



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:30 PM UTC

PDB ID : 5TB4 / pdb_00005tb4
EMDB ID : EMD-8395
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-11
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

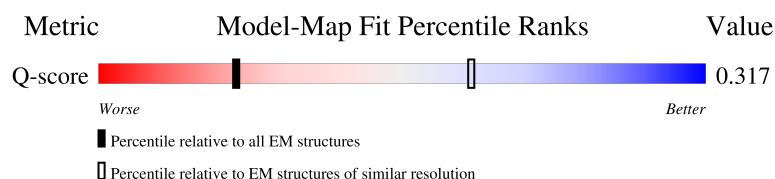
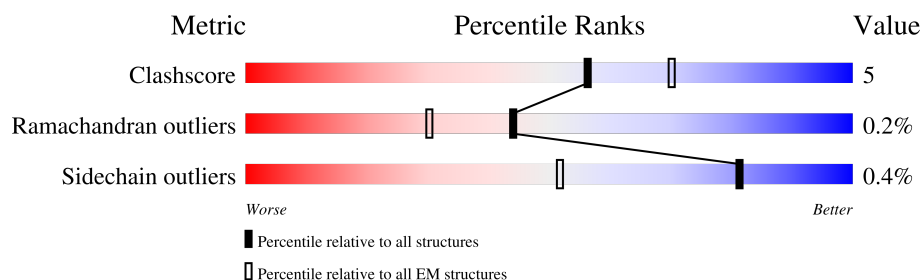
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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

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

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Mol	Chain	Length	Quality of chain			
2	B	4416	39%			
2	E	4416	84%			
2	G	4416	11%			
2	I	4416	5%			

2 Entry composition

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

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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

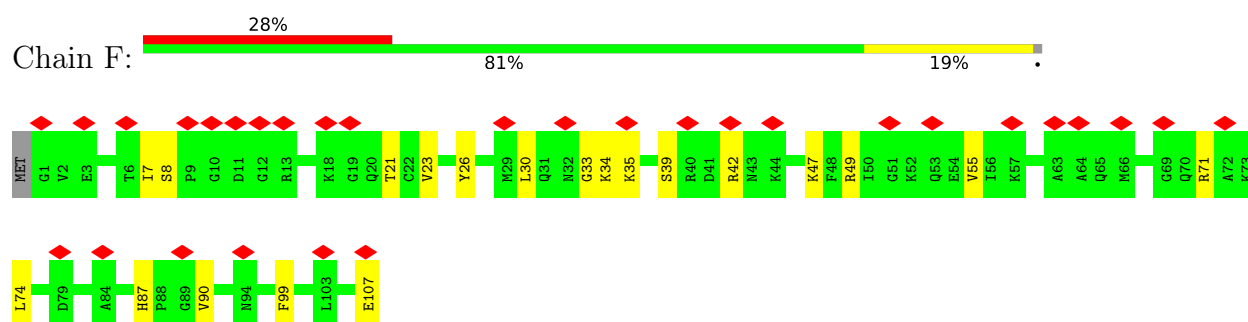
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

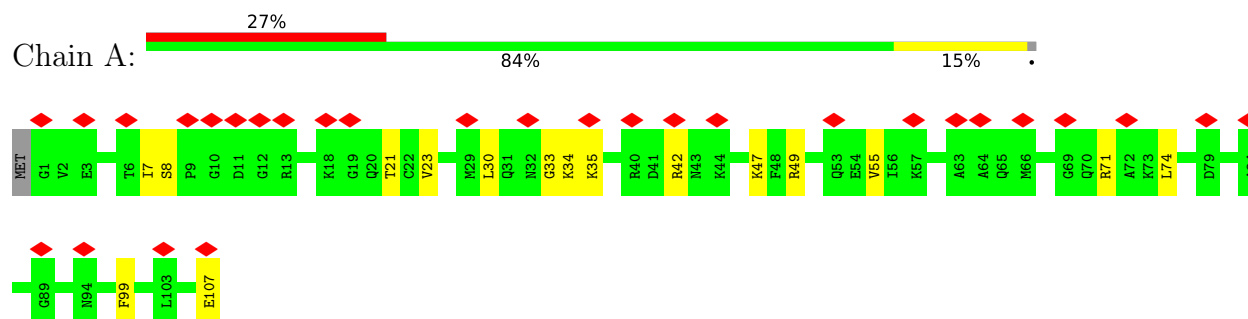
3 Residue-property plots [i](#)

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

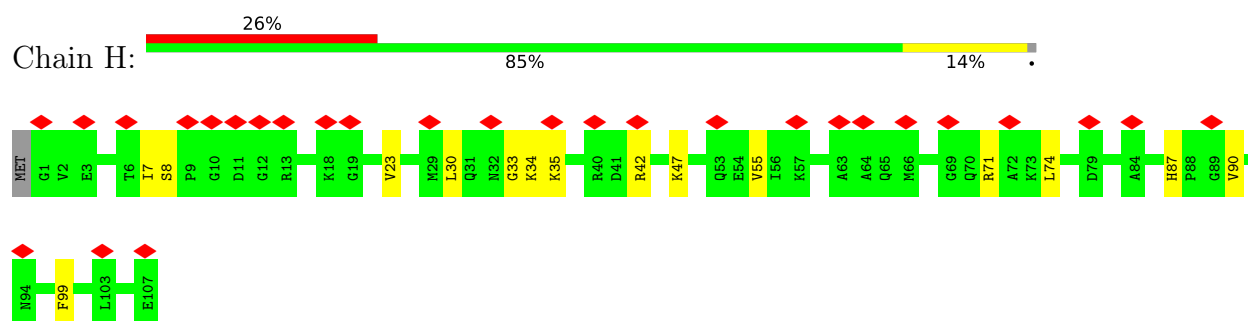
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



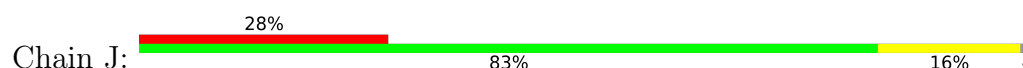
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

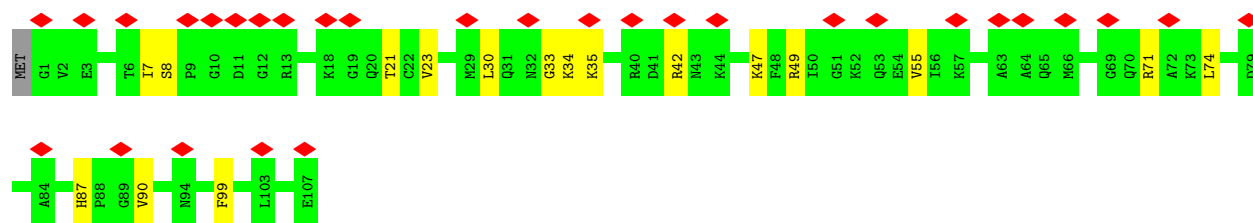


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

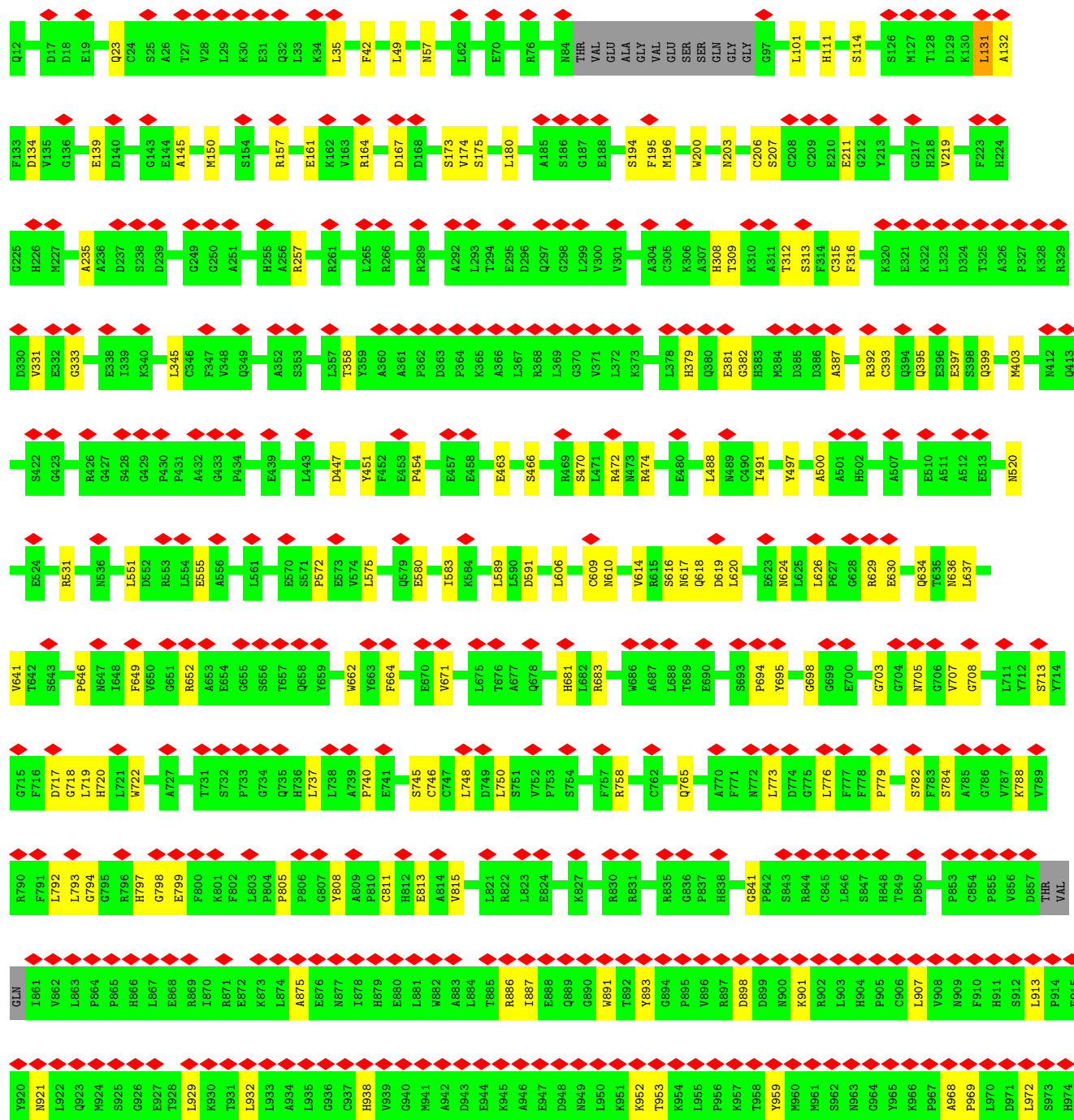
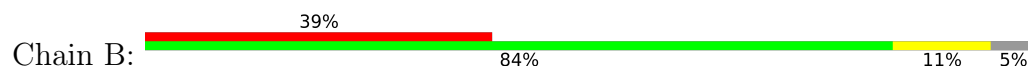


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1



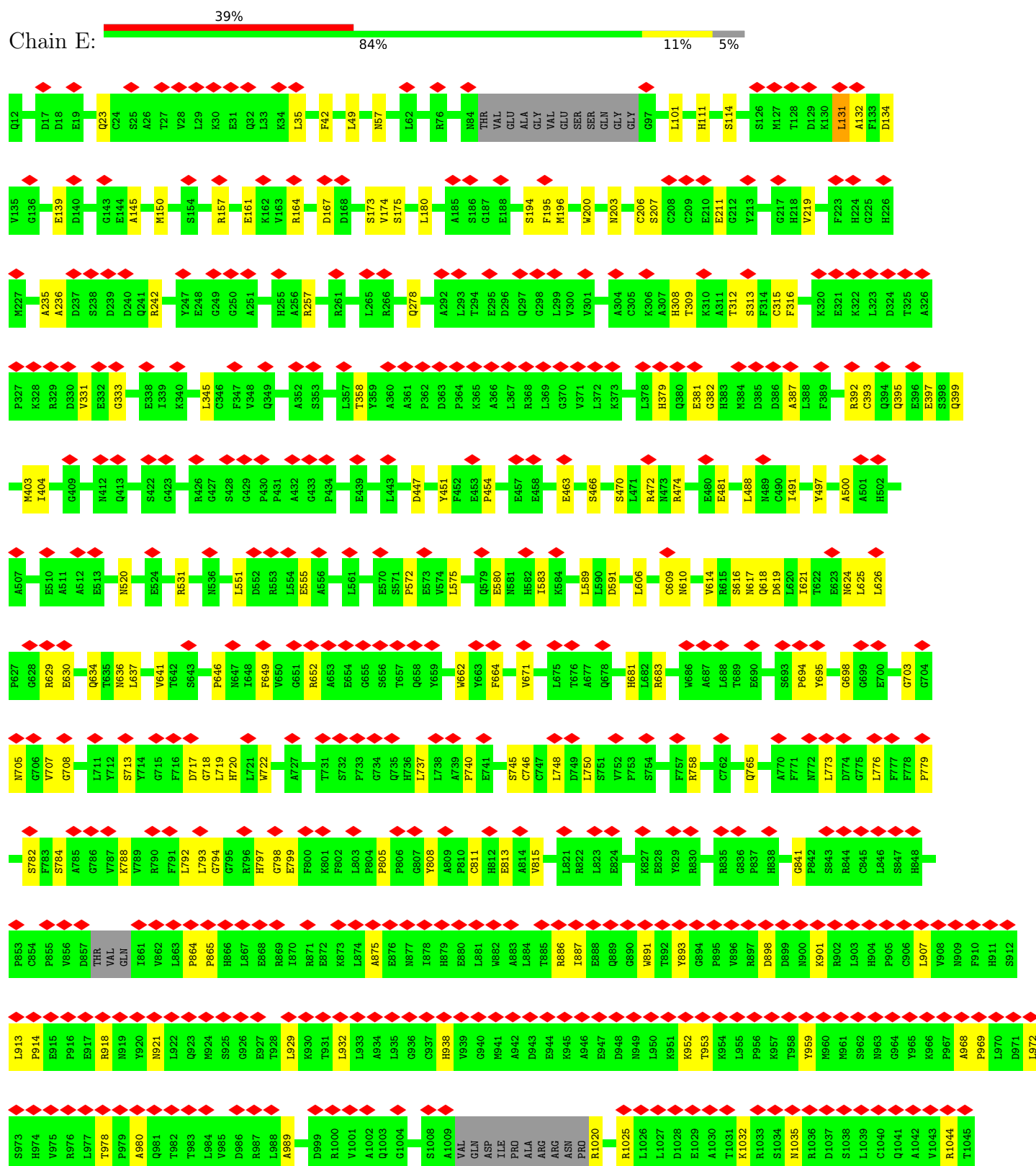






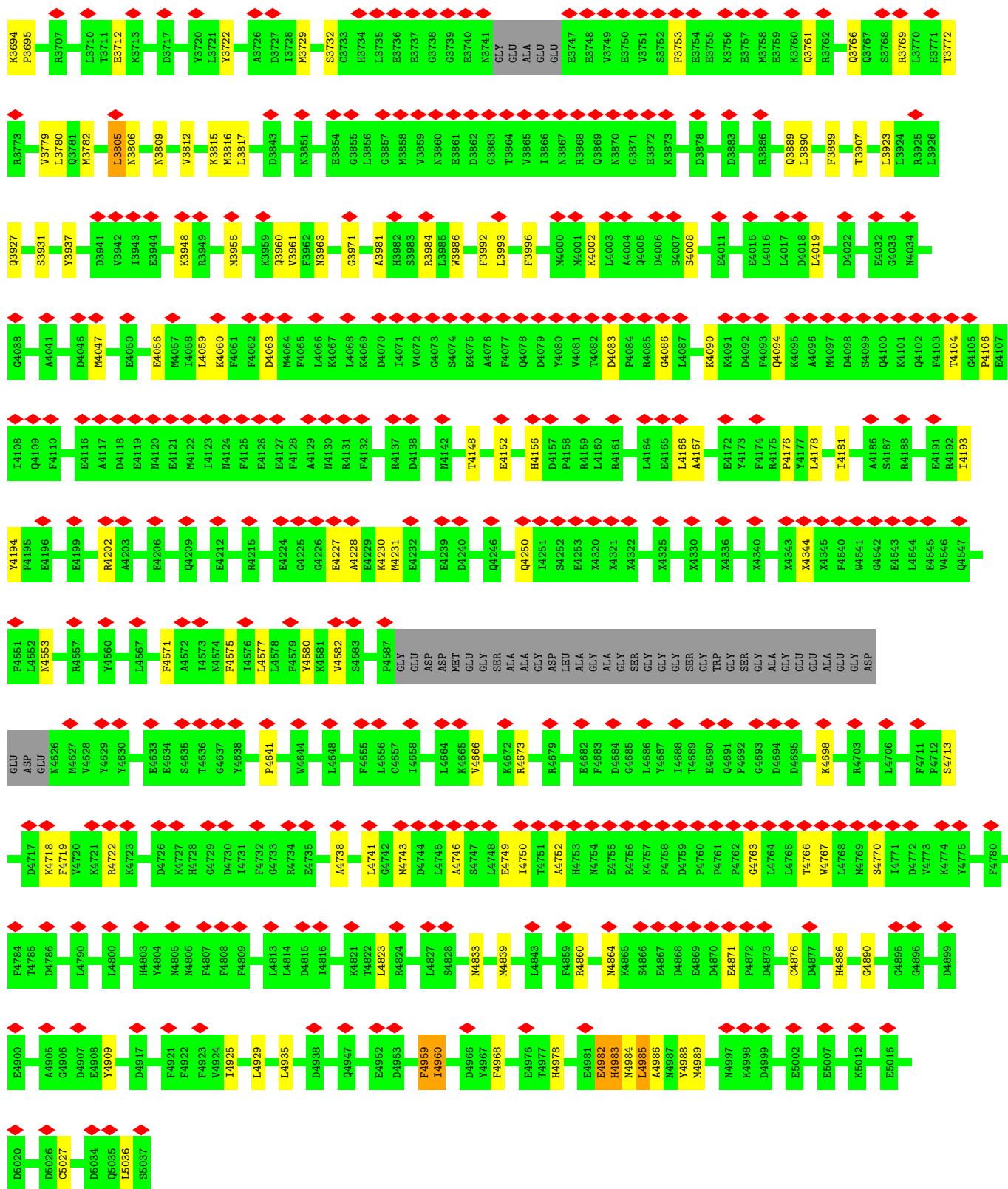
• Molecule 2: Ryanodine receptor 1

Chain E:





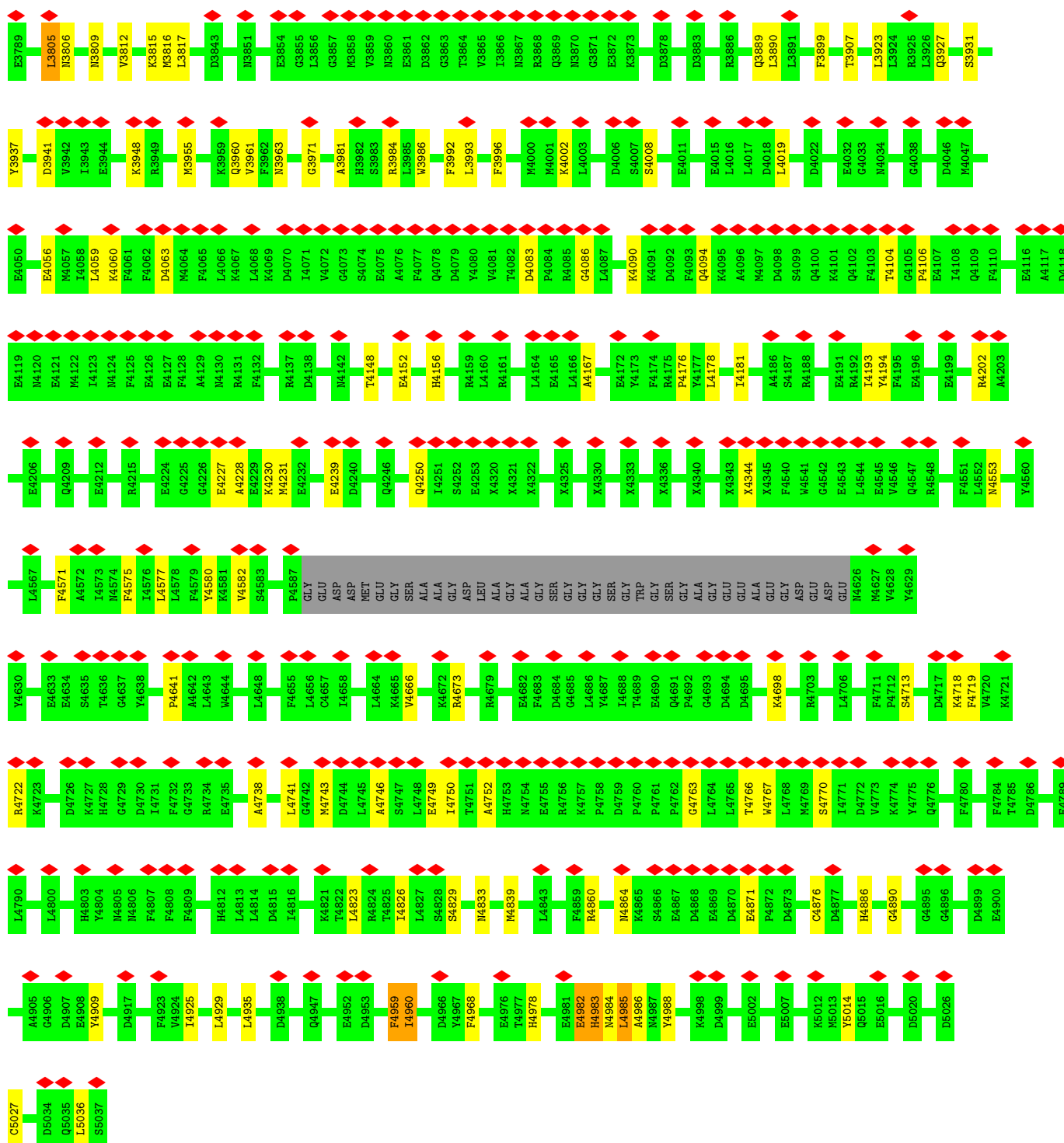
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X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3518	X3519	X3520	X3433	X3434	X3435	X3436	X3437	X3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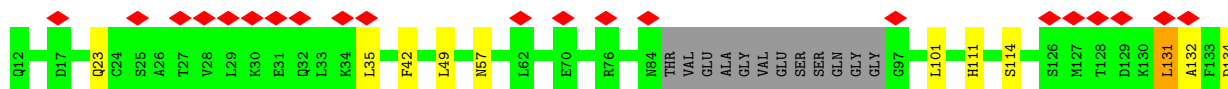


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D3717	X3606	X3400	X3337	X3265	X3046	X2952	K2890	E2830	K2770	X2672
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D3726	X3608	X3402	X3339	X3267	X3048	X2954	Q2892	ARG	Q2772	X2674
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		X3412	X3349	X3277	X3065	X2964	H2902	GLN	D2782	X2692
		X3413	X3350	X3278	X3066	X2965	P2903	ALA	E2783	X2693
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		X3493		X3337						
		X3494		X3338						
		X3495		X3339						
		X3496		X3340						
		X3497		X3341						
		X3498		X3342						
		X3499		X3343						
		X3500		X3344						
		X3501		X3345						
		X3502		X3346						
		X3503		X3347						
		X3504		X3348						
		X3505		X3349						
		X3506		X3350						
		X3507		X3351						
		X3508		X3352						
		X3509		X3353						
		X3510		X3354						
		X3511		X3355						
		X3512		X3356						
		X3513		X3357						
		X3514		X3358						
		X3515		X3359						
		X3516		X3360						
		X3517		X3361						
		X3518		X3362						
		X3519		X3363						
		X3520		X3364						
		X3521		X3365						
		X3522		X3366						
		X3523		X3367						
		X3524		X3368						
		X3525		X3369						
		X3526		X3370						
		X3527		X3371						
		X3528		X3372						
		X3529		X3373						
		X3530		X3374						
		X3531		X3375						
		X3532		X3376						
		X3533		X3377						
		X3534		X3378						
		X3535		X3379						
		X3536		X3380						
		X3537		X3381						
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		X3541		X3385						
		X3542		X3386						
		X3543		X3387						
		X3544		X3388						
		X3545		X3389						
		X3546		X3390						
		X3547		X3391						
		X3548		X3392						
		X3549		X3393						
		X3550		X3394						
		X3551		X3395						
		X3552		X3396						
		X3553		X3397						
		X3554		X3398						
		X3555		X3399						
		X3556		X3400						
		X3557		X3401						
		X3558		X3402						
		X3559		X3403						
		X3560		X3404						
		X3561		X3405						
		X3562		X3406						
		X3563		X3407						
		X3564		X3408						
		X3565		X3409						
		X3566		X3410						
		X3567		X3411						
		X3568		X3412						
		X3569		X3413						
		X3570		X3414						
		X3571		X3415						
		X3572		X3416						
		X3573		X3417						
		X3574		X3418						
		X3575		X3419						
		X3576		X3420						
		X3577		X3421						
		X3578		X3422						
		X3579		X3423						
		X3580		X3424						
		X3581		X3425						
		X3582		X3426						
		X3583		X3427						
		X3584		X3428						
		X3585		X3429						
		X3586		X3430						
		X3587		X3431						
		X3588		X3432						
		X3589		X3433						
		X3590		X3434						
		X3591		X3435						
		X3592		X3436						
		X3593		X3437						
		X3594		X3438						
		X3595								

