



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:52 PM UTC

PDB ID : 5T9R / pdb_00005t9r
EMDB ID : EMD-8374
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 5.80 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:

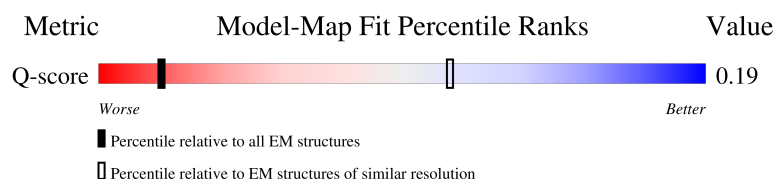
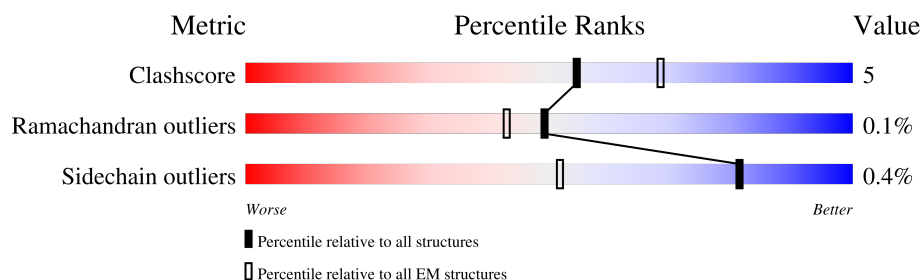
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 5.80 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	511 (5.30 - 6.30)

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	60% 80% 19%
1	F	108	56% 80% 19%
1	H	108	57% 81% 18%
1	J	108	57% 81% 18%

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Mol	Chain	Length	Quality of chain
2	B	4676	46% 78% 11% 11%
2	E	4676	46% 78% 10% 11%
2	G	4676	46% 78% 11% 11%
2	I	4676	46% 78% 11% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	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	

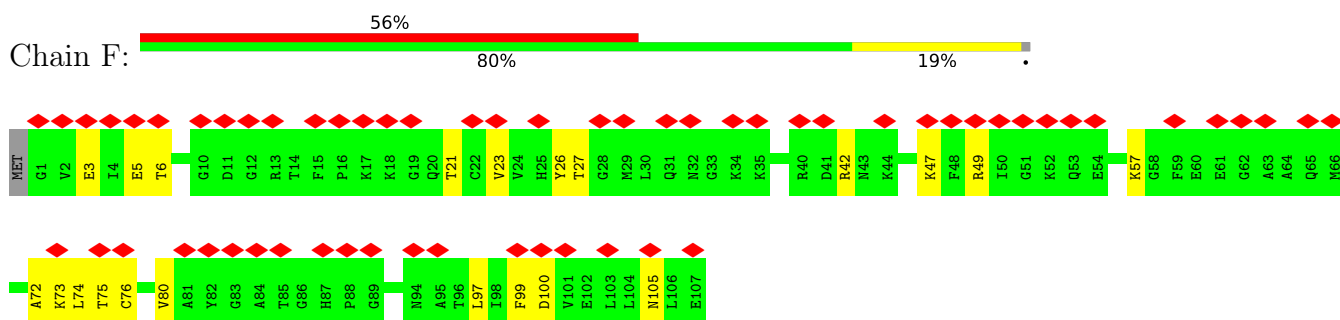
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

3 Residue-property plots [i](#)

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

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



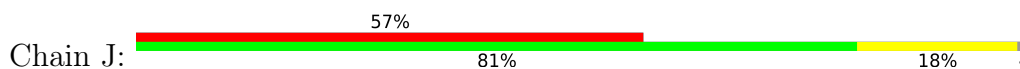
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- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



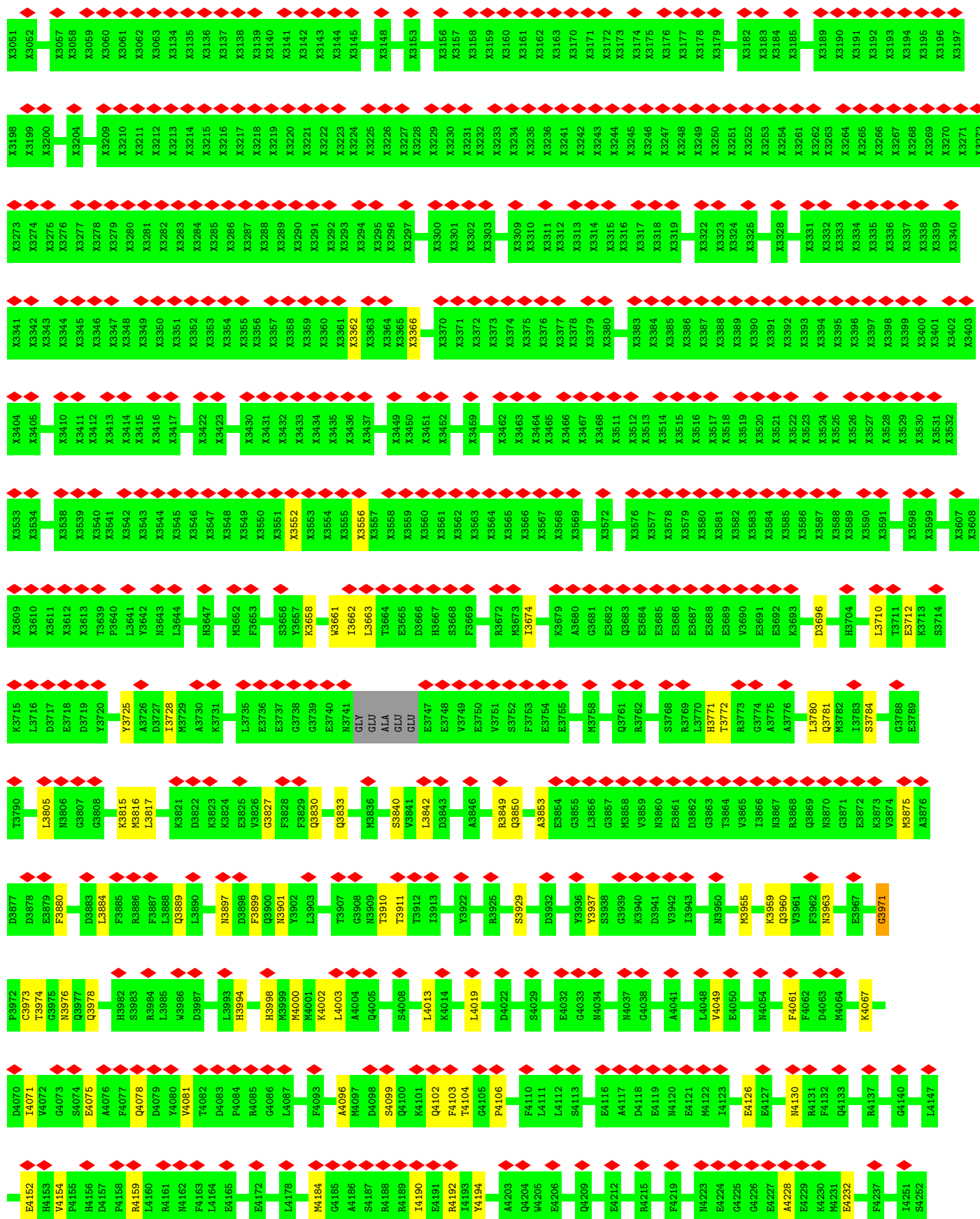
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

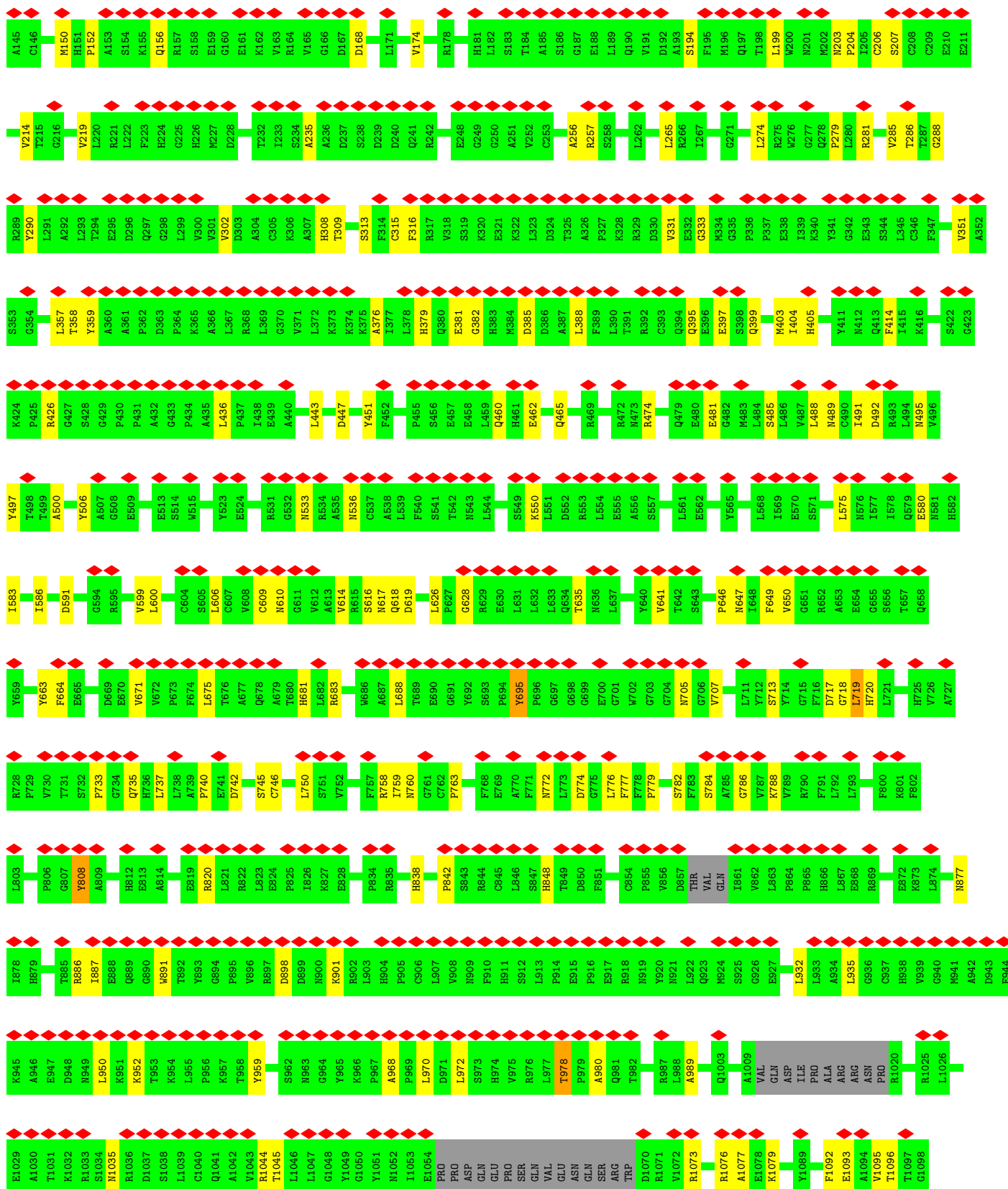




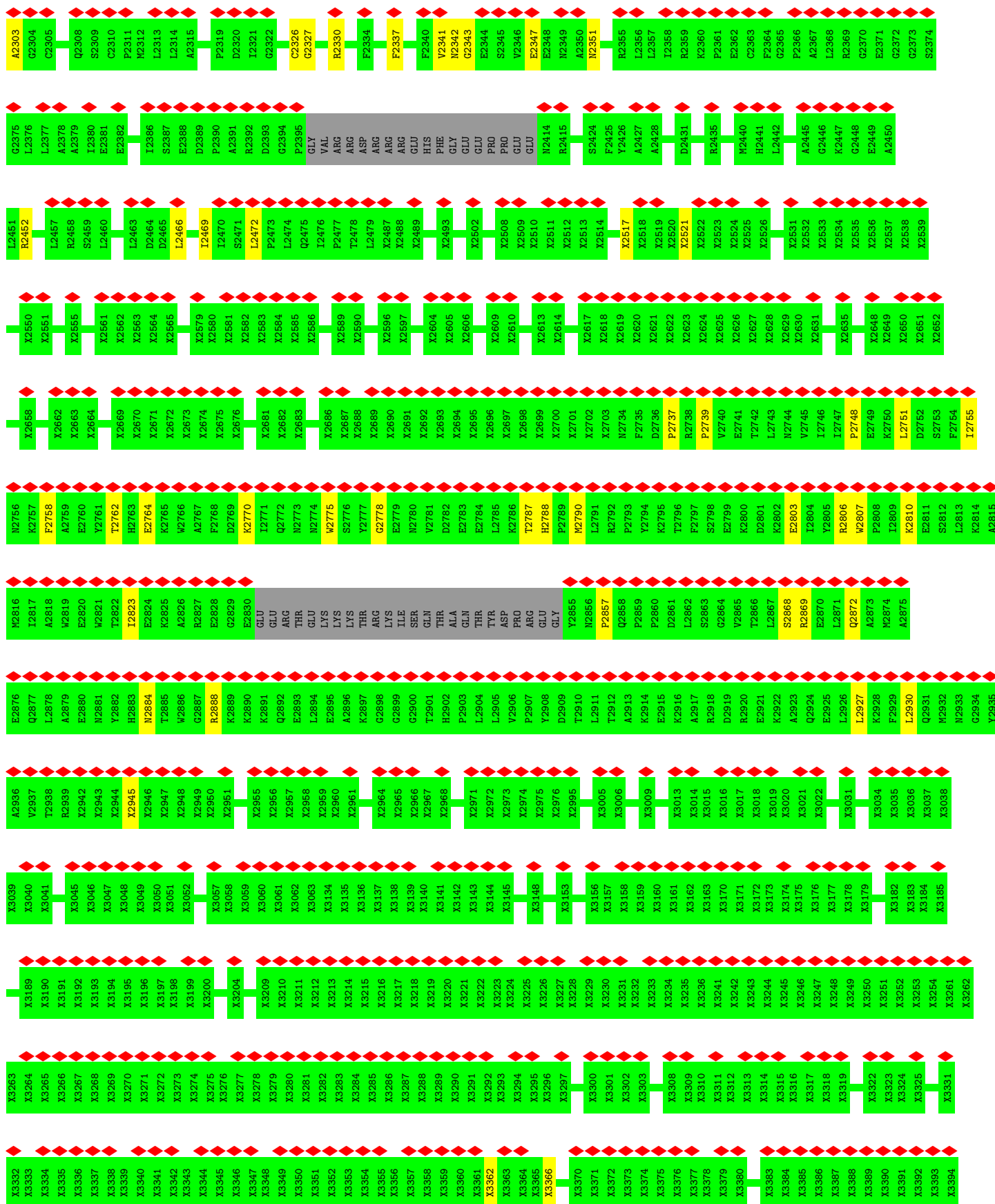


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R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	P2861	L2862	S2863	S2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	E2875	Q2876	Q2877	L2878	A2879	E2880	N2881	Y2882	N2883	N2884	T2885	N2886	
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K2221	E2222	F2225	M2228	L2236	Q2247	R2248	D2252	H2253	Y2256	N2280	S2281	G2282	I2283	G2284	L2285	G2286	M2287	Q2288	G2289	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	R2355	L2356	L2357	I2358	L2359	K2360	P2361	E2362	G2363	F2364	A2367	L2368	A2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378						
Q2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	P2319	D2320	I2321	G2322	C2326	G2327	R2330	F2334	F2337	A2338	V2339	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	R2355	L2356	L2357	I2358	L2359	K2360	P2361	E2362	G2363	F2364	A2367	L2368	A2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378							
A2379	I2380	E2381	E2382	I2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	GLU	N2414	R2415	V2416	S2424	F2425	Y2426	A2427	A2428	D2431	R2435	M2440	H2441	L2442	A2445	G2446	L2447	G2448	E2449	A2450	L2451	R2452									
L2457	R2458	S2459	L2460	L2463	D2464	D2465	L2466	I2470	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	L2478	X2487	X2488	X2489	X2493	X2509	X2510	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2550	X2551	X2555	X2561										
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R2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	P2861	L2862	S2863	S2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	E2875	Q2876	Q2877	L2878	A2879	E2880	N2881	Y2882	N2883	N2884	T2885	N2886		
K2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	E2896	K2897	K2898	G2899	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	P2908	P2909	T2910	T2912	A2913	K2914	E2915	E2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	N2932	N2933	Q2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948
X2949	X2950	X2951	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2964	X2965	X2966	X2967	X2968	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X3005	X3006	X3009	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3031	X3034	X3035	X3036	X3037	X3040	X3041	X3045	X3046	X3047	X3048	X3049	X3050										



