



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:25 AM UTC

PDB ID : 5TAU / pdb_00005tau
EMDB ID : EMD-8385
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

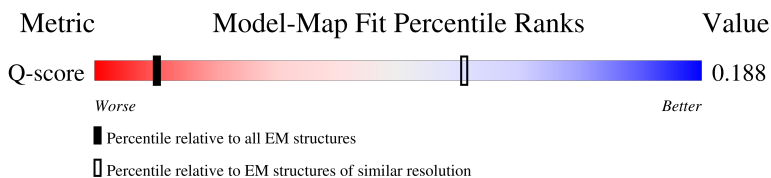
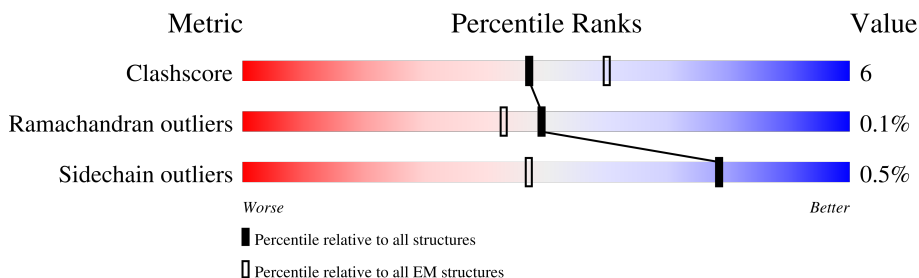
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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.



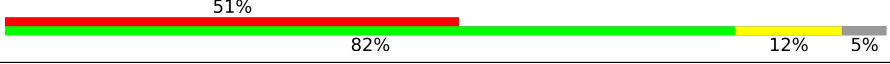
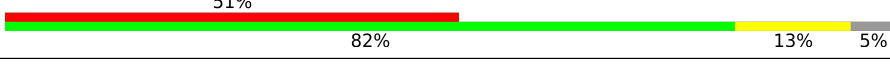
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

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	51% 70% 29%
1	F	108	52% 69% 30%
1	H	108	52% 72% 27%
1	J	108	53% 72% 27%

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121436 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.

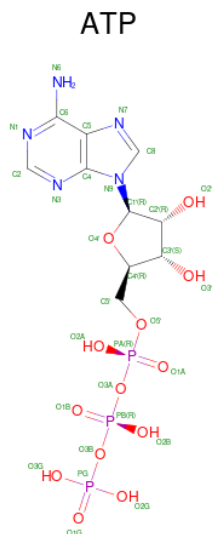
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

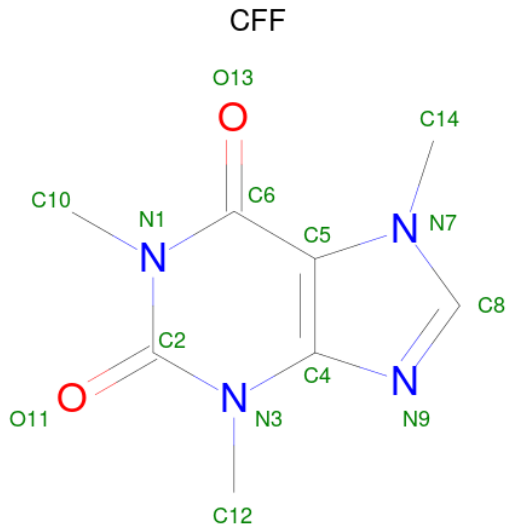
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		

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



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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



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

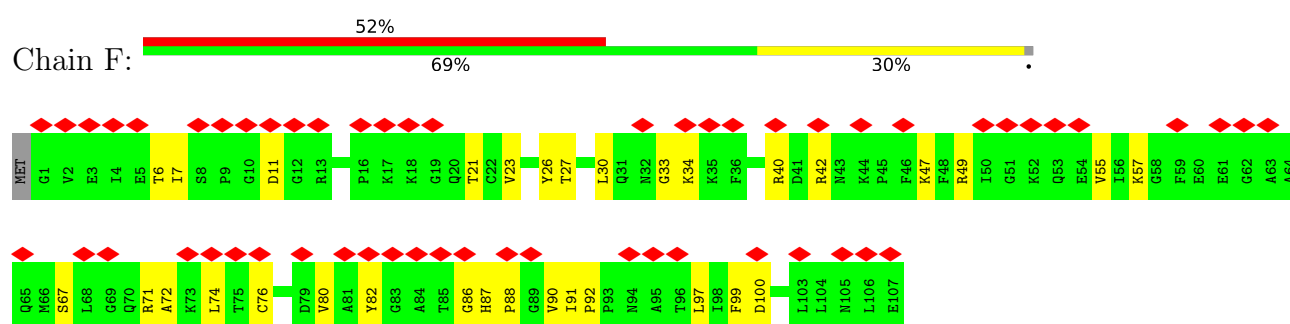
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

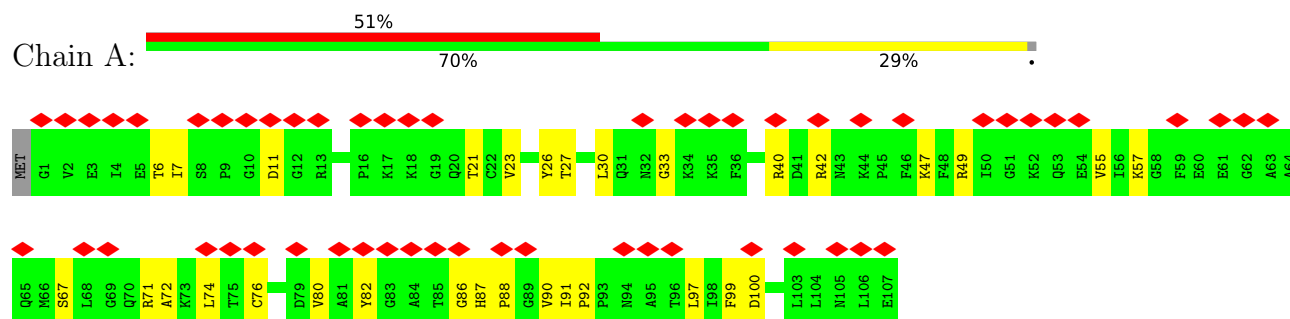
3 Residue-property plots [i](#)

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.

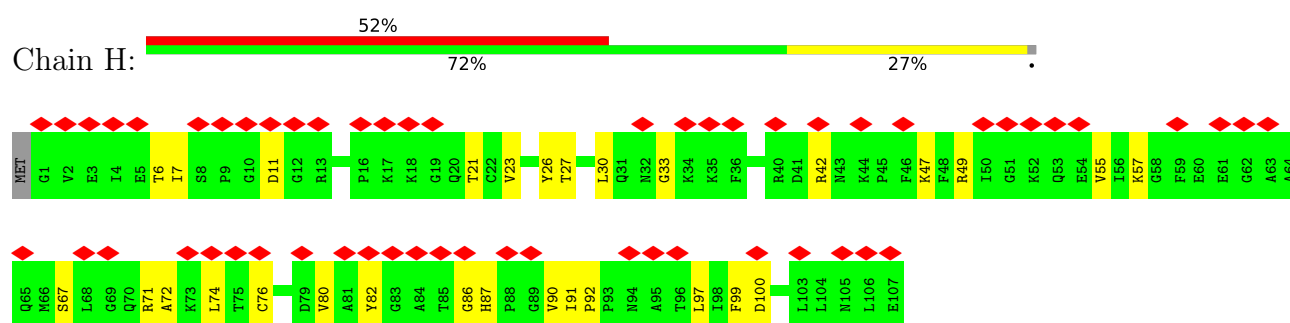
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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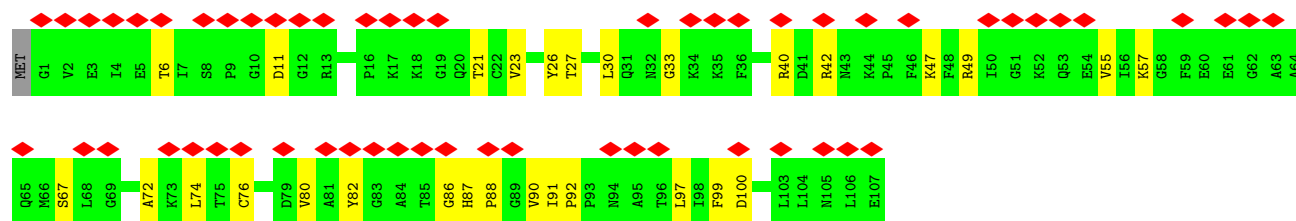


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

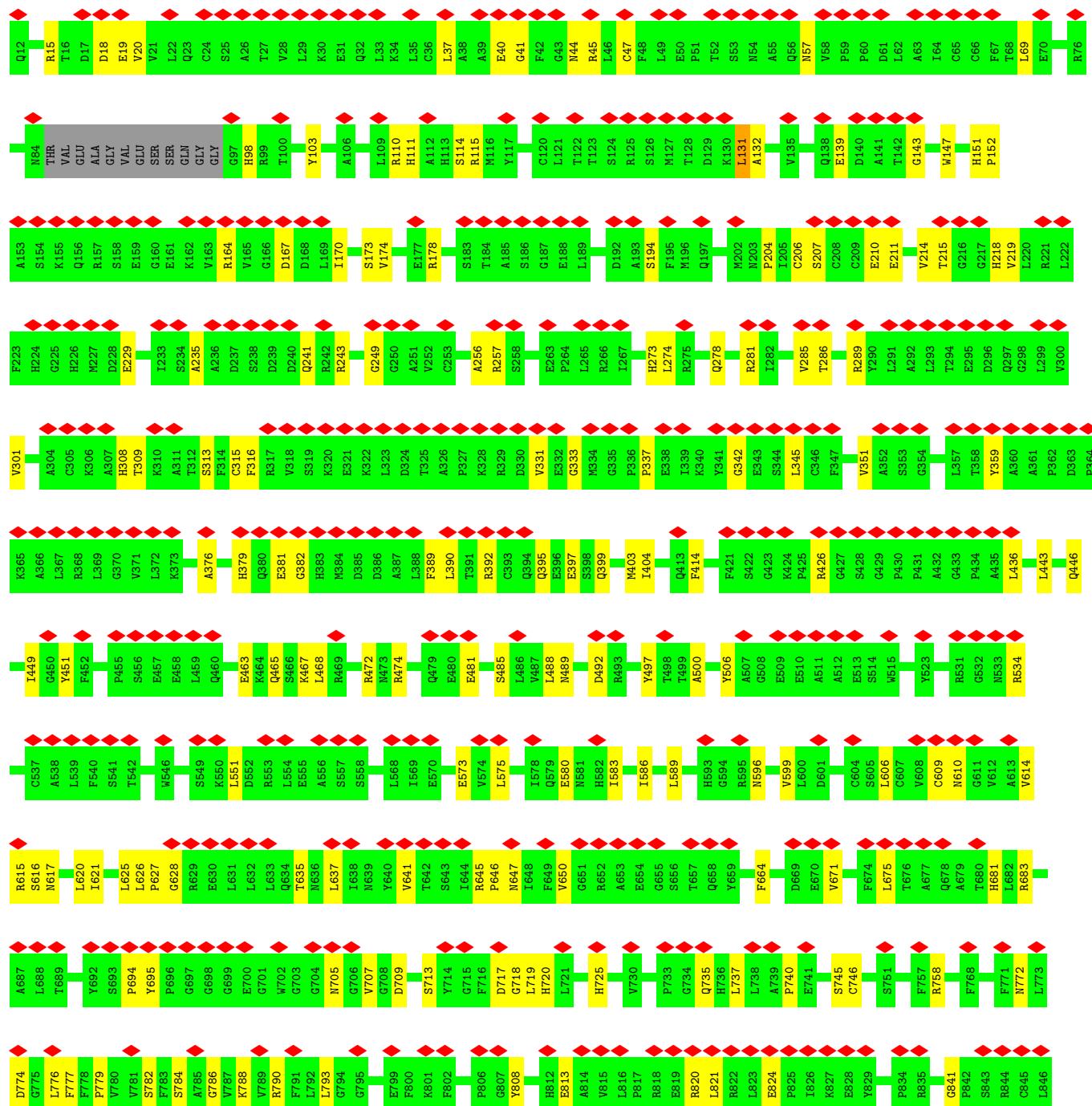
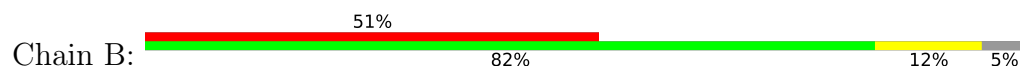


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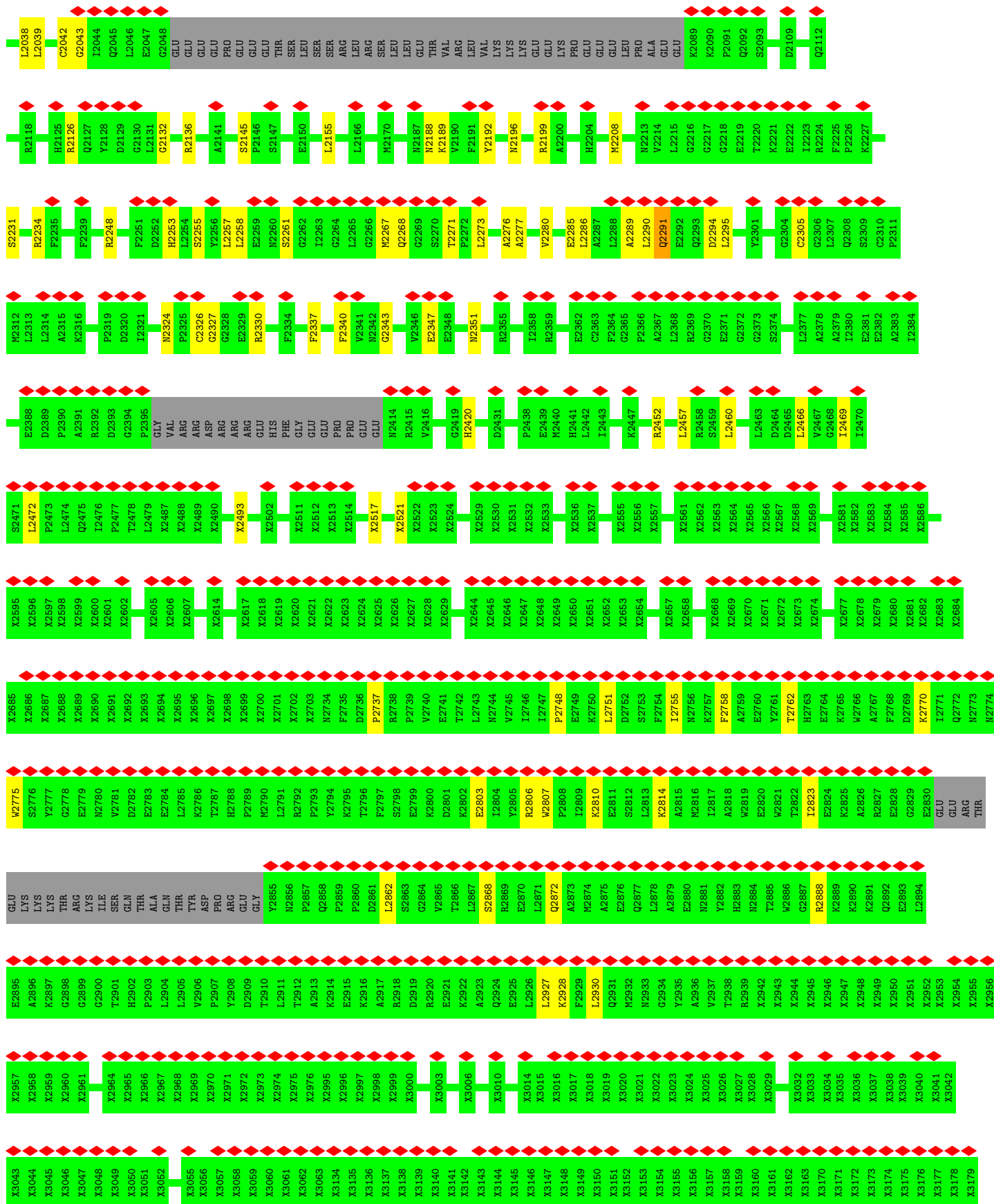


