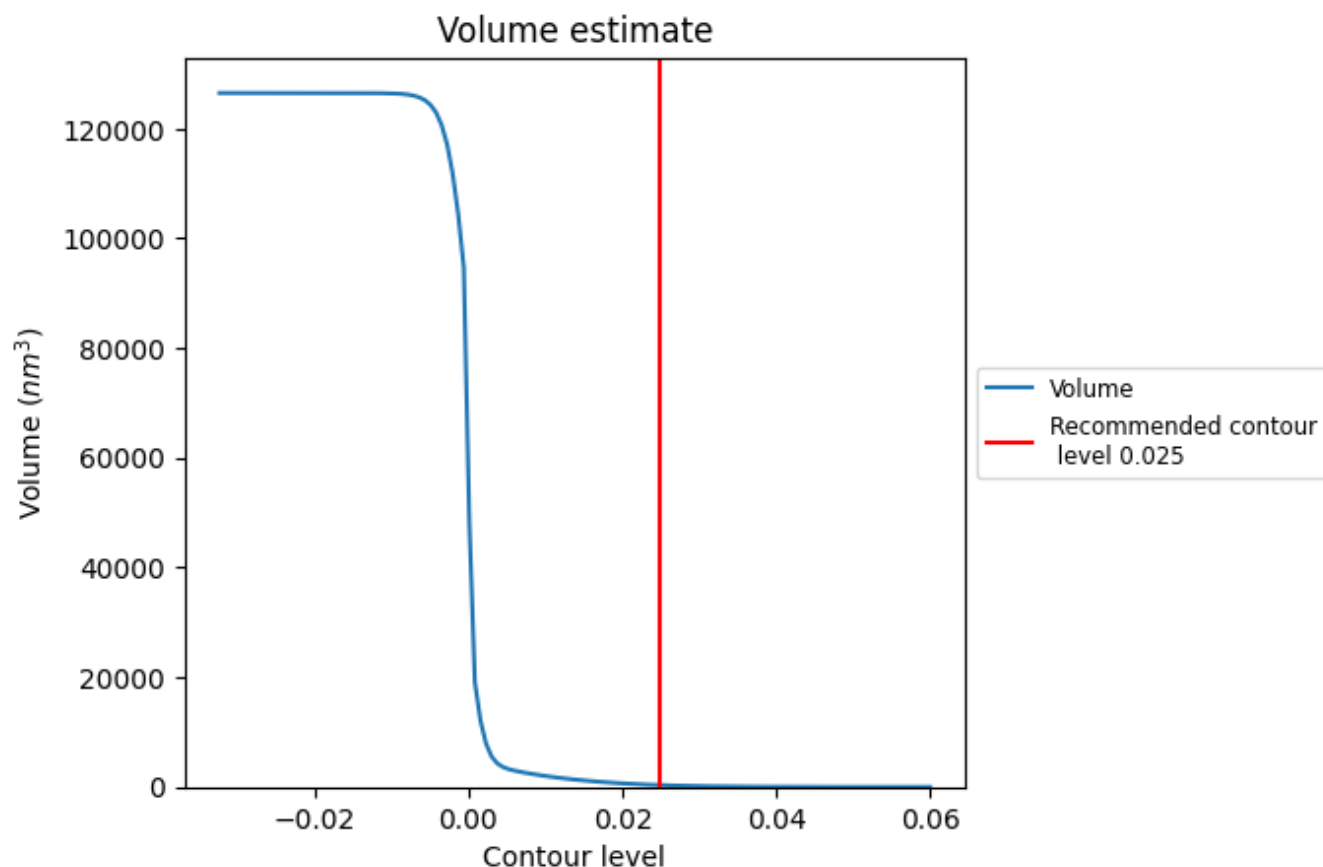
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

