



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 07:45 AM EDT

PDB ID : 5TB2
EMDB ID : EMD-8393
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

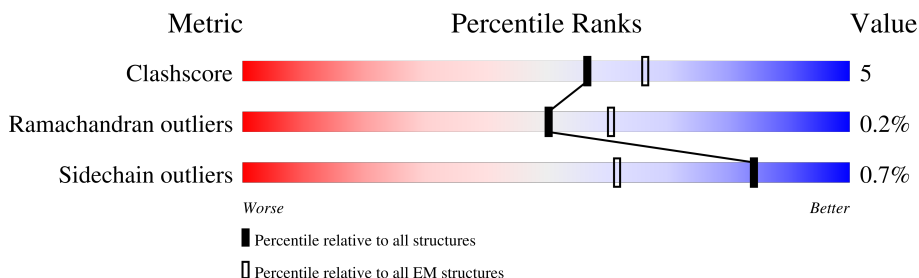
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	108	<div> <div>61%</div> <div>87%12%</div> </div>
1	F	108	<div> <div>62%</div> <div>87%12%</div> </div>
1	H	108	<div> <div>61%</div> <div>87%12%</div> </div>
1	J	108	<div> <div>60%</div> <div>90%9%</div> </div>
2	B	4416	<div> <div>51%</div> <div>84%11%5%</div> </div>
2	E	4416	<div> <div>51%</div> <div>84%11%5%</div> </div>
2	G	4416	<div> <div>51%</div> <div>84%11%5%</div> </div>
2	I	4416	<div> <div>52%</div> <div>84%11%5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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

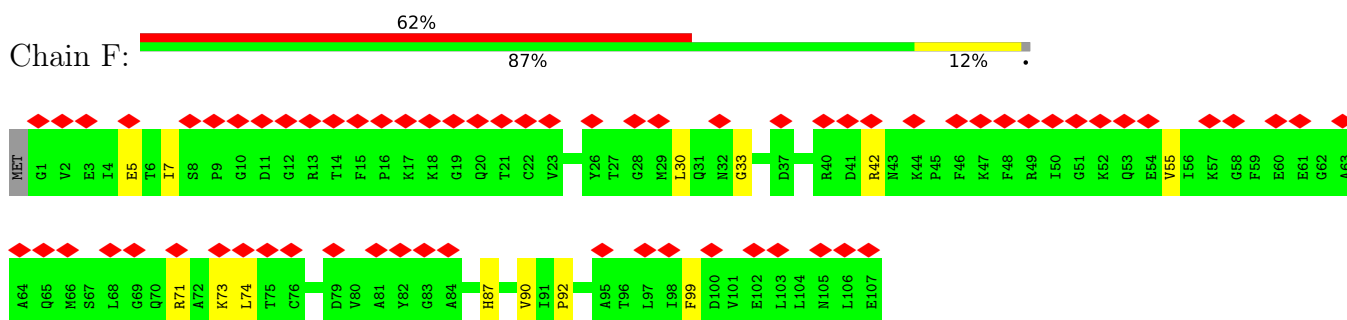
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

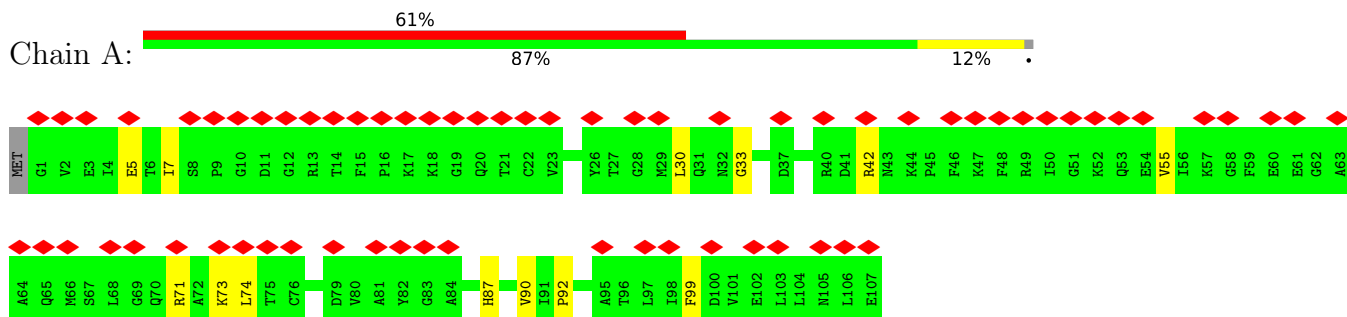
3 Residue-property plots [i](#)

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.

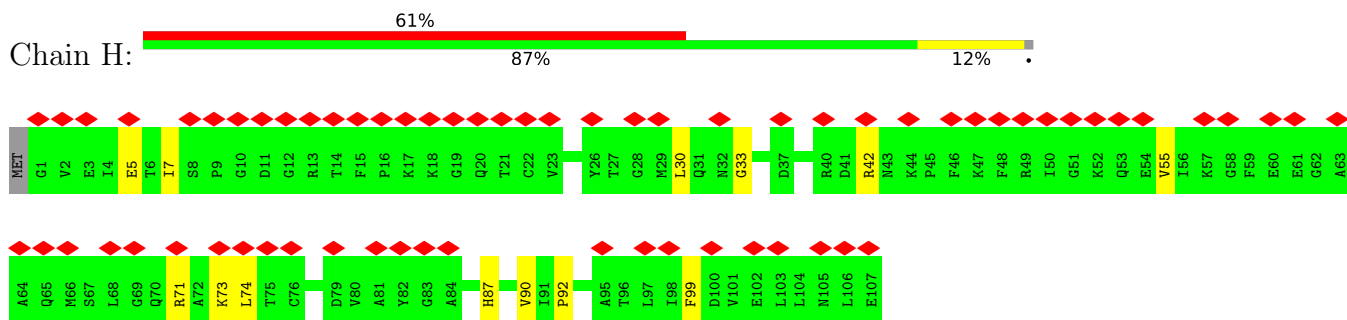
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



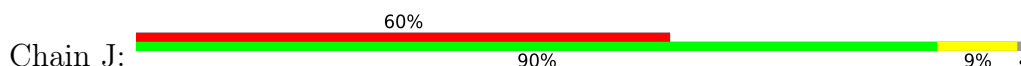
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

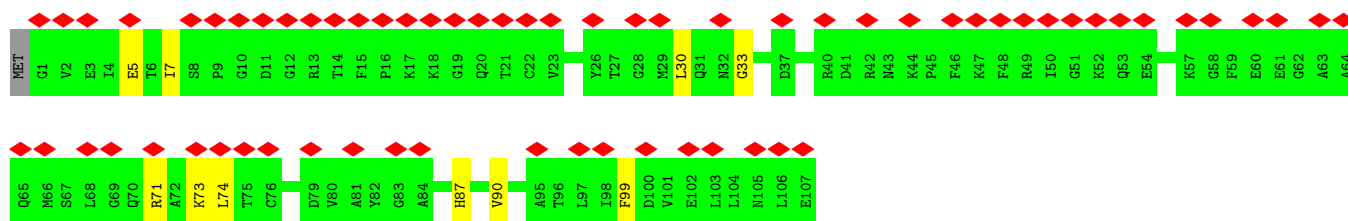


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

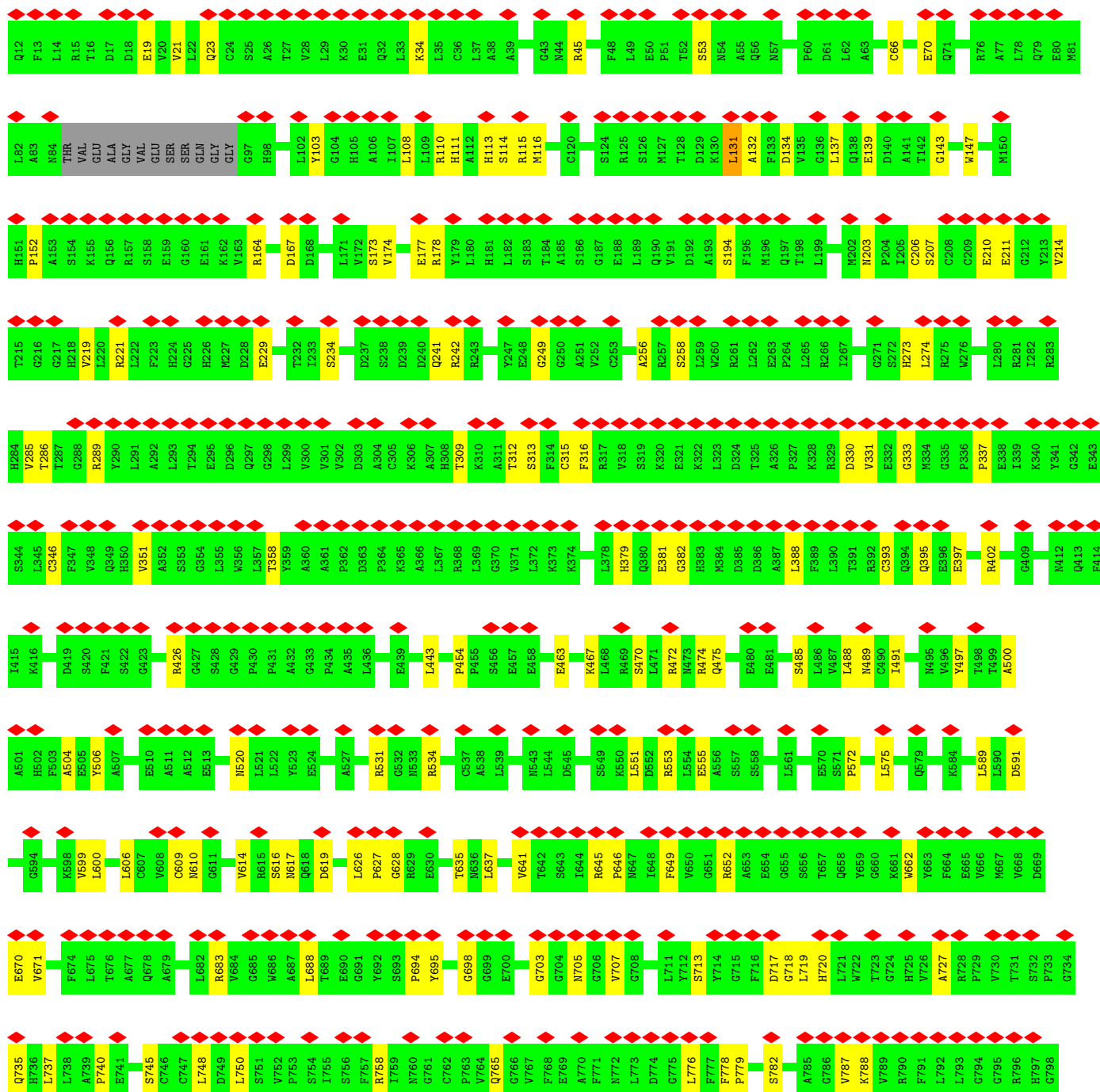
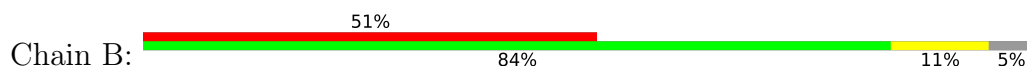


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





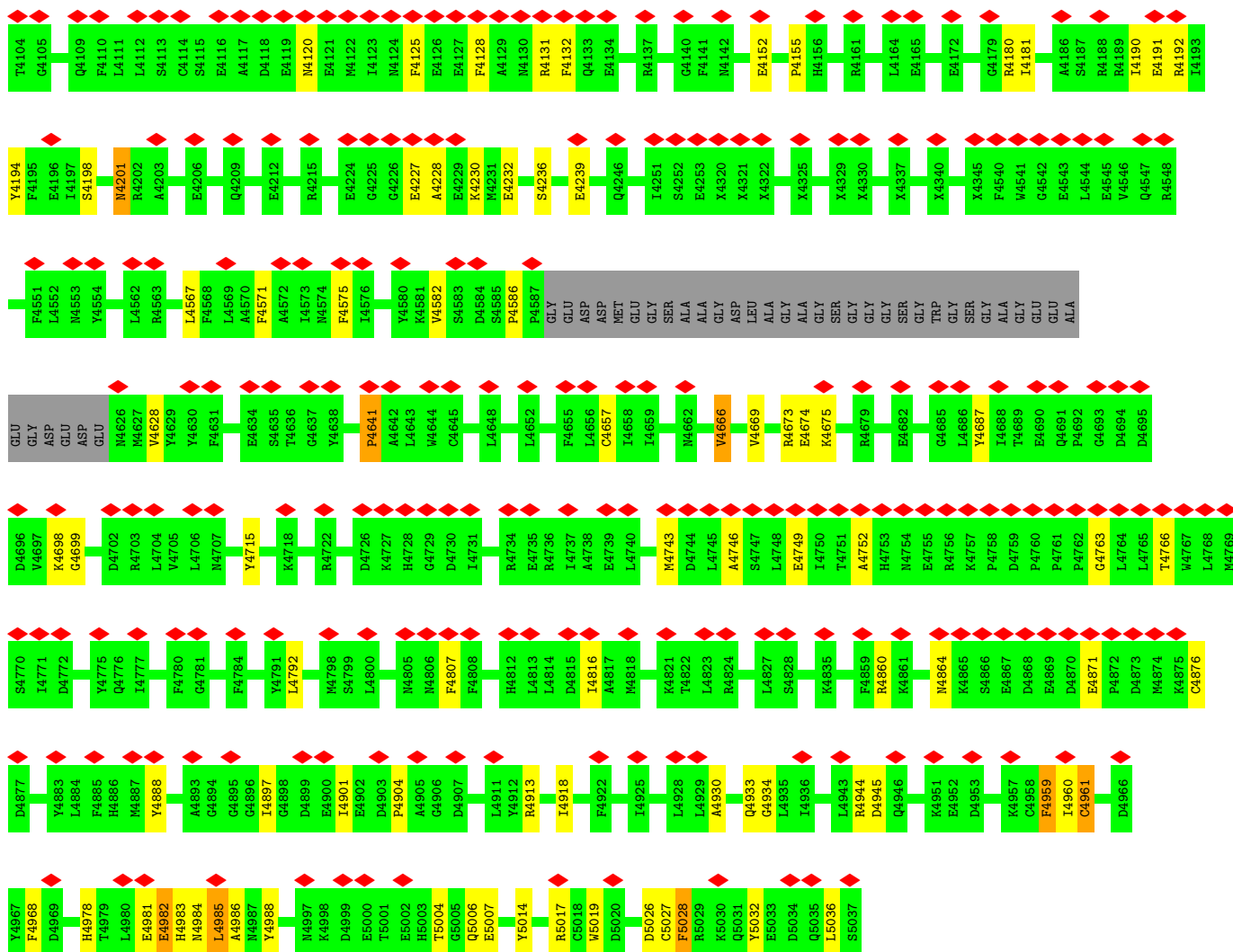
• Molecule 2: Ryanodine receptor 1





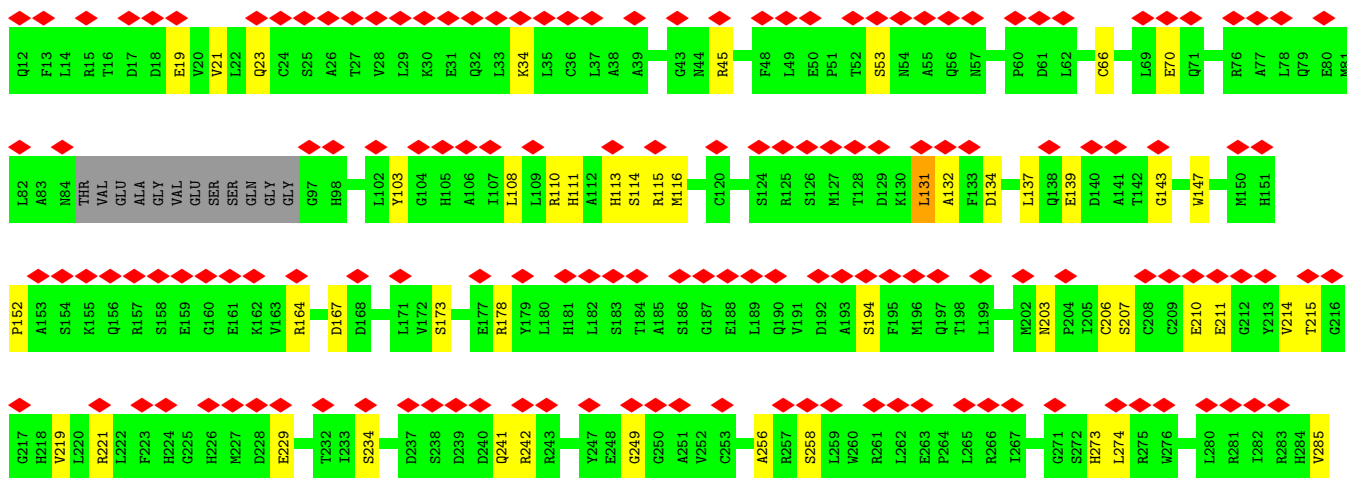






• Molecule 2: Ryanodine receptor 1

Chain I:

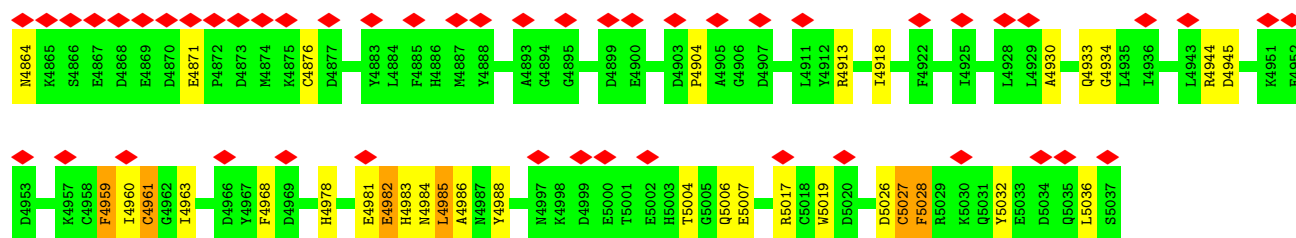




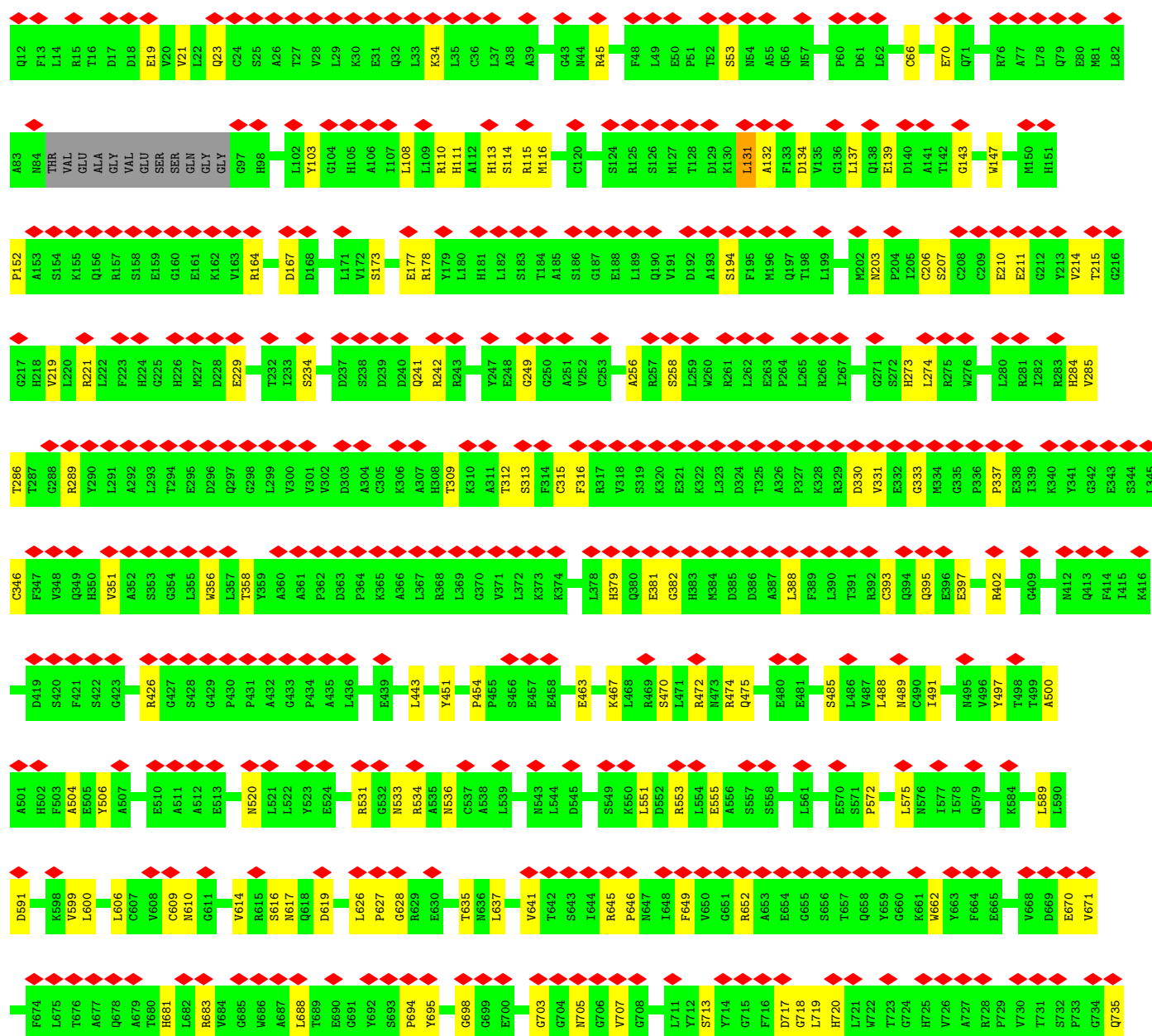
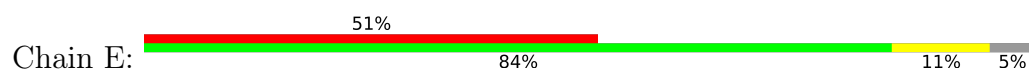




D4759	D4760	P4761	P4762	G4763	L4764	L4765	T4766	L4767	L4768	L4769	S4770	L4771	D4772	L4775	D4776	L4777	F4780	F4784	L4791	L4792	L4798	S4799	L4800	M4805	M4806	F4807	F4808	H4812	L4813	L4814	D4815	L4816	L4817	M4818	K4821	R4824	T4825	L4826	L4827	S4828	S4829	K4835	L4844	F4859	R4860	K4861									
I4688	T4689	E4690	Q4691	P4692	G4693	D4694	D4695	D4696	D4697	K4698	Q4699	D4702	R4703	L4704	L4705	L4706	Y4715	E4634	S4635	T4636	G4637	Y4638	P4641	L4642	L4643	L4644	C4645	L4648	L4652	F4655	L4656	C4657	T4658	Y4661	V4666	Y4669	R4673	E4674	L4675	R4679	E4682	G4685	L4686	Y4687											
X4330	X4340	X4341	X4345	F4340	M4341	F4342	E4343	L4344	E4345	F4346	E4347	E4348	F4351	L4352	M4353	L4356	F4357	L4358	F4359	L4360	F4361	A4362	M4363	F4364	F4365	L4366	F4367	GLY	GLY	ASP	ASP	MET	GLY	GLY	SER	ALA	GLY	ASP	LEU	ALA	GLY	GLY	GLY	GLY	GLY										
X3538	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3597	X3598	X3599	X3600
X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	P3640	L3641	Y3642	N3643	L3644	R3648	N3651	N3652	F3653	L3654	E3655	K3658	A3659	A3660	L3661	L3663	L3664	E3665	D3666	H3667	S3668	F3669	D3675	D3676	K3679	A3680	Q3681	Q3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	E3712	K3713	S3714				
K3715	E3718	D3719	Y3720	M3723	A3724	Y3725	A3726	K3731	S3732	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLY	ALA	GLU	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	E3759	K3760	Q3761	R3762	L3763	Q3766	R3769	T3772	R3773	V3779	L3780	E3693	K3787	S3803	L3804	L3805					
N3809	E3810	E3811	K3815	M3816	L3817	K3821	D3822	Q3830	Q3833	L3842	D3843	R3849	Q3850	E3854	G3855	L3856	G3857	M3858	V3859	N3860	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873	V3874	M3875	A3876	D3877	D3878	Q3882	R3886	Q3889	E3893	N3896	N3897	D3898	F3899										
T3907	D3921	Y3922	L3923	E3928	S3929	D3932	F3933	Y3934	Y3937	S3938	G3939	K3940	D3941	V3942	I3943	E3944	E3945	Q3946	G3947	K3948	R3949	N3950	K3953	K3959	Q3960	V3961	F3962	N3963	Q3970	Q3978	S3979	L3980	A3981	H3982	L3985	L3993	A3997	M4000	M4001	L4003	A4004	Q4005	D4006	S4007	S4008										
Q4009	L4010	E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	D4022	L4031	E4032	G4033	N4034	V4035	G4038	A4041	E4050	E4056	M4057	L4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	L4071	V4072	G4073	S4074	E4075	A4076	F4077	Q4078	D4079	V4080	Y4081	T4082	D4083	P4084	L4085	G4086	L4087	I4088	K4091			
D4092	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	L4108	Q4109	F4110	L4111	L4112	S4113	C4114	S4115	E4116	A4117	D4118	E4119	N4120	E4121	M4122	L4123	N4124	F4125	E4126	F4127	F4128	A4129	N4130	R4131	F4132	Q4133	E4134	R4137	C4140	F4141	N4142	L4147	E4152	P4155	H4156	D4157	P4158	R4161				
L4164	E4165	E4172	R4180	I4181	A4186	S4187	R4188	R4189	T4190	E4191	L4192	Y4193	Y4194	F4195	E4196	I4197	S4198	M4201	R4202	A4203	E4206	Q4209	E4212	R4215	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	S4236	E4239	E4244	I4251	S4252	E4253	X4320	X4321	X4322	X4325	X4329											
X4330	X4340	X4341	X4345	F4340	M4341	F4342	E4343	L4344	E4345	F4346	E4347	E4348	F4351	L4352	M4353	L4356	F4357	L4358	F4359	L4360	F4361	A4362	M4363	F4364	F4365	L4366	F4367	GLY	GLY	ASP	ASP	MET	GLY	GLY	SER	ALA	GLY	ASP	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY							
TRP	GLY	SER	ALA	GLY	GLY	GLY	GLY	ASP	ASP	GLY	N4626	M4627	Y4628	Y4629	Y4630	F4631	E4634	S4635	T4636	G4637	Y4638	P4641	L4642	L4643	L4644	C4645	L4648	L4652	F4655	L4656	C4657	T4658	Y4661	V4666	Y4669	R4673	E4674	L4675	R4679	E4682	G4685	L4686	Y4687												
D4759	P4760	P4761	P4762	G4763	L4764	L4765	T4766	L4767	L4768	L4769	S4770	L4771	D4772	D4775	D4776	L4777	F4780	F4784	L4791	L4792	L4798	S4799	L4800	M4805	M4806	F4807	F4808	H4812	L4813	L4814	D4815	L4816	L4817	M4818	K4821	R4824	T4825	L4826	L4827	S4828	S4829	K4835	L4844	F4859	R4860	K4861									



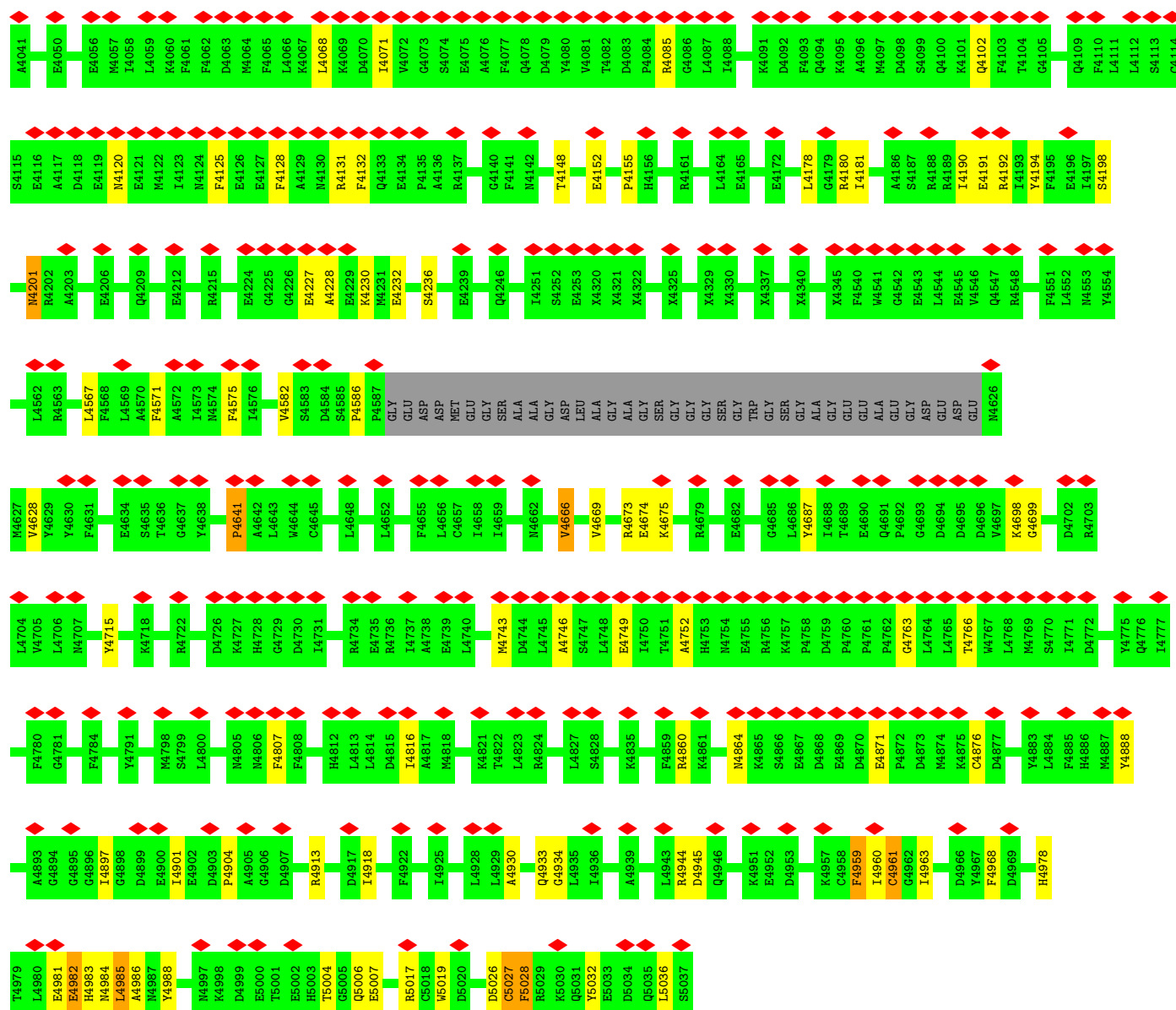
• Molecule 2: Ryanodine receptor 1



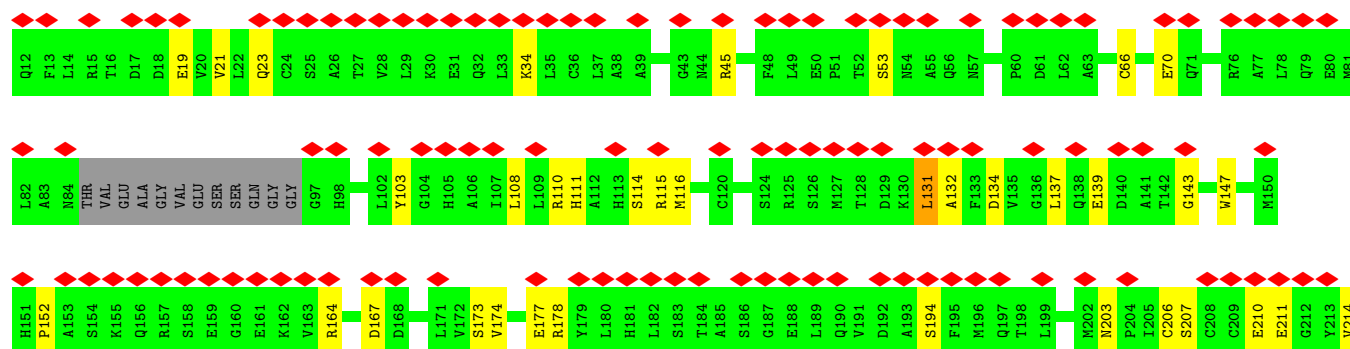
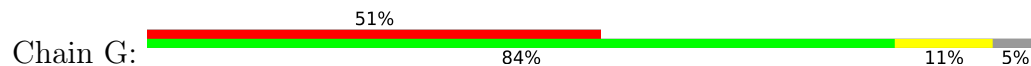