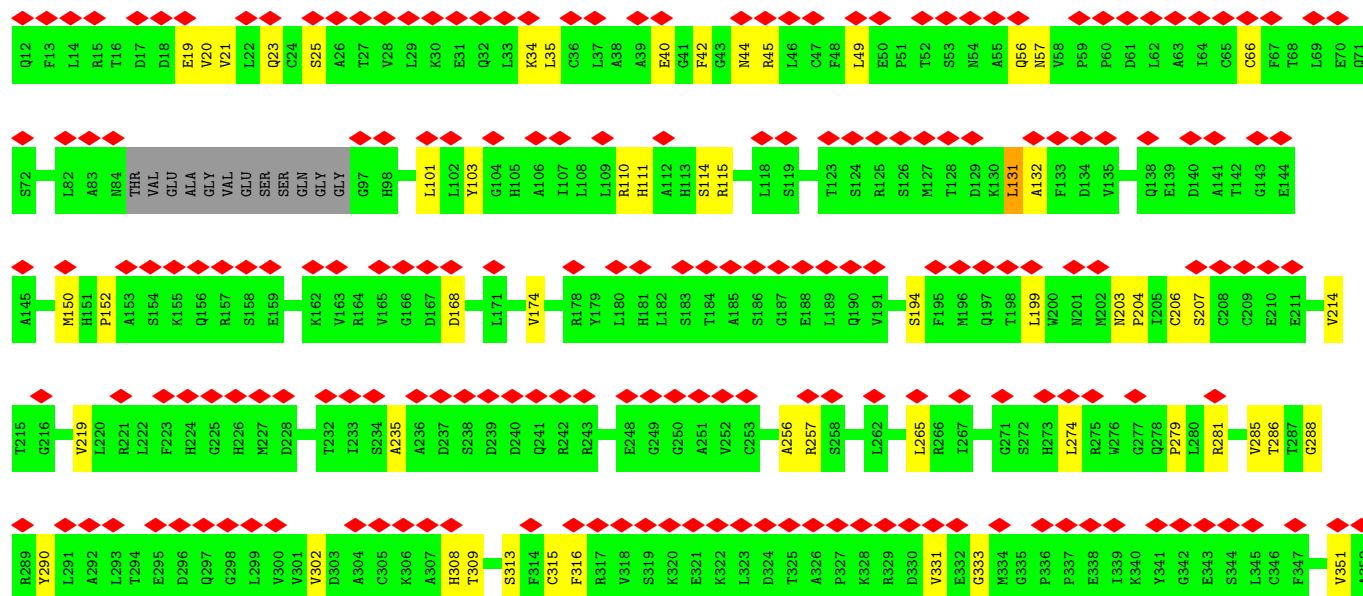
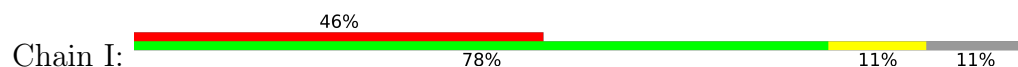


