



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:45 AM UTC

PDB ID : 5TB2 / pdb_00005tb2
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:

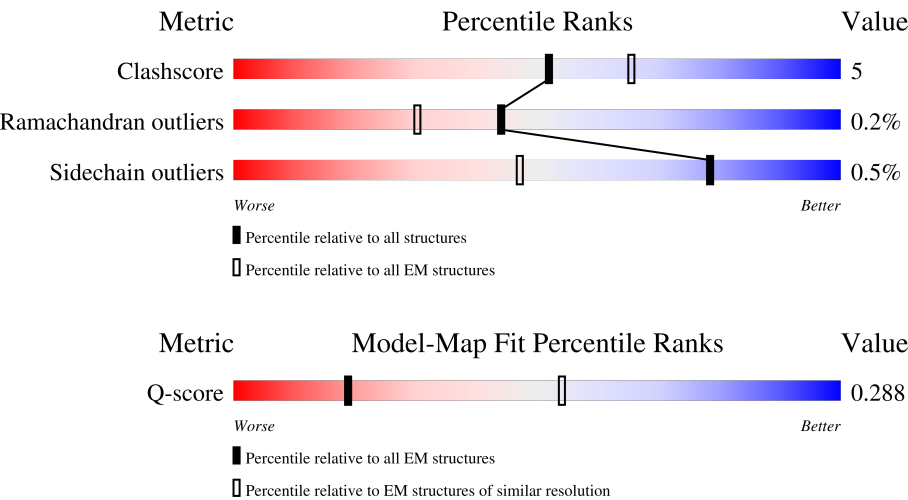
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber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

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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

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

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Mol	Chain	Length	Quality of chain
2	B	4416	51% 84% 11% 5%
2	E	4416	51% 83% 11% 5%
2	G	4416	51% 83% 11% 5%
2	I	4416	52% 84% 11% 5%

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		

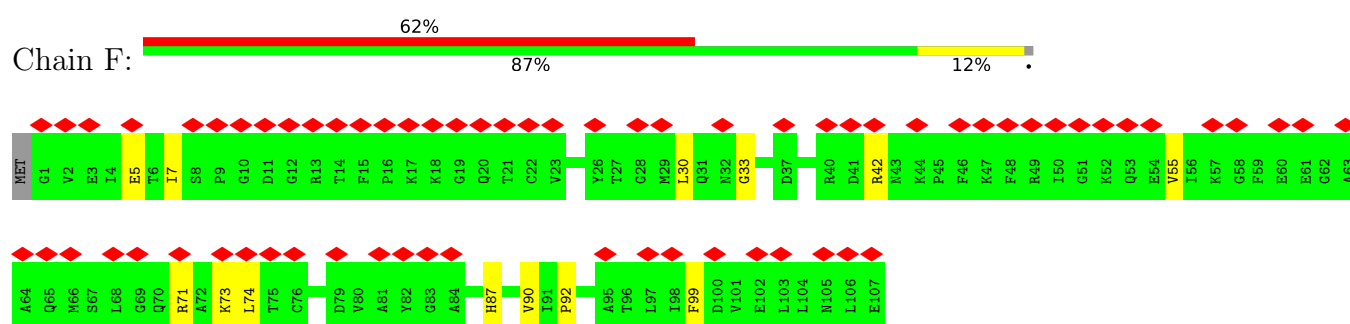
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

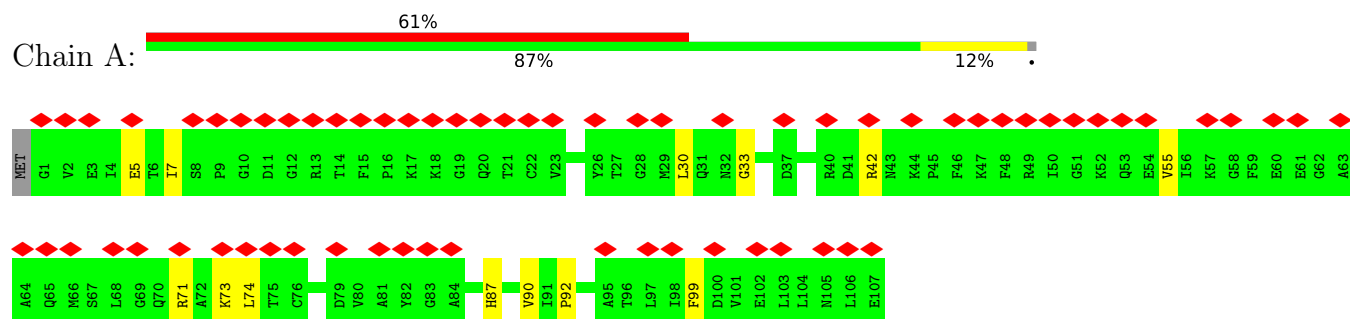
3 Residue-property plots [i](#)

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.

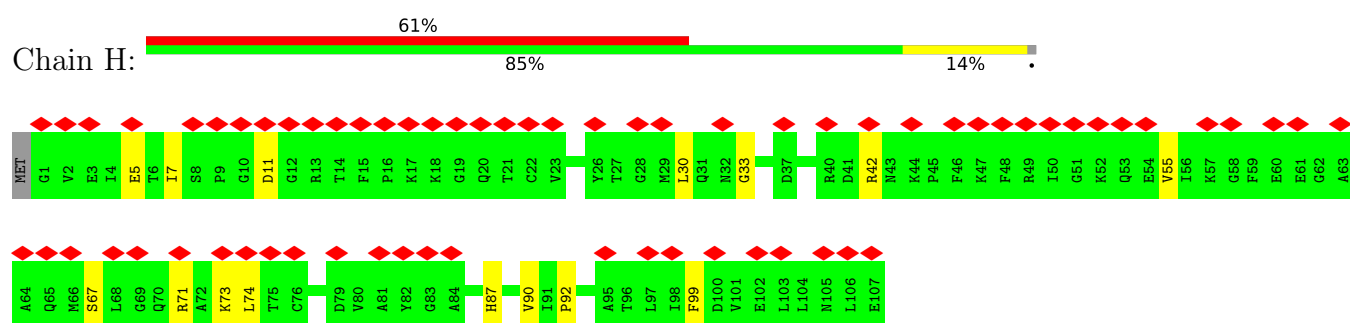
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



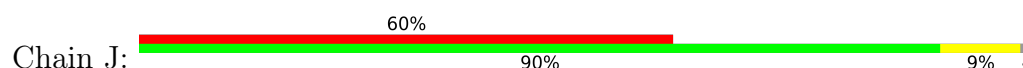
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

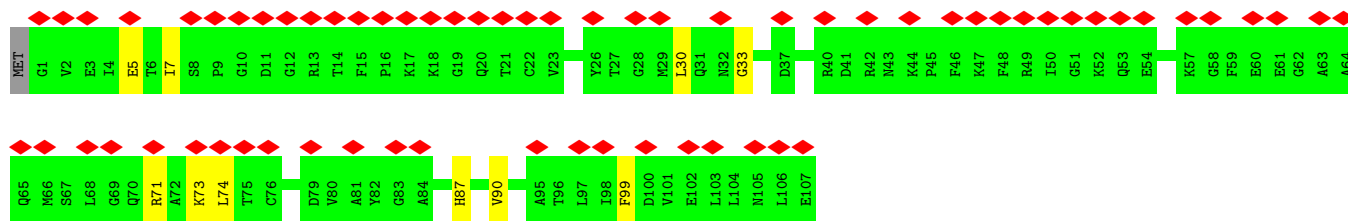


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

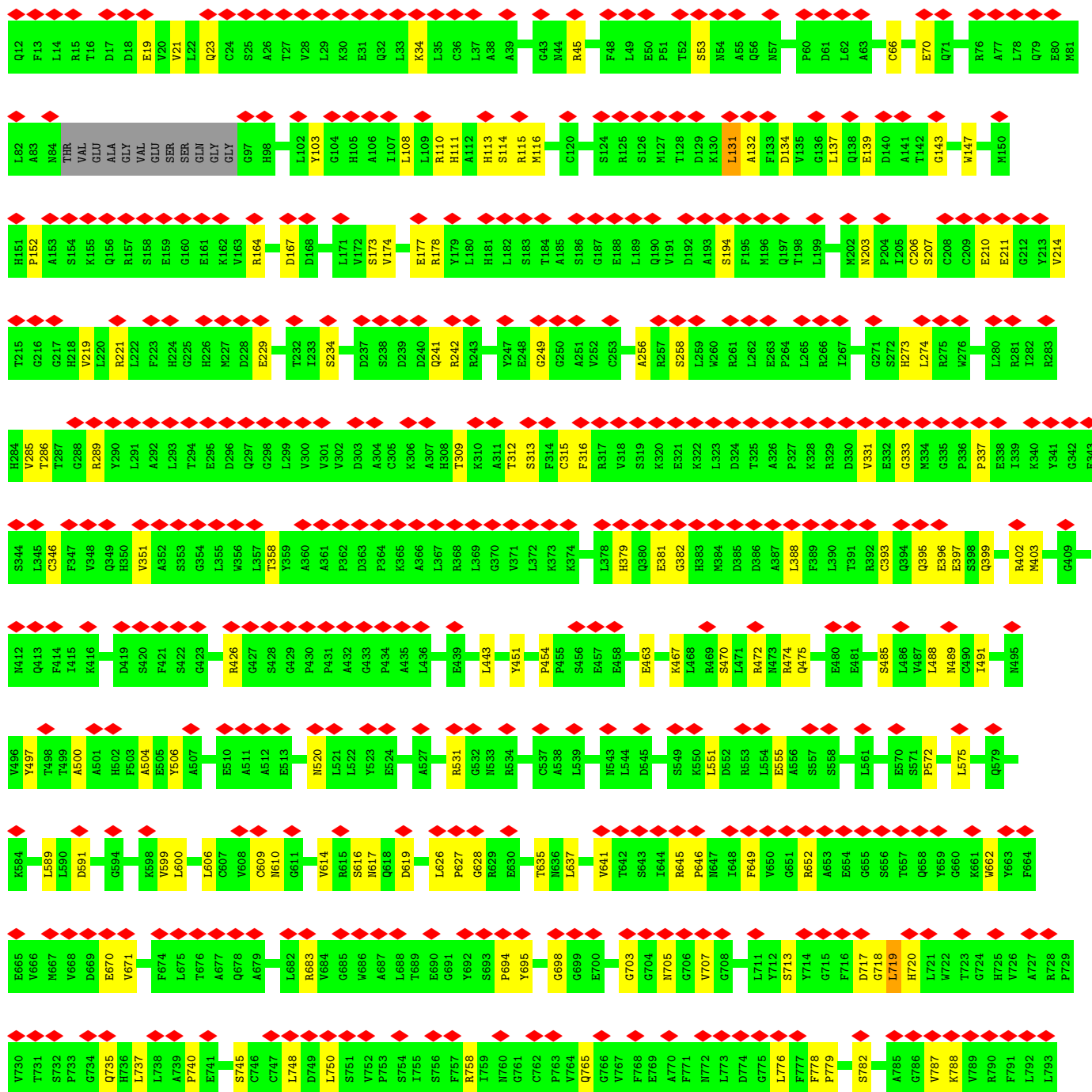
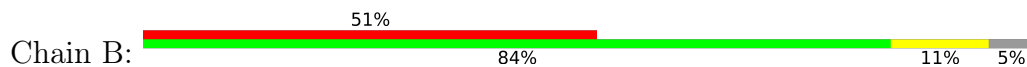