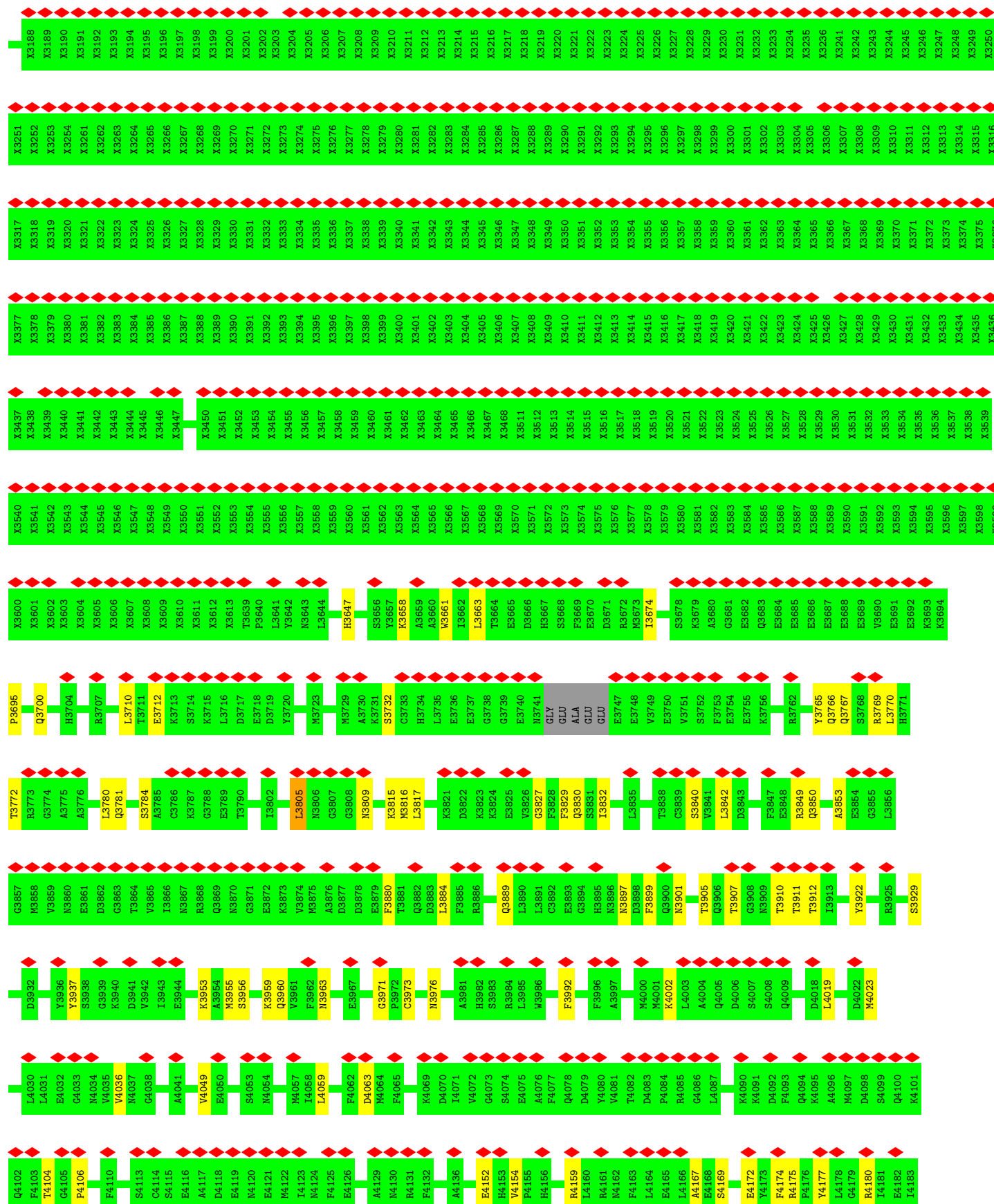


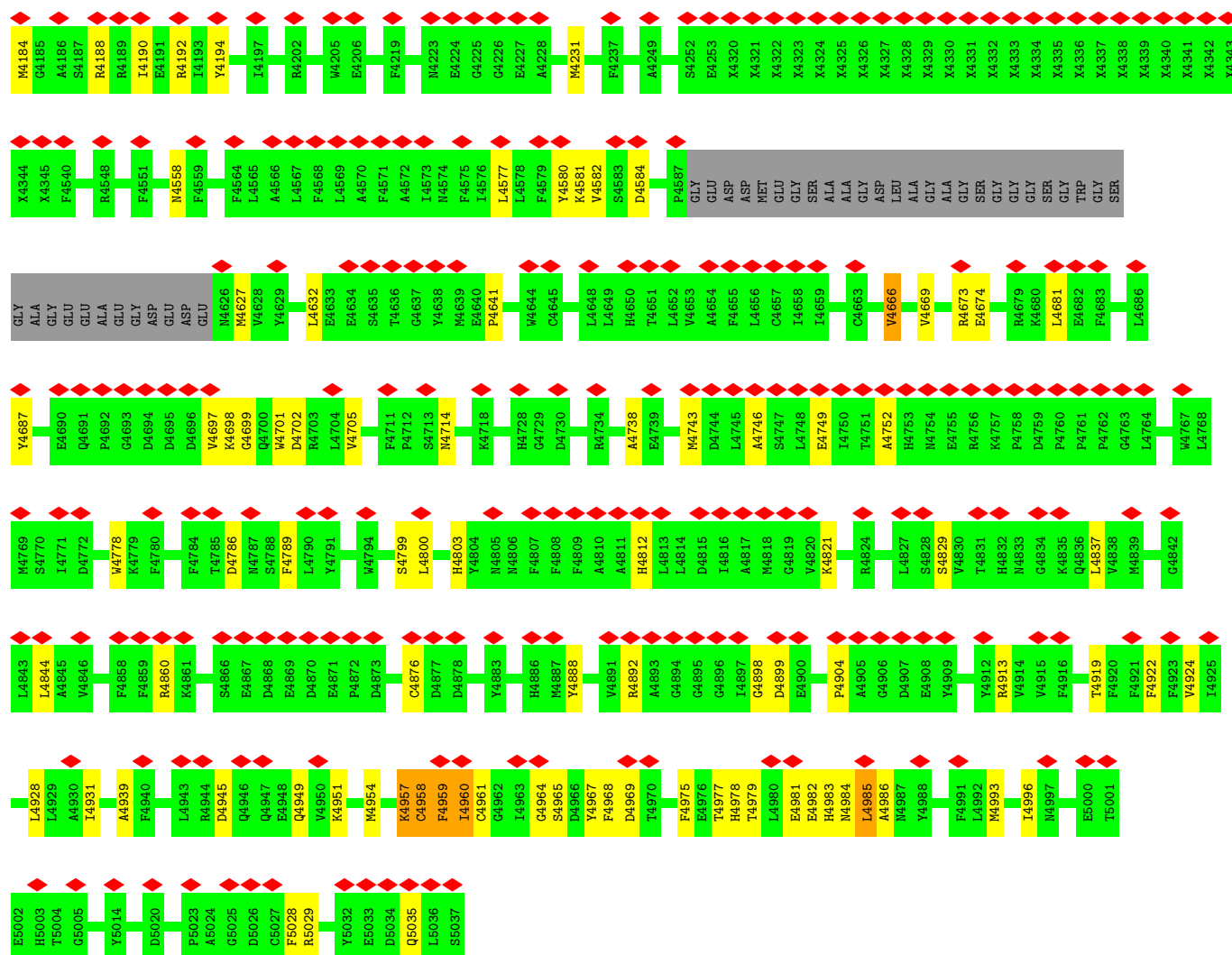
• Molecule 2: Ryanodine receptor 1



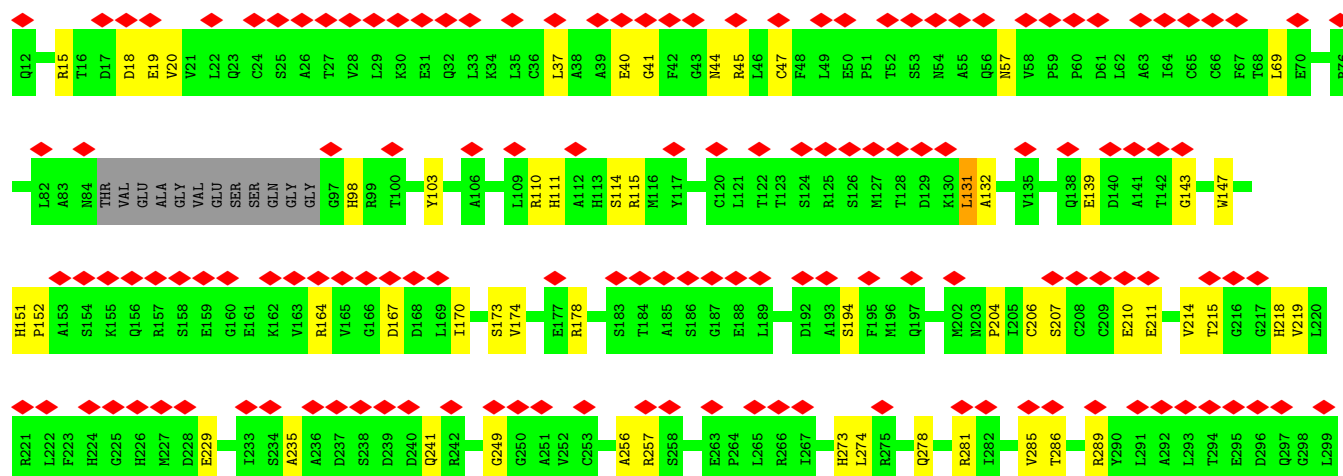
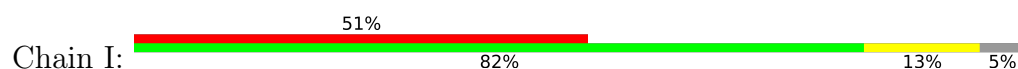


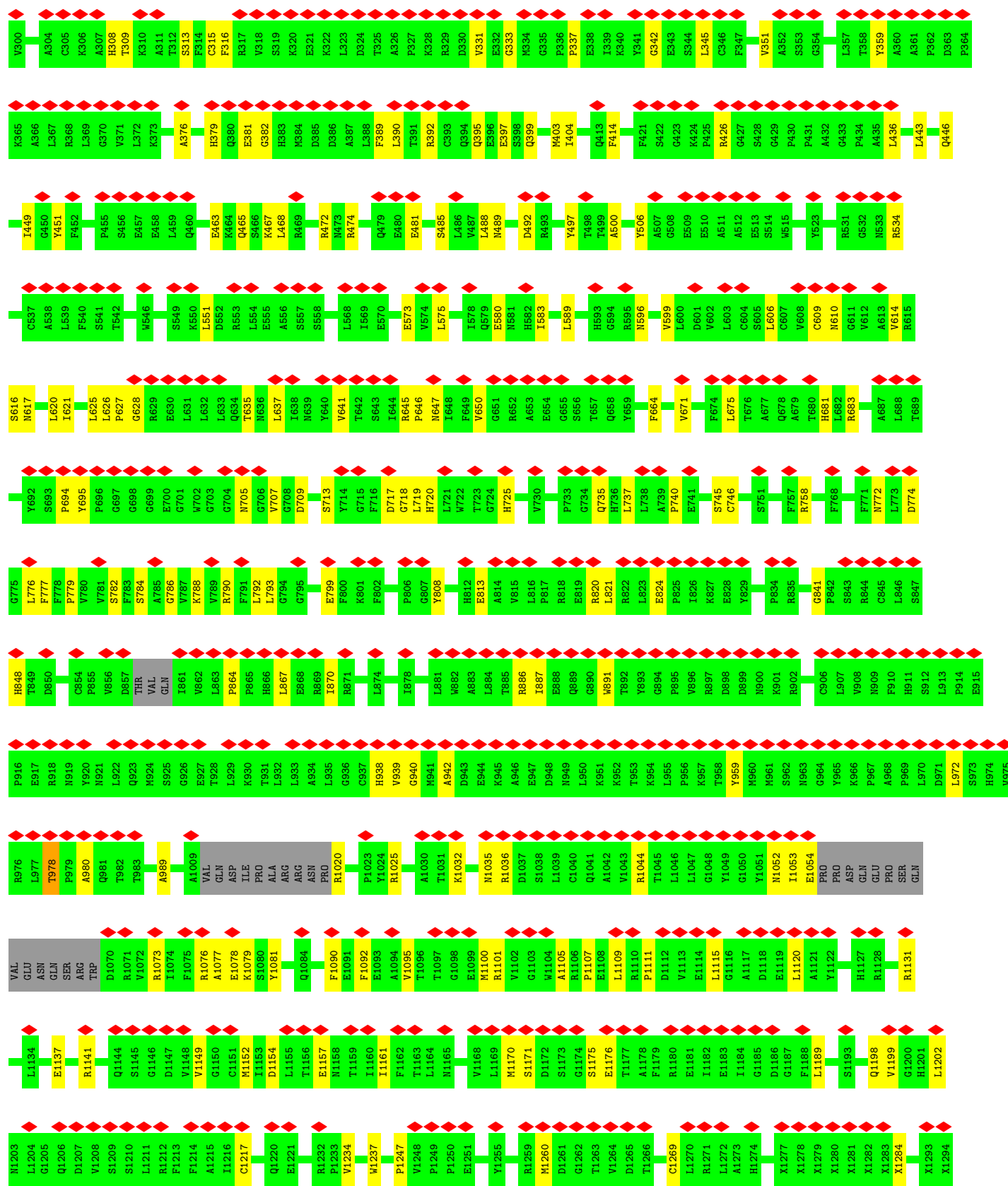






• Molecule 2: Ryanodine receptor 1

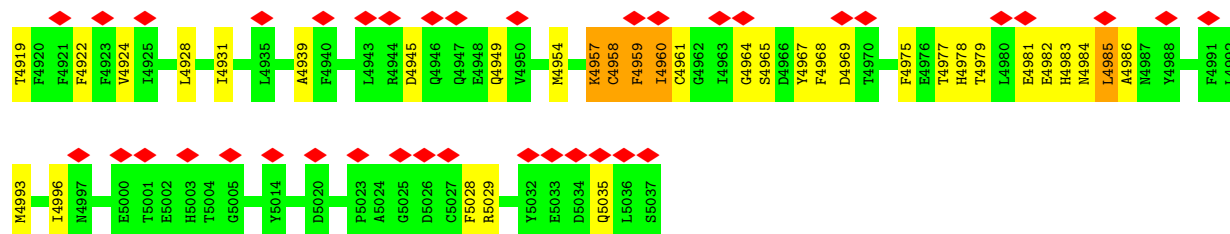




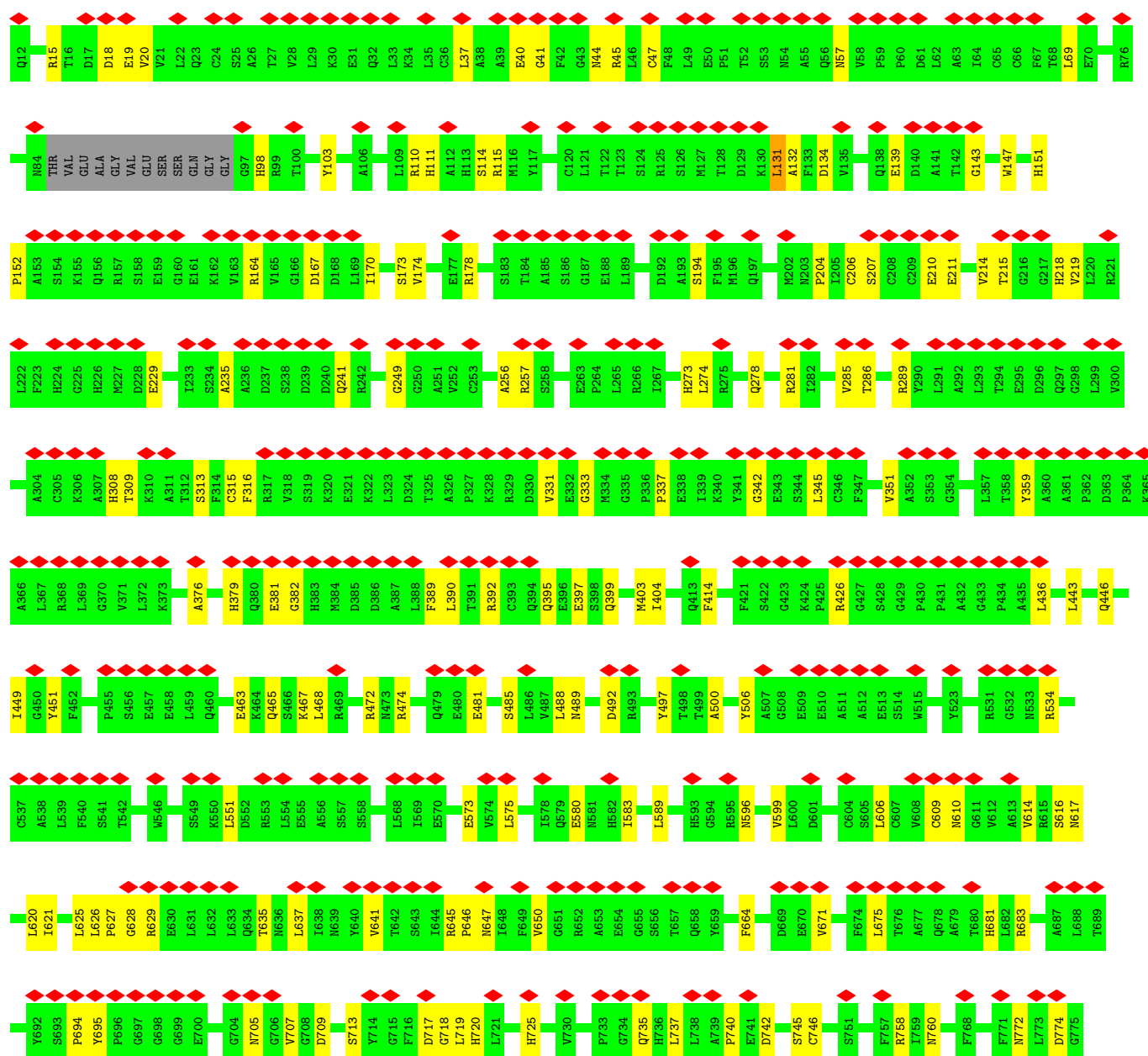
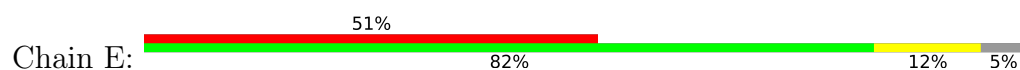


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X3535	X3432	X3372	X3312	X3246	X3175	X3038	X2952	K2890	E2830	K2770	X2680	X2582
X3536	X3433	X3373	X3313	X3247	X3176	X3039	X2953	K2891	GLU	I2771	X2681	X2583
X3537	X3434	X3374	X3314	X3248	X3177	X3040	X2954	K2892	ARG	Q2772	X2682	X2584
X3538	X3435	X3375	X3315	X3249	X3178	X3041	X2955	E2893	THR	Q2773	X2683	X2585
X3539	X3436	X3376	X3316	X3250	X3179	X3042	X2956	L2894	GLU	W2774	X2684	X2586
X3437	X3377	X3251	X3317	X3251	X3180	X3043	X2957	E2895	LYS	W2775	X2685	X2586
X3438	X3378	X3252	X3318	X3252	X3181	X3044	X2958	A2896	LYS	S2776	X2686	X2595
X3439	X3379	X3253	X3319	X3253	X3182	X3045	X2959	K2897	THR	Y2777	X2687	X2596
X3440	X3380	X3254	X3320	X3254	X3190	X3046	X2960	G2898	ARG	G2778	X2688	X2597
X3441	X3381	X3261	X3321	X3261	X3191	X3047	X2961	G2899	LYS	E2779	X2689	X2598
X3442	X3382	X3262	X3322	X3262	X3192	X3048	X2962	G2900	ILE		X2690	X2599
X3443	X3383	X3263	X3323	X3263	X3193	X3049	X2963	T2901	GLN	W2781	X2691	X2600
X3444	X3384	X3264	X3324	X3264	X3194	X3050	X2964	H2902	THR	D2782	X2692	X2601
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X3446	X3386	X3266	X3326	X3266	X3196	X3052	X2966	L2904	GLN	E2784	X2694	
X3447	X3387	X3267	X3327	X3267	X3197	X3053	X2967	L2905	THR	E2785	X2695	X2605
X3450	X3388	X3268	X3328	X3268	X3198	X3054	X2968	V2906	ASP	L2786	X2696	X2606
X3451	X3389	X3269	X3329	X3269	X3199	X3055	X2969	P2907	PRO	K2786	X2697	X2607
X3452	X3390	X3270	X3330	X3270	X3200	X3056	X2970	Y2908	ARG	T2787	X2698	
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X3454	X3392	X3272	X3332	X3272	X3202	X3058	X2972	T2910		M2789	X2700	X2618
X3455	X3393	X3273	X3333	X3273	X3203	X3059	X2973	L2911		M2790	X2701	X2619
X3456	X3394	X3274	X3334	X3274	X3204	X3060	X2974	L2912		L2791	X2702	X2620
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X3458	X3396	X3276	X3336	X3276	X3206	X3062	X2976	K2914		P2793	X2704	X2622
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X3468	X3406	X3286	X3346	X3286	X3216	X3072	X2986	Q2924		E2803	X2714	X2645
X3511	X3511	X3287	X3347	X3287	X3217	X3073	X2987	Q2925		I2804	X2715	X2646
X3512	X3512	X3288	X3348	X3288	X3218	X3074	X2988	L2926		K2806	X2716	X2647
X3513	X3513	X3289	X3349	X3289	X3219	X3075	X2989	L2927		W2807	X2717	X2648
X3514	X3514	X3290	X3350	X3290	X3220	X3076	X2990	K2928		P2808	X2718	X2649
X3515	X3515	X3291	X3351	X3291	X3221	X3077	X2991	A2929		E2749	X2719	X2650
X3516	X3516	X3292	X3352	X3292	X3222	X3078	X2992	F2929		K2750	X2651	X2652
X3517	X3517	X3293	X3353	X3293	X3223	X3079	X2993	L2930		L2751	X2653	X2654
X3518	X3518	X3294	X3354	X3294	X3224	X3080	X2994	Q2931		D2752	X2654	
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X3522	X3522	X3298	X3358	X3298	X3228	X3084	X2998	A2873		K2755	X2658	
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X3524	X3524	X3300	X3360	X3300	X3230	X3086	X3000	A2875		K2756	X2660	X2669
X3525	X3525	X3301	X3361	X3301	X3231	X3087	X3001	A2876		Y2757	X2670	X2670
X3526	X3526	X3302	X3362	X3302	X3232	X3088	X3002	Q2877		A2759	X2671	X2672
X3527	X3527	X3303	X3363	X3303	X3233	X3089	X3003	L2878		E2760	X2672	X2673
X3528	X3528	X3304	X3364	X3304	X3234	X3090	X3004	A2879		Y2761	X2673	X2674
X3529	X3529	X3305	X3365	X3305	X3235	X3091	X3005	E2880		T2762	X2674	X2677
X3530	X3530	X3306	X3366	X3306	X3236	X3092	X3006	N2881		H2763	X2675	
X3531	X3531	X3307	X3367	X3307	X3237	X3093	X3007	Y2882		E2764	X2676	
X3532	X3532	X3308	X3368	X3308	X3238	X3094	X3008	H2883		K2765	X2677	
		X3428	X3369	X3309	X3239	X3095	X3009	W2886		W2766	X2678	
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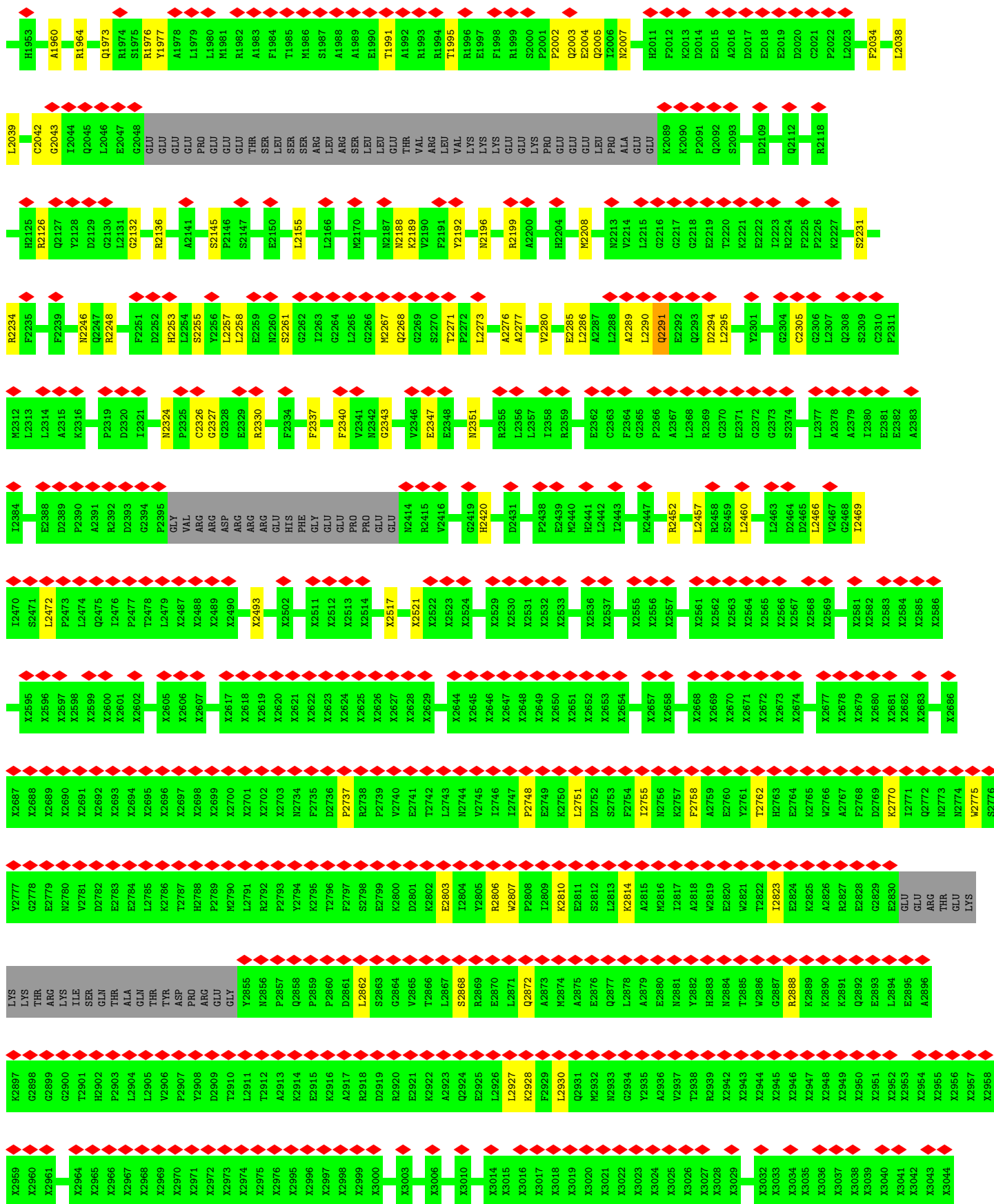