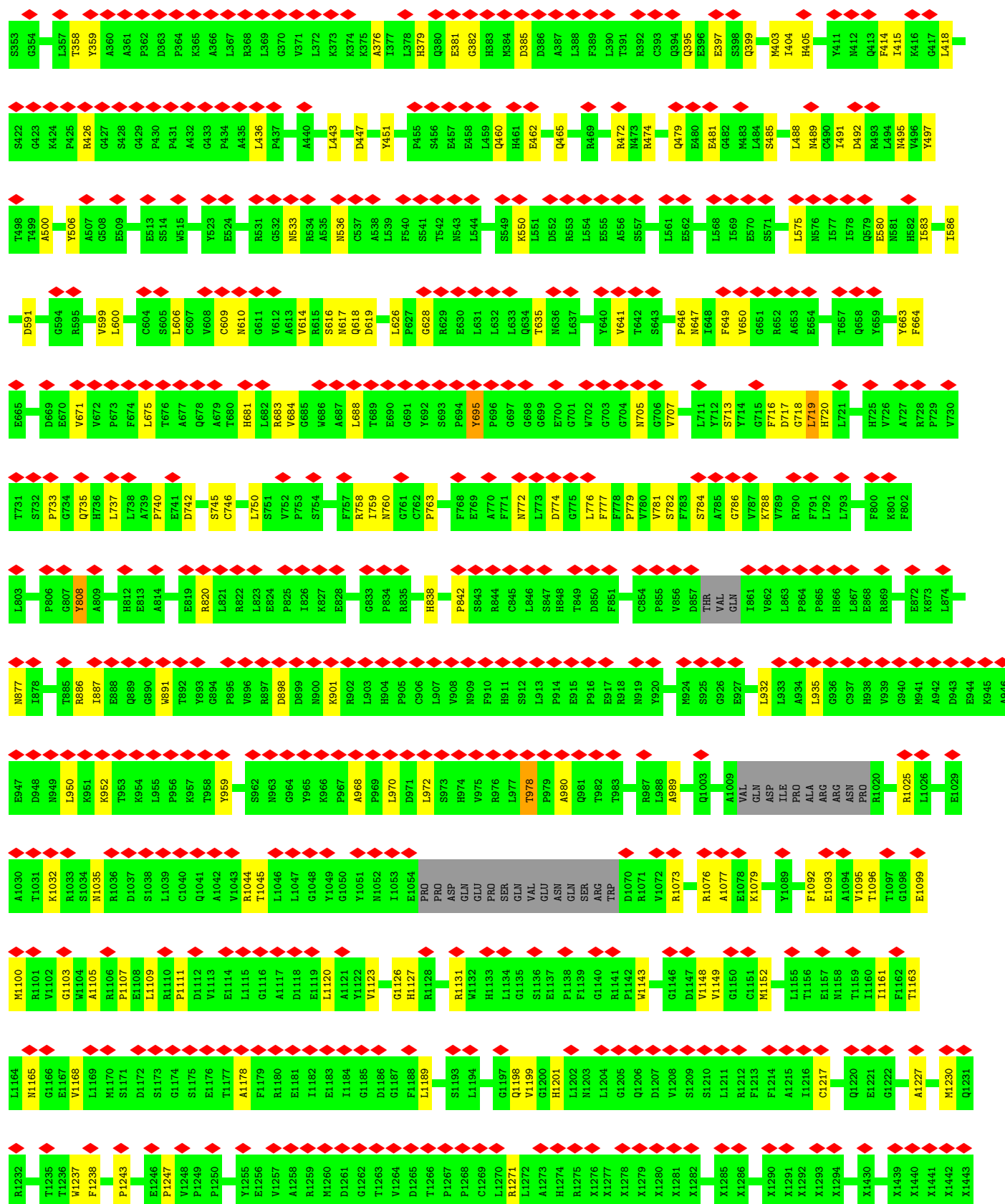


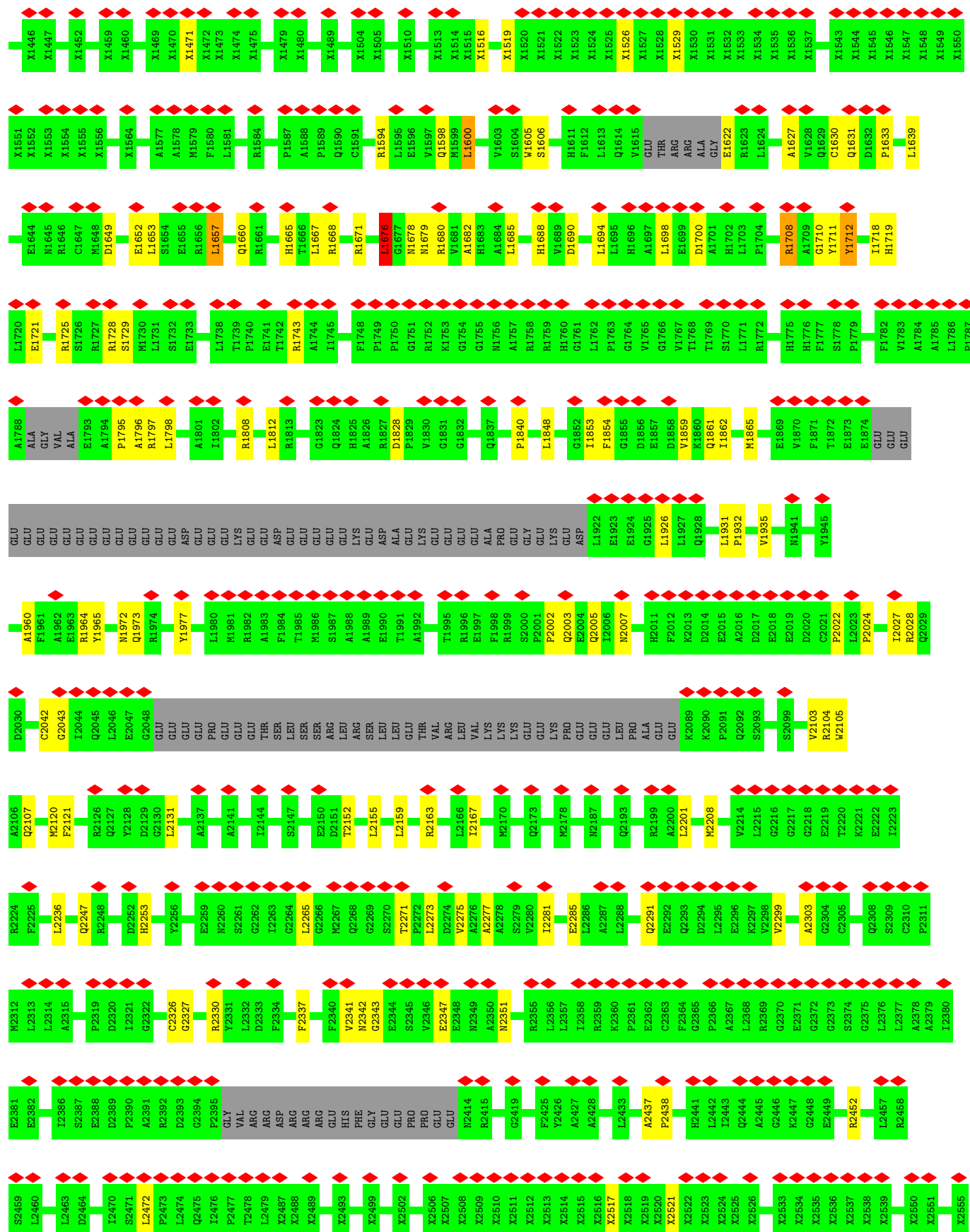




- Molecule 2: Ryanodine receptor 1

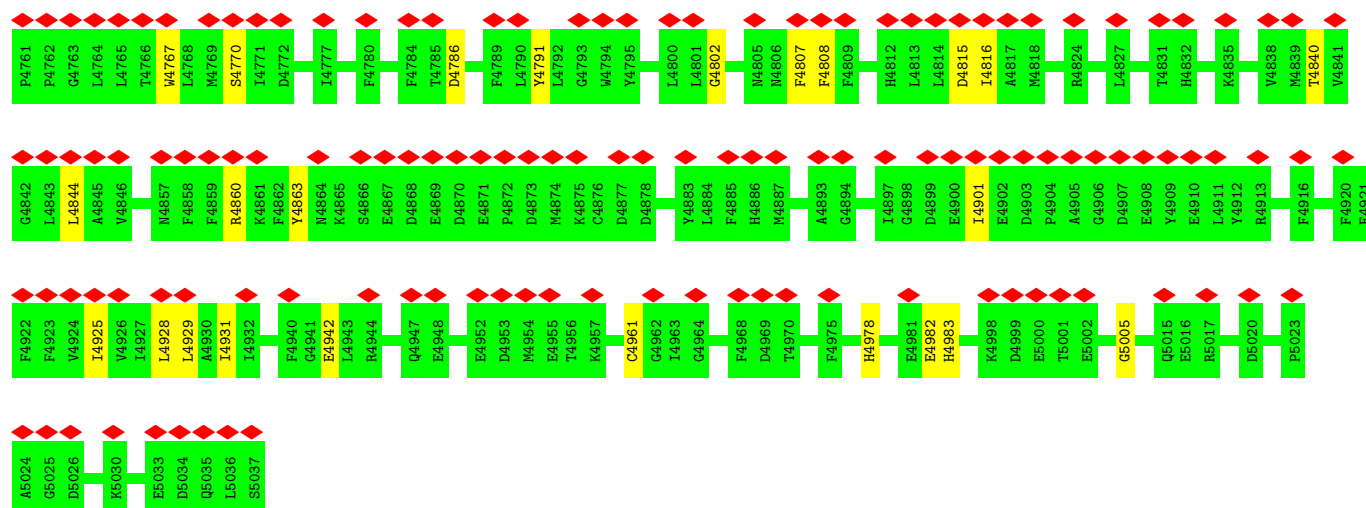




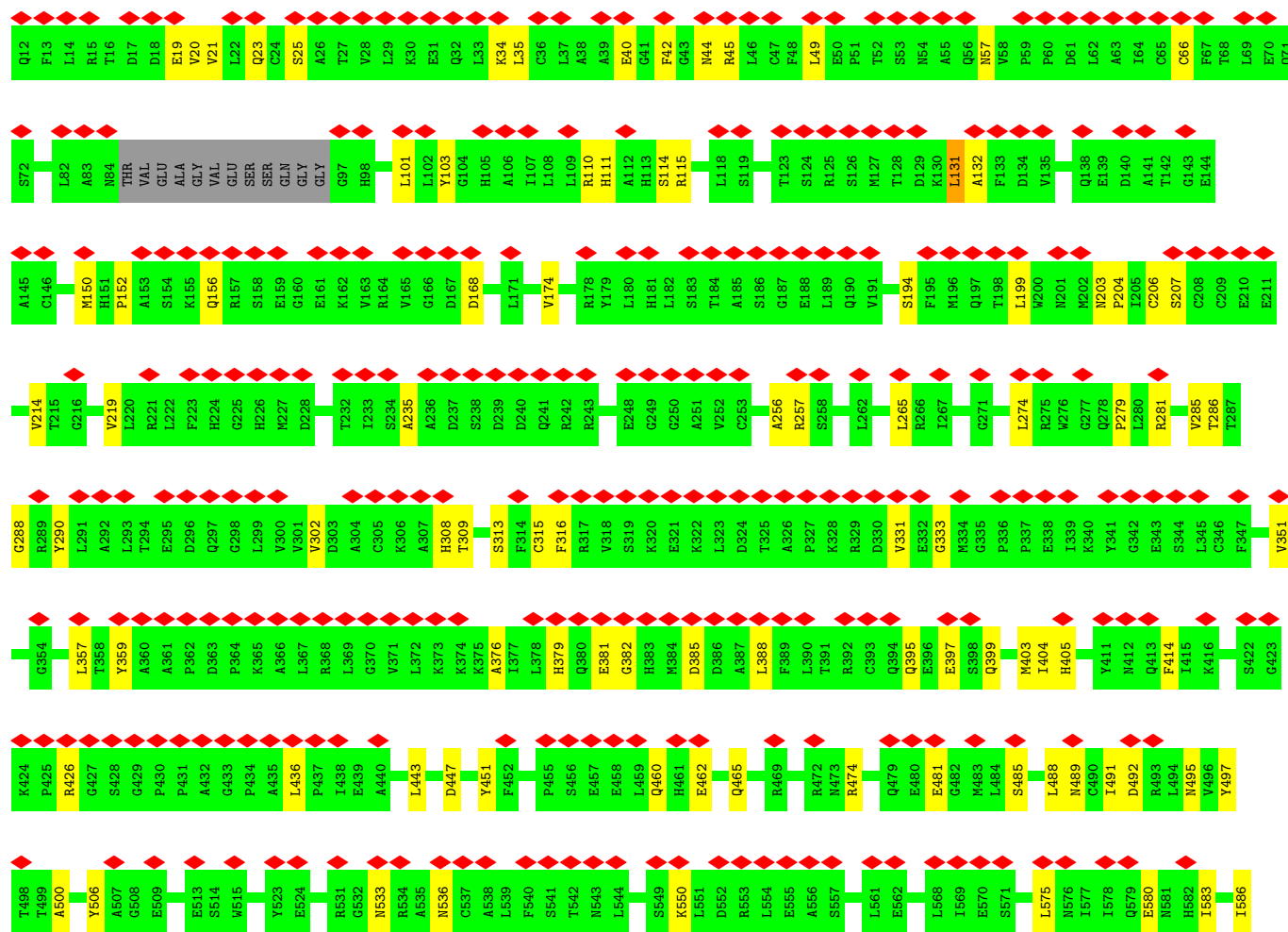
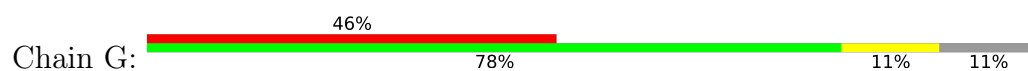


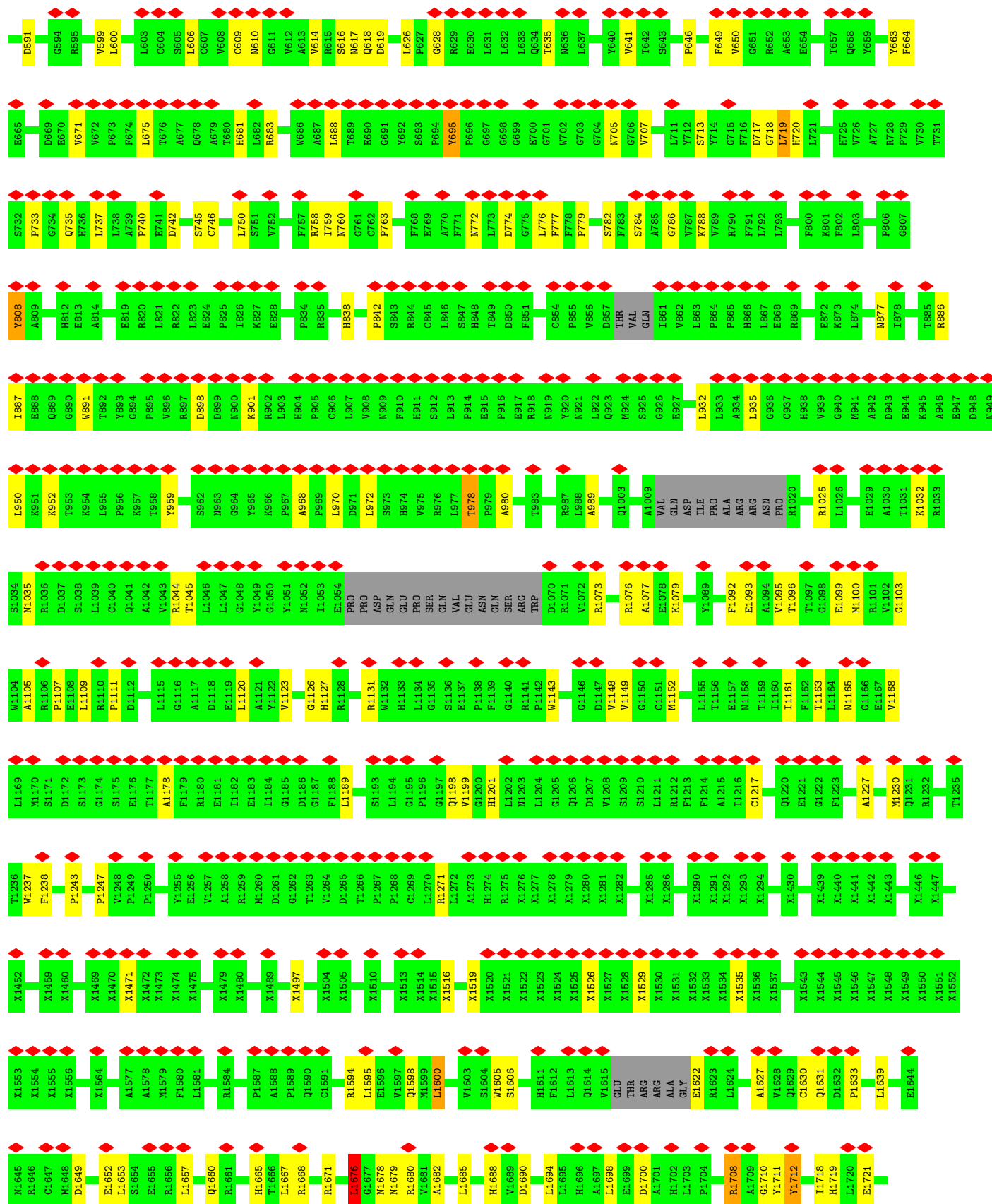






• Molecule 2: Ryanodine receptor 1

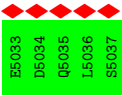






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X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398
X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3422	X3423	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3449	X3450	X3451	X3452	X3458	X3459	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526				
X3336	X3337	X3338	X3339	X3340	X																																																				





