



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:45 AM UTC

PDB ID : 5TB3 / pdb_00005tb3
EMDB ID : EMD-8394
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.70 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:

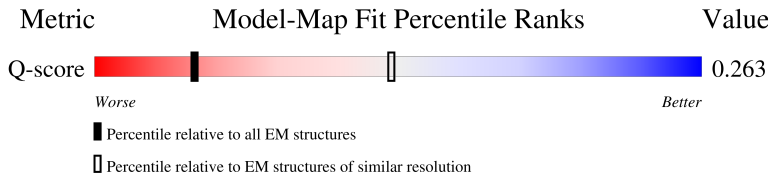
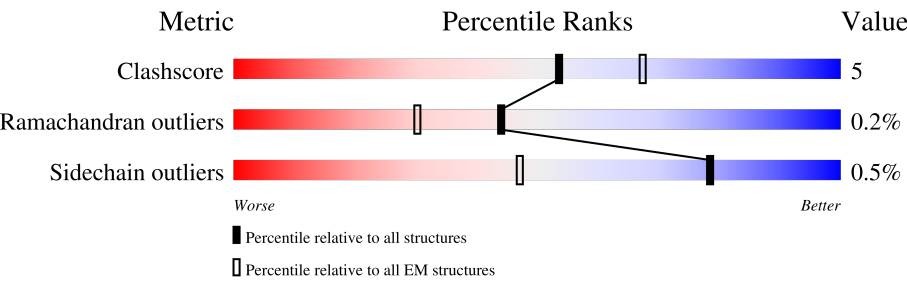
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.70 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	1989 (4.20 - 5.20)

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	4416	66% 83% 12% 5%
2	E	4416	67% 84% 11% 5%
2	G	4416	66% 83% 12% 5%
2	I	4416	67% 83% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121312 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	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	E	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	I	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	G	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		

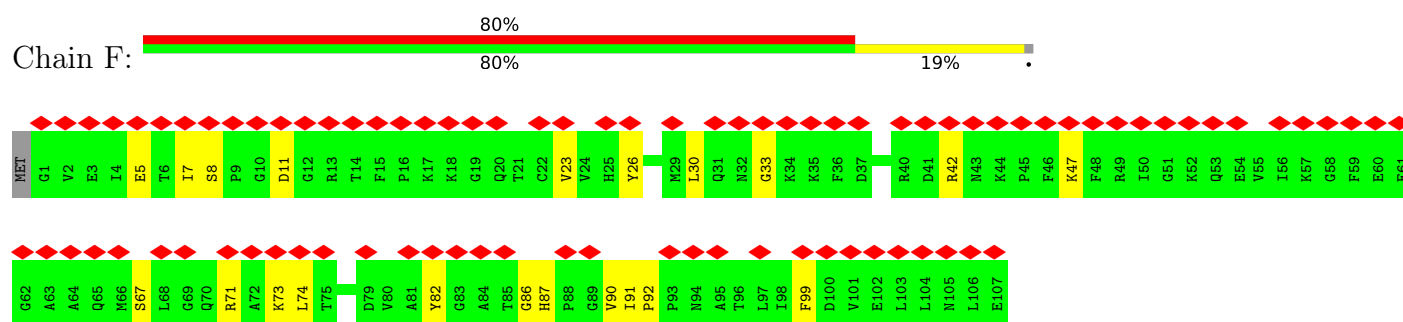
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

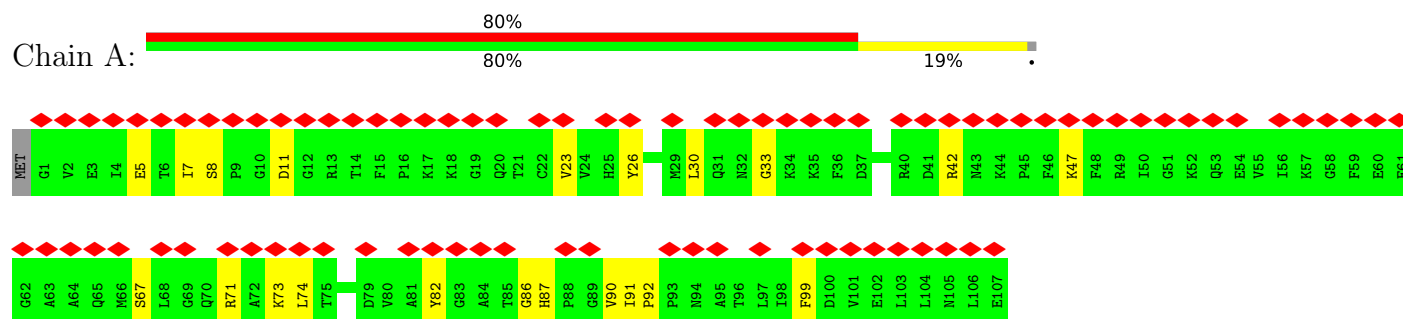
3 Residue-property plots [i](#)

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

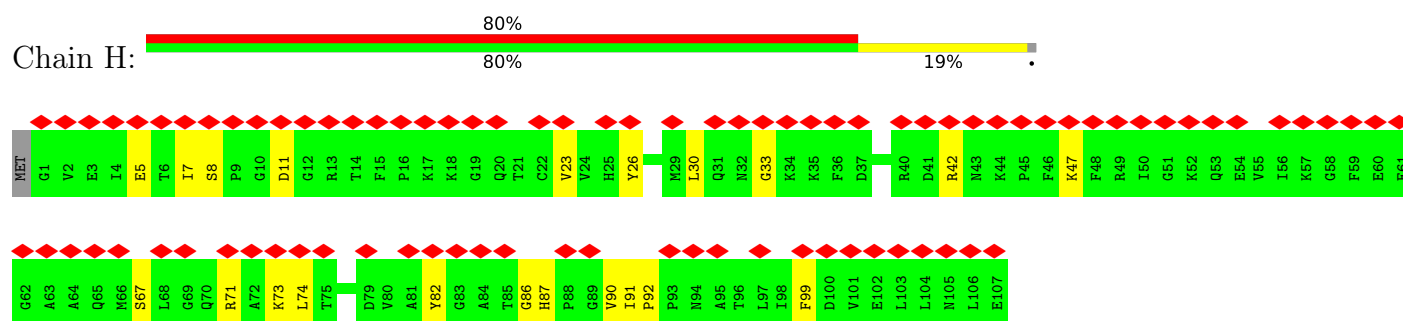
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



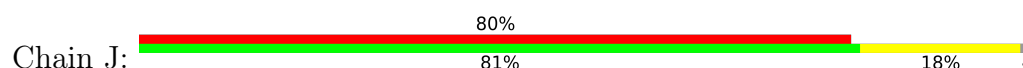
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

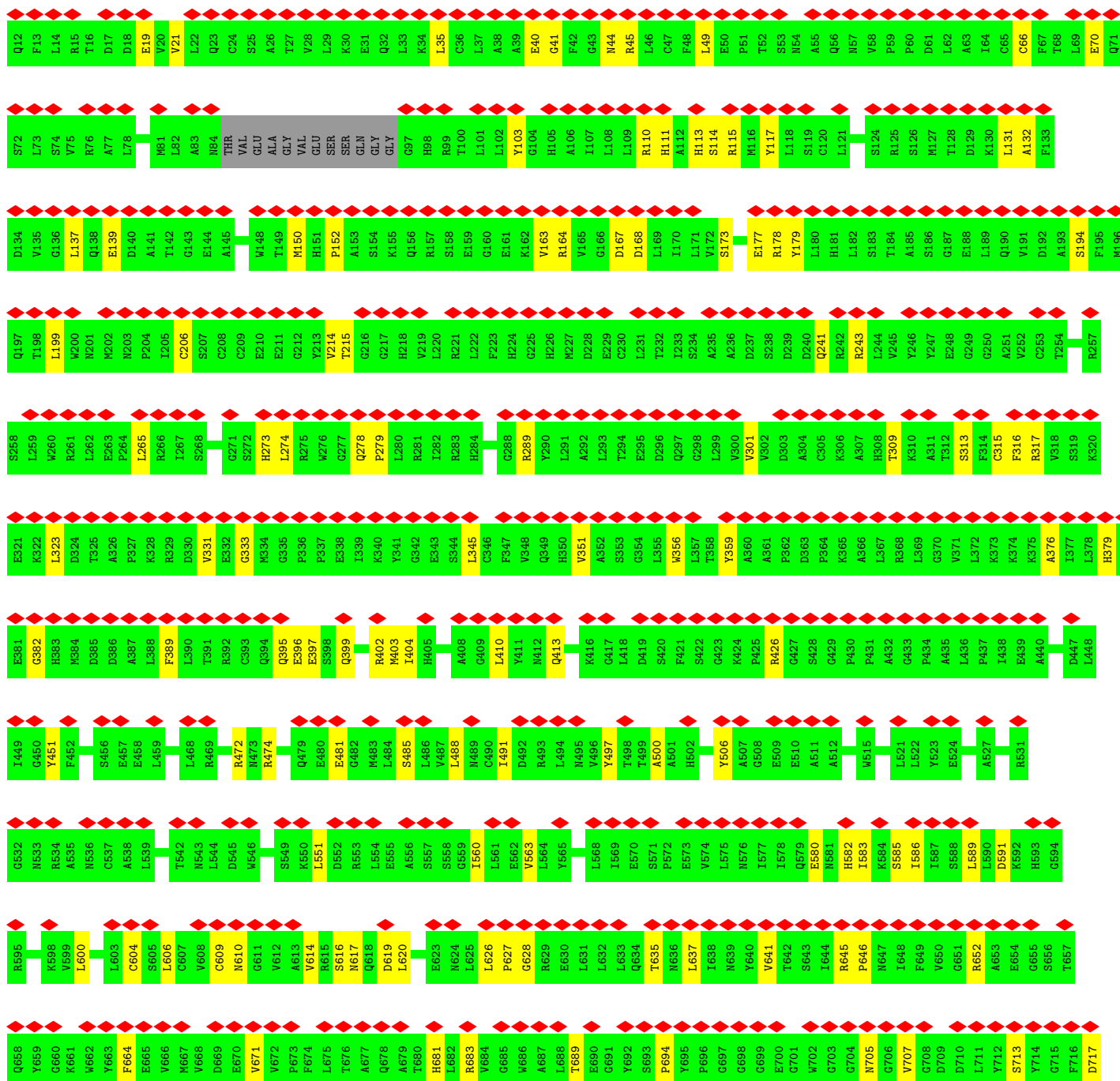


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

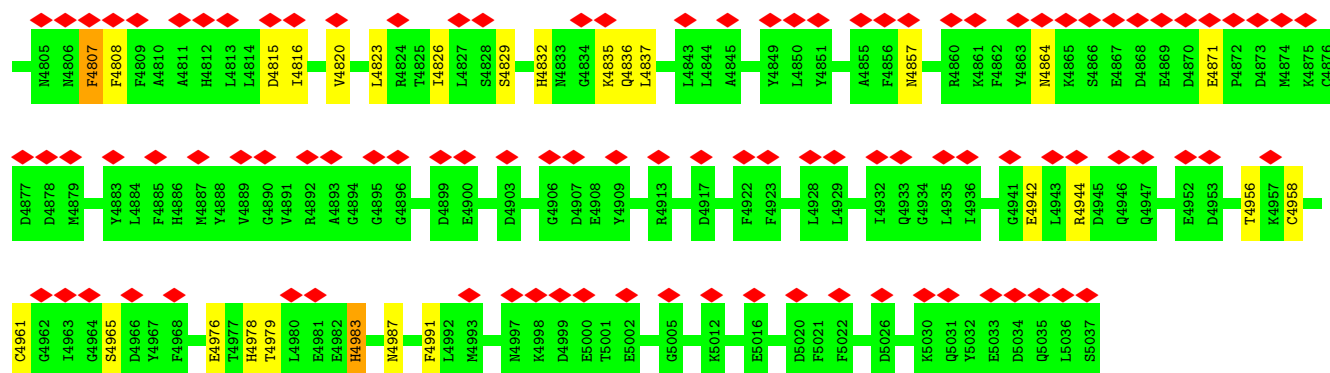


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

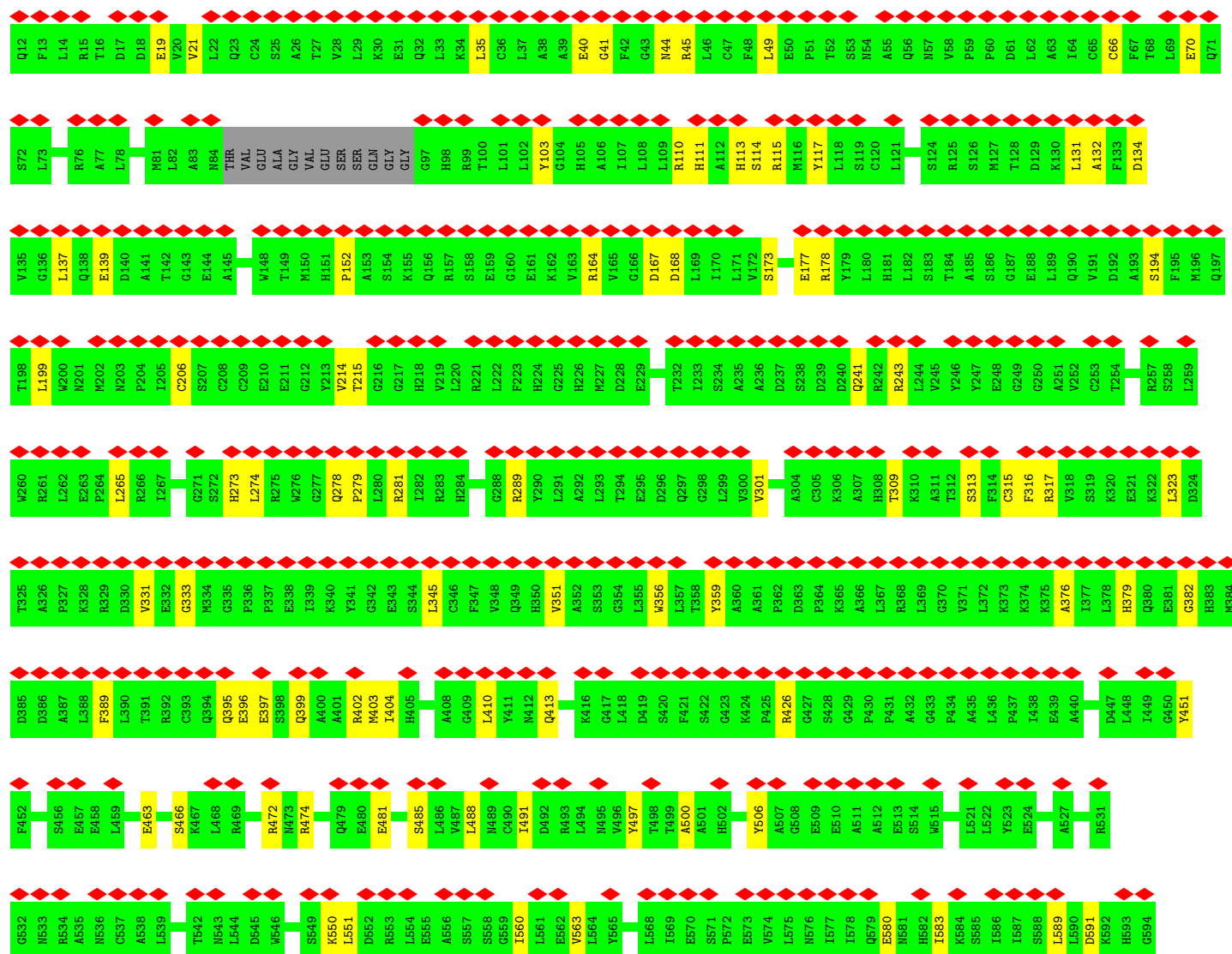
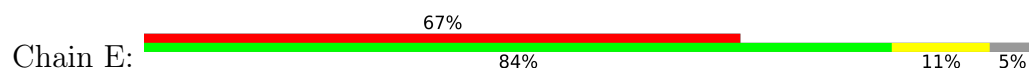