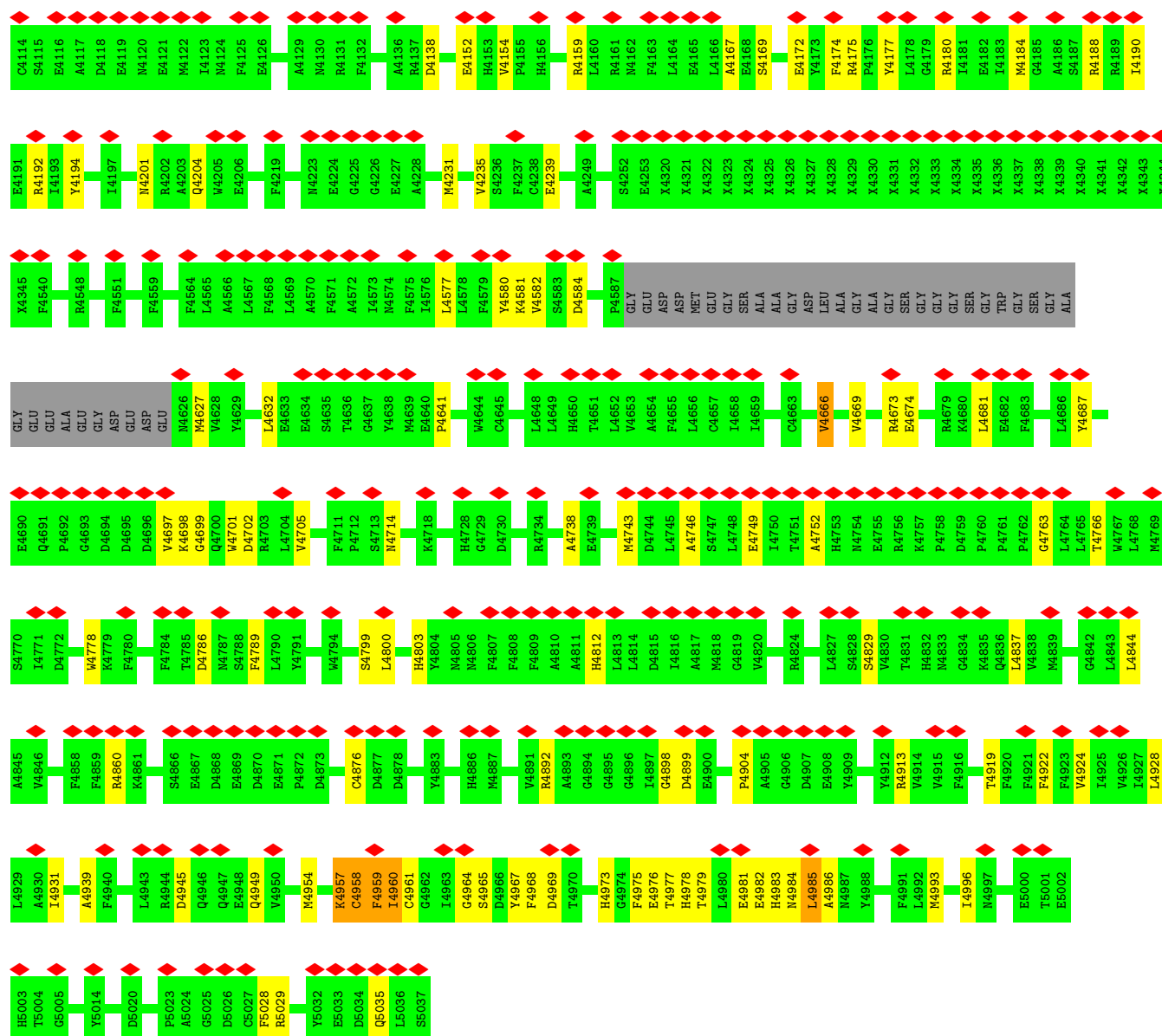
• Molecule 2: Ryanodine receptor 1



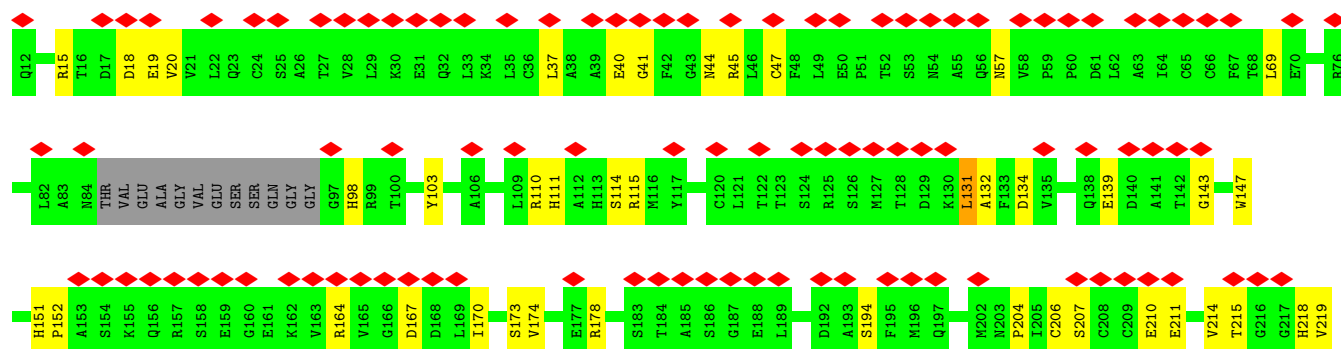
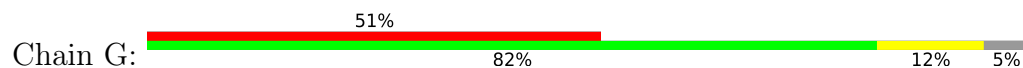
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GLU	A1796	R1727	E1651	X1551	X1446	S1210	Q1145	THR	T982	L922	V856	F778
GLU	R1797	R1728	L1653	X1554	X1447	L1211	G1146	D1070	T983	Q923	D857	P779
GLU	I1802	E1733	S1654	X1555	X1448	R1212	D1147	R1071	A989	N924	VAL	V780
GLU	P1803	Y1734	E1655	X1556	X1449	F1213	D1148	V1072	A1009	S925	GLN	V781
GLU	A1806	I1735	R1656	X1561	X1450	F1214	V1149	R1073	VAL	Q926	S783	S784
GLU	R1808	L1738	D1657	X1562	X1455	I1216	V1150	F1074	GLN	E927	A785	A785
GLU	L1812	T1739	L1659	X1567	X1458	C1217	G1151	R1075	ASP	T928	P864	K788
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GLU	L1815	T1742	H1663	X1577	X1474	P1233	L1155	S1080	ALA	L932	L867	F791
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ALA	V1840	L1762	D1690	L1614	X1516	R1271	I1182	D1112	T1045	K951	E890	R820
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		GLY			X1547	X1443		E1137	GLN	R976	E917	
		VAL			X1548	X1443		E1137	GLN	L977	R918	
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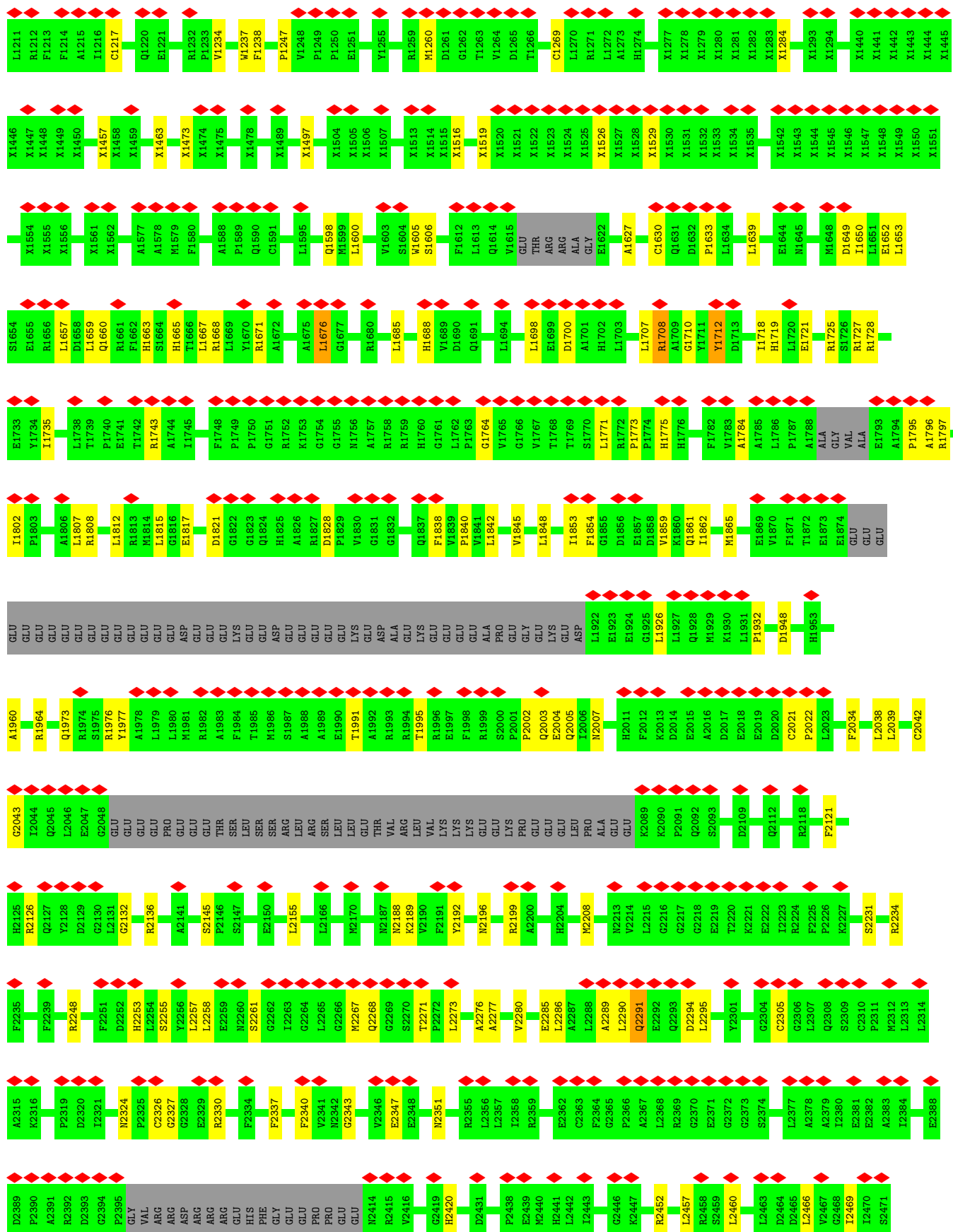
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	F3828	N3897	E3665	GLU	X3468	X3406	X3346	X3286	X3216	X3073
F3996	Q3829	H3895	D3666	GLU	X3469	X3407	X3347	X3287	X3217	X3074
A3997	Q3830	N3896	H3667	ALA	X3511	X3408	X3348	X3288	X3218	X3075
M4000	S3831	N3897	S3668	GLU	X3512	X3409	X3349	X3289	X3219	X3076
M4001	I3832	F3899	S3669	GLU	X3513	X3410	X3350	X3290	X3220	X3077
K4002	L3835	Q3900	E3670	E3747	X3514	X3411	X3351	X3291	X3221	X3078
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	G3857	L3770	E3690	L3770	X3530	X3427	X3367	X3307	X3237	X3094
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	V3859	T3772	E3691	T3772	X3532	X3429	X3369	X3309	X3239	X3096
	N3860	R3773	E3692	G3773	X3533	X3430	X3370	X3310	X3240	X3097
	G3774	A3775	K3693	A3775	X3534	X3431	X3371	X3311	X3241	X3098
	E3861	A3776	P3695	G3776	X3535	X3432	X3372	X3312	X3242	X3099
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• Molecule 2: Ryanodine receptor 1

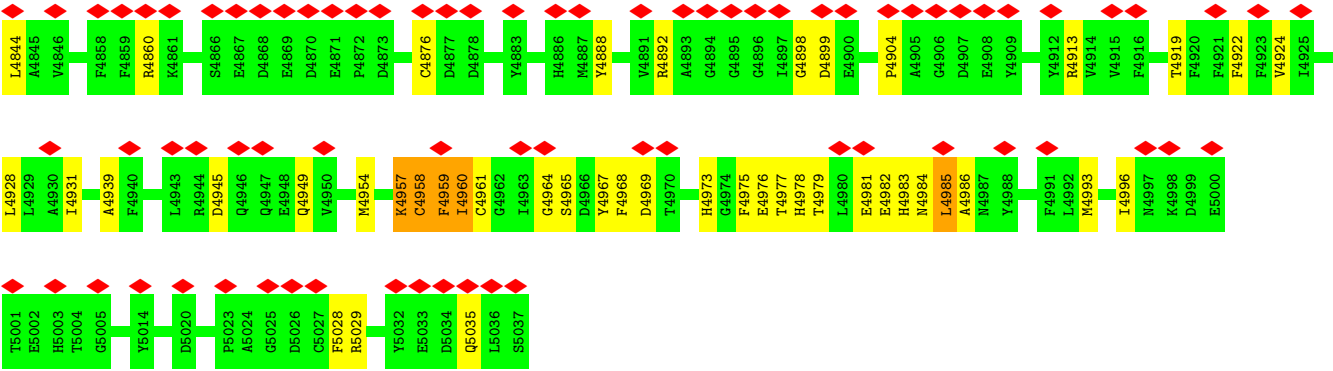






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4 Experimental information

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	0.076	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.032	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: CFF, ATP, 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	0.19	0/834	0.47	0/1123
1	F	0.19	0/834	0.46	0/1123
1	H	0.19	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.20	0/25424	0.52	4/34530 (0.0%)
2	E	0.20	0/25424	0.52	4/34530 (0.0%)
2	G	0.20	0/25424	0.52	4/34530 (0.0%)
2	I	0.20	0/25424	0.52	4/34530 (0.0%)
All	All	0.20	0/105032	0.51	16/142612 (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	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4958	CYS	CA-C-N	5.46	131.97	121.54
2	E	4958	CYS	C-N-CA	5.46	131.97	121.54
2	I	4958	CYS	CA-C-N	5.44	131.93	121.54
2	I	4958	CYS	C-N-CA	5.44	131.93	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4958	CYS	CA-C-N	5.43	131.91	121.54
2	B	4958	CYS	C-N-CA	5.43	131.91	121.54
2	G	4958	CYS	CA-C-N	5.43	131.91	121.54
2	G	4958	CYS	C-N-CA	5.43	131.91	121.54
2	I	2280	VAL	N-CA-C	-5.29	108.12	113.20
2	G	2280	VAL	N-CA-C	-5.29	108.12	113.20
2	B	2280	VAL	N-CA-C	-5.28	108.13	113.20
2	E	2280	VAL	N-CA-C	-5.28	108.14	113.20
2	B	131	LEU	CA-CB-CG	5.13	134.26	116.30
2	E	131	LEU	CA-CB-CG	5.13	134.25	116.30
2	I	131	LEU	CA-CB-CG	5.12	134.24	116.30
2	G	131	LEU	CA-CB-CG	5.12	134.22	116.30

There are no chirality outliers.

All (52) 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	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	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	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	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	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	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	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	19	0
1	F	818	0	824	20	0
1	H	818	0	824	16	0
1	J	818	0	824	17	0
2	B	29495	0	24734	325	0
2	E	29495	0	24734	324	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	29495	0	24734	323	0
2	I	29495	0	24734	327	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121436	0	102320	1341	0

