



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:44 PM UTC

PDB ID : 8SEN / pdb_00008sen
EMDB ID : EMD-40422
Title : Cryo-EM Structure of RyR1
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.49 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:

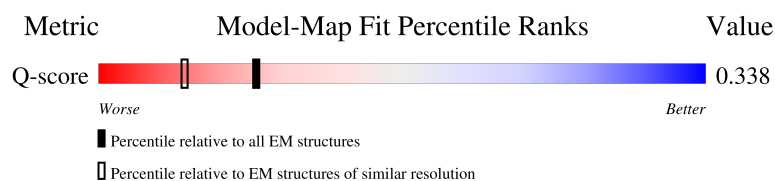
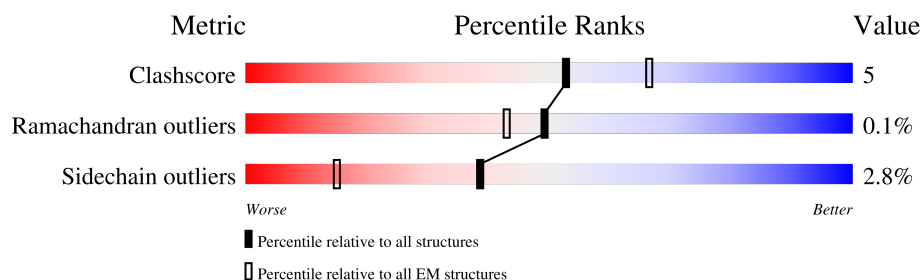
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.49 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	13600 (2.99 - 3.99)

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	5037	16% 73% 14% 13%
1	B	5037	16% 73% 14% 13%
1	C	5037	16% 73% 14% 13%
1	D	5037	16% 73% 14% 13%

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Mol	Chain	Length	Quality of chain
2	E	350	 24% 6% 69%
2	F	350	 24% 7% 69%
2	G	350	 24% 6% 69%
2	H	350	 24% 7% 69%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 142960 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		
1	B	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		
1	C	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		
1	D	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

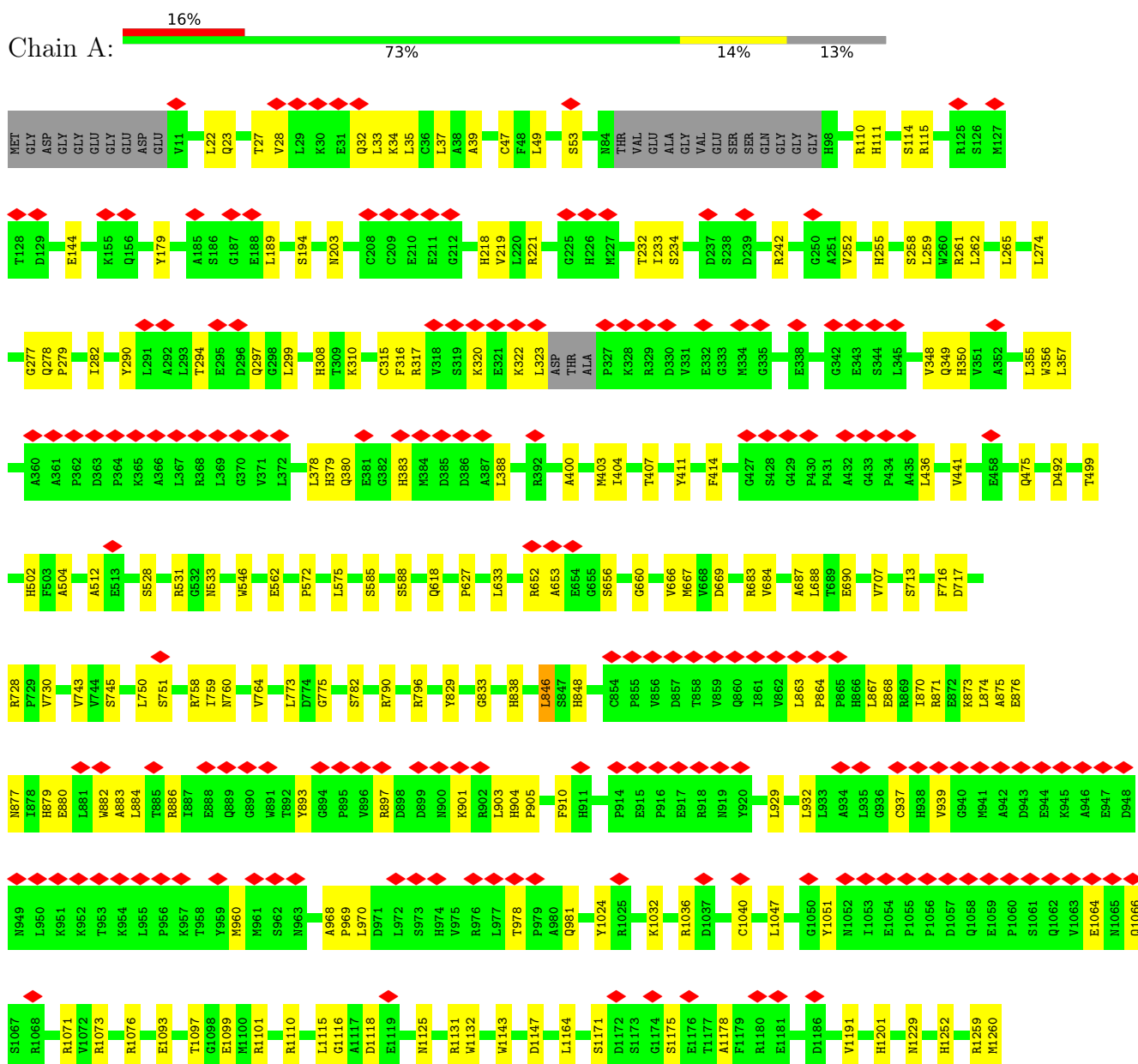
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

3 Residue-property plots

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: Ryanodine receptor 1



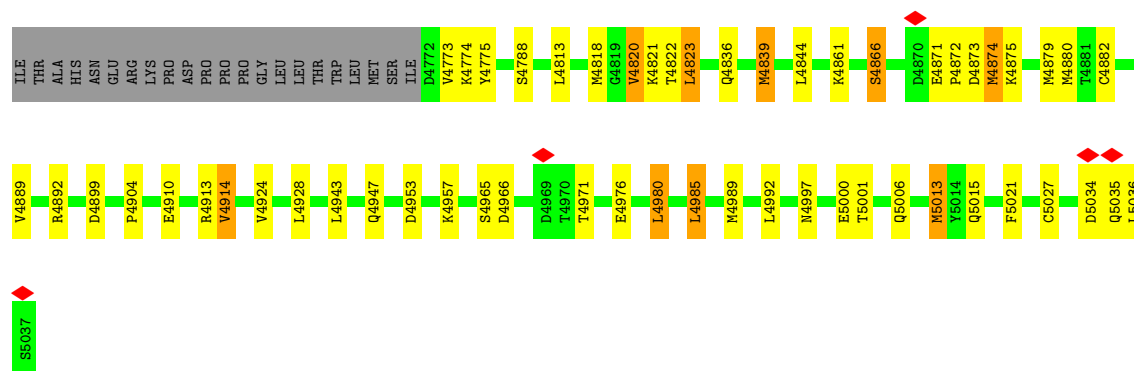


S4089	M3875	GLY	H3449	V3346	K3247	D3154	H3052	M2967	P2903	SER
K4090	A3876	GLU	N3450	S3347	R3248	D3155	R3053	S2970	L2904	GLN
K4091	D3877	ALA	R3453	L3354	L3249	V3156	V3054			THR
D4092	F3880	GLU				I3157	S3055		L2905	ALA
F4093	L3891	GLU	V3459	F3358	L3256	L3158	L3056	F2973	V2906	GLN
D4094		GLU	V3460	I3359	T3264	D3159	T3059	A2975	P2907	THR
K4095	F3899		Q3461	T3361	E3265	S3164	P3062	H2976	P2908	TYR
K4096	Q3900		N3462	T3360	K3266	R3167	V3065	L2977	D2909	ASP
M4097	N3901		E3463	F3364	H3268	L3169	D3076	E2978	L2977	PRO
D4098	R3904		T3464	R3364	T3272	S3171	A3077		T2910	ARG
S4099	F3753		N3465	L3365	L3277	S3172	V3080	V2980	T2911	GLU
S4100	E3754		N3466	K3371		S3173	K3081	V2981	T2912	GLY
K4101	E3755		N3467	A3374	K3284	S3174	V3082	S2982	A2913	
F4102	K3756		S3468	E3375	E3285	L3175	K3082	K2983	K2914	
F4103	E3757		F3469	Q3378	M3286	G3176	S3083	G2984	K2915	
T4104			L3470	L3379	R3287	T3177	G3084	V2986	K2916	
F4106	H3771		T3471	R3380	E3290	T3178	P3085	E2987	A2917	
T4108	R3773		A3472	L3381	A3291	K3179	K3085	K2988	R2918	
D4109	G3801		S3473	E3382	A3291	N3180	E3086	S2989	R2920	
F4110	L3805		K3474	E3383	P3292	T3181	E3087	P2990	E2921	
L4111			S3476	K3384	P3293	G3182	V3088	H2991	K2922	
L4112	N3976		S3477	A3385	P3294	V3183	E3089	E2992	A2923	
M4001			K3478	E3387	A3295	E3184	A3099	Q2993	Q2924	
K4002			A3479	E3388	L3296	L3194	V3107	F2997	E2925	
D4006			LYS	E3389	P3297	A3195		F2998	L2926	
L4017			ALA	E3390	A3298	R3196			L2927	
M4044			GLY	G3390	G3299	L3206		I3001	K2928	
F4061			ASP	E3391	A3300			L3002	F2929	
K4067			ALA	L3392	P3301	E3212		I3006	L2930	
L4068			GLN	L3393	P3302	G3213		F3009	Q2872	
K4069			SER	L3394	P3303	N3214		F3010	A2873	
D4070			GLY	R3395	C3304	A3215			M2874	
I4071			ASP	D3396	T3305	C3216		F3017	A2875	
V4072			GLN	R3403	L3316	S3217			Q2876	
G4073			ARG	L3408	I3322	V3218		A3022	Q2877	
S4074			THR	L3414	I3323	Y3219		K3023	L2878	
E4075			LYS	R3417	V3324	T3220		V3024	E2879	
A4076			LYS	D3417	N3325	T3221		L3025	E2880	
D4079			R3498	R3420	D3330	K3222		G3026	N2881	
Y4080			R3499	R3424	E3331	P3224		S3027	Y2882	
T4082			G3500	R3437	K3335	R3225		G3028	H2883	
D4083			D3501	L3424	K3336	E3226		G3029	T2884	
P4084			R3502	N3430	K3337	R3227		H3030	V2886	
R4085			S3504	E3433	R3337	A3228		K3034	Q2887	
I4089			V3505	L3434	L3338	I3229		E3035	R2888	
			Q3506	F3435	A3339	L3230		K3036	T2889	
			T3507	R3437	V3340	G3231		E3037	K2891	
			V3511	M3437	F3341	L3232		K3045	Q2892	
			T3520	F3442	P3344	P3233		A3048	E2893	
			M3524		Q3343	N3234		L3049	L2894	
					T3345			V3050	E2895	
					H3621			R3051	A2896	
									K2897	
									Q2961	
									Q2962	
									L2963	
									L2964	
									G2899	
									G2900	
									T2901	
									H2902	