G4733	L4656	GLU	D4022	K3948	L3716	X3559
R4734	C4657	ASP	L4028	R3949	D3717	X3560
E4735	I4658	ASP	L4028	N3950	E3718	X3561
A4738	I4659	GLU	E4032	K3953	D3719	X3562
E4739	S4252	E4032	G4033	A3954	D3720	X3563
L4740	E4253	G4033	G4034	X3955	L3721	X3564
L4741	X4320	D4100	E4034	K3955	Y3722	X3565
L4742	X4321	K4101	G4038	K3959	Y3725	X3566
L4743	X4322	Q4102	F4174	Q3960	A3726	X3567
L4744	X4325	F4103	R4175	Y3961	L3803	X3568
L4745	X4325	T4104	L4040	X3962	L3805	X3569
L4746	X4331	G4105	A4041	X3963	N3806	X3570
L4747	X4331	P4106	E4041	S3964	N3809	X3571
L4748	X4334	E4107	D4046	L3965	L3816	X3572
L4749	X4340	L4108	M4047	T3966	L3817	X3573
L4750	X4341	Q4109	E4050	E3967	K3821	X3574
L4751	X4342	F4110	S4051	Y3968	L3735	X3575
L4752	X4343	L4111	E4056	T3969	D3822	X3576
L4753	X4344	L4112	N4064	Q3970	E3825	X3577
L4754	X4345	S4113	E4055	G3971	Q3830	X3578
L4755	X4345	E4114	M4057	Q3978	Q3833	X3579
L4756	X4346	S4115	I4058	K3984	Q3834	X3580
L4757	X4347	E4116	L4059	L3985	A3834	X3581
L4758	X4348	A4117	E4060	L3986	L3842	X3582
L4759	X4349	D4118	F4061	Y3990	L3843	X3583
L4760	X4350	E4119	D4062	F3991	A3846	X3584
L4761	X4351	N4120	E4063	F3992	Q3850	X3585
L4762	X4352	E4121	M4064	L3993	K3849	X3586
L4763	X4353	L4122	F4065	L3994	Q3850	X3587
L4764	X4354	L4123	L4066	V3995	V3750	X3588
L4765	X4355	N4124	K4067	F3996	V3751	X3589
L4766	X4356	F4125	L4068	A3997	S3752	X3590
L4767	X4357	E4126	K4069	H3998	F3753	X3591
L4768	X4358	E4127	D4070	X3999	E3682	X3592
L4769	X4359	F4128	L4071	N4000	Q3683	X3593
L4770	X4360	A4129	V4072	M4001	E3754	X3594
L4771	X4361	N4130	G4073	K4002	K3756	X3595
L4772	X4362	R4131	S4074	L4003	E3757	X3596
L4773	X4363	Q4132	E4075	L4004	M3758	X3597
L4774	X4364	E4133	A4076	Q4005	E3759	X3598
L4775	X4365	E4134	F4077	D4006	K3760	X3599
L4776	X4366	R4137	Q4078	S4007	R3761	X3600
L4777	X4367	D4138	D4079	S4008	L3762	X3601
L4778	X4368	T4139	Y4080	Q4009	L3763	X3602
L4779	X4369	G4140	V4081	E4011	L3764	X3605
L4780	X4370	F4141	T4082	L4012	Q3766	X3606
L4781	X4371	N4142	D4083	L4013	Q3767	X3607
L4782	X4372	L4147	P4084	K4014	S3768	X3608
L4783	X4373	E4152	R4085	E4015	R3769	X3609
L4784	X4374	H4156	E4088	L4016	L3770	X3610
L4785	X4375	R4159	I4089	L4017	H3771	X3611
L4786	X4376	L4160	K4230	D4018	T3772	X3612
L4787	X4377	E4239	M4231	L4019	G3773	X3613
L4788	X4378	L4233	E4232	Q4020	A3775	X3614
L4789	X4379	D4233	E4239	K4021	E3777	X3615
L4790	X4380	S4583	E4232	K4021	E3777	X3616
L4791	X4381	D4584	E4232	K4021	E3777	X3617
L4792	X4382	S4585	E4232	K4021	E3777	X3618
L4793	X4383	P4586	E4232	K4021	E3777	X3619
L4794	X4384	GLY	E4232	K4021	E3777	X3620
L4795	X4385	GLY	E4232	K4021	E3777	X3621
L4796	X4386	GLY	E4232	K4021	E3777	X3622
L4797	X4387	GLY	E4232	K4021	E3777	X3623
L4798	X4388	GLY	E4232	K4021	E3777	X3624
L4799	X4389	GLY	E4232	K4021	E3777	X3625
L4800	X4390	GLY	E4232	K4021	E3777	X3626
L4801	X4391	GLY	E4232	K4021	E3777	X3627
L4802	X4392	GLY	E4232	K4021	E3777	X3628



• Molecule 2: Ryanodine receptor 1

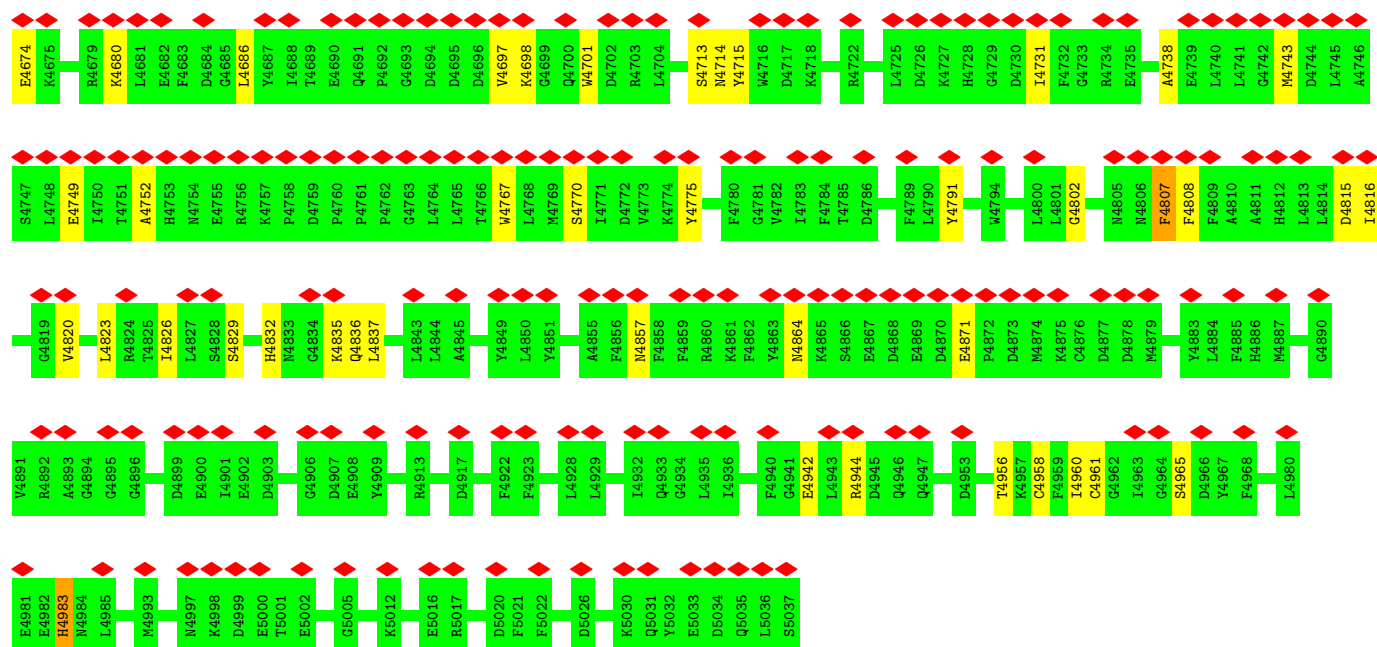


X1504	X1505	X1506	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1517	X1518	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1537	X1538	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1561	X1562	X1563	X1564	X1573	X1574	X1575	X1576	X1577				
X1290	X1291	X1292	X1293	X1294	X1295	X1430	X1431	X1434	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1455	X1456	X1457	X1458	X1459	X1460	X1464	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1484	X1485	X1486	X1487	X1488	X1489	X1492	X1497									
Q1220	E1221	G1222	F1223	E1224	A1227	I1228	Q1231	R1232	T1235	T1236	W1237	F1238	S1239	K1240	S1241	F1245	E1246	E1251	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	P1267	P1268	C1269	L1270	R1271	L1272	A1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1285	X1286	X1287	X1288	X1289							
E1157	M1158	T1159	I1160	T1161	F1162	T1163	L1164	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	T1182	E1183	T1184	G1185	D1186	G1187	F1188	L1189	P1190	V1191	C1192	S1193	L1194	G1195	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216	C1217	G1218	L1219		
T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	T1122	G1123	F1124	N1125	G1126	H1127	R1128	C1192	Q1129	R1131	W1132	H1133	L1134	G1135	S1136	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	V1149	G1150	C1151	M1152	I1153	D1154	L1155	T1156	
N963	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	D999	Q1003	G1004	W1005	S1006	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1026	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033				
L904	H903	P905	C906	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	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M961	S962		
S943	R944	C945	L946	S947	H948	T949	D950	F951	R952	P953	C954	P955	R956	D957	THR	VAL	GLN	I961	V962	L963	P964	P965	H966	L967	E968	R969	I970	R971	E972	K973	L974	A975	E976	N977	I978	H979	E980	L981	A982	A983	L984	T985	R986	I987	E988	Q989	G990	W991	T992	Y993	G994	P995	V996	R997	D998	D999	N990	K901	R902
F783	S784	A785	G786	V787	K788	V789	R790	F791	L792	G793	G794	G795	R796	H797	G798	E799	F900	K901	F902	L903	P904	P905	P906	Y908	A909	P910	C911	H912	E913	A914	V915	L916	P917	R918	E919	R920	L921	R922	L923	E924	P925	I926	K927	E928	Y929	R930	R931	E932	G933	P934	R935	G936	P937	H938	L939	G941	P942		
H720	L721	G724	H725	A727	V726	M728	P729	V730	T731	S732	P733	G734	Q735	H736	L737	L738	F739	T740	P741	E741	S745	C746	C747	L748	D749	L750	S751	V752	P753	S754	I755	S756	F757	R758	I759	N760	G761	C762	P763	V764	G765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	V781	S782	
G660	K661	W662	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	G691	Y692	S693	P694	Y695	P696	G697	G698	G699	E700	G701	W702	G703	G704	N705	G706	I648	F649	V650	G651	R652	A653	E654	G655	S656	T657	Q658	Y659	

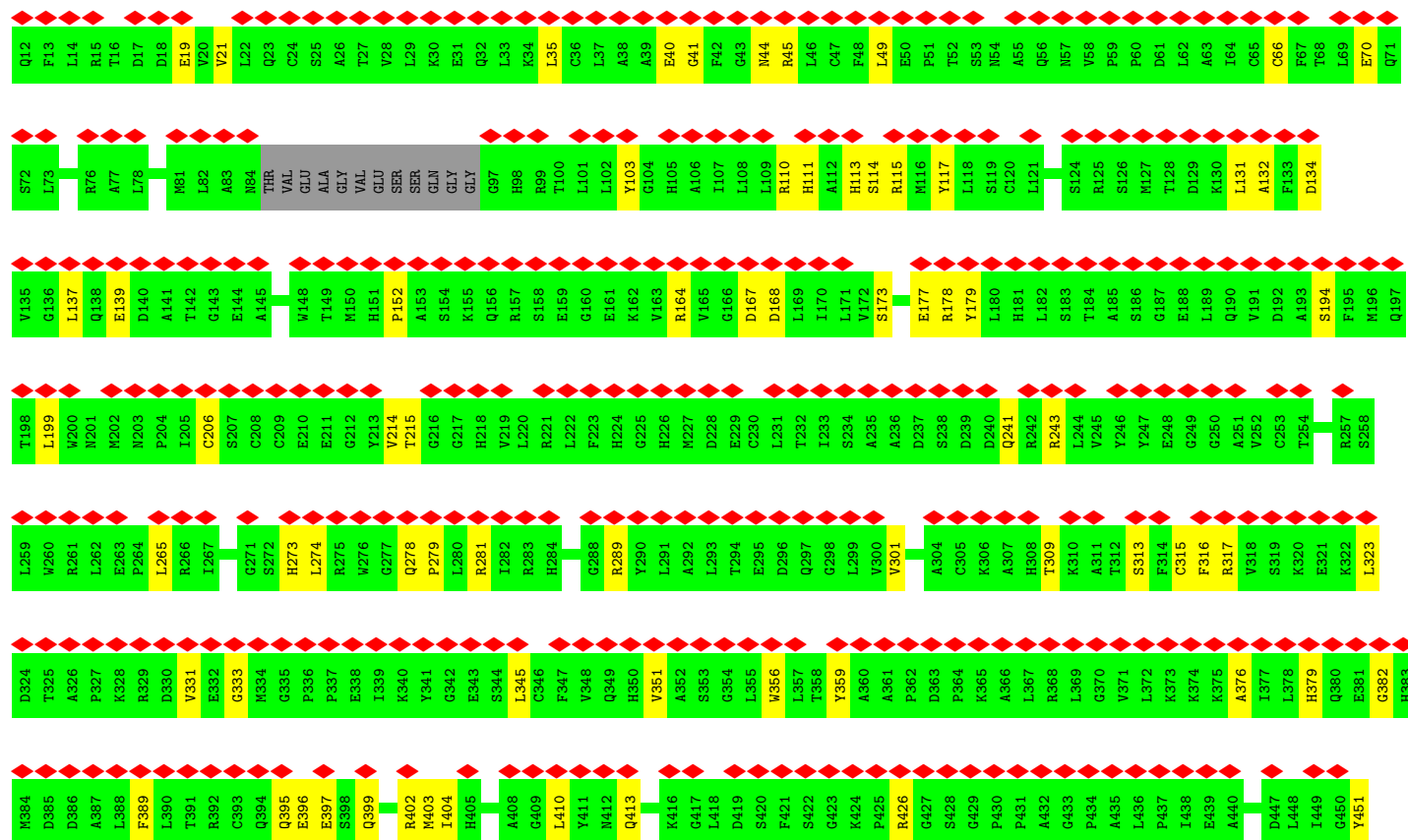
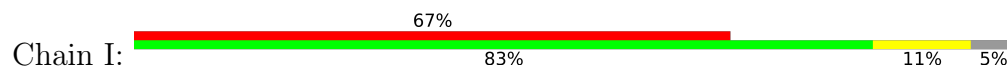


X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401																														
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	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341																													
X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211																													
X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	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
G2934	Y2935	A2936	V2937	T2938	R2939	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	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013												
M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933																														
M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933																														
X2814	A2815	M2816	T2817	A2818	X2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	D2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	V2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	S2867	S2868	R2869	E2870	L2871	Q2872	A2873																																
F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	X2766	X2767	X2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Z2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	D2786	T2787	H2788	T2789	M2790	L2791	R2792	P2793	Y2794	K2795	L2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813																														
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	X2641	X2644	X2645	X2646	X2647	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	R2708	P2709	V2710	E2711	T2712	N2713	V2714	L2715	N2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	E2749	K2750	L2751	D2752	S2753
X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2541	X2542	X2543	X2544	X2550	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601																																		
L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	L2470	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	L2478	L2479	L2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2506	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533																																		

ALA	X3402	X3467	X3657	X3731	X3809	X3889	X3963	D4046	Q4109	M4184	G4185	X4334	ALA
GLY	X3403	X3468	X3658	X3732	X3816	X3890	T3966	M4047	F4110	G4186	A4187	X4340	GLY
SER	X3404	X3511	A3660	C3733	L3817	L3891	X3967	E4050	L4111	A4188	S4187	X4341	GLY
GLY	X3405	X3512	W3661	H3734	X3821	C3892	X3968	S4051	L4112	R4189	R4188	X4342	GLY
SER	X3406	X3513	I3662	L3735	D3822	E3893	T3969	M4054	S4113	R4190	S4187	X4343	GLY
TRP	X3407	X3514	L3663	E3736	X3827	X3896	X3970	G3971	C4114	S4115	R4189	X4344	GLY
GLY	X3408	X3515	T3664	X3737	X3827	N3897	G3978	M4054	S4116	S4115	R4189	X4345	GLY
GLY	X3409	X3516	E3665	G3738	X3825	X3897	X3978	M4057	A4117	E4191	E4191	X4346	GLY
GLY	X3410	X3517	D3666	X3739	X3826	X3898	X3978	L4058	D4118	E4192	R4189	F4540	GLY
ALA	X3411	X3518	H3667	G3740	G3827	X3900	X3978	K4060	E4119	E4192	E4192	W4541	GLY
GLY	X3412	X3519	S3668	N3741	Q3830	X3901	R3884	F4061	M4120	E4196	E4196	G4542	GLY
GLY	X3413	X3520	F3669	GLU	S3831	Y3902	L3985	F4062	E4121	I4197	I4197	G4542	GLY
ALA	X3414	X3521	X3670	ALA	X3832	L3903	W3986	D4063	M4122	S4198	S4198	E4543	GLY
GLY	X3415	X3522	X3671	GLU	Q3833	R3904	X3986	M4064	I4123	E4199	E4199	L4544	GLY
ASP	X3416	X3523	R3672	GLU	A3834	T3905	Y3990	M4064	M4124	T4200	T4200	E4545	GLY
GLY	X3417	X3524	X3673	E3747	X3842	Q3906	G3991	F4065	M4125	N4201	N4201	V4546	GLY
ASP	X3418	X3525	E3748	X3748	L3842	X3906	F3992	L4066	F4126	R4202	R4202	Q4547	GLY
ASP	X3419	X3526	D3675	X3749	D3843	T3910	L3993	K4067	E4127	A4203	A4203	R4548	GLY
GLU	X3420	X3527	X3676	X3750	X3846	X3912	V3995	L4068	E4128	Q4204	Q4204	F4551	GLY
GLU	X3421	X3528	X3676	X3751	X3846	X3913	F3996	L4068	A4129	W4205	W4205	Y4551	GLY
X3422	X3529	X3591	X3679	X3752	R3849	I3913	X3997	D4070	M4130	E4206	E4206	F4551	GLY
X3423	X3530	X3592	X3679	F3753	Q3850	C3918	H3998	I4071	M4131	A4207	A4207	Y4551	GLY
X3427	X3531	X3593	X3681	E3754	N3851	D3921	M4000	I4072	F4131	Q4208	Q4208	Y4554	GLY
X3428	X3532	X3595	Q3683	E3755	X3852	X3921	M4001	G4073	F4132	Q4209	Q4209	L4555	GLY
X3429	X3533	X3596	Q3684	X3756	X3853	R3926	K4002	S4074	Q4133	E4211	E4211	S4556	GLY
X3430	X3534	X3597	E3685	E3757	E3854	X3928	L4003	E4075	E4134	E4212	E4212	R4557	GLY
X3431	X3535	X3598	E3686	M3758	E3854	E3928	A4004	A4076	R4137	R4215	R4215	L4562	GLY
X3432	X3536	X3598	E3686	X3759	G3855	E3928	A4004	F4077	D4138	F4219	F4219	L4567	GLY
X3433	X3537	X3599	E3687	X3760	L3856	X3932	Q4005	Q4078	L4139	F4219	F4219	F4568	GLY
X3434	X3538	X3600	E3688	X3761	X3857	F3933	D4006	D4079	C4140	G4223	G4223	F4571	GLY
X3435	X3539	X3601	E3689	R3762	M3858	Y3934	S4007	Y4080	F4141	E4224	E4224	A4572	GLY
X3436	X3540	X3602	V3690	X3763	V3860	W3935	S4008	V4081	M4142	G4225	G4225	I4573	GLY
X3437	X3541	X3603	E3691	L3764	X3860	Y3936	Q4009	T4082	F4147	G4226	G4226	M4574	GLY
X3438	X3542	X3604	E3692	X3765	X3861	X3937	D4010	D4083	L4147	E4227	E4227	I4575	GLY
X3439	X3543	X3607	X3693	X3766	D3862	S3938	E4011	P4084	E4152	A4228	A4228	I4576	GLY
X3440	X3544	X3607	X3693	X3767	G3863	G3939	L4012	R4085	H4153	E4229	E4229	I4577	GLY
X3441	X3545	X3608	H3704	S3768	T3864	X3940	L4013	G4086	H4153	E4229	E4229	W4582	GLY
X3442	X3546	X3609	H3704	L3770	V3865	D3941	K4014	L4087	H4156	E4230	E4230	S4583	GLY
X3443	X3547	X3610	S3706	H3771	X3866	V3942	E4015	S4089	H4156	E4231	E4231	D4584	GLY
X3446	X3548	X3611	R3707	X3772	X3867	I3943	L4016	L4089	R4159	E4232	E4232	S4585	GLY
X3447	X3549	X3612	R3707	X3773	X3868	E3944	L4017	K4090	L4160	E4233	E4233	S4586	GLY
X3448	X3550	X3613	T3711	X3774	X3869	E3945	D4018	K4091	R4161	E4239	E4239	P4587	GLY
X3449	X3551	X3613	E3712	A3776	N3870	Q3946	L4019	D4092	R4162	E4239	E4239	GLY	GLY
X3450	X3552	X3613	E3713	X3777	G3871	X3947	Q4020	F4093	F4163	Q4250	Q4250	GLY	GLY
X3451	X3553	X3614	S3714	X3778	X3872	K3948	K4021	Q4094	L4164	I4251	I4251	ASP	ASP
X3452	X3554	X3614	R3642	M3778	E3873	R3949	D4022	K4095	L4166	S4252	S4252	GLY	GLY
X3453	X3555	X3615	X3643	X3779	X3874	N3950	L4028	M4097	L4167	E4253	E4253	GLY	GLY
X3454	X3556	X3616	L3644	X3715	X3875	X3953	L4028	M4097	L4167	X4320	X4320	GLY	GLY
X3455	X3557	X3617	D3716	L3716	X3876	K3953	E4032	M4097	L4167	X4321	X4321	GLY	GLY
X3456	X3558	X3618	P3645	D3717	X3876	A3954	E4033	M4097	L4167	X4322	X4322	GLY	GLY
X3457	X3559	X3619	H3647	D3718	X3877	M3955	Q4034	M4097	L4167	X4323	X4323	GLY	GLY
X3458	X3560	X3620	H3647	E3719	D3878	X3959	M4034	M4097	L4167	X4324	X4324	GLY	GLY
X3459	X3561	X3621	X3648	L3721	E3879	Q3960	Q4038	M4097	L4167	X4325	X4325	GLY	GLY
X3460	X3562	X3622	A3649	Y3722	F3880	V3961	Q4038	M4097	L4167	X4326	X4326	GLY	GLY
X3464	X3563	X3623	C3650	Y3722	T3881	F3962	Q4038	M4097	L4167	X4327	X4327	GLY	GLY
X3465	X3564	X3624	N3651	Y3725	L3805	F3962	Q4038	M4097	L4167	X4328	X4328	GLY	GLY
X3466	X3565	X3625	F3653	M3729	N3806	F3962	Q4038	M4097	L4167	X4329	X4329	GLY	GLY
X3467	X3566	X3626	L3654	A3730	X3886	F3962	Q4038	M4097	L4167	X4330	X4330	GLY	GLY