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	0.093	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/834	0.44	0/1123
1	F	0.17	0/834	0.44	0/1123
1	H	0.17	0/834	0.44	0/1123
1	J	0.17	0/834	0.44	0/1123
2	B	0.20	1/25428 (0.0%)	0.52	3/34534 (0.0%)
2	E	0.20	1/25428 (0.0%)	0.52	3/34534 (0.0%)
2	G	0.20	1/25428 (0.0%)	0.52	3/34534 (0.0%)
2	I	0.20	1/25428 (0.0%)	0.52	3/34534 (0.0%)
All	All	0.20	4/105048 (0.0%)	0.52	12/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	10.84	1.59	1.33
2	I	695	TYR	C-N	10.83	1.59	1.33
2	B	695	TYR	C-N	10.83	1.59	1.33
2	E	695	TYR	C-N	10.83	1.59	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4666	VAL	CA-C-N	-7.29	110.73	119.84
2	E	4666	VAL	C-N-CA	-7.29	110.73	119.84
2	B	4666	VAL	CA-C-N	-7.28	110.74	119.84
2	B	4666	VAL	C-N-CA	-7.28	110.74	119.84
2	I	4666	VAL	CA-C-N	-7.27	110.75	119.84
2	I	4666	VAL	C-N-CA	-7.27	110.75	119.84
2	G	4666	VAL	CA-C-N	-7.26	110.77	119.84
2	G	4666	VAL	C-N-CA	-7.26	110.77	119.84
2	B	131	LEU	CA-CB-CG	5.11	134.19	116.30
2	I	131	LEU	CA-CB-CG	5.11	134.18	116.30
2	G	131	LEU	CA-CB-CG	5.11	134.17	116.30
2	E	131	LEU	CA-CB-CG	5.10	134.16	116.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	12	0
1	H	818	0	824	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	818	0	824	10	0
2	B	29369	0	24721	275	0
2	E	29369	0	24720	272	0
2	G	29369	0	24720	277	0
2	I	29369	0	24720	277	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
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102177	1128	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 (1128) 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:788:LYS:HG2	2:G:1630:CYS:H	1.52	0.74
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.53	0.72
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.53	0.72
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.53	0.72
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.66
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.65
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.78	0.65
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.79	0.65
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.78	0.64
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.79	0.64
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.79	0.64
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.63	0.64
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.79	0.64
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.79	0.63
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.63	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.81	0.62
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.81	0.62
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.81	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.63	0.62
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.81	0.62
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.63	0.62
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.81	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.61
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.81	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.81	0.61
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.81	0.61
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.61
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.32	0.61
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.81	0.61
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.83	0.61
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.83	0.60
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.84	0.60
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.84	0.60
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.60
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.60
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.84	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
1:A:27:THR:HB	1:A:100:ASP:HB3	1.84	0.60
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.82	0.60
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.84	0.60
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.82	0.60
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.83	0.60
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.59
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.59
1:F:27:THR:HB	1:F:100:ASP:HB3	1.84	0.59
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.49	0.59
1:J:27:THR:HB	1:J:100:ASP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.84	0.59
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.84	0.59
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.85	0.59
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.85	0.59
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.36	0.59
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.68	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.59
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.49	0.59
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.85	0.59
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.83	0.59
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.85	0.59
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.84	0.59
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.84	0.59
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.85	0.59
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.68	0.59
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.36	0.58
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.36	0.58
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.37	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.86	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.85	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58
1:H:27:THR:HB	1:H:100:ASP:HB3	1.84	0.58
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.68	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.85	0.58
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.36	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.85	0.58
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.84	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.36	0.58
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.85	0.58
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.36	0.58
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.84	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.36	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.86	0.57
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.68	0.57
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.86	0.57
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.36	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.36	0.57
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.86	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.78	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.84	0.57
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.87	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.86	0.57
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.37	0.57
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.37	0.57
1:F:3:GLU:HB2	1:F:75:THR:HB	1.86	0.57
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.78	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.57
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.78	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.87	0.57
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.86	0.57
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.32	0.57
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.78	0.57
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.87	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.37	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.37	0.56
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.56
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.87	0.56
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.87	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.86	0.56
2:I:359:TYR:HA	2:I:376:ALA:HA	1.88	0.56
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.87	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.88	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.56
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	1.88	0.56
2:B:4067:LYS:NZ	2:B:4102:GLN:O	2.39	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.88	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
1:A:3:GLU:HB2	1:A:75:THR:HB	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.86	0.56
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.56
2:I:4067:LYS:NZ	2:I:4102:GLN:O	2.39	0.56
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.88	0.56
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.56
2:B:4928:LEU:HD23	2:B:4931:ILE:HD12	1.87	0.56
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.88	0.56
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.56
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.56
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.56
2:G:4928:LEU:HD23	2:G:4931:ILE:HD12	1.87	0.56
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.88	0.56
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.88	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.88	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	1.88	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
1:H:3:GLU:HB2	1:H:75:THR:HB	1.86	0.55
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.86	0.55
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.88	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.55
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	1.88	0.55
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.87	0.55
2:E:4067:LYS:NZ	2:E:4102:GLN:O	2.39	0.55
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:GLU:HB2	1:J:75:THR:HB	1.86	0.55
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.88	0.55
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.55
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.31	0.55
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.55
2:I:385:ASP:HB2	2:G:156:GLN:HE21	1.71	0.55
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.89	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.88	0.55
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.88	0.55
2:E:4928:LEU:HD23	2:E:4931:ILE:HD12	1.87	0.55
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.87	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.89	0.55
2:G:359:TYR:HA	2:G:376:ALA:HA	1.88	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.39	0.55
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.40	0.55
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.89	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.55
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.88	0.55
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.55
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.55
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.55
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.40	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.55
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.55
2:G:4067:LYS:NZ	2:G:4102:GLN:O	2.39	0.55
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.89	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.88	0.55
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.55
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.87	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.55
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.54
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.89	0.54
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.54
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.88	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.40	0.54
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.89	0.54
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.89	0.54
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.88	0.54
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.31	0.54
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.41	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.54
2:G:331:VAL:HG12	2:G:333:GLY:H	1.72	0.54
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.90	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.54
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.40	0.54
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.89	0.54
2:E:2758:PHE:O	2:E:2762:THR:N	2.41	0.54
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.41	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.41	0.54
2:B:2758:PHE:O	2:B:2762:THR:N	2.41	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.73	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.90	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.54
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.90	0.54
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.41	0.54
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.89	0.54
2:I:4928:LEU:HD23	2:I:4931:ILE:HD12	1.87	0.54
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.90	0.54
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.90	0.54
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.90	0.54
2:I:331:VAL:HG12	2:I:333:GLY:H	1.72	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.73	0.54
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.54
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.89	0.53
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.42	0.53
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.88	0.53
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.74	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.41	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.91	0.53
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.42	0.53
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.90	0.53
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.42	0.53
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.89	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.72	0.53
2:B:1973:GLN:O	2:B:1977:TYR:N	2.42	0.53
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.42	0.53
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.90	0.53
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.42	0.53
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.53
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.42	0.53
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.42	0.53
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.90	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.90	0.53
2:I:4925:ILE:HA	2:I:4929:LEU:HD13	1.91	0.53
2:B:4925:ILE:HA	2:B:4929:LEU:HD13	1.91	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.42	0.53
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.91	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.90	0.53
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.41	0.53
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.91	0.53
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.90	0.53
2:E:331:VAL:HG12	2:E:333:GLY:H	1.72	0.53
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.42	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.90	0.53
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.41	0.53
2:G:1622:GLU:N	2:G:1627:ALA:O	2.42	0.53
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.74	0.53
2:G:4925:ILE:HA	2:G:4929:LEU:HD13	1.91	0.53
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.42	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.53
2:E:4925:ILE:HA	2:E:4929:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.42	0.53
2:I:2868:SER:O	2:I:2872:GLN:N	2.42	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.90	0.52
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.90	0.52
2:B:1622:GLU:N	2:B:1627:ALA:O	2.42	0.52
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.74	0.52
2:E:1973:GLN:O	2:E:1977:TYR:N	2.42	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.91	0.52
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.52
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.91	0.52
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.91	0.52
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.38	0.52
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.91	0.52
2:E:1622:GLU:N	2:E:1627:ALA:O	2.42	0.52
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.91	0.52
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.91	0.52
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.91	0.52
1:H:6:THR:HA	1:H:72:ALA:HA	1.91	0.52
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.91	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.91	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.91	0.52
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.40	0.52
2:B:156:GLN:HE21	2:E:385:ASP:HB2	1.74	0.52
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.41	0.52
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.75	0.52
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.74	0.52
2:I:1622:GLU:N	2:I:1627:ALA:O	2.42	0.52
1:A:6:THR:HA	1:A:72:ALA:HA	1.91	0.52
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.52
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.42	0.52
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.52
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.52
2:I:2758:PHE:O	2:I:2762:THR:N	2.41	0.52
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.75	0.51
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.38	0.51
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.91	0.51
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.51
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.75	0.51
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.91	0.51
2:I:1973:GLN:O	2:I:1977:TYR:N	2.42	0.51
2:G:2758:PHE:O	2:G:2762:THR:N	2.41	0.51
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.93	0.51
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.93	0.51
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.92	0.51
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.93	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.51
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.93	0.51
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.93	0.51
1:F:6:THR:HA	1:F:72:ALA:HA	1.91	0.51
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.93	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.51
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.93	0.51
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.93	0.51
2:E:451:TYR:O	2:E:474:ARG:NH1	2.44	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.93	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.42	0.51
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.93	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.93	0.51
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.93	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.29	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.29	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.51
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.29	0.51
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.75	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.51
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.92	0.51
2:G:1973:GLN:O	2:G:1977:TYR:N	2.42	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.29	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.76	0.50
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.50
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.50
2:E:4942:GLU:HG3	2:G:4944:ARG:HH11	1.77	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.93	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.50
1:J:6:THR:HA	1:J:72:ALA:HA	1.91	0.50
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.50
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.93	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.40	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.42	0.50
2:I:451:TYR:O	2:I:474:ARG:NH1	2.44	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.45	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.50
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.92	0.50
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.76	0.50
2:E:2347:GLU:O	2:E:2351:ASN:N	2.45	0.50
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.93	0.50
2:G:451:TYR:O	2:G:474:ARG:NH1	2.44	0.50
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.50
2:G:2347:GLU:O	2:G:2351:ASN:N	2.45	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.93	0.50
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.76	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.93	0.50
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.94	0.50
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.76	0.50
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.50
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.50
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.50
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.50
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.38	0.50
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.93	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.42	0.50
2:I:488:LEU:O	2:I:492:ASP:N	2.43	0.50
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.77	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.93	0.50
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.77	0.49
2:B:3974:THR:O	2:B:3978:GLN:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.94	0.49
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.93	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.45	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.94	0.49
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.49
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.95	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.49
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.78	0.49
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.94	0.49
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.92	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.49
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.93	0.49
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.49
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.95	0.49
2:E:156:GLN:HE21	2:G:385:ASP:HB2	1.78	0.49
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.95	0.49
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.77	0.49
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.95	0.49
2:B:451:TYR:O	2:B:474:ARG:NH1	2.44	0.49
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.94	0.49
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.95	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.95	0.49
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.49
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.49
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.93	0.49
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.77	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.94	0.49
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.95	0.49
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.94	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.49
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.95	0.49
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.93	0.49
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.94	0.49
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.46	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.49
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.95	0.48
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.38	0.48
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.46	0.48
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.95	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.48
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.95	0.48
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.46	0.48
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.95	0.48
2:I:4741:LEU:HB2	2:I:4743:MET:HE2	1.95	0.48
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.94	0.48
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.44	0.48
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.95	0.48
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.95	0.48
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.30	0.48
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.94	0.48
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.95	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.48
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.95	0.48
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.96	0.48
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.46	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.31	0.48
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.48
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.48
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.95	0.48
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.78	0.48
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.46	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.48
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.48
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.95	0.48
2:G:3974:THR:O	2:G:3978:GLN:N	2.40	0.48
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.96	0.48
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.96	0.48
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.95	0.48
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.94	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.94	0.48
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.95	0.48
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.96	0.48
2:I:21:VAL:HG12	2:I:66:CYS:HA	1.96	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.95	0.48
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.46	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.48
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.78	0.48
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.96	0.48
2:I:3974:THR:O	2:I:3978:GLN:N	2.40	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.48
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.96	0.48
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.48
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.95	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.38	0.48
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.78	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.95	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.31	0.48
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.95	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.47	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.96	0.48
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.38	0.48
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.46	0.48
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.96	0.48
2:G:206:CYS:SG	2:G:207:SER:N	2.87	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	1.96	0.48
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	1.96	0.48
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.95	0.48
2:G:21:VAL:HG12	2:G:66:CYS:HA	1.96	0.48
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.46	0.48
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.44	0.47
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.47	0.47
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.46	0.47
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	1.96	0.47
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.95	0.47
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.95	0.47
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.46	0.47
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.95	0.47
2:B:206:CYS:SG	2:B:207:SER:N	2.87	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4192:ARG:HH12	2:B:4982:GLU:HG2	1.80	0.47
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.97	0.47
2:B:4944:ARG:HH11	2:I:4942:GLU:HG3	1.78	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.44	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.47
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.79	0.47
2:I:206:CYS:SG	2:I:207:SER:N	2.87	0.47
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.42	0.47
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.79	0.47
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.97	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.47	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.47
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.96	0.47
2:E:4741:LEU:HB2	2:E:4743:MET:HE2	1.95	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.47	0.47
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.44	0.47
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.47
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.96	0.47
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.79	0.47
2:G:4741:LEU:HB2	2:G:4743:MET:HE2	1.95	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.47
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.28	0.47
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.96	0.47
2:E:488:LEU:O	2:E:492:ASP:N	2.43	0.47
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.47
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.79	0.47
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.47	0.47
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.95	0.47
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.97	0.47
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.47
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.96	0.47
2:E:206:CYS:SG	2:E:207:SER:N	2.87	0.47
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.97	0.47
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.96	0.47
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.96	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.47
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.47
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.96	0.47
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.95	0.47
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.47
2:G:4192:ARG:HH12	2:G:4982:GLU:HG2	1.80	0.47
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	1.96	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:E:4192:ARG:HH12	2:E:4982:GLU:HG2	1.80	0.47
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.48	0.47
2:I:1238:PHE:O	2:I:1606:SER:N	2.48	0.47
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.47
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.96	0.47
2:B:21:VAL:HG12	2:B:66:CYS:HA	1.96	0.47
2:E:647:ASN:ND2	2:E:820:ARG:O	2.39	0.47
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.96	0.47
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.47
2:I:4192:ARG:HH12	2:I:4982:GLU:HG2	1.80	0.47
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.48	0.47
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.48	0.47
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.95	0.47
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.79	0.47
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.47
2:E:21:VAL:HG12	2:E:66:CYS:HA	1.96	0.47
2:G:733:PRO:HD2	2:G:763:PRO:HD2	1.97	0.47
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.47	0.47
2:E:733:PRO:HD2	2:E:763:PRO:HD2	1.97	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.47
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.95	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.47
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:G:3757:GLU:HA	2:G:3760:LYS:HZ1	1.80	0.47
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.96	0.47
2:B:309:THR:O	2:B:313:SER:OG	2.33	0.46
2:B:2105:TRP:HE3	2:B:2120:MET:HE3	1.80	0.46
2:E:309:THR:O	2:E:313:SER:OG	2.33	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.97	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:G:488:LEU:O	2:G:492:ASP:N	2.43	0.46
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.81	0.46
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.47	0.46
2:B:4741:LEU:HB2	2:B:4743:MET:HE2	1.95	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.46
2:I:733:PRO:HD2	2:I:763:PRO:HD2	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.79	0.46
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.46	0.46
2:G:309:THR:O	2:G:313:SER:OG	2.33	0.46
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.79	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.97	0.46
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.48	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.96	0.46
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.97	0.46
2:B:4661:TYR:OH	2:B:4786:ASP:OD2	2.34	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.96	0.46
2:E:3757:GLU:HA	2:E:3760:LYS:HZ1	1.80	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.81	0.46
2:E:4096:ALA:HA	2:E:4099:SER:HB2	1.98	0.46
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.80	0.46
2:G:4661:TYR:OH	2:G:4786:ASP:OD2	2.34	0.46
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.80	0.46
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.97	0.46
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.46
2:B:111:HIS:CD2	2:B:114:SER:H	2.31	0.46
2:B:733:PRO:HD2	2:B:763:PRO:HD2	1.97	0.46
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.80	0.46
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.97	0.46
2:I:309:THR:O	2:I:313:SER:OG	2.33	0.46
2:I:4096:ALA:HA	2:I:4099:SER:HB2	1.98	0.46
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.80	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.80	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.96	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.81	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:G:4096:ALA:HA	2:G:4099:SER:HB2	1.98	0.46
2:B:488:LEU:O	2:B:492:ASP:N	2.43	0.46
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.48	0.46
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.96	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.79	0.46
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.49	0.46
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.81	0.46
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.44	0.46
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.29	0.46
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.46
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.81	0.46
2:B:4096:ALA:HA	2:B:4099:SER:HB2	1.98	0.46
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.46
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.80	0.46
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.81	0.46
2:I:4661:TYR:OH	2:I:4786:ASP:OD2	2.34	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.45
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.44	0.45
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.81	0.45
2:G:2105:TRP:HE3	2:G:2120:MET:HE3	1.80	0.45
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.80	0.45
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.46	0.45
2:E:4661:TYR:OH	2:E:4786:ASP:OD2	2.34	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.47	0.45
2:G:2152:THR:HA	2:G:2155:LEU:HB2	1.99	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.45
2:E:111:HIS:CD2	2:E:114:SER:H	2.31	0.45
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.97	0.45
2:I:3757:GLU:HA	2:I:3760:LYS:HZ1	1.81	0.45
2:B:647:ASN:ND2	2:B:820:ARG:O	2.39	0.45
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.97	0.45
2:E:2105:TRP:HE3	2:E:2120:MET:HE3	1.80	0.45
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.45
2:I:2105:TRP:HE3	2:I:2120:MET:HE3	1.80	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.80	0.45
2:I:4071:ILE:HG13	2:I:4103:PHE:HZ	1.81	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.45
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.45
2:E:4071:ILE:HG13	2:E:4103:PHE:HZ	1.81	0.45
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.45
2:B:4000:MET:HE2	2:B:4061:PHE:HB3	1.99	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.99	0.45
2:E:3974:THR:O	2:E:3978:GLN:N	2.40	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:G:4071:ILE:HG13	2:G:4103:PHE:HZ	1.81	0.45
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.81	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.45
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.45
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	0.45
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.29	0.45
2:B:4863:TYR:HA	2:B:4901:ILE:HG23	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.99	0.45
2:I:2152:THR:HA	2:I:2155:LEU:HB2	1.99	0.45
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.97	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.45
2:G:3880:PHE:O	2:G:3884:LEU:N	2.50	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.45
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.99	0.45
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.99	0.45
2:I:4863:TYR:HA	2:I:4901:ILE:HG23	1.98	0.45
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.97	0.45
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.99	0.45
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.82	0.44
2:B:3880:PHE:O	2:B:3884:LEU:N	2.50	0.44
2:B:4071:ILE:HG13	2:B:4103:PHE:HZ	1.81	0.44
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.44	0.44
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.44
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.98	0.44
2:B:2152:THR:HA	2:B:2155:LEU:HB2	1.99	0.44
2:E:3880:PHE:O	2:E:3884:LEU:N	2.50	0.44
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.82	0.44
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.53	0.44
2:I:4000:MET:HE2	2:I:4061:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:SER:HB3	2:B:351:VAL:HB	1.99	0.44
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.83	0.44
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.52	0.44
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.44
2:I:647:ASN:ND2	2:I:820:ARG:O	2.39	0.44
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.82	0.44
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.99	0.44
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.44
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.00	0.44
2:G:4000:MET:HE2	2:G:4061:PHE:HB3	1.99	0.44
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.82	0.44
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.00	0.44
2:E:4000:MET:HE2	2:E:4061:PHE:HB3	1.99	0.44
2:I:1865:MET:SD	2:I:1865:MET:N	2.91	0.44
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.44
2:G:1238:PHE:O	2:G:1606:SER:N	2.48	0.44
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.44
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.82	0.44
2:E:1238:PHE:O	2:E:1606:SER:N	2.48	0.44
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.81	0.44
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.53	0.44
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.00	0.44
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.47	0.44
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.99	0.44
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.36	0.44
2:E:313:SER:HB3	2:E:351:VAL:HB	1.99	0.44
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.53	0.44
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	2.00	0.44
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.00	0.44
2:E:4863:TYR:HA	2:E:4901:ILE:HG23	1.98	0.44
2:I:3880:PHE:O	2:I:3884:LEU:N	2.50	0.44
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.82	0.44
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.81	0.44
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.36	0.44
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.99	0.44
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.82	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.44	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:313:SER:HB3	2:I:351:VAL:HB	1.99	0.44
2:I:460:GLN:HG2	2:I:462:GLU:H	1.83	0.44
2:I:1639:LEU:HD12	2:I:1653:LEU:HD21	2.00	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.44
2:G:290:TYR:O	2:G:302:VAL:N	2.51	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.91	0.44
2:G:4863:TYR:HA	2:G:4901:ILE:HG23	1.98	0.44
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.43
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.43
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.43
2:E:2152:THR:HA	2:E:2155:LEU:HB2	1.99	0.43
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.00	0.43
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.42	0.43
2:E:290:TYR:O	2:E:302:VAL:N	2.51	0.43
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.43
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.43
2:I:1271:ARG:HA	2:I:1471:UNK:HA	2.00	0.43
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.43
2:B:3840:SER:OG	2:B:3875:MET:O	2.34	0.43
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.43
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.99	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.43
2:E:1865:MET:SD	2:E:1865:MET:N	2.91	0.43
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.99	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.00	0.43
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.00	0.43
2:E:460:GLN:HG2	2:E:462:GLU:H	1.83	0.43
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.52	0.43
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.99	0.43
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	2.00	0.43
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.82	0.43
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.99	0.43
2:B:3696:ASP:OD2	2:B:3771:HIS:NE2	2.52	0.43
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	2.01	0.43
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	2.00	0.43
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.36	0.43
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.01	0.43
2:I:290:TYR:O	2:I:302:VAL:N	2.51	0.43
2:G:1639:LEU:HD12	2:G:1653:LEU:HD21	2.00	0.43
2:E:2299:VAL:O	2:E:2303:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.01	0.43
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.37	0.43
2:I:3696:ASP:OD2	2:I:3771:HIS:NE2	2.52	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.43
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.01	0.43
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.99	0.43
1:J:23:VAL:HB	1:J:105:ASN:HA	2.01	0.43
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.99	0.43
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.01	0.43
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.37	0.43
2:E:3696:ASP:OD2	2:E:3771:HIS:NE2	2.52	0.43
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	2.01	0.43
2:G:3696:ASP:OD2	2:G:3771:HIS:NE2	2.52	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.46	0.43
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.52	0.43
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	2.00	0.43
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.52	0.43
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	2.00	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:G:485:SER:HA	2:G:488:LEU:HB2	2.01	0.43
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.01	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.43
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.43
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.01	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.00	0.43
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.42	0.43
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.54	0.43
2:G:626:LEU:HG	2:G:628:GLY:H	1.84	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.52	0.43
2:G:2437:ALA:HA	2:G:2438:PRO:HD3	1.92	0.43
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	2.01	0.43
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.36	0.43
1:H:23:VAL:HB	1:H:105:ASN:HA	2.01	0.42
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.01	0.42
2:E:485:SER:HA	2:E:488:LEU:HB2	2.01	0.42
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.52	0.42
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.42
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	2.00	0.42
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.00	0.42
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.42
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.01	0.42
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.42
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.42
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.37	0.42
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.42
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.42
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.42
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.42
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.52	0.42
2:G:2236:LEU:HD23	2:G:2275:VAL:HG11	2.01	0.42
2:G:4840:THR:O	2:G:4844:LEU:N	2.47	0.42
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.42
2:B:2299:VAL:O	2:B:2303:ALA:N	2.52	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.00	0.42
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.52	0.42
2:E:1804:LEU:O	2:E:1808:ARG:N	2.45	0.42
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.42
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	2.02	0.42
2:I:485:SER:HA	2:I:488:LEU:HB2	2.01	0.42
2:I:626:LEU:HG	2:I:628:GLY:H	1.85	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:4056:GLU:O	2:I:4060:LYS:N	2.52	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	1.99	0.42
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.84	0.42
2:G:460:GLN:HG2	2:G:462:GLU:H	1.83	0.42
1:H:21:THR:HA	1:H:49:ARG:HA	2.01	0.42
2:B:460:GLN:HG2	2:B:462:GLU:H	1.83	0.42
2:B:1639:LEU:HD12	2:B:1653:LEU:HD21	2.00	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.42
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.37	0.42
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.54	0.42
2:E:950:LEU:HB3	2:E:970:LEU:HD22	2.02	0.42
2:E:1639:LEU:HD12	2:E:1653:LEU:HD21	2.00	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.42
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.54	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.00	0.42
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.52	0.42
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.85	0.42
2:B:914:PRO:O	2:B:918:ARG:N	2.51	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.01	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.42
2:E:2236:LEU:HD23	2:E:2275:VAL:HG11	2.01	0.42
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.54	0.42
2:I:25:SER:HA	2:I:34:LYS:HA	2.02	0.42
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.84	0.42
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.01	0.42
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.42
2:I:2517:UNK:O	2:I:2521:UNK:N	2.52	0.42
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.42
1:F:21:THR:HA	1:F:49:ARG:HA	2.01	0.42
2:B:25:SER:HA	2:B:34:LYS:HA	2.02	0.42
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	2.02	0.42
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.42
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.32	0.42
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.42
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.02	0.42
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	2.01	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.47	0.42
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	2.02	0.42
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.42
2:B:1238:PHE:O	2:B:1606:SER:N	2.48	0.42
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.84	0.42
2:E:626:LEU:HG	2:E:628:GLY:H	1.84	0.42
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.85	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.02	0.42
2:G:25:SER:HA	2:G:34:LYS:HA	2.02	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.42
2:G:950:LEU:HB3	2:G:970:LEU:HD22	2.02	0.42
1:A:23:VAL:HB	1:A:105:ASN:HA	2.01	0.42
2:B:626:LEU:HG	2:B:628:GLY:H	1.84	0.42
2:B:950:LEU:HB3	2:B:970:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:THR:O	2:B:987:ARG:N	2.51	0.42
2:B:4942:GLU:HG3	2:E:4944:ARG:HH11	1.84	0.42
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.42
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.01	0.42
2:I:663:TYR:HB2	2:I:808:TYR:HB3	2.02	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG11	2.01	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.02	0.42
2:B:485:SER:HA	2:B:488:LEU:HB2	2.01	0.42
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.85	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.47	0.42
2:E:838:HIS:HA	2:E:1201:HIS:HB3	2.01	0.42
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.42
1:J:21:THR:HA	1:J:49:ARG:HA	2.01	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.01	0.41
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.84	0.41
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.41
2:I:1148:VAL:N	2:I:1165:ASN:OD1	2.53	0.41
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.53	0.41
2:I:2299:VAL:O	2:I:2303:ALA:N	2.52	0.41
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.02	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.85	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.31	0.41
2:B:759:ILE:HG22	2:B:760:ASN:H	1.86	0.41
2:B:1148:VAL:N	2:B:1165:ASN:OD1	2.54	0.41
2:E:25:SER:HA	2:E:34:LYS:HA	2.02	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.02	0.41
1:F:23:VAL:HB	1:F:105:ASN:HA	2.01	0.41
2:B:663:TYR:HB2	2:B:808:TYR:HB3	2.02	0.41
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.85	0.41
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.03	0.41
2:E:1271:ARG:HA	2:E:1471:UNK:HA	2.02	0.41
2:I:23:GLN:HE21	2:I:34:LYS:HB3	1.85	0.41
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.03	0.41
2:I:759:ILE:HG22	2:I:760:ASN:H	1.86	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.48	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.02	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4056:GLU:O	2:G:4060:LYS:N	2.52	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.03	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.85	0.41
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.41
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:E:4840:THR:O	2:E:4844:LEU:N	2.47	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.19	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.02	0.41
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.30	0.41
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.92	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.02	0.41
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.01	0.41
2:B:1041:GLN:O	2:B:1045:THR:OG1	2.30	0.41
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	2.03	0.41
2:B:4918:ILE:HD11	2:E:4888:TYR:HA	2.03	0.41
2:E:759:ILE:HG22	2:E:760:ASN:H	1.86	0.41
2:I:56:GLN:O	2:I:309:THR:OG1	2.30	0.41
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.41
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.44	0.41
2:G:759:ILE:HG22	2:G:760:ASN:H	1.86	0.41
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.01	0.41
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.44	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.02	0.41
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.38	0.41
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.02	0.41
2:B:4840:THR:O	2:B:4844:LEU:N	2.47	0.41
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.02	0.41
2:I:950:LEU:HB3	2:I:970:LEU:HD22	2.02	0.41
1:A:21:THR:HA	1:A:49:ARG:HA	2.02	0.41
2:B:290:TYR:O	2:B:302:VAL:N	2.50	0.41
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.01	0.41
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.28	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.37	0.41
2:I:4840:THR:O	2:I:4844:LEU:N	2.47	0.41
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.85	0.41
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	2.03	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.19	0.41
2:B:776:LEU:HG	2:B:848:HIS:HA	2.03	0.41
2:B:2236:LEU:HD23	2:B:2275:VAL:HG11	2.01	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.03	0.41
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.53	0.41
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.95	0.41
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.02	0.41
2:I:2103:VAL:O	2:I:2107:GLN:N	2.48	0.41
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	2.03	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.03	0.41
2:G:1148:VAL:N	2:G:1165:ASN:OD1	2.53	0.41
2:G:1804:LEU:O	2:G:1808:ARG:N	2.45	0.41
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.94	0.41
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.53	0.41
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.41
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.38	0.41
2:G:4977:THR:O	2:G:4981:GLU:N	2.41	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.03	0.41
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.54	0.41
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.38	0.41
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.38	0.41
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.34	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.03	0.40
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.40
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.03	0.40
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.02	0.40
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.40
2:E:1663:HIS:O	2:E:1667:LEU:N	2.53	0.40
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.03	0.40
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.40
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.02	0.40
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.04	0.40
2:I:1729:SER:O	2:I:2163:ARG:NH1	2.54	0.40
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.56	0.40
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1271:ARG:HA	2:G:1471:UNK:HA	2.04	0.40
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.96	0.40
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.87	0.40
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.56	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.40
2:B:1729:SER:O	2:B:2163:ARG:NH1	2.54	0.40
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.40
2:I:684:VAL:HA	2:I:781:VAL:HA	2.03	0.40
2:I:1657:LEU:HD13	2:I:1657:LEU:HA	1.97	0.40
2:G:1497:UNK:HA	2:G:1535:UNK:HA	2.03	0.40
2:G:2208:MET:HE2	2:G:2208:MET:HB3	1.99	0.40
1:F:5:GLU:HB2	1:F:73:LYS:HB3	2.04	0.40
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.03	0.40
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.04	0.40
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.04	0.40
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.86	0.40
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.40
2:E:1729:SER:O	2:E:2163:ARG:NH1	2.54	0.40
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.03	0.40
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.54	0.40
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.38	0.40
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.04	0.40
1:A:5:GLU:HB2	1:A:73:LYS:HB3	2.04	0.40
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.04	0.40
2:E:1148:VAL:N	2:E:1165:ASN:OD1	2.54	0.40
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	2.03	0.40
2:I:716:PHE:HE2	2:I:759:ILE:HD11	1.87	0.40
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.86	0.40
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.04	0.40
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.04	0.40
2:B:2290:LEU:HB3	2:B:3849:ARG:NH1	2.37	0.40
2:B:3662:ILE:H	2:B:3662:ILE:HG13	1.77	0.40
2:E:3902:TYR:O	2:E:3906:GLN:NE2	2.55	0.40
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	2.02	0.40
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.40
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.04	0.40
2:I:415:ILE:HA	2:I:418:LEU:HD13	2.04	0.40
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.40
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.86	0.40
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.02	0.40
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2034:PHE:O	2:G:2038:LEU:N	2.55	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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2923 (90%)	308 (10%)	4 (0%)	48	83
2	E	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	48	83
2	G	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	48	83
2	I	3235/4676 (69%)	2924 (90%)	307 (10%)	4 (0%)	48	83
All	All	13360/19136 (70%)	12064 (90%)	1280 (10%)	16 (0%)	49	83