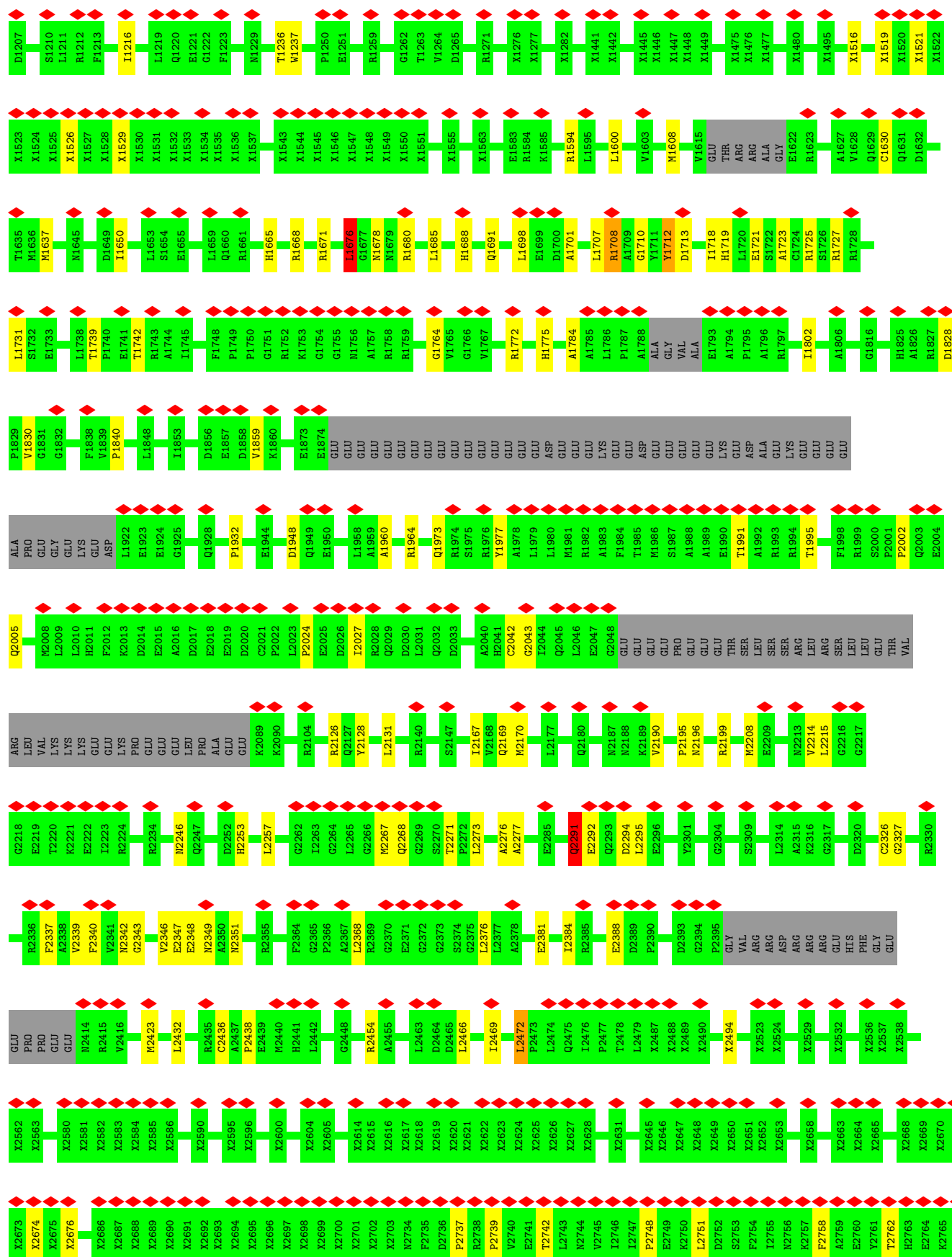


• Molecule 2: Ryanodine receptor 1

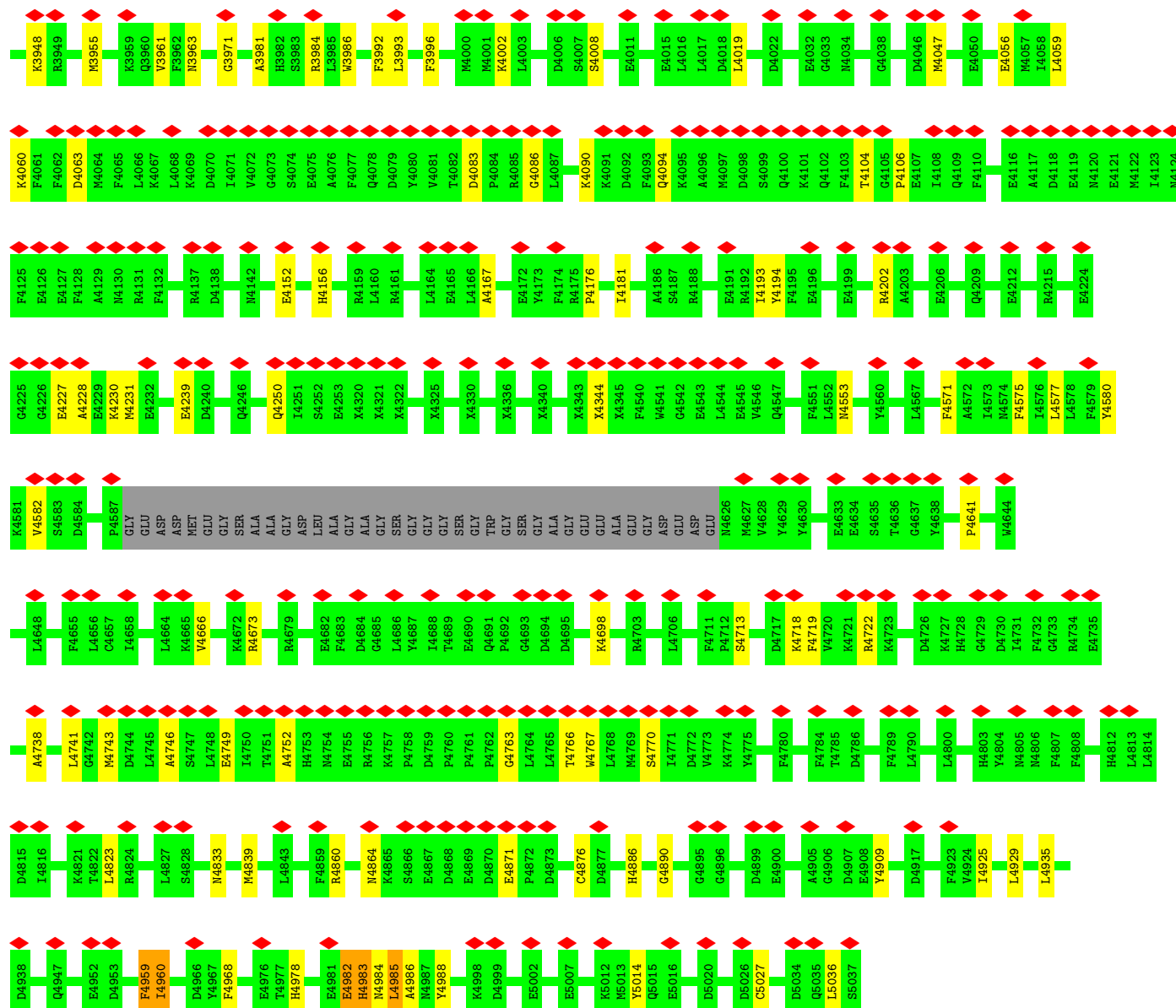
Chain G: 39% 84% 11% 5%







V3812	L3710	X3600	X3401	X3338	X3266	X3194	X3047	X2953	K2891	GLU	Q2771
X3815	T3711	X3606	X3402	X3339	X3267	X3195	X3048	X2954	Q2892	GLU	Q2772
X3816	E3712	X3607	X3403	X3340	X3268	X3196	X3049	X2955	E2893	ARG	Q2773
L3817	X3713	X3608	X3404	X3341	X3269	X3197	X3051	X2956	L2894	THR	Q2774
		X3609	X3405	X3342	X3270	X3198	X3052	X2957	E2895	GLU	Q2775
		X3610	X3406	X3343	X3271	X3199	X3053	X2958	L2896	LYS	Q2776
		X3611	X3407	X3344	X3272	X3200	X3057	X2959	A2897	LYS	Q2777
		X3612	X3408	X3345	X3273			X2960	K2897	THR	Q2778
		X3613	X3409	X3346	X3274			X2961	Q2898	ARG	Q2779
			X3410	X3347	X3275	X3203	X3060	X2962	Q2899	LYS	E2779
			X3411	X3348	X3276	X3204	X3061	X2963	Q2900	ILE	E2780
			X3412	X3349	X3277	X3205	X3062	X2964	T2901	SER	E2781
			X3413	X3350	X3278	X3206	X3063		H2902	GLN	E2782
			X3414	X3351	X3279	X3207	X3134	X2968	P2903	ALA	E2783
			X3415	X3352	X3280	X3208	X3135	X2969	L2904	THR	E2784
			X3416	X3353	X3281	X3209	X3136	X2970	L2905	THR	E2785
			X3417	X3354	X3282	X3210	X3137		V2906	TVR	L2785
				X3355	X3283	X3211	X3138	X2973	Q2907	ASP	K2786
			X3421	X3356	X3284	X3212	X3139	X2974	P2908	ARG	T2787
			X3422	X3357	X3285	X3213	X3140	X2975	Y2908	GLU	H2788
				X3358	X3286	X3214	X3141	X2976	D2909	ALA	P2789
			X3433	X3359	X3287	X3215	X3142	X2996	T2910	THR	L2791
			X3434	X3360	X3288	X3216	X3143	X2997	L2911	TVR	E2792
			X3435	X3363	X3289	X3217	X3144	X2998	T2912	ASP	P2793
			X3436	X3364	X3290	X3218	X3145	X2999	A2913	THR	Y2794
				X3365	X3291	X3219		X3000	K2914	PRD	E2795
			X3439	X3366	X3292	X3220	X3148	X3001	E2915	ARG	T2796
			X3441	X3367	X3293	X3221	X3149	X3002	K2916	GLU	T2797
			X3442	X3368	X3294	X3222	X3150		A2917	THR	F2797
			X3443	X3369	X3295	X3223	X3151	X3014	R2918	ALA	S2798
								X3015	D2919	THR	G2864
								X3016	R2920	TVR	E2799
									E2921	ASP	K2800
									K2922	ARG	D2801
									L2867	GLY	K2802
									S2868		E2803
									R2869		T2804
									Q2924		E2805
									E2925		R2806
									L2926		Q2807
									L2927		P2808
									K2928		L2809
									F2929		K2810
									L2930		E2811
									Q2931		S2812
									M2932		L2813
									N2933		K2814
									Q2934		E2815
									X2935		M2816
									Y2936		L2817
									Q2937		A2818
									T2938		Q2819
									X2939		E2820
									Q2942		W2821
									X2943		T2822
									Q2944		E2823
									X2945		E2824
									K2899		K2825
									X2946		A2826
									X2947		E2827
									X2948		E2828
									X2949		Q2829
									X2950		E2830
									X2951		
									X2952		



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	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.46	0/1123
1	F	0.20	0/834	0.46	0/1123
1	H	0.20	0/834	0.46	0/1123
1	J	0.21	0/834	0.46	0/1123
2	B	0.23	0/25428	0.53	7/34534 (0.0%)
2	E	0.23	0/25428	0.53	7/34534 (0.0%)
2	G	0.23	0/25428	0.53	7/34534 (0.0%)
2	I	0.23	0/25428	0.54	8/34534 (0.0%)
All	All	0.23	0/105048	0.53	29/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2190	VAL	N-CA-C	-8.75	104.21	112.96
2	I	2190	VAL	N-CA-C	-8.75	104.21	112.96
2	G	2190	VAL	N-CA-C	-8.75	104.21	112.96
2	B	2190	VAL	N-CA-C	-8.72	104.24	112.96
2	I	2242	ILE	N-CA-C	6.02	112.66	106.21
2	E	2472	LEU	CA-C-N	5.96	127.28	119.84
2	E	2472	LEU	C-N-CA	5.96	127.28	119.84
2	I	2472	LEU	CA-C-N	5.96	127.28	119.84
2	I	2472	LEU	C-N-CA	5.96	127.28	119.84
2	B	2472	LEU	CA-C-N	5.93	127.25	119.84
2	B	2472	LEU	C-N-CA	5.93	127.25	119.84
2	G	2472	LEU	CA-C-N	5.90	127.21	119.84
2	G	2472	LEU	C-N-CA	5.90	127.21	119.84
2	E	2291	GLN	CA-C-N	5.66	132.35	121.54
2	E	2291	GLN	C-N-CA	5.66	132.35	121.54
2	B	2291	GLN	CA-C-N	5.66	132.34	121.54
2	B	2291	GLN	C-N-CA	5.66	132.34	121.54
2	I	2291	GLN	CA-C-N	5.66	132.34	121.54
2	I	2291	GLN	C-N-CA	5.66	132.34	121.54
2	G	2291	GLN	CA-C-N	5.65	132.33	121.54
2	G	2291	GLN	C-N-CA	5.65	132.33	121.54
2	B	131	LEU	CA-CB-CG	5.12	134.20	116.30
2	E	131	LEU	CA-CB-CG	5.12	134.20	116.30
2	G	131	LEU	CA-CB-CG	5.12	134.20	116.30
2	I	131	LEU	CA-CB-CG	5.11	134.18	116.30
2	B	4960	ILE	N-CA-C	-5.03	107.48	111.81
2	E	4960	ILE	N-CA-C	-5.03	107.48	111.81
2	I	4960	ILE	N-CA-C	-5.03	107.48	111.81
2	G	4960	ILE	N-CA-C	-5.02	107.49	111.81

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	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

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Mol	Chain	Res	Type	Group
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	624	ASN	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	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	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	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	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	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	11	0
1	F	818	0	824	12	0
1	H	818	0	824	9	0
1	J	818	0	824	11	0
2	B	29499	0	24757	276	0
2	E	29499	0	24757	274	0
2	G	29499	0	24757	265	0
2	I	29499	0	24757	270	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121272	0	102324	1096	0