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GLU	E1963	P2024	S2093	K2221	Q2308	S2374	L2451	X2535	X2633	X2697	T2787	THR
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GLU	V1965	D2026	Q2107	R2223	S2310	L2376	R2453	X2537	X2635	X2699	ASP	ASP
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		GLU	Q2193	L2286	L2351	N2414	L2493	X2570	X2668	H2763	L2821	
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		GLU	H2204	L2289	L2354	H2417	L2496	X2573	X2601	L2766	K2814	
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		GLU	G2217	K2297	L2359	L2432	L2501	X2578	X2606	X2615	L2819	
					L2360	L2433	L2502	X2579	X2607	X2616	E2820	
					L2361	L2434	L2503	X2580	X2608	X2617	L2821	
					L2362	G2434	L2504	X2581	X2609	X2618	L2822	
					L2363	R2435	L2505	X2582	X2610	X2619	E2823	
					L2364		L2506	X2583	X2611	X2620	L2824	
					L2365		L2507	X2584	X2612	X2621	K2825	
					L2366		L2508	X2585	X2613	X2622	A2826	
					L2367		L2509	X2586	X2614	X2623	R2827	
					L2368		L2510	X2587	X2615	X2624	E2828	
					R2369		L2511	X2588	X2616	X2625	G2829	
					G2370		L2512	X2589	X2617	X2626	E2830	
							L2513	X2590	X2618	X2627	GLU	
							L2514	X2591	X2619	X2628	ARG	
							L2515	X2592	X2620	X2629	THR	
							L2516	X2593	X2621	X2630	GLU	
							L2517	X2594	X2622	X2631	LYS	
							L2518	X2595	X2623	X2632	LYS	
							L2519	X2596	X2624	X2633	LYS	
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							L2521	X2598	X2626	X2635	LYS	
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							L2523	X2600	X2628	X2637	LYS	
							L2524	X2601	X2629	X2638	LYS	
							L2525	X2602	X2630	X2639	LYS	
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							L2530	X2607	X2635	X2644	LYS	
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							L2532	X2609	X2637	X2646	LYS	
							L2533	X2610	X2638	X2647	LYS	
							L2534	X2611	X2639	X2648	LYS	
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X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	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		
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N3651	M3652	F3653	K3658	A3659	A3660	W3661	L3662	L3663	T3664	E3665	D3666	S3667	S3668	F3669	D3675	D3676	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	F3689	V3690	E3691	E3692	K3693	R3707	E3712	K3713	S3714	K3715	E3718	D3719	V3720	M3723	A3724	V3725	K3731	S3732	C3733	H3734	L3735	G3736	E3737	G3738									
G3739	E3740	N3741	GLY	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	E3759	K3760	Q3761	R3762	L3763	Q3766	R3769	T3772	K3773	V3779	L3780	K3787	S3803	L3804	L3805	N3809	A3810	E3811	K3815	M3816	L3817	K3821	D3822	Q3830	Q3833	L3842	D3843															
R3849	Q3850	E3854	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873	V3874	M3875	A3876	D3877	D3878	E3879	Q3882	R3886	Q3889	E3893	N3896	F3899	Q3906	T3907	L3923	L3924	R3925	E3928	S3929	D3932	Y3937	S3938	G3939	K3940	D3941	V3942												
L3943	E3944	E3945	Q3946	G3947	K3948	L3949	N3950	K3953	V3961	F3962	N3963	Q3970	Q3978	S3979	L3980	A3981	H3982	L3985	L3993	F3996	A3997	M4000	M4001	K4002	L4003	A4004	Q4005	Q4006	S4007	S4008	Q4009	L4010	E4011	L4012	L4013	L4014	E4015	D4018	L4019	D4022	L4031	E4032	G4033	N4034	V4035	G4038													



• Molecule 2: Ryanodine receptor 1

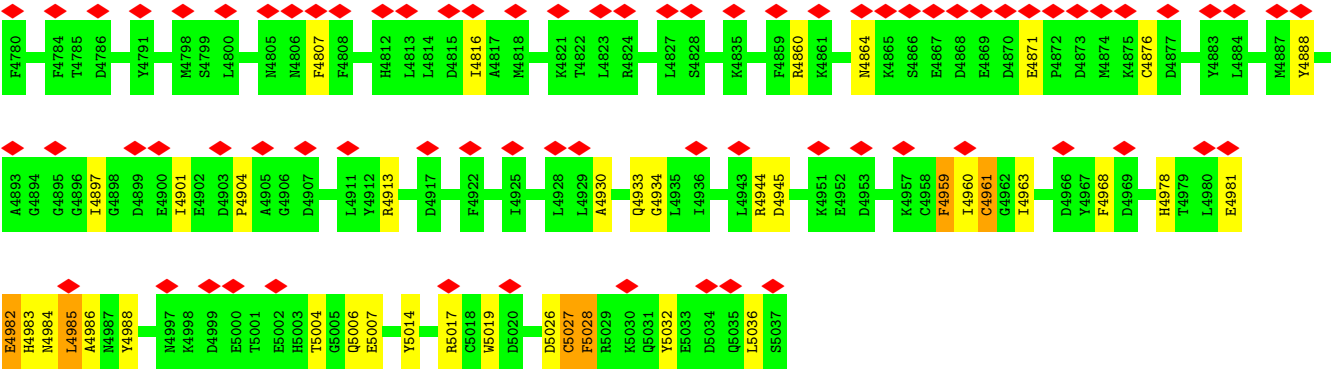


PRO	D986	G926	H866	E799	G734	D669	L589	T499	I415	S344	H984	T215
ASP	R987	E927	L867	F800	Q735	E670	L590	A500	K416	L345	V285	G216
GLN	L988	T928	E868	K801	H736	V671	D591	A501	D419	C346	T286	G217
PRO	A989	L929	R869	F802	L737	F674	K998	H502	S420	F347	G288	H218
SER	G992	K930	R870	P806	A739	L675	V599	A504	S422	V348	R289	V219
GLN	H993	T931	R871	G807	P740	L676	L606	E505	G423	H350	R290	L220
VAL	H994	L932	E872	Y808	E741	T677	C607	Y506	A292	V351	L222	R221
ASN	D999	L933	K873	A809	S745	Q678	V608	A507	R426	A352	L291	L223
GLN		A934	L874	H812	C746	Q679	G609	E510	G427	S353	A293	F223
SER	Y1007	G936	E876	E813	C747	A679	N610	A511	S428	G354	T294	H224
ARG	A1009	H938	T877	R814	L748	L682	G611	A512	G429	L355	D296	H226
TRP	VAL	H939	T878	V815	D749	R683	V614	E513	P430	W356	Q297	D228
D1070	GLN	G940	R879	L816	L750	V684	R615	N520	P431	T358	G298	E229
R1071	ASP	T940	E880	L817	S751	G685	S616	L521	A359	Y359	L299	T232
R1073	ILE	M941	L881	P817	T752	G686	N617	L522	A432	A360	V300	I233
F1074	PRO	A942	W892	R820	F753	A687	Q618	Y523	G433	A361	V301	S234
R1076	ALA	D943	A883	L821	S754	L688	D619	E524	P434	P362	D303	D237
R1078	ARG	E944	L884	L822	T755	T689	L626	R531	A435	D363	A304	S238
E1078	ARG	R822	L885	L823	S756	E690	P627	G532	E439	P364	C305	D239
K1079	ASN	K945	T885	L824	F757	G691	G628	N533	L443	A366	K306	D240
PRO	PRO	A946	R886	E824	R758	P694	R629	R534	Y451	L367	A307	Q241
Y1089	L1021	E947	T887	R827	W760	Y695	E630	A535	P454	R368	H308	R242
F1092	V1022	D948	E888	E828	G761	G699	T635	C537	P455	L369	K310	R243
E1093	P1023	N949	Q889	Y829	T762	E700	N636	L539	S456	G370	A311	Y247
A1094	Y1024	L950	C890	R830	F763	G699	L637	A538	S457	V371	T312	E248
V1095	R1025	K951	W891	R831	W764	E700	V641	L544	E458	L372	S313	G249
T1096	L1026	K952	T892	E832	Q765	G766	T642	D545	E463	K373	F314	G250
T1097	L1027	T953	Y893	G833	G766	G767	S643	N543	R317	C374	F315	A251
G1098	L1028	K954	C894	P834	F768	G767	I644	L544	K467	F316	R318	C253
E1099	E1029	L955	P895	R835	E769	G768	R645	L544	L468	R319	V318	A256
M1100	A1030	P956	V896	R836	A770	N705	R646	D552	R469	S320	S319	R257
G1103	T1031	K957	D898	P837	F771	G706	P646	R553	S470	E321	K320	S258
W1104	R1032	T958	D899	H838	W772	V707	N647	L554	L471	H383	L259	L260
A1105	R1033	Y959	N900	L839	L773	G708	I648	R555	R472	M384	R261	L262
P1107	S1034	M960	K901	S843	G775	L711	T648	A556	Q475	D385	L263	E263
E1108	D1037	S962	R902	R844	L776	Y712	F649	S557	E480	D386	P264	L265
R1110	S1038	N963	L903	R845	F777	S713	V650	S558	E481	L388	P327	L266
P1111	L1039	G964	H904	L846	P778	Y714	R652	A558	S485	F389	K328	R266
D1112	C1040	P965	C905	L846	P779	G715	A653	S558	L486	L390	R329	D330
V1113	K966	K966	C906	L847	P779	F716	E654	S558	V487	T391	D331	V331
E1114	Q1041	P967	C907	H848		D717	G655	L561	L488	R392	E332	G271
L1115	A1042	A968	V908	T849	S782	G718	G655	L561	M489	C393	G333	S272
G1116	V1043	A968	N909	D850	A785	L719	S656	E570	Q490	Q394	G333	H273
A1117	R1044	P969	F910	P853	G786	H720	T657	S571	S485	Q395	M334	L274
D1118	T1045	L970	H911	C854	W787	W722	Q658	P572	L486	E596	G335	R275
E1119	L1046	D971	P855	R856	K788	T723	G660	L575	L488	E597	P336	W276
L1120	L1047	S973	L913	D857	W789	G724	R661	N576	M489	Q395	P337	L280
A1121	H974	H974	P914	THR	R790	H725	W662	I577	Q491	Q395	E338	R281
Y1122	G1048	H975	E915	VAL	F791	W726	Y663	I578	L491	E596	I339	R282
V1123	Y1049	P976	P916	GLN	L792	A727	F664	Q579	M495	E597	K340	I282
F1124	G1050	R976	P917	T861	L793	R728	G665	K584	V496	E597	Y341	R283
M1125	Y1051	L977	E917	L861	G794	P729	V666		Y497		G342	
	M1052	T978	R918	W862	G795	V730	M667		T498		E343	
	I1053	P979	N919	L863	R796	T731						
	PRO	A980	Y920	P864		S732						
		Q981	N921	P865		P733						
		T982	L922									
		T983	N924									
		L984	S925									
		V985										



X3317	X3318	X3319	X3320	X3321	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	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																																																																		
X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	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																																																																
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	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	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	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250																																																																	
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	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047																																																
L2904	L2905	V2906	P2907	D2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2916	K2917	A2918	D2919	A2920	E2921	K2922	A2923	K2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	X2940	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966																																																																
E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	P2792	P2793	V2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	V2805	K2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	M2819	E2820	V2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	K2829	E2830	GLU	GLU	THR	ARG	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	P2783																																																																
GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	E2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903																																																																
X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	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																																																																	
X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2558	X2561	X2562	X2563	X2567	X2568	X2569	X2570	X2571	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2593	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2605	X2606	X2611	X2612	X2613	X2614	X2618	X2619	X2620	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652																																																						
K2447	G2448	L2451	R2452	L2453	R2454	A2455	R2458	S2459	L2460	L2463	L2466	I2469	S2471	L2472	P2473	L2474	Q2475	I2476	P2477	P2478	L2479	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2498	X2499	X2500	X2511	X2512	X2513	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2528	X2529	X2532	X2533																																																																												
S2374	G2375	L2376	L2377	A2378	A2379	L2380	E2381	E2382	A2383	L2384	S2387	E2388	D2389	P2390	A2391	D2392	D2393	G2394	P2395	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	GLU	N2414	R2415	V2416	H2417	L2418	G2419	M2423	L2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	H2440	H2441																																																																										





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	0.068	Depositor
Minimum map value	-0.038	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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	33/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	17
2	E	0	17
2	G	0	16
2	I	0	16
All	All	0	66