All (16) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3202 (78%)	2482 (100%)	11 (0%)	84	84
2	E	2493/3202 (78%)	2482 (100%)	11 (0%)	84	84
2	G	2493/3202 (78%)	2482 (100%)	11 (0%)	84	84
2	I	2493/3202 (78%)	2482 (100%)	11 (0%)	84	84
All	All	10324/13164 (78%)	10280 (100%)	44 (0%)	81	84

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	688	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	3663	LEU

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Mol	Chain	Res	Type
2	B	3805	LEU
2	B	4081	VAL
2	B	4154	VAL
2	E	131	LEU
2	E	688	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4081	VAL
2	E	4154	VAL
2	I	131	LEU
2	I	688	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1657	LEU
2	I	1676	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4154	VAL
2	G	131	LEU
2	G	688	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4154	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	87	HIS

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Mol	Chain	Res	Type
1	A	32	ASN
1	A	87	HIS
1	H	32	ASN
1	H	87	HIS
1	J	32	ASN
1	J	87	HIS
2	B	23	GLN
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	156	GLN
2	B	203	ASN
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	461	HIS
2	B	465	GLN
2	B	479	GLN
2	B	489	ASN
2	B	495	ASN
2	B	582	HIS
2	B	797	HIS
2	B	838	HIS
2	B	866	HIS
2	B	877	ASN
2	B	1220	GLN
2	B	1598	GLN
2	B	1665	HIS
2	B	1679	ASN
2	B	1693	GLN
2	B	1719	HIS
2	B	1949	GLN
2	B	1972	ASN
2	B	1973	GLN
2	B	2032	GLN
2	B	2194	HIS
2	B	2260	ASN
2	B	2773	ASN
2	B	2788	HIS

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Mol	Chain	Res	Type
2	B	2877	GLN
2	B	3761	GLN
2	B	3814	GLN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3906	GLN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4246	GLN
2	B	4691	GLN
2	B	4728	HIS
2	B	4776	GLN
2	B	4864	ASN
2	B	4947	GLN
2	B	4949	GLN
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	156	GLN
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	461	HIS
2	E	465	GLN
2	E	479	GLN
2	E	489	ASN
2	E	495	ASN
2	E	582	HIS
2	E	797	HIS
2	E	838	HIS
2	E	866	HIS
2	E	877	ASN

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Mol	Chain	Res	Type
2	E	1598	GLN
2	E	1665	HIS
2	E	1679	ASN
2	E	1693	GLN
2	E	1719	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	2194	HIS
2	E	2773	ASN
2	E	2788	HIS
2	E	2877	GLN
2	E	3761	GLN
2	E	3814	GLN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3906	GLN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4246	GLN
2	E	4691	GLN
2	E	4728	HIS
2	E	4776	GLN
2	E	4864	ASN
2	E	4947	GLN
2	E	4949	GLN
2	E	5015	GLN
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	113	HIS
2	I	156	GLN
2	I	203	ASN
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN

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Mol	Chain	Res	Type
2	I	405	HIS
2	I	413	GLN
2	I	461	HIS
2	I	465	GLN
2	I	479	GLN
2	I	489	ASN
2	I	495	ASN
2	I	582	HIS
2	I	765	GLN
2	I	797	HIS
2	I	838	HIS
2	I	866	HIS
2	I	877	ASN
2	I	1598	GLN
2	I	1665	HIS
2	I	1679	ASN
2	I	1693	GLN
2	I	1719	HIS
2	I	1861	GLN
2	I	1972	ASN
2	I	2005	GLN
2	I	2194	HIS
2	I	2260	ASN
2	I	2773	ASN
2	I	2788	HIS
2	I	2877	GLN
2	I	3761	GLN
2	I	3814	GLN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3906	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4691	GLN

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Mol	Chain	Res	Type
2	I	4728	HIS
2	I	4776	GLN
2	I	4864	ASN
2	I	4947	GLN
2	I	4949	GLN
2	I	5015	GLN
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	156	GLN
2	G	203	ASN
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	461	HIS
2	G	465	GLN
2	G	479	GLN
2	G	489	ASN
2	G	495	ASN
2	G	582	HIS
2	G	797	HIS
2	G	838	HIS
2	G	866	HIS
2	G	877	ASN
2	G	1220	GLN
2	G	1598	GLN
2	G	1665	HIS
2	G	1679	ASN
2	G	1693	GLN
2	G	1719	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2194	HIS
2	G	2773	ASN
2	G	2788	HIS
2	G	2877	GLN
2	G	3761	GLN