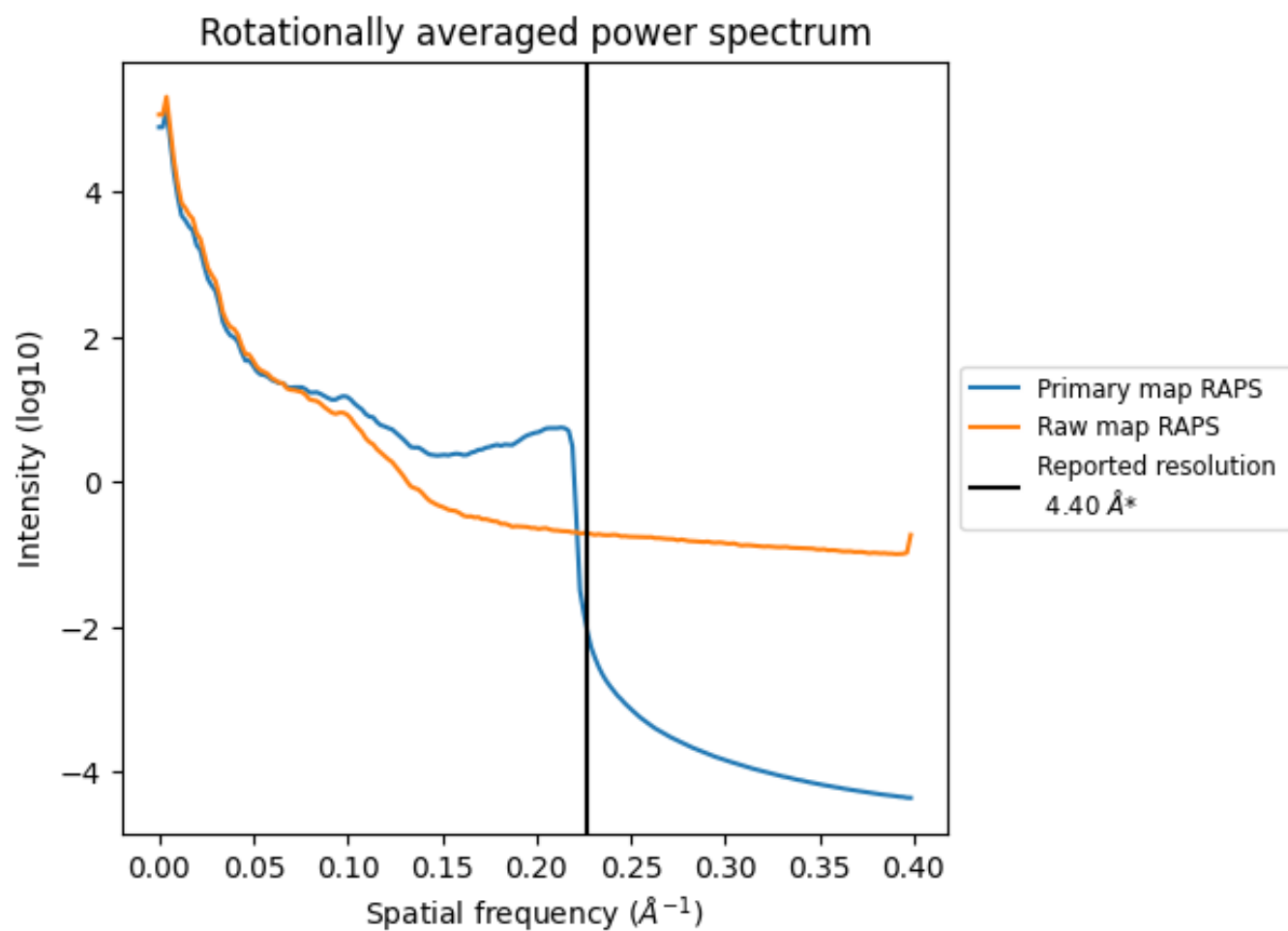
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm^3 ; this corresponds to an approximate mass of 299 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 ⓘ