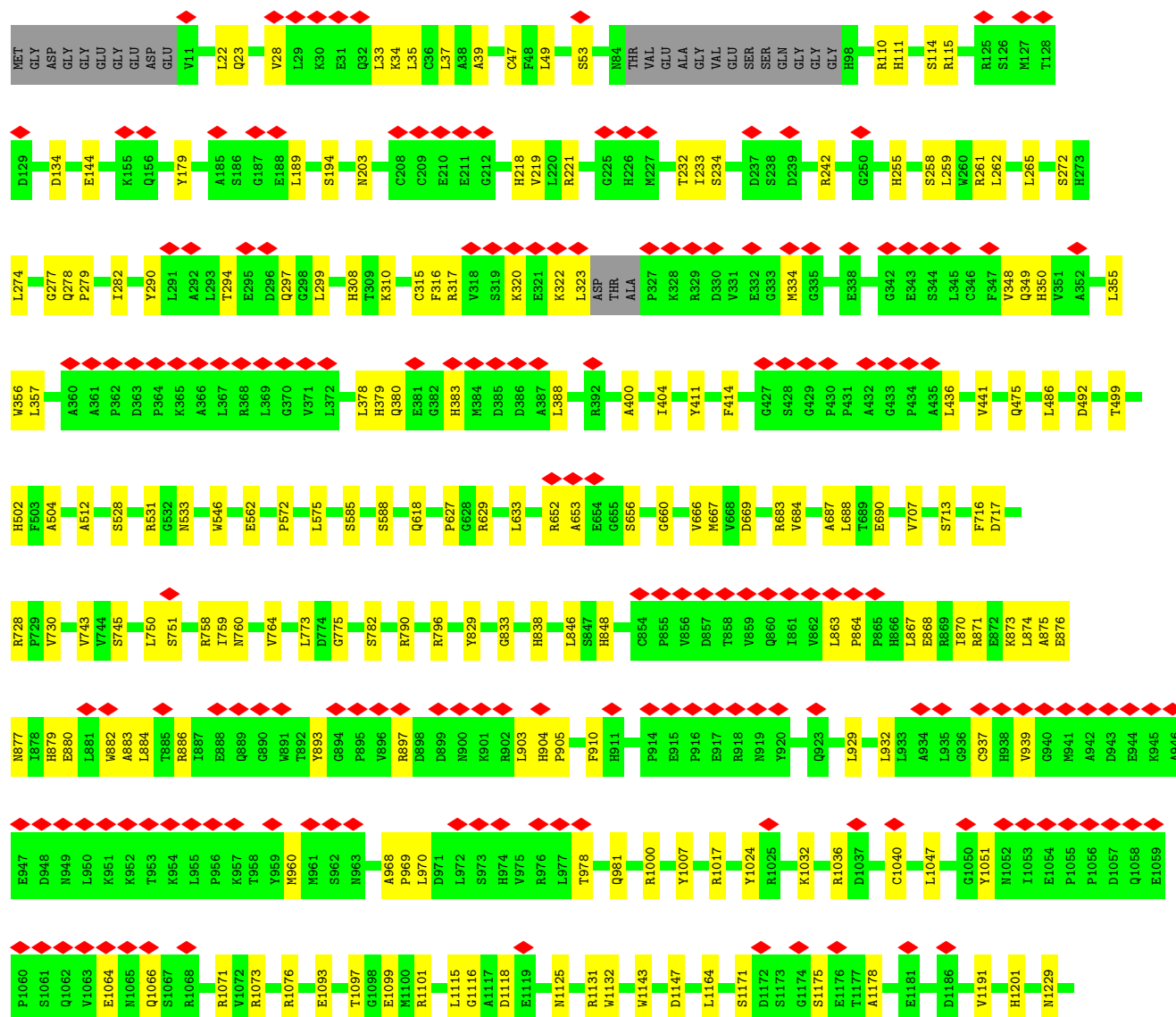








• Molecule 1: Ryanodine receptor 1



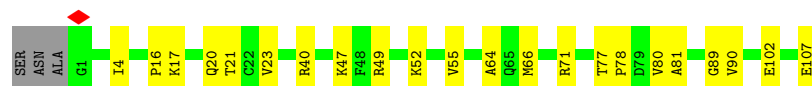


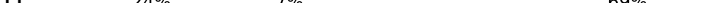
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Q3869	N3870	G3871	E3872	K3873	V3874	K3875	A3876	D3877	F3880	L3888	L3891	F3899	Q3900	N3901	R3904	S3929	Y3937	D3941	E3945	K3948	R3949	Y3968	N3976	M4001	K4002	D4006	L4017	F4061	L4068	K4069	D4070	L4071	V4072	G4073	S4074	E4075	A4076	D4079	Y4080	V4081	T4082	E4165	P4176	R4180													
E3736	GLY	GLU	GLY	GLU	ASN	GLY	GLU	ALA	GLU	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	S3768	R3769	L3770	H3771	T3772	R3773	G3801	L3805	L3817	K3821	D3822	K3823	L3835	S3840	V3841	L3842	K3852	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	K3865	L3866	N3867	R3868								
K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	Y3642	R3648	M3652	E3655	A3659	L3663	D3676	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	K3694	P3695	H3699	F3705	T3708										
V3511	I3520	M3524	T3528	I3533	M3534	A3541	L3542	K3543	D3544	T3545	E3548	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	M3573	L3579	P3580	G3581	E3583	E3584	D3585	A3586	D3587	I3592	V3593	R3594	L3595	V3596	H3605	L3606	T3609	E3610	H3611	F3612	Y3613	K3614	S3615												
F3435	R3436	M3437	F3442	H3449	N3450	R3453	V3459	V3460	Q3461	N3462	E3463	I3464	N3465	N3466	M3467	S3468	F3469	T3471	A3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	Q3506	T3507				
A3339	V3340	F3341	Q3342	Q3343	P3344	I3345	V3346	L3354	F3358	I3359	P3360	T3361	R3364	L3365	K3371	A3374	E3375	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	R3403	L3408	R3414	D3417	R3420	L3424	N3430	E3433	L3434												
A3228	T3229	L3230	G3231	L3232	P3233	N3234	V3245	L3246	D3247	R3248	L3256	T3264	E3265	K3266	P3267	H3268	I3272	K3284	W3285	E3286	F3287	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	L3316	T3322	L3323	V3324	N3325	N3326	D3330	E3331	K3335	K3336	R3337	L3338								
T3133	V3134	A3135	L3136	Q3145	Q3149	Q3151	D3154	P3155	V3156	I3157	L3158	D3159	S3164	R3167	T3168	L3169	G3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	N3180	T3181	Y3182	V3183	E3184	L3194	A3195	R3196	L3206	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	P3224	R3225	E3226	R3227									
K3034	E3035	K3036	E3037	K3045	A3048	L3049	V3050	H3052	R3053	V3054	S3055	L3056	T3059	P3062	V3065	D3076	A3077	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	K2988	S2989	P2990	L2991	F2992	Q2993	F2998	L3002	I3006	Y3009	F3010	F3017	A3022	K3023	V3024	L3025	G3026	S3027	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU				
G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	A2922	Q2923	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	L2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU
R2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	LYS	LYS	THR	ARG	LYS	THR	ILE	SER	GLN	THR	ALA	GLN	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	F2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886

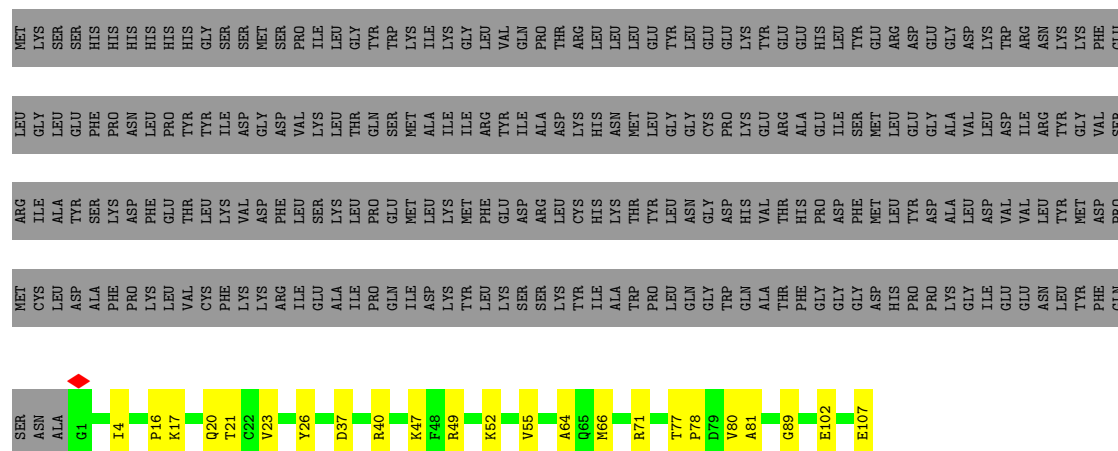








- Chain H:  24% 7% 69%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.402	Depositor
Minimum map value	-0.437	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.428	Depositor
Map size ($\text{\AA}$)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/35738	0.59	9/48398 (0.0%)
1	B	0.27	0/35738	0.59	9/48398 (0.0%)
1	C	0.27	0/35738	0.59	9/48398 (0.0%)
1	D	0.27	0/35738	0.59	9/48398 (0.0%)
2	E	0.21	0/834	0.52	0/1123
2	F	0.21	0/834	0.52	0/1123
2	G	0.21	0/834	0.52	0/1123
2	H	0.21	0/834	0.52	0/1123
All	All	0.27	0/146288	0.59	36/198084 (0.0%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3301	PRO	N-CD-CG	-7.38	92.12	103.20
1	B	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	C	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	D	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	A	3301	PRO	CA-N-CD	-7.25	101.85	112.00
1	B	3301	PRO	CA-N-CD	-7.22	101.89	112.00
1	C	3301	PRO	CA-N-CD	-7.22	101.89	112.00
1	D	3301	PRO	CA-N-CD	-7.22	101.89	112.00
1	B	2412	GLU	CA-C-N	5.61	132.25	121.54
1	B	2412	GLU	C-N-CA	5.61	132.25	121.54
1	C	2412	GLU	CA-C-N	5.61	132.25	121.54
1	C	2412	GLU	C-N-CA	5.61	132.25	121.54
1	D	2412	GLU	CA-C-N	5.61	132.25	121.54
1	D	2412	GLU	C-N-CA	5.61	132.25	121.54
1	A	2412	GLU	CA-C-N	5.58	132.20	121.54
1	A	2412	GLU	C-N-CA	5.58	132.20	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4693	GLY	CA-C-N	5.32	131.71	121.54
1	A	4693	GLY	C-N-CA	5.32	131.71	121.54
1	D	4693	GLY	CA-C-N	5.32	131.69	121.54
1	D	4693	GLY	C-N-CA	5.32	131.69	121.54
1	B	4693	GLY	CA-C-N	5.30	131.67	121.54
1	B	4693	GLY	C-N-CA	5.30	131.67	121.54
1	C	4693	GLY	CA-C-N	5.30	131.67	121.54
1	C	4693	GLY	C-N-CA	5.30	131.67	121.54
1	B	3615	SER	CA-C-N	5.15	131.38	121.54
1	B	3615	SER	C-N-CA	5.15	131.38	121.54
1	C	3615	SER	CA-C-N	5.15	131.38	121.54
1	C	3615	SER	C-N-CA	5.15	131.38	121.54
1	D	3615	SER	CA-C-N	5.15	131.38	121.54
1	D	3615	SER	C-N-CA	5.15	131.38	121.54
1	A	3615	SER	CA-C-N	5.14	131.37	121.54
1	A	3615	SER	C-N-CA	5.14	131.37	121.54
1	A	905	PRO	N-CA-C	5.10	122.98	112.47
1	B	905	PRO	N-CA-C	5.09	122.96	112.47
1	C	905	PRO	N-CA-C	5.09	122.96	112.47
1	D	905	PRO	N-CA-C	5.09	122.96	112.47

There are no chirality outliers.

There are no planarity outliers.