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Mol	Chain	Res	Type
2	G	3814	GLN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3906	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4691	GLN
2	G	4728	HIS
2	G	4776	GLN
2	G	4864	ASN
2	G	4947	GLN
2	G	4949	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	12
2	G	12
2	E	12
2	I	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	43.37
1	G	3613:UNK	C	3639:THR	N	43.37
1	E	3613:UNK	C	3639:THR	N	43.34
1	I	3613:UNK	C	3639:THR	N	43.32
1	B	3163:UNK	C	3170:UNK	N	16.45
1	E	3163:UNK	C	3170:UNK	N	16.45
1	I	3163:UNK	C	3170:UNK	N	16.45
1	G	3163:UNK	C	3170:UNK	N	16.45
1	B	3468:UNK	C	3511:UNK	N	15.10
1	E	3468:UNK	C	3511:UNK	N	15.10
1	I	3468:UNK	C	3511:UNK	N	15.10
1	G	3468:UNK	C	3511:UNK	N	15.10
1	I	3063:UNK	C	3134:UNK	N	14.88
1	B	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.86
1	I	2703:UNK	C	2734:ASN	N	14.34
1	E	2703:UNK	C	2734:ASN	N	14.33
1	B	2703:UNK	C	2734:ASN	N	14.32
1	G	2703:UNK	C	2734:ASN	N	14.32
1	B	3236:UNK	C	3241:UNK	N	13.55

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3236:UNK	C	3241:UNK	N	13.55
1	I	3236:UNK	C	3241:UNK	N	13.55
1	G	3236:UNK	C	3241:UNK	N	13.55
1	I	1564:UNK	C	1573:MET	N	12.87
1	E	1564:UNK	C	1573:MET	N	12.85
1	G	1564:UNK	C	1573:MET	N	12.85
1	B	1564:UNK	C	1573:MET	N	12.84
1	B	2976:UNK	C	2995:UNK	N	12.50
1	E	2976:UNK	C	2995:UNK	N	12.50
1	I	2976:UNK	C	2995:UNK	N	12.50
1	G	2976:UNK	C	2995:UNK	N	12.50
1	B	3254:UNK	C	3261:UNK	N	8.64
1	E	3254:UNK	C	3261:UNK	N	8.64
1	I	3254:UNK	C	3261:UNK	N	8.64
1	G	3254:UNK	C	3261:UNK	N	8.64
1	I	1297:UNK	C	1430:UNK	N	5.73
1	B	1297:UNK	C	1430:UNK	N	5.72
1	E	1297:UNK	C	1430:UNK	N	5.72
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	2939:ARG	C	2942:UNK	N	3.71
1	E	2939:ARG	C	2942:UNK	N	3.71
1	I	2939:ARG	C	2942:UNK	N	3.71
1	G	2939:ARG	C	2942:UNK	N	3.71
1	G	2479:LEU	C	2487:UNK	N	3.27
1	B	2479:LEU	C	2487:UNK	N	3.26
1	E	2479:LEU	C	2487:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.25

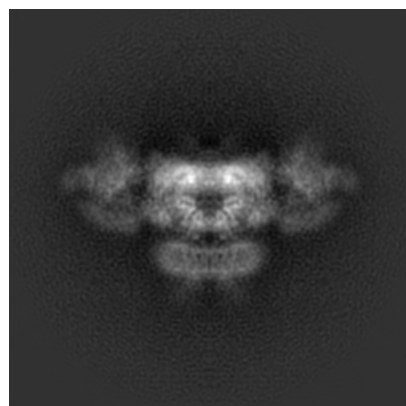
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8374. These allow visual inspection of the internal detail of the map and identification of artifacts.

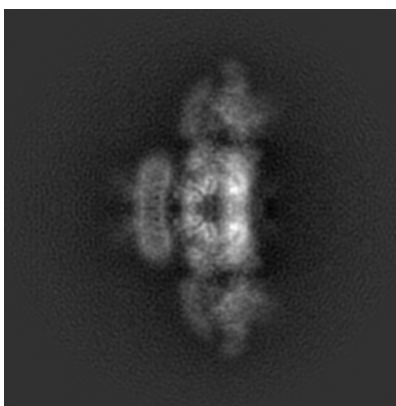
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

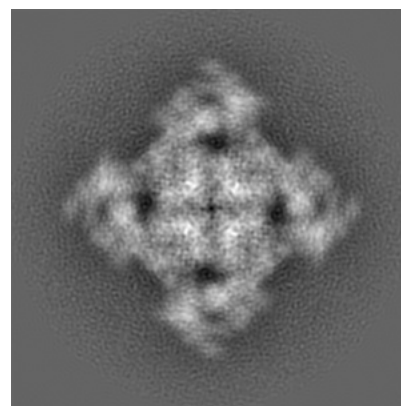
6.1.1 Primary map



X

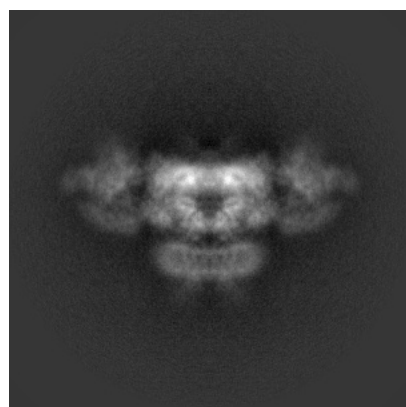


Y

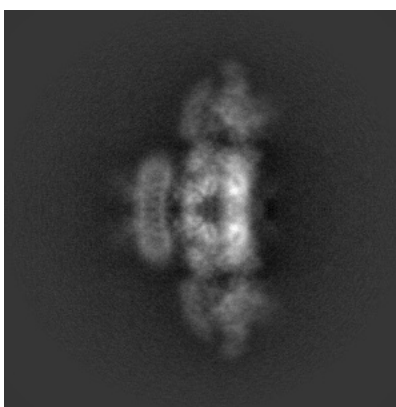


Z

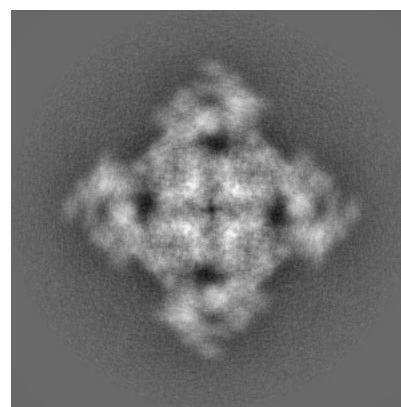
6.1.2 Raw map



X



Y

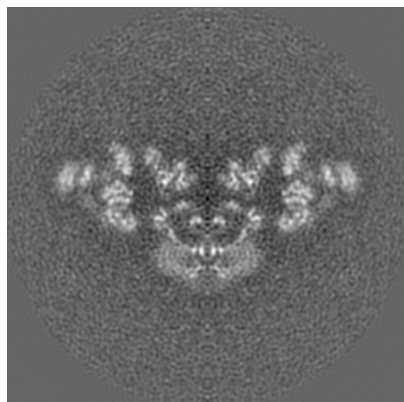


Z

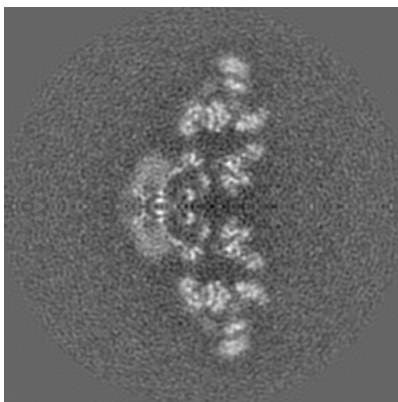
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

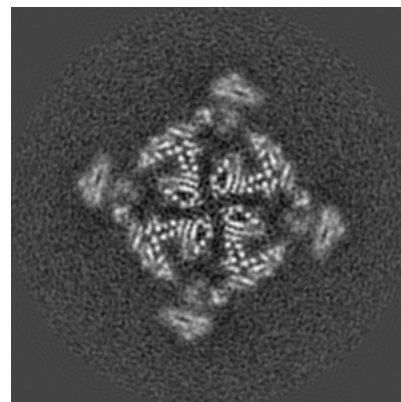
6.2.1 Primary map



X Index: 200

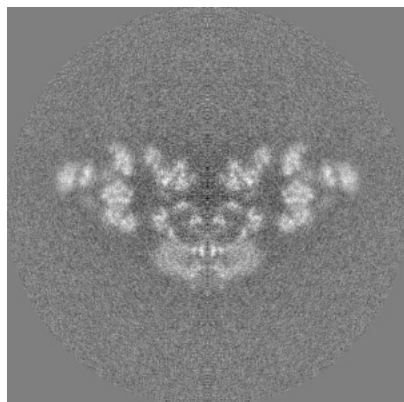


Y Index: 200

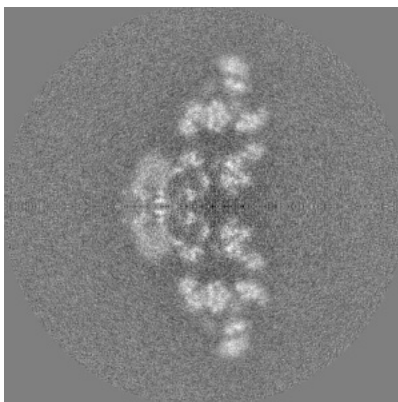


Z Index: 200

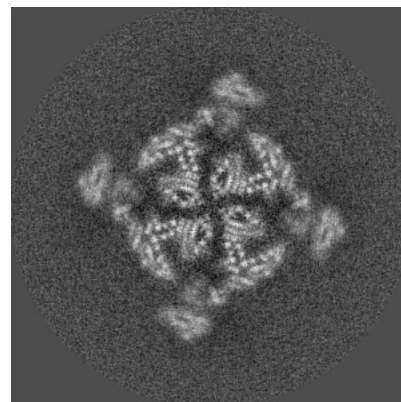
6.2.2 Raw map



X Index: 200



Y Index: 200

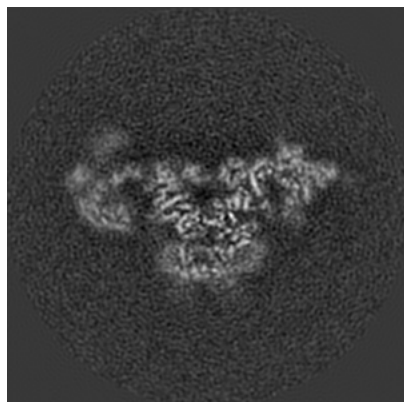


Z Index: 200

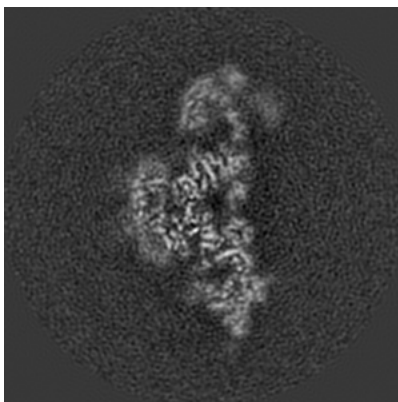
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

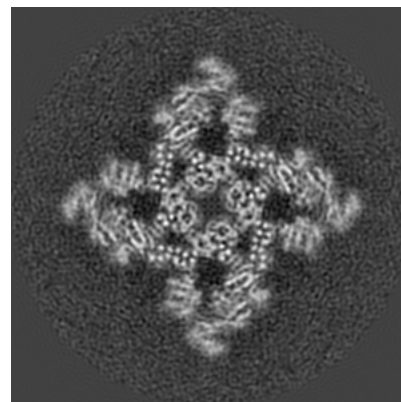
6.3.1 Primary map



X Index: 184

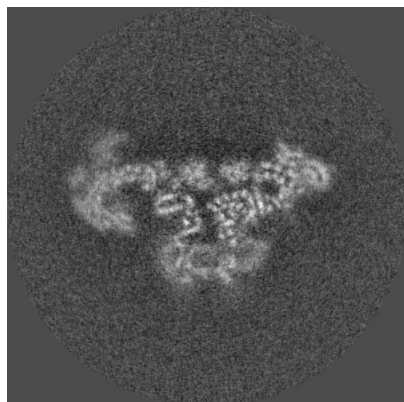


Y Index: 184

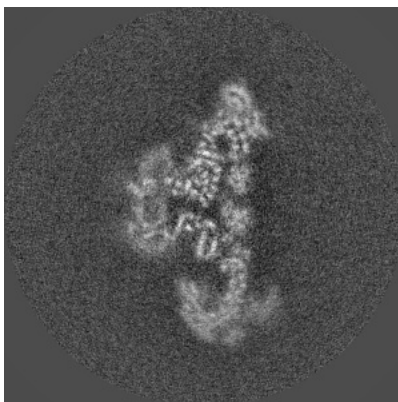


Z Index: 227

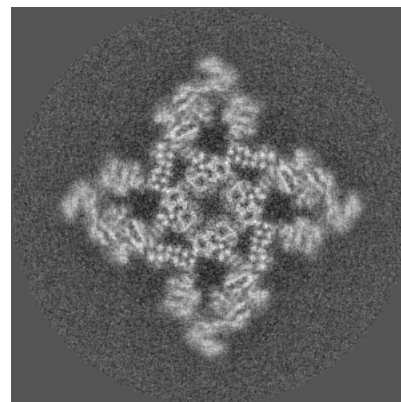
6.3.2 Raw map



X Index: 179



Y Index: 221

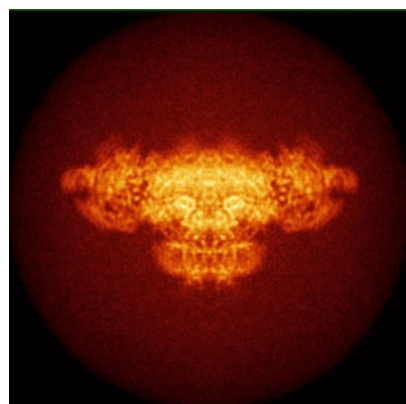


Z Index: 227

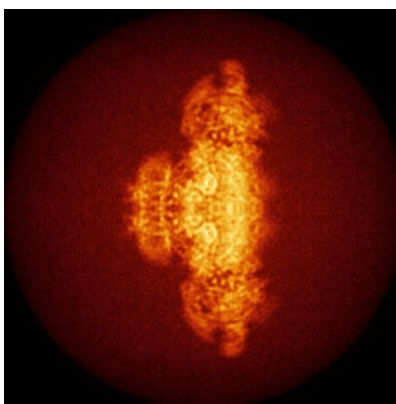
The images above show the largest variance slices of the map in three orthogonal directions.