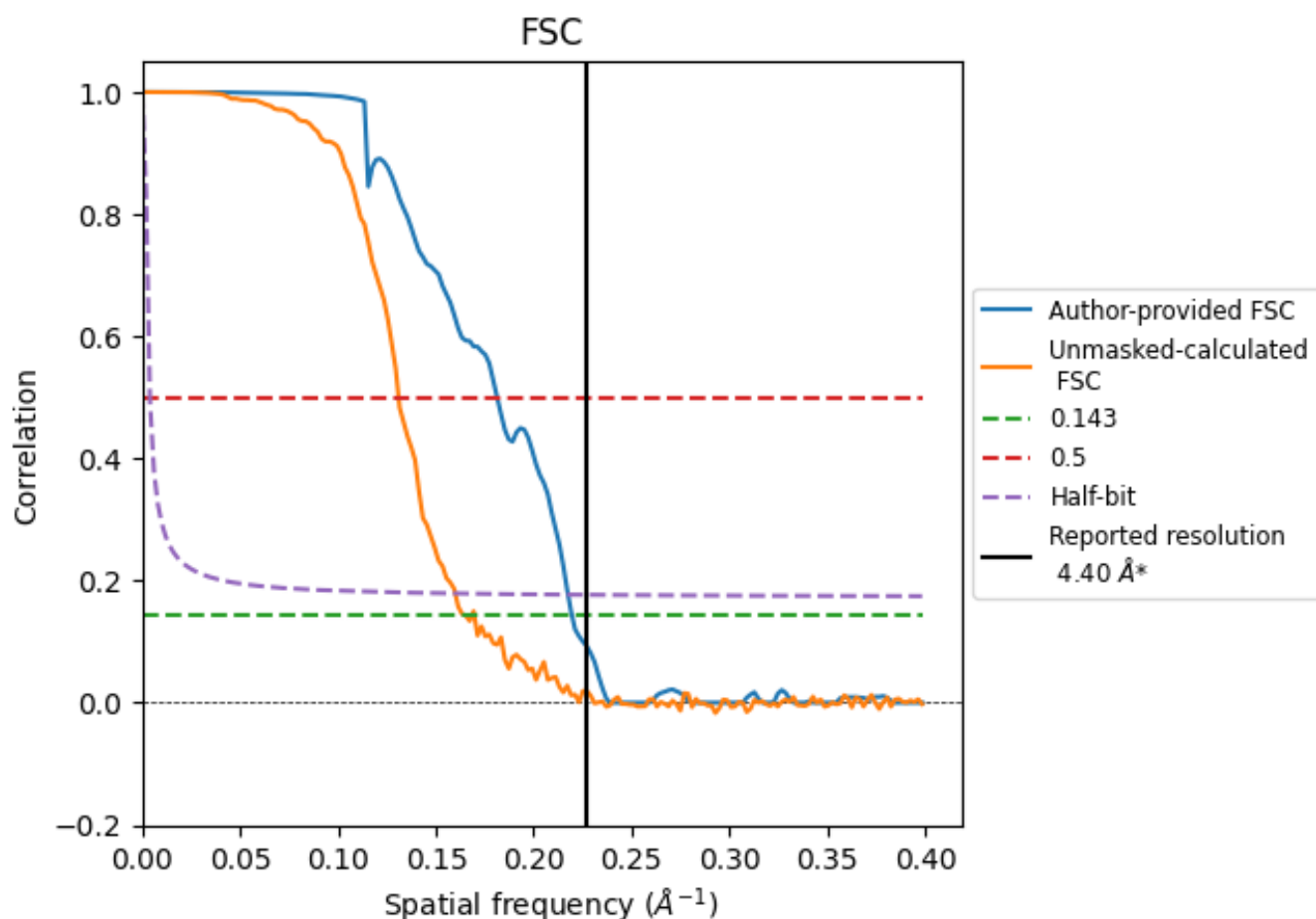


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

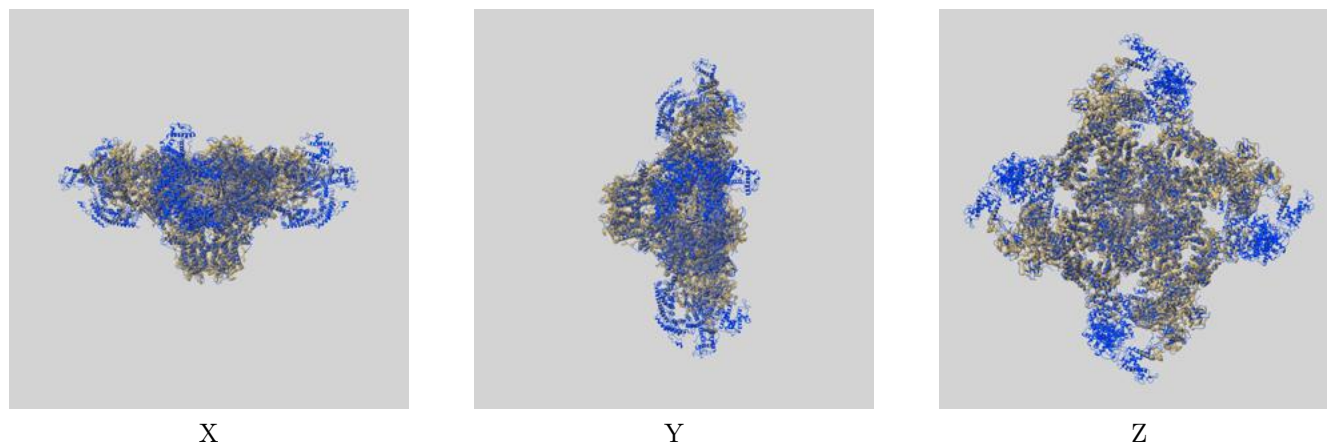
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.56	5.52	4.60
Unmasked-calculated*	6.06	7.64	6.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.06 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