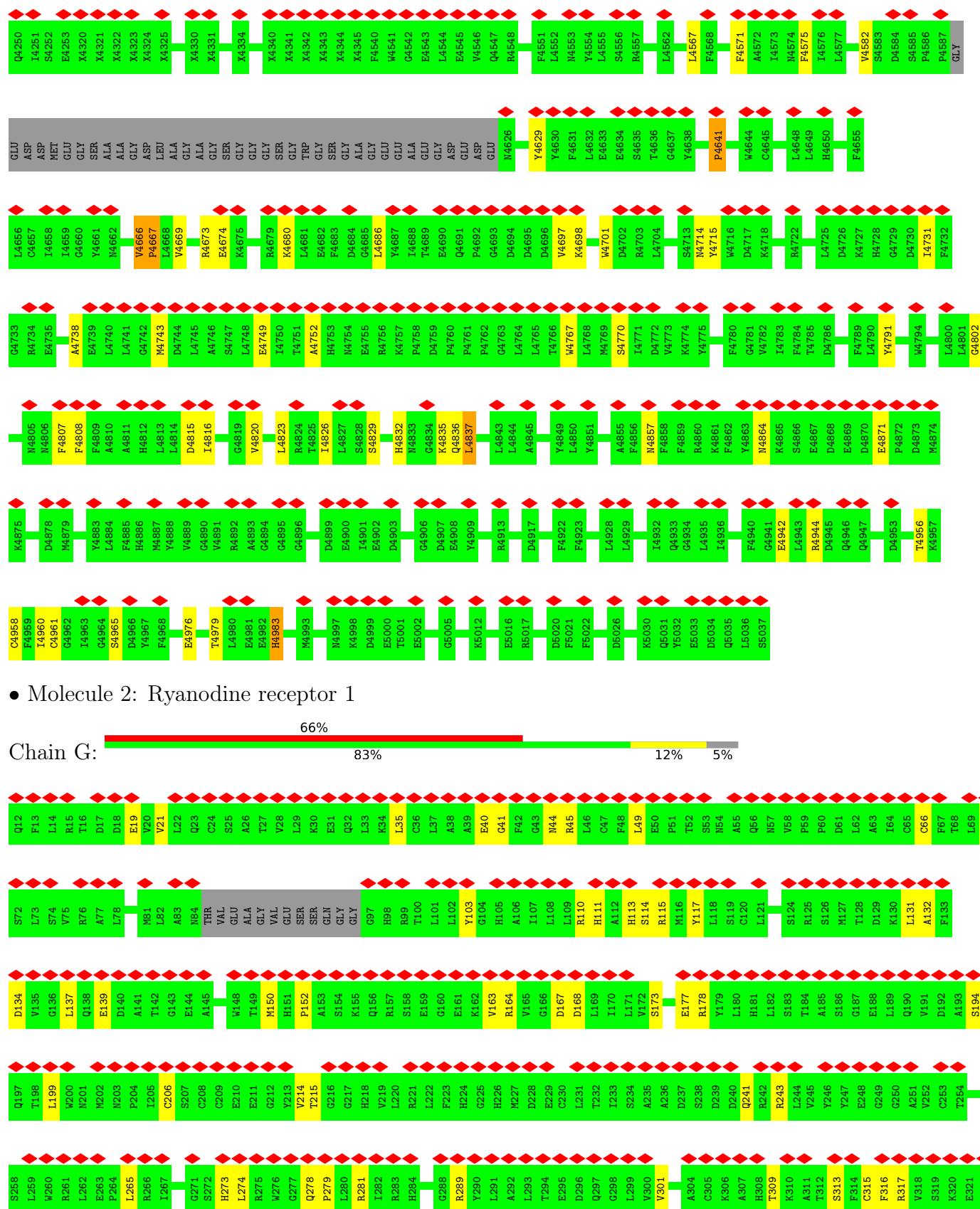


• Molecule 2: Ryanodine receptor 1





E4165	E4166	L4166	A4167	E4168	S4169	E4172	E4173	F4174	R4175	P4176	R4180	N4184	G4185	A4186	S4187	R4188	R4189	I4190	E4191	R4192	E4196	I4197	S4198	E4199	T4200	N4201	R4202	I4203	N4204	W4205	E4206	N4207	P4208	Q4209	V4210	E4211	E4212	R4215	F4219	N4223	E4224	G4225	G4226	E4227	A4228	E4229	R4230	W4231	E4232	L4233	E4239										
K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	I4107	I4108	Q4109	F4110	L4111	L4112	S4113	C4114	S4115	E4116	D4117	A4118	L4119	E4119	N4120	E4121	M4122	I4123	N4124	F4125	E4126	E4127	F4128	A4129	V4072	G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	S4088	K4089	K4090	K4091	L4156	R4159	L4160	R4161	F4093	Q4094
K4021	D4022	L4028	E4032	G4033	N4034	G4038	M4039	I4040	A4041	D4046	M4047	E4050	S4051	M4054	M4057	I4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072	G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	S4088	K4089	K4090	K4091	L4019	Q4020										
G3947	K3948	E3949	N3950	K3953	A3954	L3955	K3959	V3961	F3962	N3963	S3964	L3965	T3966	E3967	Y3968	I3969	Q3970	Q3971	Q3978	R3984	L3985	V3986	V3990	F3992	L3993	H3994	V3995	F3996	K3997	H3998	K3999	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	S4007	S4008	Q4009	I4010	E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	L4019	Q4020									
M3875	A3876	D3877	E3878	F3880	Q3881	Q3882	D3883	R3886	Q3889	L3890	L3891	C3892	E3893	N3896	N3897	D3898	F3899	Q3900	N3901	Y3902	L3903	R3904	T3905	Q3906	T3910	T3911	T3912	I3913	C3918	D3921	R3925	L3926	Q3927	E3928	S3931	D3932	F3933	Y3934	V3935	Y3936	Y3937	S3938	G3939	K3940	D3941	V3942	R3943	E3944	E3945	Q3946											
L3780	S3785	K3799	S3803	L3804	L3805	N3806	N3809	M3816	L3817	K3821	D3822	E3825	V3826	G3827	Q3830	S3831	I3832	Q3833	A3834	L3842	D3843	A3846	R3849	Q3850	N3851	K3852	A3853	E3854	G3855	L3856	C3857	H3858	V3859	N3860	E3861	D3862	C3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	C3871	E3872	K3873	V3874													
D3717	E3718	D3719	Y3720	L3721	Y3722	Y3725	M3729	A3730	K3731	S3732	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	D3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	E3759	K3760	Q3761	R3762	L3763	L3764	Y3765	Q3766	Q3767	S3768	R3769	L3770	H3771	T3772	R3773	G3774	A3775	C3776	H3777	V3779						
T3646	H3647	R3648	C3649	C3650	N3651	K3652	F3653	L3654	E3655	S3656	Y3657	K3658	A3659	A3660	W3661	L3662	T3663	T3664	E3665	G3666	H3667	S3668	F3669	E3670	D3671	K3672	R3673	L3674	D3675	D3676	K3679	A3680	Q3681	E3682	K3683	E3684	E3685	E3686	E3687	K3688	E3689	E3690	V3690	E3691	Y3692	Q3693	L3703	H3704	F3705	S3706	R3707	T3711	E3712	K3713	S3714	K3715	L3716				
X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	T3639	P3640	L3641	Y3642	N3643	L3644	P3645				
X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557			
X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453				
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	X3384	X3385	X3386	X3387	X3388	X3389	X3390		
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	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330			



L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	G335	P336	P337	E338	I339	K340	Y341	G342	E343	S344	L345	C346	F347	V348	Q349	H350	V351	A352	S353	G354	L355	W356	L357	T358	Y359	A360	A361	P362	P363	D364	K365	A366	L367	R368	L369	G370	V371	L372	K373	K374	K375	A376	I377	L378	H379	Q380	E381	G382
H383	M384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	Q395	E396	E397	S398	Q399	R402	M403	I404	H405	A408	G409	L410	Y411	M412	Q413	K416	G417	L418	D419	S420	F421	S422	G423	K424	P425	R426	G427	S428	G429	P431	A432	G433	P434	A435	L436	P437	I438	E439	A440	D447	L448	I449	G450					
Y451	F452	S456	E457	E458	L459	E463	S466	L467	L468	R469	R472	M473	R474	Q479	E480	E481	S485	L486	V487	L488	M489	G490	I491	D492	R493	L494	T498	T499	A500	A501	H502	Y506	A507	G508	E509	E510	A511	A512	E513	S514	W515	L521	L522	Y523	E524	A527	L521	L522	Y523	E524	A527	L521	L522	Y523	E524	A527			
R531	G532	N533	R534	A535	N536	C537	A538	L539	T542	N543	L544	D545	W546	S549	K550	L551	D552	R553	L554	E555	A556	S557	S558	G559	I560	L561	E562	V563	L564	L568	I569	E570	S571	P572	E573	V574	L575	N576	I577	I578	Q579	E580	N581	H582	I583	K584	S585	L586	I587	S588	L589	D591	K592	H593					
G594	R595	K598	G600	L600	L603	C604	S605	L606	C607	V608	C609	N610	G611	V612	A613	R615	S616	Q618	D619	L620	E623	N624	L625	L626	P627	G628	R629	L631	L632	L633	Q634	T635	N636	L637	T638	N639	Y640	V641	T642	S643	L644	R645	P646	N647	T648	F649	V650	G651	R652	Y651	A653	E654	G655						
T657	Q658	Y659	G660	T661	W662	Y663	F664	E665	V666	W667	W668	D669	E670	V671	V672	P673	F674	L675	S676	A677	Q678	A679	T680	H681	L682	R683	V684	G685	W686	A687	L688	T689	E690	G691	Y692	S693	P694	Y695	P696	W697	T698	G699	E700	G701	W702	G703	G704	W705	G706	T707	G708	D709	D710	L711	Y712	S713	Y714	G715	F716
D717	G718	L719	H720	L721	G724	H725	V726	A727	R728	F729	W730	T731	S732	F733	G734	Q735	H736	L737	A739	P740	E741	S745	C746	G747	L748	L750	S751	V752	F753	S754	I755	S756	F757	Y758	L759	W760	G761	G762	C763	V764	G765	G766	V767	F768	E769	A770	F771	W772	L773	D774	G775	L776	F777	F778	P779				
V780	V781	S782	F783	S784	A785	G786	W787	K788	W789	R790	F791	L792	L793	G794	G795	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809	H812	E813	A814	W815	L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	L826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	Y840	
G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	W852	P853	C854	P855	W856	D857	THR	VAL	GLN	I861	W862	L863	P864	P865	H866	L867	R869	T870	R871	E872	K873	L874	A875	E876	R877	L878	H879	E880	L881	W882	A883	T885	R886	L887	R888	Q889	C890	W891	T892	Y893	C894	P895	W896	R897	D898	D899	N900		
K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	E927	T928	L929	K930	T931	L932	L933	A934	L935	Q936	C937	H938	V939	G940	Y941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	Y959	N960		
M961	S962	N963	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	D999	Q1003	G1004	W1005	Y1007	S1008	VAL	GLN	ASP	ILE	PRD	ALA	ARG	ARG	ASN	PRD	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	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	T1052	T1053	E1054	PRD	PRD	ASP	GLN	GLU	PRD	GLN	VAL	E1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	Y1089	F1090	E1091	F1092	M1152									
E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	P1110	P1111	D1112	V1113	E1114	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	M1125	G1126	H1127	R1128	S1006	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	Y1089	F1090	E1091	F1092	M1152				



X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	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
L2927	K2928	F2929	L2930	M2931	M2932	N2933	G2934	N2935	A2936	V2937	T2938	R2939	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	X3003	X3004	X3005	X3006																																																			
L2867	S2868	R2869	E2870	L2871	L2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	K2892	E2893	L2894	E2895	L2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	T2909	T2910	T2911	T2912	A2913	K2914	E2915	K2916	L2917	S2918	R2919	D2920	E2921	K2922	A2923	Q2924	E2925	L2926																																																																					
W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	L2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866																																																																								
L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	E2759	E2760	Y2761	T2762	H2763	E2764	K2765	V2766	F2767	E2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	L2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	R2800	D2801	K2802	E2803	Y2805	R2806																																																																						
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	X2641	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655																																																																						
X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2541	X2542	X2543	X2544	X2550	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590	X2593																																																																									
T2453	R2454	A2455	L2456	R2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	I2469	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2506	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526																																																																										
A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HTS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	R2415	L2416	H2417	L2418	G2419	H2420	A2421	L2422	N2423	S2424	F2425	V2426	A2427	T2430	D2431	L2432	L2433	G2434	R2435	C2436	A2437	P2438	E2439	M2440	H2441	L2442	A2445	G2446	G2447	G2448	E2449	L2451	R2452																																																																											
G2328	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	A2338	V2339	P2340	N2342	G2343	E2344	S2345	V2346	E2347	N2348	N2349	A2350	R2355	L2356	L2357	L2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	G2369	C2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	T2380	E2381	E2382	L2383	L2384	R2385	L2386	S2387	E2388	D2389	P2390																																																																							
G2264	L2265	G2266	M2267	Q2268	D2269	S2270	T2271	P2272	L2273	D2274	E2275	A2276	A2277	A2278	S2279	V2280	I2281	D2282	N2283	N2284	E2285	L2288	A2289	L2290	Q2291	E2292	Q2293	D2294	L2295	E2296	K2297	S2300	Y2301	L2302	A2303	G2304	C2305	G2306	G2307	G2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	K2316	G2317	Y2318	P2319	D2320	L2321	P2325	G2326	G2327																																																																								
Y2192	P2195	N2196	L2199	A2200	L2201	H2204	M2208	E2209	V2210	N2213	G2216	G2217	G2218	E2219	T2220	K2221	E2222	L2223	R2224	F2225	P2226	H2228	V2229	T2230	S2231	R2234	F2235	V2238	F2239	S2243	R2244	Q2245	N2246	Q2247	R2248	S2249	N2250	F2251	D2252	H2253	V2256	L2257	L2258	E2259	N2260	S2261	G2262	L2263																																																																																