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	34921	0	34541	370	0
1	B	34921	0	34541	371	0
1	C	34921	0	34541	363	0
1	D	34921	0	34541	371	0
2	E	818	0	824	12	0
2	F	818	0	824	14	0
2	G	818	0	824	13	0
2	H	818	0	824	13	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	142960	0	141460	1508	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 (1508) 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)
1:A:1561:VAL:HG12	1:A:1562:ILE:HG12	1.73	0.71
1:C:1561:VAL:HG12	1:C:1562:ILE:HG12	1.73	0.71
1:B:1561:VAL:HG12	1:B:1562:ILE:HG12	1.73	0.71
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.56	0.70
1:D:1561:VAL:HG12	1:D:1562:ILE:HG12	1.73	0.70
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.56	0.70
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.56	0.70
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.56	0.69
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.76	0.68
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.76	0.67
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.77	0.67
1:A:3256:LEU:HB3	1:A:3266:MET:HE1	1.78	0.66
1:B:3256:LEU:HB3	1:B:3266:MET:HE1	1.78	0.66
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.77	0.66
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.76	0.66
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.77	0.66
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.76	0.66
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.78	0.66
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.78	0.66
1:C:3256:LEU:HB3	1:C:3266:MET:HE1	1.78	0.66
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.77	0.65
1:D:3256:LEU:HB3	1:D:3266:MET:HE1	1.78	0.65
1:B:666:VAL:HG21	1:B:684:VAL:HG21	1.79	0.65
1:D:666:VAL:HG21	1:D:684:VAL:HG21	1.79	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.78	0.65
1:C:666:VAL:HG21	1:C:684:VAL:HG21	1.79	0.65
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.78	0.65
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.78	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.79	0.65
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.79	0.64
1:A:666:VAL:HG21	1:A:684:VAL:HG21	1.79	0.64
1:D:1476:MET:HB2	1:D:1485:SER:HB3	1.80	0.64
1:B:1476:MET:HB2	1:B:1485:SER:HB3	1.80	0.64
1:A:1476:MET:HB2	1:A:1485:SER:HB3	1.80	0.64
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.79	0.64
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.78	0.64
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.31	0.64
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.31	0.64
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.78	0.63
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.31	0.63
1:C:1476:MET:HB2	1:C:1485:SER:HB3	1.80	0.63
1:B:667:MET:HE1	1:B:743:VAL:HG22	1.81	0.63
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.79	0.63
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.31	0.63
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.81	0.63
1:D:4001:MET:HE1	1:D:4061:PHE:HB2	1.80	0.63
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.81	0.62
1:B:4001:MET:HE1	1:B:4061:PHE:HB2	1.80	0.62
1:C:667:MET:HE1	1:C:743:VAL:HG22	1.81	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:D:667:MET:HE1	1:D:743:VAL:HG22	1.81	0.62
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.62
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.81	0.62
1:C:4001:MET:HE1	1:C:4061:PHE:HB2	1.80	0.62
1:A:4001:MET:HE1	1:A:4061:PHE:HB2	1.80	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:A:667:MET:HE1	1:A:743:VAL:HG22	1.81	0.61
1:A:34:LYS:H	1:A:53:SER:HB3	1.66	0.61
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.34	0.61
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.81	0.61
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.34	0.61
1:B:34:LYS:H	1:B:53:SER:HB3	1.66	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.34	0.61
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.65	0.61
1:A:688:LEU:HD23	1:A:690:GLU:H	1.66	0.61
1:A:3172:ILE:HD11	1:A:3194:LEU:HD13	1.83	0.61
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.83	0.61
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.33	0.61
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.74	0.61
1:B:3172:ILE:HD11	1:B:3194:LEU:HD13	1.83	0.61
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.74	0.61
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.34	0.61
1:A:4892:ARG:NH1	1:B:4899:ASP:OD1	2.34	0.61
1:C:3681:GLY:O	1:C:3683:GLN:NE2	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.83	0.60
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.65	0.60
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.65	0.60
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.34	0.60
1:D:3172:ILE:HD11	1:D:3194:LEU:HD13	1.83	0.60
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.60
1:B:3681:GLY:O	1:B:3683:GLN:NE2	2.34	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.60
1:C:2175:GLU:HG3	1:C:2228:MET:HB2	1.82	0.60
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.74	0.60
1:D:34:LYS:H	1:D:53:SER:HB3	1.66	0.60
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.34	0.60
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.83	0.60
1:B:688:LEU:HD23	1:B:690:GLU:H	1.65	0.60
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.32	0.60
1:C:34:LYS:H	1:C:53:SER:HB3	1.66	0.60
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	1.82	0.60
1:C:1252:HIS:O	1:C:1275:ARG:NH2	2.34	0.60
1:A:2175:GLU:HG3	1:A:2228:MET:HB2	1.82	0.60
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.35	0.59
1:A:3681:GLY:O	1:A:3683:GLN:NE2	2.34	0.59
1:D:2175:GLU:HG3	1:D:2228:MET:HB2	1.82	0.59
1:C:688:LEU:HD23	1:C:690:GLU:H	1.65	0.59
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.83	0.59
1:C:3172:ILE:HD11	1:C:3194:LEU:HD13	1.83	0.59
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.32	0.59
1:D:688:LEU:HD23	1:D:690:GLU:H	1.65	0.59
1:D:317:ARG:HD3	1:D:323:LEU:HD23	1.84	0.59
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.34	0.59
1:D:3681:GLY:O	1:D:3683:GLN:NE2	2.34	0.59
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.85	0.59
1:A:3324:VAL:HG11	1:A:3361:THR:HG22	1.85	0.59
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3354:LEU:HA	1:C:3358:PHE:HB2	1.85	0.59
1:A:317:ARG:HD3	1:A:323:LEU:HD23	1.84	0.58
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.36	0.58
1:C:3324:VAL:HG11	1:C:3361:THR:HG22	1.85	0.58
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.36	0.58
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.36	0.58
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.85	0.58
1:B:317:ARG:HD3	1:B:323:LEU:HD23	1.84	0.58
1:C:317:ARG:HD3	1:C:323:LEU:HD23	1.84	0.58
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.77	0.58
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.85	0.58
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.74	0.58
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.85	0.58
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	1.85	0.58
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.34	0.58
1:D:3354:LEU:HA	1:D:3358:PHE:HB2	1.85	0.58
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.77	0.58
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.77	0.58
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.77	0.58
1:B:3354:LEU:HA	1:B:3358:PHE:HB2	1.85	0.58
1:D:2093:SER:OG	1:D:2096:GLU:OE1	2.21	0.58
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.36	0.58
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.32	0.58
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.33	0.58
1:D:1252:HIS:O	1:D:1275:ARG:NH2	2.34	0.58
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	1.85	0.58
1:D:3324:VAL:HG11	1:D:3361:THR:HG22	1.85	0.57
1:B:3324:VAL:HG11	1:B:3361:THR:HG22	1.85	0.57
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	1.85	0.57
1:A:2624:ARG:HH12	1:A:2911:LEU:HA	1.70	0.57
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.38	0.57
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.85	0.57
1:C:3937:TYR:O	1:C:4002:LYS:NZ	2.38	0.57
1:A:3354:LEU:HA	1:A:3358:PHE:HB2	1.85	0.57
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.38	0.57
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.87	0.57
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	1.87	0.57
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.87	0.57
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.85	0.57
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.87	0.57
1:B:475:GLN:NE2	1:B:528:SER:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.85	0.57
1:C:2624:ARG:HH12	1:C:2911:LEU:HA	1.70	0.57
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	1.87	0.57
1:D:1097:THR:HA	1:D:1143:TRP:HE1	1.70	0.57
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.38	0.57
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	1.85	0.57
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.87	0.57
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.86	0.57
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.38	0.57
1:C:475:GLN:NE2	1:C:528:SER:O	2.38	0.57
1:D:475:GLN:NE2	1:D:528:SER:O	2.38	0.57
1:A:475:GLN:NE2	1:A:528:SER:O	2.38	0.56
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.86	0.56
1:B:4866:SER:HB2	1:B:4873:ASP:H	1.70	0.56
1:D:3937:TYR:O	1:D:4002:LYS:NZ	2.38	0.56
1:B:882:TRP:O	1:B:886:ARG:NH1	2.38	0.56
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.87	0.56
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.87	0.56
1:A:882:TRP:O	1:A:886:ARG:NH1	2.38	0.56
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.86	0.56
1:D:2624:ARG:HH12	1:D:2911:LEU:HA	1.70	0.56
1:B:1097:THR:HA	1:B:1143:TRP:HE1	1.70	0.56
1:C:1097:THR:HA	1:C:1143:TRP:HE1	1.70	0.56
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.32	0.56
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.79	0.56
1:D:2214:VAL:HG21	1:D:2228:MET:HE1	1.87	0.56
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.86	0.56
1:B:3006:ILE:O	1:B:3010:PHE:HB2	2.06	0.56
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.88	0.56
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.88	0.56
1:C:882:TRP:O	1:C:886:ARG:NH1	2.38	0.56
1:A:1097:THR:HA	1:A:1143:TRP:HE1	1.70	0.56
1:A:1252:HIS:O	1:A:1275:ARG:NH2	2.34	0.56
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.88	0.56
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.79	0.56
1:D:882:TRP:O	1:D:886:ARG:NH1	2.38	0.56
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.87	0.56
1:A:2093:SER:OG	1:A:2096:GLU:OE1	2.21	0.56
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.39	0.56
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	1.87	0.56
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.39	0.56
1:A:2214:VAL:HG21	1:A:2228:MET:HE1	1.87	0.56
1:B:2624:ARG:HH12	1:B:2911:LEU:HA	1.70	0.56
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.33	0.56
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.38	0.56
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.79	0.56
1:A:3006:ILE:O	1:A:3010:PHE:HB2	2.06	0.56
1:A:3945:GLU:OE1	1:A:3949:ARG:NH1	2.40	0.56
1:A:4866:SER:HB2	1:A:4873:ASP:H	1.70	0.56
1:A:475:GLN:OE1	1:A:533:ASN:ND2	2.39	0.55
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.35	0.55
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	1.87	0.55
1:B:357:LEU:HD11	1:B:388:LEU:HD11	1.89	0.55
1:B:475:GLN:OE1	1:B:533:ASN:ND2	2.39	0.55
1:B:3107:VAL:HG21	1:B:3171:SER:HB2	1.88	0.55
1:C:2214:VAL:HG21	1:C:2228:MET:HE1	1.87	0.55
1:C:4866:SER:HB2	1:C:4873:ASP:H	1.70	0.55
1:D:357:LEU:HD11	1:D:388:LEU:HD11	1.89	0.55
1:D:3206:LEU:HB3	1:D:3246:LEU:HB2	1.88	0.55
1:B:3206:LEU:HB3	1:B:3246:LEU:HB2	1.88	0.55
1:B:294:THR:HG23	1:B:297:GLN:H	1.72	0.55
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.40	0.55
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.39	0.55
1:A:357:LEU:HD11	1:A:388:LEU:HD11	1.89	0.55
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.39	0.55
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.79	0.55
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.39	0.55
1:C:357:LEU:HD11	1:C:388:LEU:HD11	1.89	0.55
1:C:4214:LYS:HD2	1:C:4985:LEU:HD11	1.89	0.55
1:D:2368:LEU:HD11	1:D:2376:LEU:HD12	1.88	0.55
1:D:3107:VAL:HG21	1:D:3171:SER:HB2	1.88	0.55
1:A:2538:THR:HG23	1:A:2540:THR:H	1.71	0.55
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.88	0.55
1:B:2214:VAL:HG21	1:B:2228:MET:HE1	1.87	0.55
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.72	0.55
1:C:2538:THR:HG23	1:C:2540:THR:H	1.71	0.55
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.35	0.55
1:D:4866:SER:HB2	1:D:4873:ASP:H	1.70	0.55
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.39	0.55
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.39	0.55
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.88	0.55
1:D:4068:LEU:HD22	1:D:4111:LEU:HD11	1.89	0.55
1:D:4214:LYS:HD2	1:D:4985:LEU:HD11	1.89	0.55
1:B:1260:MET:HB2	1:B:1269:CYS:HB2	1.89	0.55
1:C:3006:ILE:O	1:C:3010:PHE:HB2	2.06	0.55
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.89	0.55
1:A:4214:LYS:HD2	1:A:4985:LEU:HD11	1.89	0.55
1:C:2368:LEU:HD11	1:C:2376:LEU:HD12	1.88	0.55
1:C:2912:THR:O	1:C:2916:LYS:HB2	2.07	0.55
1:C:3206:LEU:HB3	1:C:3246:LEU:HB2	1.88	0.55
1:A:499:THR:HG23	1:A:502:HIS:H	1.72	0.55
1:A:4068:LEU:HD22	1:A:4111:LEU:HD11	1.89	0.55
1:B:2368:LEU:HD11	1:B:2376:LEU:HD12	1.88	0.55
1:B:3945:GLU:OE1	1:B:3949:ARG:NH1	2.40	0.55
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.89	0.55
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.89	0.55
1:D:3006:ILE:O	1:D:3010:PHE:HB2	2.06	0.55
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.89	0.54
1:A:1260:MET:HB2	1:A:1269:CYS:HB2	1.89	0.54
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.40	0.54
1:A:3107:VAL:HG21	1:A:3171:SER:HB2	1.88	0.54
1:A:3145:GLN:OE1	1:A:3196:ARG:NE	2.40	0.54
1:A:3206:LEU:HB3	1:A:3246:LEU:HB2	1.88	0.54
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.89	0.54
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.89	0.54
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.40	0.54
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.40	0.54
1:D:1272:LEU:HD22	1:D:1289:LEU:HD11	1.90	0.54
1:D:3145:GLN:OE1	1:D:3196:ARG:NE	2.40	0.54
1:A:2368:LEU:HD11	1:A:2376:LEU:HD12	1.88	0.54
1:B:4214:LYS:HD2	1:B:4985:LEU:HD11	1.89	0.54
1:C:232:THR:HG22	1:C:258:SER:HB3	1.89	0.54
1:C:1260:MET:HB2	1:C:1269:CYS:HB2	1.89	0.54
1:C:3145:GLN:OE1	1:C:3196:ARG:NE	2.40	0.54
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.90	0.54
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.89	0.54
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.72	0.54
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.90	0.54
1:A:2912:THR:O	1:A:2916:LYS:HB2	2.07	0.54
1:B:499:THR:HG23	1:B:502:HIS:H	1.72	0.54
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:THR:HG22	1:D:258:SER:HB3	1.89	0.54
1:D:294:THR:HG23	1:D:297:GLN:H	1.72	0.54
1:D:1260:MET:HB2	1:D:1269:CYS:HB2	1.89	0.54
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.40	0.54
1:D:499:THR:HG23	1:D:502:HIS:H	1.72	0.54
1:D:3945:GLU:OE1	1:D:3949:ARG:NH1	2.40	0.54
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.41	0.54
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.33	0.54
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.40	0.54
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.41	0.54
1:B:2912:THR:O	1:B:2916:LYS:HB2	2.07	0.54
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.39	0.54
1:C:2967:MET:HE2	1:C:3045:LYS:HB3	1.90	0.54
1:A:294:THR:HG23	1:A:297:GLN:H	1.72	0.54
1:B:110:ARG:HH21	1:B:115:ARG:HB3	1.72	0.54
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.90	0.54
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.88	0.54
1:D:110:ARG:HH21	1:D:115:ARG:HB3	1.72	0.54
1:D:2538:THR:HG23	1:D:2540:THR:H	1.71	0.54
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.88	0.54
1:D:2967:MET:HE2	1:D:3045:LYS:HB3	1.90	0.54
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.41	0.54
1:A:3414:ARG:HE	1:A:3472:ALA:HB3	1.73	0.54
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.89	0.54
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.24	0.54
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.39	0.54
2:E:17:LYS:HE3	2:E:20:GLN:HE22	1.73	0.54
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.41	0.54
1:B:3145:GLN:OE1	1:B:3196:ARG:NE	2.40	0.54
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.41	0.54
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.35	0.54
1:C:3414:ARG:HE	1:C:3472:ALA:HB3	1.73	0.54
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.39	0.54
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.90	0.54
1:D:2912:THR:O	1:D:2916:LYS:HB2	2.07	0.54
1:C:499:THR:HG23	1:C:502:HIS:H	1.72	0.54
1:C:4068:LEU:HD22	1:C:4111:LEU:HD11	1.89	0.54
2:F:17:LYS:HE3	2:F:20:GLN:HE22	1.73	0.54
1:B:1272:LEU:HD22	1:B:1289:LEU:HD11	1.90	0.54
1:C:3945:GLU:OE1	1:C:3949:ARG:NH1	2.40	0.54
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.38	0.54
2:H:17:LYS:HE3	2:H:20:GLN:HE22	1.73	0.54
1:B:3414:ARG:HE	1:B:3472:ALA:HB3	1.73	0.53
1:B:4068:LEU:HD22	1:B:4111:LEU:HD11	1.89	0.53
1:C:294:THR:HG23	1:C:297:GLN:H	1.72	0.53
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.89	0.53
1:D:3414:ARG:HE	1:D:3472:ALA:HB3	1.73	0.53
1:A:110:ARG:HH21	1:A:115:ARG:HB3	1.72	0.53
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.90	0.53
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.90	0.53
1:B:2093:SER:OG	1:B:2096:GLU:OE1	2.21	0.53
1:B:2967:MET:HE2	1:B:3045:LYS:HB3	1.90	0.53
1:C:3107:VAL:HG21	1:C:3171:SER:HB2	1.88	0.53
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.40	0.53
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.91	0.53
1:B:2538:THR:HG23	1:B:2540:THR:H	1.71	0.53
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.40	0.53
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.90	0.53
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.41	0.53
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.91	0.53
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.40	0.53
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.26	0.53
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.91	0.53
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.40	0.53
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.72	0.53
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.40	0.53
1:A:232:THR:HG22	1:A:258:SER:HB3	1.89	0.53
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.91	0.53
1:A:2534:ALA:O	1:A:2588:ARG:NH1	2.42	0.53
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.41	0.53
1:D:1864:LYS:NZ	1:D:1871:PHE:O	2.39	0.53
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.41	0.53
1:D:3111:ARG:NH2	1:D:3174:SER:OG	2.42	0.53
2:G:17:LYS:HE3	2:G:20:GLN:HE22	1.73	0.53
1:A:627:PRO:HD3	2:E:89:GLY:HA2	1.89	0.53
1:A:1450:VAL:HG22	1:A:1552:VAL:HG22	1.91	0.53
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.89	0.53
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.72	0.53
1:D:350:HIS:HB2	1:D:378:LEU:HD21	1.91	0.53
1:A:3111:ARG:NH2	1:A:3174:SER:OG	2.42	0.53