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

All (1096) 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:G:2291:GLN:HB3	2:G:2294:ASP:H	1.51	0.76
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.51	0.75
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.51	0.74
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.57	0.70
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.57	0.69
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.57	0.69
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.57	0.68
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.75	0.68
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.75	0.68
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.75	0.67
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.76	0.67
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.76	0.66
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.75	0.66
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.31	0.66
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.31	0.66
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.31	0.65
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.76	0.65
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.31	0.65
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.76	0.65
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.80	0.63
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.82	0.62
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.82	0.62
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.62
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.65	0.62
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.73	0.62
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.73	0.62
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.73	0.61
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.82	0.61
1:F:35:LYS:HD3	2:E:636:ASN:HD21	1.65	0.61
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.61
1:H:35:LYS:HD3	2:G:636:ASN:HD21	1.65	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.61
2:I:379:HIS:HD2	2:I:382:GLY:H	1.49	0.61
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.82	0.61
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.82	0.61
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.82	0.61
1:A:35:LYS:HD3	2:B:636:ASN:HD21	1.65	0.61
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.83	0.60
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.73	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:HIS:HD2	2:B:382:GLY:H	1.49	0.60
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.60
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.84	0.60
2:E:379:HIS:HD2	2:E:382:GLY:H	1.49	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.67	0.60
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.82	0.60
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.82	0.59
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.84	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.83	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.59
2:I:331:VAL:HG12	2:I:333:GLY:H	1.67	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.59
2:E:626:LEU:HD23	2:E:630:GLU:H	1.68	0.59
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.59
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.84	0.58
2:E:331:VAL:HG12	2:E:333:GLY:H	1.67	0.58
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.84	0.58
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.84	0.58
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.58
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.58
2:I:626:LEU:HD23	2:I:630:GLU:H	1.68	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.67	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.58
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.86	0.58
2:G:379:HIS:HD2	2:G:382:GLY:H	1.49	0.58
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.58
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.36	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.86	0.57
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:626:LEU:HD23	2:G:630:GLU:H	1.68	0.57
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.40	0.57
2:B:626:LEU:HD23	2:B:630:GLU:H	1.68	0.57
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.87	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.40	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.57
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.57
2:B:652:ARG:HD3	2:B:773:LEU:HD13	1.87	0.57
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.57
2:I:315:CYS:SG	2:I:316:PHE:N	2.78	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.57
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.57
2:I:652:ARG:HD3	2:I:773:LEU:HD13	1.87	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.87	0.56
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.87	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.87	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.56
2:E:652:ARG:HD3	2:E:773:LEU:HD13	1.87	0.56
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.87	0.56
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.39	0.56
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.86	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.86	0.56
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.87	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.87	0.56
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.56
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.88	0.56
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.56
2:E:1076:ARG:HB3	2:E:1191:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.55
2:I:1671:ARG:HH21	2:I:1713:ASP:HB3	1.71	0.55
2:G:652:ARG:HD3	2:G:773:LEU:HD13	1.87	0.55
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.88	0.55
2:E:3993:LEU:HA	2:E:3996:PHE:HB2	1.88	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.55
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.87	0.55
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.40	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.55
2:G:1076:ARG:HB3	2:G:1191:VAL:HG23	1.89	0.55
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.89	0.55
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.89	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.89	0.55
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	1.88	0.55
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.89	0.55
2:I:3993:LEU:HA	2:I:3996:PHE:HB2	1.89	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.75	0.55
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.88	0.55
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.87	0.55
2:G:3993:LEU:HA	2:G:3996:PHE:HB2	1.89	0.55
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.40	0.55
2:B:1076:ARG:HB3	2:B:1191:VAL:HG23	1.88	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.75	0.55
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.40	0.55
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.40	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.40	0.55
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.55
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.88	0.55
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.40	0.55
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.89	0.54
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.40	0.54
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.89	0.54
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.72	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:E:1671:ARG:HH21	2:E:1713:ASP:HB3	1.71	0.54
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.75	0.54
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.88	0.54
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.40	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.40	0.54
2:G:1671:ARG:HH21	2:G:1713:ASP:HB3	1.71	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.75	0.54
2:B:3993:LEU:HA	2:B:3996:PHE:HB2	1.88	0.54
2:E:161:GLU:OE2	2:G:3984:ARG:NH2	2.41	0.54
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.40	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.88	0.54
2:B:1671:ARG:HH21	2:B:1713:ASP:HB3	1.71	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.41	0.54
2:E:3732:SER:O	2:E:3766:GLN:NE2	2.41	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.41	0.54
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.72	0.54
2:G:4960:ILE:HG21	2:G:4988:TYR:HE2	1.73	0.54
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.89	0.54
2:G:3732:SER:O	2:G:3766:GLN:NE2	2.41	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.80	0.53
2:I:3732:SER:O	2:I:3766:GLN:NE2	2.41	0.53
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.41	0.53
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.40	0.53
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.40	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.72	0.53
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.72	0.53
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.42	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.53
2:B:1052:ASN:ND2	2:B:1054:GLU:OE2	2.42	0.53
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.90	0.53
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.41	0.53
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.91	0.53
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.91	0.53
2:B:3732:SER:O	2:B:3766:GLN:NE2	2.41	0.53
2:B:4056:GLU:O	2:B:4060:LYS:N	2.36	0.53
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.53
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.89	0.53
2:B:161:GLU:OE2	2:E:3984:ARG:NH2	2.42	0.53
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.91	0.53
2:I:4960:ILE:HG21	2:I:4988:TYR:HE2	1.73	0.53
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.91	0.53
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.53
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.74	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.53
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.42	0.53
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.74	0.52
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.52
2:E:4960:ILE:HG21	2:E:4988:TYR:HE2	1.73	0.52
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.90	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:E:1052:ASN:ND2	2:E:1054:GLU:OE2	2.42	0.52
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.91	0.52
2:I:1052:ASN:ND2	2:I:1054:GLU:OE2	2.42	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.90	0.52
2:G:1052:ASN:ND2	2:G:1054:GLU:OE2	2.42	0.52
2:B:173:SER:OG	2:B:174:VAL:N	2.43	0.52
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.91	0.52
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.52
2:I:4056:GLU:O	2:I:4060:LYS:N	2.36	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.42	0.52
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.74	0.52
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.42	0.52
2:G:4090:LYS:O	2:G:4094:GLN:N	2.42	0.52
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.90	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.92	0.52
2:B:4960:ILE:HG21	2:B:4988:TYR:HE2	1.73	0.52
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.52
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.91	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:I:173:SER:OG	2:I:174:VAL:N	2.43	0.52
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.43	0.52
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:G:4056:GLU:O	2:G:4060:LYS:N	2.36	0.52
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.41	0.51
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.51
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.74	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.80	0.51
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.92	0.51
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.41	0.51
2:E:173:SER:OG	2:E:174:VAL:N	2.43	0.51
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.90	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.80	0.51
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.43	0.51
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.51
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.51
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.51
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.43	0.51
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.92	0.51
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.93	0.51
2:B:3984:ARG:NH2	2:I:161:GLU:OE2	2.43	0.51
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.43	0.51
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.92	0.51
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.93	0.51
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.92	0.51
2:B:2195:PRO:HB3	2:B:2246:ASN:HD21	1.76	0.51
2:E:2195:PRO:HB3	2:E:2246:ASN:HD21	1.76	0.51
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.93	0.51
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.93	0.51
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.44	0.51
2:G:173:SER:OG	2:G:174:VAL:N	2.43	0.51
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.50
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.43	0.50
2:I:3984:ARG:NH2	2:G:161:GLU:OE2	2.43	0.50
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.92	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.94	0.50
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.50
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.94	0.50
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.41	0.50
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.50
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.50
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.42	0.50
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.94	0.50
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.77	0.50
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.77	0.50
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.94	0.50
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.94	0.50
2:E:4059:LEU:O	2:E:4063:ASP:N	2.45	0.50
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.94	0.50
2:I:2195:PRO:HB3	2:I:2246:ASN:HD21	1.76	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:E:4056:GLU:O	2:E:4060:LYS:N	2.36	0.49
2:I:913:LEU:O	2:I:918:ARG:NH2	2.45	0.49
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.93	0.49
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.49
2:B:913:LEU:O	2:B:918:ARG:NH2	2.45	0.49
2:E:609:CYS:SG	2:E:610:ASN:N	2.85	0.49
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.94	0.49
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.49
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.49
2:G:609:CYS:SG	2:G:610:ASN:N	2.85	0.49
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.76	0.49
2:G:2195:PRO:HB3	2:G:2246:ASN:HD21	1.76	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.43	0.49
2:I:4059:LEU:O	2:I:4063:ASP:N	2.45	0.49
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.94	0.49
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.49
2:B:3753:PHE:HE2	2:B:4718:LYS:HB2	1.77	0.49
2:B:4059:LEU:O	2:B:4063:ASP:N	2.45	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.49
2:E:1991:THR:O	2:E:1995:THR:OG1	2.30	0.49
2:E:4090:LYS:O	2:E:4094:GLN:N	2.42	0.49
2:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.77	0.49
2:G:1991:THR:O	2:G:1995:THR:OG1	2.30	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.94	0.49
2:E:913:LEU:O	2:E:918:ARG:NH2	2.45	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.77	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.49
2:I:609:CYS:SG	2:I:610:ASN:N	2.85	0.49
2:I:3992:PHE:O	2:I:3996:PHE:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:913:LEU:O	2:G:918:ARG:NH2	2.45	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.93	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.49
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.36	0.49
2:I:132:ALA:HA	2:I:194:SER:HB2	1.95	0.49
2:G:132:ALA:HA	2:G:194:SER:HB2	1.95	0.49
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.49
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.49
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.94	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.76	0.49
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.49
2:E:2868:SER:O	2:E:2872:GLN:N	2.39	0.49
2:I:683:ARG:NH1	2:I:707:VAL:O	2.44	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.49
2:I:4090:LYS:O	2:I:4094:GLN:N	2.42	0.49
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.49
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.49
2:I:3753:PHE:HE2	2:I:4718:LYS:HB2	1.77	0.49
2:G:4059:LEU:O	2:G:4063:ASP:N	2.45	0.49
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.27	0.49
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.36	0.49
2:B:1991:THR:O	2:B:1995:THR:OG1	2.30	0.49
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.36	0.49
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.49
2:E:3753:PHE:HE2	2:E:4718:LYS:HB2	1.77	0.49
2:I:1991:THR:O	2:I:1995:THR:OG1	2.30	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.49
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.94	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.94	0.48
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.36	0.48
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.44	0.48
2:G:683:ARG:NH1	2:G:707:VAL:O	2.44	0.48
2:B:609:CYS:SG	2:B:610:ASN:N	2.85	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.48
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:G:3753:PHE:HE2	2:G:4718:LYS:HB2	1.78	0.48
2:E:132:ALA:HA	2:E:194:SER:HB2	1.95	0.48
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:B:132:ALA:HA	2:B:194:SER:HB2	1.95	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.48
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.47	0.48
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.29	0.48
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.48
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.47	0.48
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.48
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.96	0.48
2:B:683:ARG:NH1	2:B:707:VAL:O	2.44	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.42	0.48
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.47	0.48
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.48
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.96	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.48
2:I:1973:GLN:HE22	2:I:2005:GLN:HE22	1.62	0.48
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.42	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.41	0.48
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.48
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.79	0.48
2:B:929:LEU:HD23	2:B:932:LEU:HD12	1.96	0.48
2:B:4090:LYS:O	2:B:4094:GLN:N	2.42	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.47	0.48
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.44	0.48
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.47	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.39	0.48
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.79	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.47
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.44	0.47
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.47
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.47
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.47	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.47
2:B:1973:GLN:HE22	2:B:2005:GLN:HE22	1.62	0.47
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.32	0.47
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.47	0.47
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.32	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:1973:GLN:HE22	2:G:2005:GLN:HE22	1.62	0.47
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.47
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.79	0.47
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.97	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.47
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.96	0.47
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.96	0.47
2:B:2423:MET:HE3	2:B:2494:UNK:HA	1.97	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.79	0.47
2:I:929:LEU:HD23	2:I:932:LEU:HD12	1.96	0.47
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.47	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.97	0.47
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.96	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.79	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.96	0.47
2:B:2810:LYS:HB3	2:B:2814:LYS:HE3	1.97	0.47
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.47
2:E:1723:ALA:HB1	2:E:1775:HIS:HD2	1.80	0.47
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.79	0.47
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.96	0.47
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.47
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.97	0.47
2:B:219:VAL:O	2:B:392:ARG:NH1	2.48	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.32	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.47	0.47
2:G:219:VAL:O	2:G:392:ARG:NH1	2.48	0.47
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.29	0.47
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.32	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.97	0.47
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.29	0.47
2:E:1973:GLN:HE22	2:E:2005:GLN:HE22	1.62	0.47
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.42	0.47
2:I:219:VAL:O	2:I:392:ARG:NH1	2.48	0.47
2:I:345:LEU:HD22	2:I:387:ALA:HB1	1.97	0.47
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.47
2:E:345:LEU:HD22	2:E:387:ALA:HB1	1.97	0.47
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.88	0.47
2:E:2810:LYS:HB3	2:E:2814:LYS:HE3	1.97	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.88	0.47
2:I:2423:MET:HE3	2:I:2494:UNK:HA	1.97	0.47
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.79	0.47
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.97	0.47
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.47
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.47
2:B:345:LEU:HD22	2:B:387:ALA:HB1	1.97	0.46
2:B:1701:ALA:HB1	2:B:1830:VAL:HG22	1.97	0.46
2:B:1723:ALA:HB1	2:B:1775:HIS:HD2	1.80	0.46
2:B:3806:ASN:HA	2:B:3890:LEU:HD13	1.98	0.46
2:I:1701:ALA:HB1	2:I:1830:VAL:HG22	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.47	0.46
2:G:345:LEU:HD22	2:G:387:ALA:HB1	1.97	0.46
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.46
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.49	0.46
2:B:792:LEU:HD22	2:B:799:GLU:H	1.80	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.39	0.46
2:B:4826:ILE:O	2:B:4829:SER:OG	2.30	0.46
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.98	0.46
2:E:929:LEU:HD23	2:E:932:LEU:HD12	1.96	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.46
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.46
2:G:792:LEU:HD22	2:G:799:GLU:H	1.80	0.46
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.96	0.46
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.98	0.46
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.46
2:E:1701:ALA:HB1	2:E:1830:VAL:HG22	1.97	0.46
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.97	0.46
2:E:219:VAL:O	2:E:392:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.79	0.46
2:E:2423:MET:HE3	2:E:2494:UNK:HA	1.97	0.46
2:E:2913:ALA:HA	2:E:2916:LYS:HB2	1.98	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.97	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.47	0.46
2:G:2913:ALA:HA	2:G:2916:LYS:HB2	1.98	0.46
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.97	0.46
2:I:4982:GLU:HB3	2:I:4983:HIS:CD2	2.51	0.46
2:G:2810:LYS:HB3	2:G:2814:LYS:HE3	1.97	0.46
2:B:463:GLU:O	2:B:466:SER:OG	2.30	0.46
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.98	0.46
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.49	0.46
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.88	0.46
2:B:2913:ALA:HA	2:B:2916:LYS:HB2	1.98	0.46
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.98	0.46
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.28	0.46
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.98	0.46
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.97	0.46
2:G:1723:ALA:HB1	2:G:1775:HIS:HD2	1.80	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	3.04	0.46
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.98	0.46
2:B:1516:UNK:N	2:B:1529:UNK:O	2.49	0.46
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.46
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.48	0.46
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.98	0.46
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.46
2:I:3927:GLN:O	2:I:3931:SER:N	2.47	0.46
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.98	0.46
2:G:929:LEU:HD23	2:G:932:LEU:HD12	1.96	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.46
2:E:683:ARG:NH1	2:E:707:VAL:O	2.44	0.46
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.49	0.46
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.46
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.46
2:G:1516:UNK:N	2:G:1529:UNK:O	2.49	0.46
2:G:1701:ALA:HB1	2:G:1830:VAL:HG22	1.97	0.46
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.46
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.46
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.46
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.88	0.46
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.79	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.96	0.46
2:B:195:PHE:HB3	2:B:196:MET:HG2	1.98	0.46
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	1.98	0.46
2:B:3992:PHE:O	2:B:3996:PHE:N	2.43	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:4344:UNK:N	2:I:4909:TYR:OH	2.49	0.46
2:I:1516:UNK:N	2:I:1529:UNK:O	2.49	0.46
2:I:2913:ALA:HA	2:I:2916:LYS:HB2	1.98	0.46
2:G:2423:MET:HE3	2:G:2494:UNK:HA	1.97	0.46
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.81	0.45
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.81	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.45
2:I:2810:LYS:HB3	2:I:2814:LYS:HE3	1.97	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.45
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.49	0.45
2:I:3806:ASN:HA	2:I:3890:LEU:HD13	1.98	0.45
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	3.04	0.45
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.99	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.98	0.45
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.45
2:B:4982:GLU:HB3	2:B:4983:HIS:CD2	2.51	0.45
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.45
2:E:4982:GLU:HB3	2:E:4983:HIS:CD2	2.51	0.45
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.52	0.45
2:G:2346:VAL:HG13	2:G:2349:ASN:H	1.82	0.45
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	1.99	0.45
2:E:195:PHE:HB3	2:E:196:MET:HG2	1.98	0.45
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	1.98	0.45
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.49	0.45
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.49	0.45
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.99	0.45
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.97	0.45
2:I:4826:ILE:O	2:I:4829:SER:OG	2.30	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.49	0.45
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.99	0.45
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.45
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.49	0.45
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.82	0.45
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.49	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.28	0.45
2:G:3806:ASN:HA	2:G:3890:LEU:HD13	1.98	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.45
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.49	0.45
2:E:662:TRP:H	2:E:748:LEU:HB3	1.82	0.45
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.45
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	3.04	0.45
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.45
2:I:1723:ALA:HB1	2:I:1775:HIS:HD2	1.80	0.45
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.98	0.45
2:G:662:TRP:H	2:G:748:LEU:HB3	1.82	0.45
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.49	0.45
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.98	0.45
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.82	0.45
2:E:792:LEU:HD22	2:E:799:GLU:H	1.80	0.45
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	1.99	0.45
2:E:2346:VAL:HG13	2:E:2349:ASN:H	1.82	0.45
2:I:792:LEU:HD22	2:I:799:GLU:H	1.80	0.45
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	1.98	0.45
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.99	0.45
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.50	0.45
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.50	0.45
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.52	0.45
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.98	0.45
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.99	0.45
2:E:3806:ASN:HA	2:E:3890:LEU:HD13	1.98	0.45
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.50	0.45
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	1.99	0.45
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.52	0.45
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.99	0.45
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.50	0.45
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.99	0.45
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.49	0.45
2:G:4982:GLU:HB3	2:G:4983:HIS:CD2	2.51	0.45
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.97	0.45
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.50	0.45
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	1.99	0.45
2:G:4047:MET:HE3	2:G:4047:MET:HB2	1.93	0.45
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.50	0.44
2:I:195:PHE:HB3	2:I:196:MET:HG2	1.98	0.44
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.00	0.44
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.99	0.44
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.99	0.44
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.77	0.44
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.35	0.44
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.50	0.44
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.99	0.44
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.99	0.44
2:E:875:ALA:HB1	2:E:921:ASN:HB3	1.99	0.44
2:E:3927:GLN:O	2:E:3931:SER:N	2.47	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.44
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.44
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	2.00	0.44
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.81	0.44
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.82	0.44
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.00	0.44
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	2.00	0.44
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.99	0.44
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.35	0.44
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.81	0.44
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.98	0.44
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.44
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.99	0.44
1:F:55:VAL:HA	2:E:1784:ALA:HA	2.00	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.47	0.44
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.50	0.44
2:E:4047:MET:HE3	2:E:4047:MET:HB2	1.93	0.44
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.44
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.99	0.44
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.52	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.80	0.44
2:B:4344:UNK:N	2:G:4909:TYR:OH	2.50	0.44
2:E:463:GLU:O	2:E:466:SER:OG	2.30	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.44
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	2.00	0.44
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.00	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.71	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.82	0.44
2:G:3941:ASP:OD1	2:G:3941:ASP:N	2.50	0.44
2:G:4886:HIS:O	2:G:4890:GLY:N	2.50	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.53	0.44
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	2.00	0.44
2:I:875:ALA:HB1	2:I:921:ASN:HB3	1.99	0.44
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	1.99	0.44
2:I:2902:HIS:HB3	2:I:2905:LEU:HG	2.00	0.44
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.30	0.44
2:B:875:ALA:HB1	2:B:921:ASN:HB3	1.99	0.44
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.51	0.44
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	1.99	0.44
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.98	0.44
2:E:3729:MET:O	2:E:3732:SER:OG	2.35	0.44
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.43	0.44
2:G:875:ALA:HB1	2:G:921:ASN:HB3	1.99	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.50	0.44
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.44
2:B:662:TRP:H	2:B:748:LEU:HB3	1.82	0.44
2:B:811:CYS:HB3	2:B:815:VAL:HG11	2.00	0.44
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.50	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.44
2:I:2868:SER:O	2:I:2872:GLN:N	2.39	0.44
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	2.00	0.44
2:B:4909:TYR:OH	2:G:4344:UNK:N	2.51	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.71	0.43
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	2.00	0.43
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.51	0.43
2:G:111:HIS:HD2	2:G:114:SER:H	1.65	0.43
2:G:4181:ILE:HG23	2:G:4193:ILE:HB	2.00	0.43
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.43
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.99	0.43
2:E:811:CYS:HB3	2:E:815:VAL:HG11	2.00	0.43
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.51	0.43
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.00	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.84	0.43
2:E:4713:SER:HA	2:E:4718:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.82	0.43
2:G:195:PHE:HB3	2:G:196:MET:HG2	1.98	0.43
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.00	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.43
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.00	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:B:4989:MET:HE3	2:B:4989:MET:HB3	1.92	0.43
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.00	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.53	0.43
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.43
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.77	0.43
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.29	0.43
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.50	0.43
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.00	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.99	0.43
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.01	0.43
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.00	0.43
2:E:3992:PHE:O	2:E:3996:PHE:N	2.43	0.43
2:E:4741:LEU:HB2	2:E:4743:MET:HE2	2.00	0.43
2:I:662:TRP:H	2:I:748:LEU:HB3	1.82	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.53	0.43
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.00	0.43
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.50	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.53	0.43
2:B:938:HIS:N	2:B:1054:GLU:O	2.52	0.43
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.43
2:E:4989:MET:HE3	2:E:4989:MET:HB3	1.92	0.43
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.43
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.00	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.43
2:G:811:CYS:HB3	2:G:815:VAL:HG11	2.00	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.82	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.84	0.43
2:E:111:HIS:HD2	2:E:114:SER:H	1.66	0.43
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.00	0.43
2:I:4181:ILE:HG23	2:I:4193:ILE:HB	2.00	0.43
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.84	0.43
2:E:134:ASP:N	2:E:134:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3761:GLN:NE2	2:E:4750:ILE:O	2.50	0.43
2:I:811:CYS:HB3	2:I:815:VAL:HG11	2.00	0.43
2:G:180:LEU:O	2:G:200:TRP:NE1	2.43	0.43
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.51	0.43
2:G:4713:SER:HA	2:G:4718:LYS:HE2	2.00	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.43
2:B:4738:ALA:HA	2:B:4743:MET:HE3	2.00	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.84	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.00	0.43
2:B:111:HIS:HD2	2:B:114:SER:H	1.65	0.43
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.43
2:B:1152:MET:HB2	2:B:1161:ILE:HB	2.00	0.43
2:B:4713:SER:HA	2:B:4718:LYS:HE2	2.00	0.43
2:E:938:HIS:N	2:E:1054:GLU:O	2.52	0.43
2:E:4181:ILE:HG23	2:E:4193:ILE:HB	2.00	0.43
2:I:111:HIS:HD2	2:I:114:SER:H	1.65	0.43
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.43
2:I:4713:SER:HA	2:I:4718:LYS:HE2	2.00	0.43
2:I:4738:ALA:HA	2:I:4743:MET:HE3	2.00	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.43
2:G:3927:GLN:O	2:G:3931:SER:N	2.47	0.43
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.84	0.43
2:B:1936:LYS:O	2:B:1940:CYS:N	2.48	0.43
2:B:2170:MET:HG3	2:B:2214:VAL:HG12	2.01	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.28	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.43
2:E:4909:TYR:OH	2:I:4344:UNK:N	2.52	0.43
2:I:3729:MET:O	2:I:3732:SER:OG	2.35	0.43
2:G:1101:ARG:HG2	2:G:1125:ASN:HA	2.01	0.43
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.72	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.00	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.42
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.00	0.42
2:I:4181:ILE:HG13	2:I:4988:TYR:CE1	2.54	0.42
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.30	0.42
2:G:1152:MET:HB2	2:G:1161:ILE:HB	2.00	0.42
2:G:2438:PRO:HG2	2:G:2454:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.50	0.42
2:B:4181:ILE:HG13	2:B:4988:TYR:CE1	2.54	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:4886:HIS:O	2:E:4890:GLY:N	2.50	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.01	0.42
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.46	0.42
2:I:2170:MET:HG3	2:I:2214:VAL:HG12	2.01	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.46	0.42
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.49	0.42
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.93	0.42
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.42
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	2.02	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.02	0.42
2:B:4741:LEU:HB2	2:B:4743:MET:HE2	2.00	0.42
2:E:893:TYR:HD1	2:E:907:LEU:HB2	1.85	0.42
2:E:2170:MET:HG3	2:E:2214:VAL:HG12	2.01	0.42
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.00	0.42
2:E:4181:ILE:HG13	2:E:4988:TYR:CE1	2.54	0.42
2:E:4250:GLN:O	2:E:4553:ASN:ND2	2.53	0.42
2:E:4738:ALA:HA	2:E:4743:MET:HE3	2.00	0.42
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.72	0.42
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	2.02	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.02	0.42
2:I:4959:PHE:CD1	2:I:4959:PHE:O	2.72	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.00	0.42
2:G:2170:MET:HG3	2:G:2214:VAL:HG12	2.01	0.42
2:G:4741:LEU:HB2	2:G:4743:MET:HE2	2.00	0.42
2:B:893:TYR:HD1	2:B:907:LEU:HB2	1.85	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.42
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.00	0.42
2:E:145:ALA:HA	2:E:175:SER:HB3	2.01	0.42
2:E:180:LEU:O	2:E:200:TRP:NE1	2.43	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.42
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.42
2:I:145:ALA:HA	2:I:175:SER:HB3	2.01	0.42
2:I:652:ARG:HD2	2:I:750:LEU:HB3	2.02	0.42
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.42	0.42
2:I:758:ARG:HH22	2:I:805:PRO:HD3	1.84	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.42
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.50	0.42
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.84	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.42
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.42
1:J:30:LEU:HB3	1:J:33:GLY:HA3	2.01	0.42
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.72	0.42
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.93	0.42
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.42
2:E:2438:PRO:HG2	2:E:2454:ARG:HB2	2.01	0.42
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.02	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.00	0.42
2:I:708:GLY:HA3	2:I:722:TRP:HB3	2.01	0.42
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.42
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.53	0.42
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.02	0.42
2:G:794:GLY:H	2:G:798:GLY:HA3	1.84	0.42
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.99	0.42
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.53	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.85	0.42
1:F:30:LEU:HB3	1:F:33:GLY:HA3	2.01	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.01	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.42
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.42
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.42
2:I:794:GLY:H	2:I:798:GLY:HA3	1.84	0.42
2:I:2432:LEU:O	2:I:2436:CYS:N	2.52	0.42
2:I:4741:LEU:HB2	2:I:4743:MET:HE2	2.00	0.42
2:G:793:LEU:HD12	2:G:797:HIS:H	1.85	0.42
2:G:4738:ALA:HA	2:G:4743:MET:HE3	2.00	0.42
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.42
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.42
2:B:1101:ARG:HG2	2:B:1125:ASN:HA	2.01	0.42
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.02	0.42
2:B:3927:GLN:O	2:B:3931:SER:N	2.47	0.42
2:B:4181:ILE:HG23	2:B:4193:ILE:HB	2.00	0.42
2:E:621:ILE:O	2:E:625:LEU:N	2.49	0.42
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.01	0.42
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.53	0.42
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2438:PRO:HG2	2:I:2454:ARG:HB2	2.01	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.42
2:G:621:ILE:O	2:G:625:LEU:N	2.49	0.42
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.02	0.42
1:A:30:LEU:HB3	1:A:33:GLY:HA3	2.01	0.42
2:B:652:ARG:HD2	2:B:750:LEU:HB3	2.02	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.02	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.02	0.42
2:B:2432:LEU:O	2:B:2436:CYS:N	2.52	0.42
2:B:4839:MET:HE2	2:E:4823:LEU:HD11	2.01	0.42
2:E:758:ARG:HH22	2:E:805:PRO:HD3	1.85	0.42
2:E:793:LEU:HD12	2:E:797:HIS:H	1.85	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.46	0.42
2:E:2432:LEU:O	2:E:2436:CYS:N	2.52	0.42
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.02	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.02	0.42
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.35	0.42
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.01	0.42
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.42
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.00	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.02	0.42
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.42	0.42
2:G:3992:PHE:O	2:G:3996:PHE:N	2.43	0.42
2:B:145:ALA:HA	2:B:175:SER:HB3	2.01	0.42
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.42
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.53	0.42
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	2.02	0.42
2:B:3729:MET:O	2:B:3732:SER:OG	2.35	0.42
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.38	0.42
2:I:4250:GLN:O	2:I:4553:ASN:ND2	2.53	0.42
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.42
2:G:914:PRO:O	2:G:918:ARG:N	2.52	0.42
2:B:758:ARG:HH22	2:B:805:PRO:HD3	1.84	0.42
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.42
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.30	0.42
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.42
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.42
2:G:893:TYR:HD1	2:G:907:LEU:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.93	0.42
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.42
2:G:2128:TYR:HB3	2:G:3669:PHE:HB3	2.02	0.42
2:G:4250:GLN:O	2:G:4553:ASN:ND2	2.53	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.03	0.41
2:B:4250:GLN:O	2:B:4553:ASN:ND2	2.53	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.85	0.41
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.41
2:G:758:ARG:HH22	2:G:805:PRO:HD3	1.84	0.41
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.85	0.41
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.86	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.02	0.41
2:B:2384:ILE:O	2:B:2388:GLU:N	2.53	0.41
2:I:621:ILE:O	2:I:625:LEU:N	2.49	0.41
2:I:2384:ILE:O	2:I:2388:GLU:N	2.53	0.41
2:G:652:ARG:HD2	2:G:750:LEU:HB3	2.02	0.41
1:F:21:THR:HA	1:F:49:ARG:HA	2.03	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:3556:UNK:O	2:B:3560:UNK:N	2.54	0.41
2:E:1101:ARG:HG2	2:E:1125:ASN:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.02	0.41
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.03	0.41
2:G:157:ARG:HH21	2:G:164:ARG:HD2	1.86	0.41
2:G:708:GLY:HA3	2:G:722:TRP:HB3	2.01	0.41
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.02	0.41
2:G:2384:ILE:O	2:G:2388:GLU:N	2.53	0.41
2:G:4181:ILE:HG13	2:G:4988:TYR:CE1	2.54	0.41
2:G:4719:PHE:HD1	2:G:4722:ARG:HD3	1.85	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.00	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:B:708:GLY:HA3	2:B:722:TRP:HB3	2.01	0.41
2:B:793:LEU:HD12	2:B:797:HIS:H	1.85	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.38	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.02	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.03	0.41
2:E:2384:ILE:O	2:E:2388:GLU:N	2.53	0.41
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.71	0.41
2:I:3556:UNK:O	2:I:3560:UNK:N	2.54	0.41
2:I:3941:ASP:OD1	2:I:3941:ASP:N	2.50	0.41
2:G:145:ALA:HA	2:G:175:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.02	0.41
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.02	0.41
1:H:30:LEU:HB3	1:H:33:GLY:HA3	2.01	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.85	0.41
2:B:2777:TYR:HD1	2:B:2791:LEU:HB2	1.86	0.41
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.54	0.41
2:B:4886:HIS:O	2:B:4890:GLY:N	2.50	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
2:E:708:GLY:HA3	2:E:722:TRP:HB3	2.01	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.02	0.41
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.49	0.41
1:F:21:THR:N	1:F:107:GLU:OE1	2.43	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.41
2:B:2438:PRO:HG2	2:B:2454:ARG:HB2	2.01	0.41
2:B:4156:HIS:CE1	2:B:5036:LEU:HD11	2.56	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.41
2:E:3556:UNK:O	2:E:3560:UNK:N	2.54	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.02	0.41
2:I:157:ARG:HH21	2:I:164:ARG:HD2	1.86	0.41
2:I:793:LEU:HD12	2:I:797:HIS:H	1.85	0.41
2:I:893:TYR:HD1	2:I:907:LEU:HB2	1.85	0.41
2:I:1101:ARG:HG2	2:I:1125:ASN:HA	2.01	0.41
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.93	0.41
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.85	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.41
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	2.02	0.41
2:B:1931:LEU:HD13	2:B:1935:VAL:HG11	2.03	0.41
2:B:3761:GLN:NE2	2:B:4750:ILE:O	2.50	0.41
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.85	0.41
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	2.02	0.41
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	2.02	0.41
2:I:3761:GLN:NE2	2:I:4750:ILE:O	2.50	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.03	0.41
1:A:21:THR:N	1:A:107:GLU:OE1	2.43	0.41
1:J:21:THR:HA	1:J:49:ARG:HA	2.03	0.41
2:B:2128:TYR:HB3	2:B:3669:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.36	0.41
2:E:652:ARG:HD2	2:E:750:LEU:HB3	2.02	0.41
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.54	0.41
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.03	0.41
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.41
2:I:4156:HIS:CE1	2:I:5036:LEU:HD11	2.56	0.41
2:G:938:HIS:N	2:G:1054:GLU:O	2.52	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.38	0.41
1:F:26:TYR:N	1:F:39:SER:OG	2.48	0.41
1:A:21:THR:HA	1:A:49:ARG:HA	2.03	0.41
2:B:157:ARG:HH21	2:B:164:ARG:HD2	1.86	0.41
2:B:180:LEU:O	2:B:200:TRP:NE1	2.43	0.41
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.03	0.41
2:B:4056:GLU:HG2	2:B:4166:LEU:HD23	2.03	0.41
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.53	0.41
2:B:4823:LEU:HD11	2:I:4839:MET:HE2	2.01	0.41
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.38	0.41
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	2.02	0.41
2:E:3722:TYR:CZ	2:E:3782:MET:HE3	2.56	0.41
2:E:4719:PHE:HD1	2:E:4722:ARG:HD3	1.85	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.91	0.41
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.02	0.41
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.41
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.02	0.41
2:I:2777:TYR:HD1	2:I:2791:LEU:HB2	1.86	0.41
2:I:4823:LEU:HD11	2:G:4839:MET:HE2	2.02	0.41
2:G:236:ALA:HA	2:G:242:ARG:HD2	2.03	0.41
2:G:953:THR:HB	2:G:969:PRO:HD2	2.03	0.41
2:G:2777:TYR:HD1	2:G:2791:LEU:HB2	1.86	0.41
2:G:3556:UNK:O	2:G:3560:UNK:N	2.54	0.41
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.85	0.41
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.71	0.41
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.86	0.41
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.54	0.41
2:B:4148:THR:HG21	2:B:4178:LEU:HD21	2.03	0.41
2:B:4719:PHE:HD1	2:B:4722:ARG:HD3	1.85	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.41
2:E:1931:LEU:HD13	2:E:1935:VAL:HG11	2.03	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.03	0.41
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.02	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:I:2128:TYR:HB3	2:I:3669:PHE:HB3	2.02	0.41
2:I:4719:PHE:HD1	2:I:4722:ARG:HD3	1.85	0.41
2:G:2432:LEU:O	2:G:2436:CYS:N	2.52	0.41
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.02	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:B:3722:TYR:CZ	2:B:3782:MET:HE3	2.56	0.40
2:E:206:CYS:SG	2:E:207:SER:N	2.94	0.40
2:E:278:GLN:N	2:E:315:CYS:SG	2.91	0.40
2:E:953:THR:HB	2:E:969:PRO:HD2	2.03	0.40
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.96	0.40
2:E:4839:MET:HE2	2:G:4823:LEU:HD11	2.02	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.94	0.40
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.03	0.40
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.85	0.40
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.02	0.40
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.96	0.40
1:J:7:ILE:HD13	1:J:71:ARG:HG2	2.04	0.40
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.03	0.40
2:B:953:THR:HB	2:B:969:PRO:HD2	2.03	0.40
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.02	0.40
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	2.02	0.40
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.49	0.40
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.35	0.40
2:E:1171:SER:OG	2:E:1175:SER:N	2.44	0.40
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.02	0.40
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.03	0.40
2:I:232:THR:OG1	2:I:233:ILE:N	2.55	0.40
2:I:1931:LEU:HD13	2:I:1935:VAL:HG11	2.03	0.40
2:I:1936:LYS:O	2:I:1940:CYS:N	2.48	0.40
2:I:4886:HIS:O	2:I:4890:GLY:N	2.50	0.40
2:G:404:ILE:HD13	2:G:481:GLU:HG3	2.03	0.40
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.85	0.40
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.40
2:G:4156:HIS:CE1	2:G:5036:LEU:HD11	2.56	0.40
1:A:7:ILE:HD13	1:A:71:ARG:HG2	2.04	0.40
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.85	0.40
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.04	0.40
2:E:404:ILE:HD13	2:E:481:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.77	0.40
2:E:4056:GLU:HG2	2:E:4166:LEU:HD23	2.03	0.40
2:I:485:SER:O	2:I:489:ASN:N	2.44	0.40
2:I:914:PRO:O	2:I:918:ARG:N	2.52	0.40
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.54	0.40
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.03	0.40
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.03	0.40
2:B:206:CYS:SG	2:B:207:SER:N	2.94	0.40
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.86	0.40
2:E:914:PRO:O	2:E:918:ARG:N	2.52	0.40
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	2.02	0.40
2:E:2777:TYR:HD1	2:E:2791:LEU:HB2	1.86	0.40
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.85	0.40
2:I:236:ALA:HA	2:I:242:ARG:HD2	2.03	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.40
2:I:4148:THR:HG21	2:I:4178:LEU:HD21	2.03	0.40
2:I:4984:ASN:C	2:I:4986:ALA:N	2.80	0.40
2:G:206:CYS:SG	2:G:207:SER:N	2.94	0.40
2:G:2674:UNK:O	2:G:2676:UNK:N	2.55	0.40
2:B:2776:SER:OG	2:B:2786:LYS:O	2.39	0.40
2:B:4060:LYS:NZ	2:B:4107:GLU:OE2	2.41	0.40
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.94	0.40
2:E:157:ARG:HH21	2:E:164:ARG:HD2	1.86	0.40
2:E:236:ALA:HA	2:E:242:ARG:HD2	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.37	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.55	0.40
2:I:953:THR:HB	2:I:969:PRO:HD2	2.03	0.40
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	43	77
2	E	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	43	77
2	G	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	43	77
2	I	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	43	77
All	All	13360/18096 (74%)	11956 (90%)	1376 (10%)	28 (0%)	44	77