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





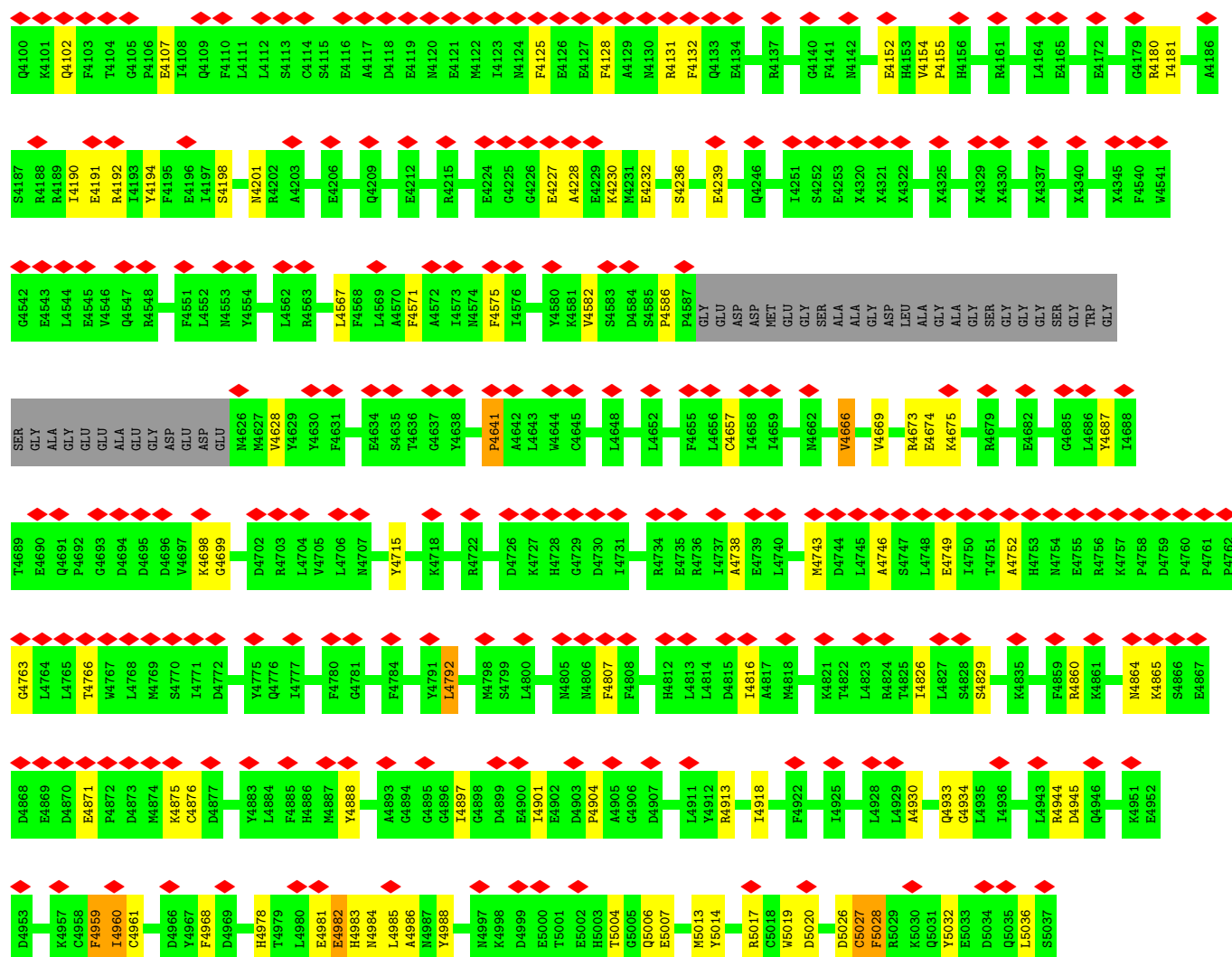
• Molecule 2: Ryanodine receptor 1



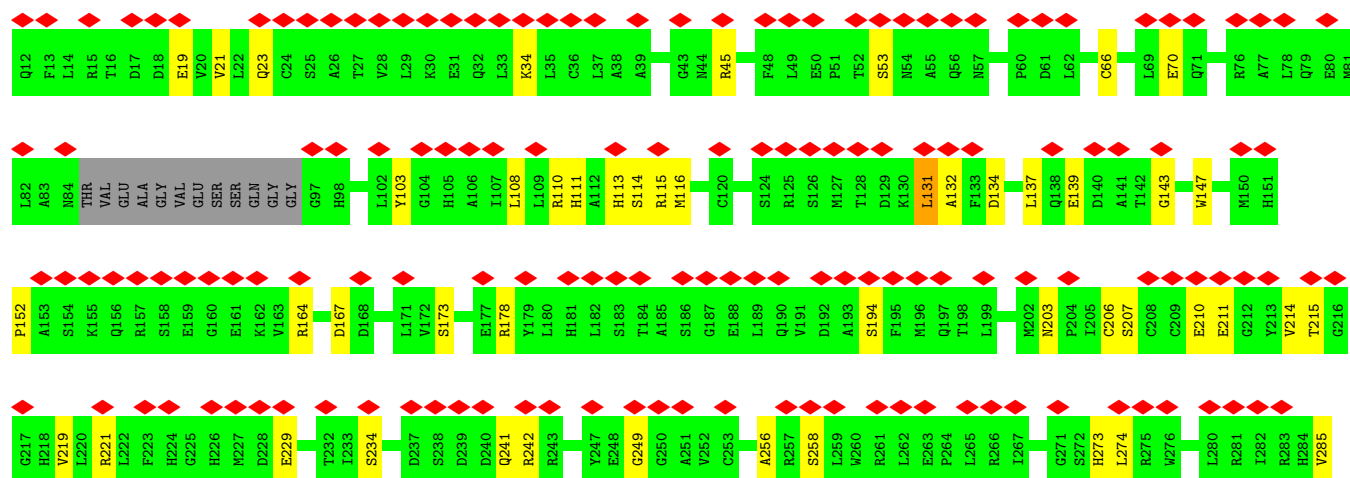


L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	P2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	R2924	E2925	L2926	L2927	K2928	P2929	L2930	K2931	M2932	L2933	G2934	V2935	E2880	M2881	V2882	H2883	M2884	T2885	V2886	Q2887	K2888	K2889	K2890	K2891	A2892	F2893	K2894	K2895	K2896	K2897	K2898	K2899	K2900	K2901	K2902	K2903	K2904	K2905	K2906	K2907	K2908	K2909	K2910	K2911	K2912	K2913	K2914	K2915	K2916	K2917	K2918	K2919	K2920	K2921	K2922	K2923	K2924	K2925	K2926	K2927	K2928	K2929	K2930	K2931	K2932	K2933	K2934	K2935	K2936	K2937	K2938	K2939	K2940	K2941	K2942	K2943	K2944	K2945	K2946	K2947	K2948	K2949	K2950	K2951	K2952	K2953	K2954	K2955	K2956																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
THR	GLU	LVS	LVS	THR	ARG	ARG	GLN	THR	ALA	GLN	THR	ASP	PRO	ARG	GLU	GLY	T2855	M2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	G2879	E2880	M2881	V2882	H2883	M2884	T2885	V2886	Q2887	K2888	K2889	K2890	K2891	A2892	F2893	K2894	K2895	K2896	K2897	K2898	K2899	K2900	K2901	K2902	K2903	K2904	K2905	K2906	K2907	K2908	K2909	K2910	K2911	K2912	K2913	K2914	K2915	K2916	K2917	K2918	K2919	K2920	K2921	K2922	K2923	K2924	K2925	K2926	K2927	K2928	K2929	K2930	K2931	K2932	K2933	K2934	K2935	K2936	K2937	K2938	K2939	K2940	K2941	K2942	K2943	K2944	K2945	K2946	K2947	K2948	K2949	K2950	K2951	K2952	K2953	K2954	K2955	K2956																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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D3932	Y3937	S3938	G3939	K3940	D3941	V3942	I3943	E3944	E3945	Q3946	K3947	K3948	R3949	N3950	K3953	K3959	Q3960	V3961	F3962	N3963	Q3970	Q3976	S3979	L3980	A3981	H3982	L3985	L3993	F3996	A3997	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	S4007	S4008	Q4009	I4010	E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	D4019									
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X3434	X3435	X3436	X3437	X3441	X3442	X3443	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3463	X3464	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	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			
X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3420	X3421	X3428	X3429	X3430	X3431	X3432	X3433		
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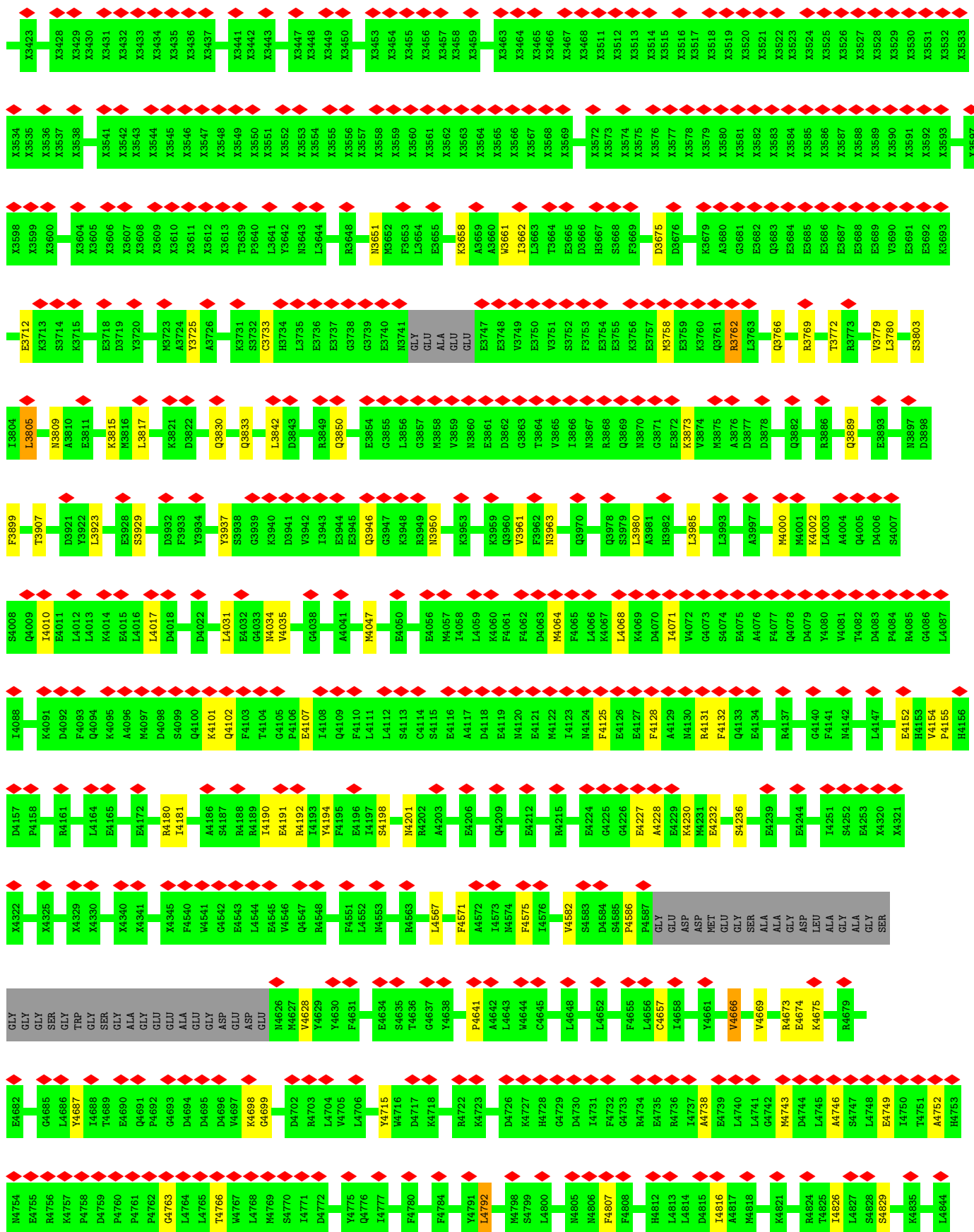
Chain I: 52% 84% 11% 5%