1:B:232:THR:HG22	1:B:258:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4112:LEU:O	1:B:4115:SER:OG	2.26	0.53
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.91	0.53
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.90	0.53
1:B:3111:ARG:NH2	1:B:3174:SER:OG	2.42	0.53
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.39	0.53
1:D:2534:ALA:O	1:D:2588:ARG:NH1	2.42	0.53
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.89	0.53
1:C:2093:SER:OG	1:C:2096:GLU:OE1	2.21	0.53
1:C:2534:ALA:O	1:C:2588:ARG:NH1	2.42	0.53
1:A:2967:MET:HE2	1:A:3045:LYS:HB3	1.90	0.53
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.89	0.53
1:B:1450:VAL:HG22	1:B:1552:VAL:HG22	1.91	0.53
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.91	0.53
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.89	0.53
1:C:320:LYS:NZ	1:C:383:HIS:O	2.42	0.52
1:C:3036:LYS:NZ	1:C:3076:ASP:OD2	2.37	0.52
1:C:3111:ARG:NH2	1:C:3174:SER:OG	2.42	0.52
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.75	0.52
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.91	0.52
1:A:350:HIS:HB2	1:A:378:LEU:HD21	1.91	0.52
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.24	0.52
1:C:2628:PHE:HE2	1:C:2735:PHE:HA	1.74	0.52
1:B:2628:PHE:HE2	1:B:2735:PHE:HA	1.74	0.52
1:C:1450:VAL:HG22	1:C:1552:VAL:HG22	1.91	0.52
1:C:4088:ILE:O	1:C:4123:ILE:N	2.43	0.52
1:C:4112:LEU:O	1:C:4115:SER:OG	2.26	0.52
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.42	0.52
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.42	0.52
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.75	0.52
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.26	0.52
1:A:4088:ILE:O	1:A:4123:ILE:N	2.43	0.52
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.42	0.52
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.75	0.52
1:B:350:HIS:HB2	1:B:378:LEU:HD21	1.91	0.52
1:B:4088:ILE:O	1:B:4123:ILE:N	2.43	0.52
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.42	0.52
1:D:2628:PHE:HE2	1:D:2735:PHE:HA	1.74	0.52
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.91	0.52
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.42	0.52
1:D:1671:ARG:O	1:D:1675:ALA:HB2	2.10	0.52
1:A:2628:PHE:HE2	1:A:2735:PHE:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.91	0.52
1:B:504:ALA:HB2	1:B:512:ALA:HB2	1.92	0.52
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.35	0.52
1:D:1450:VAL:HG22	1:D:1552:VAL:HG22	1.91	0.52
1:D:4088:ILE:O	1:D:4123:ILE:N	2.43	0.52
2:F:71:ARG:HG2	2:F:102:GLU:HB2	1.92	0.52
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.92	0.52
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.92	0.52
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.92	0.52
2:E:71:ARG:HG2	2:E:102:GLU:HB2	1.92	0.52
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.51
1:B:2534:ALA:O	1:B:2588:ARG:NH1	2.42	0.51
1:C:111:HIS:ND1	1:C:114:SER:OG	2.39	0.51
1:C:350:HIS:HB2	1:C:378:LEU:HD21	1.91	0.51
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.92	0.51
1:A:320:LYS:NZ	1:A:383:HIS:O	2.42	0.51
1:B:2604:GLU:HG2	1:B:2639:MET:HG3	1.92	0.51
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.44	0.51
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.44	0.51
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.91	0.51
1:A:2109:ASP:HA	1:A:3694:LYS:HD2	1.93	0.51
1:B:1671:ARG:O	1:B:1675:ALA:HB2	2.10	0.51
1:D:2109:ASP:HA	1:D:3694:LYS:HD2	1.93	0.51
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.92	0.51
1:B:1969:LEU:HD11	1:B:2009:LEU:HD13	1.93	0.51
1:C:504:ALA:HB2	1:C:512:ALA:HB2	1.92	0.51
1:C:1969:LEU:HD11	1:C:2009:LEU:HD13	1.93	0.51
1:D:504:ALA:HB2	1:D:512:ALA:HB2	1.92	0.51
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.26	0.51
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.92	0.51
1:D:1969:LEU:HD11	1:D:2009:LEU:HD13	1.93	0.51
1:C:1864:LYS:NZ	1:C:1871:PHE:O	2.39	0.51
1:D:2827:ARG:NH2	1:D:2935:TYR:OH	2.44	0.51
1:A:743:VAL:HB	1:A:760:ASN:HA	1.93	0.51
1:A:1671:ARG:O	1:A:1675:ALA:HB2	2.10	0.51
1:A:1969:LEU:HD11	1:A:2009:LEU:HD13	1.93	0.51
1:B:1658:ASP:N	1:B:1658:ASP:OD1	2.44	0.51
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.92	0.51
1:C:743:VAL:HB	1:C:760:ASN:HA	1.93	0.51
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.75	0.51
1:D:4689:THR:HG22	1:D:4690:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4729:GLY:HA2	1:D:4737:ILE:HG13	1.93	0.51
2:H:71:ARG:HG2	2:H:102:GLU:HB2	1.92	0.51
1:A:2604:GLU:HG2	1:A:2639:MET:HG3	1.92	0.51
1:A:4689:THR:HG22	1:A:4690:GLU:HG3	1.93	0.51
1:C:1695:LEU:HA	1:C:1698:LEU:HG	1.93	0.51
1:D:320:LYS:NZ	1:D:383:HIS:O	2.42	0.51
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.92	0.51
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.93	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.91	0.51
2:F:21:THR:N	2:F:107:GLU:OE2	2.44	0.51
1:B:403:MET:O	1:B:407:THR:OG1	2.23	0.51
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.91	0.51
1:C:2624:ARG:NH2	1:C:2915:GLU:OE2	2.44	0.51
1:C:3545:THR:HG22	1:C:3548:GLU:HG3	1.93	0.51
1:C:4680:LYS:HD2	1:C:4686:LEU:HD22	1.92	0.51
1:C:4689:THR:HG22	1:C:4690:GLU:HG3	1.93	0.51
1:D:111:HIS:ND1	1:D:114:SER:OG	2.39	0.51
1:A:3036:LYS:NZ	1:A:3076:ASP:OD2	2.37	0.51
1:A:4112:LEU:O	1:A:4115:SER:OG	2.26	0.51
1:B:2827:ARG:NH2	1:B:2935:TYR:OH	2.44	0.51
1:B:4689:THR:HG22	1:B:4690:GLU:HG3	1.93	0.51
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.42	0.51
1:D:2624:ARG:NH2	1:D:2915:GLU:OE2	2.44	0.51
1:A:2624:ARG:NH2	1:A:2915:GLU:OE2	2.44	0.50
1:A:2827:ARG:NH2	1:A:2935:TYR:OH	2.44	0.50
1:C:1291:LEU:HD13	1:C:1595:LEU:HD11	1.94	0.50
1:C:2109:ASP:HA	1:C:3694:LYS:HD2	1.93	0.50
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.45	0.50
1:D:2604:GLU:HG2	1:D:2639:MET:HG3	1.92	0.50
2:G:21:THR:N	2:G:107:GLU:OE2	2.44	0.50
1:B:1695:LEU:HA	1:B:1698:LEU:HG	1.93	0.50
1:B:3036:LYS:NZ	1:B:3076:ASP:OD2	2.37	0.50
1:C:1671:ARG:O	1:C:1675:ALA:HB2	2.10	0.50
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.45	0.50
1:A:504:ALA:HB2	1:A:512:ALA:HB2	1.92	0.50
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.45	0.50
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.76	0.50
1:A:4729:GLY:HA2	1:A:4737:ILE:HG13	1.93	0.50
1:B:320:LYS:NZ	1:B:383:HIS:O	2.42	0.50
1:B:3545:THR:HG22	1:B:3548:GLU:HG3	1.93	0.50
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2856:ASN:ND2	1:C:2858:GLN:OE1	2.44	0.50
1:A:2856:ASN:ND2	1:A:2858:GLN:OE1	2.44	0.50
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.94	0.50
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.36	0.50
1:C:2604:GLU:HG2	1:C:2639:MET:HG3	1.92	0.50
1:D:218:HIS:O	1:D:261:ARG:HA	2.12	0.50
1:D:2394:GLY:HA3	1:D:2415:ARG:HH21	1.77	0.50
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.94	0.50
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.42	0.50
1:A:1291:LEU:HD13	1:A:1595:LEU:HD11	1.94	0.50
1:B:2109:ASP:HA	1:B:3694:LYS:HD2	1.93	0.50
1:B:2624:ARG:NH2	1:B:2915:GLU:OE2	2.44	0.50
1:B:2856:ASN:ND2	1:B:2858:GLN:OE1	2.44	0.50
1:C:218:HIS:O	1:C:261:ARG:HA	2.12	0.50
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.76	0.50
1:D:743:VAL:HB	1:D:760:ASN:HA	1.93	0.50
1:D:1698:LEU:HA	1:D:1712:TYR:HE1	1.77	0.50
1:D:4680:LYS:HD2	1:D:4686:LEU:HD22	1.92	0.50
2:E:21:THR:N	2:E:107:GLU:OE2	2.44	0.50
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.94	0.50
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.42	0.50
1:A:2394:GLY:HA3	1:A:2415:ARG:HH21	1.77	0.50
1:A:2490:MET:SD	1:A:2490:MET:N	2.85	0.50
1:B:4729:GLY:HA2	1:B:4737:ILE:HG13	1.93	0.50
1:D:3545:THR:HG22	1:D:3548:GLU:HG3	1.93	0.50
1:A:2003:GLN:NE2	1:A:3655:GLU:OE2	2.45	0.50
1:B:585:SER:O	1:B:588:SER:OG	2.29	0.50
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.94	0.50
1:C:1698:LEU:HA	1:C:1712:TYR:HE1	1.77	0.50
1:C:4924:VAL:HA	1:C:4928:LEU:HD12	1.94	0.50
1:D:4112:LEU:O	1:D:4115:SER:OG	2.26	0.50
2:G:71:ARG:HG2	2:G:102:GLU:HB2	1.92	0.50
1:A:1229:ASN:HB2	1:A:1827:ARG:HG3	1.94	0.50
1:A:1695:LEU:HA	1:A:1698:LEU:HG	1.93	0.50
1:B:4680:LYS:HD2	1:B:4686:LEU:HD22	1.92	0.50
1:B:4924:VAL:HA	1:B:4928:LEU:HD12	1.94	0.50
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.76	0.50
1:A:111:HIS:ND1	1:A:114:SER:OG	2.39	0.50
1:A:3545:THR:HG22	1:A:3548:GLU:HG3	1.93	0.50
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.45	0.50
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2003:GLN:NE2	1:D:3655:GLU:OE2	2.45	0.50
1:D:2856:ASN:ND2	1:D:2858:GLN:OE1	2.44	0.50
2:H:21:THR:N	2:H:107:GLU:OE2	2.44	0.50
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.94	0.49
1:B:2394:GLY:HA3	1:B:2415:ARG:HH21	1.77	0.49
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.93	0.49
1:C:2003:GLN:NE2	1:C:3655:GLU:OE2	2.45	0.49
1:C:2394:GLY:HA3	1:C:2415:ARG:HH21	1.77	0.49
1:C:2827:ARG:NH2	1:C:2935:TYR:OH	2.44	0.49
1:A:218:HIS:O	1:A:261:ARG:HA	2.12	0.49
1:B:3450:ASN:OD1	1:B:3453:ARG:NH1	2.39	0.49
1:D:1291:LEU:HD13	1:D:1595:LEU:HD11	1.94	0.49
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.93	0.49
1:B:218:HIS:O	1:B:261:ARG:HA	2.12	0.49
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.94	0.49
1:A:4680:LYS:HD2	1:A:4686:LEU:HD22	1.92	0.49
1:B:743:VAL:HB	1:B:760:ASN:HA	1.93	0.49
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.49
1:B:3097:GLU:OE1	1:B:3167:ARG:NH2	2.46	0.49
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.94	0.49
1:A:2128:TYR:OH	1:A:3676:ASP:OD2	2.31	0.49
1:B:1291:LEU:HD13	1:B:1595:LEU:HD11	1.94	0.49
1:C:2128:TYR:OH	1:C:3676:ASP:OD2	2.31	0.49
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	1.94	0.49
1:D:3036:LYS:NZ	1:D:3076:ASP:OD2	2.37	0.49
1:A:3817:LEU:HD11	1:A:3821:LYS:HE3	1.95	0.49
1:A:4924:VAL:HA	1:A:4928:LEU:HD12	1.93	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.95	0.49
1:B:2245:GLN:NE2	1:B:3861:GLU:OE1	2.46	0.49
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.76	0.49
1:C:1586:ASN:ND2	1:C:1590:GLN:OE1	2.46	0.49
1:C:3097:GLU:OE1	1:C:3167:ARG:NH2	2.46	0.49
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.95	0.49
1:A:3583:GLU:HB2	1:A:3586:ALA:HB2	1.95	0.49
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.94	0.49
1:B:1586:ASN:ND2	1:B:1590:GLN:OE1	2.46	0.49
1:B:2003:GLN:NE2	1:B:3655:GLU:OE2	2.45	0.49
1:B:2128:TYR:OH	1:B:3676:ASP:OD2	2.31	0.49
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.95	0.49
1:C:3817:LEU:HD11	1:C:3821:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.49
1:D:1695:LEU:HA	1:D:1698:LEU:HG	1.93	0.49
1:A:2245:GLN:NE2	1:A:3861:GLU:OE1	2.46	0.49
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.49
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.95	0.49
1:D:4924:VAL:HA	1:D:4928:LEU:HD12	1.94	0.49
1:A:3097:GLU:OE1	1:A:3167:ARG:NH2	2.46	0.49
1:A:4976:GLU:O	1:A:4980:LEU:HB2	2.13	0.49
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.95	0.49
1:D:2387:SER:OG	1:D:2492:ALA:O	2.31	0.49
1:D:2490:MET:SD	1:D:2490:MET:N	2.85	0.49
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.95	0.49
1:A:3862:ASP:OD1	1:A:3862:ASP:N	2.46	0.49
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.94	0.49
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.46	0.49
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.93	0.49
1:C:3862:ASP:OD1	1:C:3862:ASP:N	2.46	0.49
1:C:4976:GLU:O	1:C:4980:LEU:HB2	2.13	0.49
1:D:2128:TYR:OH	1:D:3676:ASP:OD2	2.31	0.49
1:D:3097:GLU:OE1	1:D:3167:ARG:NH2	2.46	0.49
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.46	0.48
1:B:660:GLY:HA2	1:B:750:LEU:HD12	1.95	0.48
1:B:3583:GLU:HB2	1:B:3586:ALA:HB2	1.95	0.48
1:B:3968:TYR:O	1:B:3976:ASN:ND2	2.42	0.48
1:B:4976:GLU:O	1:B:4980:LEU:HB2	2.13	0.48
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.95	0.48
1:C:4729:GLY:HA2	1:C:4737:ILE:HG13	1.93	0.48
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.24	0.48
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.46	0.48
1:B:652:ARG:NH1	1:B:751:SER:O	2.46	0.48
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.94	0.48
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.95	0.48
1:B:3817:LEU:HD11	1:B:3821:LYS:HE3	1.95	0.48
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.95	0.48
1:C:4017:LEU:HD13	1:C:4135:PRO:HB2	1.95	0.48
1:D:660:GLY:HA2	1:D:750:LEU:HD12	1.95	0.48
1:D:1586:ASN:ND2	1:D:1590:GLN:OE1	2.46	0.48
1:A:1698:LEU:HA	1:A:1712:TYR:HE1	1.77	0.48
1:A:2387:SER:OG	1:A:2492:ALA:O	2.31	0.48
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.95	0.48
1:B:1698:LEU:HA	1:B:1712:TYR:HE1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2280:VAL:HG21	1:B:2290:LEU:HD12	1.95	0.48
1:B:3371:LYS:NZ	1:B:3375:GLU:OE2	2.45	0.48
1:C:2280:VAL:HG21	1:C:2290:LEU:HD12	1.95	0.48
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.26	0.48
1:D:627:PRO:HD3	2:H:89:GLY:HA2	1.96	0.48
1:D:1293:LEU:HD11	1:D:1594:ARG:HD3	1.95	0.48
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.43	0.48
1:D:3817:LEU:HD11	1:D:3821:LYS:HE3	1.95	0.48
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.95	0.48
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.95	0.48
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	1.94	0.48
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.36	0.48
1:D:28:VAL:HG22	1:D:33:LEU:HD22	1.96	0.48
1:D:652:ARG:NH1	1:D:751:SER:O	2.46	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.48
1:A:1293:LEU:HD11	1:A:1594:ARG:HD3	1.95	0.48
1:A:3433:GLU:HG3	1:A:3437:MET:HE3	1.96	0.48
1:B:1293:LEU:HD11	1:B:1594:ARG:HD3	1.95	0.48
1:D:1743[A]:ARG:NH1	1:D:1963:GLU:OE2	2.47	0.48
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.96	0.48
1:B:1743[A]:ARG:NH1	1:B:1963:GLU:OE2	2.47	0.48
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.95	0.48
1:C:652:ARG:NH1	1:C:751:SER:O	2.46	0.48
1:D:3433:GLU:HG3	1:D:3437:MET:HE3	1.96	0.48
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.96	0.48
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.44	0.48
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:C:2245:GLN:NE2	1:C:3861:GLU:OE1	2.46	0.48
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.37	0.48
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.95	0.48
1:A:1586:ASN:ND2	1:A:1590:GLN:OE1	2.46	0.48
1:A:3371:LYS:NZ	1:A:3375:GLU:OE2	2.45	0.48
1:B:1864:LYS:NZ	1:B:1871:PHE:O	2.39	0.48
1:C:3583:GLU:HB2	1:C:3586:ALA:HB2	1.95	0.48
1:D:3583:GLU:HB2	1:D:3586:ALA:HB2	1.95	0.48
1:D:4976:GLU:O	1:D:4980:LEU:HB2	2.13	0.48
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.42	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.48
1:B:2387:SER:OG	1:B:2492:ALA:O	2.31	0.48
1:B:4017:LEU:HD13	1:B:4135:PRO:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1743[A]:ARG:NH1	1:C:1963:GLU:OE2	2.47	0.48
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	1.96	0.48
1:C:4627:MET:HB2	1:C:4627:MET:HE3	1.76	0.48
1:D:221:ARG:NH2	1:D:255:HIS:O	2.46	0.48
1:D:3606:LEU:O	1:D:3609:THR:OG1	2.31	0.48
1:A:1743[A]:ARG:NH1	1:A:1963:GLU:OE2	2.46	0.48
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.95	0.48
1:A:3968:TYR:O	1:A:3976:ASN:ND2	2.41	0.48
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.96	0.48
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.95	0.48
1:B:2998:PHE:HD1	1:B:3002:LEU:HD22	1.79	0.48
1:C:627:PRO:HD3	2:G:89:GLY:HA2	1.96	0.48
1:C:1293:LEU:HD11	1:C:1594:ARG:HD3	1.95	0.48
1:C:3450:ASN:OD1	1:C:3453:ARG:NH1	2.39	0.48
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.96	0.48
1:D:2420:HIS:HB2	1:D:2492:ALA:HA	1.96	0.48
1:A:28:VAL:HG22	1:A:33:LEU:HD22	1.96	0.47
1:A:585:SER:O	1:A:588:SER:OG	2.29	0.47
1:A:1864:LYS:NZ	1:A:1871:PHE:O	2.39	0.47
1:A:4722:ARG:H	1:A:4722:ARG:HG2	1.43	0.47
1:B:2813:LEU:HA	1:B:2816:MET:HG3	1.97	0.47
1:B:3433:GLU:HG3	1:B:3437:MET:HE3	1.96	0.47
1:C:28:VAL:HG22	1:C:33:LEU:HD22	1.96	0.47
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.96	0.47
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.47	0.47
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.95	0.47
1:D:2245:GLN:NE2	1:D:3861:GLU:OE1	2.46	0.47
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.95	0.47
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.95	0.47
1:A:4017:LEU:HD13	1:A:4135:PRO:HB2	1.95	0.47
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.96	0.47
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	1.94	0.47
1:A:1171:SER:HG	1:A:1175:SER:HG	1.62	0.47
1:A:1494:MET:HE3	1:A:1494:MET:HB2	1.66	0.47
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.96	0.47
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.46	0.47
1:A:652:ARG:NH1	1:A:751:SER:O	2.46	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:A:2280:VAL:HG21	1:A:2290:LEU:HD12	1.95	0.47
1:A:2813:LEU:HA	1:A:2816:MET:HG3	1.96	0.47
1:A:3420:ARG:HG3	1:A:3520:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.95	0.47
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.96	0.47
1:B:3380:ARG:HH22	1:B:3394:VAL:HG21	1.79	0.47
1:B:3420:ARG:HG3	1:B:3520:ILE:HD11	1.97	0.47
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.96	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.97	0.47
1:C:2387:SER:OG	1:C:2492:ALA:O	2.31	0.47
1:C:2813:LEU:HA	1:C:2816:MET:HG3	1.97	0.47
1:C:2998:PHE:HD1	1:C:3002:LEU:HD22	1.79	0.47
1:D:2998:PHE:HD1	1:D:3002:LEU:HD22	1.79	0.47
1:D:3420:ARG:HG3	1:D:3520:ILE:HD11	1.97	0.47
1:D:4017:LEU:HD13	1:D:4135:PRO:HB2	1.95	0.47
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.96	0.47
1:A:2420:HIS:HB2	1:A:2492:ALA:HA	1.96	0.47
1:A:3132:THR:HA	1:A:3136:LEU:HB3	1.96	0.47
1:B:28:VAL:HG22	1:B:33:LEU:HD22	1.96	0.47
1:B:572:PRO:HA	1:B:575:LEU:HD13	1.96	0.47
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.46	0.47
1:C:660:GLY:HA2	1:C:750:LEU:HD12	1.95	0.47
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.43	0.47
1:D:274:LEU:HD23	1:D:278:GLN:HE21	1.79	0.47
1:D:1118:ASP:N	1:D:1118:ASP:OD1	2.47	0.47
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.95	0.47
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.97	0.47
1:A:3380:ARG:HH22	1:A:3394:VAL:HG21	1.79	0.47
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.46	0.47
1:D:572:PRO:HA	1:D:575:LEU:HD13	1.96	0.47
1:D:2280:VAL:HG21	1:D:2290:LEU:HD12	1.95	0.47
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.46	0.47
1:A:274:LEU:HD23	1:A:278:GLN:HE21	1.79	0.47
1:A:2463:LEU:HA	1:A:2466:LEU:HD12	1.97	0.47
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.95	0.47
1:A:4880:MET:HE2	1:A:4880:MET:HB2	1.73	0.47
1:B:2420:HIS:HB2	1:B:2492:ALA:HA	1.96	0.47
1:B:2490:MET:SD	1:B:2490:MET:N	2.85	0.47
1:C:322:LYS:HZ1	1:C:356:TRP:HE1	1.61	0.47
1:C:572:PRO:HA	1:C:575:LEU:HD13	1.96	0.47
1:C:2490:MET:SD	1:C:2490:MET:N	2.85	0.47
1:C:2660:GLY:HA3	1:C:2666:VAL:HG22	1.97	0.47
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.95	0.47
1:D:2463:LEU:HA	1:D:2466:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2660:GLY:HA3	1:D:2666:VAL:HG22	1.97	0.47
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.95	0.47
1:D:3037:GLU:HG2	1:D:3085:PRO:HD3	1.97	0.47
1:D:3380:ARG:HH22	1:D:3394:VAL:HG21	1.79	0.47
1:D:3450:ASN:OD1	1:D:3453:ARG:NH1	2.39	0.47
1:A:3037:GLU:HG2	1:A:3085:PRO:HD3	1.97	0.47
1:A:4006:ASP:N	1:A:4006:ASP:OD1	2.48	0.47
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.47	0.47
1:C:3380:ARG:HH22	1:C:3394:VAL:HG21	1.79	0.47
1:C:3433:GLU:HG3	1:C:3437:MET:HE3	1.96	0.47