Q4038	K3959	L3886	L3805	L3721	C3650	X3562	X3458	X3395	X3274	X3204	X3138
Q4039	Q3960	L3889	M3806	Y3722	N3651	X3563	X3459	X3396	X3275	X3205	X3139
L4040	F3962	L3890	N3809	M3729	M3652	X3564	X3460	X3397	X3276	X3206	X3140
N3963	S3964	L3891	M3816	A3730	F3653	X3565	X3464	X3398	X3277	X3207	X3141
L3965	C3892	L3892	L3817	K3731	E3655	X3566	X3465	X3399	X3278	X3208	X3142
T3966	L3965	C3733	L3817	S3732	S3656	X3567	X3466	X3400	X3279	X3209	X3143
E3967	T3966	C3733	K3821	H3734	K3658	X3568	X3467	X3401	X3280	X3210	X3144
Y3968	N3896	D3022	D3022	H3734	A3659	X3569	X3468	X3402	X3281	X3211	X3145
I3969	N3897	F3825	F3825	L3735	A3660	X3570	X3511	X3403	X3282	X3212	X3146
Q3970	F3899	F3825	F3825	E3737	E3737	X3571	X3512	X3404	X3283	X3213	X3147
G3971	Q3900	G3827	G3827	G3738	L3662	X3572	X3513	X3405	X3284	X3214	X3148
Q3978	N3901	Q3830	Q3830	G3739	L3663	X3573	X3514	X3406	X3285	X3215	X3149
R3984	Y3902	Q3830	Q3830	E3740	T3664	X3574	X3515	X3407	X3286	X3216	X3150
L3985	L3903	Q3833	Q3833	E3740	E3665	X3575	X3516	X3408	X3287	X3217	X3151
M3986	R3904	A3834	A3834	N3741	D3666	X3576	X3517	X3409	X3288	X3218	X3152
V3990	T3905	L3842	L3842	GLU	H3667	X3577	X3518	X3410	X3289	X3219	X3153
G3991	GLU	D3843	D3843	ALA	S3668	X3578	X3519	X3411	X3290	X3220	X3154
F3992	GLU	A3846	A3846	GLU	F3669	X3579	X3520	X3412	X3291	X3221	X3155
L3993	E3748	E3748	E3748	E3748	E3670	X3580	X3521	X3413	X3292	X3222	X3156
H3994	V3749	E3749	E3749	V3749	D3671	X3581	X3522	X3414	X3293	X3223	X3157
V3995	E3750	E3750	E3750	E3750	R3672	X3582	X3523	X3415	X3294	X3224	X3158
F3996	V3751	Q3850	Q3850	V3751	M3673	X3583	X3524	X3416	X3295	X3225	X3159
A3997	F3752	N3851	N3851	F3752	D3674	X3584	X3525	X3417	X3296	X3226	X3160
H3998	F3753	F3852	F3852	F3753	D3676	X3585	X3526	X3418	X3297	X3227	X3161
M4000	E3754	A3853	A3853	E3754	K3679	X3586	X3527	X3419	X3298	X3228	X3162
M4001	E3755	E3854	E3854	E3755	A3680	X3587	X3528	X3420	X3299	X3229	X3163
S4002	K3756	K3855	K3855	K3756	G3681	X3588	X3529	X3421	X3300	X3230	X3170
L4003	E3757	L3856	L3856	E3757	E3682	X3589	X3530	X3422	X3301	X3231	X3171
A4004	M3758	Q3857	Q3857	M3758	Q3683	X3590	X3531	X3423	X3302	X3232	X3172
Q4005	F3932	N3858	N3858	F3932	X3594	X3591	X3532	X3427	X3303	X3233	X3173
D4006	F3933	N3860	N3860	F3933	X3595	X3592	X3533	X3428	X3304	X3234	X3174
S4007	Y3934	E3861	E3861	Y3934	E3685	X3596	X3534	X3429	X3305	X3235	X3175
S4008	Y3935	D3862	D3862	Y3935	E3686	X3597	X3535	X3430	X3306	X3236	X3176
Q4009	Y3936	G3863	G3863	L3763	E3687	X3598	X3536	X3431	X3307	X3237	X3177
I4010	S3937	T3864	T3864	Q3765	E3688	X3599	X3537	X3432	X3308	X3242	X3178
E4011	G3939	V3965	V3965	Q3766	E3689	X3600	X3538	X3433	X3309	X3243	X3179
L4012	K3940	I3866	I3866	Q3767	V3690	X3601	X3539	X3434	X3310	X3244	X3180
L4013	D3941	N3867	N3867	S3768	E3691	X3602	X3540	X3435	X3311	X3245	X3181
K4014	V3942	E3868	E3868	L3770	E3692	X3605	X3541	X3436	X3312	X3246	X3182
E4015	I3943	Q3869	Q3869	H3771	L3703	X3606	X3542	X3437	X3313	X3247	X3183
L4016	I3943	N3870	N3870	T3772	H3704	X3607	X3543	X3438	X3314	X3248	X3184
L4017	E3944	G3871	G3871	R3773	F3705	X3608	X3544	X3439	X3315	X3249	X3185
D4018	E3945	E3872	E3872	R3773	S3706	X3609	X3545	X3440	X3316	X3250	X3186
L4019	Q3946	E3873	E3873	E3777	R3707	X3610	X3546	X3441	X3317	X3251	X3187
Q4020	G3947	K3873	K3873	M3778	B3707	X3611	X3547	X3442	X3318	X3252	X3188
K4021	R3948	V3874	V3874	F3779	T3711	X3612	X3548	X3443	X3319	X3253	X3189
D4022	N3950	M3875	M3875	L3780	E3712	X3613	X3550	X3444	X3320	X3254	X3190
L4028	K3953	D3877	D3877	S3795	P3640	X3614	X3551	X3445	X3321	X3255	X3191
E4032	A3954	D3878	D3878	K3799	X3552	X3615	X3552	X3446	X3322	X3256	X3192
G4033	M3955	L3716	L3716	L3643	X3553	X3616	X3553	X3447	X3323	X3257	X3193
N4034		D3717	D3717	L3644	X3554	X3617	X3554	X3448	X3324	X3258	X3194
		E3718	E3718	N3645	X3555	X3618	X3555	X3449	X3325	X3259	X3195
		D3719	D3719	H3646	X3556	X3619	X3556	X3450	X3326	X3260	X3196
		Y3720	Y3720	H3647	X3557	X3620	X3557	X3451	X3327	X3261	X3197
				R3648	X3558	X3621	X3558	X3452	X3328	X3262	X3198
				A3649	X3559	X3622	X3559	X3453	X3329	X3263	X3199
					X3560	X3623	X3560	X3454	X3330	X3264	X3200
					X3561	X3624	X3561	X3455	X3331	X3265	X3201
						X3625		X3456	X3332	X3266	X3202
						X3626		X3457	X3333	X3267	X3203
						X3627			X3334	X3272	
						X3628				X3273	

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	-0.030	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

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	0.46	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.22	0/25438	0.53	6/34548 (0.0%)
2	E	0.22	0/25438	0.53	6/34548 (0.0%)
2	G	0.22	0/25438	0.53	6/34548 (0.0%)
2	I	0.22	0/25438	0.53	6/34548 (0.0%)
All	All	0.22	0/105088	0.53	24/142684 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2807	TRP	CA-C-N	-6.65	113.36	120.94
2	E	2807	TRP	C-N-CA	-6.65	113.36	120.94
2	B	2807	TRP	CA-C-N	-6.62	113.40	120.94
2	B	2807	TRP	C-N-CA	-6.62	113.40	120.94
2	I	2807	TRP	CA-C-N	-6.61	113.40	120.94
2	I	2807	TRP	C-N-CA	-6.61	113.40	120.94
2	G	2807	TRP	CA-C-N	-6.61	113.40	120.94
2	G	2807	TRP	C-N-CA	-6.61	113.40	120.94
2	G	2808	PRO	N-CA-C	-5.43	107.73	114.68
2	B	2808	PRO	N-CA-C	-5.42	107.75	114.68
2	E	2808	PRO	N-CA-C	-5.41	107.76	114.68
2	I	2808	PRO	N-CA-C	-5.41	107.76	114.68
2	E	137	LEU	CA-C-N	-5.22	115.32	121.90
2	E	137	LEU	C-N-CA	-5.22	115.32	121.90
2	B	137	LEU	CA-C-N	-5.21	115.34	121.90
2	B	137	LEU	C-N-CA	-5.21	115.34	121.90
2	G	137	LEU	CA-C-N	-5.21	115.34	121.90
2	G	137	LEU	C-N-CA	-5.21	115.34	121.90
2	I	137	LEU	CA-C-N	-5.18	115.37	121.90
2	I	137	LEU	C-N-CA	-5.18	115.37	121.90
2	B	1829	PRO	N-CA-C	5.06	119.16	111.11
2	G	1829	PRO	N-CA-C	5.06	119.15	111.11
2	E	1829	PRO	N-CA-C	5.05	119.14	111.11
2	I	1829	PRO	N-CA-C	5.04	119.12	111.11