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	G	131	LEU	CA-CB-CG	8.35	134.51	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.48	115.30
2	E	131	LEU	CA-CB-CG	8.33	134.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1676	LEU	CA-CB-CG	6.33	129.86	115.30
2	G	1676	LEU	CA-CB-CG	6.33	129.86	115.30
2	B	1676	LEU	CA-CB-CG	6.32	129.84	115.30
2	E	1676	LEU	CA-CB-CG	6.32	129.84	115.30
2	E	1600	LEU	CA-CB-CG	6.29	129.77	115.30
2	B	1600	LEU	CA-CB-CG	6.29	129.75	115.30
2	I	1600	LEU	CA-CB-CG	6.29	129.76	115.30
2	B	4985	LEU	CA-CB-CG	6.28	129.75	115.30
2	E	4985	LEU	CA-CB-CG	6.28	129.74	115.30
2	G	4985	LEU	CA-CB-CG	6.28	129.74	115.30
2	G	1600	LEU	CA-CB-CG	6.28	129.74	115.30
2	I	4985	LEU	CA-CB-CG	6.27	129.73	115.30
2	G	977	LEU	CA-CB-CG	5.57	128.11	115.30
2	E	977	LEU	CA-CB-CG	5.56	128.08	115.30
2	B	977	LEU	CA-CB-CG	5.55	128.08	115.30
2	I	977	LEU	CA-CB-CG	5.54	128.04	115.30
2	I	3663	LEU	CA-CB-CG	5.22	127.30	115.30
2	E	3663	LEU	CA-CB-CG	5.21	127.27	115.30
2	G	3663	LEU	CA-CB-CG	5.20	127.26	115.30
2	B	3663	LEU	CA-CB-CG	5.20	127.25	115.30
2	E	688	LEU	CA-CB-CG	5.08	126.99	115.30
2	I	2290	LEU	CA-CB-CG	5.08	126.98	115.30
2	G	688	LEU	CA-CB-CG	5.08	126.97	115.30
2	B	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	B	2290	LEU	CA-CB-CG	5.07	126.96	115.30
2	I	688	LEU	CA-CB-CG	5.07	126.96	115.30
2	G	2290	LEU	CA-CB-CG	5.07	126.95	115.30
2	E	2290	LEU	CA-CB-CG	5.06	126.94	115.30
2	B	727	ALA	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2001	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	4031	LEU	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
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2001	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	4031	LEU	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
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2001	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	4031	LEU	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2001	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	4031	LEU	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	8	0
1	J	818	0	824	5	0
2	B	29499	0	24751	284	0
2	E	29499	0	24751	290	0
2	G	29499	0	24751	288	0
2	I	29499	0	24751	286	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	121272	0	102300	1147	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 (1147) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	1.76	1.33
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	1.77	1.33
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	1.77	1.32
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	1.76	1.31
2:B:4190:ILE:HD11	2:B:5026:ASP:OD2	1.31	1.26
2:E:4190:ILE:HD11	2:E:5026:ASP:OD2	1.31	1.19
2:G:4190:ILE:HD11	2:G:5026:ASP:OD2	1.31	1.13
2:I:4190:ILE:HD11	2:I:5026:ASP:OD2	1.31	1.11
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.78	1.02
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.78	1.01
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.78	1.01
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.78	1.00
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.31	0.99
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.30	0.99
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.30	0.98
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.30	0.98
2:I:4190:ILE:HD11	2:I:5026:ASP:CG	1.92	0.90
2:B:4190:ILE:HD11	2:B:5026:ASP:CG	1.92	0.90
2:E:4190:ILE:HD11	2:E:5026:ASP:CG	1.92	0.89
2:G:4190:ILE:HD11	2:G:5026:ASP:CG	1.92	0.89
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.61	0.89
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.61	0.89
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.61	0.88
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.61	0.88
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.61	0.88
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.61	0.88
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.61	0.87
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.61	0.87
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.66	0.83
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.60	0.83
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.66	0.82
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.61	0.82
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.49	0.81
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.49	0.81
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.66	0.81
2:B:4968:PHE:HZ	2:B:4978:HIS:CE1	1.99	0.81
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.60	0.80
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	1.81	0.80
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.61	0.80
2:E:4190:ILE:HD13	2:E:5026:ASP:OD2	1.81	0.80
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.49	0.79
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.49	0.79
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	2.01	0.78
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	2.01	0.78
2:I:4968:PHE:HZ	2:I:4978:HIS:CE1	1.99	0.78
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	2.01	0.78
2:G:4968:PHE:HZ	2:G:4978:HIS:CE1	1.99	0.78
2:E:4968:PHE:HZ	2:E:4978:HIS:CE1	1.99	0.77
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	2.01	0.76
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.33	0.76
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.01	0.75
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.33	0.75
2:B:4190:ILE:HD13	2:B:5026:ASP:OD2	1.81	0.75
2:G:4190:ILE:HD13	2:G:5026:ASP:OD2	1.81	0.74
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.33	0.74
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.01	0.74
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.01	0.74
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.01	0.73
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.33	0.72
2:I:4960:ILE:HG23	2:I:4988:TYR:HE2	1.56	0.71
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.60	0.70
2:G:4960:ILE:HG23	2:G:4988:TYR:HE2	1.56	0.70
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.59	0.70
2:B:4960:ILE:HG23	2:B:4988:TYR:HE2	1.56	0.70
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.59	0.69
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.69
2:E:4960:ILE:HG23	2:E:4988:TYR:HE2	1.56	0.69
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.57	0.69
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.59	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.68
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.57	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.57	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.57	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.67
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.29	0.65
2:B:173:SER:HB3	2:B:178:ARG:H	1.62	0.65
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.30	0.65
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.62	0.65
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.30	0.65
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.30	0.64
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	2.13	0.64
2:G:173:SER:HB3	2:G:178:ARG:H	1.62	0.64
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.62	0.64
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.62	0.64
2:I:173:SER:HB3	2:I:178:ARG:H	1.62	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.13	0.64
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.63
2:E:173:SER:HB3	2:E:178:ARG:H	1.62	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.80	0.63
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.63
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.63
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.62	0.63
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.13	0.63
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.32	0.63
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.32	0.62
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.80	0.62
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.32	0.62
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.62
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.62
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.80	0.62
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.32	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.61
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.61
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.61
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.61
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.30	0.61
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.80	0.61
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.82	0.61
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.83	0.61
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.61
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.83	0.61
2:B:2347:GLU:O	2:B:2351:ASN:N	2.34	0.61
2:E:2347:GLU:O	2:E:2351:ASN:N	2.34	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.60
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.83	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.60
2:G:2347:GLU:O	2:G:2351:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.35	0.60
2:I:2347:GLU:O	2:I:2351:ASN:N	2.34	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.60
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.35	0.59
2:G:626:LEU:HG	2:G:628:GLY:H	1.66	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.67	0.59
2:I:626:LEU:HG	2:I:628:GLY:H	1.66	0.59
2:E:626:LEU:HG	2:E:628:GLY:H	1.66	0.59
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.67	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.59
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.67	0.59
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.35	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.59
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.85	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.59
2:I:4944:ARG:NH2	2:G:4945:ASP:OD2	2.36	0.59
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.85	0.59
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.85	0.59
2:B:626:LEU:HG	2:B:628:GLY:H	1.66	0.58
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.68	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.85	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.85	0.58
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.58
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.58
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.85	0.58
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.58
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.68	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.58
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.68	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.58
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.67	0.57
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.35	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.85	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.77	0.57
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.86	0.57
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.77	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.36	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.77	0.57
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.86	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.38	0.57
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.57
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.57
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.86	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.68	0.57
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.86	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.87	0.57
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.57
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.38	0.57
2:G:4960:ILE:HG23	2:G:4988:TYR:CE2	2.40	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.87	0.57
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.87	0.56
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.38	0.56
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.87	0.56
2:I:4960:ILE:HG23	2:I:4988:TYR:CE2	2.40	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.37	0.56
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.38	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.56
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.87	0.56
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.86	0.56
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.86	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.87	0.56
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.87	0.56
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.79	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.56
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.86	0.55
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.88	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.79	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.79	0.55
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.55
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.40	0.55
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.86	0.55
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.79	0.55
2:E:4960:ILE:HG23	2:E:4988:TYR:CE2	2.40	0.55
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.88	0.55
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.55
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.87	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.89	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.55
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.55
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.40	0.55
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.40	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.79	0.55
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.55
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.89	0.55
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.87	0.55
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.88	0.55
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.40	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.37	0.55
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.39	0.55
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.40	0.55
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.39	0.55
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.40	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.72	0.55
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.89	0.54
2:B:4960:ILE:HG23	2:B:4988:TYR:CE2	2.40	0.54
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.40	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.39	0.54
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.89	0.54
2:B:606:LEU:O	2:B:617:ASN:ND2	2.41	0.54
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.89	0.54
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.89	0.54
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.89	0.54
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.54
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.89	0.54
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.90	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.41	0.54
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.72	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.54
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.54
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.72	0.54
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.90	0.54
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.54
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.54
2:B:4888:TYR:HA	2:I:4918:ILE:HD11	1.90	0.54
2:I:34:LYS:H	2:I:53:SER:HG	1.54	0.54
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.41	0.54
2:G:606:LEU:O	2:G:617:ASN:ND2	2.41	0.54
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.40	0.54
2:B:470:SER:O	2:B:474:ARG:NE	2.37	0.54
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.41	0.54
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.54
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.89	0.54
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.54
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.41	0.54
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.72	0.54
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.90	0.54
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.90	0.54
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.90	0.54
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.90	0.54
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.90	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.41	0.53
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.90	0.53
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.90	0.53
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.90	0.53
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.26	0.53
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.42	0.53
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.90	0.53
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.89	0.53
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.41	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.73	0.53
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.42	0.53
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.41	0.53
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.91	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.89	0.53
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.91	0.53
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.90	0.53
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.42	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.90	0.53
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.91	0.53
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.74	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.73	0.53
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.42	0.53
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.53
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.90	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.89	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.90	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.40	0.53
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.90	0.53
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.91	0.53
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.91	0.53
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.74	0.53
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.40	0.52
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.40	0.52
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.90	0.52
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.90	0.52
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.91	0.52
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.42	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.42	0.52
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.41	0.52
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.26	0.52
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.41	0.52
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.41	0.52
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.91	0.52
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.42	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.42	0.52
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.91	0.52
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.91	0.52
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.52
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.90	0.52
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.92	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.89	0.52
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.92	0.52
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.41	0.52
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.52
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.92	0.52
2:B:4945:ASP:OD2	2:E:4944:ARG:NH2	2.42	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.73	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.42	0.52
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.42	0.52
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.92	0.52
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.42	0.52
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.74	0.52
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.92	0.52
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.92	0.52
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.52
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.26	0.52
2:I:241:GLN:O	2:I:289:ARG:NH1	2.40	0.52
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.92	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.74	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:I:470:SER:O	2:I:474:ARG:NE	2.37	0.51
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.92	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.73	0.51
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.91	0.51
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.41	0.51
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.51
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.90	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.91	0.51
2:E:34:LYS:H	2:E:53:SER:HG	1.55	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.43	0.51
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.92	0.51
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.92	0.51
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.91	0.51
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.75	0.51
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.92	0.51
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.43	0.51
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.84	0.51
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.51
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.92	0.51
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.43	0.51
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.92	0.51
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.93	0.51
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.39	0.51
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.51
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	0.51
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.76	0.51
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.26	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.51
2:E:221:ARG:NE	2:E:258:SER:OG	2.44	0.51
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.92	0.51
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.75	0.51
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.92	0.51
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.90	0.51
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.51
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.93	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.51
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.93	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.84	0.51
2:B:34:LYS:H	2:B:53:SER:HG	1.55	0.51
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.51
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.51
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.76	0.51
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.51
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.84	0.51
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.51
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.91	0.51
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.93	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.93	0.51
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.93	0.50
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.93	0.50
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.84	0.50
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.76	0.50
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.93	0.50
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.93	0.50
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.75	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.93	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.39	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.50
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.50
2:I:3758:MET:HG3	2:I:3762:ARG:HD2	1.94	0.50
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.75	0.50
2:E:309:THR:O	2:E:313:SER:OG	2.29	0.50
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.76	0.50
2:G:3758:MET:HG3	2:G:3762:ARG:HD2	1.94	0.50
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.50
2:E:4960:ILE:CG2	2:E:4988:TYR:CE2	2.95	0.50
2:G:34:LYS:H	2:G:53:SER:HG	1.55	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:B:4960:ILE:CG2	2:B:4988:TYR:CE2	2.95	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.92	0.50
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.40	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.93	0.50
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.50
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.50
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.93	0.50
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.93	0.50
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.43	0.50
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.76	0.50
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.50
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.44	0.50
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.94	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.50
2:G:241:GLN:O	2:G:289:ARG:NH1	2.40	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.94	0.50
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.43	0.50
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.93	0.50
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.94	0.50
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.94	0.50
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.93	0.50
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.94	0.50
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.93	0.50
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.50
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.44	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3758:MET:HG3	2:B:3762:ARG:HD2	1.94	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.49
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.94	0.49
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.93	0.49
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.77	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.49
2:E:3758:MET:HG3	2:E:3762:ARG:HD2	1.94	0.49
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.94	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.49
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.49
2:G:221:ARG:NE	2:G:258:SER:OG	2.44	0.49
2:G:662:TRP:HB2	2:G:748:LEU:HD23	1.94	0.49
2:B:309:THR:O	2:B:313:SER:OG	2.29	0.49
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.46	0.49
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.94	0.49
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.43	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.78	0.49
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.46	0.49
2:G:776:LEU:HG	2:G:848:HIS:HA	1.94	0.49
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.46	0.49
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.76	0.49
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.78	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.94	0.49
2:G:4960:ILE:CG2	2:G:4988:TYR:CE2	2.95	0.49
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.94	0.49
2:B:241:GLN:O	2:B:289:ARG:NH1	2.40	0.49
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.94	0.49
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.95	0.49
2:I:662:TRP:HB2	2:I:748:LEU:HD23	1.94	0.49
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.78	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.94	0.49
2:I:4960:ILE:CG2	2:I:4988:TYR:CE2	2.95	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.94	0.49
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.95	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.78	0.49
2:I:776:LEU:HG	2:I:848:HIS:HA	1.94	0.49
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.94	0.49
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.40	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.49
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.49
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.95	0.49
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.94	0.49
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.49
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.48	0.49
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.49
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.46	0.49
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.94	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.40	0.49
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.43	0.49
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.95	0.49
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.76	0.49
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.48
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.48	0.48
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.94	0.48
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.94	0.48
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.44	0.48
2:E:4945:ASP:OD2	2:G:4944:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.95	0.48
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.95	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.85	0.48
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.96	0.48
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.48
2:I:467:LYS:HA	2:I:470:SER:HB2	1.96	0.48
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.95	0.48
2:G:2880:GLU:O	2:G:2884:ASN:N	2.46	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.94	0.48
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.95	0.48
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.48
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.29	0.48
2:I:234:SER:O	2:I:242:ARG:NE	2.46	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.48
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.95	0.48