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

All (1341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.60	0.90
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.60	0.90
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.60	0.89
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.60	0.89
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.86	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.75
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.75
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.86	0.74
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.54	0.72
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.72
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.54	0.72
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.54	0.71
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.54	0.70
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.70
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.75	0.69
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.75	0.69
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.75	0.69
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.69
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.81	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.81	0.68
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.81	0.68
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.75	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.77	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.67
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.77	0.66
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.66
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.77	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.66
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.78	0.66
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.78	0.65
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.78	0.65
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.77	0.65
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.77	0.65
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.78	0.65
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.77	0.65
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.77	0.64
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.79	0.64
2:E:331:VAL:HG12	2:E:333:GLY:H	1.62	0.64
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.62	0.64
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.62	0.64
2:G:331:VAL:HG12	2:G:333:GLY:H	1.62	0.64
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.79	0.64
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.79	0.64
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.78	0.64
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.62	0.63
2:I:173:SER:HB3	2:I:178:ARG:H	1.64	0.63
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.81	0.63
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.62	0.63
2:B:173:SER:HB3	2:B:178:ARG:H	1.64	0.63
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.79	0.63
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.81	0.63
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.81	0.63
2:G:173:SER:HB3	2:G:178:ARG:H	1.64	0.63
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.63
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.82	0.62
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.32	0.62
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.81	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.62	0.62
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.82	0.62
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.32	0.62
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.80	0.62
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.32	0.62
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.80	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.32	0.62
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.82	0.62
2:E:173:SER:HB3	2:E:178:ARG:H	1.64	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.80	0.62
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.82	0.62
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.82	0.62
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.82	0.62
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.82	0.61
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.81	0.61
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.81	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.62	0.61
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.82	0.61
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.33	0.61
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.33	0.61
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.82	0.61
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.83	0.61
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.83	0.61
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.83	0.61
2:E:4968:PHE:CZ	2:E:4978:HIS:HE1	2.19	0.61
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.83	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.33	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.34	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.84	0.60
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.34	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.83	0.60
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.83	0.60
2:B:313:SER:HB3	2:B:351:VAL:HB	1.84	0.60
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.35	0.60
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.83	0.59
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.83	0.59
2:E:313:SER:HB3	2:E:351:VAL:HB	1.84	0.59
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.83	0.59
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.83	0.59
2:I:4844:LEU:HD13	2:I:4928:LEU:HG	1.84	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.83	0.59
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.59
2:B:4844:LEU:HD13	2:B:4928:LEU:HG	1.85	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.19	0.59
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.35	0.59
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.84	0.59
1:F:6:THR:HA	1:F:72:ALA:HA	1.84	0.59
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.82	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.59
2:E:4844:LEU:HD13	2:E:4928:LEU:HG	1.85	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.35	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.84	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.59
2:G:4844:LEU:HD13	2:G:4928:LEU:HG	1.84	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.59
1:A:6:THR:HA	1:A:72:ALA:HA	1.84	0.59
1:J:6:THR:HA	1:J:72:ALA:HA	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.83	0.59
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.58
1:H:6:THR:HA	1:H:72:ALA:HA	1.84	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.35	0.58
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.36	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.85	0.58
2:E:4180:ARG:HH22	2:E:4981:GLU:HA	1.68	0.58
2:G:313:SER:HB3	2:G:351:VAL:HB	1.84	0.58
2:I:313:SER:HB3	2:I:351:VAL:HB	1.84	0.58
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.34	0.58
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:B:4190:ILE:HG21	2:B:5028:PHE:HA	1.86	0.58
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.85	0.57
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.36	0.57
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.34	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:I:4180:ARG:HH22	2:I:4981:GLU:HA	1.68	0.57
2:I:4190:ILE:HG21	2:I:5028:PHE:HA	1.86	0.57
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.38	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.87	0.57
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.87	0.57
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.85	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.36	0.57
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.87	0.57
2:G:4180:ARG:HH22	2:G:4981:GLU:HA	1.68	0.57
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.85	0.57
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.70	0.57
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.38	0.57
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.38	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.87	0.56
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.70	0.56
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.70	0.56
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.56
2:B:4180:ARG:HH22	2:B:4981:GLU:HA	1.68	0.56
2:E:4190:ILE:HG21	2:E:5028:PHE:HA	1.86	0.56
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.87	0.56
2:G:4945:ASP:O	2:G:4949:GLN:NE2	2.38	0.56
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.87	0.56
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.87	0.56
2:B:4945:ASP:O	2:B:4949:GLN:NE2	2.38	0.56
2:G:4190:ILE:HG21	2:G:5028:PHE:HA	1.86	0.56
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.87	0.56
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.38	0.56
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.39	0.56
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.71	0.56
2:I:4945:ASP:O	2:I:4949:GLN:NE2	2.38	0.56
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.38	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.71	0.56
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.38	0.56
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.87	0.56
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.87	0.56
1:F:27:THR:HB	1:F:100:ASP:HB3	1.88	0.56
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.88	0.56
2:I:4892:ARG:NH2	2:G:4899:ASP:OD1	2.39	0.56
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.87	0.56
2:E:4945:ASP:O	2:E:4949:GLN:NE2	2.38	0.56
1:J:27:THR:HB	1:J:100:ASP:HB3	1.88	0.56
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.70	0.56
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.71	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.87	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:HE1	2.19	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.88	0.56
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.88	0.55
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.88	0.55
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.87	0.55
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.88	0.55
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.71	0.55
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.88	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.71	0.55
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.71	0.55
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.71	0.55
1:A:27:THR:HB	1:A:100:ASP:HB3	1.88	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.88	0.55
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.89	0.55
2:G:621:ILE:O	2:G:625:LEU:N	2.40	0.55
2:G:4829:SER:HB2	2:G:4939:ALA:HB1	1.88	0.55
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.40	0.55
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.88	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.87	0.55
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.40	0.55
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.89	0.55
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.71	0.55
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.89	0.55
1:H:27:THR:HB	1:H:100:ASP:HB3	1.88	0.55
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.39	0.55
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.40	0.55
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.89	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.87	0.55
2:I:4829:SER:HB2	2:I:4939:ALA:HB1	1.88	0.55
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.40	0.55
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.88	0.55
2:G:4968:PHE:CZ	2:G:4978:HIS:HE1	2.19	0.55
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.89	0.55
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.89	0.55
2:E:621:ILE:O	2:E:625:LEU:N	2.40	0.55
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.89	0.55
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.81	0.55
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.89	0.55
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.89	0.55
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.38	0.55
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.72	0.55
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.40	0.55
2:I:4954:MET:HE3	3:I:5101:ATP:H1'	1.90	0.54
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.88	0.54
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.40	0.54
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.80	0.54
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.41	0.54
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.40	0.54
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.40	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.54
2:E:4829:SER:HB2	2:E:4939:ALA:HB1	1.88	0.54
2:G:4954:MET:HE3	3:G:5101:ATP:H1'	1.90	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.54
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.72	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.40	0.54
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.81	0.54
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.89	0.54
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.90	0.54
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.40	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.54
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.81	0.54
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.89	0.54
2:B:4829:SER:HB2	2:B:4939:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.90	0.54
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.40	0.54
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.40	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.54
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.89	0.54
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.40	0.54
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.89	0.54
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.88	0.54
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.41	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.54
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.54
2:E:4954:MET:HE3	3:E:5101:ATP:H1'	1.90	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.40	0.54
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.90	0.54
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.89	0.54
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.89	0.54
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.41	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.40	0.54
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.40	0.54
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.89	0.54
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.41	0.54
2:I:621:ILE:O	2:I:625:LEU:N	2.40	0.54
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.89	0.54
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.89	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.40	0.54
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.40	0.54
2:B:4954:MET:HE3	3:B:5101:ATP:H1'	1.90	0.54
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.90	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.90	0.54
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.40	0.54
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.40	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.90	0.54
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.89	0.54
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.54
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.89	0.54
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.90	0.54
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.54
2:B:621:ILE:O	2:B:625:LEU:N	2.40	0.54
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.90	0.54
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.41	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.41	0.53
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.53
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.89	0.53
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.90	0.53
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.89	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.41	0.53
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.90	0.53
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.41	0.53
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.89	0.53
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.53
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.53
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.90	0.53
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.42	0.53
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.90	0.53
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.89	0.53
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.90	0.53
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.73	0.53
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.90	0.53
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.90	0.53
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.91	0.53
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.73	0.53
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.89	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.42	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.91	0.53
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.72	0.53
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.42	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.73	0.53
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.53
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.91	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.90	0.53
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.91	0.53
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.90	0.53
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.42	0.53
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.72	0.53
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.53
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.53
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.92	0.52
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.90	0.52
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.90	0.52
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.90	0.52
2:I:1457:UNK:N	2:I:1497:UNK:O	2.43	0.52
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.91	0.52
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.91	0.52
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.91	0.52
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.91	0.52
2:E:1457:UNK:N	2:E:1497:UNK:O	2.43	0.52
2:G:645:ARG:N	2:G:824:GLU:O	2.41	0.52
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.42	0.52
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.40	0.52
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.52
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.41	0.52
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.90	0.52
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.91	0.52
2:B:1457:UNK:N	2:B:1497:UNK:O	2.43	0.52
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.90	0.52
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.91	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.52
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.92	0.52
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.52
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.90	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.91	0.52
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.41	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.52
1:H:11:ASP:OD1	1:H:67:SER:OG	2.28	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.52
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.83	0.52
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.92	0.52
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.91	0.52
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.52
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.91	0.52
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.73	0.52
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.52
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.90	0.52
1:F:11:ASP:OD1	1:F:67:SER:OG	2.28	0.52
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.52
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.42	0.52
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.83	0.52
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.43	0.52
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.90	0.52
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.51
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.92	0.51
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.51
2:B:4924:VAL:HA	2:B:4928:LEU:HD23	1.93	0.51
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.92	0.51
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.42	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.92	0.51
1:J:87:HIS:H	1:J:91:ILE:HB	1.75	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.92	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.29	0.51
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.51
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.51
1:F:87:HIS:H	1:F:91:ILE:HB	1.75	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.91	0.51
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.92	0.51
2:I:645:ARG:N	2:I:824:GLU:O	2.41	0.51
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.92	0.51
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	1.93	0.51
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.92	0.51
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.29	0.51
1:H:87:HIS:H	1:H:91:ILE:HB	1.75	0.51
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.92	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.51
2:I:241:GLN:O	2:I:289:ARG:NH1	2.38	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.76	0.51
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.43	0.51
2:G:1457:UNK:N	2:G:1497:UNK:O	2.43	0.51
1:A:87:HIS:H	1:A:91:ILE:HB	1.75	0.51
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.76	0.51
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.92	0.51
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.91	0.51
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.51
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.93	0.51
1:J:11:ASP:OD1	1:J:67:SER:OG	2.28	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.93	0.51
2:E:2758:PHE:O	2:E:2762:THR:N	2.44	0.51
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	1.93	0.51
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.51
2:I:4984:ASN:C	2:I:4986:ALA:H	2.20	0.50
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.93	0.50
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.93	0.50
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.93	0.50
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.93	0.50
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.76	0.50
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.93	0.50
2:E:4924:VAL:HA	2:E:4928:LEU:HD23	1.93	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.94	0.50
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.50
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.94	0.50
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.93	0.50
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.93	0.50
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.76	0.50
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	1.93	0.50
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.93	0.50
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.94	0.50
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.94	0.50
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.93	0.50
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.93	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.93	0.50
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.50
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.29	0.50
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.93	0.50
2:G:647:ASN:ND2	2:G:820:ARG:O	2.43	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.94	0.50
2:B:4984:ASN:C	2:B:4986:ALA:H	2.20	0.50
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.50
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.94	0.50
2:E:647:ASN:ND2	2:E:820:ARG:O	2.43	0.50
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4924:VAL:HA	2:G:4928:LEU:HD23	1.93	0.50
1:J:21:THR:HA	1:J:49:ARG:HA	1.93	0.50
2:B:647:ASN:ND2	2:B:820:ARG:O	2.43	0.50
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.94	0.50
1:A:11:ASP:OD1	1:A:67:SER:OG	2.28	0.50
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.93	0.50
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.94	0.50
2:E:2290:LEU:HB3	2:E:3849:ARG:HH12	1.77	0.50
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.93	0.50
2:G:4984:ASN:C	2:G:4986:ALA:H	2.20	0.50
2:B:776:LEU:HG	2:B:848:HIS:HA	1.94	0.50
2:B:2290:LEU:HB3	2:B:3849:ARG:HH12	1.77	0.50
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.94	0.50
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.94	0.50
2:I:315:CYS:SG	2:I:316:PHE:N	2.85	0.50
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.45	0.50
2:G:241:GLN:O	2:G:289:ARG:NH1	2.38	0.50
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.45	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.83	0.50
1:H:21:THR:HA	1:H:49:ARG:HA	1.93	0.49
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.93	0.49
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.93	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.34	0.49
2:I:4924:VAL:HA	2:I:4928:LEU:HD23	1.93	0.49
2:E:645:ARG:N	2:E:824:GLU:O	2.41	0.49
2:E:3766:GLN:O	2:E:3770:LEU:N	2.45	0.49
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.94	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.49
2:B:315:CYS:SG	2:B:316:PHE:N	2.85	0.49
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.45	0.49
2:E:485:SER:O	2:E:489:ASN:N	2.40	0.49
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.94	0.49
2:E:4898:GLY:O	2:G:4892:ARG:NH2	2.45	0.49
2:G:2290:LEU:HB3	2:G:3849:ARG:HH12	1.77	0.49
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.94	0.49
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.93	0.49
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.94	0.49
2:E:315:CYS:SG	2:E:316:PHE:N	2.85	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.41	0.49
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.93	0.49
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2758:PHE:O	2:B:2762:THR:N	2.44	0.49
2:B:4928:LEU:HD13	2:B:4931:ILE:HD12	1.93	0.49
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.94	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.94	0.49
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.45	0.49
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.94	0.49
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.46	0.49
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.93	0.49
2:B:2255:SER:HA	2:B:2258:LEU:HB3	1.94	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.43	0.49
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.95	0.49
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.78	0.49
2:B:4965:SER:O	2:B:4969:ASP:N	2.45	0.49
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.94	0.49
2:I:2290:LEU:HB3	2:I:3849:ARG:HH12	1.77	0.49
2:I:4965:SER:O	2:I:4969:ASP:N	2.45	0.49
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.93	0.49
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.94	0.49
2:G:4965:SER:O	2:G:4969:ASP:N	2.45	0.49
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.94	0.49
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.94	0.49
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.86	0.49
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.94	0.49
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.45	0.49
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.93	0.49
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.45	0.49
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.93	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.49
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.78	0.49
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.45	0.49
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.94	0.49
2:B:3766:GLN:O	2:B:3770:LEU:N	2.45	0.49
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.93	0.49
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.94	0.49
2:E:485:SER:HA	2:E:488:LEU:HB2	1.95	0.49
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.95	0.49
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.83	0.49
2:E:2255:SER:HA	2:E:2258:LEU:HB3	1.94	0.49
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:485:SER:HA	2:G:488:LEU:HB2	1.95	0.49
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.49
2:G:2255:SER:HA	2:G:2258:LEU:HB3	1.94	0.49
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.49
2:I:2255:SER:HA	2:I:2258:LEU:HB3	1.94	0.49
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.86	0.49
2:I:4892:ARG:NH2	2:G:4898:GLY:O	2.46	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:G:315:CYS:SG	2:G:316:PHE:N	2.85	0.49
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.94	0.48
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.93	0.48
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.31	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.48
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.86	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.94	0.48
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.46	0.48
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.86	0.48
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.93	0.48
2:B:614:VAL:HG22	2:B:616:SER:H	1.78	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.48
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.46	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.95	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.94	0.48
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.78	0.48
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.48
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.45	0.48
2:B:1284:UNK:HA	2:B:1463:UNK:HA	1.96	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:I:485:SER:HA	2:I:488:LEU:HB2	1.95	0.48
2:I:1865:MET:SD	2:I:1865:MET:N	2.86	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.46	0.48
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.94	0.48
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.96	0.48
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.94	0.48
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.95	0.48
2:E:4984:ASN:C	2:E:4986:ALA:H	2.20	0.48
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.31	0.48
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.95	0.48
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.94	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.94	0.48
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.94	0.48
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.48
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.45	0.48
2:B:241:GLN:O	2:B:289:ARG:NH1	2.38	0.48
2:I:647:ASN:ND2	2:I:820:ARG:O	2.43	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.94	0.48
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.46	0.48
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.94	0.48
2:E:1865:MET:SD	2:E:1865:MET:N	2.87	0.48
2:E:4919:THR:HA	2:E:4922:PHE:HD2	1.79	0.48
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.96	0.48
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.47	0.48
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.95	0.48
2:E:614:VAL:HG22	2:E:616:SER:H	1.78	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.95	0.48
2:G:4800:LEU:HA	2:G:4803:HIS:HD2	1.79	0.48
2:I:614:VAL:HG22	2:I:616:SER:H	1.78	0.48
2:I:1516:UNK:N	2:I:1529:UNK:O	2.46	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.48
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.95	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:B:1865:MET:SD	2:B:1865:MET:N	2.87	0.48
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.48
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.95	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.47	0.48
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.96	0.48
2:G:4919:THR:HA	2:G:4922:PHE:HD2	1.79	0.48
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.95	0.48
2:I:1284:UNK:HA	2:I:1463:UNK:HA	1.96	0.48
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.96	0.48
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.96	0.47
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.96	0.47
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.46	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:614:VAL:HG22	2:G:616:SER:H	1.78	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.47
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.31	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.47
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.41	0.47
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.96	0.47
2:I:1105:ALA:N	2:I:1189:LEU:O	2.48	0.47
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.42	0.47
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.96	0.47
2:E:1284:UNK:HA	2:E:1463:UNK:HA	1.96	0.47
2:E:4965:SER:O	2:E:4969:ASP:N	2.45	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.47	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.96	0.47
2:B:4919:THR:HA	2:B:4922:PHE:HD2	1.79	0.47
2:B:4960:ILE:HD13	2:B:4960:ILE:H	1.79	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.47
2:I:4919:THR:HA	2:I:4922:PHE:HD2	1.79	0.47
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.96	0.47
2:E:4800:LEU:HA	2:E:4803:HIS:HD2	1.79	0.47
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.96	0.47
2:B:485:SER:HA	2:B:488:LEU:HB2	1.95	0.47
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.96	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.80	0.47
2:G:1865:MET:SD	2:G:1865:MET:N	2.87	0.47
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.96	0.47
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.49	0.47
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.97	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.47	0.47
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.79	0.47
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.47
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.47
2:I:3766:GLN:O	2:I:3770:LEU:N	2.45	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.47
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.78	0.47
2:B:488:LEU:O	2:B:492:ASP:N	2.45	0.47
2:B:1105:ALA:N	2:B:1189:LEU:O	2.48	0.47
2:B:4800:LEU:HA	2:B:4803:HIS:HD2	1.79	0.47
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.95	0.47
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.96	0.47
2:I:2758:PHE:O	2:I:2762:THR:N	2.44	0.47
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.47	0.47
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.49	0.47
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.97	0.47
2:G:1284:UNK:HA	2:G:1463:UNK:HA	1.96	0.47
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.79	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.49	0.47
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.80	0.47
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.97	0.47
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.47	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:I:4800:LEU:HA	2:I:4803:HIS:HD2	1.79	0.47
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.49	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.96	0.47
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.96	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.48	0.47
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.47
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.97	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.48	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.97	0.47
2:G:151:HIS:HB2	2:G:170:ILE:HB	1.97	0.47
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.96	0.47
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.47
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.96	0.47
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.96	0.47
2:B:3840:SER:O	2:B:3922:TYR:OH	2.33	0.47
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.96	0.47
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.80	0.47
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.31	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.46	0.47
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.96	0.47
2:E:151:HIS:HB2	2:E:170:ILE:HB	1.97	0.47
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.49	0.47
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.80	0.47
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.96	0.47
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.96	0.46
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.49	0.46
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.97	0.46
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.97	0.46
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.48	0.46
2:G:4960:ILE:HD13	2:G:4960:ILE:H	1.79	0.46
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.97	0.46
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.80	0.46
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.47	0.46
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.96	0.46
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.96	0.46
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.97	0.46
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.46
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.42	0.46
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.98	0.46
2:I:151:HIS:HB2	2:I:170:ILE:HB	1.97	0.46
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.48	0.46
2:I:4960:ILE:CD1	2:I:4985:LEU:HD23	2.46	0.46
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.80	0.46
2:E:241:GLN:O	2:E:289:ARG:NH1	2.38	0.46
2:E:488:LEU:O	2:E:492:ASP:N	2.45	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.41	0.46
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.98	0.46
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.46
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.97	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.80	0.46
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.98	0.46
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.96	0.46
2:I:3767:GLN:HA	2:I:3770:LEU:HB2	1.97	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.97	0.46
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.98	0.46
2:E:1105:ALA:N	2:E:1189:LEU:O	2.48	0.46
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.47	0.46
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.97	0.46
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.97	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.96	0.46
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.48	0.46
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.98	0.46
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.98	0.46
2:I:3953:LYS:O	2:I:3956:SER:OG	2.32	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.47	0.46
2:E:2347:GLU:O	2:E:2351:ASN:N	2.34	0.46
2:E:3840:SER:O	2:E:3922:TYR:OH	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.97	0.46
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.97	0.46
2:B:151:HIS:HB2	2:B:170:ILE:HB	1.97	0.46
2:I:342:GLY:N	2:I:390:LEU:O	2.49	0.46
2:E:342:GLY:N	2:E:390:LEU:O	2.49	0.46
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.97	0.46
2:G:4960:ILE:CD1	2:G:4985:LEU:HD23	2.46	0.46
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.98	0.46
2:E:4960:ILE:CD1	2:E:4985:LEU:HD23	2.46	0.46
2:G:3766:GLN:O	2:G:3770:LEU:N	2.45	0.46
2:G:3840:SER:O	2:G:3922:TYR:OH	2.33	0.46
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.79	0.46
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.97	0.46
2:G:488:LEU:O	2:G:492:ASP:N	2.45	0.46
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.97	0.45
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.98	0.45
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.45
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.79	0.45
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.81	0.45
2:I:4799:SER:HA	2:I:4812:HIS:HE1	1.82	0.45
2:E:2868:SER:O	2:E:2872:GLN:N	2.43	0.45
2:E:3767:GLN:HA	2:E:3770:LEU:HB2	1.98	0.45
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.81	0.45
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.80	0.45
2:G:3767:GLN:HA	2:G:3770:LEU:HB2	1.97	0.45
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.97	0.45
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.97	0.45
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.98	0.45
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.98	0.45
2:B:4960:ILE:CD1	2:B:4985:LEU:HD23	2.46	0.45
2:I:446:GLN:HA	2:I:449:ILE:HD12	1.99	0.45
2:I:790:ARG:HG2	2:I:1627:ALA:HA	1.98	0.45
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.98	0.45
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.81	0.45
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.97	0.45
2:B:940:GLY:O	2:B:1052:ASN:N	2.50	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.99	0.45
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.48	0.45
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.97	0.45
2:B:3953:LYS:O	2:B:3956:SER:OG	2.32	0.45
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4799:SER:HA	2:B:4812:HIS:HE1	1.82	0.45
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.96	0.45
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.81	0.45
2:G:1707:LEU:HG	2:G:1708:ARG:HG3	1.98	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.99	0.45
2:G:4888:TYR:O	2:G:4892:ARG:NE	2.39	0.45
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.46	0.45
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.82	0.45
2:I:359:TYR:HA	2:I:376:ALA:HA	1.98	0.45
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.45
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.45
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.99	0.45
2:G:4799:SER:HA	2:G:4812:HIS:HE1	1.82	0.45
2:B:1707:LEU:HG	2:B:1708:ARG:HG3	1.98	0.45
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.99	0.45
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.97	0.45
2:E:446:GLN:HA	2:E:449:ILE:HD12	1.99	0.45
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.98	0.45
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.82	0.45
2:I:940:GLY:O	2:I:1052:ASN:N	2.50	0.45
2:I:1707:LEU:HG	2:I:1708:ARG:HG3	1.98	0.45
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.98	0.45
2:E:940:GLY:O	2:E:1052:ASN:N	2.50	0.45
2:E:2132:GLY:O	2:E:2136:ARG:N	2.50	0.45
2:G:342:GLY:N	2:G:390:LEU:O	2.49	0.45
2:G:446:GLN:HA	2:G:449:ILE:HD12	1.99	0.45
2:B:3767:GLN:HA	2:B:3770:LEU:HB2	1.98	0.45
2:I:1663:HIS:NE2	2:I:1711:TYR:OH	2.39	0.45
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.98	0.45
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.81	0.45
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.97	0.45
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.45
2:E:1090:PHE:HD2	2:E:1202:LEU:HD11	1.82	0.45
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.99	0.45
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.98	0.45
2:B:446:GLN:HA	2:B:449:ILE:HD12	1.99	0.45
2:B:790:ARG:HG2	2:B:1627:ALA:HA	1.98	0.45
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.45
2:B:2347:GLU:O	2:B:2351:ASN:N	2.34	0.45
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.41	0.45
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:606:LEU:O	2:E:617:ASN:ND2	2.50	0.45
2:E:790:ARG:HG2	2:E:1627:ALA:HA	1.98	0.45
2:G:790:ARG:HG2	2:G:1627:ALA:HA	1.98	0.45
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.98	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.45
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.81	0.45
2:G:4702:ASP:HA	2:G:4778:TRP:HE1	1.82	0.45
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.45
2:B:342:GLY:N	2:B:390:LEU:O	2.49	0.44
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.99	0.44
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.99	0.44
2:B:4888:TYR:O	2:B:4892:ARG:NE	2.39	0.44
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.81	0.44
2:I:4702:ASP:HA	2:I:4778:TRP:HE1	1.82	0.44
2:E:359:TYR:HA	2:E:376:ALA:HA	1.98	0.44
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.99	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.99	0.44
2:G:1105:ALA:N	2:G:1189:LEU:O	2.47	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.44
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.98	0.44
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.53	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.81	0.44
2:I:4174:PHE:HA	2:I:4177:TYR:HD2	1.83	0.44
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.98	0.44
2:E:4799:SER:HA	2:E:4812:HIS:HE1	1.82	0.44
2:G:940:GLY:O	2:G:1052:ASN:N	2.50	0.44
2:B:359:TYR:HA	2:B:376:ALA:HA	1.98	0.44
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.83	0.44
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.86	0.44
2:I:1090:PHE:HD2	2:I:1202:LEU:HD11	1.82	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.91	0.44
2:E:3695:PRO:HB2	2:E:3700:GLN:HG3	2.00	0.44
2:E:4174:PHE:HA	2:E:4177:TYR:HD2	1.83	0.44
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.53	0.44
2:G:4174:PHE:HA	2:G:4177:TYR:HD2	1.83	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.91	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.42	0.44
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.83	0.44
2:B:3695:PRO:HB2	2:B:3700:GLN:HG3	2.00	0.44
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.81	0.44
2:B:4702:ASP:HA	2:B:4778:TRP:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1707:LEU:HG	2:E:1708:ARG:HG3	1.98	0.44
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.44
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.86	0.44
2:G:4231:MET:HE1	2:G:4960:ILE:HA	2.00	0.44
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.98	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.99	0.44
2:I:3695:PRO:HB2	2:I:3700:GLN:HG3	2.00	0.44
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.47	0.44
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.83	0.44
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.44
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.46	0.44
2:G:606:LEU:O	2:G:617:ASN:ND2	2.50	0.44
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	2.00	0.44
2:B:485:SER:O	2:B:489:ASN:N	2.40	0.44
2:I:606:LEU:O	2:I:617:ASN:ND2	2.50	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.83	0.44
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.99	0.44
2:I:2034:PHE:O	2:I:2038:LEU:N	2.51	0.44
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.83	0.44
2:E:709:ASP:HA	2:E:725:HIS:H	1.82	0.44
2:E:2034:PHE:O	2:E:2038:LEU:N	2.51	0.44
2:E:4702:ASP:HA	2:E:4778:TRP:HE1	1.82	0.44
2:G:359:TYR:HA	2:G:376:ALA:HA	1.98	0.44
2:G:2868:SER:O	2:G:2872:GLN:N	2.43	0.44
2:G:3695:PRO:HB2	2:G:3700:GLN:HG3	2.00	0.44
2:G:4201:ASN:ND2	2:G:4204:GLN:OE1	2.48	0.44
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.44
2:I:4201:ASN:ND2	2:I:4204:GLN:OE1	2.48	0.44
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	2.00	0.44
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.86	0.44
2:B:606:LEU:O	2:B:617:ASN:ND2	2.50	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.99	0.44
2:B:3766:GLN:HA	2:B:3769:ARG:HG2	2.00	0.44
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.99	0.44
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.50	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.00	0.44
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.37	0.44
2:E:1659:LEU:O	2:E:1663:HIS:N	2.47	0.44
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.44
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.00	0.44
2:G:2347:GLU:O	2:G:2351:ASN:N	2.34	0.44
2:B:215:THR:HG22	2:B:273:HIS:HA	2.00	0.44
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.46	0.44
2:B:645:ARG:N	2:B:824:GLU:O	2.41	0.44
2:B:709:ASP:HA	2:B:725:HIS:H	1.82	0.44
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.82	0.44
2:I:1663:HIS:O	2:I:1667:LEU:N	2.50	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.99	0.44
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.83	0.44
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.44
2:G:1090:PHE:HD2	2:G:1202:LEU:HD11	1.82	0.44
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.50	0.44
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.83	0.44
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	2.00	0.43
2:B:4993:MET:HA	2:B:4996:ILE:HB	2.00	0.43
2:I:3840:SER:O	2:I:3922:TYR:OH	2.33	0.43
2:I:4960:ILE:HD13	2:I:4960:ILE:H	1.79	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.83	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.43
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.99	0.43
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.00	0.43
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	2.00	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.36	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.91	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.99	0.43
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.37	0.43
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.43
2:I:3817:LEU:HD22	2:I:3899:PHE:HB2	2.00	0.43
2:I:4977:THR:HG22	2:I:4981:GLU:HB2	2.01	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.43
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.00	0.43
2:E:4231:MET:HE1	2:E:4960:ILE:HA	2.00	0.43
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.43
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.36	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.00	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.99	0.43
2:I:2517:UNK:O	2:I:2521:UNK:N	2.52	0.43
2:I:4231:MET:HE1	2:I:4960:ILE:HA	2.00	0.43
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.36	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.91	0.43
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.83	0.43
2:B:41:GLY:O	2:B:45:ARG:NH1	2.52	0.43
2:B:4174:PHE:HA	2:B:4177:TYR:HD2	1.83	0.43
2:I:709:ASP:HA	2:I:725:HIS:H	1.82	0.43
2:I:2039:LEU:HA	2:I:2042:CYS:HB3	2.01	0.43
2:I:3766:GLN:HA	2:I:3769:ARG:HG2	2.00	0.43
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.36	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.00	0.43
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.43
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.82	0.43
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.00	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.83	0.43
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	2.01	0.43
2:B:1817:GLU:O	2:B:1821:ASP:N	2.51	0.43
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.84	0.43
2:I:164:ARG:N	2:I:167:ASP:OD2	2.52	0.43
2:I:1154:ASP:HB3	2:I:1157:GLU:HB3	2.01	0.43
2:I:4904:PRO:HB3	2:I:4913:ARG:HD2	2.00	0.43
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.99	0.43
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	2.01	0.43
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.43
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.01	0.43
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.42	0.43
2:E:4977:THR:HG22	2:E:4981:GLU:HB2	2.01	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.84	0.43
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.41	0.43
2:G:3766:GLN:HA	2:G:3769:ARG:HG2	2.00	0.43
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.47	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.00	0.43
2:G:4977:THR:HG22	2:G:4981:GLU:HB2	2.01	0.43
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.01	0.43
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.89	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:B:3817:LEU:HD22	2:B:3899:PHE:HB2	2.00	0.43
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.83	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.43
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.43
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	2.01	0.43
2:E:41:GLY:O	2:E:45:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.99	0.43
2:E:2517:UNK:O	2:E:2521:UNK:N	2.52	0.43
2:G:1154:ASP:HB3	2:G:1157:GLU:HB3	2.01	0.43
2:G:2132:GLY:O	2:G:2136:ARG:N	2.50	0.43
2:G:4180:ARG:HH11	2:G:4192:ARG:HH12	1.67	0.43
2:G:4904:PRO:HB3	2:G:4913:ARG:HD2	2.00	0.43
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.01	0.43
2:B:1154:ASP:HB3	2:B:1157:GLU:HB3	2.01	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.43
2:I:1817:GLU:O	2:I:1821:ASP:N	2.51	0.43
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.86	0.43
2:E:215:THR:HG22	2:E:273:HIS:HA	2.00	0.43
2:E:4993:MET:HA	2:E:4996:ILE:HB	2.00	0.43
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	2.01	0.43
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.00	0.43
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	2.00	0.43
1:H:7:ILE:N	1:H:71:ARG:O	2.49	0.43
2:B:2517:UNK:O	2:B:2521:UNK:N	2.52	0.43
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.01	0.43
2:B:4180:ARG:HH11	2:B:4192:ARG:HH12	1.67	0.43
2:B:4231:MET:HE1	2:B:4960:ILE:HA	2.00	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.52	0.43
2:I:215:THR:HG22	2:I:273:HIS:HA	2.00	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.00	0.43
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.00	0.43
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.83	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:1663:HIS:O	2:E:1667:LEU:N	2.50	0.43
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	2.01	0.43
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	2.00	0.43
2:G:2517:UNK:O	2:G:2521:UNK:N	2.52	0.43
1:F:7:ILE:N	1:F:71:ARG:O	2.49	0.43
2:B:164:ARG:N	2:B:167:ASP:OD2	2.52	0.43
2:B:4958:CYS:HB2	3:B:5101:ATP:N6	2.34	0.43
2:B:4977:THR:HG22	2:B:4981:GLU:HB2	2.01	0.43
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	2.00	0.43
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.00	0.43
2:I:4958:CYS:HB2	3:I:5101:ATP:N6	2.34	0.43
2:E:164:ARG:N	2:E:167:ASP:OD2	2.52	0.43
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.01	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.01	0.43
2:E:4904:PRO:HB3	2:E:4913:ARG:HD2	2.00	0.43
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.01	0.43
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.43
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.43
2:G:4958:CYS:HB2	3:G:5101:ATP:N6	2.34	0.43
2:G:4967:TYR:HE2	2:G:5029:ARG:HG3	1.84	0.43
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.01	0.43
2:B:2132:GLY:O	2:B:2136:ARG:N	2.50	0.43
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.47	0.43
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.84	0.43
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:1269:CYS:HA	2:I:1473:UNK:HA	2.01	0.43
2:I:4967:TYR:HE2	2:I:5029:ARG:HG3	1.84	0.43
2:E:1154:ASP:HB3	2:E:1157:GLU:HB3	2.01	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:E:4180:ARG:HH11	2:E:4192:ARG:HH12	1.67	0.43
2:G:41:GLY:O	2:G:45:ARG:NH1	2.52	0.43
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.01	0.43
2:G:1659:LEU:O	2:G:1663:HIS:N	2.47	0.43
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.01	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.42
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.01	0.42
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.00	0.42
2:I:488:LEU:O	2:I:492:ASP:N	2.45	0.42
2:I:4180:ARG:HH11	2:I:4192:ARG:HH12	1.67	0.42
2:I:4236:SER:HG	2:I:4675:LYS:HZ1	1.59	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:2039:LEU:HA	2:E:2042:CYS:HB3	2.01	0.42
2:E:3766:GLN:HA	2:E:3769:ARG:HG2	2.00	0.42
2:E:4958:CYS:HB2	3:E:5101:ATP:N6	2.34	0.42
2:G:164:ARG:N	2:G:167:ASP:OD2	2.52	0.42
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.42
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.99	0.42
2:G:2039:LEU:HA	2:G:2042:CYS:HB3	2.01	0.42
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.84	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.00	0.42
2:I:2132:GLY:O	2:I:2136:ARG:N	2.50	0.42
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4959:PHE:HD2	2:I:4960:ILE:HD13	1.84	0.42
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.83	0.42
2:G:3817:LEU:HD22	2:G:3899:PHE:HB2	2.00	0.42
2:G:4183:ILE:O	2:G:4191:GLU:N	2.43	0.42
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:4904:PRO:HB3	2:B:4913:ARG:HD2	2.00	0.42
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.84	0.42
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.01	0.42
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.01	0.42
2:I:4960:ILE:HD12	2:I:4985:LEU:HD23	2.02	0.42
2:I:4993:MET:HA	2:I:4996:ILE:HB	2.00	0.42
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	2.00	0.42
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.54	0.42
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	2.00	0.42
2:E:4960:ILE:HD13	2:E:4960:ILE:H	1.79	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.84	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.85	0.42
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.99	0.42
2:B:2034:PHE:O	2:B:2038:LEU:N	2.51	0.42
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	2.01	0.42
2:B:4951:LYS:HE2	2:B:4951:LYS:HB3	1.91	0.42
2:B:4959:PHE:HD2	2:B:4960:ILE:HD13	1.84	0.42
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	2.00	0.42
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.42
2:G:709:ASP:HA	2:G:725:HIS:H	1.83	0.42
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	2.00	0.42
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.01	0.42
2:B:2039:LEU:HA	2:B:2042:CYS:HB3	2.01	0.42
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.01	0.42
2:B:2868:SER:O	2:B:2872:GLN:N	2.43	0.42
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.01	0.42
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.54	0.42
2:E:1131:ARG:N	2:E:1137:GLU:O	2.53	0.42
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.00	0.42
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.02	0.42
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.42
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.85	0.42
2:E:1077:ALA:HB1	2:E:1234:VAL:HG11	2.02	0.42
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.42
2:G:4959:PHE:HD2	2:G:4960:ILE:HD13	1.84	0.42
2:G:4993:MET:HA	2:G:4996:ILE:HB	2.00	0.42
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	2.02	0.42
2:B:256:ALA:HB1	2:B:286:THR:HG21	2.02	0.42
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.84	0.42
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.02	0.42
2:E:3817:LEU:HD22	2:E:3899:PHE:HB2	2.00	0.42
2:G:2034:PHE:O	2:G:2038:LEU:N	2.51	0.42
2:G:4826:ILE:O	2:G:4829:SER:OG	2.33	0.42
1:F:40:ARG:NH2	2:E:675:LEU:O	2.52	0.42
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.02	0.42
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	2.00	0.42
2:E:256:ALA:HB1	2:E:286:THR:HG21	2.02	0.42
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	2.02	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.42
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.00	0.42
2:E:4201:ASN:ND2	2:E:4204:GLN:OE1	2.48	0.42
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.02	0.42
2:G:1171:SER:OG	2:G:1175:SER:N	2.46	0.42
2:G:1817:GLU:O	2:G:1821:ASP:N	2.51	0.42
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.01	0.42
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	2.02	0.42
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.41	0.42
2:B:2810:LYS:O	2:B:2814:LYS:N	2.48	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.54	0.42
2:I:2021:CYS:HA	2:I:2022:PRO:HD3	1.93	0.42
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.01	0.42
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.85	0.42
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.82	0.42
1:A:40:ARG:NH2	2:B:675:LEU:O	2.52	0.42
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.85	0.42
2:B:4697:VAL:O	2:B:4701:TRP:N	2.53	0.42
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.02	0.42
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.85	0.42
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.00	0.42
2:G:4960:ILE:HD12	2:G:4985:LEU:HD23	2.02	0.42
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.41
2:I:1659:LEU:O	2:I:1663:HIS:N	2.47	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.41
2:I:2145:SER:HB2	2:I:3647:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.53	0.41
2:G:2145:SER:HB2	2:G:3647:HIS:CE1	2.55	0.41
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	2.01	0.41
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.85	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:2145:SER:HB2	2:B:3647:HIS:CE1	2.55	0.41
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.53	0.41
2:I:626:LEU:HG	2:I:628:GLY:H	1.84	0.41
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.85	0.41
2:E:626:LEU:HG	2:E:628:GLY:H	1.84	0.41
2:E:4959:PHE:HD2	2:E:4960:ILE:HD13	1.84	0.41
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.41
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.41
2:B:626:LEU:HG	2:B:628:GLY:H	1.84	0.41
2:B:1077:ALA:HB1	2:B:1234:VAL:HG11	2.02	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.56	0.41
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	2.01	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.54	0.41
2:G:256:ALA:HB1	2:G:286:THR:HG21	2.02	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.54	0.41
2:G:4984:ASN:C	2:G:4986:ALA:N	2.78	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.02	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:B:4960:ILE:HD12	2:B:4985:LEU:HD23	2.02	0.41
2:B:4967:TYR:HE2	2:B:5029:ARG:HG3	1.84	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.55	0.41
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.00	0.41
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.01	0.41
2:E:4697:VAL:O	2:E:4701:TRP:N	2.53	0.41
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.56	0.41
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.01	0.41
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.56	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.85	0.41
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.85	0.41
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	2.02	0.41
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.41
2:I:2103:VAL:O	2:I:2107:GLN:N	2.48	0.41
2:E:134:ASP:N	2:E:134:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.85	0.41
2:E:2810:LYS:O	2:E:2814:LYS:N	2.48	0.41
2:E:4967:TYR:HE2	2:E:5029:ARG:HG3	1.84	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.85	0.41
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.03	0.41
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.54	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.89	0.41
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.41
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	2.03	0.41
2:I:256:ALA:HB1	2:I:286:THR:HG21	2.02	0.41
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.85	0.41
2:I:580:GLU:HG3	2:I:620:LEU:HD22	2.03	0.41
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.85	0.41
2:E:580:GLU:HG3	2:E:620:LEU:HD22	2.03	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.85	0.41
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.02	0.41
2:B:3880:PHE:O	2:B:3884:LEU:N	2.54	0.41
2:I:1077:ALA:HB1	2:I:1234:VAL:HG11	2.02	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.85	0.41
2:I:1131:ARG:N	2:I:1137:GLU:O	2.53	0.41
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.54	0.41
2:I:4959:PHE:CD2	2:I:4959:PHE:C	2.99	0.41
2:I:4984:ASN:C	2:I:4986:ALA:N	2.78	0.41
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.03	0.41
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	2.02	0.41
2:G:939:VAL:HG22	2:G:1053:ILE:HG23	2.03	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.49	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.02	0.41
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.54	0.41
2:B:4960:ILE:N	2:B:4960:ILE:CD1	2.73	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.41	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.85	0.41
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.54	0.41
2:E:4235:VAL:O	2:E:4239:GLU:N	2.44	0.41
2:E:4960:ILE:HD12	2:E:4985:LEU:HD23	2.02	0.41
2:E:4984:ASN:C	2:E:4986:ALA:N	2.78	0.41
2:G:37:LEU:HD11	2:G:47:CYS:HB3	2.03	0.41
2:G:792:LEU:HD22	2:G:799:GLU:H	1.86	0.41
2:G:1077:ALA:HB1	2:G:1234:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.03	0.41
1:A:82:TYR:O	1:A:86:GLY:N	2.54	0.41
1:J:40:ARG:NH2	2:I:675:LEU:O	2.54	0.41
2:B:583:ILE:H	2:B:583:ILE:HG13	1.71	0.41
2:B:3765:TYR:HD2	2:B:3769:ARG:HH21	1.69	0.41
2:I:37:LEU:HD11	2:I:47:CYS:HB3	2.03	0.41
2:I:1141:ARG:HD2	2:I:1141:ARG:H	1.86	0.41
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.03	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.56	0.41
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.03	0.41
2:E:37:LEU:HD11	2:E:47:CYS:HB3	2.03	0.41
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.56	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.86	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.02	0.41
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.03	0.41
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.56	0.41
2:G:1105:ALA:O	2:G:1189:LEU:N	2.54	0.41
2:G:1238:PHE:O	2:G:1606:SER:N	2.45	0.41
2:G:3880:PHE:O	2:G:3884:LEU:N	2.54	0.41
2:B:37:LEU:HD11	2:B:47:CYS:HB3	2.03	0.41
2:I:939:VAL:HG22	2:I:1053:ILE:HG23	2.03	0.41
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.41
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.41
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.53	0.41
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	2.03	0.41
1:F:82:TYR:O	1:F:86:GLY:N	2.54	0.40
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.03	0.40
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.04	0.40
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.03	0.40
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.02	0.40
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.03	0.40
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.03	0.40
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.54	0.40
2:G:309:THR:O	2:G:313:SER:OG	2.39	0.40
2:G:618:GLN:O	2:G:622:THR:OG1	2.33	0.40
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.39	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.03	0.40
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1663:HIS:NE2	2:B:1711:TYR:OH	2.39	0.40
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.02	0.40
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.96	0.40
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.03	0.40
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.04	0.40
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.40
2:I:3880:PHE:O	2:I:3884:LEU:N	2.54	0.40
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.50	0.40
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	2.03	0.40
2:G:1154:ASP:O	2:G:1158:ASN:N	2.54	0.40
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.93	0.40
2:G:2305:CYS:O	2:G:2324:ASN:ND2	2.54	0.40
2:B:3992:PHE:HB2	2:B:4023:MET:HE1	2.03	0.40
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.54	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:379:HIS:CD2	2:I:382:GLY:H	2.30	0.40
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.02	0.40
2:I:792:LEU:HD22	2:I:799:GLU:H	1.86	0.40
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.96	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:E:309:THR:O	2:E:313:SER:OG	2.39	0.40
2:E:3765:TYR:HD2	2:E:3769:ARG:HH21	1.69	0.40
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.50	0.40
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	2.03	0.40
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.89	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.40
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.56	0.40
2:B:4984:ASN:C	2:B:4986:ALA:N	2.78	0.40
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	2.03	0.40
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.54	0.40
2:E:1154:ASP:O	2:E:1158:ASN:N	2.54	0.40
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.02	0.40
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.56	0.40
2:G:626:LEU:HG	2:G:628:GLY:H	1.85	0.40
2:G:4973:HIS:HB3	2:G:4976:GLU:HB3	2.04	0.40
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.03	0.40
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.04	0.40
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.55	0.40
2:B:1141:ARG:HD2	2:B:1141:ARG:H	1.86	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.54	0.40
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:ALA:O	2:I:1189:LEU:N	2.54	0.40
2:I:3662:ILE:H	2:I:3662:ILE:HG13	1.77	0.40
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.87	0.40
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.55	0.40
2:E:3977:GLN:NE2	2:E:4032:GLU:OE1	2.55	0.40
2:E:4973:HIS:HB3	2:E:4976:GLU:HB3	2.04	0.40
2:G:134:ASP:N	2:G:134:ASP:OD1	2.54	0.40
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.04	0.40
2:G:3765:TYR:HD2	2:G:3769:ARG:HH21	1.69	0.40
2:G:3992:PHE:HB2	2:G:4023:MET:HE1	2.03	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%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2926 (90%)	304 (9%)	5 (0%)	43	78
2	E	3235/4416 (73%)	2924 (90%)	306 (10%)	5 (0%)	43	78
2	G	3235/4416 (73%)	2925 (90%)	305 (9%)	5 (0%)	43	78
2	I	3235/4416 (73%)	2922 (90%)	308 (10%)	5 (0%)	43	78
All	All	13360/18096 (74%)	12077 (90%)	1263 (10%)	20 (0%)	49	83