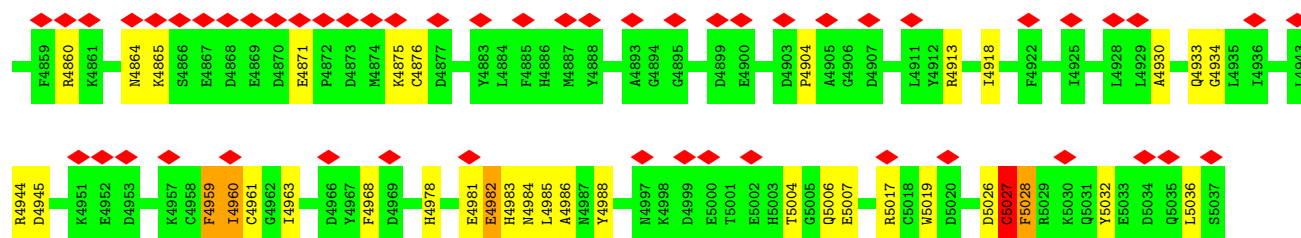


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E1114	G1048	A980	Y920	GLN	F791	A727	F664	H582	G288	G417	Q349	G288
L1115	Y1049	Q981	N921		L792	R728	E665	I583	R289	L418	H350	R289
G1116	G1050	T982	L922		L793	P729	V666	K584	Y290	D419	V351	Y290
A1117	Y1051	T983	Q923		G794	V730	M667	L589	L291	S420	A352	L291
L1118	M1052	L984	N924		G795	T731	M668	L590	A292	F421	S353	A292
E1119	I1053	V985	S925		G796	S732	D669	D591	L293	G354	L355	L293
L1120	E1054	D986	S926		R796	T733	E670	R595	L294	T294	W356	L294
A1121	PRO	R987	G927		F800	G734	V671	G598	E295	K424	L357	E295
V1122	ASP	L988	E928		R801	Q735	F674	K598	D296	R425	T358	D296
F1123	GLN	A989	T928		K802	H736	L737	V599	Q297	G427	Y359	Q297
N1125	GLU	G992	K930		L803	L738	L675	L600	G298	S428	A360	G298
G1126	PRO	H993	T931		L803	L739	T676	L506	L299	G429	A361	L299
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Q1130	ASN	R1000	A934		A875	C746	T680	C609	D303	G433	P364	D303
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W1132	SER	V1001	G936		A809	C747	H681	N610	C305	A435	L367	C305
H1133	ARG	Y1007	C937		H812	L748	L682	G611	K306	L436	R368	K306
L1134	TRP	Y1007	H938		E813	D749	R683	V614	T309	L436	R368	T309
G1135	D1070	S1008	G940		A814	L750	V684	R615	K310	E439	L369	K310
S1136	R1071	A1009	G940		W815	S751	G685	S616	A311	A440	G370	A311
E1137	V1072	VAL	N941		L816	S752	W686	N617	T312	L443	L372	T312
G1140	R1073	GLN	A942		R820	P753	A687	Q618	S313	D447	K373	S313
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F1075	F1075	ILE	D943		R822	I755	L688	L626	F315	L443	K373	F315
R1076	ALA	ARG	E944		R822	S756	L688	L626	F316	L443	K373	F316
A1077	ARG	ARG	K945		L823	S757	G691	L626	R317	L443	K373	R317
E1078	ASN	ASN	R946		E324	R758	Y692	P627	V318	L443	K373	V318
S1080	PRO	PRO	E947		R830	I759	S693	R636	S319	L443	K373	S319
Y1081	R1020	Q889	E947		R830	I759	S693	R636	K320	L443	K373	K320
L1021	L1021	Q889	D948		R830	I759	S693	R636	E321	L443	K373	E321
V1022	V1022	Q889	L950		R830	I759	S693	R636	K322	L443	K373	K322
Y1024	Y1024	Q889	K951		R830	I759	S693	R636	L323	L443	K373	L323
R1025	R1025	Q889	K952		R830	I759	S693	R636	D324	L443	K373	D324
L1026	L1026	Q889	T953		R830	I759	S693	R636	T325	L443	K373	T325
L1027	L1027	Q889	K954		R830	I759	S693	R636	A326	L443	K373	A326
D1028	D1028	Q889	K955		R830	I759	S693	R636	P327	L443	K373	P327
E1029	E1029	Q889	P956		R830	I759	S693	R636	K328	L443	K373	K328
A1030	A1030	Q889	K957		R830	I759	S693	R636	R329	L443	K373	R329
T1031	T1031	Q889	T958		R830	I759	S693	R636	D330	L443	K373	D330
K1032	K1032	Q889	N960		R830	I759	S693	R636	V331	L443	K373	V331
R1033	R1033	Q889	N961		R830	I759	S693	R636	E332	L443	K373	E332
S1034	S1034	Q889	N962		R830	I759	S693	R636	G333	L443	K373	G333
N1035	N1035	Q889	S962		R830	I759	S693	R636	H334	L443	K373	H334
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D1037	D1037	Q889	G964		R830	I759	S693	R636	P336	L443	K373	P336
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L1039	L1039	Q889	K966		R830	I759	S693	R636	E338	L443	K373	E338
C1040	C1040	Q889	P967		R830	I759	S693	R636	I339	L443	K373	I339
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V1043	V1043	Q889	L970		R830	I759	S693	R636	E342	L443	K373	E342
R1044	R1044	Q889	D971		R830	I759	S693	R636	E343	L443	K373	E343
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E1167	G1103	W1104	S973		P914	P914	P914	P914	L345	L443	K373	L345
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L1169	A1105	A1105	S973		P914	P914	P914	P914				
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S1175	A1105	A1105	S973		P914	P914	P914	P914				
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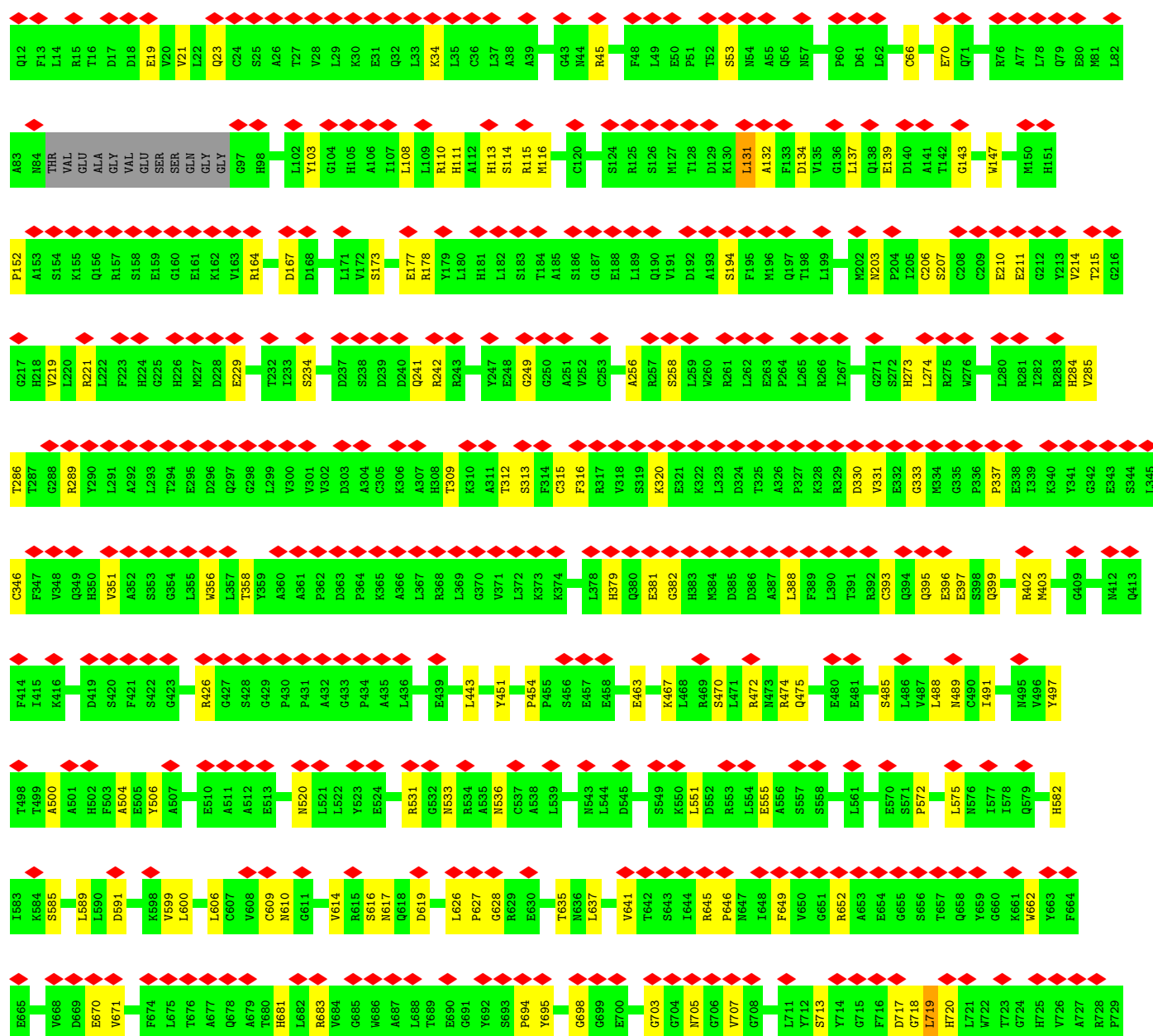
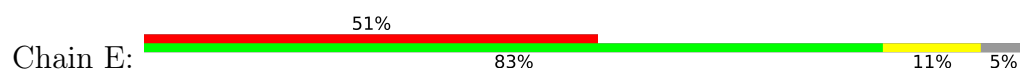


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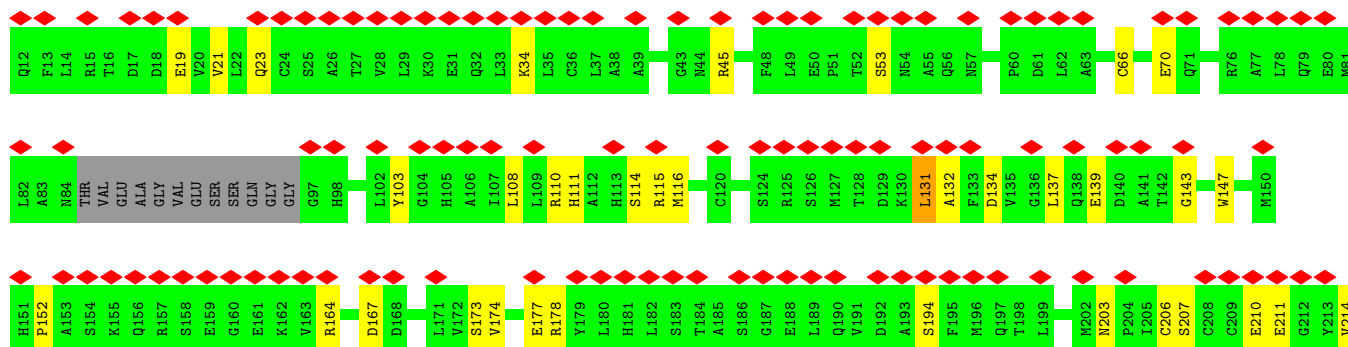
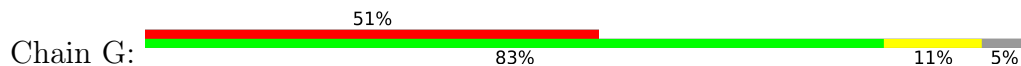
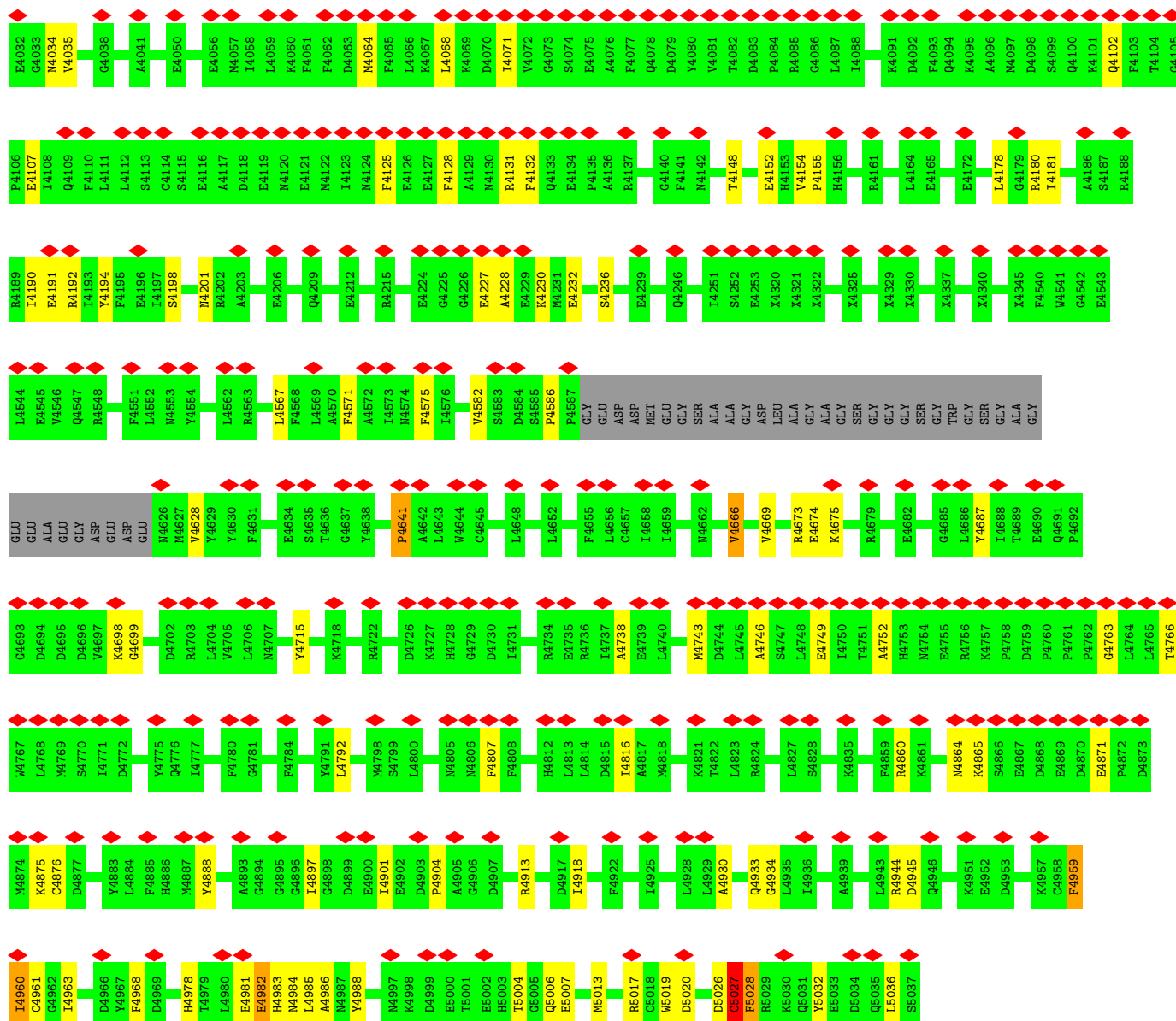
• Molecule 2: Ryanodine receptor 1