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

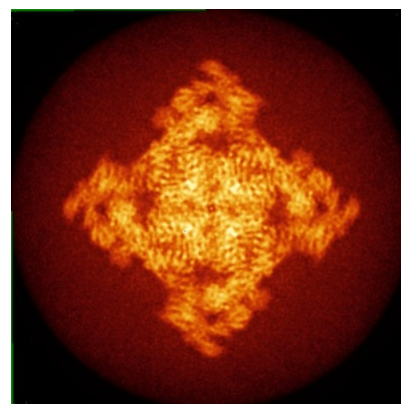
6.4.1 Primary map



X

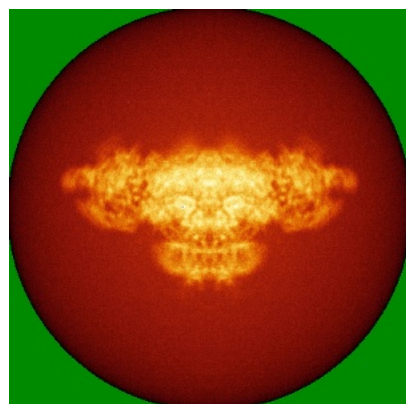


Y

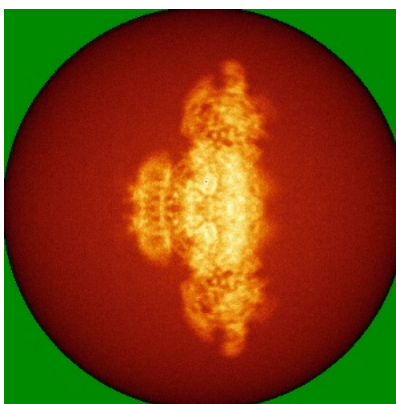


Z

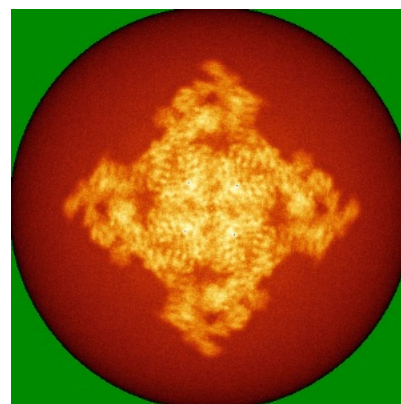
6.4.2 Raw map



X



Y

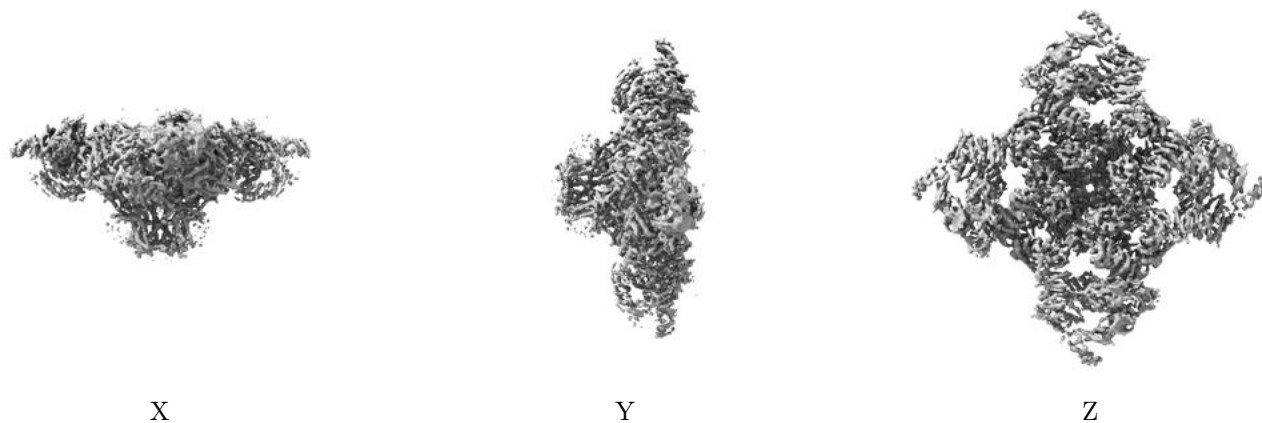


Z

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.

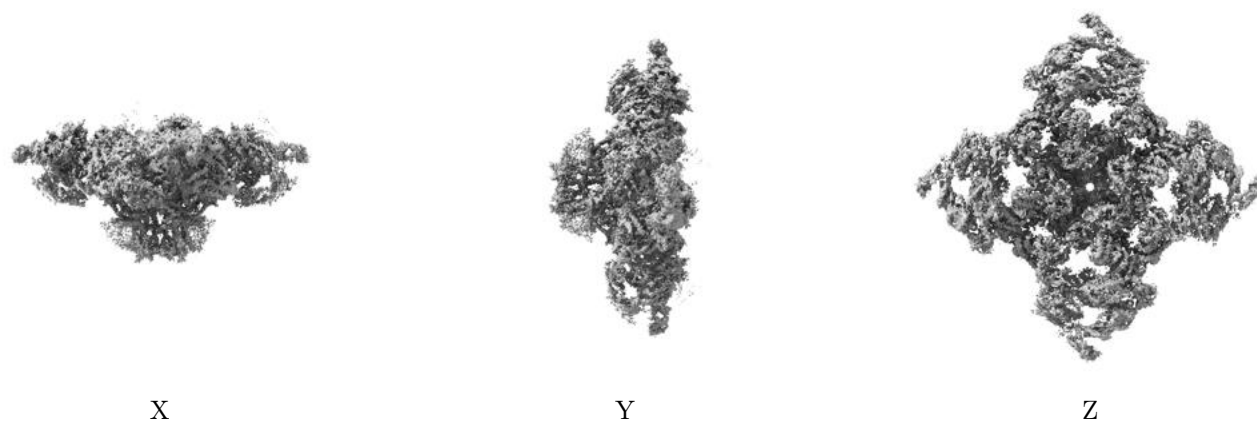
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

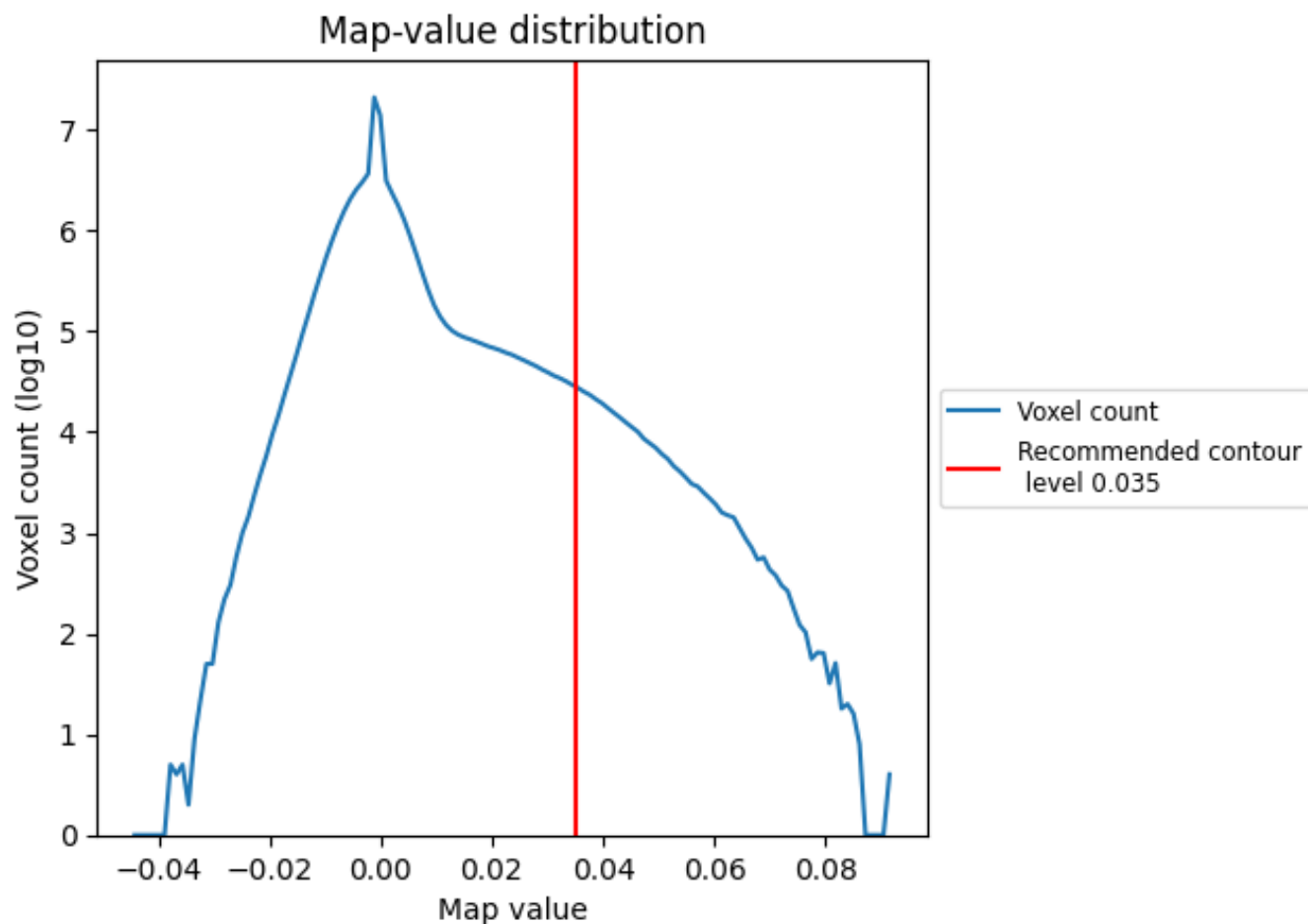
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

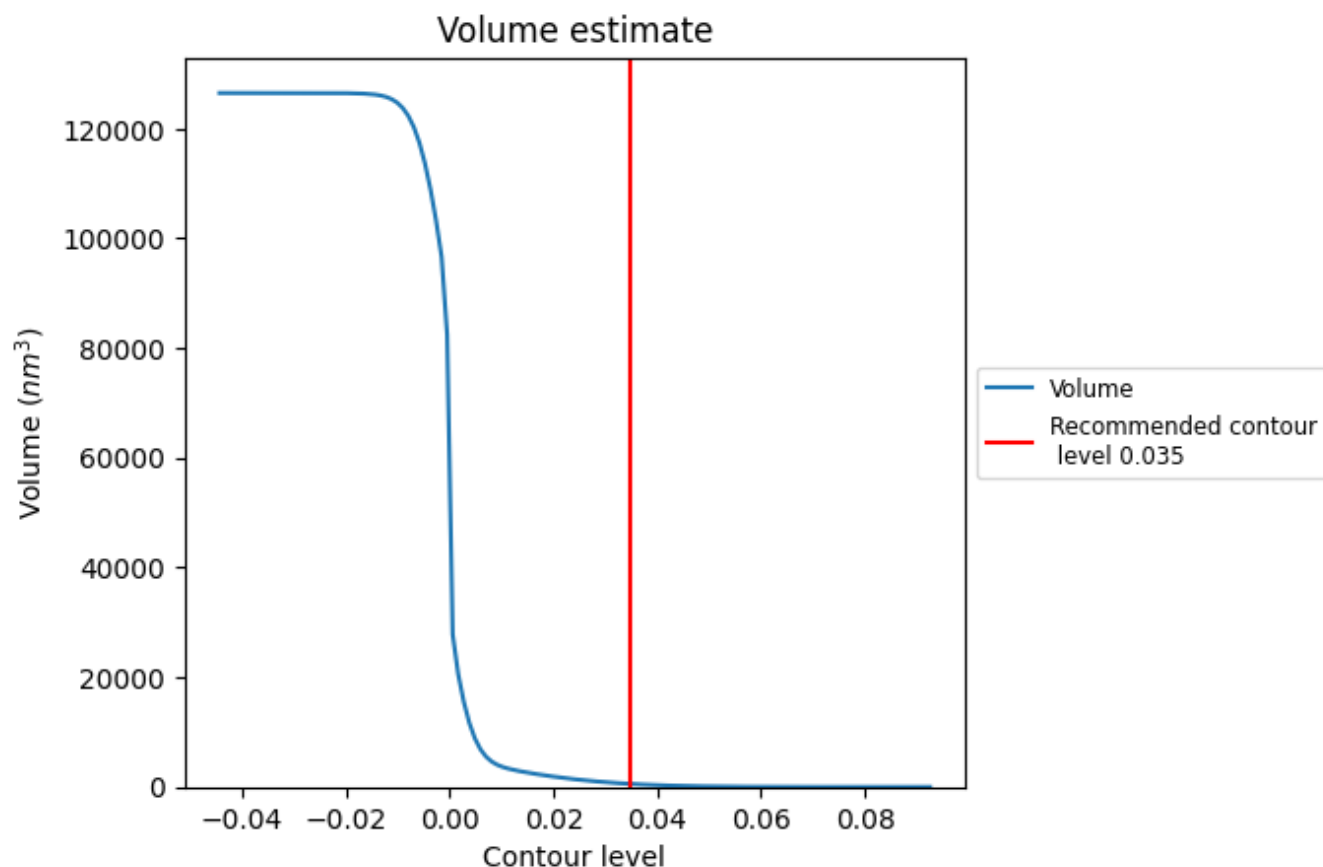
This section contains the results of statistical analysis of the map.

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.

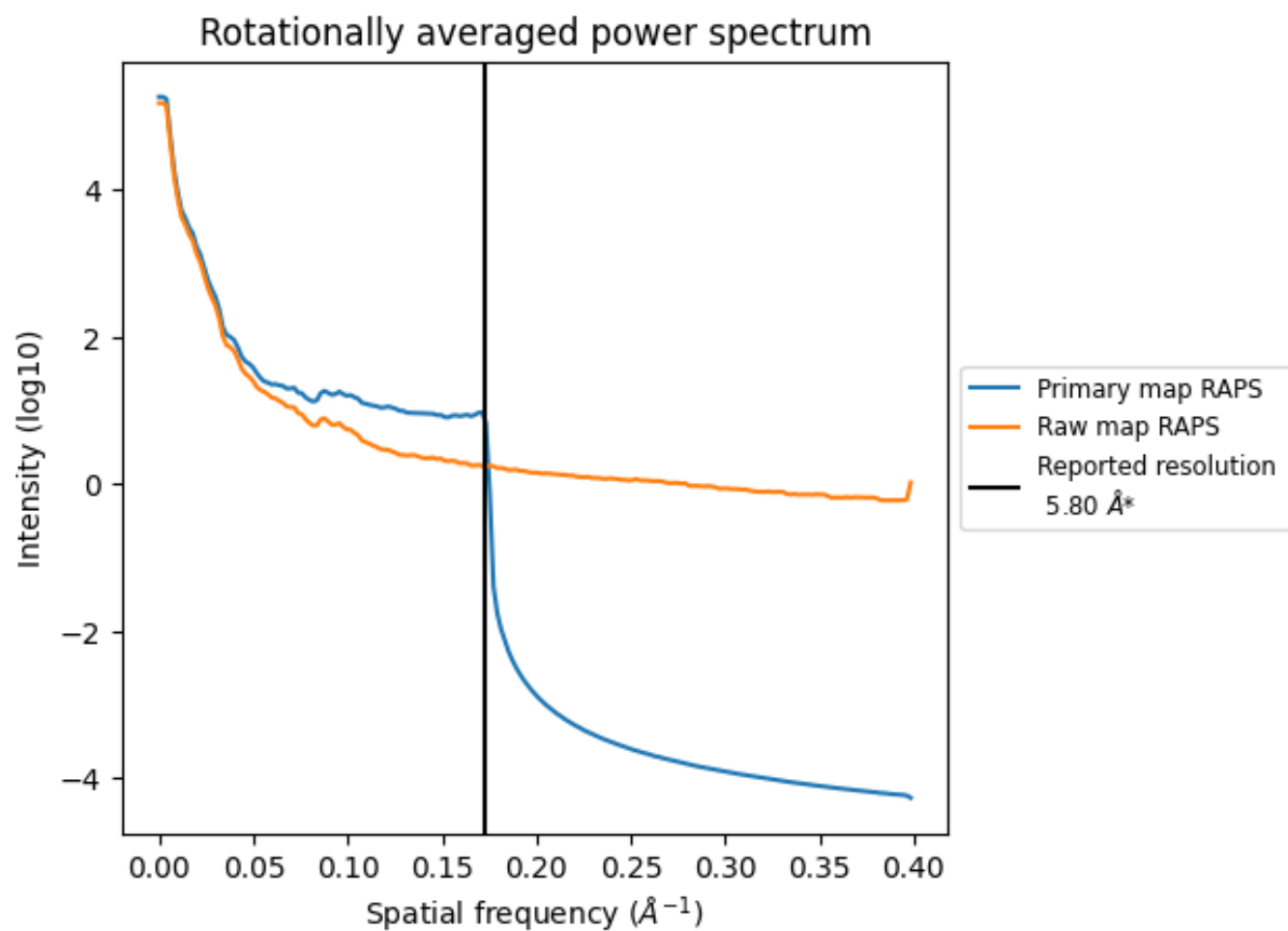
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 553 nm^3 ; this corresponds to an approximate mass of 500 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 [i](#)