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU
2	I	4985	LEU
2	E	4985	LEU
2	G	4985	LEU
2	B	1708	ARG
2	B	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	1840	PRO
2	G	1840	PRO
2	I	1840	PRO
2	E	1840	PRO
2	B	4641	PRO
2	I	4641	PRO
2	E	4641	PRO
2	G	4641	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
2	E	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
2	G	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
2	I	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
All	All	10320/12444 (83%)	10272 (100%)	48 (0%)	78	83

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

Mol	Chain	Res	Type
2	B	131	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	3663	LEU
2	B	3805	LEU
2	B	4154	VAL
2	B	4837	LEU
2	B	4957	LYS
2	B	4959	PHE
2	B	4960	ILE
2	I	131	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1657	LEU
2	I	1676	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4154	VAL
2	I	4837	LEU
2	I	4957	LYS
2	I	4959	PHE
2	I	4960	ILE
2	E	131	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4154	VAL
2	E	4837	LEU
2	E	4957	LYS
2	E	4959	PHE
2	E	4960	ILE
2	G	131	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU
2	G	3663	LEU

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Mol	Chain	Res	Type
2	G	3805	LEU
2	G	4154	VAL
2	G	4837	LEU
2	G	4957	LYS
2	G	4959	PHE
2	G	4960	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (201) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	113	HIS
2	B	151	HIS
2	B	156	GLN
2	B	201	ASN
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	520	ASN
2	B	582	HIS
2	B	597	HIS
2	B	678	GLN
2	B	765	GLN
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1640	HIS
2	B	1688	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1941	ASN

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Mol	Chain	Res	Type
2	B	1949	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	2260	ASN
2	B	2773	ASN
2	B	3771	HIS
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4109	GLN
2	B	4120	ASN
2	B	4162	ASN
2	B	4949	GLN
2	B	4987	ASN
2	B	5003	HIS
2	B	5031	GLN
2	I	57	ASN
2	I	105	HIS
2	I	113	HIS
2	I	151	HIS
2	I	156	GLN
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	520	ASN
2	I	582	HIS
2	I	597	HIS
2	I	678	GLN
2	I	765	GLN
2	I	797	HIS
2	I	838	HIS
2	I	1206	GLN

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Mol	Chain	Res	Type
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1775	HIS
2	I	1861	GLN
2	I	1949	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	2773	ASN
2	I	3771	HIS
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4109	GLN
2	I	4120	ASN
2	I	4156	HIS
2	I	4162	ASN
2	I	4949	GLN
2	I	4987	ASN
2	I	5003	HIS
2	I	5031	GLN
2	E	57	ASN
2	E	105	HIS
2	E	113	HIS
2	E	151	HIS
2	E	156	GLN
2	E	201	ASN
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	520	ASN
2	E	582	HIS