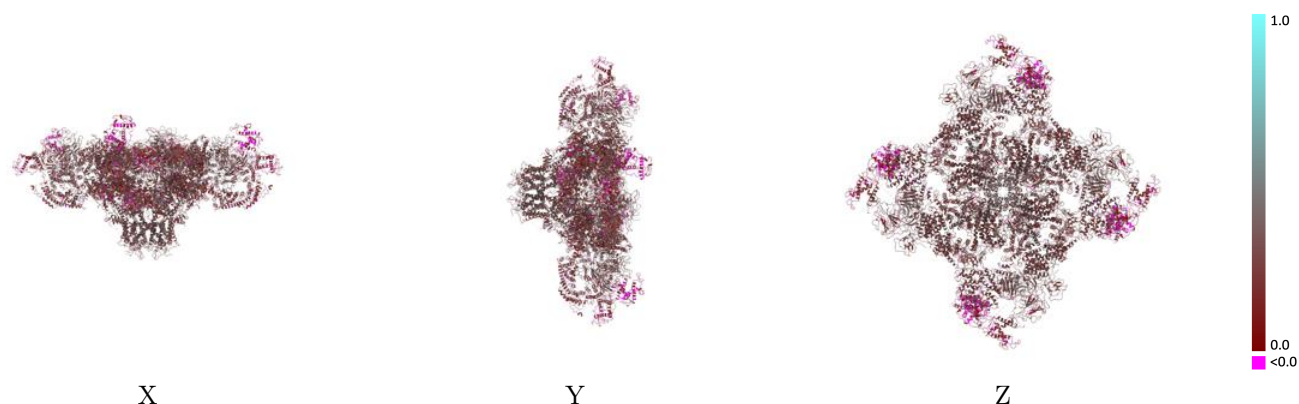
This section contains information regarding the fit between EMDB map EMD-8376 and PDB model 5T9V. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



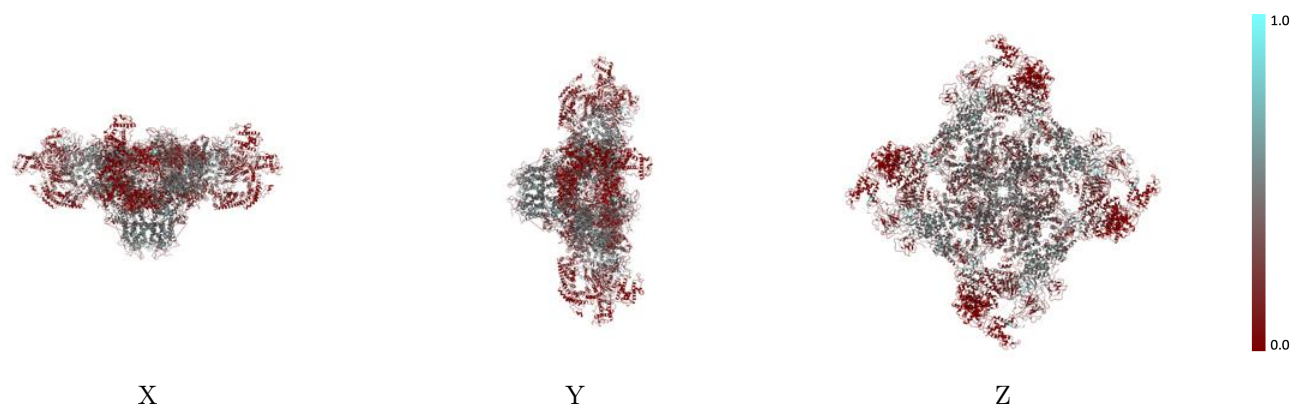
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