1:D:277:GLY:N	1:D:316:PHE:O	2.43	0.47
1:B:627:PRO:HD3	2:F:89:GLY:HA2	1.96	0.47
1:B:4006:ASP:OD1	1:B:4006:ASP:N	2.47	0.47
1:C:221:ARG:NH2	1:C:255:HIS:O	2.46	0.47
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.96	0.47
1:D:3596:VAL:O	1:D:3600:SER:OG	2.31	0.47
1:A:660:GLY:HA2	1:A:750:LEU:HD12	1.95	0.47
1:A:1776:HIS:HB3	1:A:1798:LEU:HD13	1.97	0.47
1:A:3359:ILE:HG23	1:A:3437:MET:HE1	1.97	0.47
1:A:3528:THR:HG23	1:A:3573:MET:HE1	1.97	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.97	0.47
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.97	0.47
1:B:3359:ILE:HG23	1:B:3437:MET:HE1	1.97	0.47
1:C:2452:ARG:NH1	1:D:144:GLU:OE1	2.48	0.47
1:C:3420:ARG:HG3	1:C:3520:ILE:HD11	1.97	0.47
1:D:585:SER:O	1:D:588:SER:OG	2.29	0.47
1:D:2325:PRO:HB2	1:D:2421:ALA:HB1	1.96	0.47
1:D:4006:ASP:N	1:D:4006:ASP:OD1	2.47	0.47
1:A:144:GLU:OE1	1:D:2452:ARG:NH1	2.48	0.46
1:A:2325:PRO:HB2	1:A:2421:ALA:HB1	1.96	0.46
1:B:277:GLY:N	1:B:316:PHE:O	2.43	0.46
1:B:2463:LEU:HA	1:B:2466:LEU:HD12	1.97	0.46
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.40	0.46
1:C:3037:GLU:HG2	1:C:3085:PRO:HD3	1.97	0.46
1:D:1784:ALA:HA	2:H:55:VAL:HA	1.97	0.46
1:D:4823:LEU:HD12	1:D:4823:LEU:HA	1.85	0.46
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.97	0.46
1:B:3037:GLU:HG2	1:B:3085:PRO:HD3	1.97	0.46
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.97	0.46
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.39	0.46
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2660:GLY:HA3	1:A:2666:VAL:HG22	1.96	0.46
1:A:2998:PHE:HD1	1:A:3002:LEU:HD22	1.80	0.46
1:A:3081:MET:HG3	1:A:3156:VAL:HA	1.98	0.46
1:A:4823:LEU:HD12	1:A:4823:LEU:HA	1.85	0.46
1:B:179:TYR:N	1:B:194:SER:O	2.49	0.46
1:B:1784:ALA:HA	2:F:55:VAL:HA	1.97	0.46
1:B:3081:MET:HG3	1:B:3156:VAL:HA	1.97	0.46
1:B:3085:PRO:HD2	1:B:3088:VAL:HB	1.98	0.46
1:B:3528:THR:HG23	1:B:3573:MET:HE1	1.97	0.46
1:C:274:LEU:HD23	1:C:278:GLN:HE21	1.79	0.46
1:C:3945:GLU:HA	1:C:3948:LYS:HE2	1.98	0.46
1:C:4892:ARG:NH1	1:D:4899:ASP:OD1	2.49	0.46
1:D:2813:LEU:HA	1:D:2816:MET:HG3	1.97	0.46
1:A:299:LEU:HD22	1:A:378:LEU:HB2	1.98	0.46
1:A:1970:GLN:HG2	1:A:3642:TYR:HA	1.97	0.46
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.98	0.46
1:B:1970:GLN:HG2	1:B:3642:TYR:HA	1.96	0.46
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.73	0.46
1:B:3132:THR:HA	1:B:3136:LEU:HB3	1.96	0.46
1:C:2420:HIS:HB2	1:C:2492:ALA:HA	1.96	0.46
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.97	0.46
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.97	0.46
1:C:3968:TYR:O	1:C:3976:ASN:ND2	2.42	0.46
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.41	0.46
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	1.98	0.46
1:B:3365:LEU:HD21	1:B:3408:LEU:HD12	1.97	0.46
1:C:3359:ILE:HG23	1:C:3437:MET:HE1	1.97	0.46
1:D:3081:MET:HG3	1:D:3156:VAL:HA	1.97	0.46
1:D:3176:GLY:O	1:D:3179:LYS:NZ	2.43	0.46
2:F:49:ARG:HG3	2:F:52:LYS:HD3	1.98	0.46
1:A:2316:LYS:HE2	1:A:2318:TYR:HE1	1.81	0.46
1:A:3085:PRO:HD2	1:A:3088:VAL:HB	1.98	0.46
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.98	0.46
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.97	0.46
1:C:3085:PRO:HD2	1:C:3088:VAL:HB	1.98	0.46
1:D:322:LYS:HZ1	1:D:356:TRP:HE1	1.64	0.46
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.98	0.46
1:D:3359:ILE:HG23	1:D:3437:MET:HE1	1.97	0.46
1:B:2452:ARG:NH1	1:C:144:GLU:OE1	2.48	0.46
1:C:2316:LYS:HE2	1:C:2318:TYR:HE1	1.81	0.46
1:C:3365:LEU:HD21	1:C:3408:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4722:ARG:H	1:C:4722:ARG:HG2	1.43	0.46
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.96	0.46
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.49	0.46
1:A:3176:GLY:O	1:A:3179:LYS:NZ	2.43	0.46
1:C:179:TYR:N	1:C:194:SER:O	2.49	0.46
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.98	0.46
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.98	0.46
1:C:1970:GLN:HG2	1:C:3642:TYR:HA	1.96	0.46
1:C:2265:LEU:HB3	1:C:2330:ARG:HD2	1.98	0.46
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	1.97	0.46
1:C:3132:THR:HA	1:C:3136:LEU:HB3	1.96	0.46
1:D:2316:LYS:HE2	1:D:2318:TYR:HE1	1.81	0.46
1:A:2265:LEU:HB3	1:A:2330:ARG:HD2	1.98	0.46
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.97	0.46
1:B:3945:GLU:HA	1:B:3948:LYS:HE2	1.98	0.46
1:B:4155:PRO:O	1:B:4161:ARG:NH2	2.45	0.46
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.98	0.46
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.98	0.46
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.98	0.46
1:A:3365:LEU:HD21	1:A:3408:LEU:HD12	1.97	0.46
1:B:274:LEU:HD23	1:B:278:GLN:HE21	1.79	0.46
1:B:2316:LYS:HE2	1:B:2318:TYR:HE1	1.81	0.46
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.75	0.46
1:B:4176:PRO:O	1:B:4202:ARG:NH1	2.45	0.46
1:B:4675:LYS:O	1:B:4679:ARG:HG2	2.17	0.46
1:C:4155:PRO:O	1:C:4161:ARG:NH2	2.45	0.46
1:D:3528:THR:HG23	1:D:3573:MET:HE1	1.97	0.46
1:D:4627:MET:HE3	1:D:4627:MET:HB2	1.76	0.46
1:A:221:ARG:NH2	1:A:255:HIS:O	2.46	0.45
1:A:3450:ASN:OD1	1:A:3453:ARG:NH1	2.40	0.45
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.16	0.45
1:C:4675:LYS:O	1:C:4679:ARG:HG2	2.17	0.45
1:D:299:LEU:HD22	1:D:378:LEU:HB2	1.98	0.45
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.97	0.45
1:D:3132:THR:HA	1:D:3136:LEU:HB3	1.96	0.45
1:D:4141:PHE:CE2	1:D:4196:GLU:HG2	2.52	0.45
1:A:179:TYR:N	1:A:194:SER:O	2.49	0.45
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.97	0.45
1:B:299:LEU:HD22	1:B:378:LEU:HB2	1.98	0.45
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	1.98	0.45
1:B:2660:GLY:HA3	1:B:2666:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4820:VAL:HG22	1:B:4823:LEU:HB2	1.98	0.45
1:C:411:TYR:HE1	1:C:441:VAL:HG13	1.82	0.45
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.46	0.45
1:C:3528:THR:HG23	1:C:3573:MET:HE1	1.97	0.45
1:C:4006:ASP:OD1	1:C:4006:ASP:N	2.47	0.45
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.98	0.45
1:D:1970:GLN:HG2	1:D:3642:TYR:HA	1.96	0.45
1:D:2265:LEU:HB3	1:D:2330:ARG:HD2	1.98	0.45
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.45	0.45
1:D:3945:GLU:HA	1:D:3948:LYS:HE2	1.98	0.45
2:H:49:ARG:HG3	2:H:52:LYS:HD3	1.98	0.45
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.99	0.45
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.98	0.45
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.16	0.45
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.50	0.45
1:C:1784:ALA:HA	2:G:55:VAL:HA	1.97	0.45
1:C:2014:ASP:OD1	1:C:2014:ASP:N	2.45	0.45
1:C:3371:LYS:NZ	1:C:3375:GLU:OE2	2.45	0.45
1:A:2002:PRO:O	1:A:2006:ILE:HD12	2.17	0.45
1:A:4141:PHE:CE2	1:A:4196:GLU:HG2	2.52	0.45
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.45
1:B:2002:PRO:O	1:B:2006:ILE:HD12	2.17	0.45
1:B:3359:ILE:HD11	1:B:3430:ASN:HB3	1.99	0.45
1:C:22:LEU:HD12	1:C:37:LEU:HD12	1.99	0.45
1:C:1431:THR:OG1	1:C:1521:ASP:OD1	2.32	0.45
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	1.98	0.45
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.50	0.45
1:D:411:TYR:HE1	1:D:441:VAL:HG13	1.82	0.45
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.75	0.45
1:D:4820:VAL:HG22	1:D:4823:LEU:HB2	1.98	0.45
1:A:356:TRP:O	1:A:379:HIS:N	2.50	0.45
1:A:403:MET:O	1:A:407:THR:OG1	2.23	0.45
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.98	0.45
1:A:2782:ASP:OD1	1:A:2782:ASP:N	2.50	0.45
1:B:4892:ARG:NH1	1:C:4899:ASP:OD1	2.49	0.45
1:C:3081:MET:HG3	1:C:3156:VAL:HA	1.97	0.45
1:D:22:LEU:HD12	1:D:37:LEU:HD12	1.99	0.45
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.99	0.45
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.97	0.45
1:D:3817:LEU:HD13	1:D:3899:PHE:HD1	1.82	0.45
1:A:219:VAL:HG12	1:A:259:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4675:LYS:O	1:A:4679:ARG:HG2	2.16	0.45
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.98	0.45
1:C:2765:LYS:HA	1:C:2765:LYS:HD3	1.80	0.45
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.16	0.45
1:D:2002:PRO:O	1:D:2006:ILE:HD12	2.17	0.45
1:D:3085:PRO:HD2	1:D:3088:VAL:HB	1.98	0.45
1:C:299:LEU:HD22	1:C:378:LEU:HB2	1.98	0.45
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.82	0.45
1:D:179:TYR:N	1:D:194:SER:O	2.49	0.45
1:D:2109:ASP:N	1:D:2109:ASP:OD1	2.50	0.45
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.97	0.45
1:A:4930:ALA:HB2	1:D:4933:GLN:HG2	1.99	0.45
1:B:884:LEU:HD13	1:B:968:ALA:H	1.82	0.45
1:B:2265:LEU:HB3	1:B:2330:ARG:HD2	1.98	0.45
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.97	0.45
1:B:4722:ARG:HE	1:B:4722:ARG:HB3	1.43	0.45
1:C:3206:LEU:HD13	1:C:3246:LEU:HD13	1.99	0.45
1:D:893:TYR:HB3	1:D:960:MET:HE2	1.99	0.45
1:D:1575:LEU:HB3	1:D:1579:MET:HE3	1.99	0.45
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.97	0.45
1:D:3359:ILE:HD11	1:D:3430:ASN:HB3	1.99	0.45
1:A:3945:GLU:HA	1:A:3948:LYS:HE2	1.98	0.45
1:C:219:VAL:HG12	1:C:259:LEU:HD12	1.99	0.45
1:C:4141:PHE:CE2	1:C:4196:GLU:HG2	2.52	0.45
1:D:219:VAL:HG12	1:D:259:LEU:HD12	1.99	0.45
2:F:23:VAL:HG13	2:F:47:LYS:HG2	1.99	0.45
2:G:49:ARG:HG3	2:G:52:LYS:HD3	1.98	0.45
1:A:884:LEU:HD13	1:A:968:ALA:H	1.82	0.45
1:A:893:TYR:HB3	1:A:960:MET:HE2	1.99	0.45
1:A:1474:VAL:O	1:A:1486:SER:HA	2.17	0.45
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.82	0.45
1:B:221:ARG:NH2	1:B:255:HIS:O	2.46	0.45
1:B:411:TYR:HE1	1:B:441:VAL:HG13	1.82	0.45
1:B:893:TYR:HB3	1:B:960:MET:HE2	1.99	0.45
1:B:3176:GLY:O	1:B:3179:LYS:NZ	2.43	0.45
1:B:3206:LEU:HD13	1:B:3246:LEU:HD13	1.99	0.45
1:B:3245:VAL:HG23	1:B:3248:ARG:H	1.82	0.45
1:C:356:TRP:O	1:C:379:HIS:N	2.50	0.45
1:C:4710:SER:OG	1:C:4772:ASP:OD2	2.32	0.45
1:D:1474:VAL:O	1:D:1486:SER:HA	2.17	0.45
1:D:3206:LEU:HD13	1:D:3246:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3245:VAL:HG23	1:D:3248:ARG:H	1.82	0.45
1:A:411:TYR:HE1	1:A:441:VAL:HG13	1.82	0.44
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.39	0.44
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.99	0.44
1:B:3374:ALA:O	1:B:3378:GLN:NE2	2.50	0.44
1:A:22:LEU:HD12	1:A:37:LEU:HD12	1.99	0.44
1:A:400:ALA:O	1:A:404:ILE:HD12	2.17	0.44
1:B:22:LEU:HD12	1:B:37:LEU:HD12	1.99	0.44
1:B:400:ALA:O	1:B:404:ILE:HD12	2.17	0.44
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.45	0.44
1:C:893:TYR:HB3	1:C:960:MET:HE2	1.99	0.44
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.41	0.44
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.82	0.44
1:C:3374:ALA:O	1:C:3378:GLN:NE2	2.50	0.44
1:D:3968:TYR:O	1:D:3976:ASN:ND2	2.42	0.44
1:D:4675:LYS:O	1:D:4679:ARG:HG2	2.17	0.44
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.47	0.44
1:A:2293:GLN:HA	1:A:2296:GLU:HB2	2.00	0.44
1:B:4141:PHE:CE2	1:B:4196:GLU:HG2	2.52	0.44
1:C:716:PHE:HE1	1:C:730:VAL:HG21	1.82	0.44
1:C:1474:VAL:O	1:C:1486:SER:HA	2.17	0.44
1:D:356:TRP:O	1:D:379:HIS:N	2.50	0.44
1:D:2293:GLN:HA	1:D:2296:GLU:HB2	2.00	0.44
1:D:3365:LEU:HD21	1:D:3408:LEU:HD12	1.97	0.44
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.18	0.44
1:D:4710:SER:OG	1:D:4772:ASP:OD2	2.32	0.44
2:E:23:VAL:HG13	2:E:47:LYS:HG2	1.99	0.44
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.46	0.44
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.16	0.44
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.99	0.44
1:A:3053:ARG:HA	1:A:3056:LEU:HD13	1.99	0.44
1:A:3053:ARG:HG3	1:A:3056:LEU:HD22	2.00	0.44
1:A:3359:ILE:HD11	1:A:3430:ASN:HB3	1.99	0.44
1:A:3801:GLY:O	1:A:3805:LEU:HB2	2.18	0.44
1:B:219:VAL:HG12	1:B:259:LEU:HD12	1.99	0.44
1:C:884:LEU:HD13	1:C:968:ALA:H	1.82	0.44
1:C:4820:VAL:HG22	1:C:4823:LEU:HB2	1.98	0.44
2:E:49:ARG:HG3	2:E:52:LYS:HD3	1.98	0.44
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.73	0.44
1:A:3245:VAL:HG23	1:A:3248:ARG:H	1.82	0.44
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:TRP:O	1:B:379:HIS:N	2.50	0.44
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.50	0.44
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.81	0.44
1:C:3053:ARG:HA	1:C:3056:LEU:HD13	1.99	0.44
1:C:3582:ARG:HA	1:C:3582:ARG:HD3	1.79	0.44
1:C:3606:LEU:O	1:C:3609:THR:OG1	2.31	0.44
1:D:400:ALA:O	1:D:404:ILE:HD12	2.17	0.44
1:D:3168:THR:O	1:D:3172:ILE:HG12	2.18	0.44
1:D:4827:LEU:HD23	1:D:4827:LEU:HA	1.88	0.44
1:A:35:LEU:HD11	1:A:189:LEU:HD23	2.00	0.44
1:A:716:PHE:HE1	1:A:730:VAL:HG21	1.82	0.44
1:B:1494:MET:HE3	1:B:1494:MET:HB2	1.67	0.44
1:B:3053:ARG:HG3	1:B:3056:LEU:HD22	1.99	0.44
1:B:3801:GLY:O	1:B:3805:LEU:HB2	2.18	0.44
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.82	0.44
1:C:400:ALA:O	1:C:404:ILE:HD12	2.17	0.44
1:C:1269:CYS:HA	1:C:1564:PHE:O	2.18	0.44
1:C:2951:ILE:HG21	1:C:3034:LYS:HD2	2.00	0.44
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.82	0.44
1:D:884:LEU:HD13	1:D:968:ALA:H	1.82	0.44
1:D:3374:ALA:O	1:D:3378:GLN:NE2	2.50	0.44
2:H:23:VAL:HG13	2:H:47:LYS:HG2	1.99	0.44
1:A:939:VAL:HB	1:A:1051:TYR:HB3	2.00	0.44
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.83	0.44
1:A:2452:ARG:NH1	1:B:144:GLU:OE1	2.51	0.44
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.99	0.44
1:B:1474:VAL:O	1:B:1486:SER:HA	2.17	0.44
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.83	0.44
1:C:2471:SER:HA	1:C:2525:GLY:HA2	2.00	0.44
1:C:2638:LYS:HE2	1:C:2695:LEU:HD13	1.99	0.44
1:D:716:PHE:HE1	1:D:730:VAL:HG21	1.82	0.44
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.50	0.44
1:A:2471:SER:HA	1:A:2525:GLY:HA2	2.00	0.44
1:A:2951:ILE:HG21	1:A:3034:LYS:HD2	2.00	0.44
1:A:3374:ALA:O	1:A:3378:GLN:NE2	2.50	0.44
1:A:4820:VAL:HG22	1:A:4823:LEU:HB2	1.98	0.44
1:B:308:HIS:HD2	1:B:310:LYS:HB3	1.82	0.44
1:B:716:PHE:HE1	1:B:730:VAL:HG21	1.82	0.44
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.18	0.44
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.50	0.44
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.47	0.44
1:B:2951:ILE:HG21	1:B:3034:LYS:HD2	2.00	0.44
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.37	0.44
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.83	0.44
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.82	0.44
1:C:653:ALA:HB3	1:C:656:SER:HB2	1.99	0.44
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.83	0.44
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.18	0.44
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.82	0.44
1:A:1575:LEU:HB3	1:A:1579:MET:HE3	1.99	0.44
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	2.00	0.44
1:C:3110:LEU:HB3	1:C:3175:LEU:HD11	2.00	0.44
1:C:3875:MET:HE3	1:C:3875:MET:HB3	1.84	0.44
1:D:2638:LYS:HE2	1:D:2695:LEU:HD13	1.99	0.44
1:D:2782:ASP:OD1	1:D:2782:ASP:N	2.50	0.44
1:A:3168:THR:O	1:A:3172:ILE:HG12	2.18	0.43
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.18	0.43
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.36	0.43
1:B:322:LYS:HZ1	1:B:356:TRP:HE1	1.64	0.43
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.36	0.43
1:D:2951:ILE:HG21	1:D:3034:LYS:HD2	2.00	0.43
1:A:322:LYS:HZ1	1:A:356:TRP:HE1	1.66	0.43
1:B:35:LEU:HD11	1:B:189:LEU:HD23	2.00	0.43
1:B:939:VAL:HB	1:B:1051:TYR:HB3	2.00	0.43
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.41	0.43
1:B:1575:LEU:HB3	1:B:1579:MET:HE3	1.99	0.43
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	2.00	0.43
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.54	0.43
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.18	0.43
1:C:3359:ILE:HD11	1:C:3430:ASN:HB3	1.99	0.43
1:D:939:VAL:HB	1:D:1051:TYR:HB3	2.00	0.43
2:G:23:VAL:HG13	2:G:47:LYS:HG2	1.99	0.43
1:A:3110:LEU:HB3	1:A:3175:LEU:HD11	2.00	0.43
1:A:3206:LEU:HD13	1:A:3246:LEU:HD13	1.99	0.43
1:A:3823:LYS:HD3	1:A:3823:LYS:HA	1.75	0.43
1:A:4155:PRO:O	1:A:4161:ARG:NH2	2.45	0.43
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.18	0.43
1:C:2002:PRO:O	1:C:2006:ILE:HD12	2.17	0.43
1:D:3371:LYS:NZ	1:D:3375:GLU:OE2	2.45	0.43
1:D:4722:ARG:H	1:D:4722:ARG:HG2	1.43	0.43
1:A:3466:ASN:HB3	1:A:3507:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.46	0.43
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.99	0.43
1:B:3582:ARG:HA	1:B:3582:ARG:HD3	1.79	0.43
1:B:3606:LEU:O	1:B:3609:THR:OG1	2.31	0.43
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.43
1:C:3168:THR:O	1:C:3172:ILE:HG12	2.18	0.43
1:D:728:ARG:NH2	1:D:1543:GLU:OE2	2.36	0.43
1:D:1424:PRO:HA	1:D:1427:ILE:HG22	2.01	0.43
1:D:2178:MET:HE1	1:D:2210:VAL:HG11	2.00	0.43
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	2.00	0.43
1:D:3053:ARG:HG3	1:D:3056:LEU:HD22	1.99	0.43
1:D:4155:PRO:O	1:D:4161:ARG:NH2	2.45	0.43
2:F:77:THR:HG22	2:F:80:VAL:HG22	2.00	0.43
1:A:775:GLY:H	1:A:848:HIS:CE1	2.37	0.43
1:B:111:HIS:ND1	1:B:114:SER:OG	2.39	0.43
1:B:282:ILE:O	1:B:290:TYR:HA	2.19	0.43
1:B:775:GLY:H	1:B:848:HIS:CE1	2.37	0.43
1:B:2559:LEU:HD13	1:B:2603:ILE:HG13	2.00	0.43
1:B:3110:LEU:HB3	1:B:3175:LEU:HD11	2.00	0.43
1:B:3164:SER:HA	1:B:3167:ARG:HE	1.83	0.43
1:B:3168:THR:O	1:B:3172:ILE:HG12	2.18	0.43
1:C:3801:GLY:O	1:C:3805:LEU:HB2	2.18	0.43
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.40	0.43
1:D:2687:ALA:O	1:D:2993:GLN:NE2	2.52	0.43
1:D:3110:LEU:HB3	1:D:3175:LEU:HD11	2.00	0.43
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.83	0.43
1:A:3099:ALA:HA	1:A:3136:LEU:HD21	2.00	0.43
1:B:3466:ASN:HB3	1:B:3507:THR:HB	2.00	0.43
1:C:790:ARG:HA	1:C:1626:TRP:O	2.19	0.43
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	2.01	0.43
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.47	0.43
1:C:2970:SER:HA	1:C:2973:PHE:CE2	2.54	0.43
1:C:3053:ARG:HG3	1:C:3056:LEU:HD22	1.99	0.43
1:C:4722:ARG:HE	1:C:4722:ARG:HB3	1.43	0.43
1:D:790:ARG:HA	1:D:1626:TRP:O	2.19	0.43
2:E:77:THR:HG22	2:E:80:VAL:HG22	2.00	0.43
2:H:26:TYR:OH	2:H:37:ASP:OD2	2.31	0.43
1:A:3051:ARG:HH21	1:A:3098:SER:HB3	1.83	0.43
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.54	0.43
1:B:3051:ARG:HH21	1:B:3098:SER:HB3	1.84	0.43
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:VAL:HB	1:C:1051:TYR:HB3	2.00	0.43
1:C:1575:LEU:HB3	1:C:1579:MET:HE3	1.99	0.43
1:C:2587:TYR:O	1:C:2590:SER:OG	2.26	0.43
1:C:2627:VAL:HG21	1:C:2674:LEU:HG	2.00	0.43
1:D:35:LEU:HD11	1:D:189:LEU:HD23	2.00	0.43
1:D:3888:LEU:HD23	1:D:3888:LEU:HA	1.88	0.43
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.57	0.43
1:A:282:ILE:O	1:A:290:TYR:HA	2.19	0.43
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.40	0.43
1:A:877:ASN:HA	1:A:970:LEU:H	1.84	0.43
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.54	0.43
1:A:3164:SER:HA	1:A:3167:ARG:HE	1.83	0.43
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.83	0.43
1:B:2178:MET:HE1	1:B:2210:VAL:HG11	2.00	0.43
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.54	0.43
1:C:1452:TRP:HB3	1:C:1548:LEU:HB3	2.01	0.43
1:C:2293:GLN:HA	1:C:2296:GLU:HB2	2.00	0.43
1:C:3164:SER:HA	1:C:3167:ARG:HE	1.83	0.43
1:C:4823:LEU:HD12	1:C:4823:LEU:HA	1.85	0.43
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.39	0.43
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.54	0.43
1:D:2559:LEU:HD13	1:D:2603:ILE:HG13	2.00	0.43
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.99	0.43
1:D:3199:ALA:O	1:D:3283:ARG:NE	2.46	0.43
1:D:3648:ARG:O	1:D:3652:MET:HG2	2.19	0.43
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	2.01	0.43
1:A:2178:MET:HE1	1:A:2210:VAL:HG11	2.00	0.43
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.54	0.43
1:B:1452:TRP:HB3	1:B:1548:LEU:HB3	2.01	0.43