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G1185	D1186	L1189	P1190	L1194	G1195	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	L1211	R1212	F1213	F1214	A1215	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	A1227	I1228	Q1231	R1232	T1235	T1236	W1237	Q1244	E1251	H1254	V1255	E1256	L1259	M1260	D1261	G1262	T1263	V1264	D1265	C1269																	
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Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	Y1089	F1092	E1093	A1094	V1095	T1097	G1098	E1099	M1100	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120										
P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	G992	D999	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050									
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L792	L793	G794	G795	R796	G797	G798	F799	R800	K801	F802	L803	P806	G807	Y808	A809	H812	E813	A814	V815	L816	P817	R820	L821	R822	L823	E824	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	S843	R844	C845	L846	S847	H848	T849	D850	P853	C854	P855	V856	D857	THR											
V730	T731	S732	P733	G734	Q735	H736	L737	L738	A739	P740	E741	S745	C746	G747	L748	D749	L750	S751	V752	P753	S754	I755	S756	F757	R758	I759	N760	G761	C762	P763	V764	Q765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	V781	S782	F783	S784	A785	G786	V787	K788	V789	R790	F791						





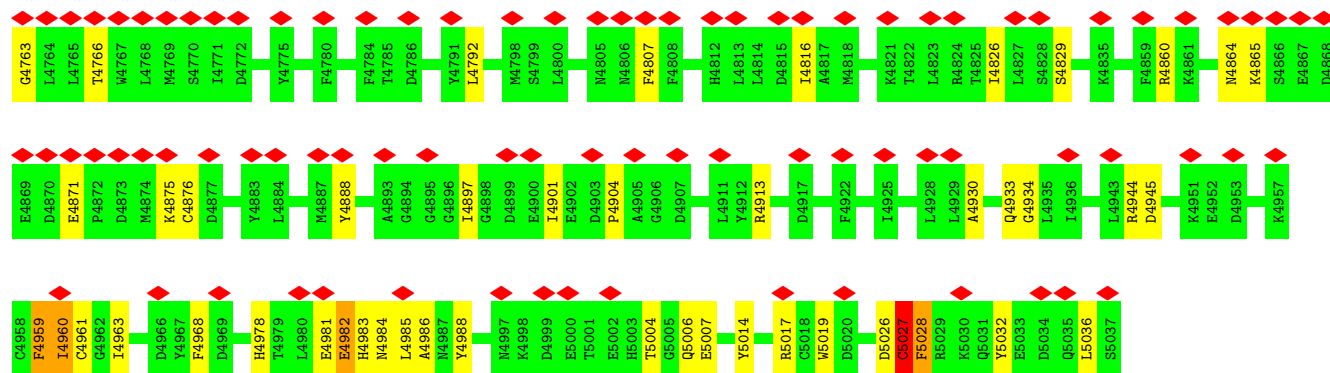


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T983	L984	V985	D986	R987	L988	A989	G992	H993	N994	D999	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	G963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	Y975	R976	L977	T978	P979	A980	Q981	T982
G795	R796	E799	F800	K801	F802	L803	P806	G807	Y808	A809	H812	E813	L814	Y815	L816	P817	R820	L821	R822	L823	E824	K827	E828	Q829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	S843	R844	C845	L846	S847	H848	T849	D850	P853	C854	P855	Y856	D857	THR	VAL	GLN	I861	Y862								
T731	S732	P733	G734	Q735	H736	L737	L738	A739	E741	S745	C746	C747	L748	D749	L750	S751	Y752	P753	S754	L755	S756	F757	R758	L759	N760	G761	C762	P763	Y764	Q765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	F776	F777	P778	P779	S782	A785	G786	Y787	K788	Y789	R790	F791	L792	L793	G794					
V666	M667	V668	D669	E670	V671	F674	L675	T676	A677	Q678	A679	L682	R683	V684	G685	G686	A687	L688	T689	E690	G691	Y692	S693	P694	Y695	G698	G699	E700	G703	G704	N705	G706	V707	G708	L711	Y712	S713	Y714	G715	F716	D717	G718	L719	H720	L721	W722	T723	G724	H725	V726	A727	R728	T729	V730						
K584	L589	L590	D591	K598	V599	L600	L606	C607	V608	C609	N610	G611	V614	R615	S616	N617	Q618	D619	L626	P627	G628	R629	E630	T635	N636	L637	V641	T642	S643	T644	R645	P646	T648	F649	V650	G651	R652	A653	G654	G655	S656	T657	Q658	Y659	G660	K661	W662	Y663	F664	E665										
V496	Y497	T498	T499	A500	A501	H502	F503	A504	Y506	A507	E510	A511	A512	E513	N520	L521	L522	Y523	E524	R531	G532	N533	R534	A535	N536	C537	A538	L539	N543	L544	D545	S549	K550	L551	D552	R553	L554	E555	A556	S557	S558	L561	E570	S571	P572	L576	N576	I577	Q579											
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S344	L345	C346	F347	V348	Q349	H350	V351	A352	E505	S353	G354	L355	W356	L357	T358	Y359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372	K373	K374	L378	H379	E381	G382	H383	M384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	Q395	E396	E397	S398	Q399	R402	M403	G409					
H284	V285	T286	T287	G288	R289	T290	L291	A292	L293	L294	T295	E296	D297	T298	L299	V300	V301	V302	D303	A304	C305	K306	A307	H308	T309	K310	A311	T312	S313	F314	C315	F316	R317	V318	S319	K320	E321	K322	L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	G335	E336	S337	E338	E339	K340	Y341	G342	E343	
T215	G216	H217	H218	V219	L220	R221	L222	F223	H224	G225	H226	M227	D228	E229	T232	L233	S234	D237	S238	D239	D240	Q241	R242	R243	Y247	E248	G249	G250	A251	V252	C253	A256	R257	S258	L259	W260	R261	L262	E263	P264	L265	R266	L267	G271	S272	H273	L274	G275	W276	L280	R281	L282	Y341	G342	E343					



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G2898	G2899	G2900	T2901	H2902	T2903	L2904	L2905	L2906	T2907	Y2908	D2909	T2910	L2911	T2912	K2913	K2914	K2915	K2916	A2917	D2918	D2919	A2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	K2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2955	X2956	X2957	X2958	X2959	X2960																																																																																																																																																																																																																																															
LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	LYS	ASP	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	E2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897																																																																																																																																																																																																																																															
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X2528	X2529	X2532	X2533	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	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652																																																																																																																																																																																																																													
P2438	E2439	M2440	H2441	K2447	G2448	L2451	R2452	I2453	R2454	A2455	R2458	S2459	L2460	L2463	L2466	I2469	I2470	S2471	L2472	P2473	Q2475	I2476	P2477	T2478	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2498	X2499	X2500	X2511	X2512	X2513	X2517	X2518	X2519	X2520	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2541	X2542	X2543	X2544	X2545	X2546	X2547	X2548	X2549	X2550	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2559	X2560	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2574	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590	X2591	X2592	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2704	X2705	X2706	X2707	X2708	X2709	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718	X2719	X2720	X2721	X2722	X2723	X2724	X2725	X2726	X2727	X2728	X2729	X2730	X2731	X2732	X2733	X2734	X2735	X2736	X2737	X2738	X2739	X2740	X2741	X2742	X2743	X2744	X2745	X2746	X2747	X2748	X2749	X2750	X2751	X2752	X2753	X2754	X2755	X2756	X2757	X2758	X2759	X2760	X2761	X2762	X2763	X2764	X2765	X2766	X2767	X2768	X2769	X2770	X2771	X2772	X2773	X2774	X2775	X2776	X2777
L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	L2380	E2381	E2382	A2383	L2384	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	N2414	R2415	V2416	H2417	L2418	G2419	M2423	L2430	L2431	L2432	L2433	G2434	R2435																																																																																																																																																																																																																																																			

E4690	Q4691	P4692	G4693	D4694	D4695	D4696	V4697	K4698	C4699	D4702	R4703	L4704	V4705	L4706	N4707	Y4715	K4716	R4722	D4726	K4727	L4643	V4644	C4645	L4646	L4652	F4655	L4656	C4657	I4658	I4659	N4662	V4666	V4669	A4673	E4674	K4675	R4679	L4750	A4752	H4753	N4754	E4755	Y4687	I4688	T4689	P4758	D4759	P4760	P4761	P4762																																																																																				
GLY	ALA	GLY	GLU	GLU	ALA	GLY	ASP	GLY	ASP	GLU	N4626	M4627	Y4628	Y4629	Y4630	F4631	E4634	S4635	T4636	G4637	Y4638	P4641	A4642	L4643	V4644	C4645	L4646	L4652	F4655	L4656	C4657	I4658	I4659	N4662	V4666	V4669	A4673	E4674	K4675	R4679	L4750	A4752	H4753	N4754	E4755	Y4687	I4688	T4689	P4758	D4759	P4760	P4761	P4762																																																																																	
W4541	G4542	E4543	L4544	E4545	V4546	Q4547	R4548	F4551	L4552	N4553	Y4554	L4562	R4563	L4567	F4568	L4569	A4570	F4571	A4572	N4574	F4575	L4576	V4582	S4583	D4584	S4585	P4586	P4587	GLY	GLU	ASP	ASP	ASP	ASP	GLY	SER	ALA	ALA	GLY	ASP	LEU	ALA	GLY	GLY	SER	GLY	GLY	GLY	SER	GLY	GLY	GLY	SER	GLY	GLY	GLY	SER																																																																													
R4188	R4189	T4190	E4191	R4192	I4193	Y4194	F4196	E4197	S4198	M4201	R4202	A4203	E4206	Q4209	E4212	R4215	E4224	Q4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	S4236	E4239	E4244	M4245	Q4246	I4251	S4252	E4253	X4320	X4321	X4322	X4325	X4329	X4330	X4337	X4340	X4345	X4346	X4347	X4348	X4349	X4350	X4351	X4352	X4353	X4354	X4355	X4356	X4357	X4358	X4359	X4360	X4361	X4362	X4363	X4364	X4365	X4366	X4367	X4368	X4369	X4370	X4371	X4372	X4373	X4374	X4375	X4376	X4377	X4378	X4379	X4380	X4381	X4382	X4383	X4384	X4385	X4386	X4387	X4388	X4389	X4390	X4391	X4392	X4393	X4394	X4395	X4396	X4397	X4398	X4399	X4400	X4401	X4402	X4403	X4404	X4405	X4406	X4407	X4408	X4409	X4410	X4411	X4412	X4413	X4414	X4415	X4416	X4417	X4418	X4419	X4420	X4421	X4422	X4423	X4424	X4425	X4426	X4427	X4428	X4429	X4430	X4431	X4432	X4433	X4434	X4435	X4436	X4437
T4104	G4105	P4106	E4107	I4108	Q4109	F4110	L4111	L4112	S4113	C4114	S4115	E4116	A4117	D4118	E4119	N4120	E4121	M4122	I4123	N4124	F4125	L4126	E4127	L4128	F4129	N4130	R4131	F4132	Q4133	E4134	P4135	A4136	R4137	G4140	F4141	N4142	E4152	H4153	W4154	P4155	H4156	R4161	L4164	E4165	E4172	Y4177	L4178	G4179	R4180	I4181	A4186	S4187																																																																																		
E4032	G4033	N4034	V4035	G4038	A4041	M4047	E4050	E4056	M4057	L4058	L4059	K4060	F4061	D4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072	S4074	E4075	A4076	F4077	Q4078	D4079	V4080	A4081	T4082	D4083	P4084	R4085	Q4086	L4087	I4088	K4091	D4092	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	K4101	Q4102	F4103																																																																																			
Y3937	S3938	G3939	K3940	D3941	V3942	I3943	E3944	E3945	Q3946	G3947	K3948	R3949	N3950	K3953	V3961	F3962	N3963	Q3970	Q3976	S3979	A3981	H3982	L3985	L3986	F3987	A3989	M4000	M4001	L4002	A4004	Q4005	D4006	S4007	S4008	Q4009	I4010	E4011	L4012	L4013	E4015	L4016	L4017	D4018	L4019	D4022	L4031																																																																																								
E3830	Q3833	L3842	D3843	R3849	Q3850	E3854	G3855	R3856	G3857	N3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	N3866	N3867	N3868	Q3869	N3870	G3871	G3872	X3873	N3874	N3875	A3876	D3877	N3878	E3879	Q3882	R3886	Q3889	E3893	F3899	Q3906	T3907	L3923	L3924	R3925	E3928	S3929	D3952																																																																																										
K3731	S3732	C3733	H3734	L3735	E3736	E3737	E3738	G3739	E3740	N3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	E3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	K3759	Q3760	Q3761	R3762	L3763	Q3766	R3769	T3772	R3773	V3779	L3780	Q3781	M3782	S3803	L3804	L3805	N3809	A3810	E3811	K3815	N3816	L3817	K3821	D3822																																																																																				
Y3642	N3643	L3644	R3648	N3651	H3652	F3653	K3658	A3659	A3660	N3661	L3663	T3664	D3666	H3667	F3669	D3675	D3676	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	E3712	K3713	S3714	K3715	E3718	T3719	V3720	L3721	Y3722	N3723	A3724	Y3725	A3726	D3727	I3728	M3729	A3730																																																																																					
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	T3639	P3640	L3641																																																																														
X3441	X3442	X3443	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3463	X3464	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551																																																																																
X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3420	X3421	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437																																																																														