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	4641	PRO
2	B	4982	GLU
2	B	4985	LEU
2	E	4641	PRO
2	E	4982	GLU
2	E	4985	LEU
2	I	4641	PRO
2	I	4982	GLU
2	I	4985	LEU
2	G	4641	PRO
2	G	4982	GLU
2	G	4985	LEU
2	B	1840	PRO
2	B	2292	GLU
2	E	1840	PRO
2	E	2292	GLU
2	I	1840	PRO
2	I	2292	GLU
2	G	1840	PRO

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Mol	Chain	Res	Type
2	G	2292	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2483 (100%)	10 (0%)	84	82
2	E	2493/3022 (82%)	2483 (100%)	10 (0%)	84	82
2	G	2493/3022 (82%)	2483 (100%)	10 (0%)	84	82
2	I	2493/3022 (82%)	2483 (100%)	10 (0%)	84	82
All	All	10324/12444 (83%)	10284 (100%)	40 (0%)	81	82

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	1600	LEU
2	B	1676	LEU
2	B	2339	VAL
2	B	3663	LEU
2	B	3805	LEU
2	B	4959	PHE
2	B	4983	HIS
2	B	4985	LEU
2	E	131	LEU
2	E	719	LEU
2	E	1600	LEU
2	E	1676	LEU

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Mol	Chain	Res	Type
2	E	2339	VAL
2	E	3663	LEU
2	E	3805	LEU
2	E	4959	PHE
2	E	4983	HIS
2	E	4985	LEU
2	I	131	LEU
2	I	719	LEU
2	I	1600	LEU
2	I	1676	LEU
2	I	2339	VAL
2	I	3663	LEU
2	I	3805	LEU
2	I	4959	PHE
2	I	4983	HIS
2	I	4985	LEU
2	G	131	LEU
2	G	719	LEU
2	G	1600	LEU
2	G	1676	LEU
2	G	2339	VAL
2	G	3663	LEU
2	G	3805	LEU
2	G	4959	PHE
2	G	4983	HIS
2	G	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	65	GLN
1	F	87	HIS
1	A	32	ASN
1	A	65	GLN
1	A	87	HIS
1	H	32	ASN
1	H	65	GLN
1	H	87	HIS
1	J	32	ASN
1	J	65	GLN
1	J	87	HIS