1:B:2002:PRO:HD3	1:B:3638:MET:HE1	2.01	0.43
1:B:2293:GLN:HA	1:B:2296:GLU:HB2	2.00	0.43
1:B:2687:ALA:O	1:B:2993:GLN:NE2	2.52	0.43
1:B:3053:ARG:HA	1:B:3056:LEU:HD13	1.99	0.43
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.52	0.43
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	2.01	0.43
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	2.01	0.43
1:D:3053:ARG:HA	1:D:3056:LEU:HD13	1.99	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.36	0.43
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.54	0.43
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.52	0.43
1:A:2627:VAL:HG21	1:A:2674:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.36	0.43
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.01	0.43
1:B:2014:ASP:N	1:B:2014:ASP:OD1	2.45	0.43
1:B:2638:LYS:HE2	1:B:2695:LEU:HD13	1.99	0.43
1:B:2675:THR:HB	1:B:2710:LEU:HD21	2.00	0.43
1:C:1812:LEU:HD23	1:C:1812:LEU:HA	1.88	0.43
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.99	0.43
1:C:3466:ASN:HB3	1:C:3507:THR:HB	2.00	0.43
1:C:3648:ARG:O	1:C:3652:MET:HG2	2.19	0.43
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.52	0.43
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.18	0.43
1:D:1828:ASP:N	1:D:1828:ASP:OD1	2.52	0.43
1:D:2627:VAL:HG21	1:D:2674:LEU:HG	2.00	0.43
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.47	0.43
1:D:3051:ARG:HH21	1:D:3098:SER:HB3	1.84	0.43
1:D:3099:ALA:HA	1:D:3136:LEU:HD21	2.00	0.43
1:D:3169:LEU:HD23	1:D:3194:LEU:HD11	2.01	0.43
1:D:3466:ASN:HB3	1:D:3507:THR:HB	2.00	0.43
1:D:3901:ASN:OD1	1:D:3904:ARG:NH1	2.36	0.43
1:A:262:LEU:HD13	1:A:274:LEU:HD11	2.01	0.42
1:A:1473:THR:HA	1:A:1487:LEU:O	2.19	0.42
1:A:2638:LYS:HE2	1:A:2695:LEU:HD13	1.99	0.42
1:B:3648:ARG:O	1:B:3652:MET:HG2	2.19	0.42
1:B:4646:LEU:HD23	1:B:4646:LEU:HA	1.87	0.42
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.39	0.42
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.01	0.42
1:C:2178:MET:HE3	1:C:2178:MET:HB2	1.86	0.42
1:C:2559:LEU:HD13	1:C:2603:ILE:HG13	2.00	0.42
1:C:2687:ALA:O	1:C:2993:GLN:NE2	2.52	0.42
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.50	0.42
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.83	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.18	0.42
1:A:3648:ARG:O	1:A:3652:MET:HG2	2.19	0.42
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.52	0.42
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	2.01	0.42
1:B:2471:SER:HA	1:B:2525:GLY:HA2	2.00	0.42
1:D:2970:SER:HA	1:D:2973:PHE:CE2	2.54	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.54	0.42
1:A:1452:TRP:HB3	1:A:1548:LEU:HB3	2.01	0.42
1:A:2002:PRO:HD3	1:A:3638:MET:HE1	2.01	0.42
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4253:GLU:OE2	1:A:4553:ASN:ND2	2.46	0.42
1:B:2712:PRO:O	1:B:2956:ALA:N	2.52	0.42
1:B:3199:ALA:O	1:B:3283:ARG:NE	2.46	0.42
1:B:4627:MET:HE3	1:B:4627:MET:HB2	1.76	0.42
1:C:3051:ARG:HH21	1:C:3098:SER:HB3	1.84	0.42
1:C:3099:ALA:HA	1:C:3136:LEU:HD21	2.00	0.42
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.36	0.42
1:D:3754:GLU:HB2	1:D:4718:LYS:HD3	2.02	0.42
2:E:26:TYR:OH	2:E:37:ASP:OD2	2.31	0.42
2:H:77:THR:HG22	2:H:80:VAL:HG22	2.00	0.42
1:A:2472:LEU:HD23	1:A:2472:LEU:HA	1.88	0.42
1:B:652:ARG:HB3	1:B:773:LEU:HD12	2.02	0.42
1:B:728:ARG:NH2	1:B:1543:GLU:OE2	2.36	0.42
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.54	0.42
1:C:35:LEU:HD11	1:C:189:LEU:HD23	2.00	0.42
1:C:282:ILE:O	1:C:290:TYR:HA	2.19	0.42
1:C:2178:MET:HE1	1:C:2210:VAL:HG11	2.00	0.42
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.36	0.42
1:D:262:LEU:HD13	1:D:274:LEU:HD11	2.02	0.42
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.53	0.42
1:D:2675:THR:HB	1:D:2710:LEU:HD21	2.00	0.42
1:D:3268:HIS:O	1:D:3272:ILE:HB	2.19	0.42
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.79	0.42
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.30	0.42
1:A:790:ARG:HA	1:A:1626:TRP:O	2.19	0.42
1:A:1432:THR:HA	1:A:1520:VAL:O	2.19	0.42
1:A:2559:LEU:HD13	1:A:2603:ILE:HG13	2.00	0.42
1:A:2687:ALA:O	1:A:2993:GLN:NE2	2.52	0.42
1:B:669:ASP:OD1	1:B:790:ARG:NH1	2.53	0.42
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	2.01	0.42
1:B:1473:THR:HA	1:B:1487:LEU:O	2.19	0.42
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.01	0.42
1:B:3099:ALA:HA	1:B:3136:LEU:HD21	2.00	0.42
1:C:585:SER:O	1:C:588:SER:OG	2.29	0.42
1:C:877:ASN:HA	1:C:970:LEU:H	1.84	0.42
1:C:2002:PRO:HD3	1:C:3638:MET:HE1	2.01	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.54	0.42
1:D:652:ARG:HB3	1:D:773:LEU:HD12	2.02	0.42
1:D:669:ASP:OD1	1:D:790:ARG:NH1	2.53	0.42
1:D:833:GLY:HA3	1:D:838:HIS:CD2	2.55	0.42
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4098:ASP:OD1	1:D:4098:ASP:N	2.53	0.42
1:D:4681:LEU:HD12	1:D:4681:LEU:HA	1.87	0.42
1:A:3582:ARG:HA	1:A:3582:ARG:HD3	1.79	0.42
1:A:3875:MET:HE3	1:A:3875:MET:HB3	1.84	0.42
1:A:4161:ARG:HD3	1:A:4161:ARG:HA	1.85	0.42
1:B:265:LEU:HD13	1:B:279:PRO:HB2	2.02	0.42
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.01	0.42
1:B:1432:THR:HA	1:B:1520:VAL:O	2.19	0.42
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.53	0.42
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.85	0.42
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.53	0.42
1:C:3169:LEU:HD23	1:C:3194:LEU:HD11	2.01	0.42
1:C:3268:HIS:O	1:C:3272:ILE:HB	2.19	0.42
1:D:282:ILE:O	1:D:290:TYR:HA	2.19	0.42
1:D:1452:TRP:HB3	1:D:1548:LEU:HB3	2.01	0.42
1:A:3169:LEU:HD23	1:A:3194:LEU:HD11	2.01	0.42
1:A:3754:GLU:HB2	1:A:4718:LYS:HD3	2.02	0.42
1:B:790:ARG:HA	1:B:1626:TRP:O	2.19	0.42
1:B:2627:VAL:HG21	1:B:2674:LEU:HG	2.00	0.42
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.47	0.42
1:B:4722:ARG:H	1:B:4722:ARG:HG2	1.43	0.42
1:B:5006:GLN:H	1:B:5006:GLN:HG2	1.64	0.42
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.37	0.42
1:D:265:LEU:HD13	1:D:279:PRO:HB2	2.02	0.42
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.01	0.42
1:A:669:ASP:OD1	1:A:790:ARG:NH1	2.53	0.42
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	2.01	0.42
1:B:877:ASN:HA	1:B:970:LEU:H	1.84	0.42
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.52	0.42
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	2.02	0.42
1:B:3754:GLU:HB2	1:B:4718:LYS:HD3	2.02	0.42
1:C:486:LEU:HD12	1:C:486:LEU:HA	1.95	0.42
1:C:775:GLY:H	1:C:848:HIS:CE1	2.37	0.42
1:C:2675:THR:HB	1:C:2710:LEU:HD21	2.00	0.42
1:C:3888:LEU:HD23	1:C:3888:LEU:HA	1.88	0.42
1:D:3164:SER:HA	1:D:3167:ARG:HE	1.83	0.42
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	2.02	0.42
2:F:4:ILE:HD11	2:F:66:MET:HB3	2.02	0.42
1:A:265:LEU:HD13	1:A:279:PRO:HB2	2.02	0.42
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.01	0.42
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2675:THR:HB	1:A:2710:LEU:HD21	2.01	0.42
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.45	0.42
1:A:3268:HIS:O	1:A:3272:ILE:HB	2.19	0.42
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.36	0.42
1:B:262:LEU:HD13	1:B:274:LEU:HD11	2.02	0.42
1:B:629:ARG:NH1	2:F:90:VAL:O	2.43	0.42
1:B:833:GLY:HA3	1:B:838:HIS:CD2	2.55	0.42
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.81	0.42
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.88	0.42
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	2.01	0.42
1:C:652:ARG:HB3	1:C:773:LEU:HD12	2.02	0.42
1:C:669:ASP:OD1	1:C:790:ARG:NH1	2.53	0.42
1:C:833:GLY:HA3	1:C:838:HIS:CD2	2.55	0.42
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.52	0.42
1:C:4910:GLU:O	1:C:4914:VAL:HG13	2.20	0.42
1:D:877:ASN:HA	1:D:970:LEU:H	1.84	0.42
1:D:880:GLU:HB3	1:D:883:ALA:HB3	2.01	0.42
1:D:3301:PRO:HA	1:D:3302:PRO:HD3	1.86	0.42
1:D:4910:GLU:O	1:D:4914:VAL:HG13	2.20	0.42
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.91	0.42
1:A:2707:ALA:HB1	1:A:3009:TYR:HD1	1.85	0.42
1:A:4899:ASP:OD1	1:D:4892:ARG:NH1	2.53	0.42
1:A:4910:GLU:O	1:A:4914:VAL:HG13	2.20	0.42
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.95	0.42
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.85	0.42
1:B:4155:PRO:HG3	1:B:5036:LEU:HD23	2.02	0.42
1:C:262:LEU:HD13	1:C:274:LEU:HD11	2.02	0.42
1:C:2677:LYS:HE2	1:C:2677:LYS:HB3	1.73	0.42
1:C:3380:ARG:NH2	1:C:3391:GLU:OE1	2.53	0.42
1:C:3852:LYS:HE3	1:C:3852:LYS:HB3	1.93	0.42
1:D:1473:THR:HA	1:D:1487:LEU:O	2.19	0.42
1:D:2002:PRO:HD3	1:D:3638:MET:HE1	2.01	0.42
1:D:2471:SER:HA	1:D:2525:GLY:HA2	2.00	0.42
2:G:77:THR:HG22	2:G:80:VAL:HG22	2.00	0.42
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	2.02	0.41
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.57	0.41
1:A:5013:MET:HE3	1:A:5021:PHE:HB3	2.02	0.41
1:B:2656:CYS:HA	1:B:2711:PRO:HG3	2.02	0.41
1:B:3132:THR:HG23	1:B:3136:LEU:HD23	2.02	0.41
1:B:3268:HIS:O	1:B:3272:ILE:HB	2.19	0.41
1:B:4910:GLU:O	1:B:4914:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1432:THR:HA	1:C:1520:VAL:O	2.19	0.41
1:C:2656:CYS:HA	1:C:2711:PRO:HG3	2.02	0.41
1:C:2707:ALA:HB1	1:C:3009:TYR:HD1	1.85	0.41
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	2.01	0.41
1:D:3380:ARG:NH2	1:D:3391:GLU:OE1	2.53	0.41
1:D:4722:ARG:HE	1:D:4722:ARG:HB3	1.43	0.41
1:A:2004:GLU:HA	1:A:2007:ASN:HB2	2.02	0.41
1:A:3852:LYS:HE3	1:A:3852:LYS:HB3	1.93	0.41
1:A:4098:ASP:OD1	1:A:4098:ASP:N	2.53	0.41
1:B:39:ALA:HB2	1:B:47:CYS:HA	2.02	0.41
1:B:181:HIS:ND1	1:B:198:THR:OG1	2.40	0.41
1:B:2004:GLU:HA	1:B:2007:ASN:HB2	2.03	0.41
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.43	0.41
1:B:3169:LEU:HD23	1:B:3194:LEU:HD11	2.01	0.41
1:B:3380:ARG:NH2	1:B:3391:GLU:OE1	2.53	0.41
1:B:3592:ILE:HA	1:B:3595:ARG:HG2	2.03	0.41
1:C:39:ALA:HB2	1:C:47:CYS:HA	2.02	0.41
1:C:687:ALA:HA	1:C:713:SER:HA	2.03	0.41
1:C:880:GLU:HB3	1:C:883:ALA:HB3	2.01	0.41
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.01	0.41
1:C:3754:GLU:HB2	1:C:4718:LYS:HD3	2.02	0.41
1:C:4874:MET:HE3	1:C:4874:MET:HB3	1.86	0.41
1:D:1968:LYS:NZ	1:D:2030:ASP:OD2	2.50	0.41
1:A:4155:PRO:HG3	1:A:5036:LEU:HD23	2.02	0.41
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.93	0.41
1:B:3813:GLN:NE2	1:B:3890:LEU:O	2.53	0.41
1:C:1171:SER:OG	1:C:1175:SER:OG	2.35	0.41
1:C:1828:ASP:OD1	1:C:1828:ASP:N	2.52	0.41
1:C:3592:ILE:HA	1:C:3595:ARG:HG2	2.03	0.41
1:D:775:GLY:H	1:D:848:HIS:CE1	2.37	0.41
1:D:2656:CYS:HA	1:D:2711:PRO:HG3	2.02	0.41
1:D:3889:GLN:OE1	1:D:3960:GLN:NE2	2.53	0.41
1:A:39:ALA:HB2	1:A:47:CYS:HA	2.02	0.41
1:A:652:ARG:HB3	1:A:773:LEU:HD12	2.02	0.41
1:B:3201:MET:HA	1:B:3202:PRO:HD3	1.98	0.41
1:B:5013:MET:HE3	1:B:5021:PHE:HB3	2.03	0.41
1:C:134:ASP:OD1	1:C:134:ASP:N	2.46	0.41
1:C:265:LEU:HD13	1:C:279:PRO:HB2	2.02	0.41
1:D:2707:ALA:HB1	1:D:3009:TYR:HD1	1.85	0.41
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.80	0.41
1:A:232:THR:HG21	1:A:252:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:GLY:HA3	1:A:838:HIS:CD2	2.55	0.41
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.01	0.41
1:A:2587:TYR:O	1:A:2590:SER:OG	2.26	0.41
1:A:2961:GLN:O	1:A:2965:ARG:HG3	2.21	0.41
1:B:134:ASP:OD1	1:B:134:ASP:N	2.46	0.41
1:B:1575:LEU:HD23	1:B:1575:LEU:HA	1.95	0.41
1:B:1828:ASP:N	1:B:1828:ASP:OD1	2.52	0.41
1:B:2924:GLN:O	1:B:2928:LYS:HG2	2.21	0.41
1:B:4943:LEU:O	1:B:4947:GLN:HG2	2.21	0.41
1:C:1473:THR:HA	1:C:1487:LEU:O	2.19	0.41
1:C:3132:THR:HG23	1:C:3136:LEU:HD23	2.02	0.41
1:C:4098:ASP:OD1	1:C:4098:ASP:N	2.53	0.41
1:C:4839:MET:HE2	1:C:4839:MET:HB2	1.94	0.41
1:D:687:ALA:HA	1:D:713:SER:HA	2.03	0.41
1:D:1432:THR:HA	1:D:1520:VAL:O	2.19	0.41
1:D:2800:LYS:HB2	1:D:2800:LYS:HE2	1.89	0.41
1:D:2865:VAL:O	1:D:2928:LYS:NZ	2.48	0.41
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	2.01	0.41
2:F:26:TYR:OH	2:F:37:ASP:OD2	2.31	0.41
1:A:4044:MET:HE2	1:A:4146:LEU:HD11	2.03	0.41
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	2.02	0.41
1:B:27:THR:OG1	1:B:32:GLN:OE1	2.30	0.41
1:B:4219:PHE:O	1:B:4223:ASN:HB2	2.21	0.41
1:C:759:ILE:HG22	1:C:764:VAL:HG22	2.03	0.41
1:C:4253:GLU:OE2	1:C:4553:ASN:ND2	2.46	0.41
1:D:259:LEU:HD13	1:D:259:LEU:HA	1.95	0.41
1:D:1494:MET:HE3	1:D:1494:MET:HB2	1.67	0.41
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.01	0.41
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.86	0.41
1:A:2924:GLN:O	1:A:2928:LYS:HG2	2.21	0.41
1:A:4822:THR:HB	1:B:4839:MET:HE3	2.02	0.41
1:B:759:ILE:HG22	1:B:764:VAL:HG22	2.03	0.41
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.85	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HB2	2.56	0.41
1:B:3256:LEU:O	1:B:3259:SER:OG	2.38	0.41
1:C:2004:GLU:HA	1:C:2007:ASN:HB2	2.03	0.41
1:C:2380:ILE:HD13	1:C:2380:ILE:HA	1.96	0.41
1:C:3695:PRO:HB3	1:C:3699:HIS:CD2	2.56	0.41
1:C:3705:PHE:HA	1:C:3708:THR:HG22	2.03	0.41
1:C:3823:LYS:HA	1:C:3823:LYS:HD3	1.75	0.41
1:C:4155:PRO:HG3	1:C:5036:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4176:PRO:O	1:C:4202:ARG:NH1	2.45	0.41
1:D:414:PHE:HE1	1:D:436:LEU:HD13	1.85	0.41
1:D:3592:ILE:HA	1:D:3595:ARG:HG2	2.03	0.41
1:D:4880:MET:HE2	1:D:4880:MET:HB2	1.73	0.41
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.86	0.41
1:A:2712:PRO:O	1:A:2956:ALA:N	2.52	0.41
1:A:4943:LEU:O	1:A:4947:GLN:HG2	2.21	0.41
1:B:2472:LEU:HD23	1:B:2472:LEU:HA	1.87	0.41
1:B:2742:THR:HB	1:B:2814:LYS:HB3	2.03	0.41
1:B:4569:LEU:HD12	1:B:4569:LEU:HA	1.95	0.41
1:C:277:GLY:N	1:C:316:PHE:O	2.43	0.41
1:C:2472:LEU:HD23	1:C:2472:LEU:HA	1.87	0.41
1:C:4161:ARG:HA	1:C:4161:ARG:HD3	1.86	0.41
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.52	0.41
1:D:3509:LEU:O	1:D:3513:THR:OG1	2.30	0.41
2:G:4:ILE:HD11	2:G:66:MET:HB3	2.02	0.41
1:A:414:PHE:HE1	1:A:436:LEU:HD13	1.85	0.41
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.85	0.41
1:A:1828:ASP:OD1	1:A:1828:ASP:N	2.52	0.41
1:A:3380:ARG:NH2	1:A:3391:GLU:OE1	2.53	0.41
1:A:3695:PRO:HB3	1:A:3699:HIS:CD2	2.56	0.41
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.56	0.41
1:A:4681:LEU:HD12	1:A:4681:LEU:HA	1.87	0.41
1:B:414:PHE:HE1	1:B:436:LEU:HD13	1.85	0.41
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.86	0.41
1:B:4874:MET:HE3	1:B:4874:MET:HB3	1.86	0.41
1:C:272:SER:HA	1:C:334:MET:HE3	2.03	0.41
1:C:414:PHE:HE1	1:C:436:LEU:HD13	1.85	0.41
1:C:629:ARG:NH1	2:G:90:VAL:O	2.43	0.41
1:C:2007:ASN:O	1:C:2011:HIS:HB2	2.21	0.41
1:C:2380:ILE:HG13	1:C:2469:ILE:HD13	2.03	0.41
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	2.02	0.41
1:D:232:THR:HG21	1:D:252:VAL:HG12	2.03	0.41
1:D:2380:ILE:HG13	1:D:2469:ILE:HD13	2.03	0.41
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.86	0.41
1:D:2997:PHE:O	1:D:3001:ILE:HB	2.21	0.41
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	2.02	0.41
1:D:3695:PRO:HB3	1:D:3699:HIS:CD2	2.56	0.41
1:A:2007:ASN:O	1:A:2011:HIS:HB2	2.21	0.41
1:A:2742:THR:HB	1:A:2814:LYS:HB3	2.03	0.41
1:A:2997:PHE:O	1:A:3001:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	2.02	0.41
1:A:3592:ILE:HA	1:A:3595:ARG:HG2	2.02	0.41
1:B:687:ALA:HA	1:B:713:SER:HA	2.03	0.41
1:B:2961:GLN:O	1:B:2965:ARG:HG3	2.21	0.41
1:B:3875:MET:HE3	1:B:3875:MET:HB3	1.84	0.41
1:C:1575:LEU:HD23	1:C:1575:LEU:HA	1.95	0.41
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.56	0.41
1:C:4219:PHE:O	1:C:4223:ASN:HB2	2.21	0.41
1:D:700:GLU:N	1:D:705:ASN:OD1	2.54	0.41
1:D:897:ARG:HH21	1:D:901:LYS:HD2	1.86	0.41
1:D:1249:PRO:HA	1:D:1250:PRO:HD3	1.95	0.41
1:D:2007:ASN:O	1:D:2011:HIS:HB2	2.21	0.41
1:D:2961:GLN:O	1:D:2965:ARG:HG3	2.21	0.41
1:D:3249:LEU:HD23	1:D:3277:LEU:HD21	2.02	0.41
1:D:3705:PHE:HA	1:D:3708:THR:HG22	2.03	0.41
2:E:16:PRO:HG2	2:E:64:ALA:HA	2.03	0.41
2:H:16:PRO:HG2	2:H:64:ALA:HA	2.03	0.41
1:A:838:HIS:CE1	1:A:1201:HIS:HB2	2.56	0.40
1:A:897:ARG:HH21	1:A:901:LYS:HD2	1.86	0.40
1:A:1492:CYS:SG	1:A:1494:MET:HE2	2.61	0.40
1:A:2656:CYS:HA	1:A:2711:PRO:HG3	2.02	0.40
1:A:2902:HIS:CE1	1:A:2904:LEU:HB2	2.56	0.40
1:B:2007:ASN:O	1:B:2011:HIS:HB2	2.21	0.40
1:B:2714:TYR:O	1:B:2955:PHE:N	2.54	0.40
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.55	0.40
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.86	0.40
1:D:39:ALA:HB2	1:D:47:CYS:HA	2.02	0.40
1:D:234:SER:HB2	1:D:242:ARG:HA	2.03	0.40
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.85	0.40
1:D:1739:THR:O	1:D:1743[B]:ARG:HG3	2.21	0.40
1:D:1983:ALA:O	1:D:1987:SER:OG	2.34	0.40
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.47	0.40
1:D:4548:ARG:HE	1:D:4548:ARG:HB3	1.74	0.40
1:D:5006:GLN:H	1:D:5006:GLN:HG2	1.64	0.40
2:H:4:ILE:HD11	2:H:66:MET:HB3	2.02	0.40
1:A:2859:PRO:HA	1:A:2860:PRO:HD3	1.99	0.40
1:A:3249:LEU:HD23	1:A:3277:LEU:HD21	2.02	0.40
1:B:3695:PRO:HB3	1:B:3699:HIS:CD2	2.56	0.40
1:B:4649:LEU:HD12	1:B:4649:LEU:HA	1.95	0.40
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.56	0.40
1:C:1492:CYS:SG	1:C:1494:MET:HE2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2924:GLN:O	1:C:2928:LYS:HG2	2.21	0.40
1:C:5013:MET:HE3	1:C:5021:PHE:HB3	2.03	0.40
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.51	0.40
1:D:2004:GLU:HA	1:D:2007:ASN:HB2	2.03	0.40
1:D:4155:PRO:HG3	1:D:5036:LEU:HD23	2.02	0.40
1:D:5013:MET:HE3	1:D:5021:PHE:HB3	2.03	0.40
1:A:759:ILE:HG22	1:A:764:VAL:HG22	2.03	0.40
1:A:4090:LYS:HE2	1:A:4090:LYS:HB3	1.89	0.40
1:A:4649:LEU:HD12	1:A:4649:LEU:HA	1.95	0.40
1:B:272:SER:HA	1:B:334:MET:HE3	2.03	0.40
1:B:1492:CYS:SG	1:B:1494:MET:HE2	2.61	0.40
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.56	0.40
1:C:234:SER:HB2	1:C:242:ARG:HA	2.03	0.40
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.86	0.40
1:C:4943:LEU:O	1:C:4947:GLN:HG2	2.21	0.40
1:D:1842:LEU:HD23	1:D:1842:LEU:HA	1.96	0.40
1:D:3875:MET:HE3	1:D:3875:MET:HB3	1.84	0.40
1:D:4219:PHE:O	1:D:4223:ASN:HB2	2.21	0.40
1:D:5029:ARG:HE	1:D:5029:ARG:HB3	1.68	0.40
1:A:234:SER:HB2	1:A:242:ARG:HA	2.03	0.40
1:A:277:GLY:N	1:A:316:PHE:O	2.43	0.40
1:A:2023:LEU:HD23	1:A:2023:LEU:HA	1.93	0.40
1:A:2682:ILE:HD13	1:A:2682:ILE:HA	1.90	0.40
1:A:4722:ARG:HE	1:A:4722:ARG:HB3	1.43	0.40
1:B:2178:MET:HE3	1:B:2178:MET:HB2	1.86	0.40
1:D:3891:LEU:HB3	1:D:3899:PHE:CE2	2.56	0.40
1:D:4569:LEU:HD12	1:D:4569:LEU:HA	1.95	0.40
1:A:687:ALA:HA	1:A:713:SER:HA	2.02	0.40
1:A:1110:ARG:HE	1:A:1110:ARG:HB3	1.78	0.40
1:A:2419:GLY:O	1:A:2423:MET:HG3	2.22	0.40
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.86	0.40
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.43	0.40
1:A:3705:PHE:HA	1:A:3708:THR:HG22	2.03	0.40
1:A:4083:ASP:OD2	1:A:4085:ARG:NH2	2.47	0.40
1:A:4219:PHE:O	1:A:4223:ASN:HB2	2.21	0.40
1:A:4627:MET:HE3	1:A:4627:MET:HB2	1.76	0.40
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.40	0.40
1:B:2182:ILE:O	1:B:2186:MET:HG2	2.22	0.40
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.56	0.40
1:D:2902:HIS:CE1	1:D:2904:LEU:HB2	2.56	0.40
2:E:4:ILE:HD11	2:E:66:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:16:PRO:HG2	2:F:64:ALA:HA	2.03	0.40
2:G:16:PRO:HG2	2:G:64:ALA:HA	2.03	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	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
1	B	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
1	C	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
1	D	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
2	E	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	F	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	G	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	H	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
All	All	17840/21548 (83%)	17332 (97%)	488 (3%)	20 (0%)	49	79