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	0.20	0/834	0.46	0/1123
1	F	0.20	0/834	0.46	0/1123
1	H	0.20	0/834	0.46	0/1123
1	J	0.20	0/834	0.46	0/1123
2	B	0.23	0/25428	0.53	2/34534 (0.0%)
2	E	0.23	0/25428	0.53	2/34534 (0.0%)
2	G	0.23	0/25428	0.53	2/34534 (0.0%)
2	I	0.23	0/25428	0.53	2/34534 (0.0%)
All	All	0.23	0/105048	0.53	8/142628 (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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5027	CYS	N-CA-C	5.52	117.59	108.49
2	E	5027	CYS	N-CA-C	5.52	117.59	108.49
2	G	5027	CYS	N-CA-C	5.50	117.57	108.49
2	I	5027	CYS	N-CA-C	5.50	117.56	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	5.21	134.52	116.30
2	G	131	LEU	CA-CB-CG	5.20	134.51	116.30
2	B	131	LEU	CA-CB-CG	5.20	134.48	116.30
2	E	131	LEU	CA-CB-CG	5.19	134.46	116.30

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
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

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Mol	Chain	Res	Type	Group
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
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	9	0
1	J	818	0	824	5	0
2	B	29499	0	24751	296	0
2	E	29499	0	24751	304	0
2	G	29499	0	24751	303	0
2	I	29499	0	24751	296	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	1199	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 (1199) 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	0.95
2:B:4190:ILE:HD11	2:B:5026:ASP:CG	1.92	0.95
2:E:4190:ILE:HD11	2:E:5026:ASP:CG	1.92	0.94
2:G:4190:ILE:HD11	2:G:5026:ASP:CG	1.92	0.94
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.49	0.86
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.49	0.86
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.49	0.83
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.49	0.83
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:4064:MET:HE3	2:E:4107:GLU:HB3	1.84	0.59
2:G:4064:MET:HE3	2:G:4107:GLU:HB3	1.84	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:I:4064:MET:HE3	2:I:4107:GLU:HB3	1.84	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:B:4064:MET:HE3	2:B:4107:GLU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4190:ILE:HD13	2:G:5026:ASP:CG	2.26	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:2267:MET:HE3	2:E:2268:GLN:HG2	1.87	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:G:2267:MET:HE3	2:G:2268:GLN:HG2	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:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.26	0.56
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.88	0.56
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:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.87	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:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:34:LYS:H	2:G:53:SER:HG	1.54	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
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: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:34:LYS:H	2:I:53:SER:HG	1.54	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:I:4738:ALA:HA	2:I:4743:MET:HE3	1.90	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4738:ALA:HA	2:B:4743:MET:HE3	1.90	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:4738:ALA:HA	2:G:4743:MET:HE3	1.90	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:E:4738:ALA:HA	2:E:4743:MET:HE3	1.90	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
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:E:23:GLN:OE1	2:E:203:ASN:ND2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.91	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:E:399:GLN:HG2	2:E:403:MET:HE3	1.92	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:399:GLN:HG2	2:I:403:MET:HE3	1.92	0.52
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.92	0.52
2:G:399:GLN:HG2	2:G:403:MET:HE3	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: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:1100:MET:HE2	2:G:1198:GLN:HB3	1.91	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
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:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.26	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:B:399:GLN:HG2	2:B:403:MET:HE3	1.92	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:34:LYS:H	2:E:53:SER:HG	1.55	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: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:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.91	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1100:MET:HE2	2:E:1198:GLN:HB3	1.91	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.77	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:34:LYS:H	2:B:53:SER:HG	1.55	0.49
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.95	0.49
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4826:ILE:O	2:G:4829:SER:OG	2.29	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:B:4826:ILE:O	2:B:4829:SER:OG	2.29	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:E:463:GLU:OE2	2:E:467:LYS:NZ	2.41	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:4865:LYS:HG3	2:B:4875:LYS:HZ3	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
1:H:11:ASP:OD1	1:H:67:SER:OG	2.31	0.46
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.97	0.46
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.80	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
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:E:4984:ASN:C	2:E:4986:ALA:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:4047:MET:HE3	2:I:4047:MET:HB2	1.86	0.45
2:I:4984:ASN:C	2:I:4986:ALA:H	2.24	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:B:4000:MET:HE3	2:B:4017:LEU:HD21	1.99	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:G:320:LYS:NZ	2:G:381:GLU:O	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4984:ASN:C	2:B:4986:ALA:H	2.24	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.50	0.45
2:I:4000:MET:HE3	2:I:4017:LEU:HD21	1.99	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
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:E:4000:MET:HE3	2:E:4017:LEU:HD21	1.99	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
2:G:4984:ASN:C	2:G:4986:ALA:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3842:LEU:O	2:E:3929:SER:OG	2.35	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
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:B:3842:LEU:O	2:B:3929:SER:OG	2.35	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:396:GLU:OE2	2:G:451:TYR:OH	2.35	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:582:HIS:O	2:E:585:SER:OG	2.30	0.44
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:211:GLU:OE2	2:G:3907:THR:OG1	2.33	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:G:4000:MET:HE3	2:G:4017:LEU:HD21	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4984:ASN:C	2:B:4986:ALA:N	2.76	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
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:I:4984:ASN:C	2:I:4986:ALA:N	2.76	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:E:4984:ASN:C	2:E:4986:ALA:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:GLU:OE2	2:E:3907:THR:OG1	2.34	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:320:LYS:NZ	2:I:381:GLU:O	2.42	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
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:4047:MET:HE3	2:B:4047:MET:HB2	1.86	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:396:GLU:OE2	2:E:451:TYR:OH	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:4984:ASN:C	2:G:4986:ALA:N	2.77	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
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:320:LYS:NZ	2:E:381:GLU:O	2.42	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:396:GLU:OE2	2:B:451:TYR:OH	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:1694:LEU:O	2:G:1712:TYR:OH	2.27	0.42
2:G:3729:MET:O	2:G:3732:SER:OG	2.34	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
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:B:4063:ASP:O	2:B:4067:LYS:NZ	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:4763:GLY:O	2:B:4766:THR:OG1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:G:4047:MET:HE3	2:G:4047:MET:HB2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1152:MET:HE1	2:G:1217:CYS:HB3	2.03	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:E:3722:TYR:CZ	2:E:3782:MET:HE3	2.57	0.40
2:E:5013:MET:HE1	2:E:5020:ASP:HB3	2.04	0.40
2:G:1029:GLU:HB3	2:G:1033:ARG:HH12	1.86	0.40
2:G:3722:TYR:CZ	2:G:3782:MET:HE3	2.57	0.40
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.03	0.40
2:B:5013:MET:HE1	2:B:5020:ASP:HB3	2.04	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:E:1152:MET:HE1	2:E:1217:CYS:HB3	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%)	43	77
2	E	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	43	77
2	G	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	43	77
2	I	3235/4416 (73%)	2891 (89%)	336 (10%)	8 (0%)	43	77
All	All	13360/18096 (74%)	11941 (89%)	1387 (10%)	32 (0%)	44	77

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
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

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Mol	Chain	Res	Type
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%)	2481 (100%)	12 (0%)	81	81
2	E	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	G	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	I	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
All	All	10324/12444 (83%)	10276 (100%)	48 (0%)	78	81

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

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	2339	VAL
2	B	3805	LEU
2	B	4154	VAL
2	B	4792	LEU
2	B	4959	PHE

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Mol	Chain	Res	Type
2	B	4960	ILE
2	B	5027	CYS
2	I	131	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1676	LEU
2	I	2339	VAL
2	I	3805	LEU
2	I	4154	VAL
2	I	4792	LEU
2	I	4959	PHE
2	I	4960	ILE
2	I	5027	CYS
2	E	131	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	2339	VAL
2	E	3805	LEU
2	E	4154	VAL
2	E	4792	LEU
2	E	4959	PHE
2	E	4960	ILE
2	E	5027	CYS
2	G	131	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	2339	VAL
2	G	3805	LEU
2	G	4154	VAL
2	G	4792	LEU
2	G	4959	PHE
2	G	4960	ILE
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (236) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	87	HIS
1	A	32	ASN
1	A	65	GLN
1	A	87	HIS
1	H	32	ASN
1	H	65	GLN
1	H	87	HIS
1	J	32	ASN
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	151	HIS
2	B	201	ASN
2	B	224	HIS
2	B	273	HIS
2	B	284	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	479	GLN
2	B	489	ASN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	838	HIS
2	B	877	ASN
2	B	1220	GLN
2	B	1611	HIS
2	B	1665	HIS
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1949	GLN
2	B	1953	HIS
2	B	1970	GLN
2	B	2005	GLN
2	B	2007	ASN
2	B	2041	HIS

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Mol	Chain	Res	Type
2	B	2194	HIS
2	B	2260	ASN
2	B	2881	ASN
2	B	3766	GLN
2	B	3781	GLN
2	B	3814	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3950	ASN
2	B	3960	GLN
2	B	3994	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4078	GLN
2	B	4102	GLN
2	B	4120	ASN
2	B	4130	ASN
2	B	4201	ASN
2	B	4553	ASN
2	B	4691	GLN
2	B	4806	ASN
2	B	4857	ASN
2	B	4864	ASN
2	B	4947	GLN
2	B	4949	GLN
2	B	5006	GLN
2	I	57	ASN
2	I	105	HIS
2	I	113	HIS
2	I	151	HIS
2	I	201	ASN
2	I	224	HIS
2	I	284	HIS
2	I	379	HIS
2	I	395	GLN
2	I	405	HIS
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	877	ASN
2	I	1220	GLN
2	I	1229	ASN

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Mol	Chain	Res	Type
2	I	1665	HIS
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1953	HIS
2	I	1970	GLN
2	I	2005	GLN
2	I	2007	ASN
2	I	2041	HIS
2	I	2194	HIS
2	I	2260	ASN
2	I	2881	ASN
2	I	3766	GLN
2	I	3781	GLN
2	I	3814	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3950	ASN
2	I	3960	GLN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4078	GLN
2	I	4102	GLN
2	I	4120	ASN
2	I	4130	ASN
2	I	4201	ASN
2	I	4553	ASN
2	I	4691	GLN
2	I	4806	ASN
2	I	4857	ASN
2	I	4864	ASN
2	I	4949	GLN
2	I	5006	GLN
2	E	57	ASN
2	E	113	HIS
2	E	151	HIS
2	E	201	ASN
2	E	224	HIS

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Mol	Chain	Res	Type
2	E	284	HIS
2	E	379	HIS
2	E	395	GLN
2	E	405	HIS
2	E	479	GLN
2	E	489	ASN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS
2	E	838	HIS
2	E	877	ASN
2	E	1220	GLN
2	E	1665	HIS
2	E	1679	ASN
2	E	1691	GLN
2	E	1693	GLN
2	E	1702	HIS
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1953	HIS
2	E	1970	GLN
2	E	2005	GLN
2	E	2007	ASN
2	E	2041	HIS
2	E	2194	HIS
2	E	2260	ASN
2	E	2773	ASN
2	E	2881	ASN
2	E	3766	GLN
2	E	3781	GLN
2	E	3814	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3950	ASN
2	E	3960	GLN
2	E	3994	HIS
2	E	4020	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4078	GLN
2	E	4102	GLN