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	113	HIS
2	B	273	HIS
2	B	284	HIS
2	B	379	HIS
2	B	383	HIS
2	B	520	ASN
2	B	582	HIS
2	B	765	GLN
2	B	877	ASN
2	B	1220	GLN
2	B	1254	HIS
2	B	1611	HIS
2	B	1678	ASN
2	B	1691	GLN
2	B	1775	HIS
2	B	1861	GLN
2	B	1952	GLN
2	B	1973	GLN
2	B	2127	GLN
2	B	2260	ASN
2	B	2349	ASN
2	B	2858	GLN
2	B	3704	HIS
2	B	3767	GLN
2	B	3809	ASN
2	B	3814	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	4102	GLN
2	B	4246	GLN
2	B	4553	ASN
2	B	4691	GLN
2	B	4832	HIS
2	B	4949	GLN
2	B	4978	HIS
2	B	4987	ASN
2	B	5031	GLN

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Mol	Chain	Res	Type
2	E	57	ASN
2	E	113	HIS
2	E	273	HIS
2	E	284	HIS
2	E	379	HIS
2	E	383	HIS
2	E	520	ASN
2	E	765	GLN
2	E	877	ASN
2	E	1220	GLN
2	E	1254	HIS
2	E	1598	GLN
2	E	1611	HIS
2	E	1678	ASN
2	E	1691	GLN
2	E	1775	HIS
2	E	1861	GLN
2	E	1952	GLN
2	E	1973	GLN
2	E	2127	GLN
2	E	2260	ASN
2	E	2324	ASN
2	E	2349	ASN
2	E	2858	GLN
2	E	3704	HIS
2	E	3767	GLN
2	E	3809	ASN
2	E	3813	GLN
2	E	3814	GLN
2	E	3895	HIS
2	E	3896	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4102	GLN
2	E	4156	HIS
2	E	4246	GLN
2	E	4553	ASN
2	E	4691	GLN
2	E	4832	HIS
2	E	4949	GLN
2	E	4978	HIS

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Mol	Chain	Res	Type
2	E	4987	ASN
2	I	57	ASN
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	520	ASN
2	I	765	GLN
2	I	877	ASN
2	I	1220	GLN
2	I	1254	HIS
2	I	1598	GLN
2	I	1611	HIS
2	I	1678	ASN
2	I	1691	GLN
2	I	1775	HIS
2	I	1861	GLN
2	I	1952	GLN
2	I	1973	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	2349	ASN
2	I	2858	GLN
2	I	3704	HIS
2	I	3767	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3895	HIS
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	4102	GLN
2	I	4120	ASN
2	I	4156	HIS
2	I	4246	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4832	HIS
2	I	4949	GLN

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Mol	Chain	Res	Type
2	I	4978	HIS
2	I	4987	ASN
2	G	57	ASN
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	520	ASN
2	G	765	GLN
2	G	877	ASN
2	G	1220	GLN
2	G	1254	HIS
2	G	1598	GLN
2	G	1611	HIS
2	G	1678	ASN
2	G	1691	GLN
2	G	1775	HIS
2	G	1861	GLN
2	G	1952	GLN
2	G	1973	GLN
2	G	2127	GLN
2	G	2260	ASN
2	G	2349	ASN
2	G	2858	GLN
2	G	3704	HIS
2	G	3767	GLN
2	G	3809	ASN
2	G	3814	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	4102	GLN
2	G	4246	GLN
2	G	4553	ASN
2	G	4691	GLN
2	G	4832	HIS
2	G	4949	GLN
2	G	4978	HIS
2	G	4987	ASN

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.04
1	E	4345:UNK	C	4540:PHE	N	74.04
1	I	4345:UNK	C	4540:PHE	N	74.04
1	G	4345:UNK	C	4540:PHE	N	74.04
1	B	3613:UNK	C	3639:THR	N	46.14
1	E	3613:UNK	C	3639:THR	N	46.14
1	I	3613:UNK	C	3639:THR	N	46.14
1	G	3613:UNK	C	3639:THR	N	46.14
1	B	4253:GLU	C	4320:UNK	N	27.75
1	E	4253:GLU	C	4320:UNK	N	27.75
1	I	4253:GLU	C	4320:UNK	N	27.75
1	G	4253:GLU	C	4320:UNK	N	27.75
1	B	3163:UNK	C	3170:UNK	N	15.37
1	E	3163:UNK	C	3170:UNK	N	15.37
1	I	3163:UNK	C	3170:UNK	N	15.37
1	G	3163:UNK	C	3170:UNK	N	15.37
1	B	3468:UNK	C	3511:UNK	N	14.99
1	E	3468:UNK	C	3511:UNK	N	14.99
1	I	3468:UNK	C	3511:UNK	N	14.99
1	G	3468:UNK	C	3511:UNK	N	14.99
1	B	3063:UNK	C	3134:UNK	N	14.98
1	E	3063:UNK	C	3134:UNK	N	14.98
1	I	3063:UNK	C	3134:UNK	N	14.98
1	G	3063:UNK	C	3134:UNK	N	14.98
1	B	2703:UNK	C	2734:ASN	N	14.84
1	E	2703:UNK	C	2734:ASN	N	14.84
1	I	2703:UNK	C	2734:ASN	N	14.84
1	G	2703:UNK	C	2734:ASN	N	14.84
1	B	3236:UNK	C	3241:UNK	N	13.23
1	E	3236:UNK	C	3241:UNK	N	13.23
1	I	3236:UNK	C	3241:UNK	N	13.23
1	G	3236:UNK	C	3241:UNK	N	13.23
1	B	2976:UNK	C	2995:UNK	N	12.15
1	E	2976:UNK	C	2995:UNK	N	12.15
1	I	2976:UNK	C	2995:UNK	N	12.15
1	G	2976:UNK	C	2995:UNK	N	12.15
1	B	1564:UNK	C	1573:MET	N	11.93
1	E	1564:UNK	C	1573:MET	N	11.93
1	I	1564:UNK	C	1573:MET	N	11.93
1	G	1564:UNK	C	1573:MET	N	11.93
1	B	3254:UNK	C	3261:UNK	N	7.98
1	E	3254:UNK	C	3261:UNK	N	7.98
1	I	3254:UNK	C	3261:UNK	N	7.98

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3254:UNK	C	3261:UNK	N	7.98
1	B	1297:UNK	C	1430:UNK	N	5.84
1	E	1297:UNK	C	1430:UNK	N	5.84
1	I	1297:UNK	C	1430:UNK	N	5.84
1	G	1297:UNK	C	1430:UNK	N	5.84
1	B	2479:LEU	C	2487:UNK	N	3.80
1	E	2479:LEU	C	2487:UNK	N	3.80
1	I	2479:LEU	C	2487:UNK	N	3.80
1	G	2479:LEU	C	2487:UNK	N	3.80
1	B	2939:ARG	C	2942:UNK	N	3.24
1	E	2939:ARG	C	2942:UNK	N	3.24
1	I	2939:ARG	C	2942:UNK	N	3.24
1	G	2939:ARG	C	2942:UNK	N	3.24

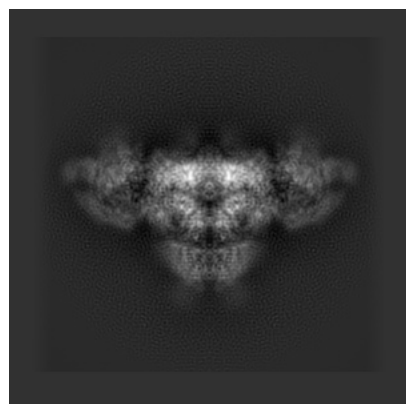
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8395. These allow visual inspection of the internal detail of the map and identification of artifacts.

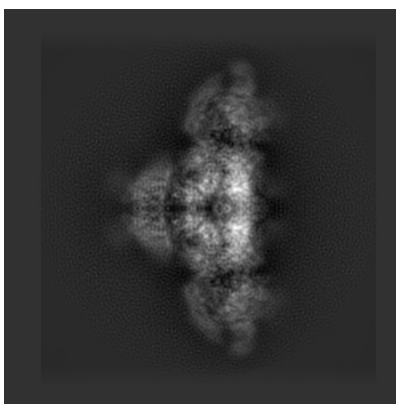
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

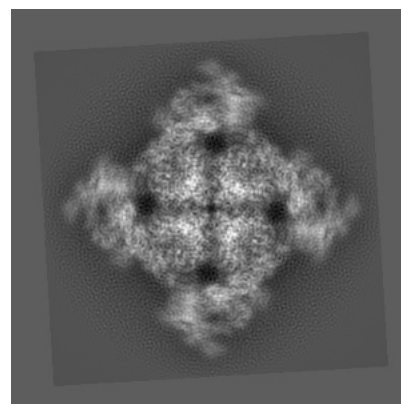
6.1.1 Primary map



X

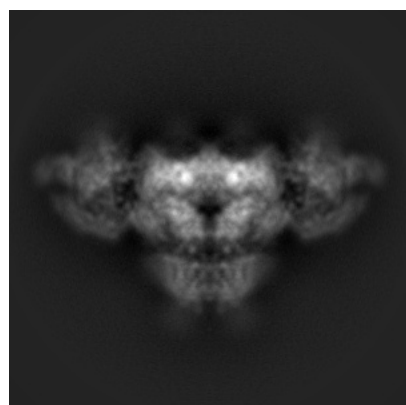


Y

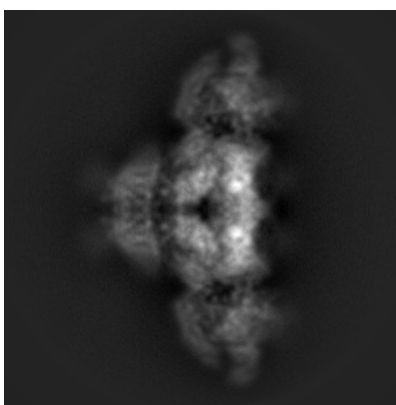


Z

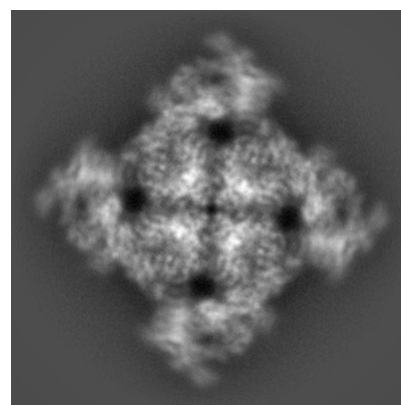
6.1.2 Raw map



X



Y

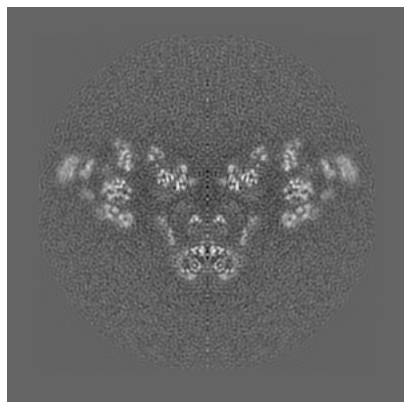


Z

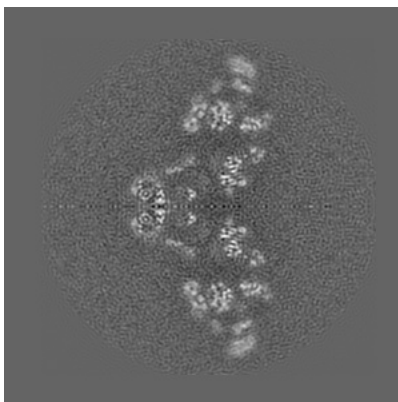
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

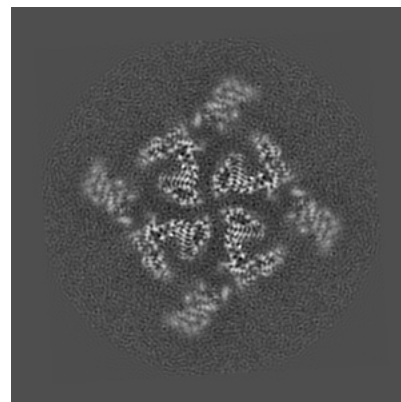
6.2.1 Primary map



X Index: 200

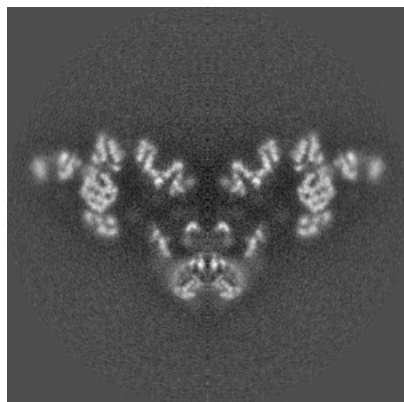


Y Index: 200

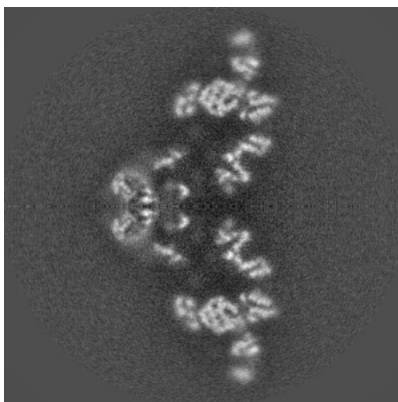


Z Index: 200

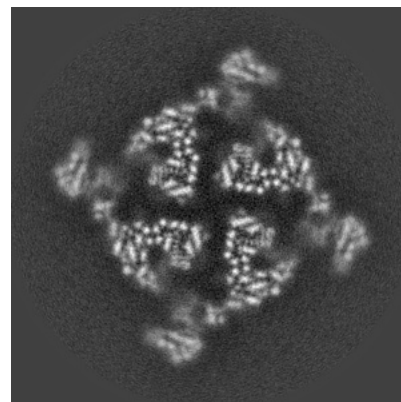
6.2.2 Raw map



X Index: 168



Y Index: 168

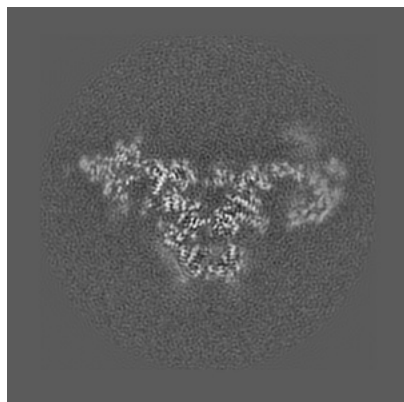


Z Index: 168

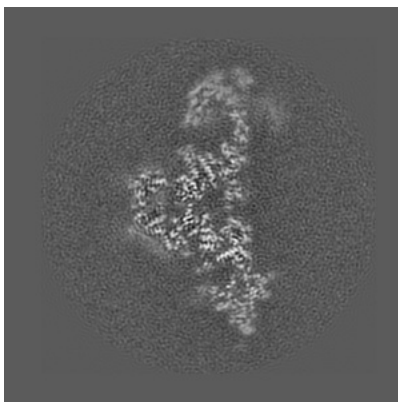
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