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	11	0
2	B	29509	0	24752	291	0
2	E	29509	0	24753	281	0
2	G	29509	0	24753	286	0
2	I	29509	0	24753	287	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121312	0	102307	1168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1168) 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:B:4983:HIS:CD2	2:B:4983:HIS:H	2.10	0.70
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.10	0.70
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.10	0.69
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.61	0.65
2:E:111:HIS:HD2	2:E:114:SER:H	1.45	0.64
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.61	0.64
2:B:111:HIS:HD2	2:B:114:SER:H	1.45	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.61	0.64
2:E:4958:CYS:SG	2:E:4961:CYS:HB2	2.38	0.64
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.80	0.63
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.79	0.63
2:I:4958:CYS:SG	2:I:4961:CYS:HB2	2.38	0.63
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.63	0.63
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.63
2:G:4958:CYS:SG	2:G:4961:CYS:HB2	2.38	0.63
2:B:4958:CYS:SG	2:B:4961:CYS:HB2	2.38	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.81	0.62
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.62
2:G:111:HIS:HD2	2:G:114:SER:H	1.45	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.62
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.63	0.62
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.64	0.62
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.80	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.63	0.62
2:I:4958:CYS:SG	2:I:4961:CYS:CB	2.88	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.45	0.62
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.82	0.62
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.64	0.62
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.82	0.61
2:B:4958:CYS:SG	2:B:4961:CYS:CB	2.88	0.61
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.82	0.61
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.82	0.61
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.61
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.64	0.61
2:E:4958:CYS:SG	2:E:4961:CYS:CB	2.88	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.81	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.80	0.61
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.64	0.61
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.61
2:E:379:HIS:HD2	2:E:382:GLY:H	1.47	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:G:4958:CYS:SG	2:G:4961:CYS:CB	2.88	0.60
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.35	0.60
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.35	0.60
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.35	0.60
2:B:173:SER:HB3	2:B:178:ARG:H	1.67	0.60
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.84	0.60
2:I:173:SER:HB3	2:I:178:ARG:H	1.67	0.60
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.35	0.60
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.84	0.59
2:G:173:SER:HB3	2:G:178:ARG:H	1.67	0.59
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.35	0.59
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.84	0.59
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.35	0.59
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.84	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.59
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.85	0.59
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.84	0.59
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.35	0.59
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.35	0.59
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.59
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.85	0.59
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.35	0.59
2:I:241:GLN:O	2:I:289:ARG:NH1	2.34	0.59
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.59
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.36	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.59
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.59
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.36	0.59
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.35	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.35	0.59
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.35	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.59
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.84	0.58
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.36	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.85	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG3	1.85	0.58
2:E:173:SER:HB3	2:E:178:ARG:H	1.67	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.36	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG3	1.85	0.58
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.58
2:B:3733:CYS:HA	2:B:3766:GLN:HG3	1.85	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.58
2:G:241:GLN:O	2:G:289:ARG:NH1	2.34	0.58
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.37	0.58
2:E:3733:CYS:HA	2:E:3766:GLN:HG3	1.84	0.58
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.85	0.58
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.85	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.58
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.58
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.85	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.57
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.38	0.57
2:I:3758:MET:HE3	2:I:3762:ARG:HE	1.69	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.57
2:G:3758:MET:HE3	2:G:3762:ARG:HE	1.69	0.57
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.37	0.57
2:E:3758:MET:HE3	2:E:3762:ARG:HE	1.69	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.37	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.57
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.85	0.57
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.37	0.57
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.37	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.38	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.57
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.38	0.57
2:B:3758:MET:HE3	2:B:3762:ARG:HE	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.36	0.57
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.87	0.57
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.37	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.87	0.57
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.78	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.57
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.78	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.57
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.38	0.56
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.37	0.56
2:I:359:TYR:HA	2:I:376:ALA:HA	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.87	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.34	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.87	0.56
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.87	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.78	0.56
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.38	0.56
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.56
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.87	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.87	0.56
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.56
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.38	0.56
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.37	0.56
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.70	0.56
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.78	0.56
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.38	0.56
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.38	0.56
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.70	0.56
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.87	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.87	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.88	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.88	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.37	0.56
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.39	0.56
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.89	0.55
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.39	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.70	0.55
2:G:359:TYR:HA	2:G:376:ALA:HA	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.87	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.87	0.55
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.39	0.55
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.87	0.55
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.55
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.39	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.70	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.89	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.89	0.55
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.89	0.55
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.89	0.55
2:E:241:GLN:O	2:E:289:ARG:NH1	2.34	0.55
2:E:978:THR:HB	2:E:980:ALA:H	1.72	0.55
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.89	0.55
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.89	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.89	0.55
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.88	0.55
2:B:978:THR:HB	2:B:980:ALA:H	1.72	0.54
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.89	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.41	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.41	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.54
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.89	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.73	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.90	0.54
2:E:451:TYR:O	2:E:474:ARG:NH1	2.41	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.90	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.73	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.54
1:F:87:HIS:H	1:F:91:ILE:HB	1.73	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.89	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.54
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.41	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.73	0.54
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.39	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.90	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.90	0.54
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.73	0.53
2:I:978:THR:HB	2:I:980:ALA:H	1.72	0.53
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.53
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.39	0.53
2:B:313:SER:HB3	2:B:351:VAL:HB	1.90	0.53
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.41	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.72	0.53
1:H:87:HIS:H	1:H:91:ILE:HB	1.73	0.53
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.90	0.53
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.53
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.91	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53
1:J:87:HIS:H	1:J:91:ILE:HB	1.73	0.53
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.37	0.53
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.91	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.91	0.53
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.57	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.41	0.53
1:A:87:HIS:H	1:A:91:ILE:HB	1.73	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.90	0.53
2:G:451:TYR:O	2:G:474:ARG:NH1	2.41	0.53
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.57	0.53
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.91	0.53
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.52
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.52
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.91	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.91	0.52
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.74	0.52
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.37	0.52
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.92	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.52
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.74	0.52
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.91	0.52
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.52
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.57	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.92	0.52
2:E:776:LEU:HG	2:E:848:HIS:HA	1.91	0.52
2:I:4063:ASP:O	2:I:4067:LYS:NZ	2.37	0.52
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.28	0.52
2:B:4063:ASP:O	2:B:4067:LYS:NZ	2.37	0.52
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.91	0.52
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.28	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.91	0.52
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.74	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.90	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.92	0.52
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.91	0.52
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.28	0.52
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.41	0.52
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.57	0.51
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.37	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.51
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.90	0.51
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.51
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	1.92	0.51
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.51
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.51
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.44	0.51
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.28	0.51
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.92	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.51
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.93	0.51
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.51
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.74	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.41	0.51
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.93	0.51
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.92	0.51
2:B:689:THR:H	2:B:778:PHE:HE2	1.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.93	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.51
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.92	0.51
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.93	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.74	0.51
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.51
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.92	0.51
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.93	0.51
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.93	0.51
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	1.92	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.51
2:B:4820:VAL:HB	2:B:4823:LEU:HD23	1.93	0.51
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.93	0.51
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.41	0.51
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.92	0.51
2:I:451:TYR:O	2:I:474:ARG:NH1	2.41	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.93	0.51
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.93	0.51
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.93	0.51
2:G:4820:VAL:HB	2:G:4823:LEU:HD23	1.93	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.50
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.50
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.50
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.93	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:E:1991:THR:O	2:E:1995:THR:OG1	2.29	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.59	0.50
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.93	0.50
2:E:4820:VAL:HB	2:E:4823:LEU:HD23	1.93	0.50
2:I:4820:VAL:HB	2:I:4823:LEU:HD23	1.93	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.93	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1457:UNK:N	2:E:1497:UNK:O	2.44	0.50
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.94	0.50
2:I:689:THR:H	2:I:778:PHE:HE2	1.59	0.50
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.93	0.50
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.92	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.50
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.92	0.50
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.94	0.50
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.94	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.44	0.50
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.50
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.92	0.50
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.94	0.50
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.50
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.93	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.45	0.50
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.50
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.27	0.50
2:G:1991:THR:O	2:G:1995:THR:OG1	2.29	0.50
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.92	0.50
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.93	0.50
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.93	0.50
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.94	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.50
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.93	0.50
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.39	0.50
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.50
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.93	0.50
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.93	0.50
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.41	0.50
2:E:4571:PHE:O	2:E:4575:PHE:N	2.45	0.50
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.93	0.50
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.50
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.77	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.50
2:I:1991:THR:O	2:I:1995:THR:OG1	2.29	0.50
2:G:1685:LEU:HD22	2:G:1718:ILE:HG21	1.92	0.50
2:G:4826:ILE:O	2:G:4829:SER:OG	2.29	0.50
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.93	0.50
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.94	0.50
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.94	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:E:4832:HIS:NE2	2:E:4942:GLU:OE2	2.45	0.50
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.94	0.50
2:G:911:HIS:O	2:G:918:ARG:NH2	2.45	0.50
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.77	0.50
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.93	0.50
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.94	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.44	0.49
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.94	0.49
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.94	0.49
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.49
2:G:689:THR:H	2:G:778:PHE:HE2	1.59	0.49
2:B:1991:THR:O	2:B:1995:THR:OG1	2.29	0.49
2:B:4571:PHE:O	2:B:4575:PHE:N	2.45	0.49
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.49
2:I:4832:HIS:NE2	2:I:4942:GLU:OE2	2.45	0.49
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.49
2:B:582:HIS:O	2:B:585:SER:OG	2.28	0.49
2:B:1973:GLN:O	2:B:1977:TYR:N	2.40	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.94	0.49
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.46	0.49
2:G:4063:ASP:O	2:G:4067:LYS:NZ	2.37	0.49
2:B:4832:HIS:NE2	2:B:4942:GLU:OE2	2.45	0.49
2:G:4571:PHE:O	2:G:4575:PHE:N	2.45	0.49
2:B:911:HIS:O	2:B:918:ARG:NH2	2.45	0.49
2:B:1171:SER:OG	2:B:1175:SER:N	2.43	0.49
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.46	0.49
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.77	0.49
2:E:1685:LEU:HD22	2:E:1718:ILE:HG21	1.93	0.49
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.46	0.49
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.94	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.49
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.49
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.94	0.49
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.49
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.77	0.49
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.95	0.49
2:G:4832:HIS:NE2	2:G:4942:GLU:OE2	2.45	0.49
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.46	0.49
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.93	0.49
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.94	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.46	0.49
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.94	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.49
2:I:4571:PHE:O	2:I:4575:PHE:N	2.45	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.48
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.46	0.48
2:E:4063:ASP:O	2:E:4067:LYS:NZ	2.37	0.48
2:I:911:HIS:O	2:I:918:ARG:NH2	2.45	0.48
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.27	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.43	0.48
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.95	0.48
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.46	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.94	0.48
2:I:3755:GLU:O	2:I:3762:ARG:NH2	2.44	0.48
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.30	0.48
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.46	0.48
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.94	0.48
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.95	0.48
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.46	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.31	0.48
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.96	0.48
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.94	0.48
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.96	0.48
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.96	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.96	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.96	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.95	0.48
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.96	0.48
2:B:792:LEU:HB3	2:B:798:GLY:HA2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.41	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	1.95	0.48
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.95	0.48
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.48
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.46	0.48
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.48
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.94	0.48
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.46	0.48
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.79	0.48
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.79	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.95	0.48
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.79	0.48
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.48
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.79	0.48
2:E:4826:ILE:O	2:E:4829:SER:OG	2.29	0.48
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.48
2:G:2103:VAL:O	2:G:2107:GLN:N	2.43	0.48
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.79	0.48
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	1.96	0.48
2:E:4582:VAL:HG23	2:E:4629:TYR:HA	1.96	0.48
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.47	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.47	0.48
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.96	0.47
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.78	0.47
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.95	0.47
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	1.96	0.47
2:B:756:SER:HB3	2:B:767:VAL:HG22	1.96	0.47
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.96	0.47
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.96	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.43	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.46	0.47
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.97	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	1.95	0.47
2:E:606:LEU:O	2:E:617:ASN:ND2	2.47	0.47
2:G:756:SER:HB3	2:G:767:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.97	0.47
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.39	0.47
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.96	0.47
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.79	0.47
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.96	0.47
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	1.96	0.47
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.79	0.47
2:B:4582:VAL:HG23	2:B:4629:TYR:HA	1.96	0.47
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.97	0.47
2:G:792:LEU:HB3	2:G:798:GLY:HA2	1.95	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HE3	1.80	0.47
2:E:331:VAL:HG12	2:E:333:GLY:H	1.79	0.47
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.96	0.47
2:I:756:SER:HB3	2:I:767:VAL:HG22	1.96	0.47
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	1.95	0.47
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.96	0.47
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.97	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.48	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.80	0.47
2:B:331:VAL:HG12	2:B:333:GLY:H	1.79	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.47	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.43	0.47
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.96	0.47
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.97	0.47
2:E:792:LEU:HB3	2:E:798:GLY:HA2	1.95	0.47
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.97	0.47
2:E:4673:ARG:HH22	2:E:4698:LYS:HE3	1.80	0.47
2:I:331:VAL:HG12	2:I:333:GLY:H	1.79	0.47
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.96	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.47	0.47
2:G:331:VAL:HG12	2:G:333:GLY:H	1.79	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.79	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.80	0.47
2:I:792:LEU:HB3	2:I:798:GLY:HA2	1.95	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.47
2:I:4673:ARG:HH22	2:I:4698:LYS:HE3	1.80	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:756:SER:HB3	2:E:767:VAL:HG22	1.96	0.47
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.47
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.97	0.46
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.30	0.46
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.47	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.98	0.46
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.97	0.46
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.98	0.46
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.98	0.46
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	1.95	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.43	0.46
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.48	0.46
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.46
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.98	0.46
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.79	0.46
2:I:1976:ARG:NH1	2:I:1997:GLU:OE2	2.49	0.46
2:I:2103:VAL:O	2:I:2107:GLN:N	2.43	0.46
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	1.96	0.46
2:G:1171:SER:OG	2:G:1175:SER:N	2.43	0.46
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.47	0.46
2:B:1976:ARG:NH1	2:B:1997:GLU:OE2	2.49	0.46
2:B:4101:LYS:HE3	2:I:4731:ILE:HA	1.97	0.46
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.46
2:E:1976:ARG:NH1	2:E:1997:GLU:OE2	2.49	0.46
1:F:82:TYR:O	1:F:86:GLY:N	2.46	0.46
2:B:792:LEU:HD22	2:B:799:GLU:H	1.81	0.46
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.80	0.46
2:E:792:LEU:HD22	2:E:799:GLU:H	1.81	0.46
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.29	0.46
2:I:4582:VAL:HG23	2:I:4629:TYR:HA	1.96	0.46
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.98	0.46
2:G:4582:VAL:HG23	2:G:4629:TYR:HA	1.96	0.46
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.35	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.98	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.49	0.46
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.80	0.46
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.96	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.46
2:G:1976:ARG:NH1	2:G:1997:GLU:OE2	2.49	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.98	0.46
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.80	0.46
2:I:792:LEU:HD22	2:I:799:GLU:H	1.81	0.46
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.98	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.40	0.46
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.96	0.46
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.80	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.46
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.46
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.98	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.98	0.46
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.46
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.98	0.46
2:G:4673:ARG:HH22	2:G:4698:LYS:HE3	1.80	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.98	0.46
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.98	0.46
2:B:164:ARG:N	2:B:167:ASP:OD2	2.49	0.46
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.80	0.46
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.98	0.46
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.48	0.46
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.80	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.98	0.46
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.49	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.46
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.37	0.46
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.99	0.46
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.98	0.46
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.49	0.46
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.98	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.49	0.45
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.45
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.80	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.49	0.45
2:I:4826:ILE:O	2:I:4829:SER:OG	2.29	0.45
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.81	0.45
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.98	0.45
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.97	0.45
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.98	0.45
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.45
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.98	0.45
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.49	0.45
2:E:164:ARG:N	2:E:167:ASP:OD2	2.49	0.45
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.98	0.45
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.49	0.45
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.98	0.45
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.48	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.45
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.99	0.45
2:B:626:LEU:HG	2:B:628:GLY:H	1.82	0.45
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.98	0.45
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.98	0.45
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.45
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.98	0.45
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.35	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.98	0.45
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.98	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.49	0.45
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.98	0.45
2:B:3362:UNK:O	2:B:3366:UNK:N	2.49	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.45
2:E:626:LEU:HG	2:E:628:GLY:H	1.82	0.45
2:E:2103:VAL:O	2:E:2107:GLN:N	2.43	0.45
2:E:4835:LYS:HG3	2:E:4836:GLN:HG3	1.98	0.45
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.99	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.98	0.45
2:E:1105:ALA:N	2:E:1189:LEU:O	2.50	0.45
2:E:1973:GLN:O	2:E:1977:TYR:N	2.40	0.45
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.49	0.45
2:I:463:GLU:O	2:I:466:SER:OG	2.30	0.45
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.98	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.45
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.98	0.45
2:G:1105:ALA:N	2:G:1189:LEU:O	2.50	0.45
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.45
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.98	0.45
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.98	0.45
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.98	0.45
2:E:278:GLN:N	2:E:315:CYS:SG	2.90	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.98	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.82	0.45
2:G:792:LEU:HD22	2:G:799:GLU:H	1.81	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.43	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.98	0.45
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.99	0.45
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.45
2:E:21:VAL:HG12	2:E:66:CYS:HA	1.99	0.45
2:E:463:GLU:O	2:E:466:SER:OG	2.30	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.98	0.45
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.98	0.45
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.99	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.98	0.45
2:B:21:VAL:HG12	2:B:66:CYS:HA	1.99	0.45
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.31	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.80	0.45
2:B:4956:THR:O	2:B:4965:SER:N	2.48	0.45
2:E:215:THR:HG22	2:E:273:HIS:HA	1.99	0.45
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.99	0.45
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.98	0.45
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.99	0.45
2:I:1114:GLU:HG3	2:I:1117:ALA:HB2	1.99	0.45
2:G:70:GLU:HG3	2:G:117:TYR:HE1	1.80	0.45
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.98	0.45
2:G:4835:LYS:HG3	2:G:4836:GLN:HG3	1.98	0.45
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.50	0.45
2:B:1105:ALA:N	2:B:1189:LEU:O	2.50	0.45
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.99	0.45
2:B:4826:ILE:O	2:B:4829:SER:OG	2.29	0.45
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.99	0.45
2:E:4201:ASN:ND2	2:E:4204:GLN:OE1	2.49	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.50	0.45
2:G:1269:CYS:HA	2:G:1473:UNK:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4201:ASN:ND2	2:G:4204:GLN:OE1	2.49	0.45
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.99	0.45
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.98	0.45
2:B:1114:GLU:HG3	2:B:1117:ALA:HB2	1.99	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.99	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.45
2:B:4201:ASN:ND2	2:B:4204:GLN:OE1	2.49	0.45
2:B:4835:LYS:HG3	2:B:4836:GLN:HG3	1.98	0.45
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.99	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.98	0.45
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.99	0.45
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.99	0.45
2:B:2257:LEU:O	2:B:2261:SER:N	2.50	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:B:3755:GLU:O	2:B:3762:ARG:NH2	2.44	0.44
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.98	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.44
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.98	0.44
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.44
2:I:3992:PHE:O	2:I:3996:PHE:N	2.40	0.44
2:G:278:GLN:N	2:G:315:CYS:SG	2.90	0.44
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.98	0.44
1:J:82:TYR:O	1:J:86:GLY:N	2.46	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.98	0.44
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.99	0.44
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.44
2:I:4835:LYS:HG3	2:I:4836:GLN:HG3	1.98	0.44
2:I:4956:THR:O	2:I:4965:SER:N	2.48	0.44
2:G:21:VAL:HG12	2:G:66:CYS:HA	1.99	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.44
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.98	0.44
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.99	0.44
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.99	0.44
2:E:395:GLN:HG3	2:E:397:GLU:H	1.82	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.50	0.44
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.99	0.44
2:E:1114:GLU:HG3	2:E:1117:ALA:HB2	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.44
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.50	0.44
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.99	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.40	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.99	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.44
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.98	0.44
2:I:21:VAL:HG12	2:I:66:CYS:HA	1.99	0.44
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.99	0.44
2:I:4201:ASN:ND2	2:I:4204:GLN:OE1	2.50	0.44
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.99	0.44
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.99	0.44
2:G:1965:TYR:OH	2:G:2027:ILE:O	2.29	0.44
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.98	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44
2:B:3764:LEU:HD21	2:B:3809:ASN:HD21	1.82	0.44
2:E:2257:LEU:O	2:E:2261:SER:N	2.50	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.99	0.44
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.53	0.44
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.99	0.44
2:G:626:LEU:HG	2:G:628:GLY:H	1.82	0.44
2:G:1114:GLU:HG3	2:G:1117:ALA:HB2	1.99	0.44
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.98	0.44
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.00	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:G:4667:PRO:O	2:G:4714:ASN:ND2	2.48	0.44
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.42	0.44
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.44
2:B:395:GLN:HG3	2:B:397:GLU:H	1.82	0.44
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.99	0.44
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.53	0.44
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.98	0.44
2:B:4976:GLU:O	2:B:4979:THR:OG1	2.35	0.44
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.99	0.44
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.99	0.44
2:I:626:LEU:HG	2:I:628:GLY:H	1.82	0.44
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.35	0.44
2:I:2517:UNK:O	2:I:2521:UNK:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3764:LEU:HD21	2:I:3809:ASN:HD21	1.82	0.44
2:I:4075:GLU:O	2:I:4079:ASP:N	2.51	0.44
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.44
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.99	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.50	0.44
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.99	0.44
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.99	0.44
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.44
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.99	0.44
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.99	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.44
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.99	0.44
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.99	0.44
2:I:1105:ALA:N	2:I:1189:LEU:O	2.50	0.44
2:I:2257:LEU:O	2:I:2261:SER:N	2.50	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.99	0.44
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.44
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.00	0.44
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.99	0.44
2:B:356:TRP:O	2:B:379:HIS:N	2.51	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.44
2:B:4667:PRO:O	2:B:4714:ASN:ND2	2.48	0.44
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	1.99	0.44
2:E:2517:UNK:O	2:E:2521:UNK:N	2.51	0.44
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.51	0.44
2:E:4075:GLU:O	2:E:4079:ASP:N	2.50	0.44
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.83	0.44
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.44
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	1.99	0.44
2:G:215:THR:HG22	2:G:273:HIS:HA	1.99	0.44
2:G:2517:UNK:O	2:G:2521:UNK:N	2.51	0.44
2:G:3755:GLU:O	2:G:3762:ARG:NH2	2.44	0.44
2:G:3764:LEU:HD21	2:G:3809:ASN:HD21	1.83	0.44
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.51	0.44
2:G:4075:GLU:O	2:G:4079:ASP:N	2.51	0.44
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.00	0.43
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.99	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.43
2:E:1171:SER:OG	2:E:1175:SER:N	2.43	0.43
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.53	0.43
2:E:4956:THR:O	2:E:4965:SER:N	2.48	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.43
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.83	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.43
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.41	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
1:F:11:ASP:OD1	1:F:67:SER:OG	2.35	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.43
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.00	0.43
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.43
2:I:4667:PRO:O	2:I:4714:ASN:ND2	2.48	0.43
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.83	0.43
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.33	0.43
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.52	0.43
1:H:82:TYR:O	1:H:86:GLY:N	2.46	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.99	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	2.01	0.43
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.43
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.52	0.43
2:I:3927:GLN:O	2:I:3931:SER:N	2.51	0.43
2:I:4066:LEU:HD11	2:I:4173:TYR:CG	2.53	0.43
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.53	0.43
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.84	0.43
2:B:278:GLN:N	2:B:315:CYS:SG	2.90	0.43
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.52	0.43
2:B:2517:UNK:O	2:B:2521:UNK:N	2.51	0.43
2:B:4075:GLU:O	2:B:4079:ASP:N	2.51	0.43
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.43
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.43
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.43
2:G:4956:THR:O	2:G:4965:SER:N	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.00	0.43
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.00	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.43
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.35	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	2.01	0.43
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.01	0.43
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.52	0.43
2:B:3674:ILE:HB	2:B:3769:ARG:HH21	1.84	0.43
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	2.01	0.43
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.99	0.43
2:E:793:LEU:HB2	2:E:797:HIS:H	1.84	0.43
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.00	0.43
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.33	0.43
2:I:4976:GLU:O	2:I:4979:THR:OG1	2.35	0.43
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	1.99	0.43
2:G:4976:GLU:O	2:G:4979:THR:OG1	2.35	0.43
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.84	0.43
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.43
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.83	0.43
2:I:395:GLN:HG3	2:I:397:GLU:H	1.82	0.43
2:I:734:GLY:O	2:I:736:HIS:ND1	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
1:A:11:ASP:OD1	1:A:67:SER:OG	2.36	0.43
2:E:356:TRP:O	2:E:379:HIS:N	2.51	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.84	0.43
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.52	0.43
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.84	0.43
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.83	0.43
2:B:4066:LEU:HD11	2:B:4173:TYR:CG	2.53	0.43
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.00	0.43
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	2.01	0.43
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.51	0.43
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.99	0.43
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.84	0.43
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.52	0.43
2:G:3674:ILE:HB	2:G:3769:ARG:HH21	1.84	0.43
2:G:4066:LEU:HD11	2:G:4173:TYR:CG	2.53	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4857:ASN:HB2	2:E:4807:PHE:HZ	1.84	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.84	0.43
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	2.01	0.43
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.00	0.43
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.52	0.43
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.84	0.43
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.83	0.43
2:G:356:TRP:O	2:G:379:HIS:N	2.51	0.43
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.43
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	2.01	0.43
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.84	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.42
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.29	0.42
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.51	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.42
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.52	0.42
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.52	0.42
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.00	0.42
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.01	0.42
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.52	0.42
2:G:1954:ARG:HE	2:G:2041:HIS:HD2	1.67	0.42
2:E:1954:ARG:HE	2:E:2041:HIS:HD2	1.67	0.42
2:I:356:TRP:O	2:I:379:HIS:N	2.51	0.42
2:I:793:LEU:HB2	2:I:797:HIS:H	1.84	0.42
2:I:1954:ARG:HE	2:I:2041:HIS:HD2	1.68	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.00	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.42
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	2.01	0.42
2:G:793:LEU:HB2	2:G:797:HIS:H	1.84	0.42
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.42
2:B:600:LEU:O	2:B:604:CYS:N	2.50	0.42
2:B:793:LEU:HB2	2:B:797:HIS:H	1.84	0.42
2:E:1089:TYR:N	2:E:1224:GLU:O	2.52	0.42
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.83	0.42
2:E:3764:LEU:HD21	2:E:3809:ASN:HD21	1.83	0.42
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.52	0.42
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.84	0.42
2:I:3674:ILE:HB	2:I:3769:ARG:HH21	1.84	0.42
2:G:600:LEU:O	2:G:604:CYS:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3992:PHE:O	2:G:3996:PHE:N	2.40	0.42
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.52	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.42
2:E:560:ILE:HA	2:E:563:VAL:HG12	2.00	0.42
2:E:4066:LEU:HD11	2:E:4173:TYR:CG	2.53	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:B:1089:TYR:N	2:B:1224:GLU:O	2.52	0.42
2:B:4978:HIS:CE1	2:B:4983:HIS:NE2	2.87	0.42
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.42
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.01	0.42
2:I:1089:TYR:N	2:I:1224:GLU:O	2.52	0.42
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.02	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.00	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.02	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:B:4060:LYS:NZ	2:B:4064:MET:SD	2.93	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.35	0.42
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.02	0.42
2:E:3805:LEU:H	2:E:3805:LEU:HG	1.77	0.42
2:G:560:ILE:HA	2:G:563:VAL:HG12	2.00	0.42
2:G:3927:GLN:O	2:G:3931:SER:N	2.51	0.42
1:A:82:TYR:O	1:A:86:GLY:N	2.46	0.42
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	2.01	0.42
2:B:1954:ARG:HE	2:B:2041:HIS:HD2	1.67	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.42
2:B:3927:GLN:O	2:B:3931:SER:N	2.51	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.02	0.42
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.85	0.42
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.01	0.42
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.52	0.42
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.37	0.42
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.42
2:E:3674:ILE:HB	2:E:3769:ARG:HH21	1.84	0.42
2:I:2297:LYS:O	2:I:2300:SER:OG	2.34	0.42
2:G:1089:TYR:N	2:G:1224:GLU:O	2.52	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.35	0.42
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.42
2:G:3729:MET:O	2:G:3732:SER:OG	2.32	0.42
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.01	0.42
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.02	0.42
2:B:4056:GLU:O	2:B:4060:LYS:N	2.51	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.02	0.42
2:E:4060:LYS:NZ	2:E:4064:MET:SD	2.93	0.42
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.02	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.02	0.42
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.01	0.42
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.02	0.42
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.02	0.42
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.02	0.41
2:G:40:GLU:HB3	2:G:44:ASN:HB3	2.02	0.41
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.85	0.41
2:E:40:GLU:HB3	2:E:44:ASN:HB3	2.02	0.41
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.33	0.41
2:E:4713:SER:HG	2:E:4775:TYR:HH	1.68	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.01	0.41
2:I:317:ARG:HE	2:I:323:LEU:HD22	1.86	0.41
2:I:4060:LYS:NZ	2:I:4064:MET:SD	2.93	0.41
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.85	0.41
2:G:2867:LEU:HB3	2:G:2871:LEU:HB2	2.02	0.41
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.02	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.41	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.02	0.41
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.02	0.41
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.41	0.41
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.02	0.41
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	2.02	0.41
2:B:2867:LEU:HB3	2:B:2871:LEU:HB2	2.03	0.41
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.53	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.02	0.41
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.85	0.41
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.49	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.41
2:G:2297:LYS:O	2:G:2300:SER:OG	2.34	0.41
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.02	0.41
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.02	0.41
2:E:2867:LEU:HB3	2:E:2871:LEU:HB2	2.02	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2867:LEU:HB3	2:I:2871:LEU:HB2	2.02	0.41
2:G:317:ARG:HE	2:G:323:LEU:HD22	1.86	0.41
2:G:4060:LYS:NZ	2:G:4064:MET:SD	2.93	0.41
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.35	0.41
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	2.03	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.41
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.02	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.41
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.02	0.41
2:E:4731:ILE:HA	2:G:4101:LYS:HE3	2.02	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.03	0.41
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.86	0.41
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.02	0.41
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.02	0.41
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.85	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.35	0.41
2:B:317:ARG:HE	2:B:323:LEU:HD22	1.86	0.41
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.02	0.41
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	2.03	0.41
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.85	0.41
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.37	0.41
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.86	0.41
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.03	0.41
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.36	0.41
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.41
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.78	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.03	0.41
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.52	0.41
2:B:2103:VAL:O	2:B:2107:GLN:N	2.43	0.41
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.56	0.41
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.85	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.02	0.41
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.33	0.41
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.03	0.41
2:B:4807:PHE:HZ	2:I:4857:ASN:HB2	1.86	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.01	0.41
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.03	0.41
2:E:1154:ASP:O	2:E:1158:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.41
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.52	0.41
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.02	0.41
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.02	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.03	0.41
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	2.03	0.41
2:I:4837:LEU:HD13	2:I:4837:LEU:HA	1.96	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.54	0.41
2:G:150:MET:HE3	2:G:163:VAL:HG21	2.03	0.41
2:G:485:SER:HA	2:G:488:LEU:HB2	2.03	0.41
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.03	0.41
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.56	0.41
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.86	0.41
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.37	0.41
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.53	0.41
2:G:4231:MET:HE1	2:G:4960:ILE:HA	2.03	0.41
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.53	0.41
2:B:1154:ASP:O	2:B:1158:ASN:N	2.54	0.41
2:E:134:ASP:OD1	2:E:134:ASP:N	2.54	0.41
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.56	0.41
2:E:4090:LYS:O	2:E:4094:GLN:N	2.49	0.41
2:I:40:GLU:HB3	2:I:44:ASN:HB3	2.03	0.41
2:I:485:SER:O	2:I:489:ASN:N	2.43	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.02	0.41
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.03	0.41
2:G:4978:HIS:CE1	2:G:4983:HIS:NE2	2.87	0.41
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.02	0.40
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.03	0.40
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.40
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.86	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.53	0.40
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.40
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.03	0.40
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.40
2:G:2318:TYR:HA	2:G:2319:PRO:HD3	1.95	0.40
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.86	0.40
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.86	0.40
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.03	0.40
2:B:4731:ILE:HA	2:E:4101:LYS:HE3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:317:ARG:HE	2:E:323:LEU:HD22	1.85	0.40
2:E:3513:UNK:O	2:E:3515:UNK:N	2.55	0.40
2:E:4231:MET:HE1	2:E:4960:ILE:HA	2.03	0.40
2:E:4667:PRO:O	2:E:4714:ASN:ND2	2.48	0.40
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.02	0.40
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.03	0.40
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.03	0.40
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.02	0.40
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.86	0.40
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.40
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.03	0.40
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.04	0.40
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.56	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
2:G:3513:UNK:O	2:G:3515:UNK:N	2.55	0.40
1:H:11:ASP:OD1	1:H:67:SER:OG	2.36	0.40
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.04	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.54	0.40
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.40
2:B:3514:UNK:O	2:B:3518:UNK:N	2.55	0.40
2:B:4987:ASN:O	2:B:4991:PHE:N	2.55	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:550:LYS:HD3	2:E:550:LYS:HA	1.93	0.40
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.04	0.40
2:I:134:ASP:N	2:I:134:ASP:OD1	2.54	0.40
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.78	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.40
2:G:946:ALA:HA	2:G:949:ASN:HB2	2.03	0.40
2:G:3842:LEU:O	2:G:3929:SER:OG	2.40	0.40
2:B:150:MET:HE3	2:B:163:VAL:HG21	2.03	0.40
2:B:485:SER:HA	2:B:488:LEU:HB2	2.03	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.04	0.40
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.34	0.40
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.49	0.40
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.53	0.40
2:E:4857:ASN:HB2	2:G:4807:PHE:HZ	1.86	0.40
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.56	0.40
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.49	0.40
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.03	0.40
2:I:2025:GLU:HA	2:I:2028:ARG:NE	2.37	0.40
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.53	0.40
2:I:4231:MET:HE1	2:I:4960:ILE:HA	2.03	0.40
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	43	78
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	43	78
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	43	78
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	43	78
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	44	78