2:E:662:TRP:HB2	2:E:748:LEU:HD23	1.94	0.48
2:E:776:LEU:HG	2:E:848:HIS:HA	1.94	0.48
2:E:2880:GLU:O	2:E:2884:ASN:N	2.46	0.48
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.95	0.48
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.78	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.42	0.48
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.78	0.48
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.95	0.48
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.48	0.48
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.43	0.48
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.96	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.48	0.48
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	1.95	0.48
2:B:134:ASP:OD1	2:B:134:ASP:N	2.47	0.48
2:B:206:CYS:SG	2:B:207:SER:N	2.87	0.48
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.96	0.48
2:I:221:ARG:NE	2:I:258:SER:OG	2.44	0.48
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.95	0.48
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.40	0.48
2:E:206:CYS:SG	2:E:207:SER:N	2.87	0.48
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.48
2:G:467:LYS:HA	2:G:470:SER:HB2	1.96	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.95	0.48
2:B:467:LYS:HA	2:B:470:SER:HB2	1.96	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.48
2:I:4930:ALA:O	2:I:4934:GLY:N	2.47	0.48
2:E:467:LYS:HA	2:E:470:SER:HB2	1.95	0.48
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.96	0.48
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.94	0.48
2:G:234:SER:O	2:G:242:ARG:NE	2.46	0.48
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	1.96	0.48
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.94	0.47
2:B:4930:ALA:O	2:B:4934:GLY:N	2.47	0.47
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.96	0.47
2:E:241:GLN:O	2:E:289:ARG:NH1	2.40	0.47
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.78	0.47
2:G:4930:ALA:O	2:G:4934:GLY:N	2.47	0.47
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.96	0.47
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.47
2:E:234:SER:O	2:E:242:ARG:NE	2.46	0.47
2:E:939:VAL:HG22	2:E:1053:ILE:HG23	1.96	0.47
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.30	0.47
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.95	0.47
2:I:4068:LEU:HD13	2:I:4132:PHE:HE2	1.79	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.47	0.47
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.96	0.47
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.96	0.47
2:B:234:SER:O	2:B:242:ARG:NE	2.46	0.47
2:B:662:TRP:HB2	2:B:748:LEU:HD23	1.94	0.47
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.96	0.47
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.30	0.47
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.95	0.47
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.96	0.47
2:B:939:VAL:HG22	2:B:1053:ILE:HG23	1.96	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.80	0.47
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.80	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.47
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.33	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.85	0.47
2:B:4068:LEU:HD13	2:B:4132:PHE:HE2	1.80	0.47
2:I:939:VAL:HG22	2:I:1053:ILE:HG23	1.96	0.47
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.47
2:G:206:CYS:SG	2:G:207:SER:N	2.87	0.47
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.96	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.80	0.47
2:G:4068:LEU:HD13	2:G:4132:PHE:HE2	1.80	0.47
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.28	0.47
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.47
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	1.95	0.47
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.96	0.47
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.79	0.47
2:I:2880:GLU:O	2:I:2884:ASN:N	2.46	0.47
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.80	0.47
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	1.95	0.47
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.47
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.33	0.47
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.97	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.42	0.47
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.96	0.47
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.46
2:B:4944:ARG:NH2	2:I:4945:ASP:OD2	2.48	0.46
2:I:206:CYS:SG	2:I:207:SER:N	2.87	0.46
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	1.97	0.46
2:G:134:ASP:OD1	2:G:134:ASP:N	2.47	0.46
2:B:2880:GLU:O	2:B:2884:ASN:N	2.46	0.46
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.97	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.46
2:E:4068:LEU:HD13	2:E:4132:PHE:HE2	1.79	0.46
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.97	0.46
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.97	0.46
2:B:4034:ASN:ND2	2:B:4035:VAL:O	2.49	0.46
2:E:3766:GLN:HE22	2:E:3769:ARG:HH11	1.64	0.46
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.33	0.46
2:G:3766:GLN:HE22	2:G:3769:ARG:HH11	1.64	0.46
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.96	0.46
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.97	0.46
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.96	0.46
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3766:GLN:HE22	2:I:3769:ARG:HH11	1.64	0.46
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.97	0.46
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.30	0.46
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.34	0.46
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.97	0.46
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.97	0.46
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.49	0.46
2:G:939:VAL:HG22	2:G:1053:ILE:HG23	1.96	0.46
2:B:1516:UNK:N	2:B:1529:UNK:O	2.49	0.46
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.49	0.46
2:I:1516:UNK:N	2:I:1529:UNK:O	2.49	0.46
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	1.98	0.46
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.34	0.46
2:E:4034:ASN:ND2	2:E:4035:VAL:O	2.49	0.46
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.97	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.97	0.46
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.98	0.46
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.33	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.97	0.46
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.41	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.42	0.46
2:G:1516:UNK:N	2:G:1529:UNK:O	2.49	0.46
2:B:221:ARG:NE	2:B:258:SER:OG	2.44	0.46
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.97	0.46
2:I:4034:ASN:ND2	2:I:4035:VAL:O	2.49	0.46
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.39	0.46
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.49	0.46
2:B:3766:GLN:HE22	2:B:3769:ARG:HH11	1.64	0.46
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.47	0.46
2:G:4034:ASN:ND2	2:G:4035:VAL:O	2.49	0.46
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.97	0.45
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.49	0.45
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.45
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.49	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.97	0.45
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.85	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	1.98	0.45
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.45
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.49	0.45
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.99	0.45
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.98	0.45
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.45
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.98	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.50	0.45
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.97	0.45
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.34	0.45
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.49	0.45
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.97	0.45
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.49	0.45
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.50	0.45
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.97	0.45
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.99	0.45
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.99	0.45
2:I:4181:ILE:HG13	2:I:4988:TYR:HE1	1.82	0.45
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	1.98	0.45
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.45
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.99	0.45
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.99	0.45
2:B:4181:ILE:HG13	2:B:4988:TYR:HE1	1.82	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.45
2:I:1865:MET:SD	2:I:1865:MET:N	2.90	0.45
2:E:4181:ILE:HG13	2:E:4988:TYR:HE1	1.82	0.45
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.33	0.45
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.45
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.98	0.45
2:B:1707:LEU:O	2:B:1710:GLY:N	2.33	0.45
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.99	0.45
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.34	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.50	0.45
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.99	0.45
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.98	0.45
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.52	0.45
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.98	0.45
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.35	0.45
2:I:134:ASP:OD1	2:I:134:ASP:N	2.47	0.45
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.45
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.45
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.45
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.99	0.45
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.52	0.45
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.52	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.29	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.45
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.45
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.40	0.44
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.52	0.44
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.99	0.44
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.52	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.34	0.44
2:G:4181:ILE:HG13	2:G:4988:TYR:HE1	1.82	0.44
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.90	0.44
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.82	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.52	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CD1	2.70	0.44
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.98	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.99	0.44
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.44
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:I:210:GLU:H	2:I:273:HIS:HE1	1.66	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.99	0.44
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.44
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.82	0.44
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.53	0.44
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.35	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.90	0.44
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.43	0.44
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.53	0.44
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.66	0.44
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.82	0.44
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.99	0.44
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.44
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.82	0.44
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.99	0.44
2:G:5028:PHE:CG	2:G:5028:PHE:O	2.70	0.44
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.00	0.44
2:I:3842:LEU:O	2:I:3929:SER:OG	2.34	0.44
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.44	0.44
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.99	0.44
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	1.98	0.44
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.82	0.44
2:I:4826:ILE:O	2:I:4829:SER:OG	2.29	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CD1	2.70	0.44
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.85	0.44
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.99	0.44
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.82	0.44
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.00	0.44
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.99	0.44
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.83	0.44
2:E:210:GLU:H	2:E:273:HIS:HE1	1.66	0.44
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.44
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.00	0.44
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.83	0.44
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.39	0.44
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.53	0.44
2:B:210:GLU:H	2:B:273:HIS:HE1	1.66	0.44
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.66	0.44
2:B:1171:SER:OG	2:B:1175:SER:N	2.42	0.44
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.82	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:E:5028:PHE:CD1	2:E:5028:PHE:O	2.71	0.44
2:E:5028:PHE:O	2:E:5028:PHE:CG	2.70	0.44
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.99	0.44
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.82	0.44
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.83	0.44
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.00	0.44
2:B:3362:UNK:O	2:B:3366:UNK:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3842:LEU:O	2:B:3929:SER:OG	2.35	0.44
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.44
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.35	0.44
2:E:3842:LEU:O	2:E:3929:SER:OG	2.35	0.44
2:B:219:VAL:HG13	2:B:285:VAL:HG21	2.00	0.43
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.82	0.43
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.70	0.43
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.82	0.43
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.43
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.52	0.43
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	2.00	0.43
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.36	0.43
2:I:4228:ALA:O	2:I:4232:GLU:N	2.51	0.43
2:E:219:VAL:HG13	2:E:285:VAL:HG21	2.00	0.43
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.99	0.43
2:G:210:GLU:H	2:G:273:HIS:HE1	1.66	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.52	0.43
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.43
2:E:1865:MET:SD	2:E:1865:MET:N	2.90	0.43
2:E:4228:ALA:O	2:E:4232:GLU:N	2.51	0.43
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.43
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.66	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.46	0.43
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.34	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.00	0.43
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.83	0.43
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.00	0.43
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.83	0.43
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.00	0.43
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.99	0.43
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.99	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.36	0.43
2:G:471:LEU:O	2:G:475:GLN:N	2.52	0.43
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.43
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.44	0.43
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.00	0.43
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	2.00	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.00	0.43
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.99	0.43
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.52	0.43
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.99	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.00	0.43
2:G:5028:PHE:O	2:G:5028:PHE:CD1	2.71	0.43
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.53	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.99	0.43
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.43
2:G:1707:LEU:O	2:G:1710:GLY:N	2.34	0.43
2:B:21:VAL:HG12	2:B:66:CYS:HA	2.00	0.43
2:B:3733:CYS:HA	2:B:3766:GLN:HB2	2.01	0.43
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.66	0.43
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	2.00	0.43
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.84	0.43
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.52	0.43
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.83	0.43
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.00	0.43
2:B:1155:LEU:HD23	2:B:1184:ILE:HD12	2.01	0.43
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.01	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.84	0.43
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.00	0.43
2:G:1155:LEU:HD23	2:G:1184:ILE:HD12	2.00	0.43
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	2.00	0.43
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.43
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.00	0.43
2:I:3733:CYS:HA	2:I:3766:GLN:HB2	2.01	0.43
2:E:1155:LEU:HD23	2:E:1184:ILE:HD12	2.00	0.43
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.43
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.43
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.36	0.43
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.42
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.01	0.42
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.42
2:G:2883:HIS:NE2	2:G:2906:VAL:O	2.52	0.42
2:G:3733:CYS:HA	2:G:3766:GLN:HB2	2.01	0.42
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.01	0.42
2:G:4228:ALA:O	2:G:4232:GLU:N	2.51	0.42
2:I:21:VAL:HG12	2:I:66:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.01	0.42
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.46	0.42
2:I:2029:GLN:O	2:I:2033:ASP:N	2.52	0.42
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.34	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.42
2:G:219:VAL:HG13	2:G:285:VAL:HG21	2.00	0.42
2:G:3805:LEU:H	2:G:3805:LEU:HG	1.69	0.42
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.36	0.42
2:B:4228:ALA:O	2:B:4232:GLU:N	2.51	0.42
2:I:219:VAL:HG13	2:I:285:VAL:HG21	2.00	0.42
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.52	0.42
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.00	0.42
2:E:21:VAL:HG12	2:E:66:CYS:HA	2.00	0.42
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.00	0.42
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.00	0.42
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	2.02	0.42
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.01	0.42
2:I:4101:LYS:HG3	2:G:4731:ILE:HA	2.01	0.42
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.01	0.42
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.46	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.84	0.42
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.35	0.42
2:I:471:LEU:O	2:I:475:GLN:N	2.52	0.42
2:E:4125:PHE:HA	2:E:4128:PHE:HB3	2.02	0.42
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.42
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.02	0.42
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.01	0.42
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	2.02	0.42
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.01	0.42
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.52	0.42
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.02	0.42
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.34	0.42
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.85	0.42
2:G:4125:PHE:HA	2:G:4128:PHE:HB3	2.02	0.42
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.52	0.42
2:I:913:LEU:O	2:I:918:ARG:NH2	2.53	0.42
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.85	0.42
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	2.02	0.42
2:G:164:ARG:N	2:G:167:ASP:OD2	2.53	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.52	0.42
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	2.02	0.42
2:I:2883:HIS:NE2	2:I:2906:VAL:O	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.42
2:E:3733:CYS:HA	2:E:3766:GLN:HB2	2.01	0.42
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.83	0.42
2:G:21:VAL:HG12	2:G:66:CYS:HA	2.00	0.42
2:G:472:ARG:HA	2:G:475:GLN:HB2	2.02	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.53	0.42
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.42
2:B:913:LEU:O	2:B:918:ARG:NH2	2.53	0.42
2:I:1155:LEU:HD23	2:I:1184:ILE:HD12	2.01	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.55	0.42
2:E:2776:SER:O	2:E:2788:HIS:N	2.53	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:G:2776:SER:O	2:G:2788:HIS:N	2.53	0.42
2:B:472:ARG:HA	2:B:475:GLN:HB2	2.02	0.42
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.85	0.42
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.02	0.42
2:B:2029:GLN:O	2:B:2033:ASP:N	2.51	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.55	0.42
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.84	0.42
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.43	0.42
2:G:451:TYR:O	2:G:474:ARG:NH1	2.53	0.42
2:B:313:SER:HB3	2:B:351:VAL:HB	2.02	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:I:472:ARG:HA	2:I:475:GLN:HB2	2.02	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.53	0.41
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.52	0.41
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.85	0.41
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	2.01	0.41
2:G:4897:ILE:HG12	2:G:4901:ILE:HD13	2.02	0.41
2:B:1972:ASN:O	2:B:1976:ARG:N	2.52	0.41
2:B:4897:ILE:HG12	2:B:4901:ILE:HD13	2.02	0.41
2:I:1041:GLN:O	2:I:1045:THR:OG1	2.31	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.43	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4125:PHE:HA	2:B:4128:PHE:HB3	2.02	0.41
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	2.01	0.41
2:E:356:TRP:O	2:E:379:HIS:N	2.52	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.42	0.41
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.02	0.41
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.41
2:G:346:CYS:N	2:G:388:LEU:O	2.52	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.55	0.41
2:B:70:GLU:HB2	2:B:108:LEU:HD23	2.03	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.01	0.41
2:I:4125:PHE:HA	2:I:4128:PHE:HB3	2.02	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.53	0.41
2:E:472:ARG:HA	2:E:475:GLN:HB2	2.02	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.93	0.41
2:E:2285:GLU:HG3	2:E:2286:LEU:HG	2.03	0.41
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.03	0.41
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	2.01	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:G:913:LEU:O	2:G:918:ARG:NH2	2.53	0.41
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.41
2:I:116:MET:HB2	2:I:137:LEU:HD12	2.03	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.02	0.41
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.03	0.41
2:I:2776:SER:O	2:I:2788:HIS:N	2.53	0.41
2:E:164:ARG:N	2:E:167:ASP:OD2	2.53	0.41
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.86	0.41
2:E:346:CYS:N	2:E:388:LEU:O	2.52	0.41
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.41
2:E:913:LEU:O	2:E:918:ARG:NH2	2.53	0.41
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.41
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.41
2:G:1936:LYS:O	2:G:1940:CYS:N	2.49	0.41
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.53	0.41
2:B:346:CYS:N	2:B:388:LEU:O	2.52	0.41
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	2.02	0.41
2:B:3694:LYS:HA	2:B:3695:PRO:HD3	1.95	0.41
2:B:4918:ILE:HD11	2:E:4888:TYR:HA	2.03	0.41
2:B:4961:CYS:O	2:B:4961:CYS:SG	2.79	0.41
2:I:70:GLU:HB2	2:I:108:LEU:HD23	2.03	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3361:UNK:O	2:I:3365:UNK:N	2.54	0.41
2:E:284:HIS:N	2:E:289:ARG:O	2.42	0.41
2:E:2883:HIS:NE2	2:E:2906:VAL:O	2.52	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.55	0.41
2:G:116:MET:HB2	2:G:137:LEU:HD12	2.03	0.41
2:G:2285:GLU:HG3	2:G:2286:LEU:HG	2.03	0.41
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.03	0.41
2:G:4236:SER:HG	2:G:4675:LYS:HZ1	1.64	0.41
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	2.01	0.41
2:B:2285:GLU:HG3	2:B:2286:LEU:HG	2.03	0.41
2:B:3361:UNK:O	2:B:3365:UNK:N	2.54	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:I:1739:THR:H	2:I:1742:THR:HB	1.86	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.54	0.41
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.03	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.54	0.41
2:E:1739:THR:H	2:E:1742:THR:HB	1.86	0.41
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.53	0.41
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.53	0.41
2:G:2517:UNK:O	2:G:2521:UNK:N	2.54	0.41
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.43	0.41
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.03	0.41
2:I:313:SER:HB3	2:I:351:VAL:HB	2.02	0.41
2:I:451:TYR:O	2:I:474:ARG:NH1	2.53	0.41
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.41
2:I:4961:CYS:O	2:I:4961:CYS:SG	2.79	0.41
2:I:5004:THR:H	2:I:5007:GLU:HB2	1.86	0.41
2:E:70:GLU:HB2	2:E:108:LEU:HD23	2.03	0.41
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.86	0.41
2:E:1972:ASN:O	2:E:1976:ARG:N	2.52	0.41
2:E:4984:ASN:C	2:E:4986:ALA:H	2.24	0.41
2:G:70:GLU:HB2	2:G:108:LEU:HD23	2.03	0.41
2:G:894:GLY:HA3	2:G:903:LEU:HD22	2.03	0.41
2:G:4961:CYS:O	2:G:4961:CYS:SG	2.79	0.41
2:B:116:MET:HB2	2:B:137:LEU:HD12	2.03	0.41
2:B:330:ASP:N	2:B:330:ASP:OD1	2.54	0.41
2:B:670:GLU:H	2:B:740:PRO:HB3	1.86	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.85	0.41
2:B:2517:UNK:O	2:B:2521:UNK:N	2.54	0.41
2:B:5004:THR:H	2:B:5007:GLU:HB2	1.86	0.41
2:I:670:GLU:H	2:I:740:PRO:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1657:LEU:HD13	2:I:1657:LEU:HA	1.94	0.41
2:I:1972:ASN:O	2:I:1976:ARG:N	2.52	0.41
2:I:4657:CYS:HB3	2:I:4792:LEU:HD11	2.03	0.41
2:I:4960:ILE:CG2	2:I:4988:TYR:OH	2.69	0.41
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	2.02	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.24	0.41
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.03	0.41
2:E:3361:UNK:O	2:E:3365:UNK:N	2.54	0.41
2:E:4897:ILE:HG12	2:E:4901:ILE:HD13	2.02	0.41
2:E:4960:ILE:CG2	2:E:4988:TYR:OH	2.69	0.41
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.61	0.41
2:G:330:ASP:OD1	2:G:330:ASP:N	2.54	0.41
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.52	0.41
2:G:670:GLU:H	2:G:740:PRO:HB3	1.86	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.54	0.41
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.86	0.41
2:G:1739:THR:H	2:G:1742:THR:HB	1.86	0.41
2:G:2029:GLN:O	2:G:2033:ASP:N	2.51	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.24	0.41
2:B:2883:HIS:NE2	2:B:2906:VAL:O	2.52	0.41
2:B:4960:ILE:CG2	2:B:4988:TYR:OH	2.69	0.41
2:I:164:ARG:N	2:I:167:ASP:OD2	2.53	0.41
2:I:1663:HIS:O	2:I:1667:LEU:N	2.53	0.41
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.86	0.41
2:I:2285:GLU:HG3	2:I:2286:LEU:HG	2.03	0.41
2:E:313:SER:HB3	2:E:351:VAL:HB	2.02	0.41
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.54	0.41
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.52	0.41
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.43	0.41
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40
2:B:1029:GLU:HB3	2:B:1033:ARG:HH12	1.86	0.40
2:B:1739:THR:H	2:B:1742:THR:HB	1.86	0.40
2:B:4010:ILE:HD12	2:B:4131:ARG:HD2	2.03	0.40
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.40
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.40
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.35	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.03	0.40
2:E:4010:ILE:HD12	2:E:4131:ARG:HD2	2.03	0.40
2:E:4961:CYS:O	2:E:4961:CYS:SG	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5004:THR:H	2:E:5007:GLU:HB2	1.86	0.40
2:G:3361:UNK:O	2:G:3365:UNK:N	2.54	0.40
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.40
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.86	0.40
2:B:2448:GLY:HA2	2:B:2451:LEU:HD12	2.04	0.40
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.61	0.40
2:E:116:MET:HB2	2:E:137:LEU:HD12	2.03	0.40
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.40
2:E:670:GLU:H	2:E:740:PRO:HB3	1.86	0.40
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.04	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.85	0.40
2:E:1707:LEU:O	2:E:1710:GLY:N	2.33	0.40
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.04	0.40
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.93	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2776:SER:O	2:B:2788:HIS:N	2.53	0.40
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.56	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.03	0.40
2:I:1141:ARG:HD2	2:I:1141:ARG:H	1.86	0.40
2:I:2448:GLY:HA2	2:I:2451:LEU:HD12	2.04	0.40
2:E:330:ASP:OD1	2:E:330:ASP:N	2.54	0.40
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.40
2:E:2517:UNK:O	2:E:2521:UNK:N	2.54	0.40
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.52	0.40
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.61	0.40
2:B:4657:CYS:HB3	2:B:4792:LEU:HD11	2.03	0.40
2:I:346:CYS:N	2:I:388:LEU:O	2.52	0.40
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.54	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:894:GLY:HA3	2:E:903:LEU:HD22	2.03	0.40
2:E:1029:GLU:HB3	2:E:1033:ARG:HH12	1.86	0.40
2:G:1029:GLU:HB3	2:G:1033:ARG:HH12	1.86	0.40
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.03	0.40
2:B:4984:ASN:C	2:B:4986:ALA:H	2.24	0.40
2:I:894:GLY:HA3	2:I:903:LEU:HD22	2.03	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.40
2:I:4010:ILE:HD12	2:I:4131:ARG:HD2	2.03	0.40
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.54	0.40
2:G:5004:THR:H	2:G:5007:GLU:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	335 (10%)	8 (0%)	47	81
2	E	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	47	81
2	G	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	336 (10%)	8 (0%)	47	81
All	All	13360/18096 (74%)	11941 (89%)	1387 (10%)	32 (0%)	50	81