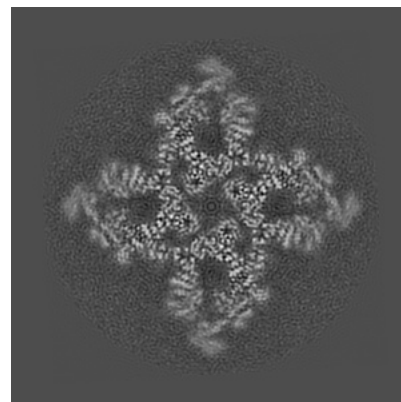
6.3.1 Primary map



X Index: 217

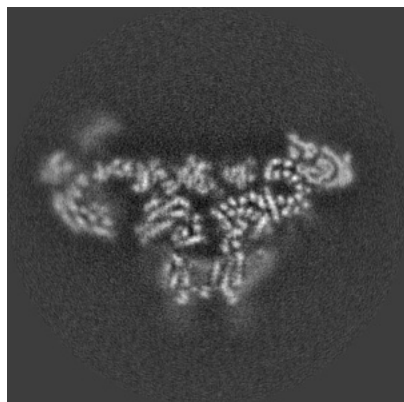


Y Index: 183

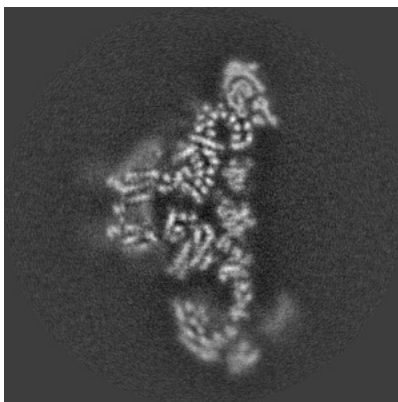


Z Index: 232

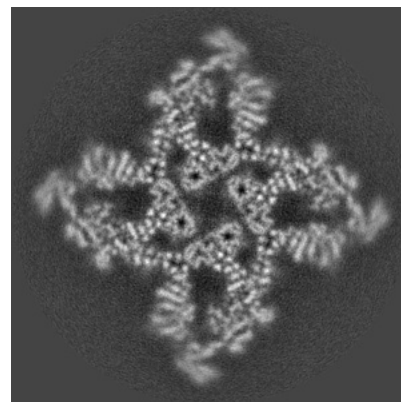
6.3.2 Raw map



X Index: 147



Y Index: 189

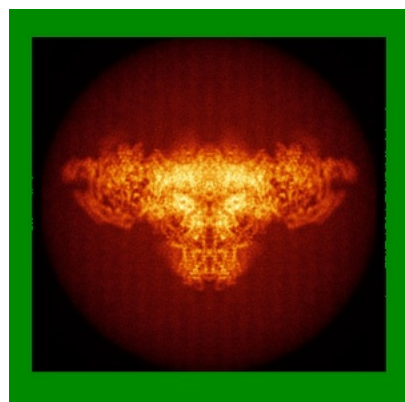


Z Index: 195

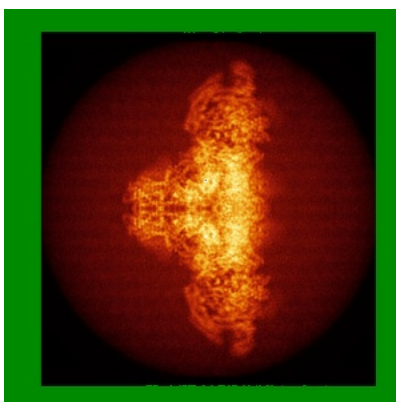
The images above show the largest variance slices of the map in three orthogonal directions.

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

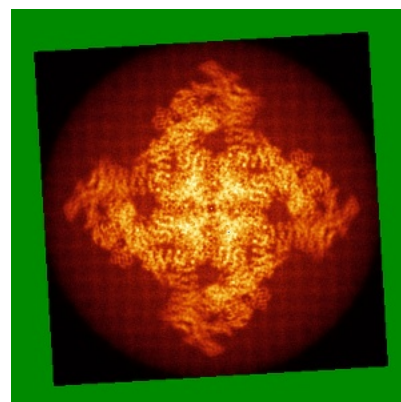
6.4.1 Primary map



X



Y

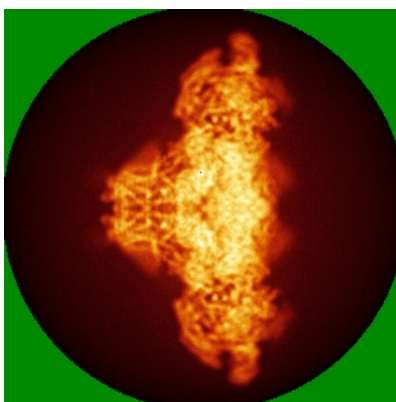


Z

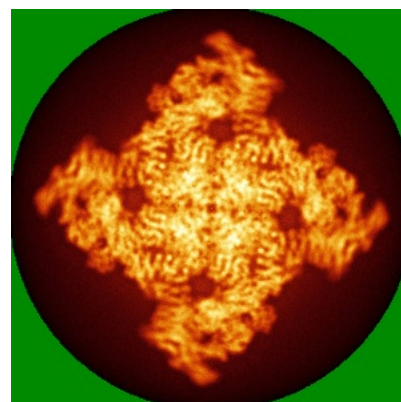
6.4.2 Raw map



X



Y

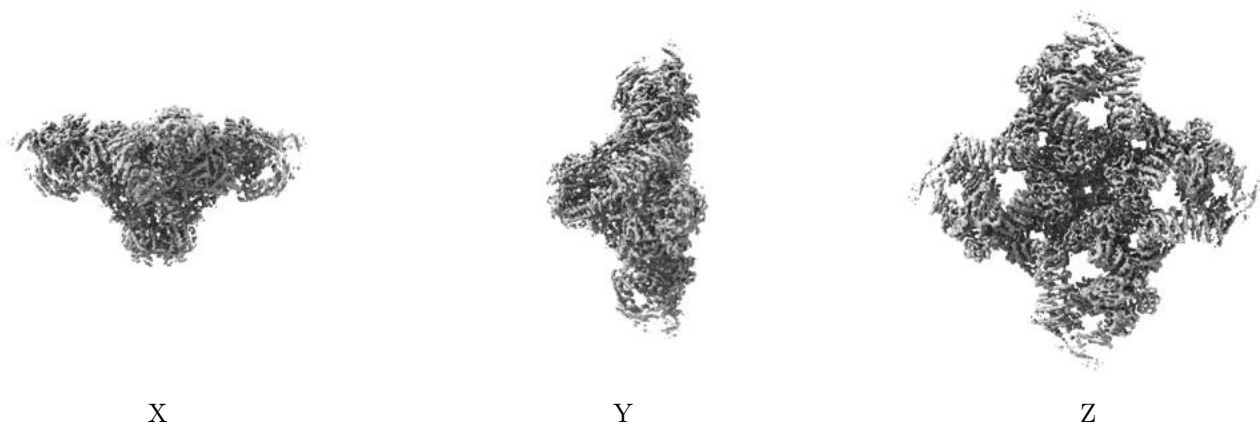


Z

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

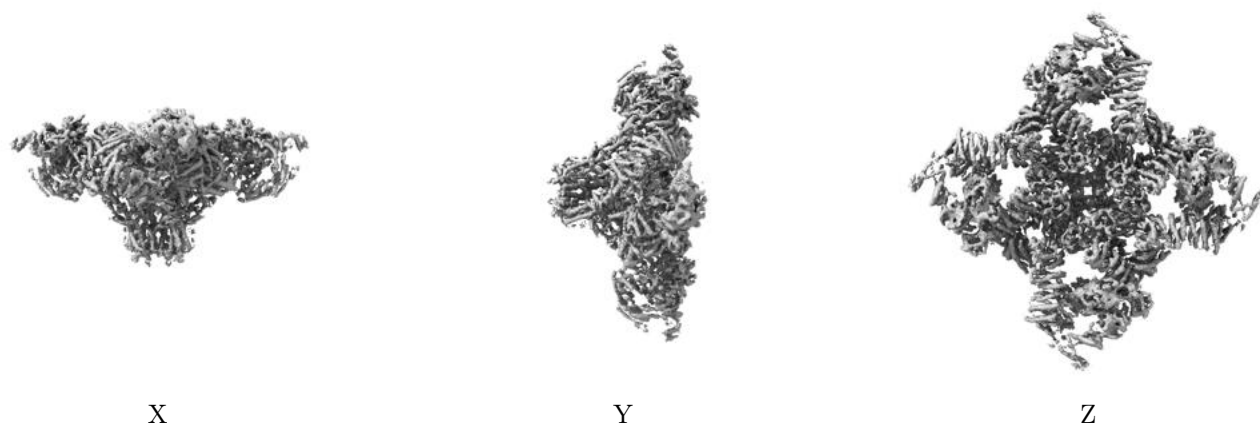
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

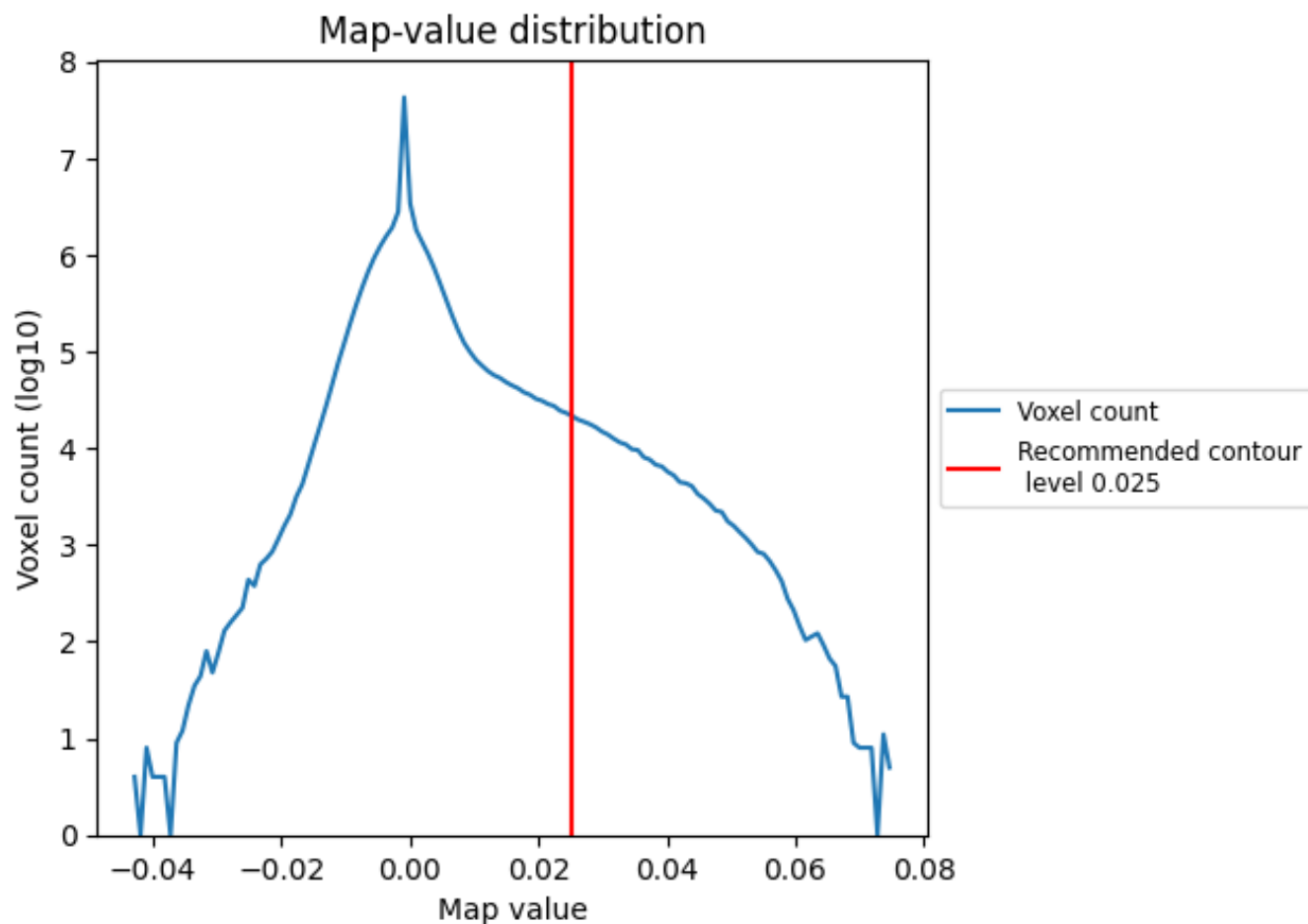
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

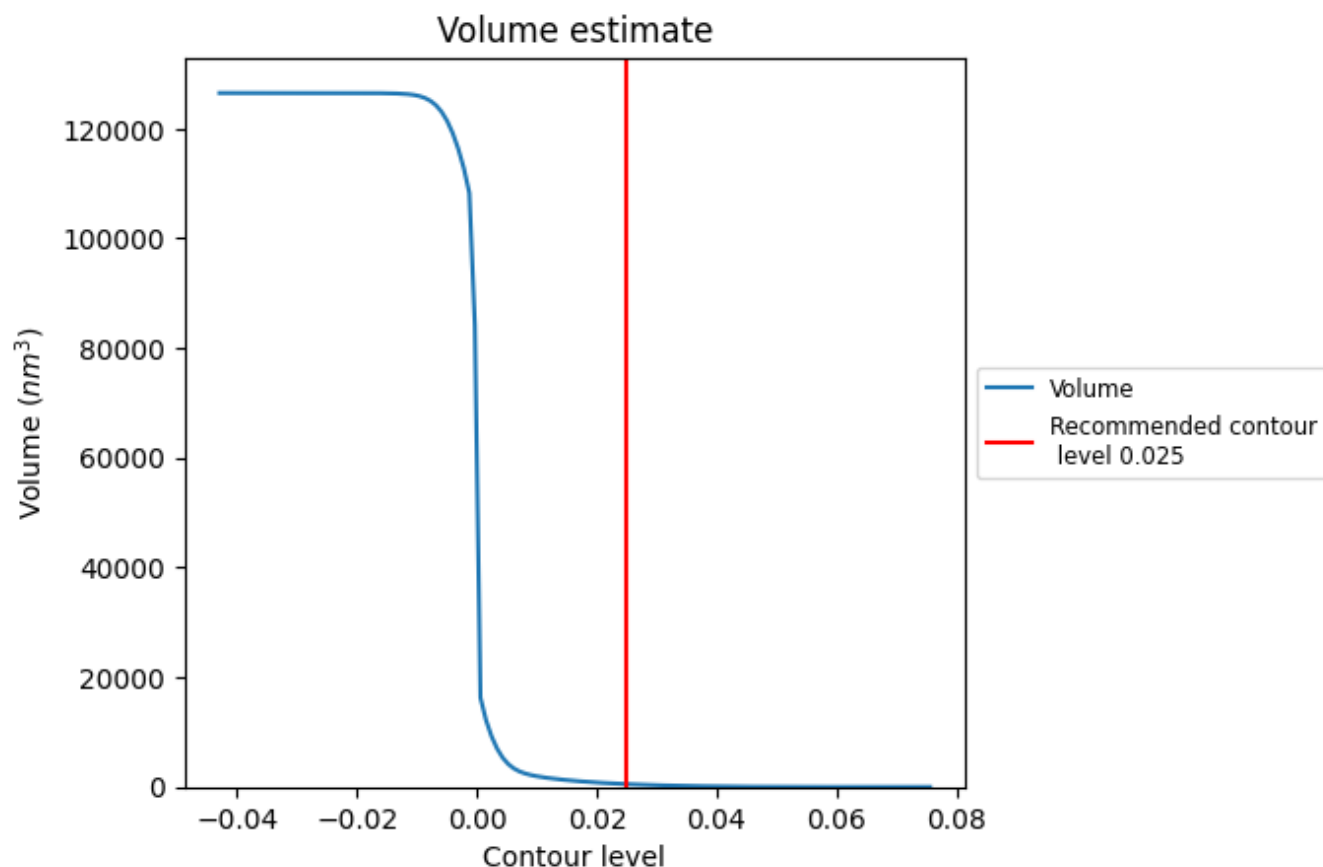
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