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	B	3615	SER
1	C	3615	SER
1	D	3615	SER
1	A	3616	LYS
1	B	3616	LYS
1	C	3616	LYS
1	D	3616	LYS

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Mol	Chain	Res	Type
1	A	4691	GLN
1	A	4712	PRO
1	B	4691	GLN
1	B	4712	PRO
1	C	4691	GLN
1	C	4712	PRO
1	D	4691	GLN
1	D	4712	PRO
1	A	4872	PRO
1	B	4872	PRO
1	C	4872	PRO
1	D	4872	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	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
1	B	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
1	C	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
1	D	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15580/18320 (85%)	15140 (97%)	440 (3%)	38	61

All (440) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	LEU
1	A	1743[A]	ARG
1	A	1743[B]	ARG

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Mol	Chain	Res	Type
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	4180	ARG
1	A	4181	ILE
1	A	4196	GLU
1	A	4198	SER
1	A	4199	GLU
1	A	4200	THR
1	A	4202	ARG
1	A	4207	MET
1	A	4211	LYS
1	A	4213	SER
1	A	4221	VAL
1	A	4223	ASN
1	A	4227	GLU
1	A	4231	MET
1	A	4232	GLU
1	A	4543	GLU
1	A	4544	LEU
1	A	4545	GLU
1	A	4548	ARG
1	A	4549	VAL
1	A	4550	LYS
1	A	4552	LEU
1	A	4555	LEU
1	A	4557	ARG
1	A	4569	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4584	ASP
1	A	4585	SER
1	A	4587	PRO
1	A	4627	MET
1	A	4628	VAL
1	A	4634	GLU
1	A	4635	SER
1	A	4641	PRO
1	A	4647	SER
1	A	4651	THR
1	A	4658	ILE