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	4641	PRO
2	E	1932	PRO
2	E	4641	PRO
2	I	1932	PRO
2	I	4641	PRO
2	G	1932	PRO
2	G	4641	PRO
2	B	1840	PRO
2	B	2291	GLN
2	E	2291	GLN
2	I	1840	PRO
2	I	2291	GLN
2	G	1840	PRO
2	G	2291	GLN
2	E	1840	PRO
2	B	4667	PRO
2	E	4667	PRO
2	I	4667	PRO
2	G	4667	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
2	E	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
2	G	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
2	I	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
All	All	10324/12444 (83%)	10276 (100%)	48 (0%)	78	82

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	2339	VAL
2	B	3663	LEU
2	B	3805	LEU
2	B	4837	LEU
2	B	4983	HIS
2	E	131	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	2339	VAL
2	E	3663	LEU
2	E	3805	LEU
2	E	4837	LEU
2	E	4983	HIS
2	I	131	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1657	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	2339	VAL
2	I	3663	LEU
2	I	3805	LEU
2	I	4837	LEU
2	I	4983	HIS
2	G	131	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	2010	LEU
2	G	2339	VAL
2	G	3663	LEU
2	G	3805	LEU
2	G	4837	LEU
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	31	GLN
1	F	65	GLN
1	F	87	HIS
1	A	31	GLN
1	A	65	GLN
1	A	87	HIS
1	H	31	GLN
1	H	65	GLN
1	H	87	HIS
1	J	31	GLN
1	J	43	ASN
1	J	65	GLN
1	J	87	HIS
2	B	71	GLN
2	B	113	HIS
2	B	156	GLN
2	B	201	ASN
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	582	HIS
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1970	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2127	GLN
2	B	2260	ASN
2	B	2773	ASN
2	B	2877	GLN
2	B	3647	HIS
2	B	3766	GLN
2	B	3771	HIS
2	B	3809	ASN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4037	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4691	GLN
2	B	4728	HIS
2	B	4947	GLN
2	E	113	HIS
2	E	156	GLN
2	E	201	ASN
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	461	HIS
2	E	479	GLN
2	E	582	HIS
2	E	797	HIS
2	E	838	HIS
2	E	1220	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	1970	GLN
2	E	2127	GLN
2	E	2260	ASN
2	E	2877	GLN
2	E	3647	HIS
2	E	3766	GLN
2	E	3771	HIS
2	E	3809	ASN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3994	HIS
2	E	4034	ASN
2	E	4037	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4553	ASN
2	E	4691	GLN
2	E	4728	HIS
2	E	4947	GLN
2	I	113	HIS
2	I	151	HIS
2	I	156	GLN
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	399	GLN
2	I	413	GLN
2	I	461	HIS
2	I	479	GLN
2	I	582	HIS
2	I	797	HIS
2	I	838	HIS
2	I	1220	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1970	GLN
2	I	2260	ASN
2	I	2788	HIS
2	I	2877	GLN
2	I	3766	GLN
2	I	3771	HIS
2	I	3809	ASN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4037	ASN
2	I	4102	GLN
2	I	4120	ASN
2	I	4553	ASN
2	I	4691	GLN
2	I	4728	HIS
2	I	4947	GLN
2	G	71	GLN
2	G	113	HIS
2	G	151	HIS
2	G	156	GLN
2	G	273	HIS
2	G	379	HIS
2	G	399	GLN
2	G	413	GLN
2	G	461	HIS
2	G	479	GLN
2	G	582	HIS
2	G	765	GLN
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1679	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	1688	HIS
2	G	1691	GLN
2	G	1775	HIS
2	G	1861	GLN
2	G	1970	GLN
2	G	2005	GLN
2	G	2260	ASN
2	G	2788	HIS
2	G	2877	GLN
2	G	3766	GLN
2	G	3771	HIS
2	G	3809	ASN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4037	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4553	ASN
2	G	4691	GLN
2	G	4728	HIS
2	G	4947	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.38
1	E	4345:UNK	C	4540:PHE	N	73.38
1	I	4345:UNK	C	4540:PHE	N	73.38
1	G	4345:UNK	C	4540:PHE	N	73.38
1	B	3613:UNK	C	3639:THR	N	48.21
1	E	3613:UNK	C	3639:THR	N	48.21
1	I	3613:UNK	C	3639:THR	N	48.21
1	G	3613:UNK	C	3639:THR	N	48.21
1	B	4253:GLU	C	4320:UNK	N	27.50
1	E	4253:GLU	C	4320:UNK	N	27.50
1	I	4253:GLU	C	4320:UNK	N	27.50
1	G	4253:GLU	C	4320:UNK	N	27.50
1	B	3163:UNK	C	3170:UNK	N	16.06

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3163:UNK	C	3170:UNK	N	16.06
1	I	3163:UNK	C	3170:UNK	N	16.06
1	G	3163:UNK	C	3170:UNK	N	16.06
1	B	3063:UNK	C	3134:UNK	N	14.88
1	E	3063:UNK	C	3134:UNK	N	14.88
1	I	3063:UNK	C	3134:UNK	N	14.88
1	G	3063:UNK	C	3134:UNK	N	14.88
1	B	3468:UNK	C	3511:UNK	N	14.29
1	E	3468:UNK	C	3511:UNK	N	14.29
1	I	3468:UNK	C	3511:UNK	N	14.29
1	G	3468:UNK	C	3511:UNK	N	14.29
1	B	2703:UNK	C	2734:ASN	N	13.58
1	E	2703:UNK	C	2734:ASN	N	13.58
1	I	2703:UNK	C	2734:ASN	N	13.58
1	G	2703:UNK	C	2734:ASN	N	13.58
1	B	3236:UNK	C	3241:UNK	N	13.52
1	E	3236:UNK	C	3241:UNK	N	13.52
1	I	3236:UNK	C	3241:UNK	N	13.52
1	G	3236:UNK	C	3241:UNK	N	13.52
1	B	1564:UNK	C	1573:MET	N	12.58
1	E	1564:UNK	C	1573:MET	N	12.58
1	I	1564:UNK	C	1573:MET	N	12.58
1	G	1564:UNK	C	1573:MET	N	12.58
1	B	2976:UNK	C	2995:UNK	N	12.37
1	E	2976:UNK	C	2995:UNK	N	12.37
1	I	2976:UNK	C	2995:UNK	N	12.37
1	G	2976:UNK	C	2995:UNK	N	12.37
1	B	3254:UNK	C	3261:UNK	N	8.09
1	E	3254:UNK	C	3261:UNK	N	8.09
1	I	3254:UNK	C	3261:UNK	N	8.09
1	G	3254:UNK	C	3261:UNK	N	8.09
1	B	1297:UNK	C	1430:UNK	N	5.89
1	I	1297:UNK	C	1430:UNK	N	5.89
1	E	1297:UNK	C	1430:UNK	N	5.88
1	G	1297:UNK	C	1430:UNK	N	5.88
1	B	2479:LEU	C	2487:UNK	N	3.66
1	E	2479:LEU	C	2487:UNK	N	3.66
1	I	2479:LEU	C	2487:UNK	N	3.66
1	G	2479:LEU	C	2487:UNK	N	3.66
1	B	2939:ARG	C	2942:UNK	N	3.38
1	E	2939:ARG	C	2942:UNK	N	3.38
1	I	2939:ARG	C	2942:UNK	N	3.38

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2939:ARG	C	2942:UNK	N	3.38

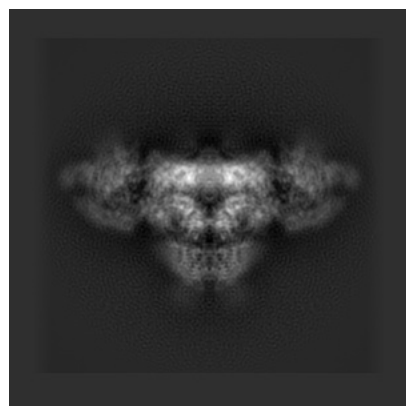
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8394. These allow visual inspection of the internal detail of the map and identification of artifacts.

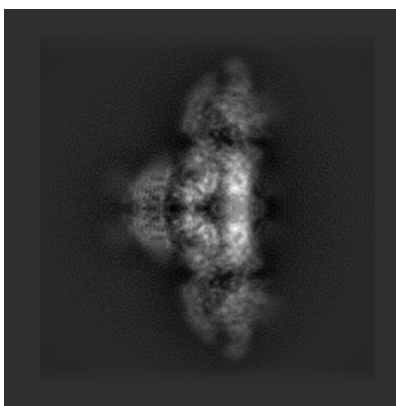
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

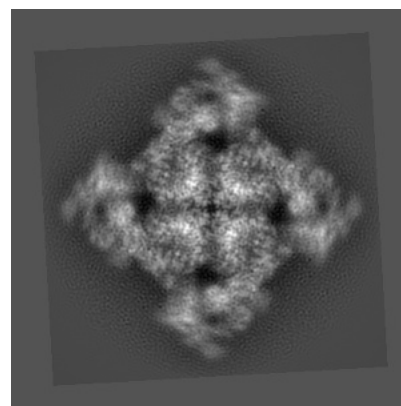
6.1.1 Primary map



X

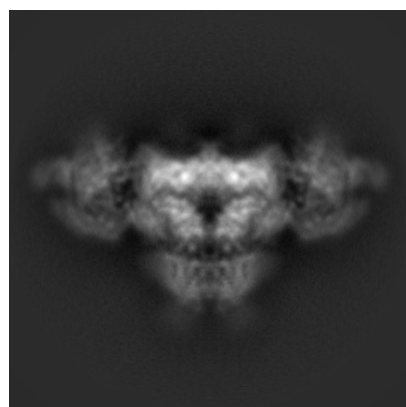


Y

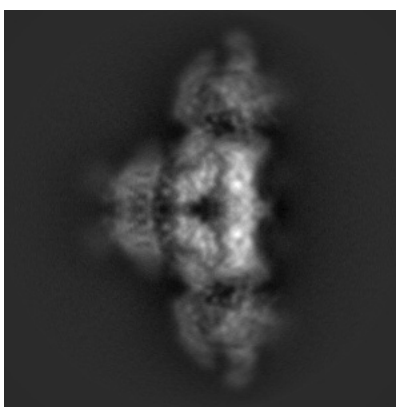


Z

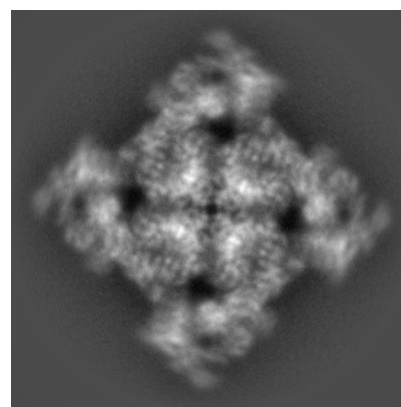
6.1.2 Raw map



X



Y

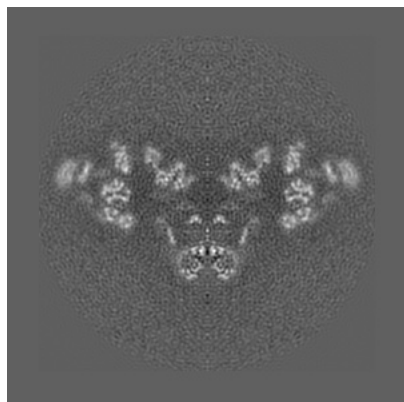


Z

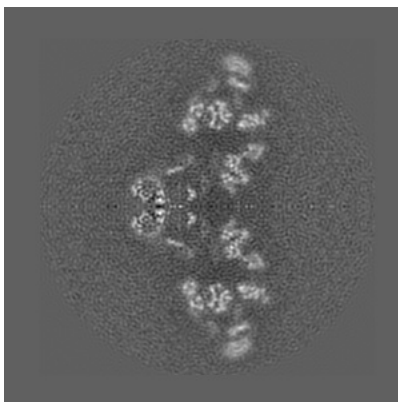
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