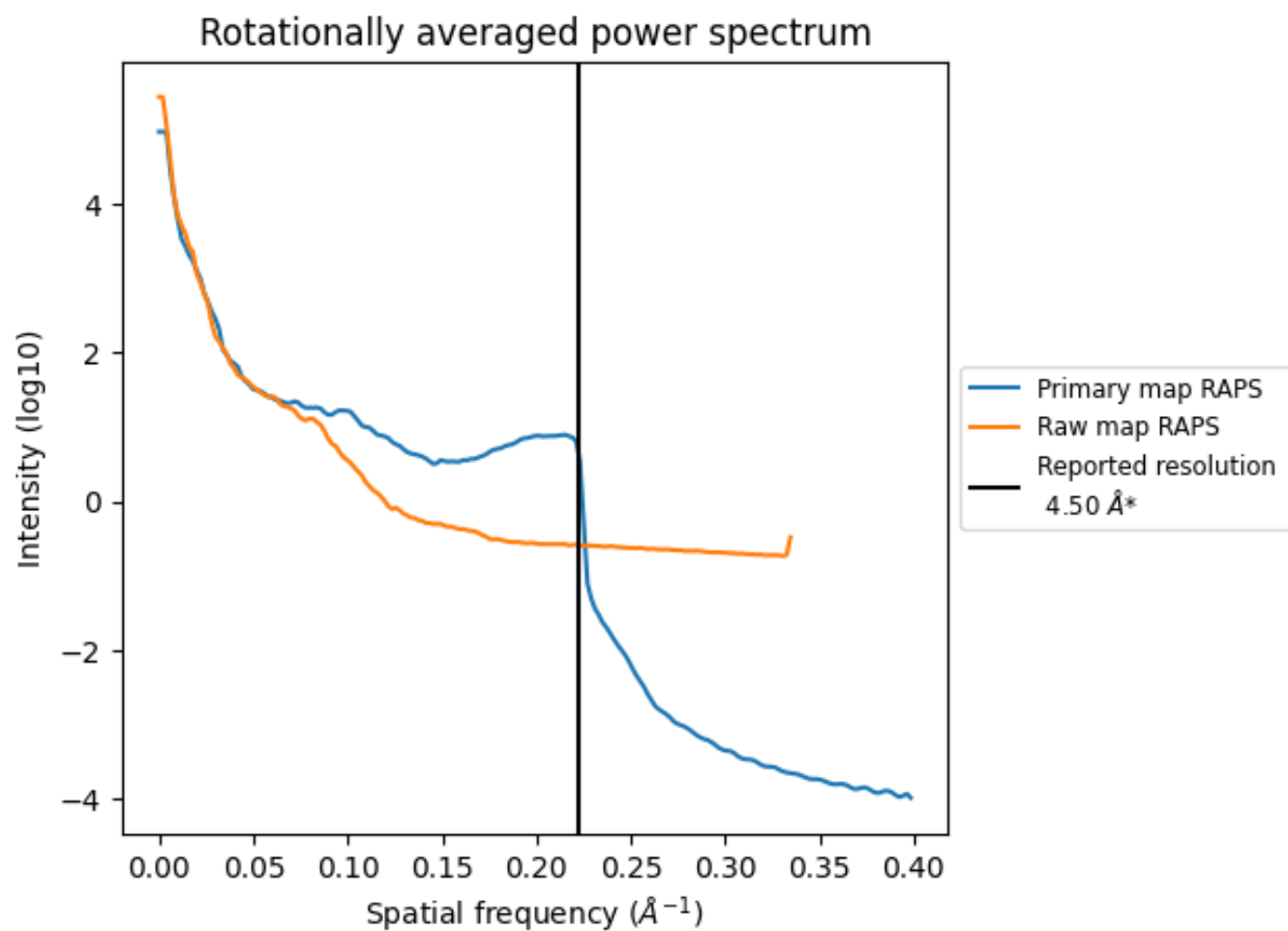
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm³; this corresponds to an approximate mass of 466 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 ⓘ

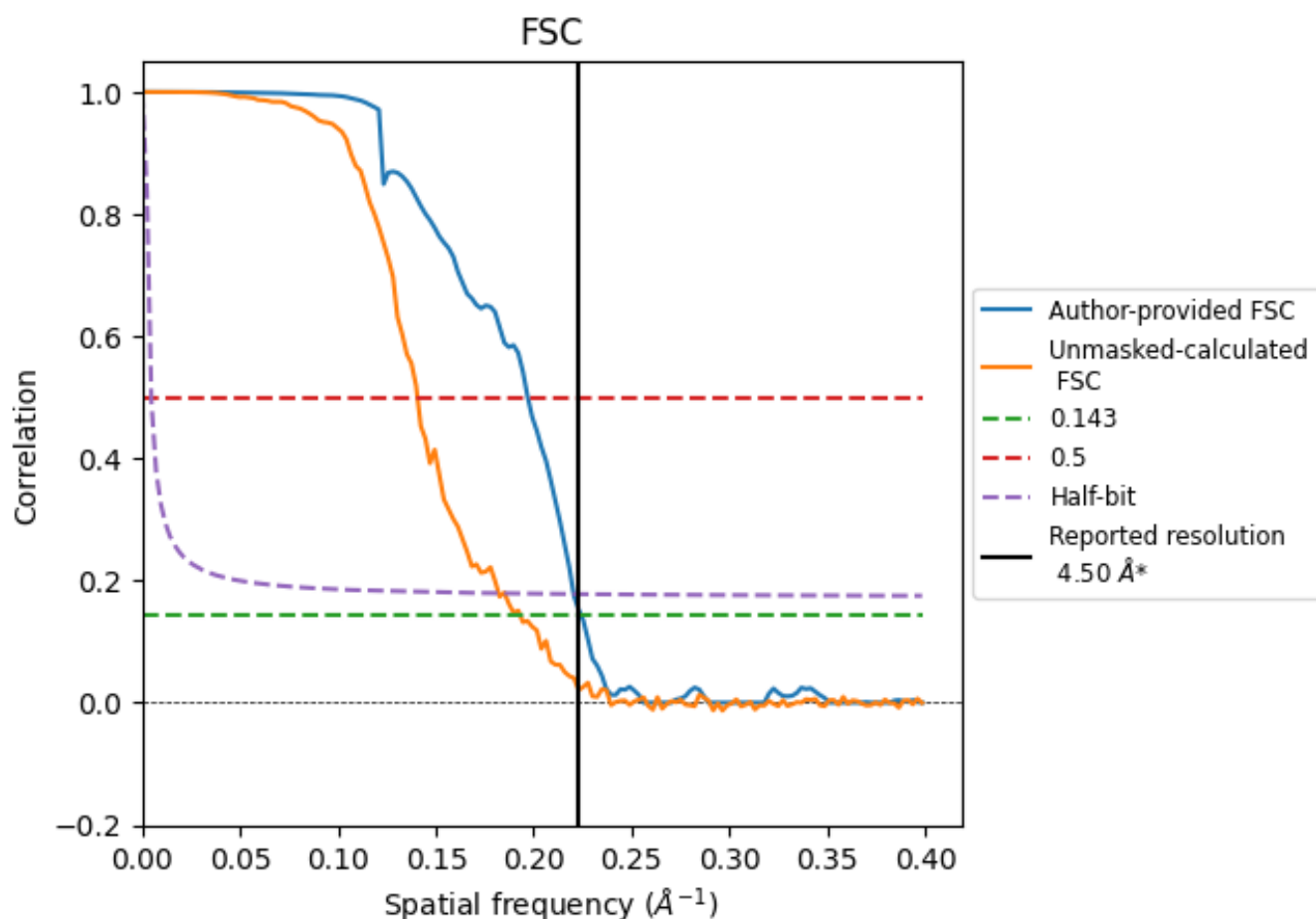


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

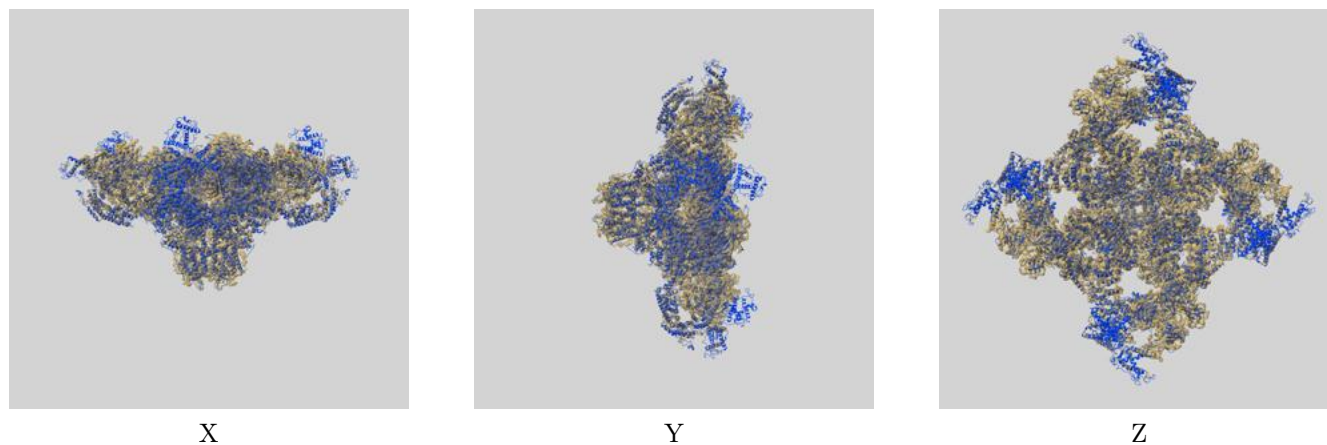
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	5.08	4.54
Unmasked-calculated*	5.18	7.11	5.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.18 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

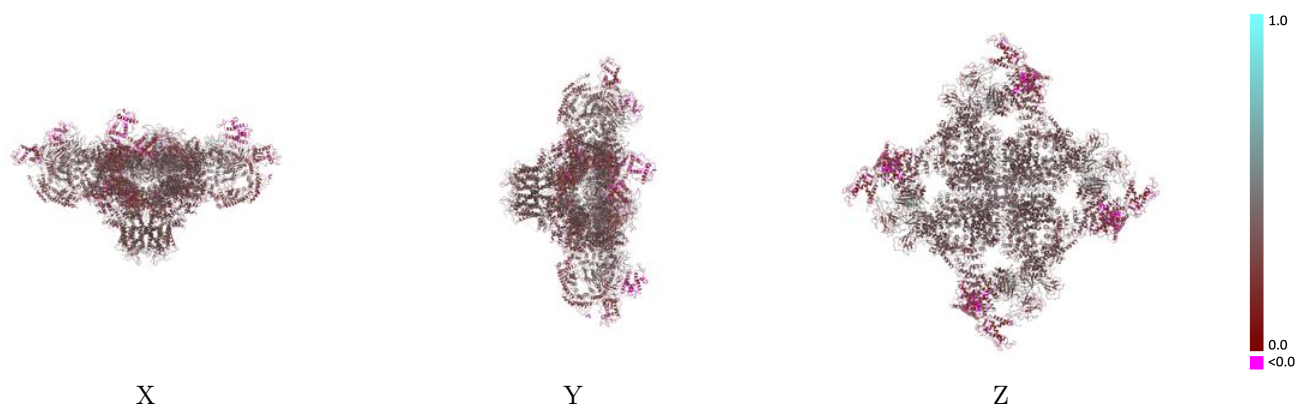
This section contains information regarding the fit between EMDB map EMD-8395 and PDB model 5TB4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



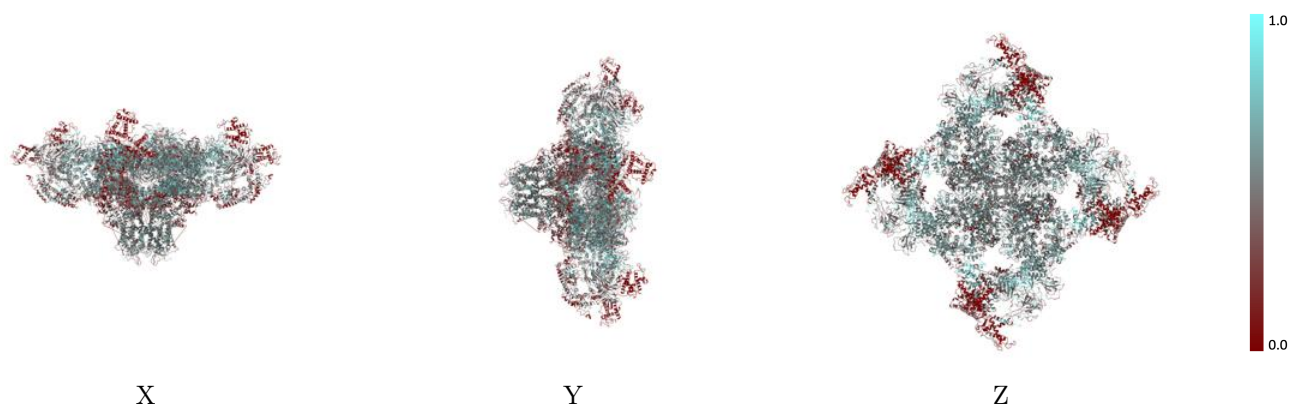
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



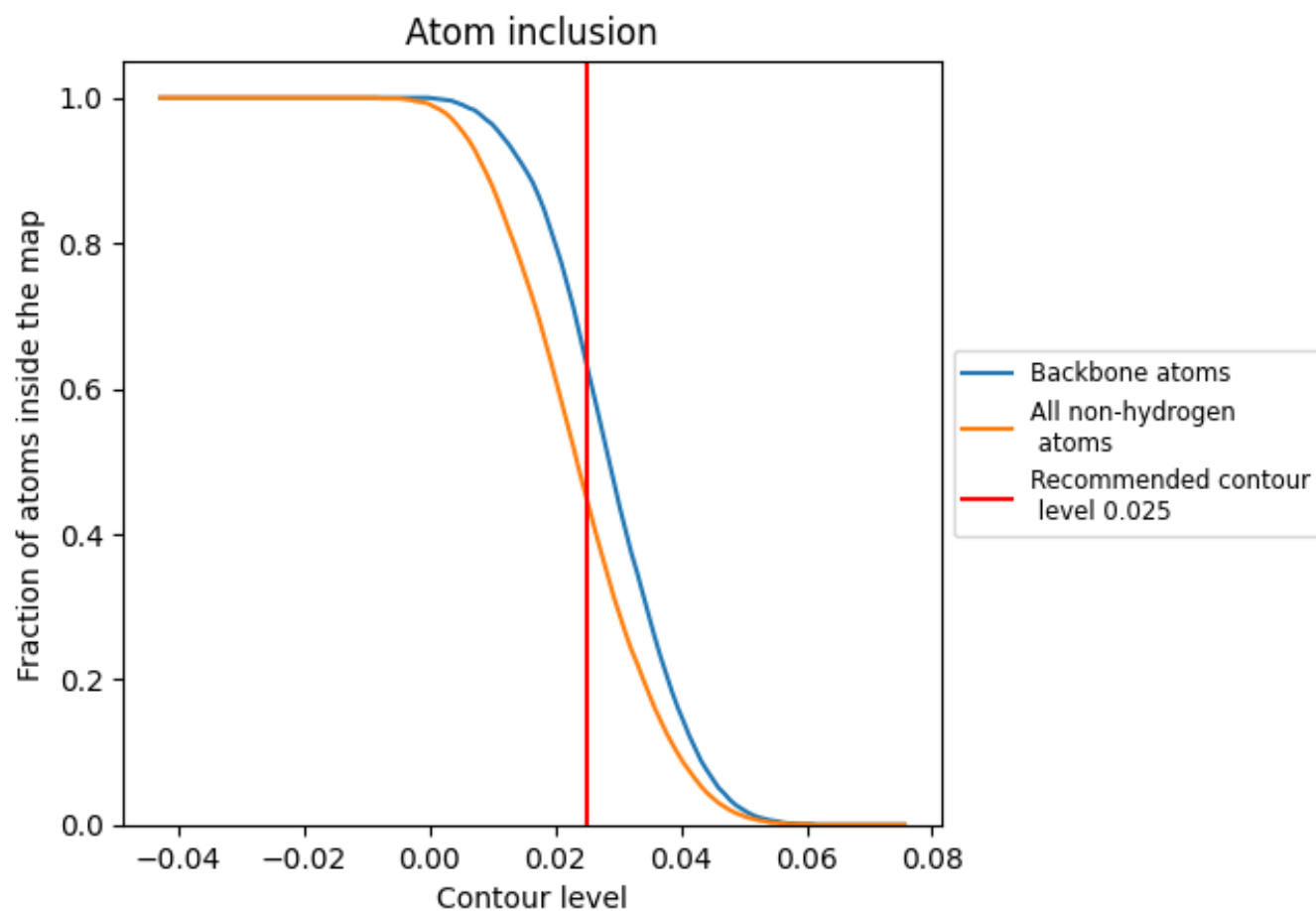
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.4480	0.3170
A	0.4810	0.3380
B	0.4470	0.3160
E	0.4470	0.3160
F	0.4740	0.3420
G	0.4470	0.3160
H	0.4790	0.3410
I	0.4470	0.3160
J	0.4800	0.3400

1.0

0.0

<0.0