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	I	5028	PHE
2	E	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	1932	PRO
2	B	4982	GLU
2	I	1708	ARG
2	I	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	E	4982	GLU
2	G	1708	ARG
2	G	1932	PRO
2	G	4982	GLU
2	I	4982	GLU
2	B	1840	PRO

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Mol	Chain	Res	Type
2	B	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	B	2291	GLN
2	B	3762	ARG
2	I	2291	GLN
2	I	3762	ARG
2	E	2291	GLN
2	E	3762	ARG
2	G	2291	GLN
2	G	3762	ARG

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%)	2474 (99%)	19 (1%)	81	89
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	84	90

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4201	ASN
2	B	4959	PHE
2	B	4961	CYS
2	B	5027	CYS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4201	ASN
2	I	4959	PHE
2	I	4961	CYS
2	I	5027	CYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG

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Mol	Chain	Res	Type
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4201	ASN
2	E	4959	PHE
2	E	4961	CYS
2	E	5027	CYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4201	ASN
2	G	4959	PHE
2	G	4961	CYS
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN

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Mol	Chain	Res	Type
2	B	111	HIS
2	B	113	HIS
2	B	151	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	479	GLN
2	B	520	ASN
2	B	582	HIS
2	B	1158	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2041	HIS
2	B	2127	GLN
2	B	3766	GLN
2	B	3781	GLN
2	B	3896	ASN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4153	HIS
2	B	4201	ASN
2	B	4553	ASN
2	B	4806	ASN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	151	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	1158	ASN
2	I	1691	GLN
2	I	1719	HIS

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Mol	Chain	Res	Type
2	I	1775	HIS
2	I	2041	HIS
2	I	2127	GLN
2	I	3766	GLN
2	I	3781	GLN
2	I	3896	ASN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4102	GLN
2	I	4120	ASN
2	I	4153	HIS
2	I	4201	ASN
2	I	4553	ASN
2	I	4806	ASN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	151	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	1158	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2041	HIS
2	E	2127	GLN
2	E	3766	GLN
2	E	3781	GLN
2	E	3896	ASN
2	E	3950	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4153	HIS
2	E	4201	ASN

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Mol	Chain	Res	Type
2	E	4553	ASN
2	E	4806	ASN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	1158	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2007	ASN
2	G	2041	HIS
2	G	2127	GLN
2	G	3766	GLN
2	G	3781	GLN
2	G	3896	ASN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4153	HIS
2	G	4553	ASN
2	G	4806	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	I	14
2	E	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	73.35
1	I	4345:UNK	C	4540:PHE	N	73.35
1	E	4345:UNK	C	4540:PHE	N	73.35
1	G	4345:UNK	C	4540:PHE	N	73.35
1	B	3613:UNK	C	3639:THR	N	45.90
1	I	3613:UNK	C	3639:THR	N	45.90
1	E	3613:UNK	C	3639:THR	N	45.90
1	G	3613:UNK	C	3639:THR	N	45.90
1	B	4253:GLU	C	4320:UNK	N	27.05

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4253:GLU	C	4320:UNK	N	27.05
1	E	4253:GLU	C	4320:UNK	N	27.05
1	G	4253:GLU	C	4320:UNK	N	27.05
1	B	3163:UNK	C	3170:UNK	N	15.84
1	I	3163:UNK	C	3170:UNK	N	15.84
1	E	3163:UNK	C	3170:UNK	N	15.84
1	G	3163:UNK	C	3170:UNK	N	15.84
1	B	3063:UNK	C	3134:UNK	N	14.98
1	I	3063:UNK	C	3134:UNK	N	14.98
1	E	3063:UNK	C	3134:UNK	N	14.98
1	G	3063:UNK	C	3134:UNK	N	14.98
1	B	3468:UNK	C	3511:UNK	N	14.61
1	I	3468:UNK	C	3511:UNK	N	14.61
1	E	3468:UNK	C	3511:UNK	N	14.61
1	G	3468:UNK	C	3511:UNK	N	14.61
1	B	2703:UNK	C	2734:ASN	N	14.05
1	I	2703:UNK	C	2734:ASN	N	14.05
1	E	2703:UNK	C	2734:ASN	N	14.05
1	G	2703:UNK	C	2734:ASN	N	14.05
1	I	3236:UNK	C	3241:UNK	N	13.51
1	B	3236:UNK	C	3241:UNK	N	13.50
1	E	3236:UNK	C	3241:UNK	N	13.50
1	G	3236:UNK	C	3241:UNK	N	13.50
1	B	2976:UNK	C	2995:UNK	N	12.34
1	I	2976:UNK	C	2995:UNK	N	12.34
1	E	2976:UNK	C	2995:UNK	N	12.34
1	G	2976:UNK	C	2995:UNK	N	12.34
1	B	1564:UNK	C	1573:MET	N	11.71
1	I	1564:UNK	C	1573:MET	N	11.71
1	E	1564:UNK	C	1573:MET	N	11.71
1	G	1564:UNK	C	1573:MET	N	11.71
1	B	3254:UNK	C	3261:UNK	N	8.48
1	I	3254:UNK	C	3261:UNK	N	8.48
1	E	3254:UNK	C	3261:UNK	N	8.48
1	G	3254:UNK	C	3261:UNK	N	8.48
1	B	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	B	2939:ARG	C	2942:UNK	N	3.79
1	I	2939:ARG	C	2942:UNK	N	3.79
1	E	2939:ARG	C	2942:UNK	N	3.79

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2939:ARG	C	2942:UNK	N	3.79
1	B	2479:LEU	C	2487:UNK	N	3.33
1	I	2479:LEU	C	2487:UNK	N	3.33
1	E	2479:LEU	C	2487:UNK	N	3.33
1	G	2479:LEU	C	2487:UNK	N	3.33

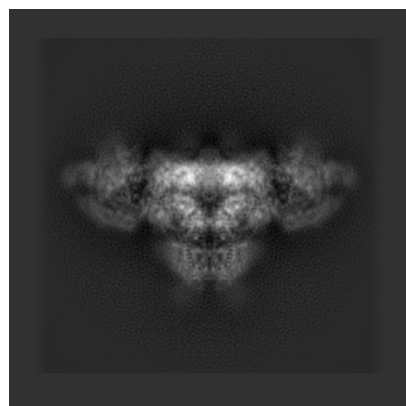
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8393. These allow visual inspection of the internal detail of the map and identification of artifacts.

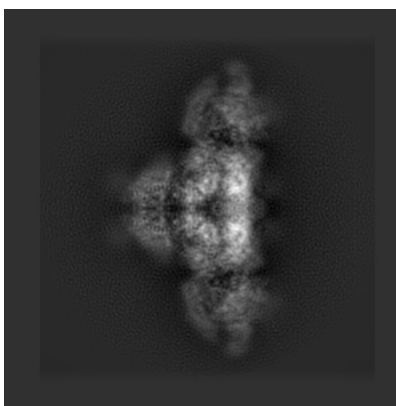
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

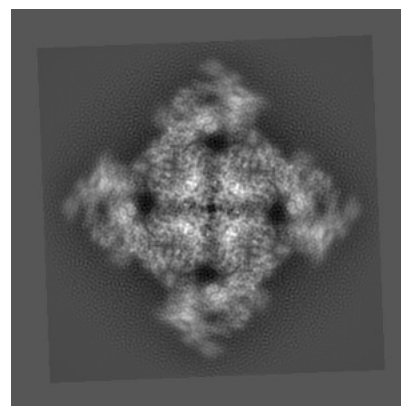
6.1.1 Primary map



X

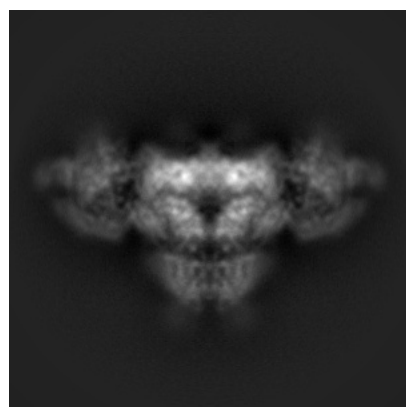


Y

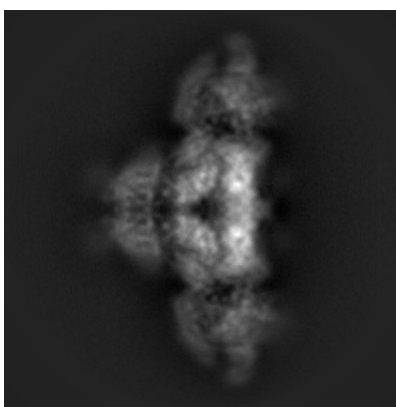


Z

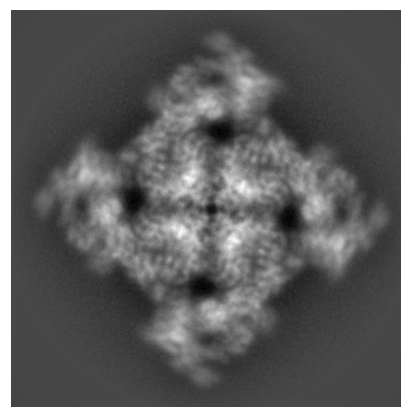
6.1.2 Raw map



X



Y

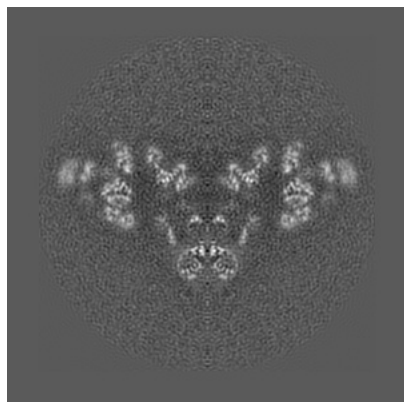


Z

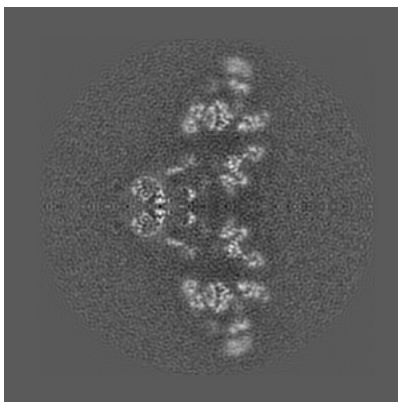
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

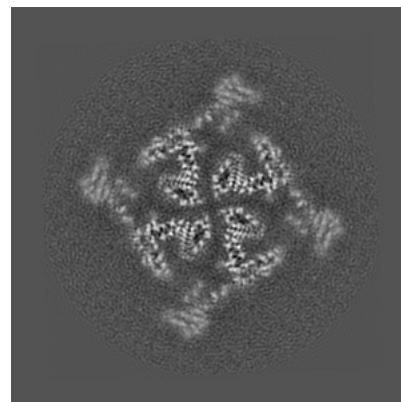
6.2.1 Primary map



X Index: 200

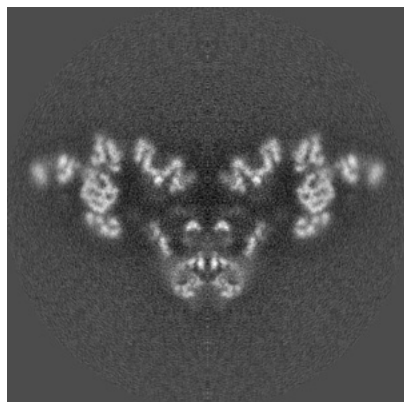


Y Index: 200

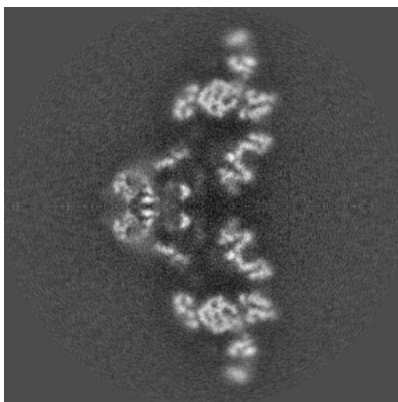


Z Index: 200

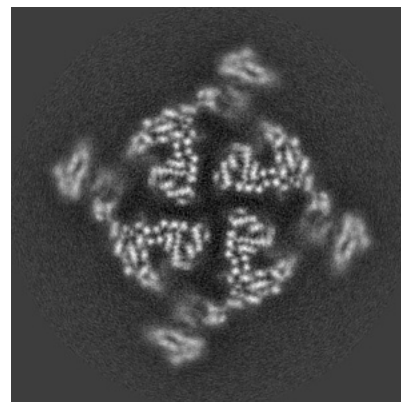
6.2.2 Raw map



X Index: 168



Y Index: 168

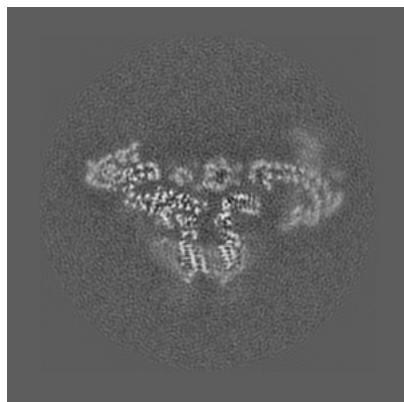


Z Index: 168

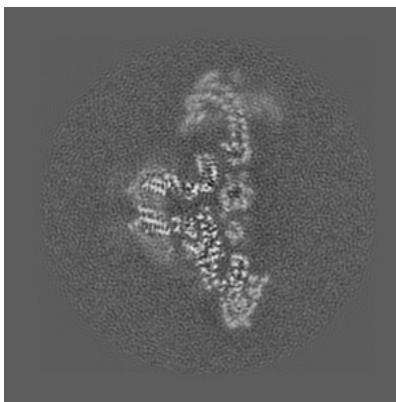
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