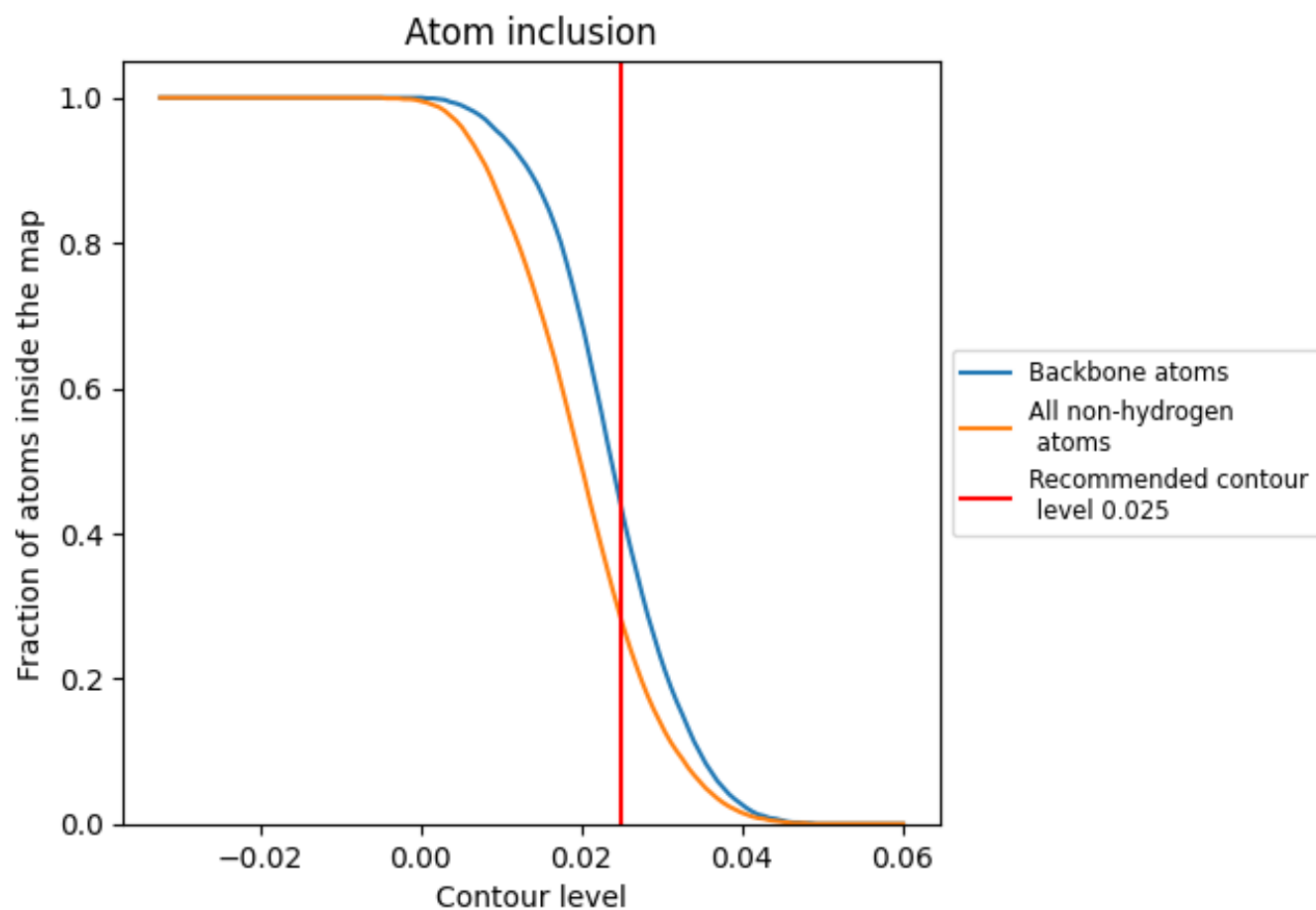
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 28% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2800	0.2680
A	0.2690	0.3040
B	0.2810	0.2690
E	0.2800	0.2650
F	0.2680	0.3070
G	0.2800	0.2680
H	0.2710	0.3040
I	0.2800	0.2660
J	0.2720	0.3050

1.0

0.0

<0.0