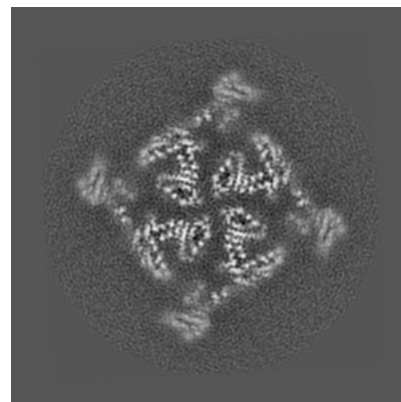
6.2.1 Primary map



X Index: 200

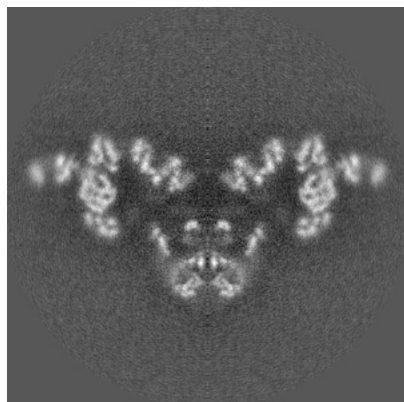


Y Index: 200

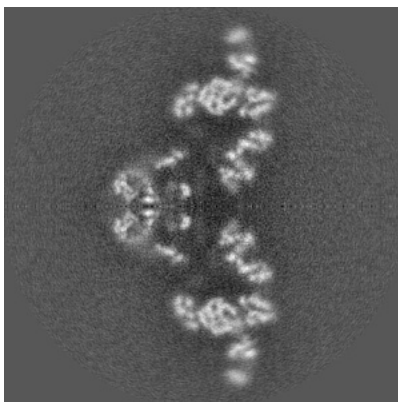


Z Index: 200

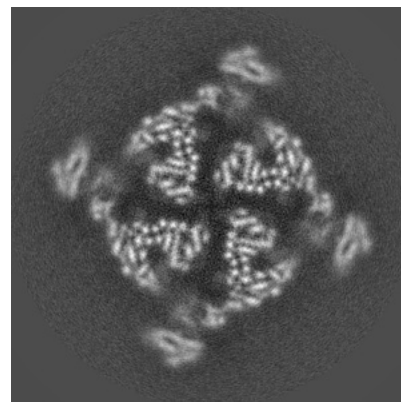
6.2.2 Raw map



X Index: 168



Y Index: 168

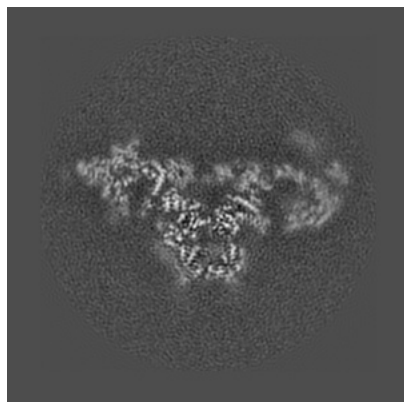


Z Index: 168

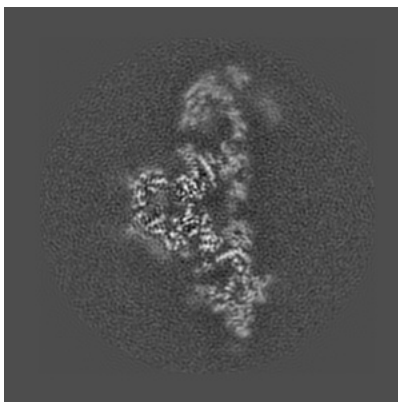
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

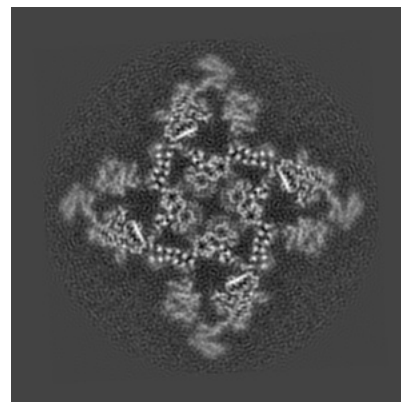
6.3.1 Primary map



X Index: 217

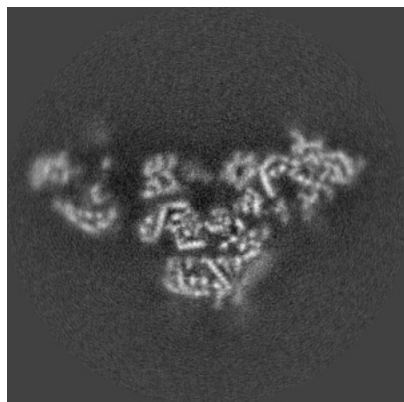


Y Index: 183

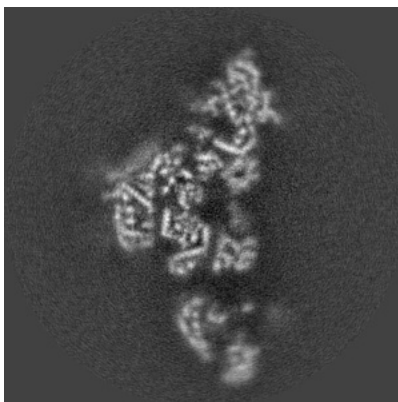


Z Index: 227

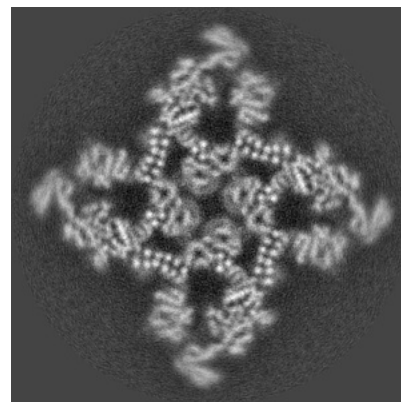
6.3.2 Raw map



X Index: 154



Y Index: 182

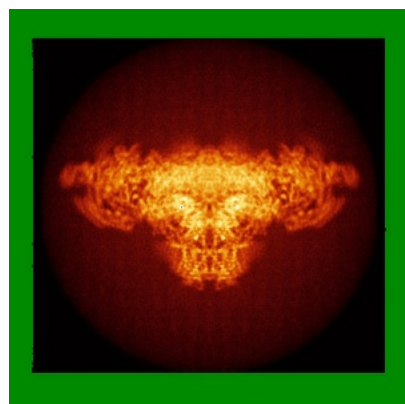


Z Index: 193

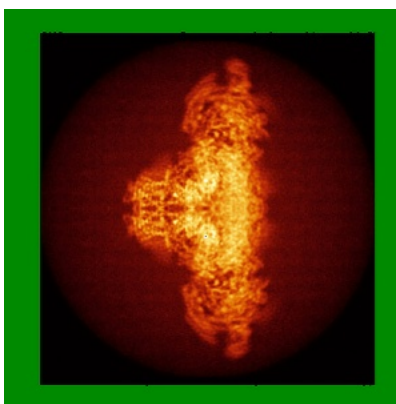
The images above show the largest variance slices of the map in three orthogonal directions.

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

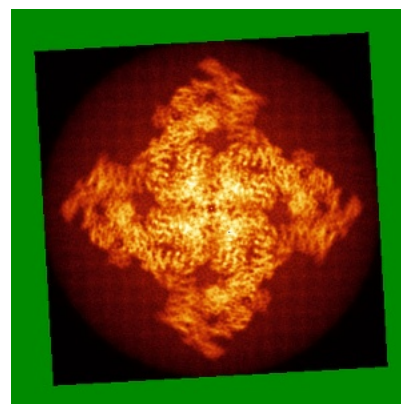
6.4.1 Primary map



X



Y

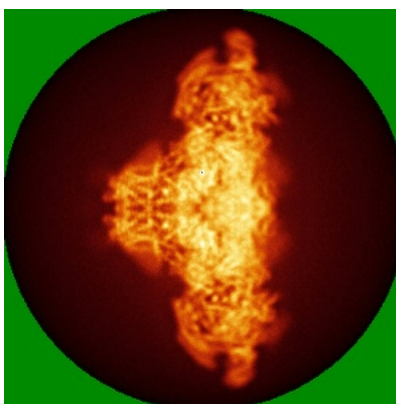


Z

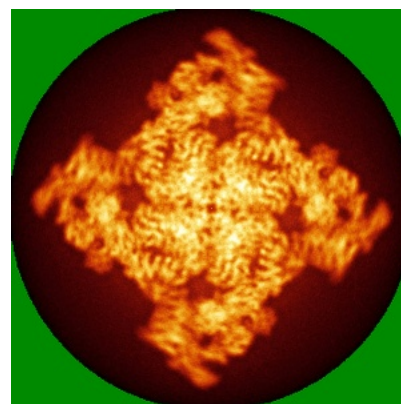
6.4.2 Raw map



X



Y

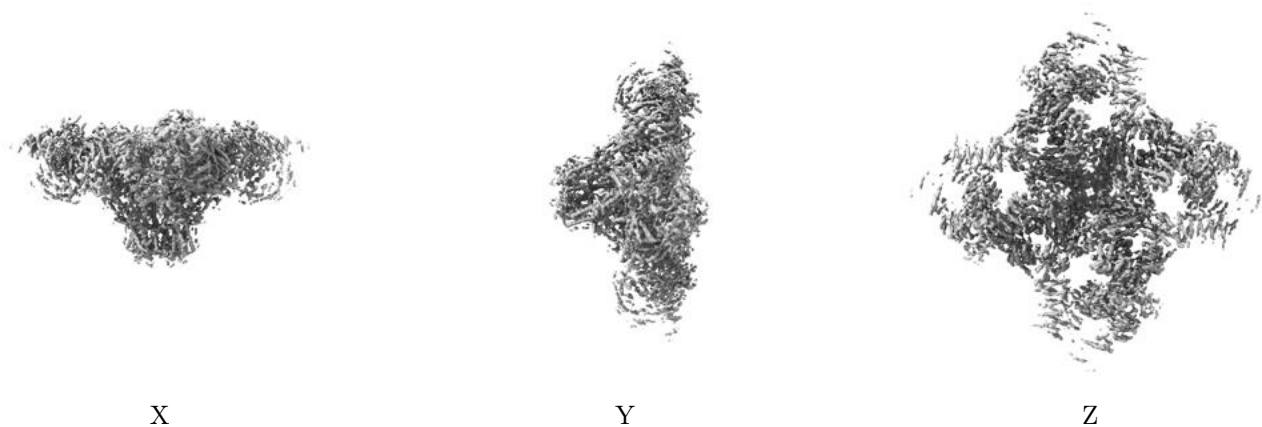


Z

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.

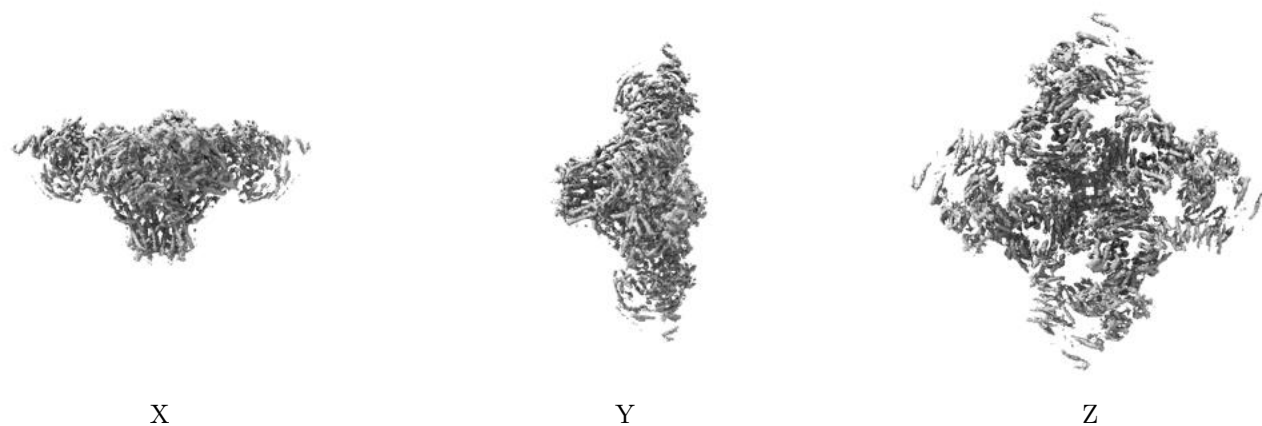
6.5 Orthogonal surface views [i](#)

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.

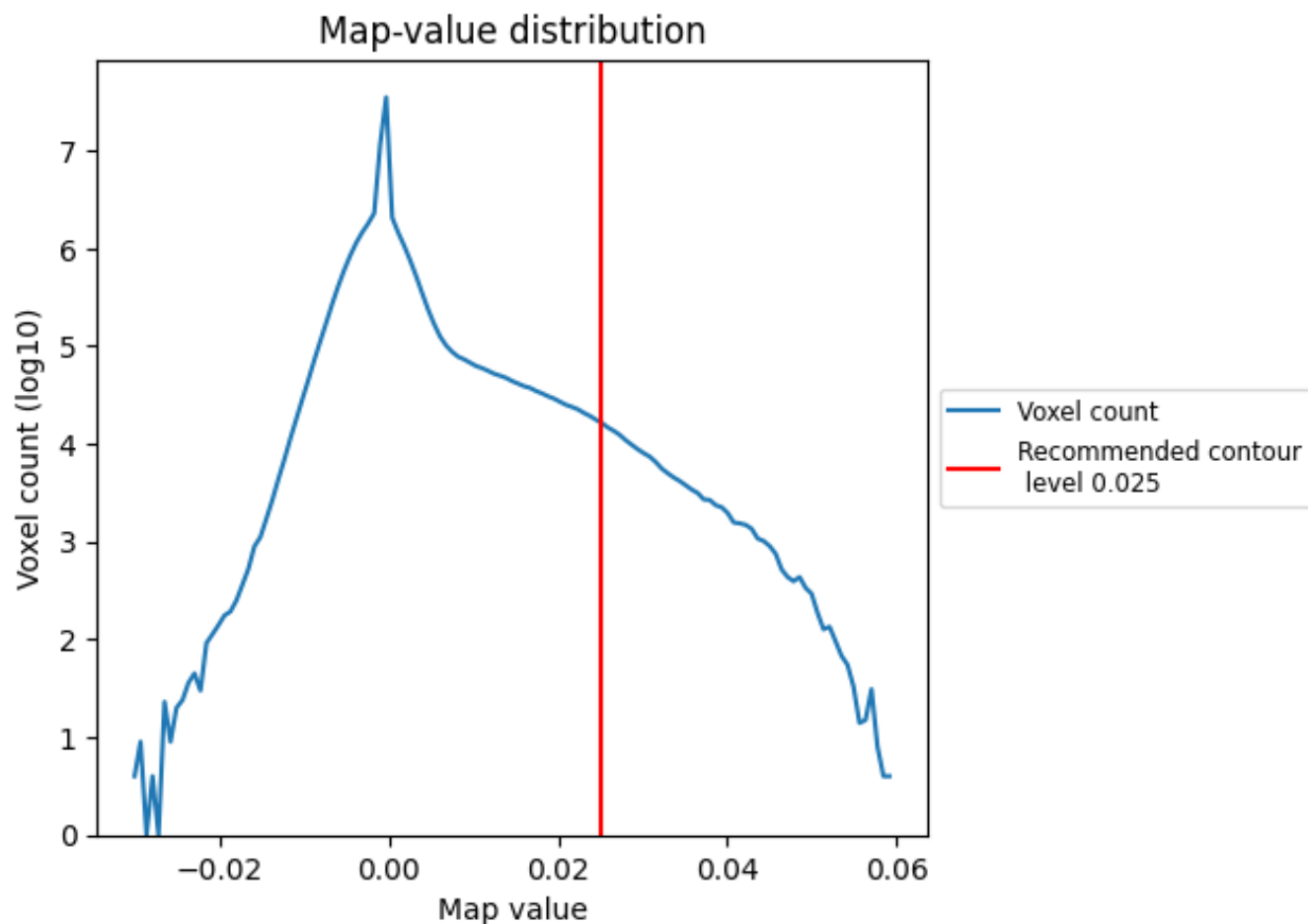
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

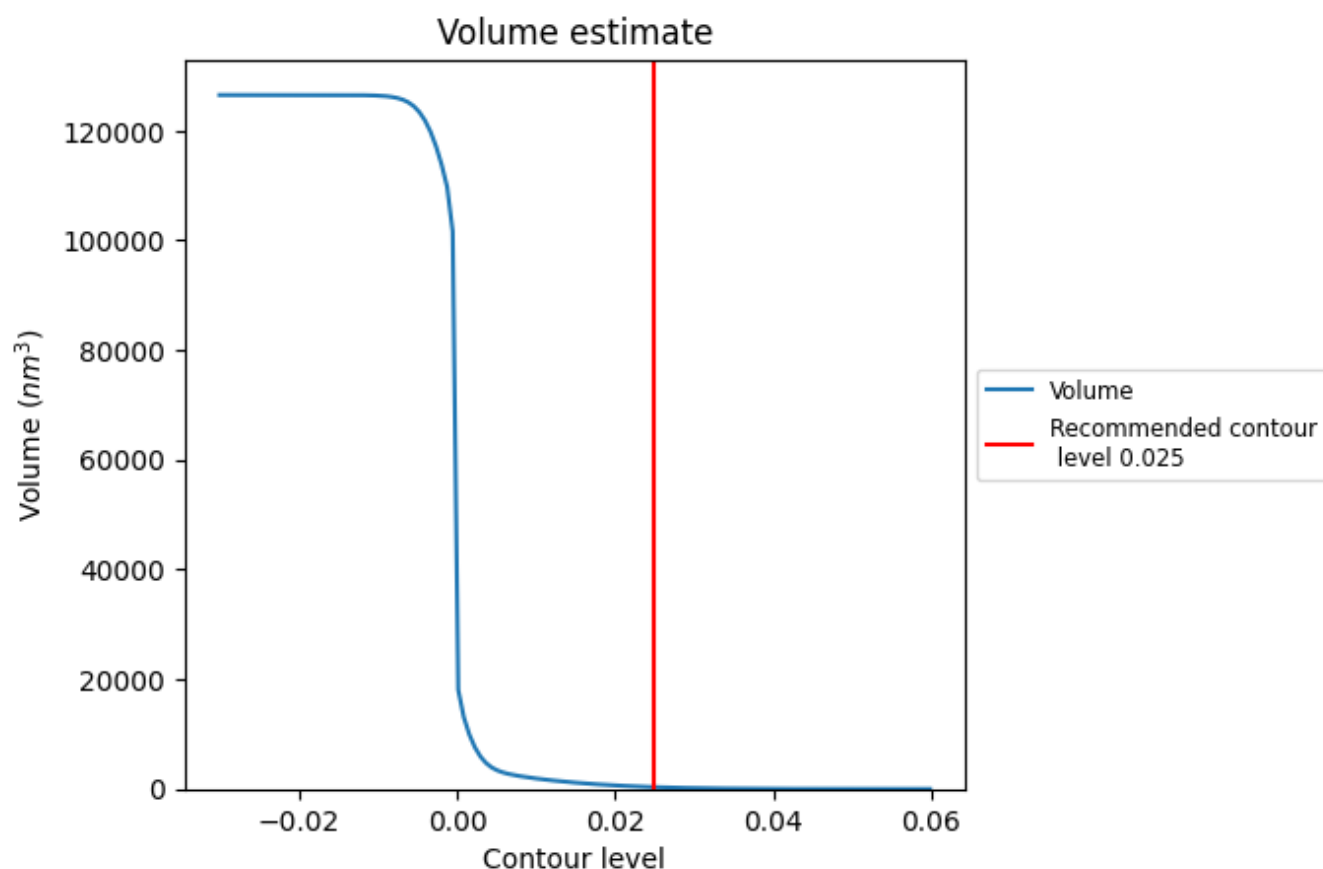
This section contains the results of statistical analysis of the map.