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Mol	Chain	Res	Type
2	E	4120	ASN
2	E	4130	ASN
2	E	4201	ASN
2	E	4553	ASN
2	E	4691	GLN
2	E	4806	ASN
2	E	4857	ASN
2	E	4864	ASN
2	E	4946	GLN
2	E	4949	GLN
2	E	5006	GLN
2	G	57	ASN
2	G	113	HIS
2	G	151	HIS
2	G	201	ASN
2	G	224	HIS
2	G	273	HIS
2	G	284	HIS
2	G	379	HIS
2	G	395	GLN
2	G	405	HIS
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	838	HIS
2	G	877	ASN
2	G	1220	GLN
2	G	1229	ASN
2	G	1665	HIS
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1949	GLN
2	G	1953	HIS
2	G	1973	GLN
2	G	2005	GLN
2	G	2007	ASN
2	G	2041	HIS
2	G	2194	HIS

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Mol	Chain	Res	Type
2	G	2260	ASN
2	G	2773	ASN
2	G	3766	GLN
2	G	3781	GLN
2	G	3814	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3950	ASN
2	G	3960	GLN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4078	GLN
2	G	4102	GLN
2	G	4120	ASN
2	G	4130	ASN
2	G	4201	ASN
2	G	4553	ASN
2	G	4691	GLN
2	G	4806	ASN
2	G	4857	ASN
2	G	4864	ASN
2	G	4949	GLN
2	G	5003	HIS
2	G	5006	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2479:LEU	C	2487:UNK	N	3.33

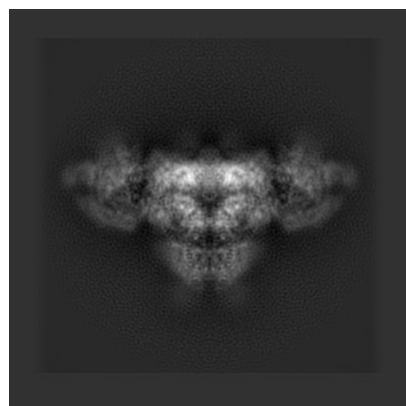
6 Map visualisation [i](#)

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.

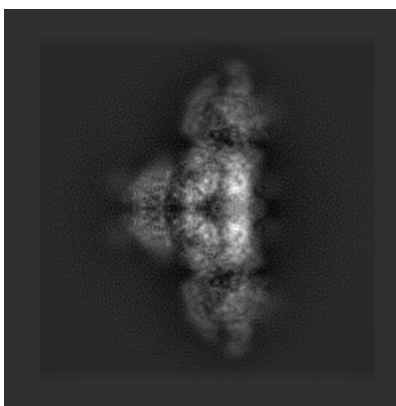
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

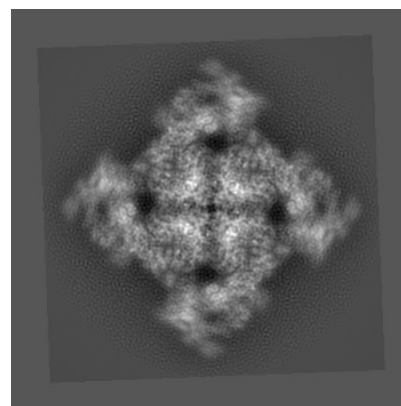
6.1.1 Primary map



X

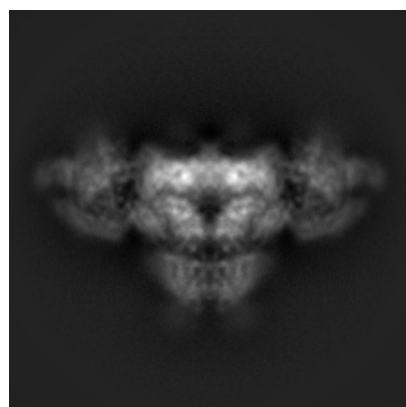


Y

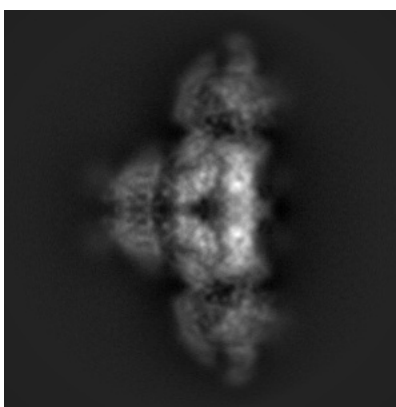


Z

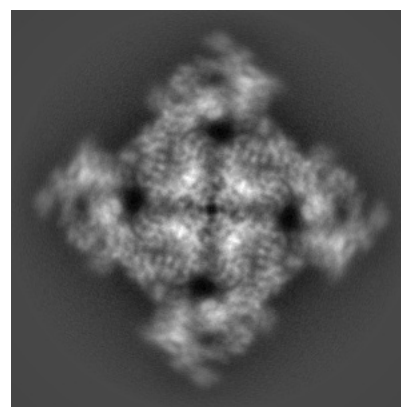
6.1.2 Raw map



X



Y

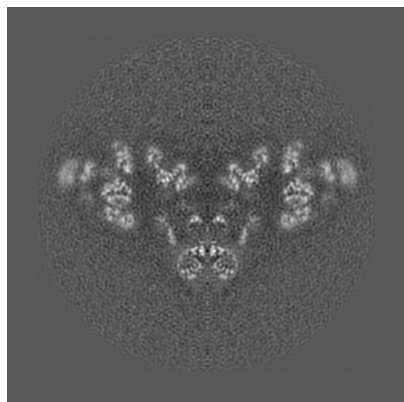


Z

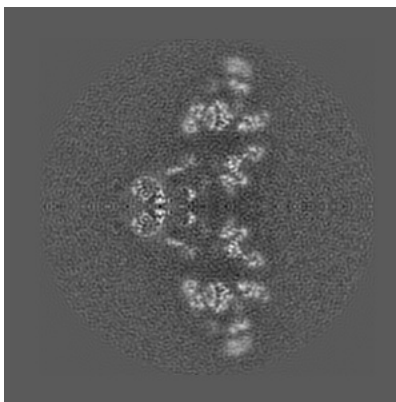
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

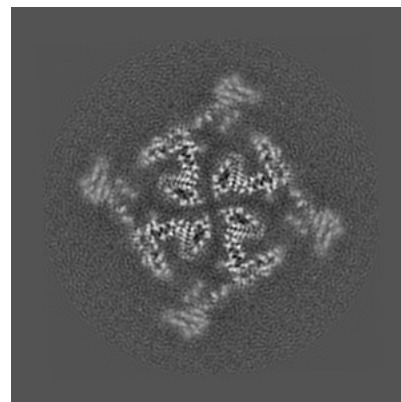
6.2.1 Primary map



X Index: 200

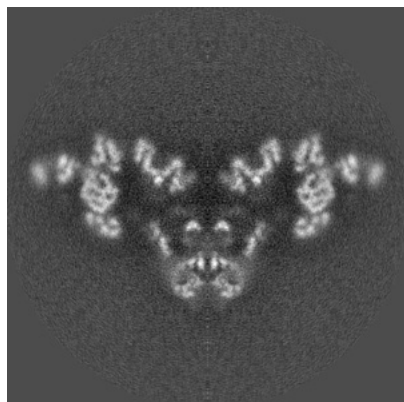


Y Index: 200

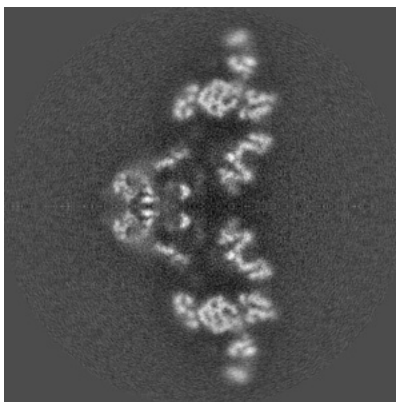


Z Index: 200

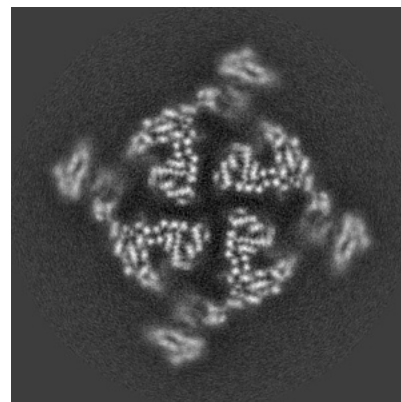
6.2.2 Raw map



X Index: 168



Y Index: 168

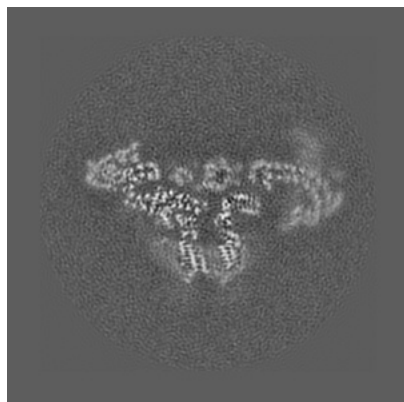


Z Index: 168

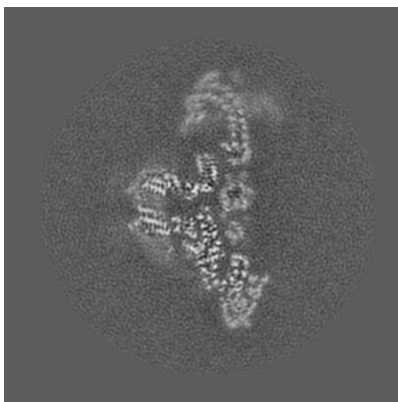
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

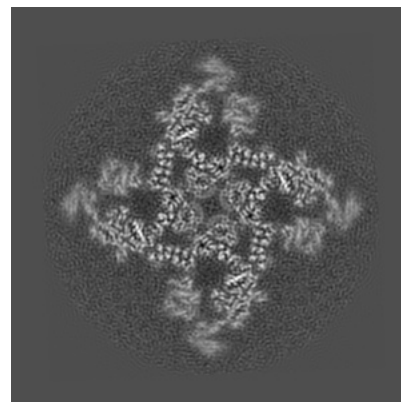
6.3.1 Primary map



X Index: 224

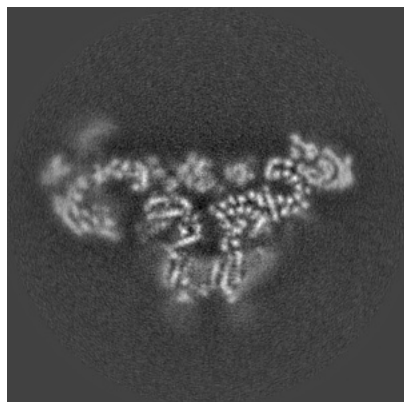


Y Index: 176

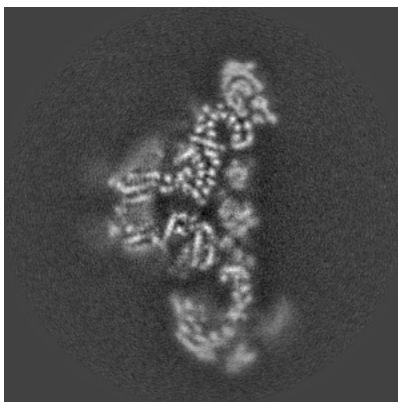


Z Index: 228

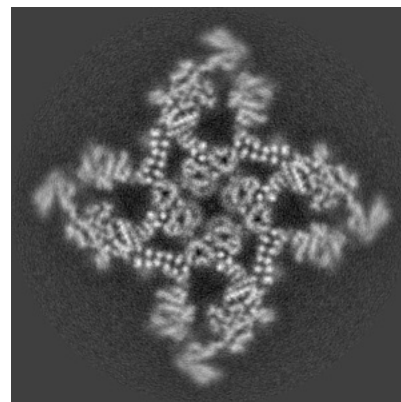
6.3.2 Raw map



X Index: 146



Y Index: 190

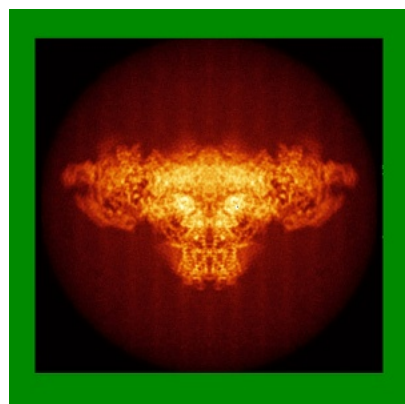


Z Index: 193

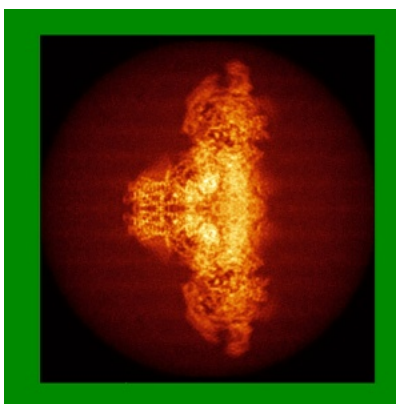
The images above show the largest variance slices of the map in three orthogonal directions.