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Mol	Chain	Res	Type
2	E	597	HIS
2	E	678	GLN
2	E	765	GLN
2	E	797	HIS
2	E	838	HIS
2	E	1206	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1949	GLN
2	E	2127	GLN
2	E	2260	ASN
2	E	2773	ASN
2	E	2902	HIS
2	E	3771	HIS
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4109	GLN
2	E	4120	ASN
2	E	4156	HIS
2	E	4162	ASN
2	E	4949	GLN
2	E	4987	ASN
2	E	5003	HIS
2	E	5031	GLN
2	G	57	ASN
2	G	105	HIS
2	G	113	HIS
2	G	151	HIS
2	G	156	GLN

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Mol	Chain	Res	Type
2	G	201	ASN
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	520	ASN
2	G	582	HIS
2	G	597	HIS
2	G	678	GLN
2	G	765	GLN
2	G	797	HIS
2	G	838	HIS
2	G	1206	GLN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1949	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	2260	ASN
2	G	2773	ASN
2	G	2902	HIS
2	G	3771	HIS
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4162	ASN
2	G	4949	GLN
2	G	4987	ASN
2	G	5003	HIS

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Mol	Chain	Res	Type
2	G	5031	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	5101	-	32,33,33	1.39	4 (12%)	48,52,52	1.80	8 (16%)
3	ATP	G	5101	-	32,33,33	1.39	4 (12%)	48,52,52	1.80	8 (16%)
4	CFF	B	5102	-	15,15,15	1.87	5 (33%)	23,23,23	2.79	8 (34%)
4	CFF	E	5102	-	15,15,15	1.88	6 (40%)	23,23,23	2.78	8 (34%)
3	ATP	I	5101	-	32,33,33	1.40	4 (12%)	48,52,52	1.80	8 (16%)
3	ATP	B	5101	-	32,33,33	1.39	4 (12%)	48,52,52	1.80	8 (16%)
4	CFF	I	5102	-	15,15,15	1.88	5 (33%)	23,23,23	2.79	8 (34%)
4	CFF	G	5102	-	15,15,15	1.87	5 (33%)	23,23,23	2.79	8 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	G	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.44	1.47	1.39
3	I	5101	ATP	C5-C4	4.44	1.47	1.39
3	E	5101	ATP	C5-C4	4.42	1.47	1.39
3	G	5101	ATP	C5-C4	4.42	1.47	1.39
4	I	5102	CFF	C6-N1	-3.77	1.32	1.40
4	E	5102	CFF	C6-N1	-3.75	1.32	1.40
4	G	5102	CFF	C6-N1	-3.74	1.32	1.40
4	B	5102	CFF	C6-N1	-3.74	1.32	1.40
4	E	5102	CFF	C4-N3	-2.62	1.33	1.38
3	I	5101	ATP	C5-N7	-2.61	1.34	1.39
3	G	5101	ATP	C5-N7	-2.61	1.34	1.39
3	B	5101	ATP	C5-N7	-2.61	1.34	1.39
3	B	5101	ATP	C5-C6	2.60	1.48	1.41
3	I	5101	ATP	C5-C6	2.60	1.48	1.41
3	E	5101	ATP	C5-C6	2.59	1.48	1.41
3	G	5101	ATP	C5-C6	2.59	1.48	1.41
3	E	5101	ATP	C5-N7	-2.57	1.34	1.39
4	G	5102	CFF	C4-N3	-2.57	1.33	1.38
4	B	5102	CFF	C4-N3	-2.56	1.33	1.38
4	I	5102	CFF	C4-N3	-2.56	1.33	1.38
4	I	5102	CFF	C5-N7	-2.32	1.34	1.38
4	B	5102	CFF	C5-N7	-2.31	1.34	1.38
4	G	5102	CFF	C5-N7	-2.30	1.34	1.38
4	E	5102	CFF	C5-N7	-2.29	1.34	1.38
4	B	5102	CFF	O13-C6	-2.15	1.18	1.23
4	I	5102	CFF	O13-C6	-2.15	1.18	1.23
4	E	5102	CFF	O13-C6	-2.15	1.18	1.23
4	G	5102	CFF	O13-C6	-2.15	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	PA-O3A	2.11	1.61	1.59
4	B	5102	CFF	C2-N3	-2.09	1.34	1.39
4	E	5102	CFF	C2-N3	-2.08	1.34	1.39
4	I	5102	CFF	C2-N3	-2.08	1.34	1.39
4	G	5102	CFF	C2-N3	-2.06	1.35	1.39
3	E	5101	ATP	PA-O3A	2.05	1.61	1.59
3	B	5101	ATP	PA-O3A	2.04	1.61	1.59
4	E	5102	CFF	O11-C2	-2.02	1.18	1.22
3	G	5101	ATP	PA-O3A	2.00	1.61	1.59

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.59	112.07	126.28
4	B	5102	CFF	C14-N7-C8	-7.57	112.11	126.28
4	I	5102	CFF	C14-N7-C8	-7.57	112.11	126.28
4	E	5102	CFF	C14-N7-C8	-7.55	112.14	126.28
3	E	5101	ATP	C5-C4-N3	-5.80	118.73	126.72
3	B	5101	ATP	C5-C4-N3	-5.77	118.77	126.72
3	G	5101	ATP	C5-C4-N3	-5.76	118.79	126.72
3	I	5101	ATP	C5-C4-N3	-5.75	118.80	126.72
4	G	5102	CFF	C14-N7-C5	5.09	139.87	127.77
4	I	5102	CFF	C14-N7-C5	5.08	139.85	127.77
4	E	5102	CFF	C14-N7-C5	5.07	139.84	127.77
4	B	5102	CFF	C14-N7-C5	5.07	139.83	127.77
3	I	5101	ATP	N3-C4-N9	4.79	135.31	127.17
3	B	5101	ATP	N3-C4-N9	4.78	135.30	127.17
3	E	5101	ATP	N3-C4-N9	4.77	135.29	127.17
3	G	5101	ATP	N3-C4-N9	4.76	135.27	127.17
4	I	5102	CFF	C5-C6-N1	4.46	120.23	112.06
4	B	5102	CFF	C5-C6-N1	4.44	120.20	112.06
4	G	5102	CFF	C5-C6-N1	4.44	120.19	112.06
4	E	5102	CFF	C5-C6-N1	4.42	120.16	112.06
3	E	5101	ATP	C4-C5-N7	-3.66	106.39	110.58
3	B	5101	ATP	C4-C5-N7	-3.65	106.41	110.58
3	G	5101	ATP	C4-C5-N7	-3.64	106.42	110.58
3	I	5101	ATP	C4-C5-N7	-3.60	106.47	110.58
3	E	5101	ATP	C2-N3-C4	3.59	120.60	111.83
3	I	5101	ATP	C2-N3-C4	3.58	120.57	111.83
3	B	5101	ATP	C2-N3-C4	3.58	120.56	111.83
3	G	5101	ATP	C2-N3-C4	3.57	120.54	111.83
4	B	5102	CFF	C6-N1-C2	-3.44	120.06	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C6-N1-C2	-3.44	120.07	125.66
4	I	5102	CFF	C6-N1-C2	-3.44	120.07	125.66
4	E	5102	CFF	C6-N1-C2	-3.40	120.13	125.66
3	I	5101	ATP	C4-N9-C8	3.24	109.14	105.74
3	B	5101	ATP	C4-N9-C8	3.20	109.09	105.74
3	G	5101	ATP	C4-N9-C8	3.20	109.09	105.74
3	E	5101	ATP	C4-N9-C8	3.15	109.04	105.74
3	G	5101	ATP	N3-C2-N1	-3.14	123.83	128.58
3	E	5101	ATP	N3-C2-N1	-3.11	123.87	128.58
3	I	5101	ATP	N3-C2-N1	-3.11	123.88	128.58
3	B	5101	ATP	N3-C2-N1	-3.11	123.88	128.58
4	G	5102	CFF	N3-C4-N9	3.08	131.12	126.27
4	E	5102	CFF	N3-C4-N9	3.08	131.12	126.27
4	B	5102	CFF	N3-C4-N9	3.06	131.08	126.27
4	I	5102	CFF	N3-C4-N9	3.06	131.08	126.27
4	E	5102	CFF	O13-C6-C5	-3.03	120.17	126.38
4	B	5102	CFF	O13-C6-C5	-3.02	120.19	126.38
4	I	5102	CFF	O13-C6-C5	-3.02	120.19	126.38
4	G	5102	CFF	O13-C6-C5	-3.02	120.19	126.38
4	I	5102	CFF	N7-C8-N9	-2.99	108.06	113.48
4	G	5102	CFF	N7-C8-N9	-2.99	108.06	113.48
4	B	5102	CFF	N7-C8-N9	-2.97	108.09	113.48
3	G	5101	ATP	C5-N7-C8	2.96	108.10	103.45
3	B	5101	ATP	C5-N7-C8	2.96	108.09	103.45
4	I	5102	CFF	C6-C5-C4	-2.95	119.20	122.92
4	E	5102	CFF	N7-C8-N9	-2.95	108.13	113.48
3	E	5101	ATP	C5-N7-C8	2.94	108.07	103.45
3	I	5101	ATP	C5-N7-C8	2.93	108.06	103.45
4	E	5102	CFF	C6-C5-C4	-2.93	119.22	122.92
4	B	5102	CFF	C6-C5-C4	-2.92	119.24	122.92
4	G	5102	CFF	C6-C5-C4	-2.88	119.29	122.92
3	I	5101	ATP	N9-C8-N7	-2.46	110.44	113.94
3	G	5101	ATP	N9-C8-N7	-2.46	110.45	113.94
3	B	5101	ATP	N9-C8-N7	-2.45	110.46	113.94
3	E	5101	ATP	N9-C8-N7	-2.41	110.51	113.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A

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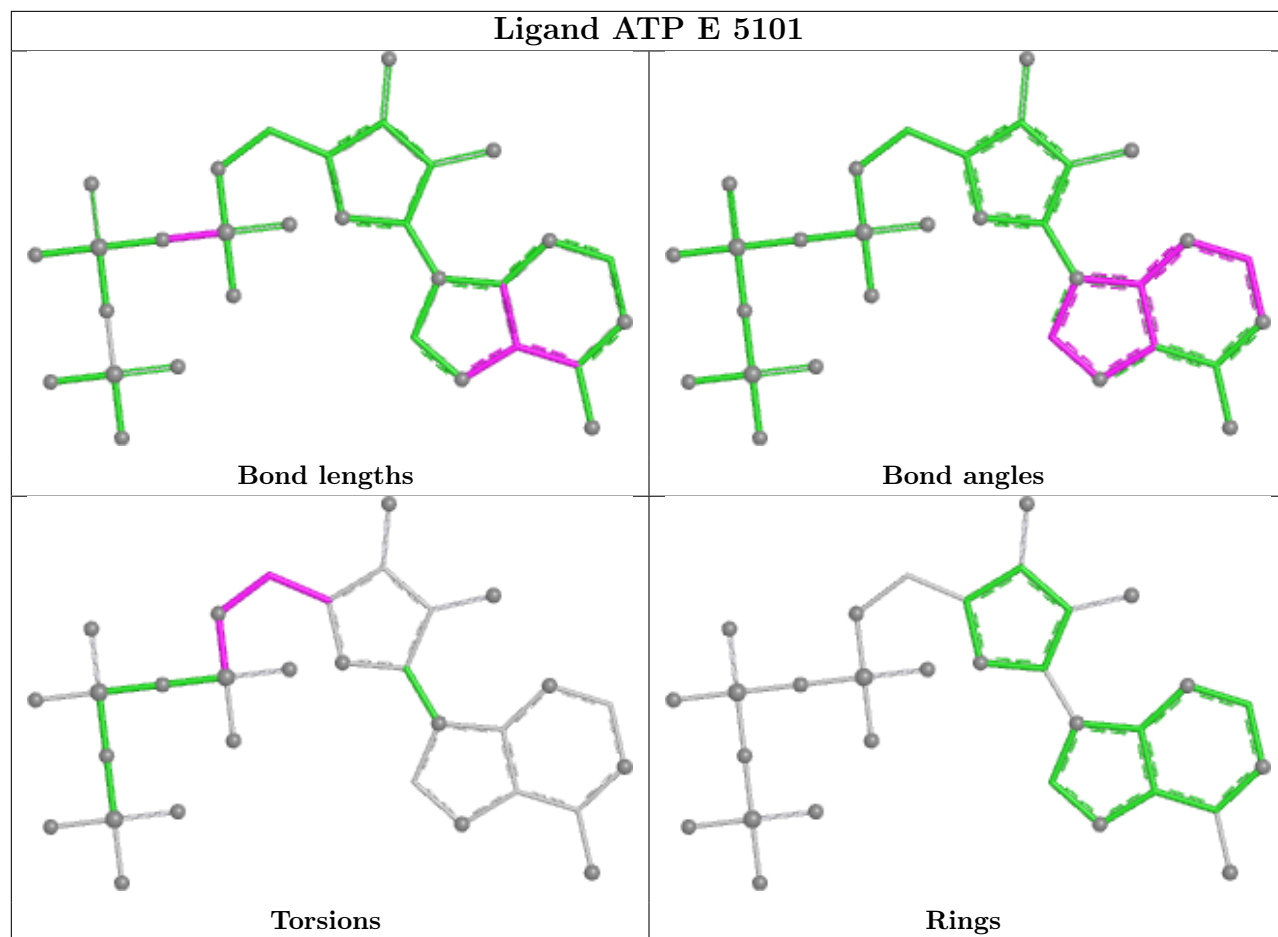
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA

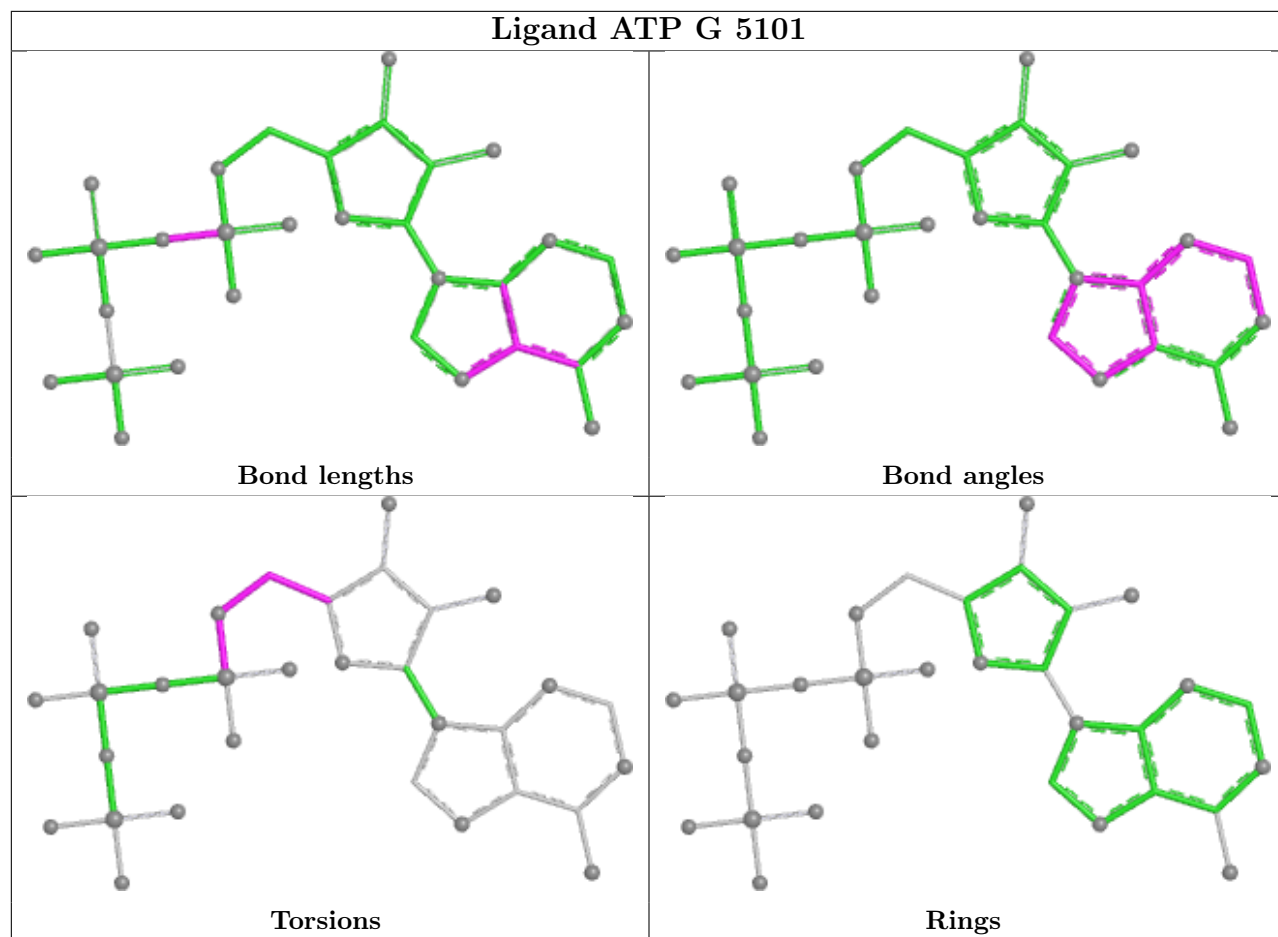
There are no ring outliers.

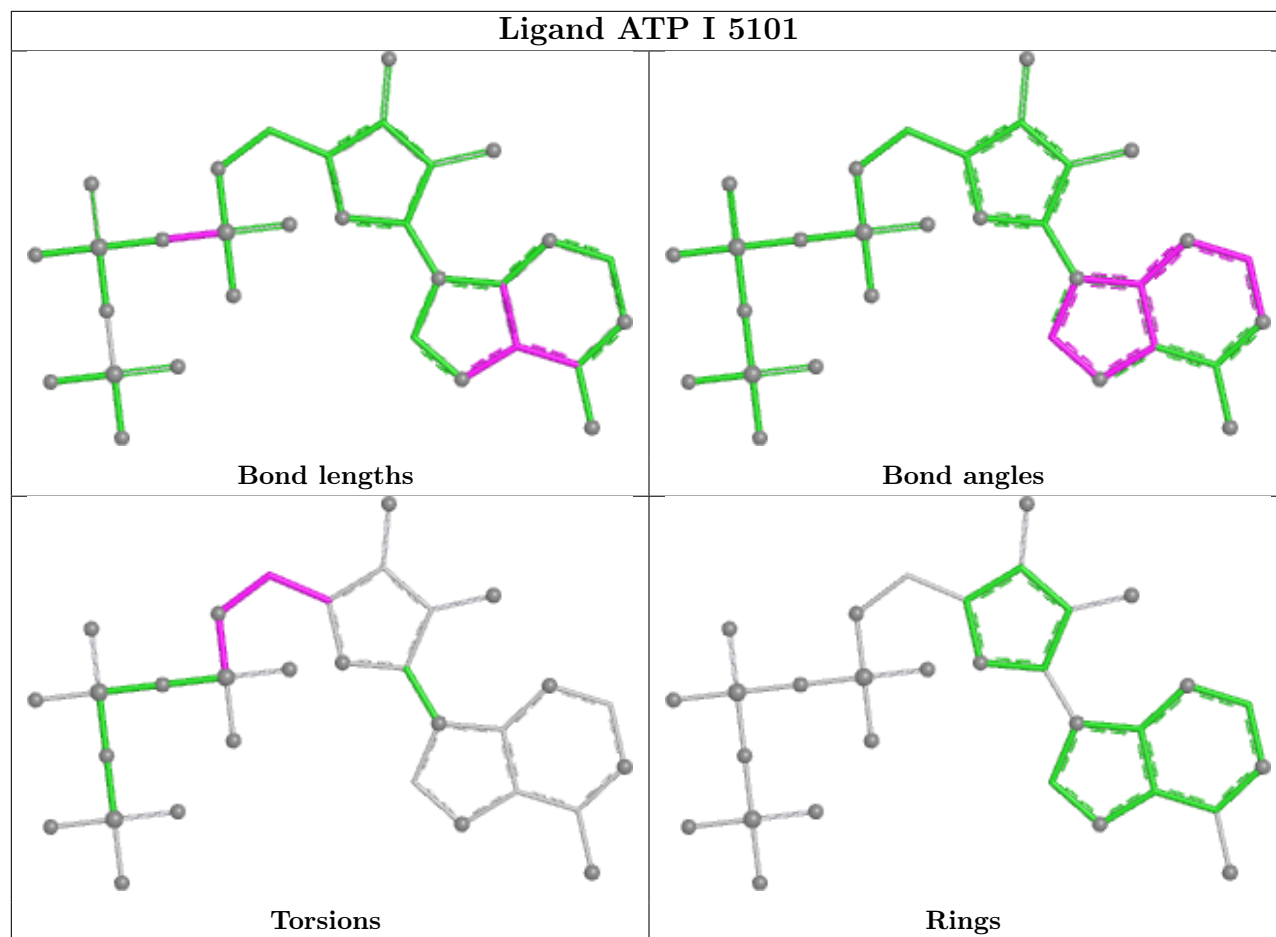
4 monomers are involved in 8 short contacts:

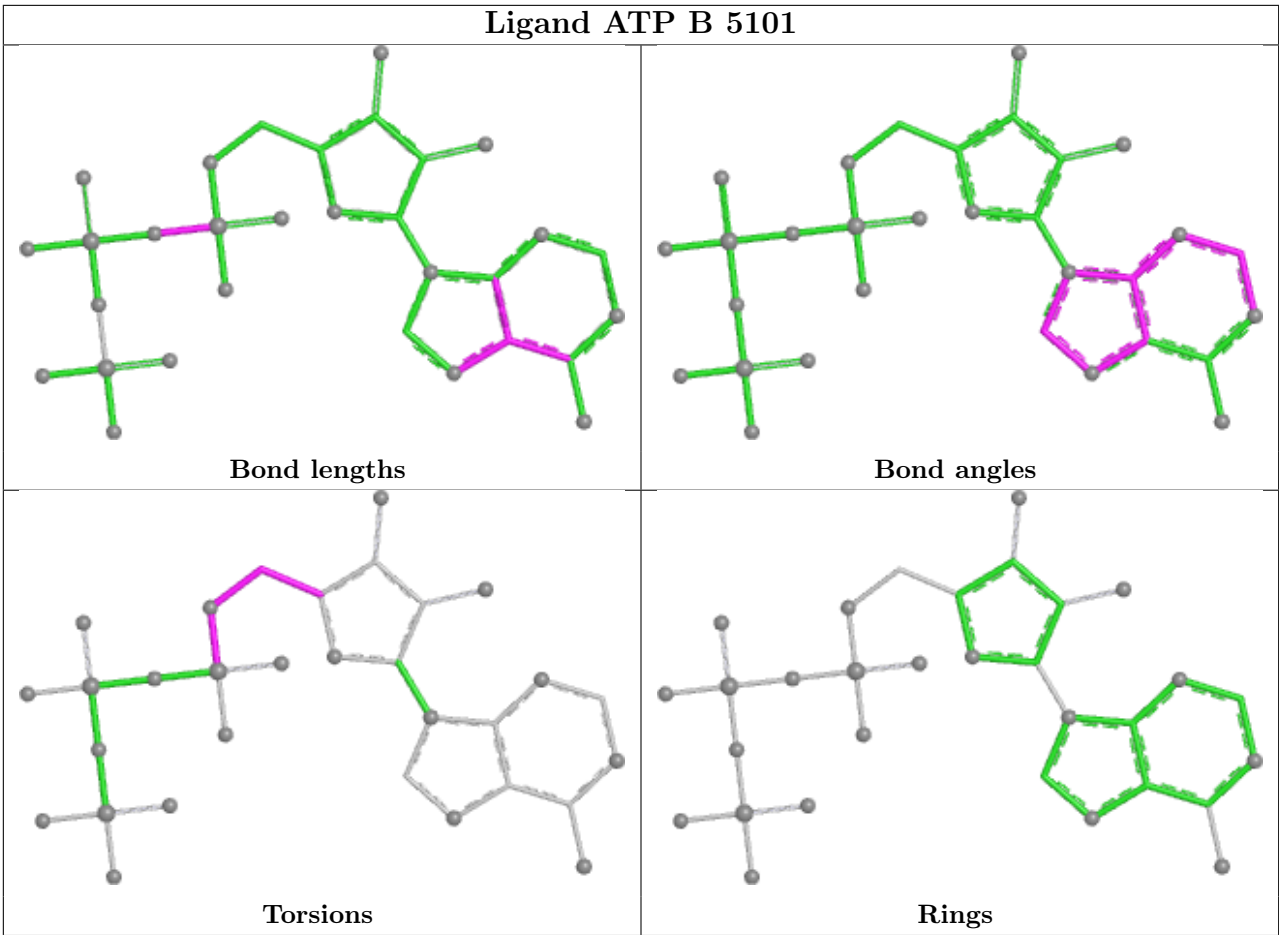
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	0
3	B	5101	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	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	72.97
1	I	4345:UNK	C	4540:PHE	N	72.97

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.97
1	G	4345:UNK	C	4540:PHE	N	72.97
1	B	3613:UNK	C	3639:THR	N	44.25
1	I	3613:UNK	C	3639:THR	N	44.25
1	E	3613:UNK	C	3639:THR	N	44.25
1	G	3613:UNK	C	3639:THR	N	44.25
1	B	4253:GLU	C	4320:UNK	N	27.48
1	I	4253:GLU	C	4320:UNK	N	27.48
1	E	4253:GLU	C	4320:UNK	N	27.48
1	G	4253:GLU	C	4320:UNK	N	27.48
1	B	3163:UNK	C	3170:UNK	N	16.07
1	I	3163:UNK	C	3170:UNK	N	16.07
1	E	3163:UNK	C	3170:UNK	N	16.07
1	G	3163:UNK	C	3170:UNK	N	16.07
1	B	3063:UNK	C	3134:UNK	N	15.01
1	I	3063:UNK	C	3134:UNK	N	15.01
1	E	3063:UNK	C	3134:UNK	N	15.01
1	G	3063:UNK	C	3134:UNK	N	15.01
1	B	3468:UNK	C	3511:UNK	N	14.60
1	I	3468:UNK	C	3511:UNK	N	14.60
1	E	3468:UNK	C	3511:UNK	N	14.60
1	G	3468:UNK	C	3511:UNK	N	14.60
1	B	2703:UNK	C	2734:ASN	N	14.12
1	I	2703:UNK	C	2734:ASN	N	14.12
1	E	2703:UNK	C	2734:ASN	N	14.12
1	G	2703:UNK	C	2734:ASN	N	14.12
1	B	3236:UNK	C	3241:UNK	N	13.51
1	I	3236:UNK	C	3241:UNK	N	13.51
1	E	3236:UNK	C	3241:UNK	N	13.51
1	G	3236:UNK	C	3241:UNK	N	13.51
1	B	1564:UNK	C	1573:MET	N	12.36
1	I	1564:UNK	C	1573:MET	N	12.36
1	E	1564:UNK	C	1573:MET	N	12.36
1	G	1564:UNK	C	1573:MET	N	12.36
1	B	2976:UNK	C	2995:UNK	N	12.31
1	I	2976:UNK	C	2995:UNK	N	12.31
1	E	2976:UNK	C	2995:UNK	N	12.31
1	G	2976:UNK	C	2995:UNK	N	12.31
1	I	3254:UNK	C	3261:UNK	N	8.30
1	B	3254:UNK	C	3261:UNK	N	8.29
1	E	3254:UNK	C	3261:UNK	N	8.29
1	G	3254:UNK	C	3261:UNK	N	8.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.73
1	I	1297:UNK	C	1430:UNK	N	5.73
1	E	1297:UNK	C	1430:UNK	N	5.73
1	G	1297:UNK	C	1430:UNK	N	5.73
1	B	2939:ARG	C	2942:UNK	N	3.51
1	I	2939:ARG	C	2942:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.51
1	G	2939:ARG	C	2942:UNK	N	3.51
1	B	2479:LEU	C	2487:UNK	N	3.41
1	I	2479:LEU	C	2487:UNK	N	3.41
1	E	2479:LEU	C	2487:UNK	N	3.41
1	G	2479:LEU	C	2487:UNK	N	3.41

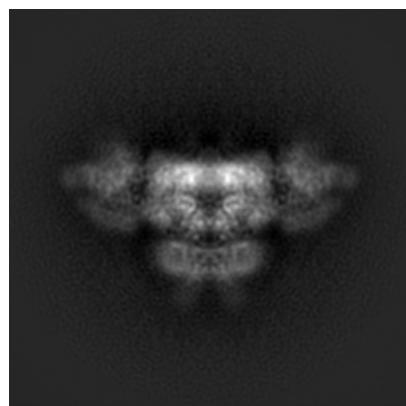
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8385. These allow visual inspection of the internal detail of the map and identification of artifacts.

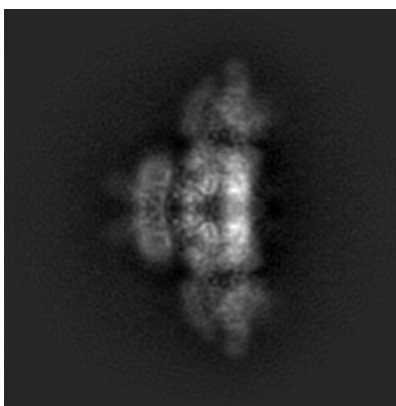
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

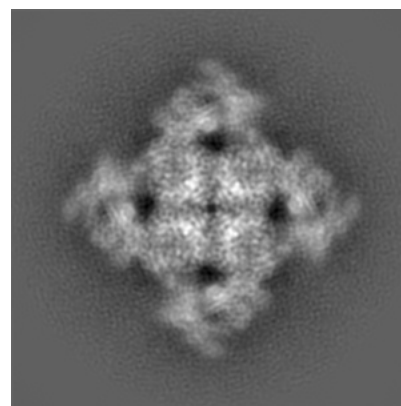
6.1.1 Primary map



X

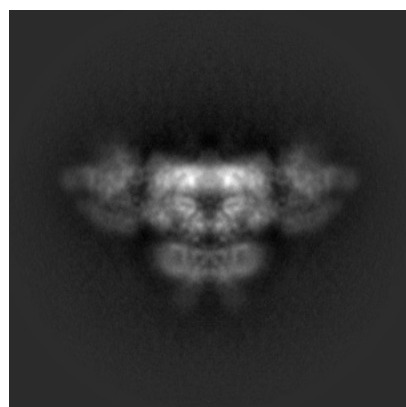


Y

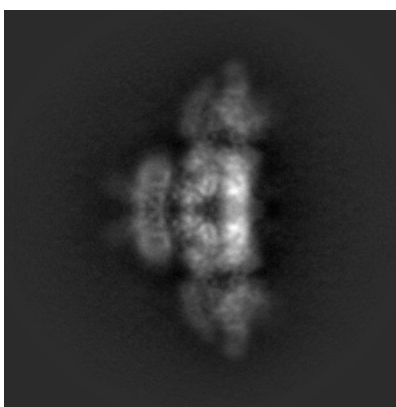


Z

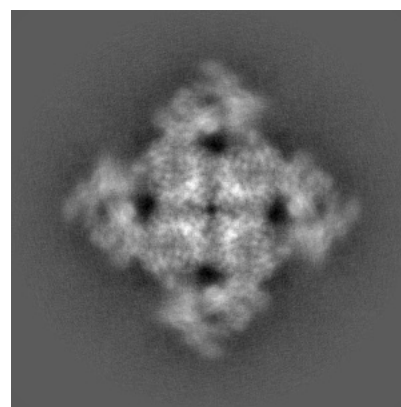
6.1.2 Raw map



X



Y

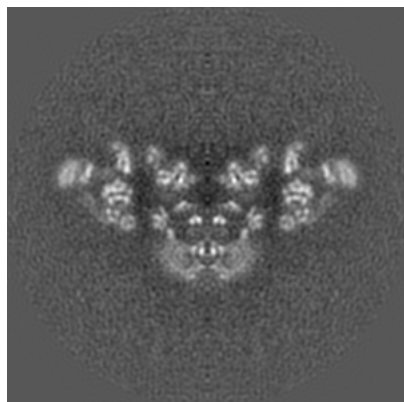


Z

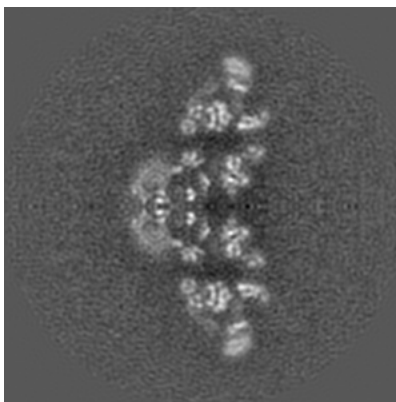
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

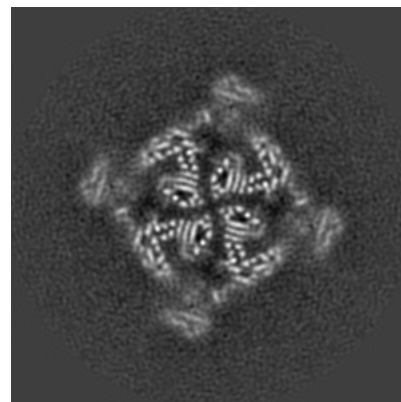
6.2.1 Primary map



X Index: 200

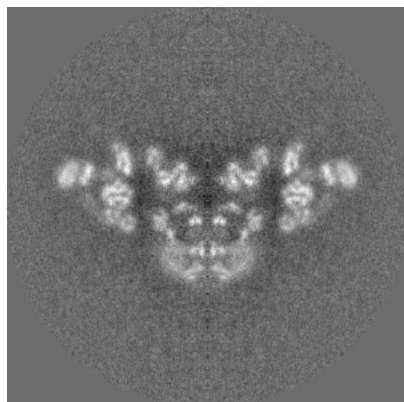


Y Index: 200

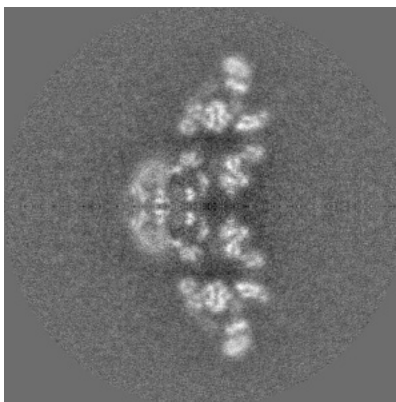


Z Index: 200

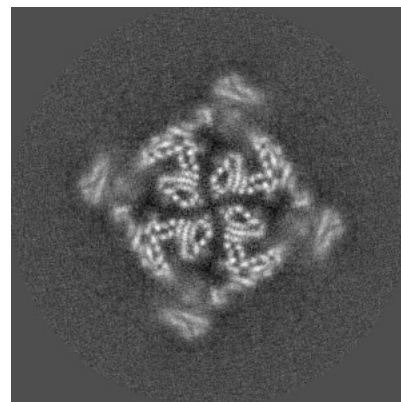
6.2.2 Raw map



X Index: 200



Y Index: 200

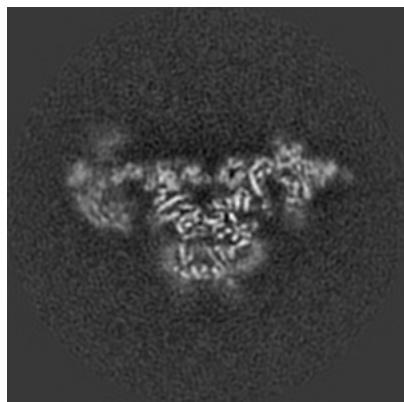


Z Index: 200

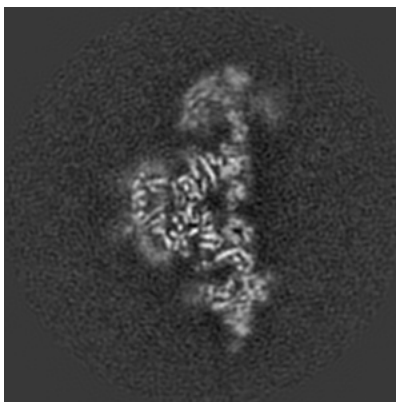
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

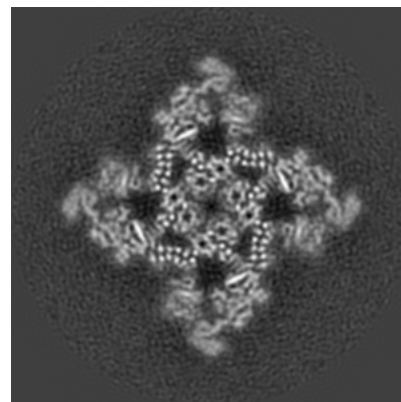
6.3.1 Primary map



X Index: 184

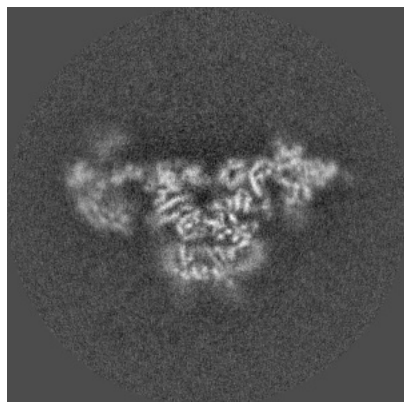


Y Index: 184

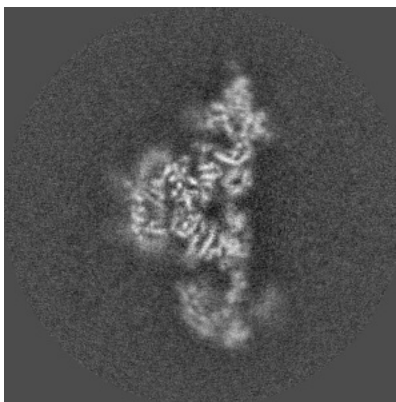


Z Index: 227

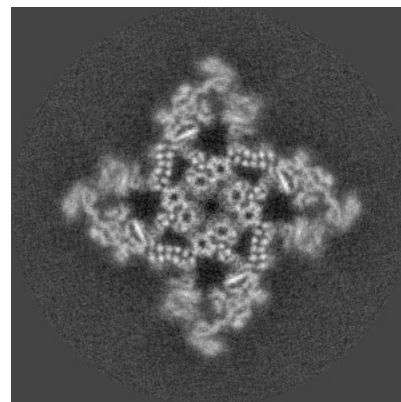
6.3.2 Raw map



X Index: 184



Y Index: 216

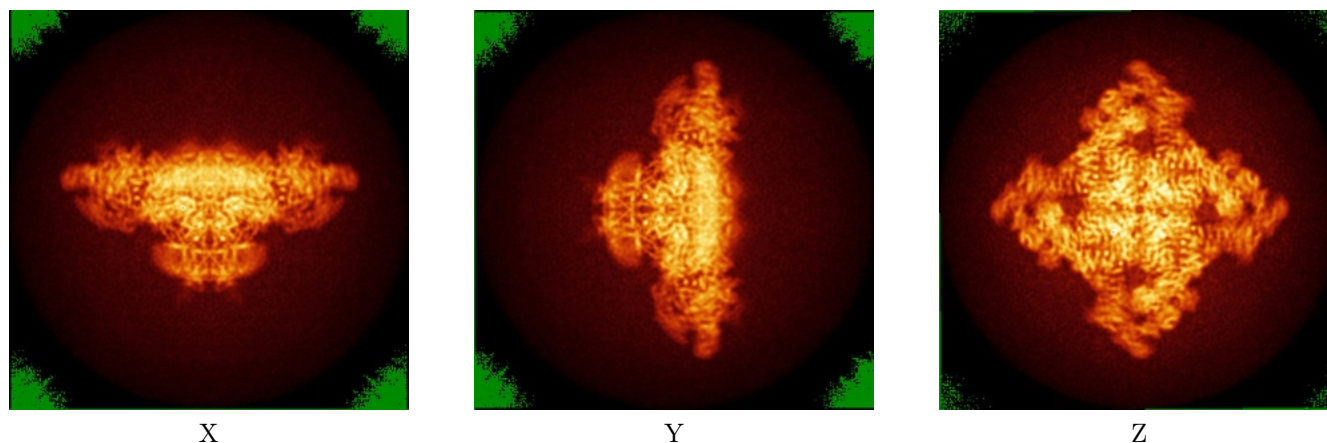


Z Index: 226

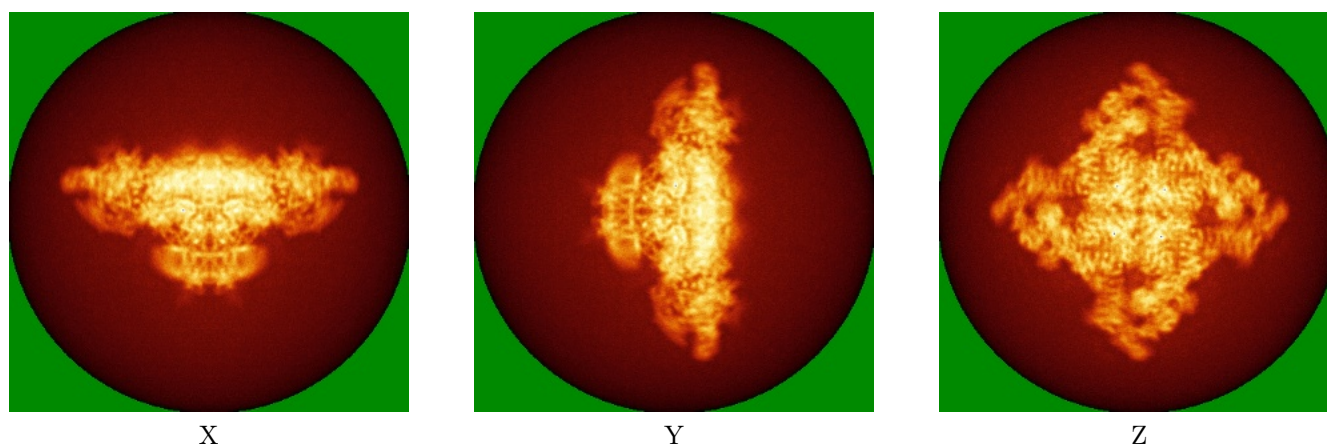
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