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.

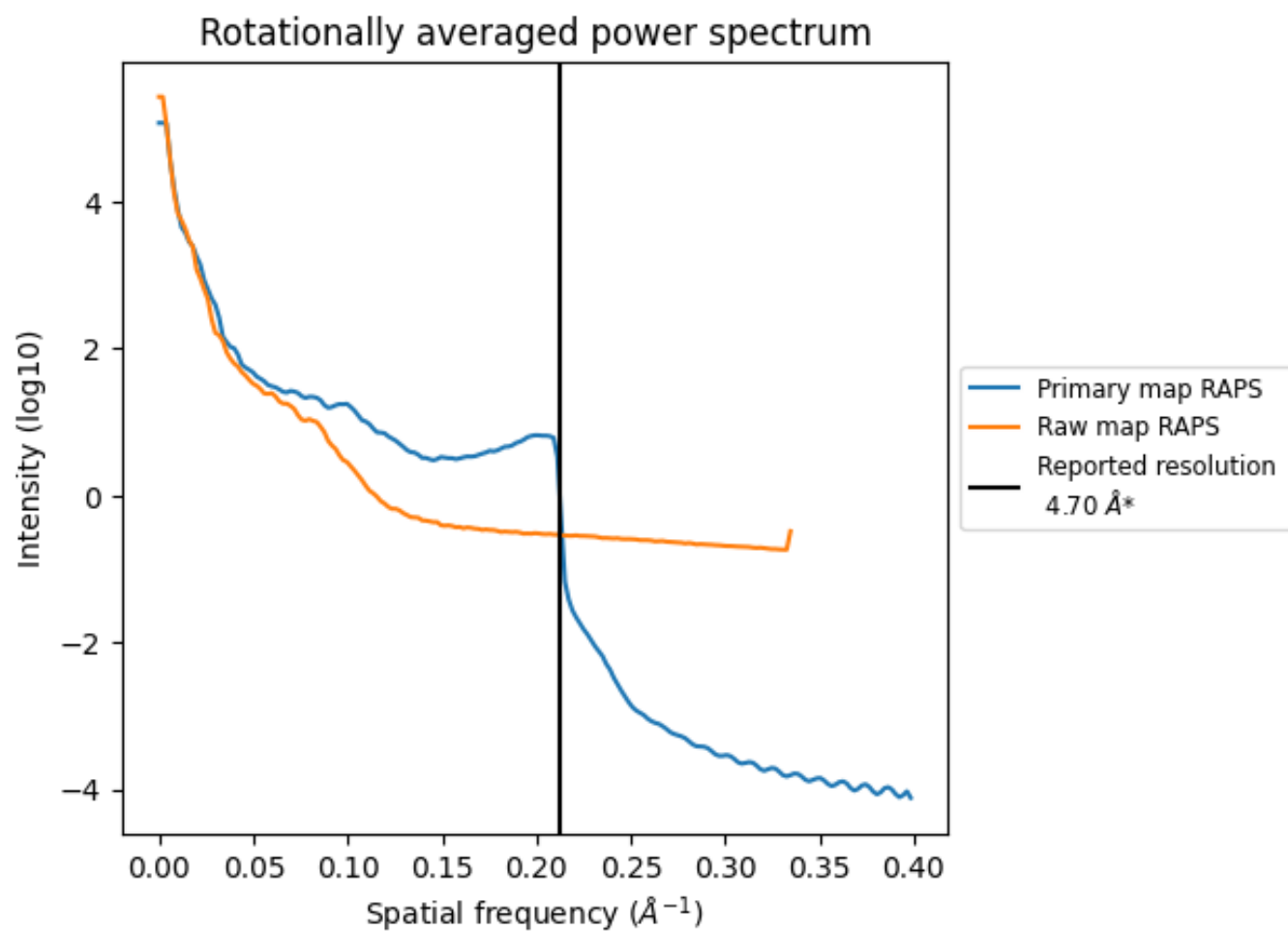
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm³; 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 ⓘ

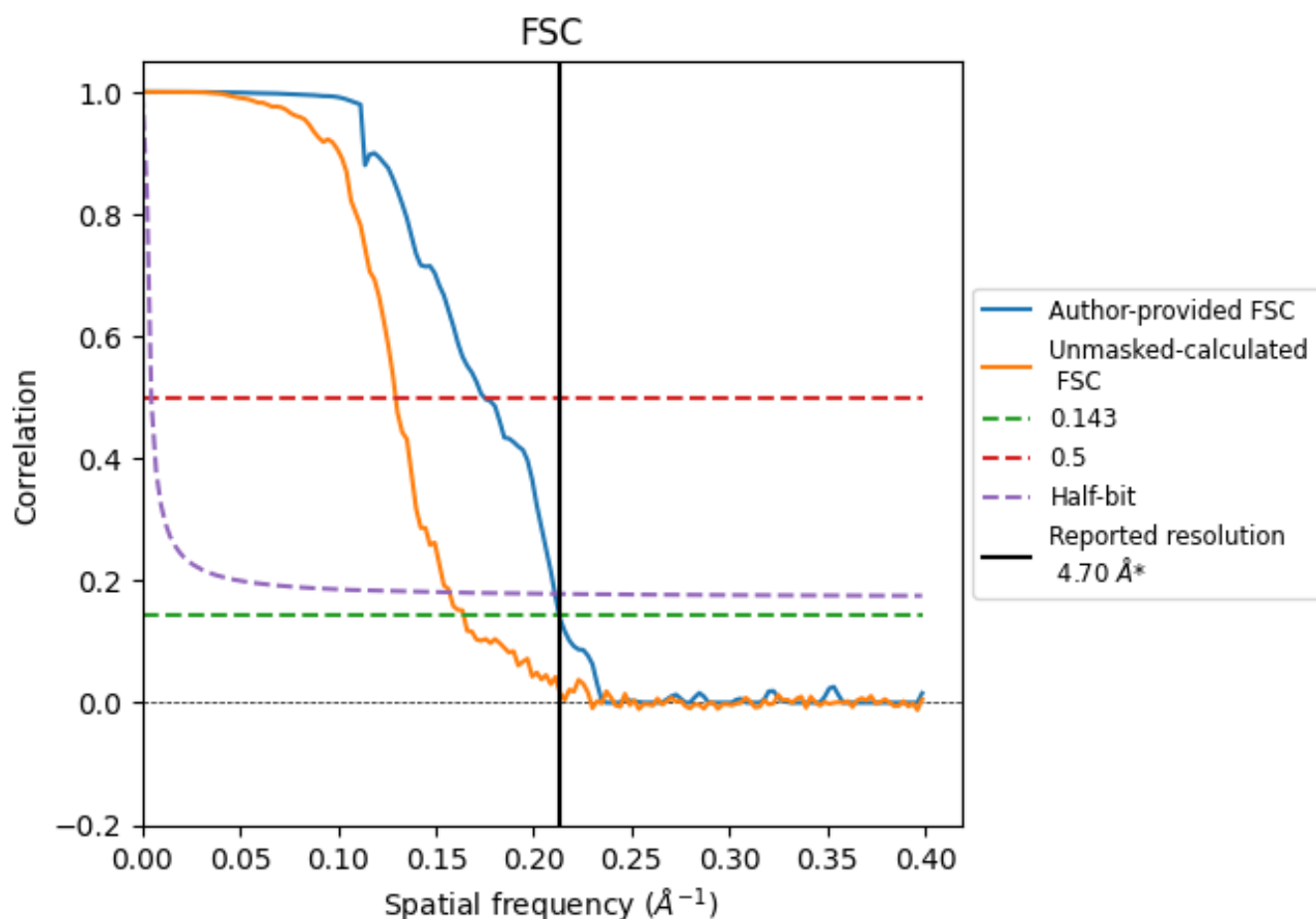


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

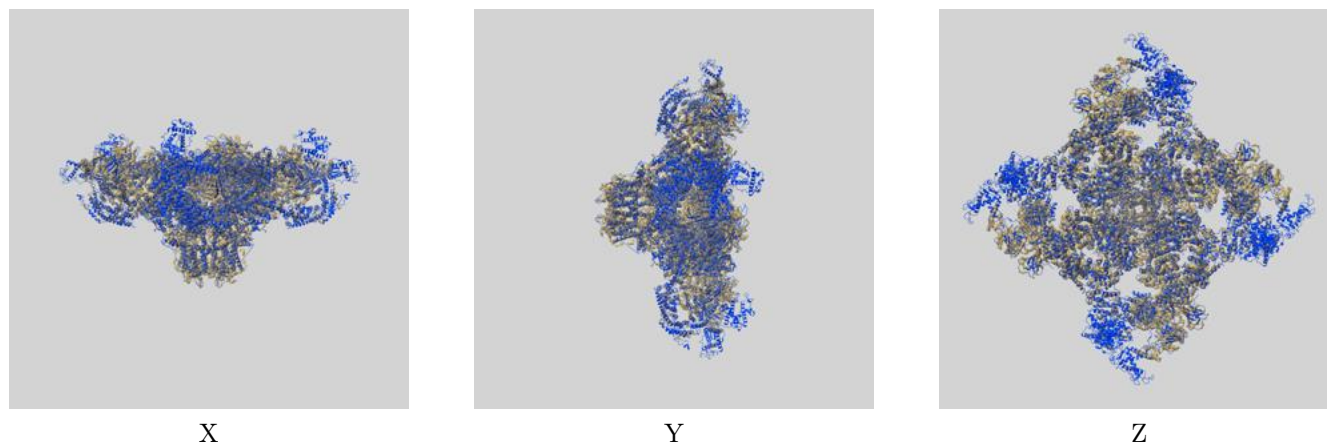
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.69	5.73	4.74
Unmasked-calculated*	6.09	7.73	6.37

*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 6.09 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

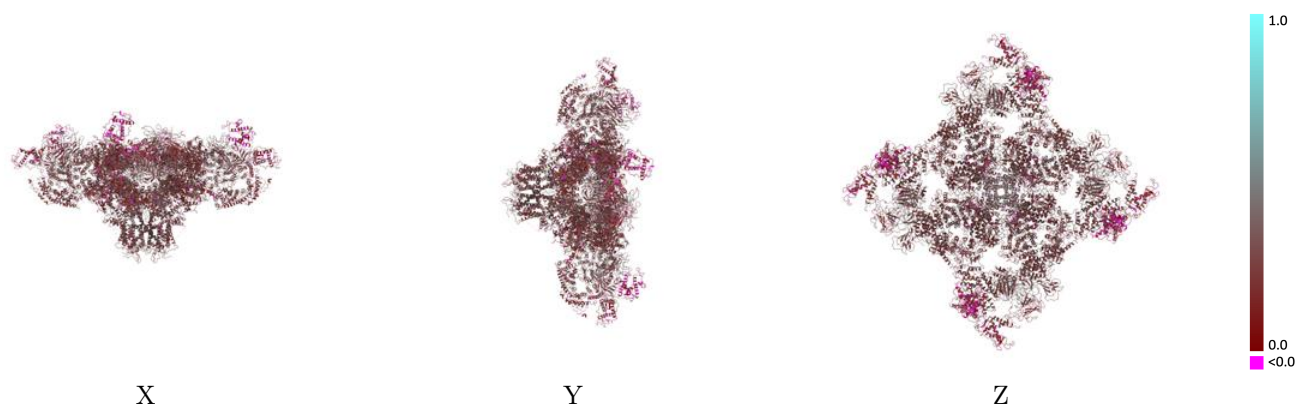
This section contains information regarding the fit between EMDB map EMD-8394 and PDB model 5TB3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



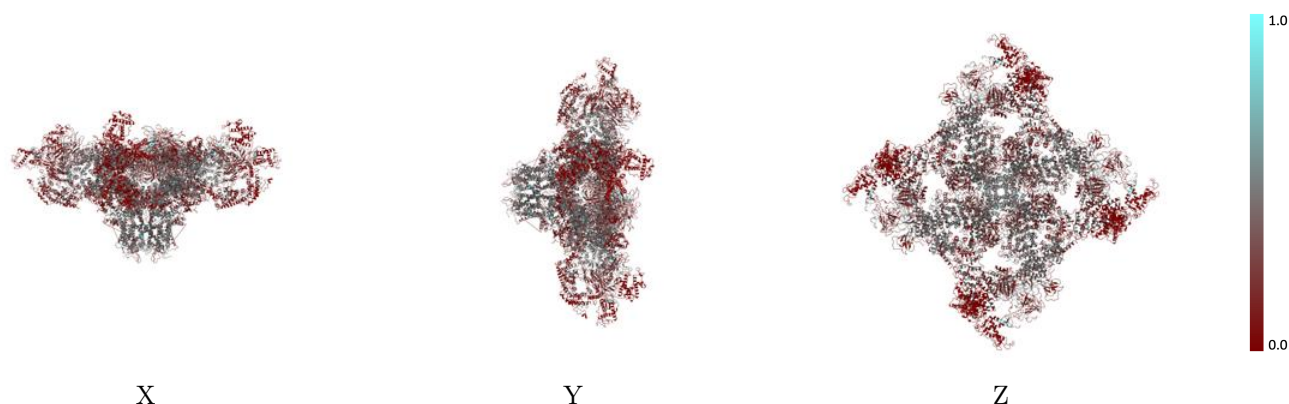
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



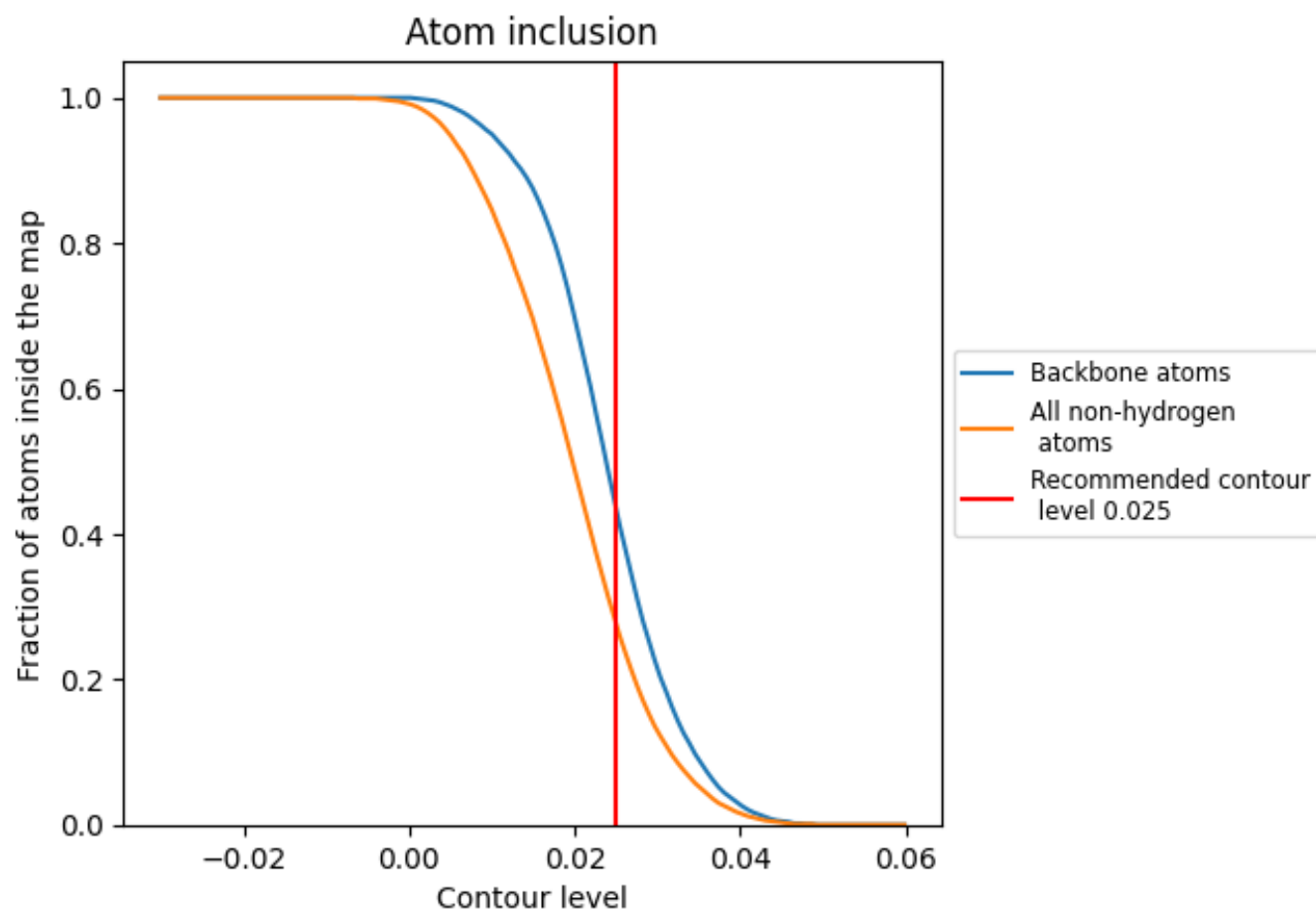
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 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	0.2760	0.2630
A	0.2390	0.2880
B	0.2780	0.2620
E	0.2770	0.2620
F	0.2380	0.2900
G	0.2770	0.2620
H	0.2390	0.2920
I	0.2770	0.2620
J	0.2390	0.2900

1.0

0.0

<0.0