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

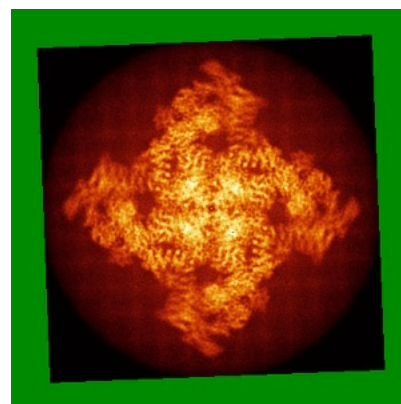
6.4.1 Primary map



X



Y

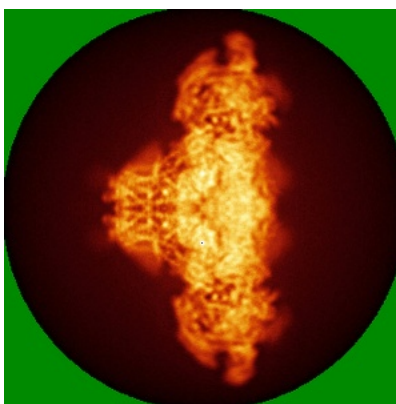


Z

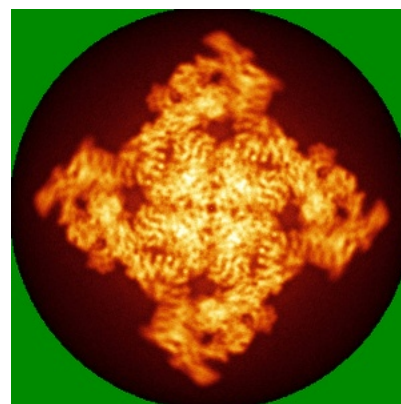
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

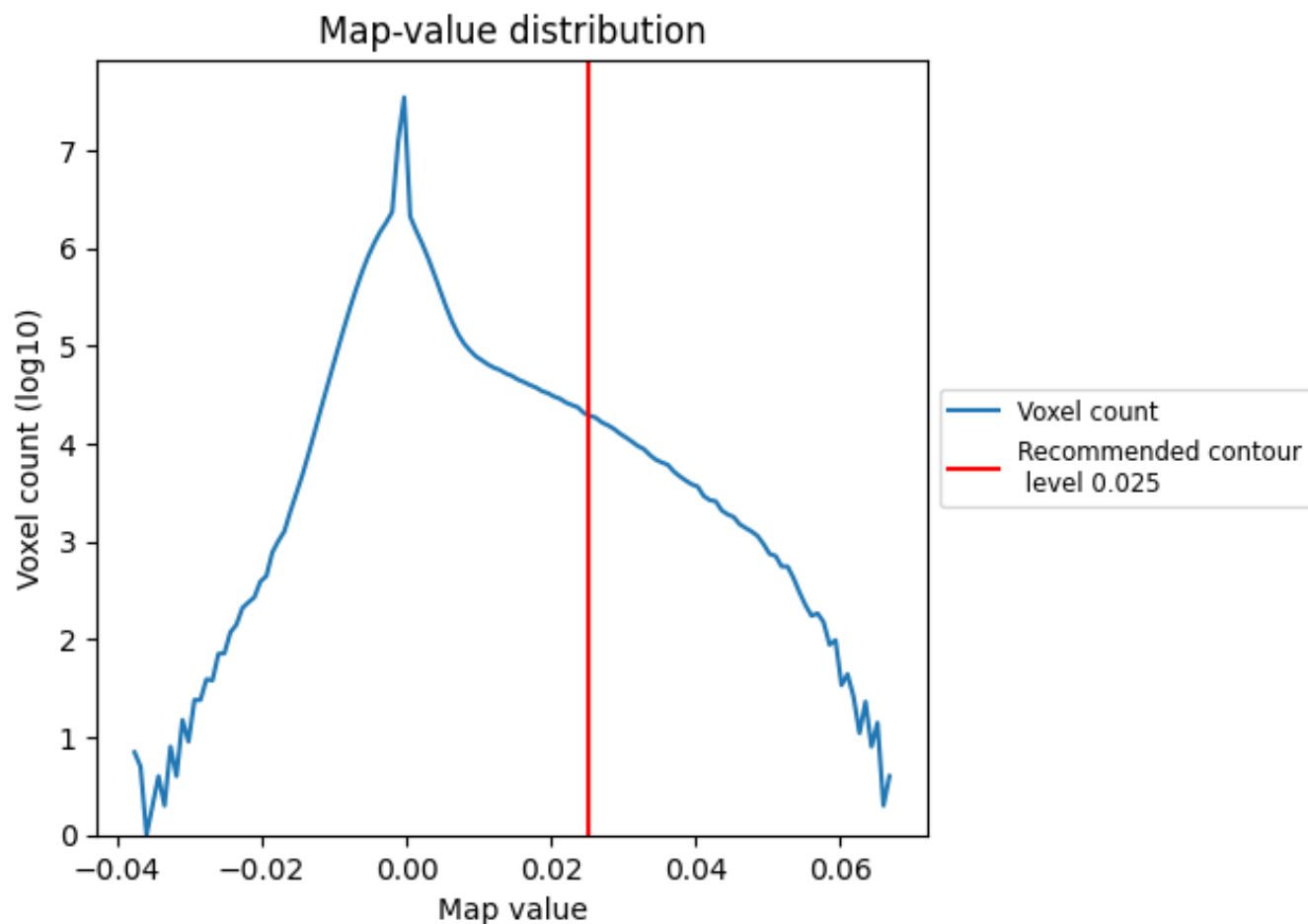
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

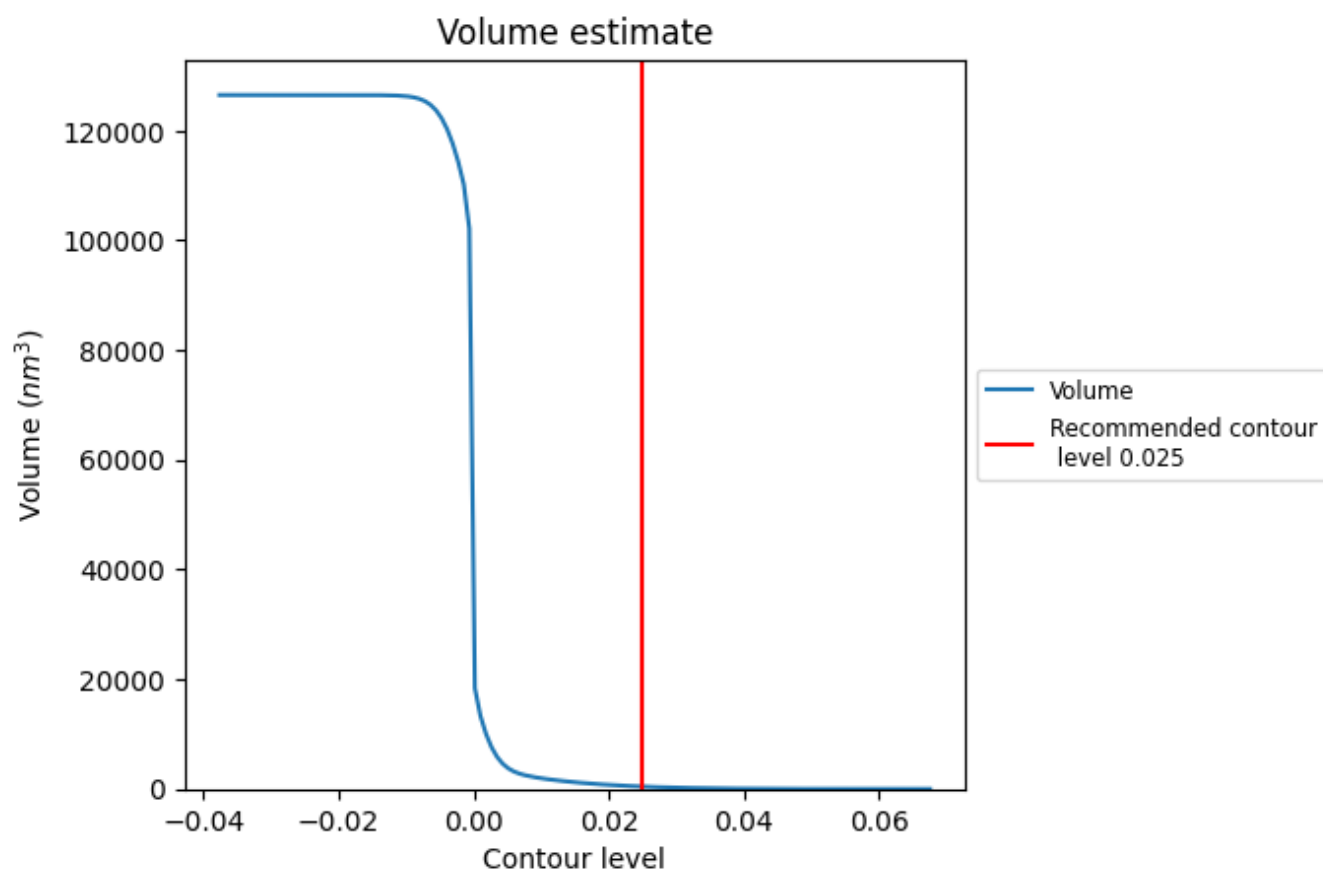
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

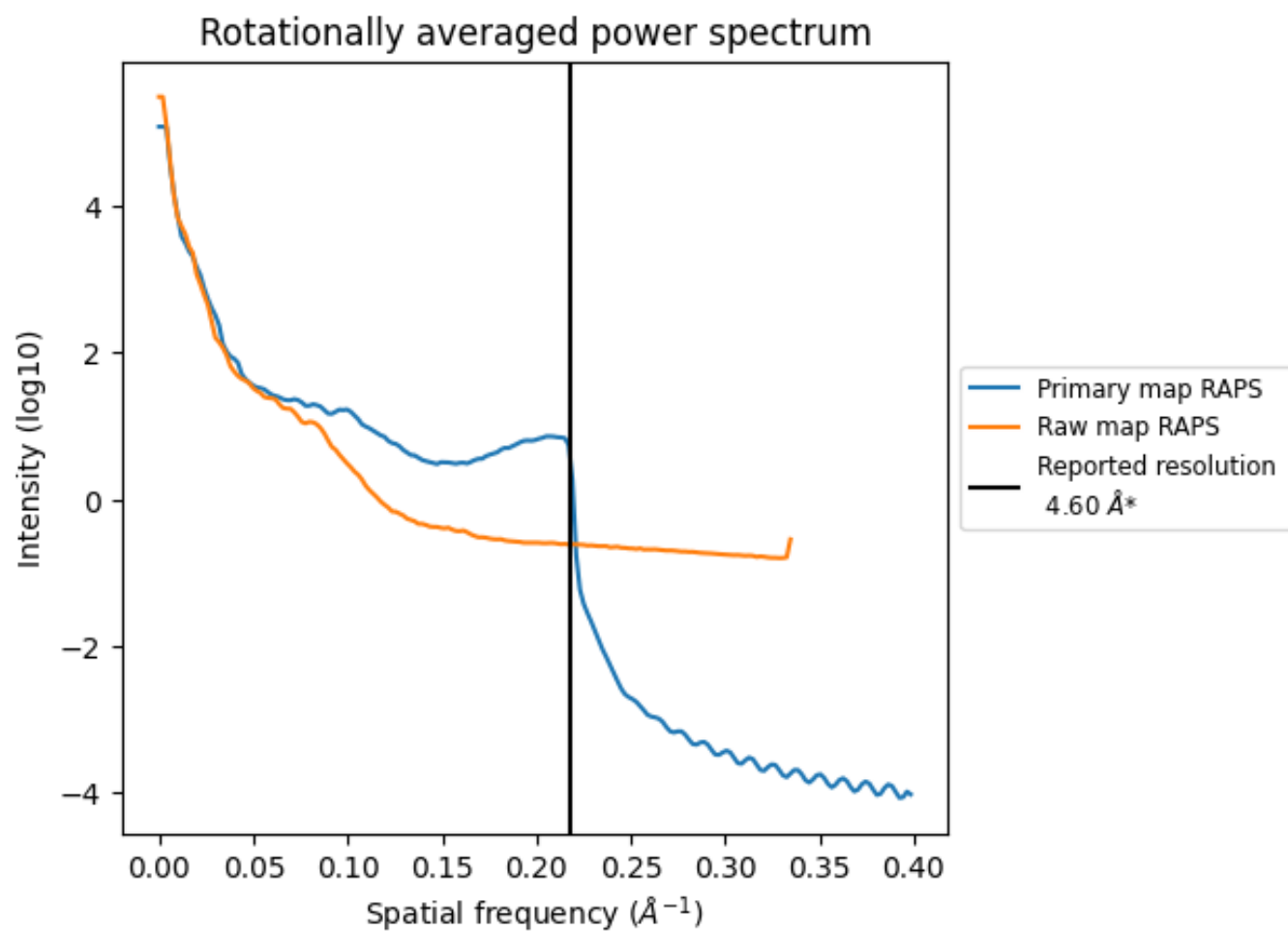
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