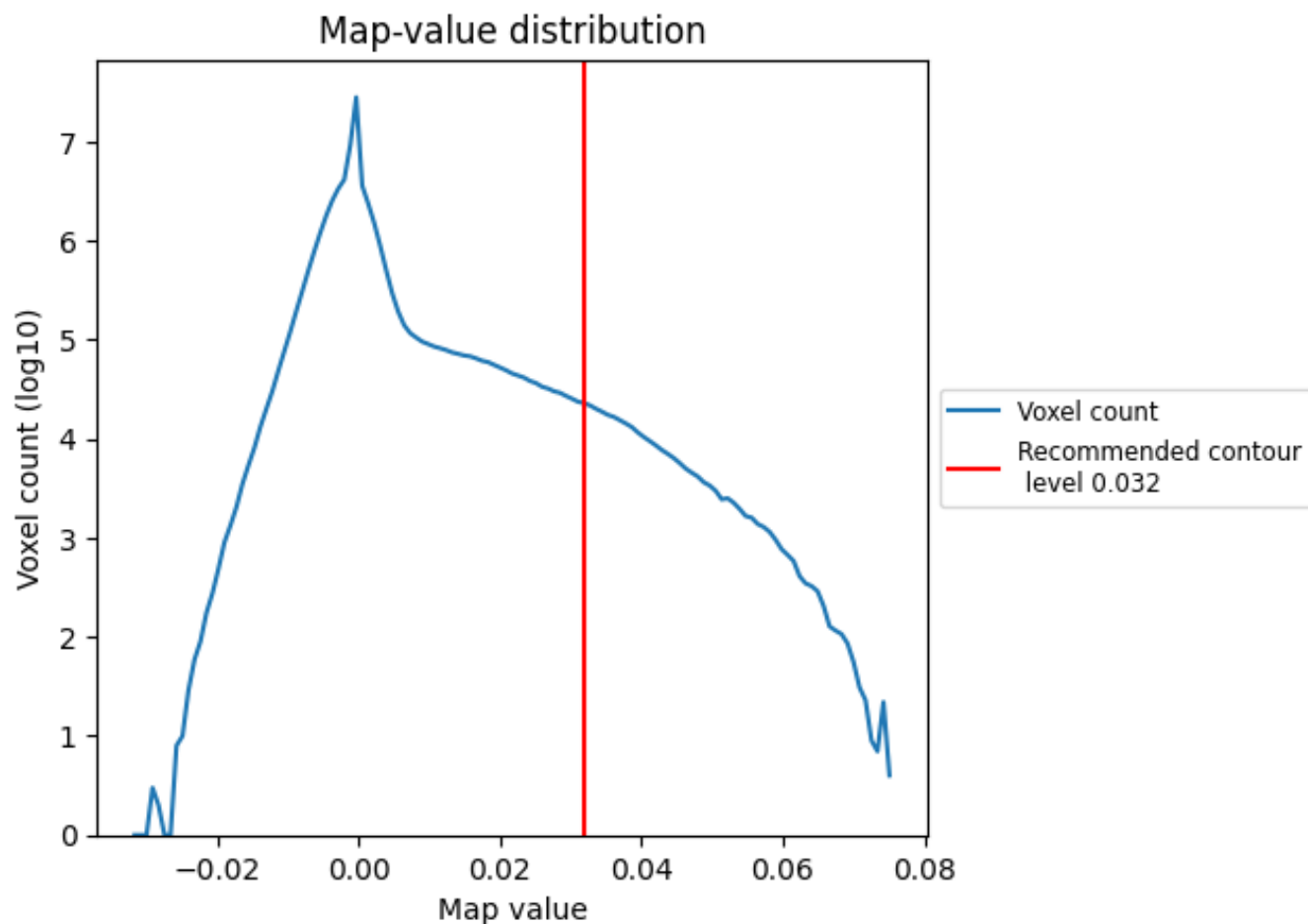
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

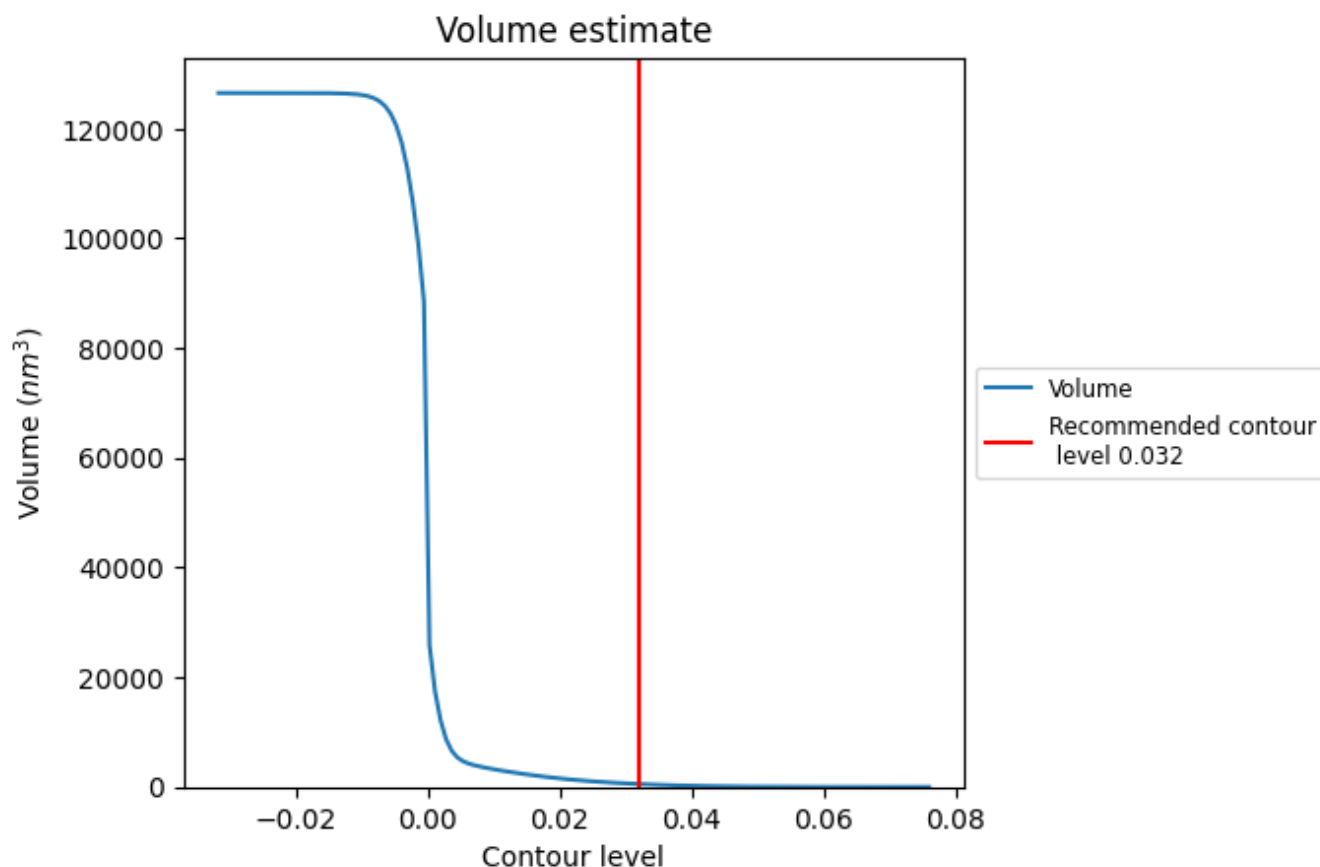
This section contains the results of statistical analysis of the map.

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.

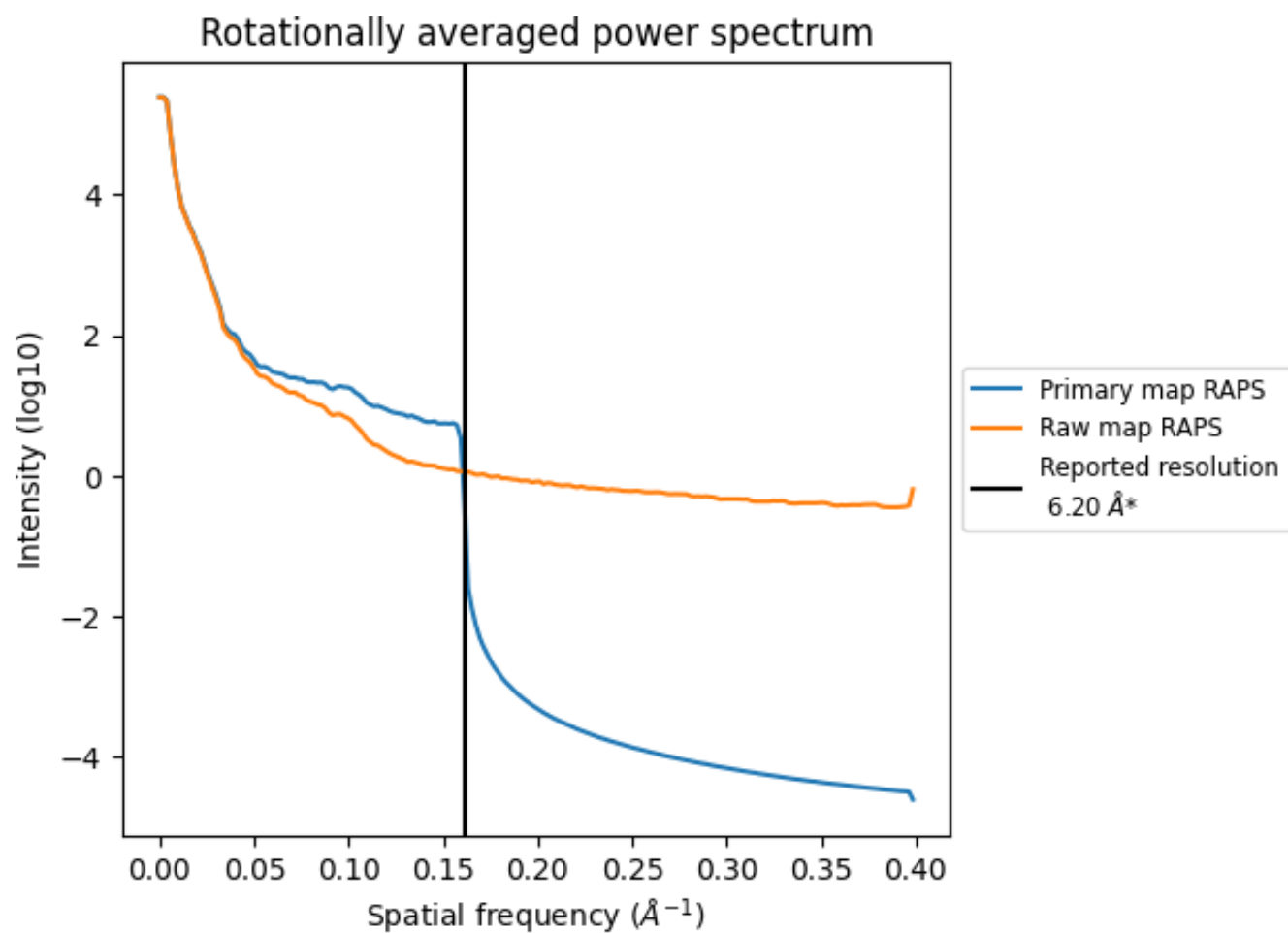
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 482 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 ⓘ

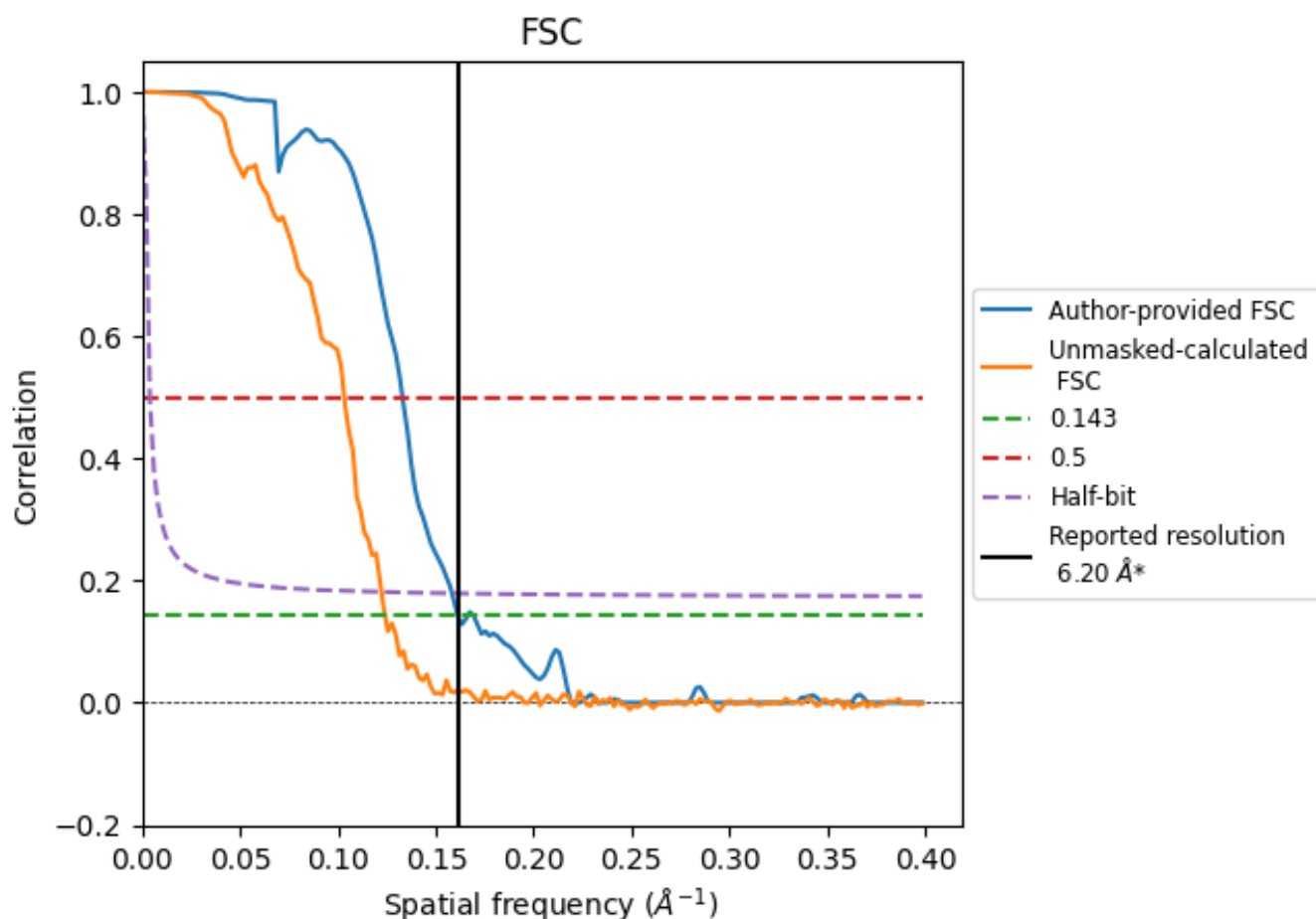


*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

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 $0.161 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.21	7.52	6.32
Unmasked-calculated*	8.06	9.69	8.18

*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 8.06 differs from the reported value 6.2 by more than 10 %

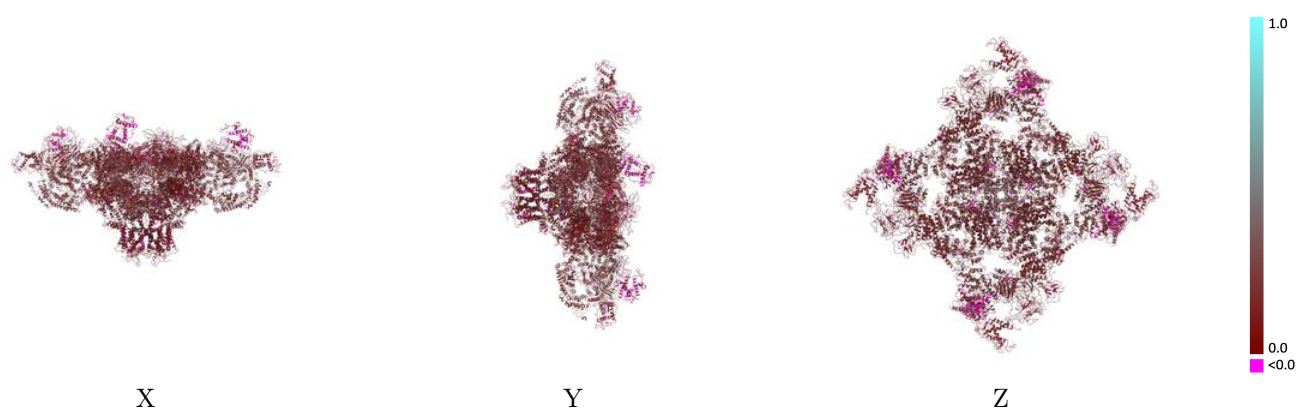
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8385 and PDB model 5TAU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

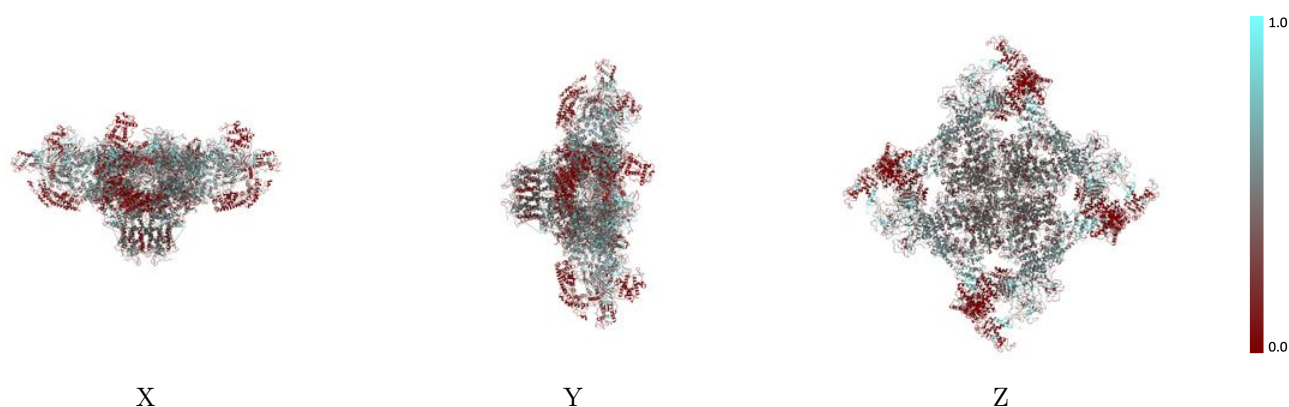
This section was not generated.

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



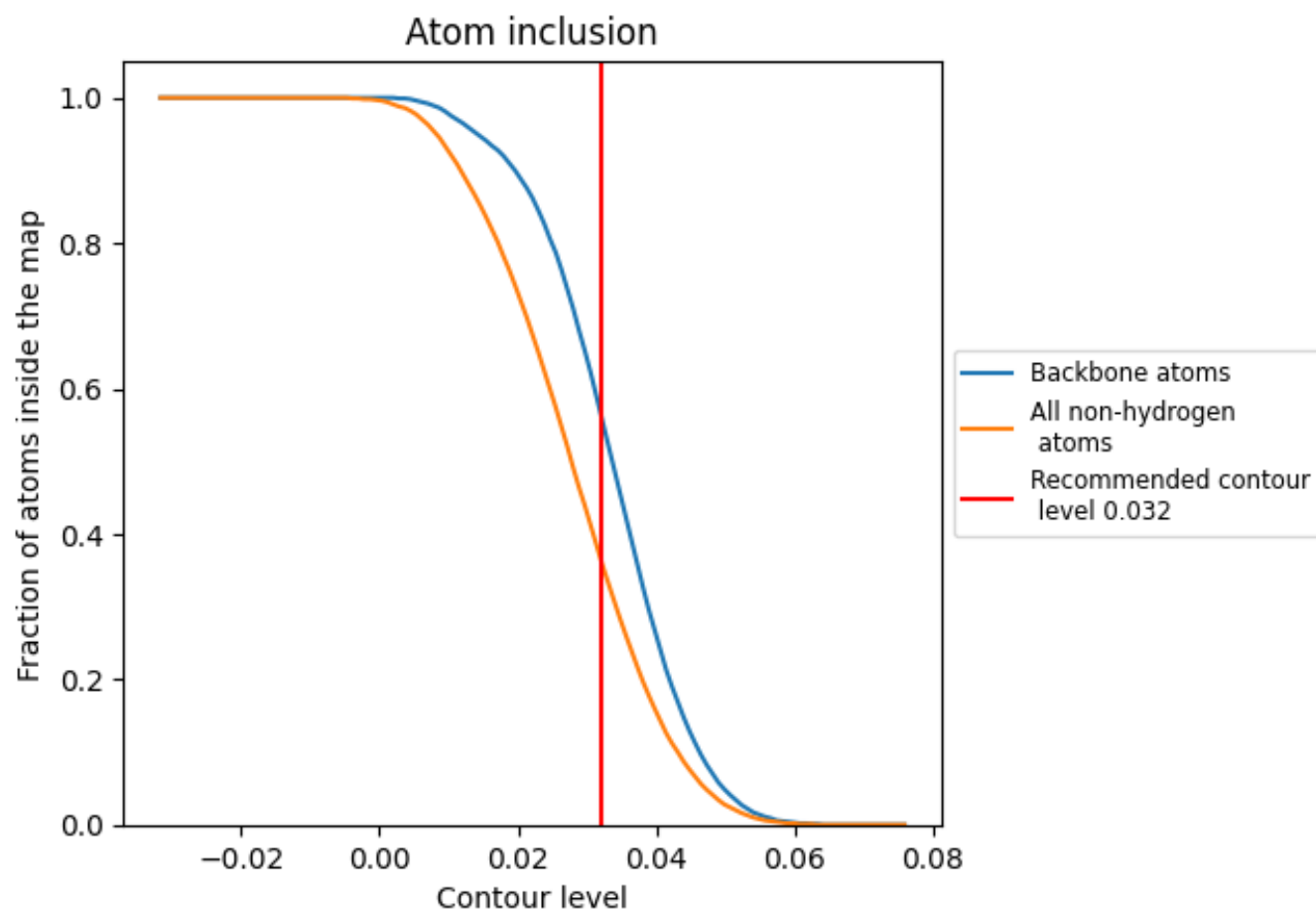
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3660	0.1880
A	0.3960	0.1860
B	0.3640	0.1880
E	0.3640	0.1880
F	0.3980	0.1900
G	0.3650	0.1880
H	0.3930	0.1880
I	0.3650	0.1880
J	0.3870	0.1880

1.0

0.0

<0.0