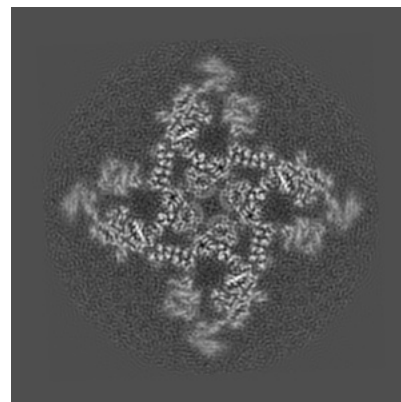
6.3.1 Primary map



X Index: 224

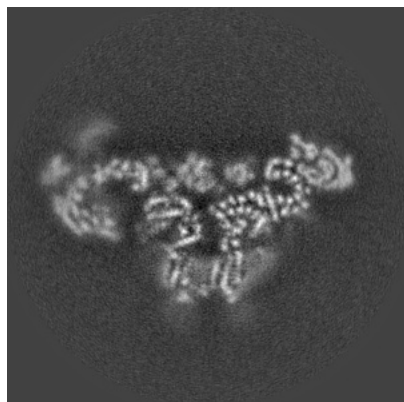


Y Index: 176

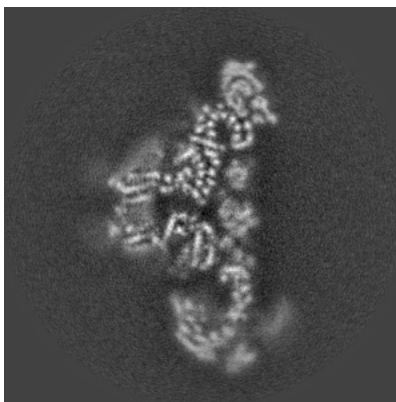


Z Index: 228

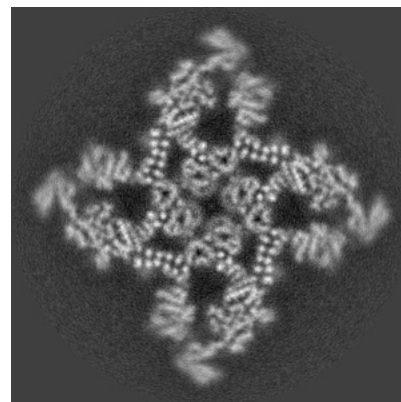
6.3.2 Raw map



X Index: 146



Y Index: 190

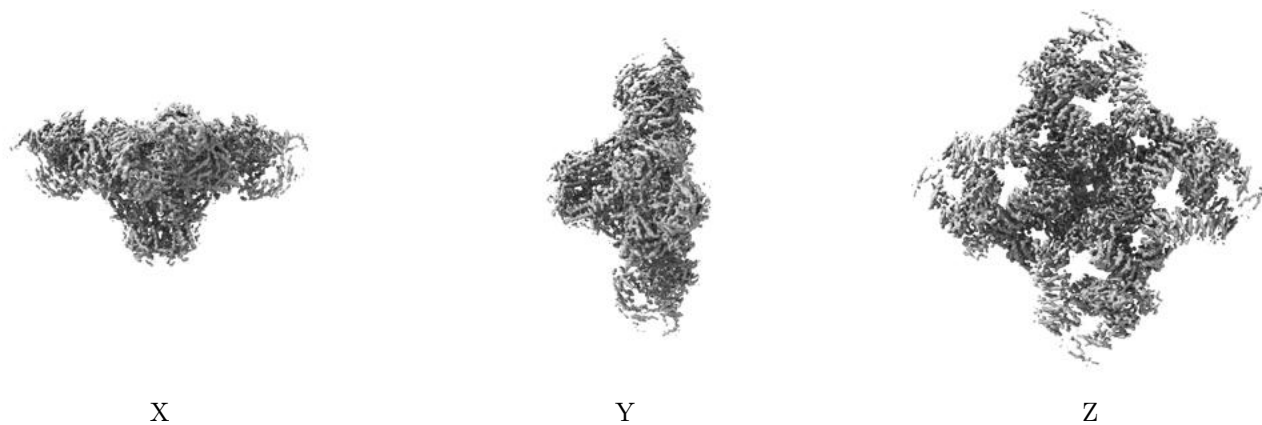


Z Index: 193

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

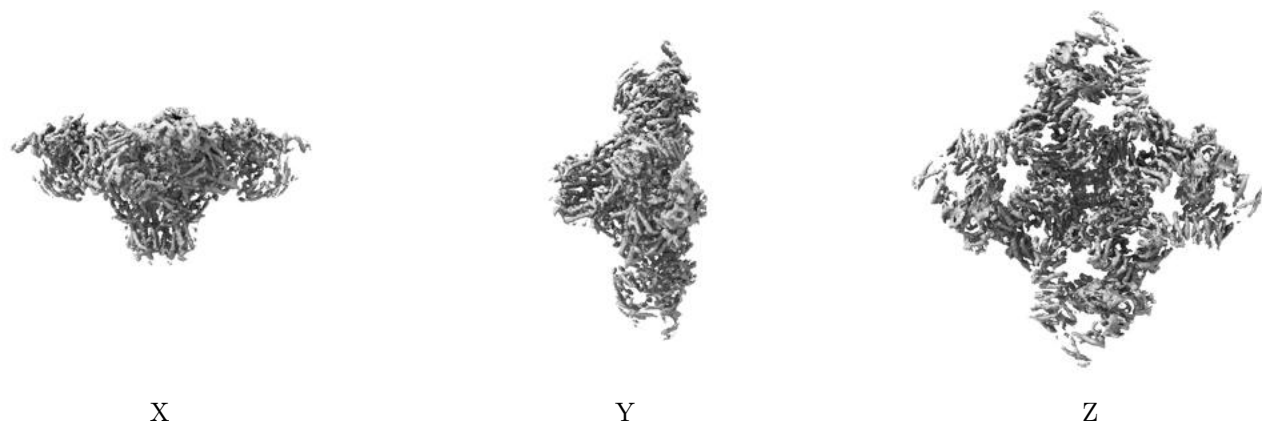
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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.

6.4.2 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.

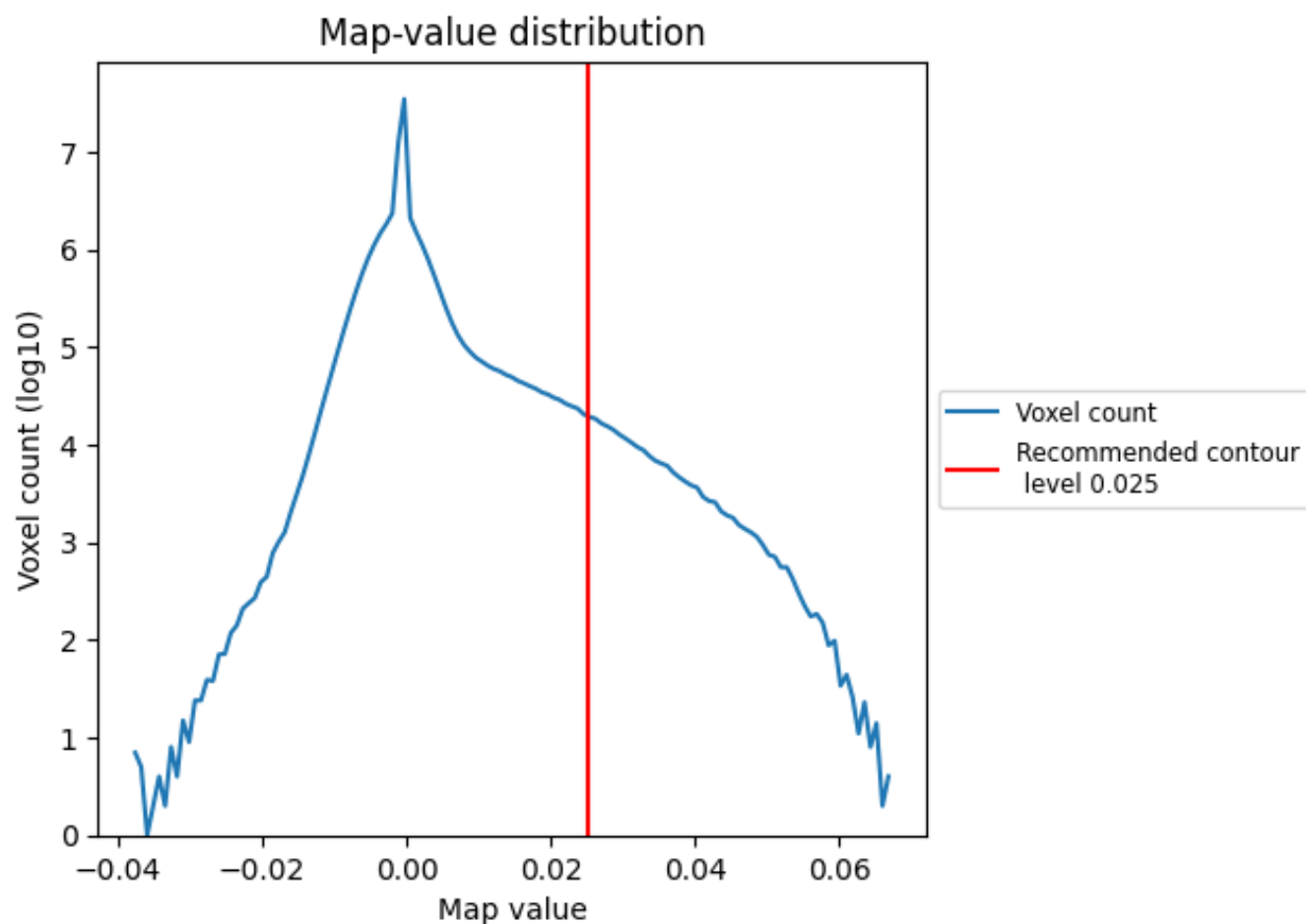
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

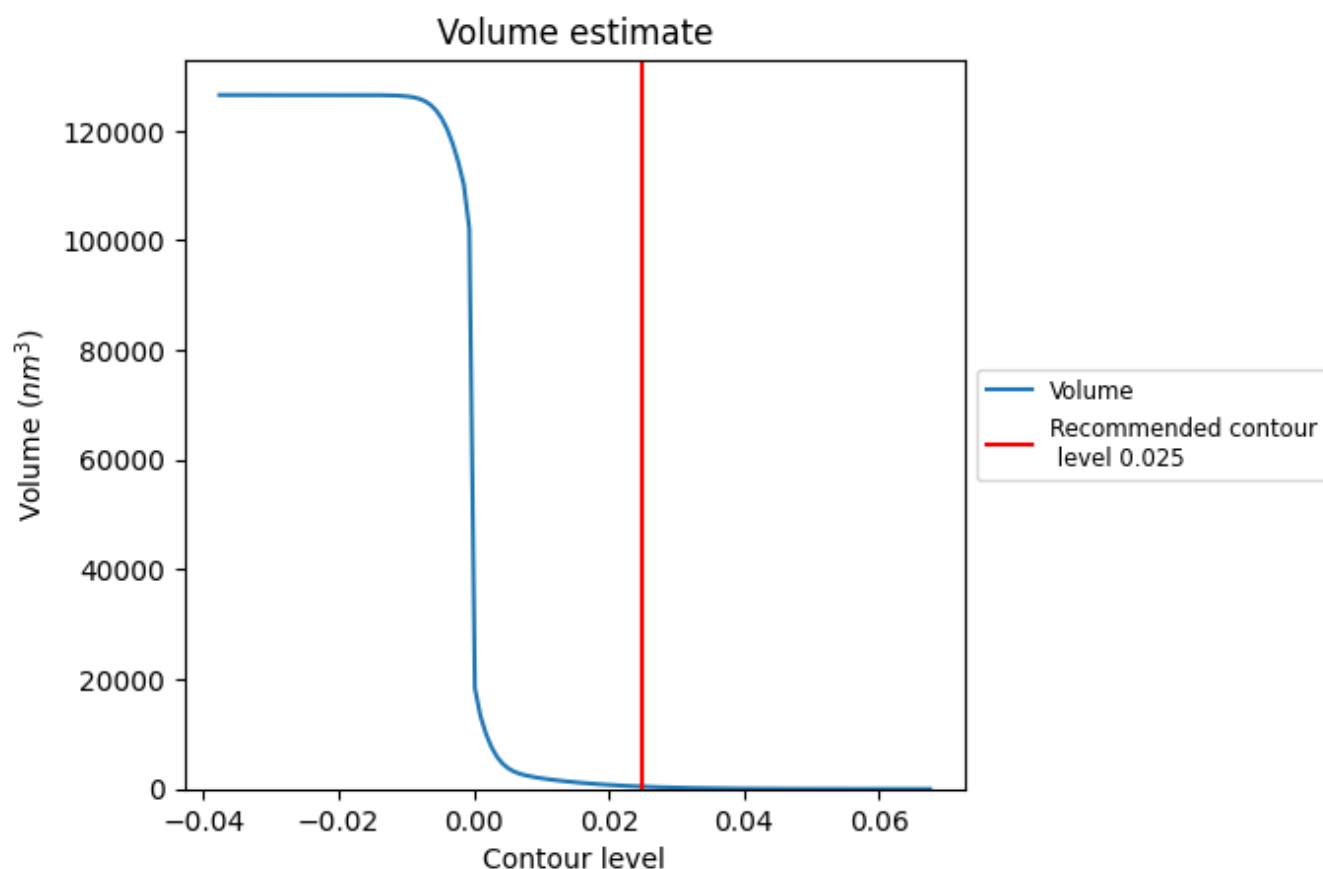
This section contains the results of statistical analysis of the map.

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.