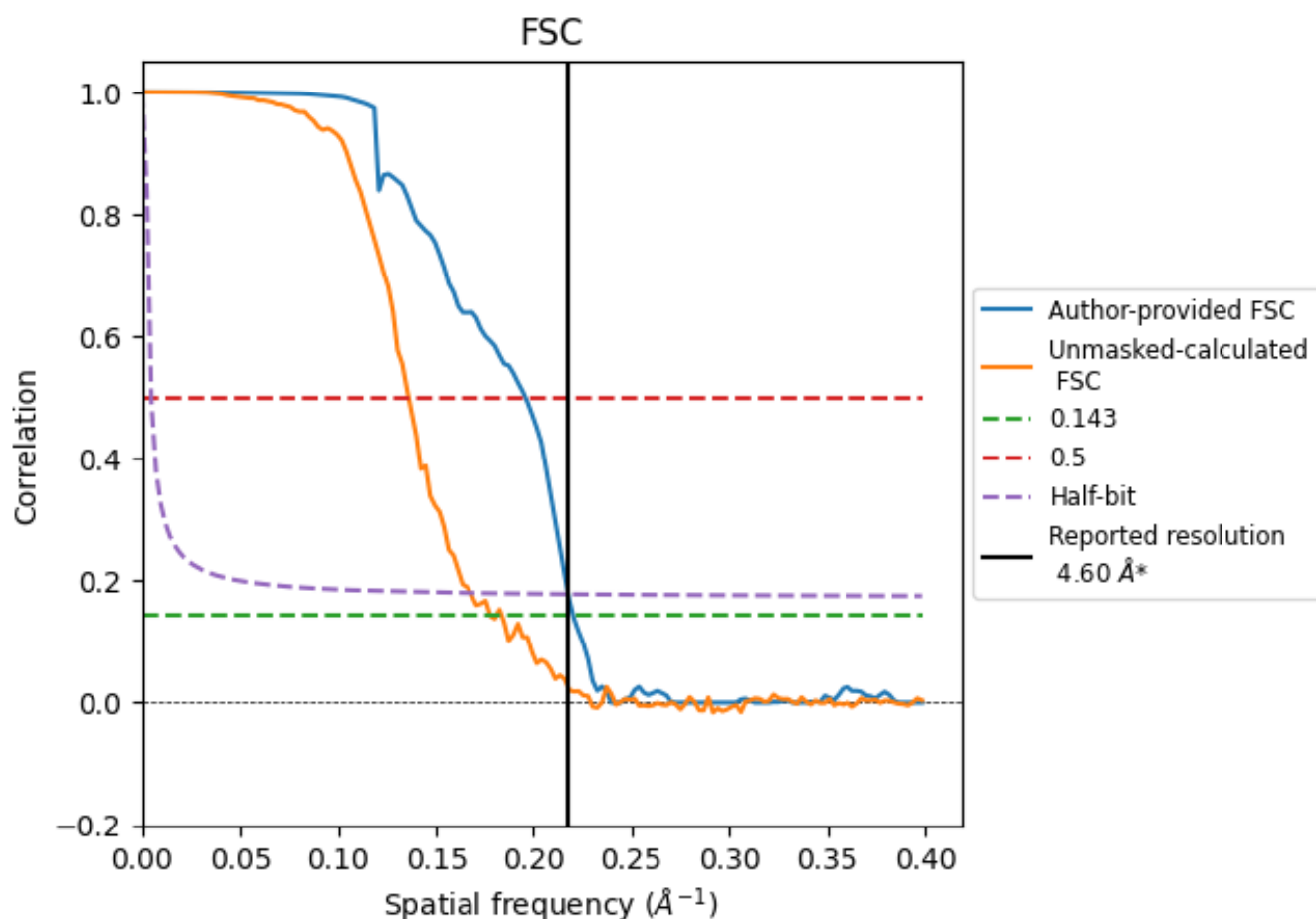


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
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 %

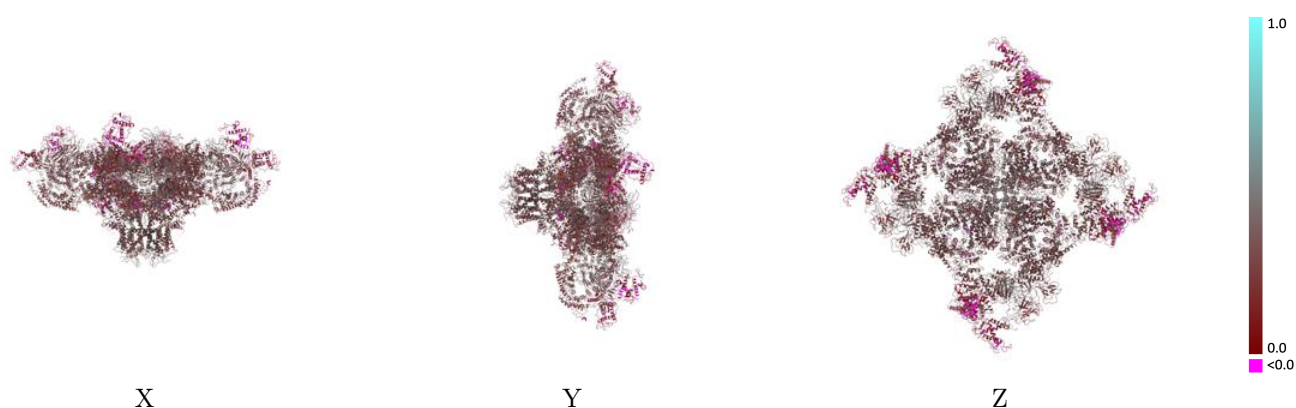
9 Map-model fit [i](#)

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 5.

9.1 Map-model overlay [i](#)

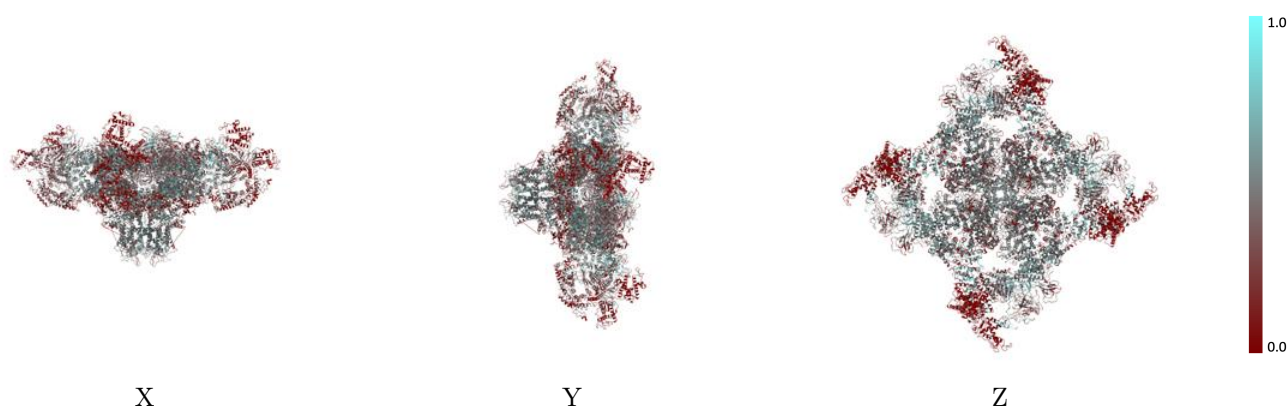
This section was not generated.

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



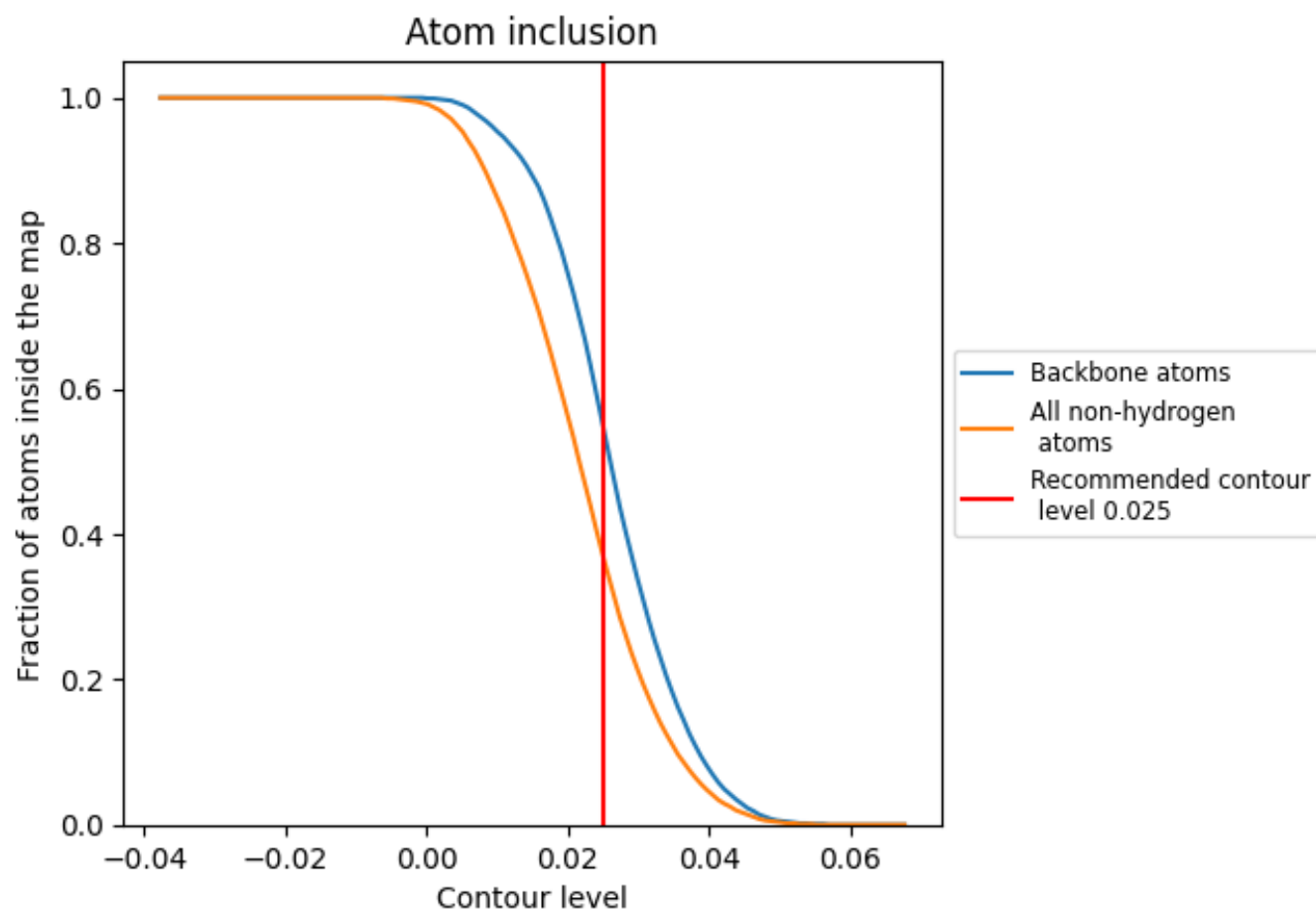
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 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	0.3690	0.2880
A	0.3500	0.3000
B	0.3700	0.2880
E	0.3690	0.2880
F	0.3440	0.3030
G	0.3700	0.2880
H	0.3490	0.3040
I	0.3700	0.2870
J	0.3500	0.3030

1.0

0.0

<0.0