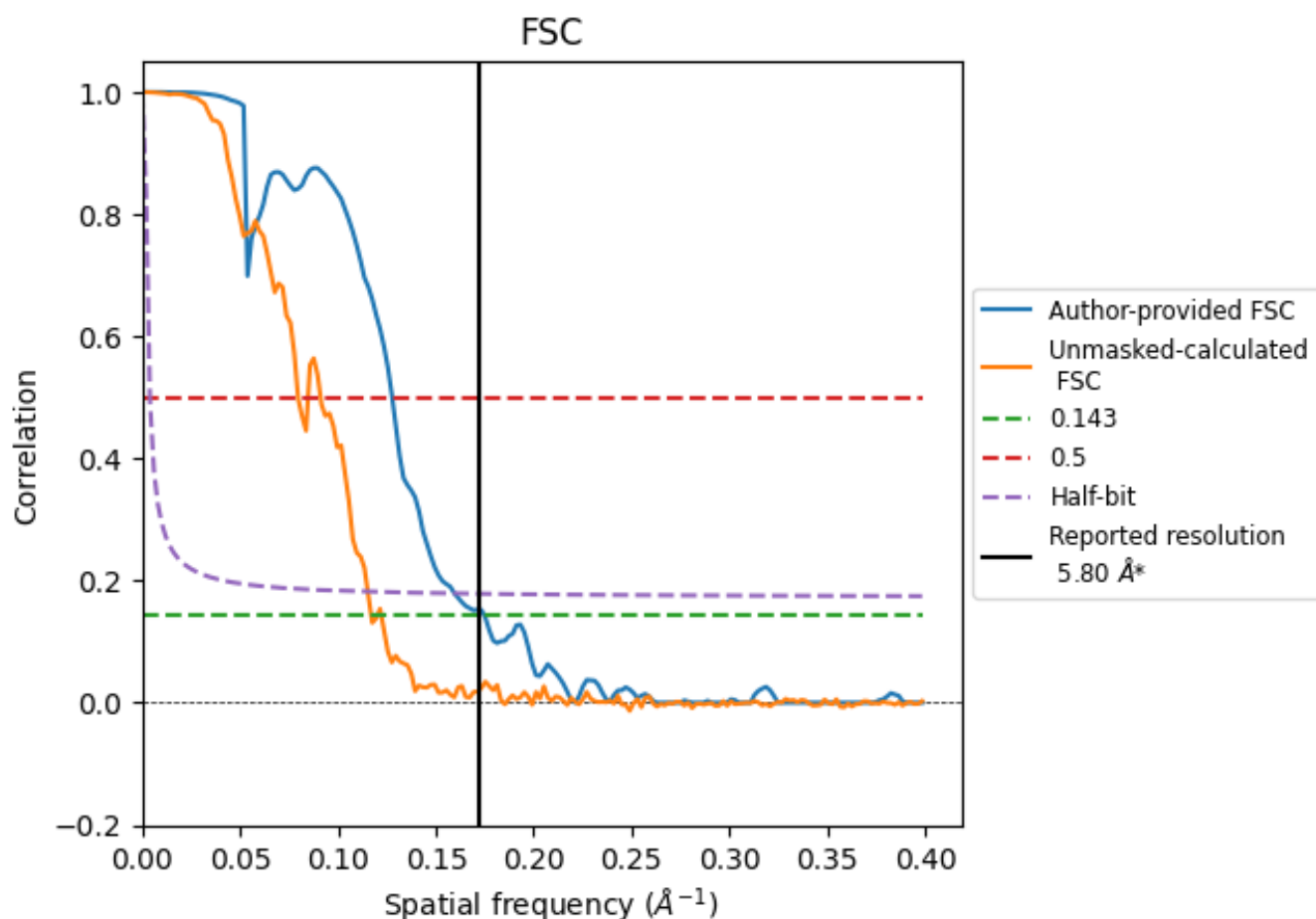


*Reported resolution corresponds to spatial frequency of 0.172 $\text{\AA}^{-1}$

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 0.172 Å⁻¹

8.2 Resolution estimates [i](#)

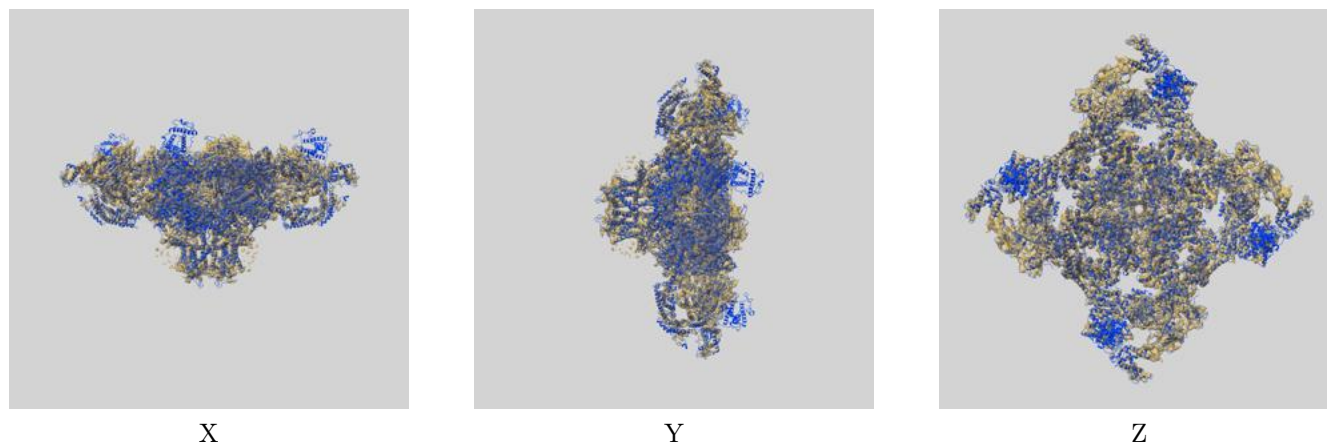
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.72	7.83	6.27
Unmasked-calculated*	8.55	12.56	8.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.55 differs from the reported value 5.8 by more than 10 %

9 Map-model fit [i](#)

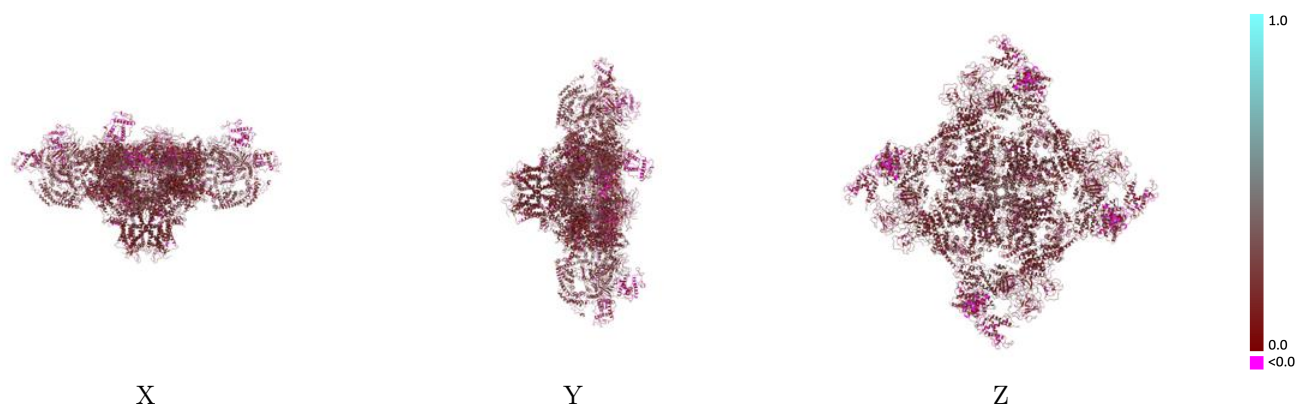
This section contains information regarding the fit between EMDB map EMD-8374 and PDB model 5T9R. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



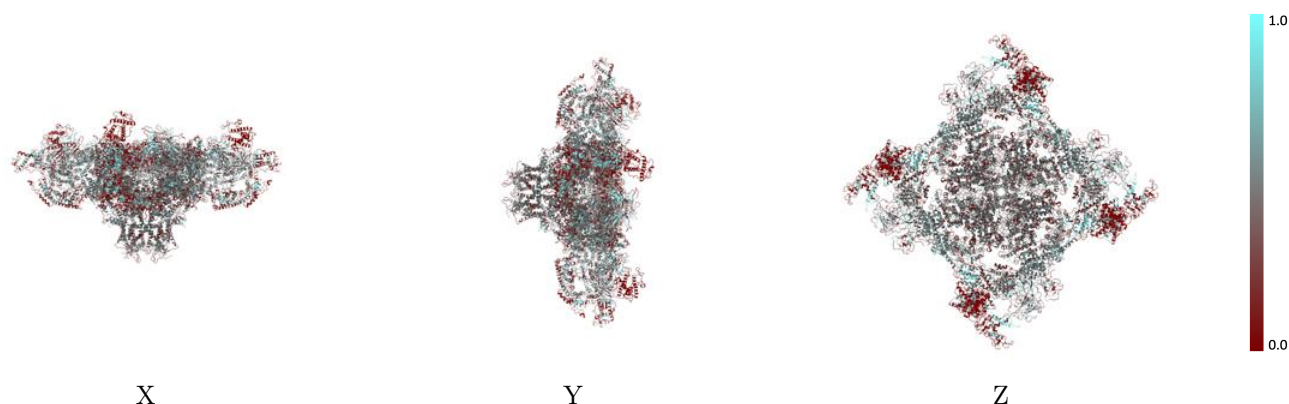
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



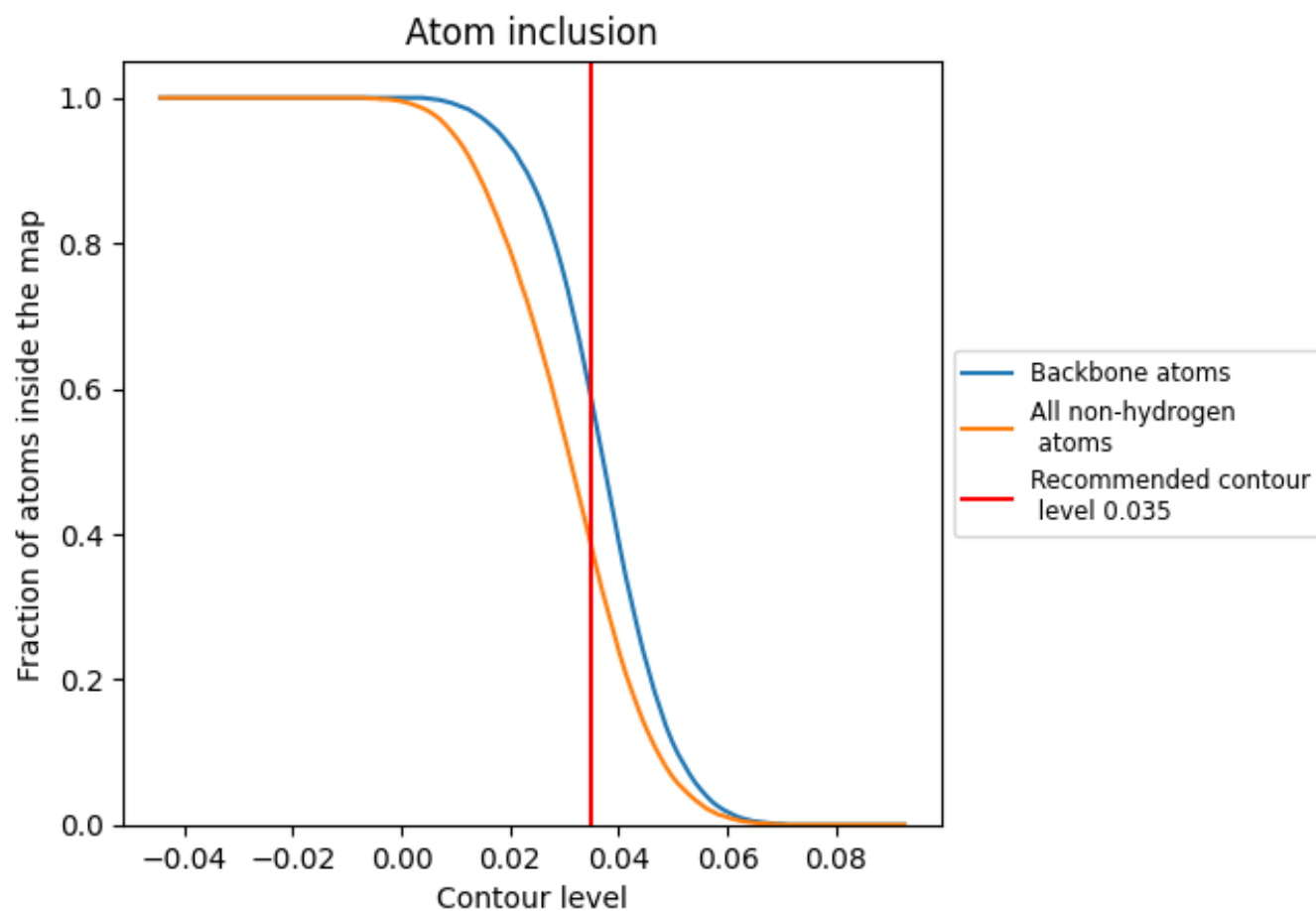
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 38% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3810	0.1900
A	0.3330	0.1720
B	0.3830	0.1910
E	0.3820	0.1910
F	0.3350	0.1750
G	0.3830	0.1900
H	0.3360	0.1740
I	0.3820	0.1910
J	0.3350	0.1740

1.0

0.0

<0.0