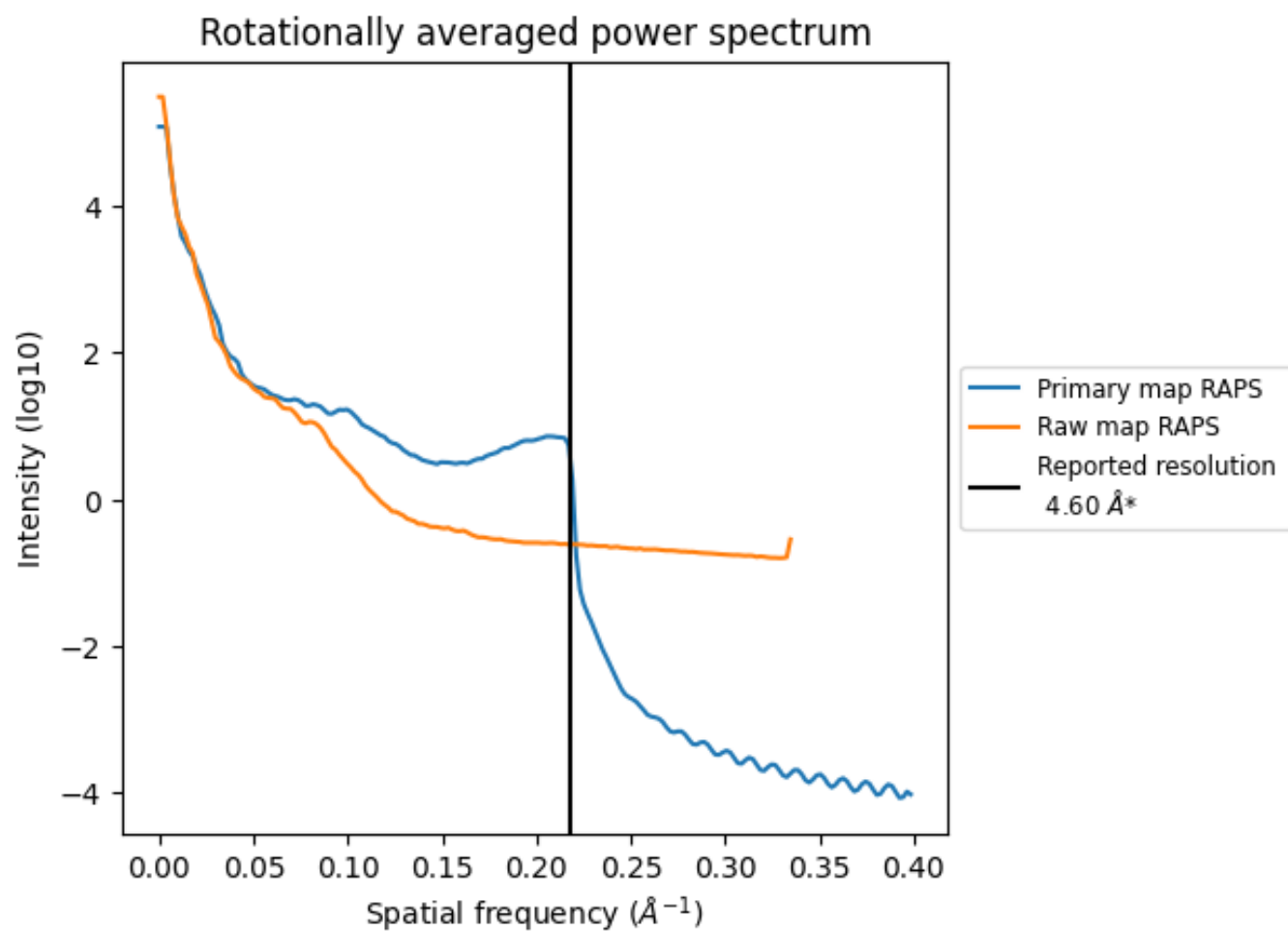
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm³; this corresponds to an approximate mass of 390 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 ⓘ

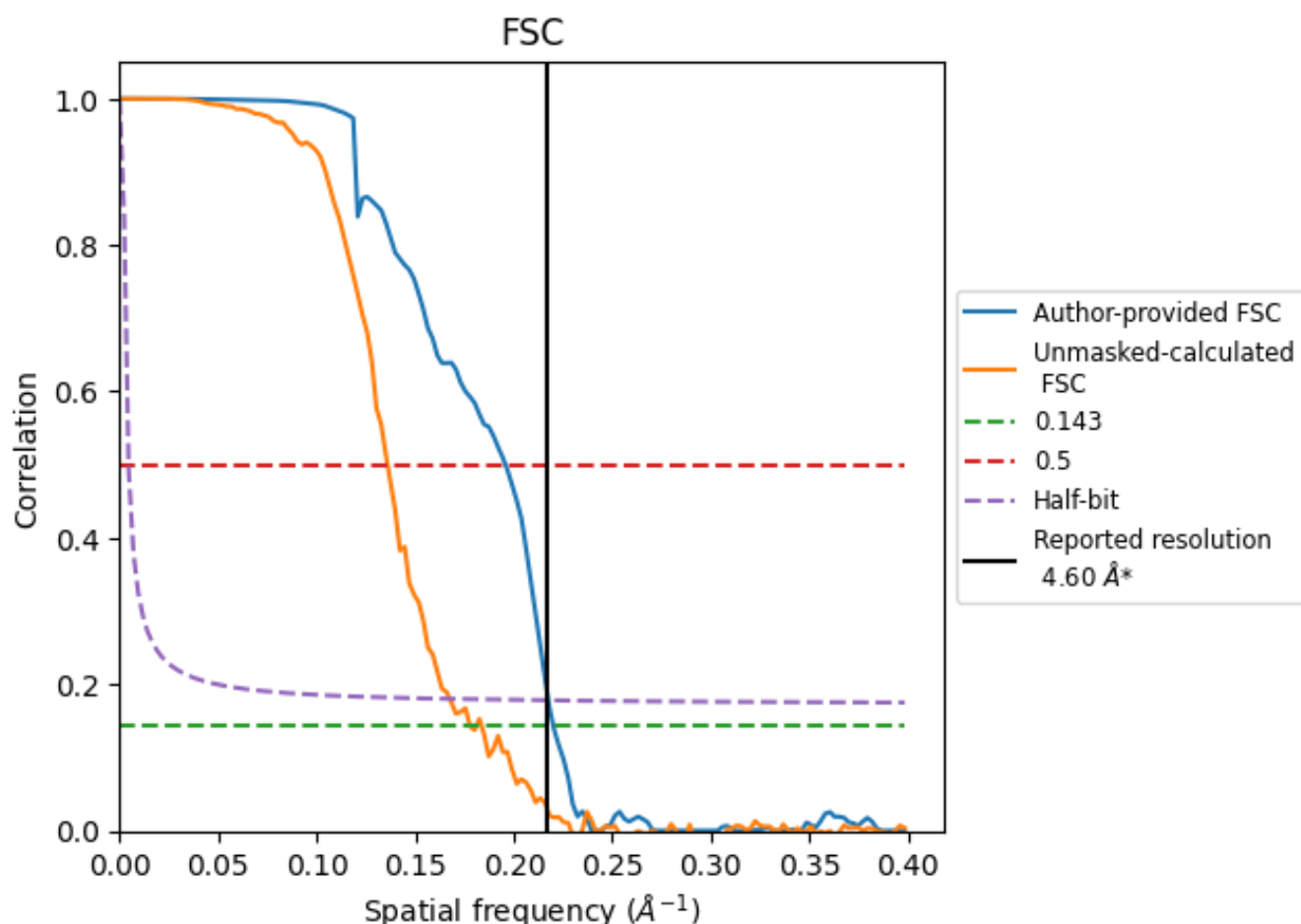


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 \AA^{-1}

8.2 Resolution estimates [i](#)

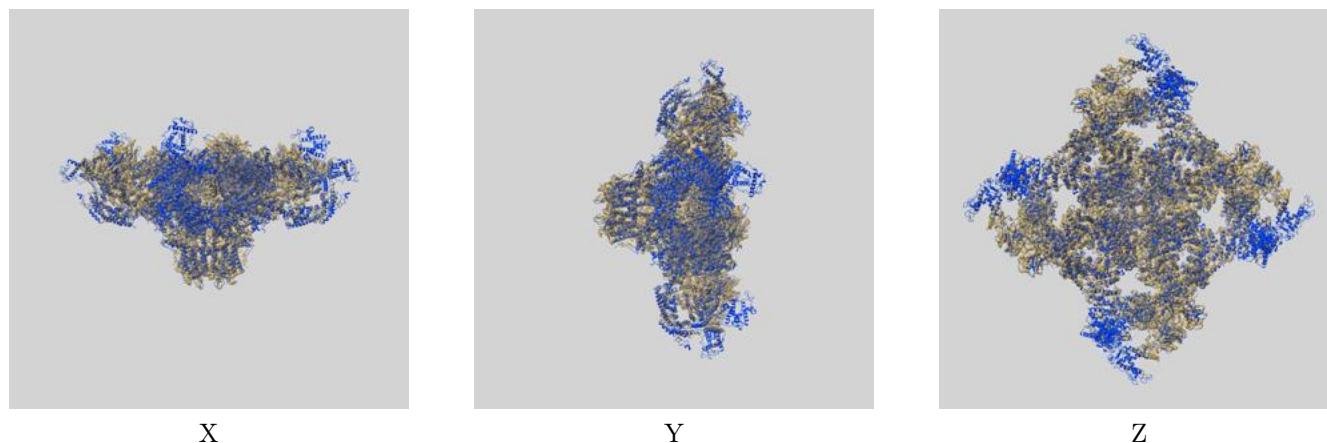
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.54	5.11	4.60
Unmasked-calculated*	5.62	7.35	5.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.62 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

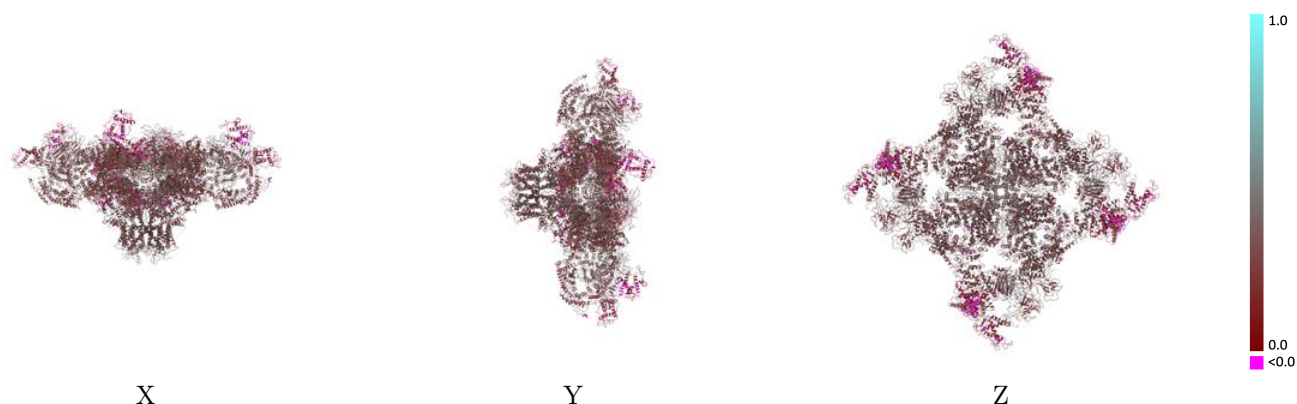
This section contains information regarding the fit between EMDB map EMD-8393 and PDB model 5TB2. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



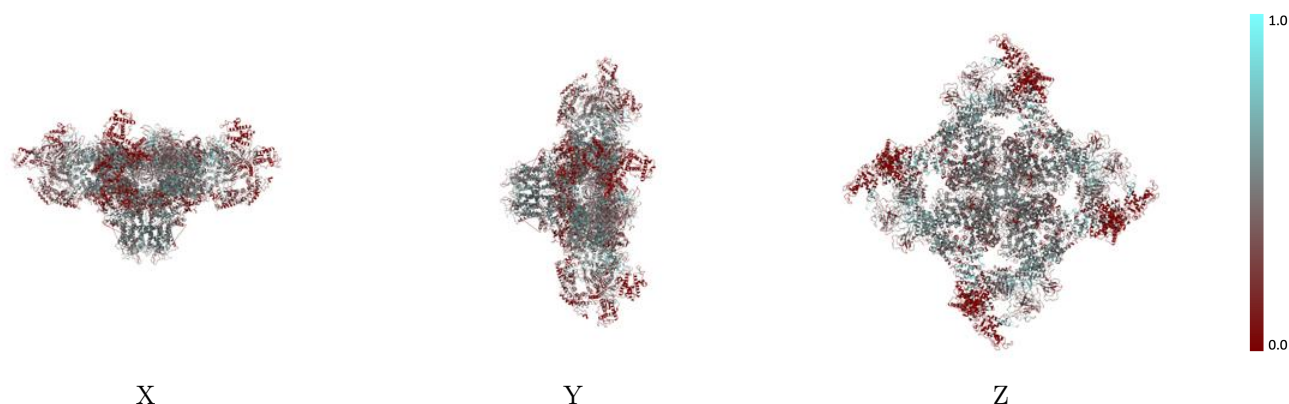
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



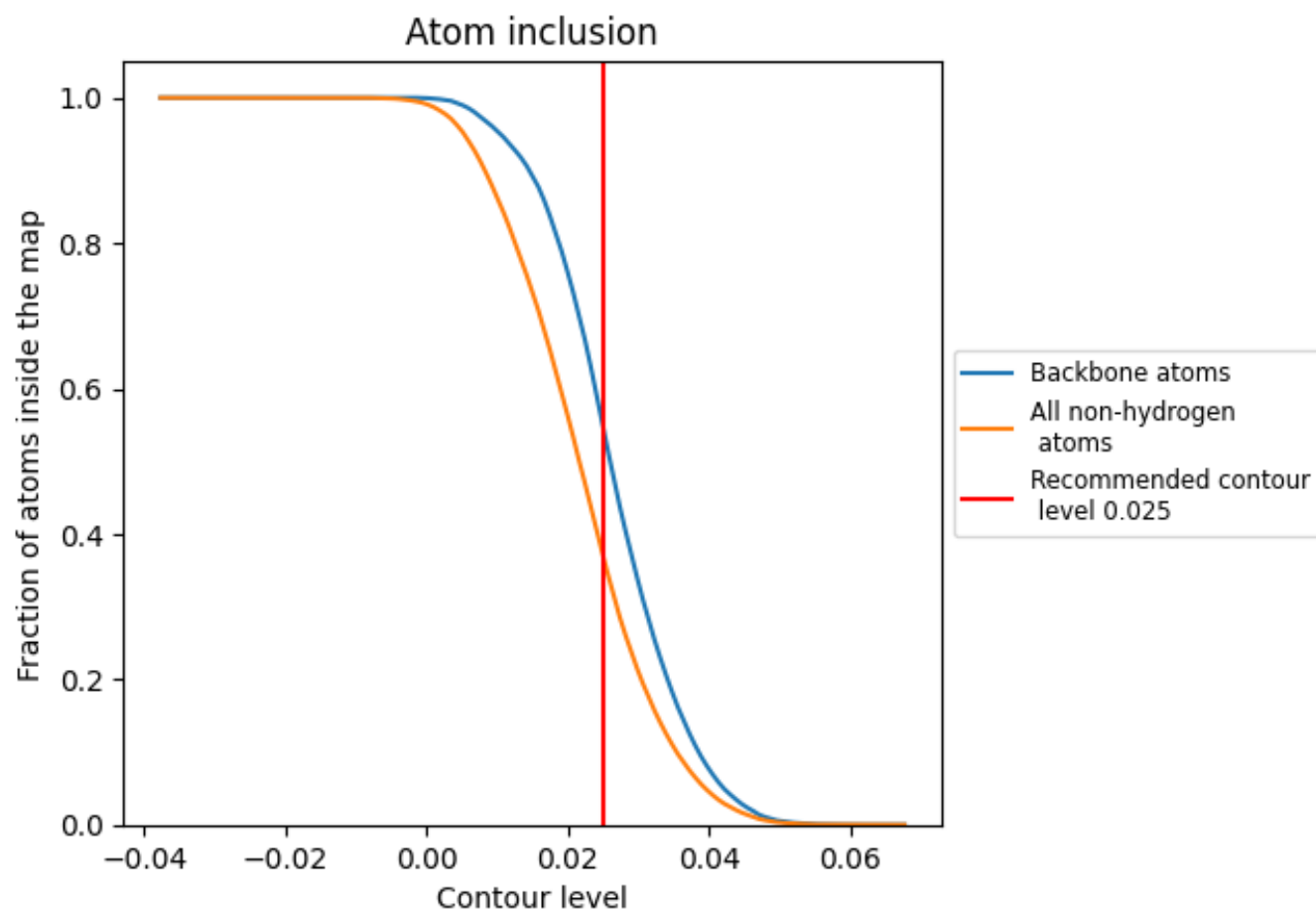
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 55% of all backbone atoms, 37% 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	<div><div></div></div> 0.3694	<div><div></div></div> 0.2880
A	<div><div></div></div> 0.3499	<div><div></div></div> 0.3000
B	<div><div></div></div> 0.3696	<div><div></div></div> 0.2880
E	<div><div></div></div> 0.3695	<div><div></div></div> 0.2880
F	<div><div></div></div> 0.3437	<div><div></div></div> 0.3030
G	<div><div></div></div> 0.3705	<div><div></div></div> 0.2880
H	<div><div></div></div> 0.3486	<div><div></div></div> 0.3040
I	<div><div></div></div> 0.3705	<div><div></div></div> 0.2870
J	<div><div></div></div> 0.3499	<div><div></div></div> 0.3030

1.0

0.0

<0.0