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Mol	Chain	Res	Type
1	A	4662	ASN
1	A	4665	LYS
1	A	4666	VAL
1	A	4675	LYS
1	A	4676	GLU
1	A	4681	LEU
1	A	4684	ASP
1	A	4689	THR
1	A	4694	ASP
1	A	4695	ASP
1	A	4697	VAL
1	A	4698	LYS
1	A	4704	LEU
1	A	4707	ASN
1	A	4708	THR
1	A	4710	SER
1	A	4717	ASP
1	A	4720	VAL
1	A	4722	ARG
1	A	4725	LEU
1	A	4731	ILE
1	A	4736	ARG
1	A	4737	ILE
1	A	4743	MET
1	A	4747	SER
1	A	4748	LEU
1	A	4773	VAL
1	A	4774	LYS
1	A	4788	SER
1	A	4813	LEU
1	A	4818	MET
1	A	4820	VAL
1	A	4821	LYS
1	A	4822	THR
1	A	4823	LEU
1	A	4836	GLN
1	A	4839	MET
1	A	4844	LEU
1	A	4861	LYS
1	A	4866	SER
1	A	4871	GLU
1	A	4874	MET

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Mol	Chain	Res	Type
1	A	4875	LYS
1	A	4879	MET
1	A	4880	MET
1	A	4882	CYS
1	A	4889	VAL
1	A	4914	VAL
1	A	4953	ASP
1	A	4957	LYS
1	A	4965	SER
1	A	4966	ASP
1	A	4971	THR
1	A	4980	LEU
1	A	4985	LEU
1	A	4989	MET
1	A	4992	LEU
1	A	4997	ASN
1	A	5000	GLU
1	A	5001	THR
1	A	5013	MET
1	A	5015	GLN
1	A	5027	CYS
1	A	5034	ASP
1	A	5035	GLN
1	B	846	LEU
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	4180	ARG
1	B	4181	ILE
1	B	4196	GLU
1	B	4198	SER
1	B	4199	GLU
1	B	4200	THR
1	B	4202	ARG
1	B	4207	MET
1	B	4211	LYS
1	B	4213	SER
1	B	4221	VAL
1	B	4223	ASN

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Mol	Chain	Res	Type
1	B	4227	GLU
1	B	4231	MET
1	B	4232	GLU
1	B	4543	GLU
1	B	4544	LEU
1	B	4545	GLU
1	B	4548	ARG
1	B	4549	VAL
1	B	4550	LYS
1	B	4552	LEU
1	B	4555	LEU
1	B	4557	ARG
1	B	4569	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4584	ASP
1	B	4585	SER
1	B	4587	PRO
1	B	4627	MET
1	B	4628	VAL
1	B	4634	GLU
1	B	4635	SER
1	B	4641	PRO
1	B	4647	SER
1	B	4651	THR
1	B	4658	ILE
1	B	4662	ASN
1	B	4665	LYS
1	B	4666	VAL
1	B	4675	LYS
1	B	4676	GLU
1	B	4681	LEU
1	B	4684	ASP
1	B	4689	THR
1	B	4694	ASP
1	B	4695	ASP
1	B	4697	VAL
1	B	4698	LYS
1	B	4704	LEU
1	B	4707	ASN
1	B	4708	THR
1	B	4710	SER

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Mol	Chain	Res	Type
1	B	4717	ASP
1	B	4720	VAL
1	B	4722	ARG
1	B	4725	LEU
1	B	4731	ILE
1	B	4736	ARG
1	B	4737	ILE
1	B	4743	MET
1	B	4747	SER
1	B	4748	LEU
1	B	4773	VAL
1	B	4774	LYS
1	B	4788	SER
1	B	4813	LEU
1	B	4818	MET
1	B	4820	VAL
1	B	4821	LYS
1	B	4822	THR
1	B	4823	LEU
1	B	4836	GLN
1	B	4839	MET
1	B	4844	LEU
1	B	4861	LYS
1	B	4866	SER
1	B	4871	GLU
1	B	4874	MET
1	B	4875	LYS
1	B	4879	MET
1	B	4880	MET
1	B	4882	CYS
1	B	4889	VAL
1	B	4914	VAL
1	B	4953	ASP
1	B	4957	LYS
1	B	4965	SER
1	B	4966	ASP
1	B	4971	THR
1	B	4980	LEU
1	B	4985	LEU
1	B	4989	MET
1	B	4992	LEU
1	B	4997	ASN

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Mol	Chain	Res	Type
1	B	5000	GLU
1	B	5001	THR
1	B	5013	MET
1	B	5015	GLN
1	B	5027	CYS
1	B	5034	ASP
1	B	5035	GLN
1	C	846	LEU
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	4180	ARG
1	C	4181	ILE
1	C	4196	GLU
1	C	4198	SER
1	C	4199	GLU
1	C	4200	THR
1	C	4202	ARG
1	C	4207	MET
1	C	4211	LYS
1	C	4213	SER
1	C	4221	VAL
1	C	4223	ASN
1	C	4227	GLU
1	C	4231	MET
1	C	4232	GLU
1	C	4543	GLU
1	C	4544	LEU
1	C	4545	GLU
1	C	4548	ARG
1	C	4549	VAL
1	C	4550	LYS
1	C	4552	LEU
1	C	4555	LEU
1	C	4557	ARG
1	C	4569	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4584	ASP

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Mol	Chain	Res	Type
1	C	4585	SER
1	C	4587	PRO
1	C	4627	MET
1	C	4628	VAL
1	C	4634	GLU
1	C	4635	SER
1	C	4641	PRO
1	C	4647	SER
1	C	4651	THR
1	C	4658	ILE
1	C	4662	ASN
1	C	4665	LYS
1	C	4666	VAL
1	C	4675	LYS
1	C	4676	GLU
1	C	4681	LEU
1	C	4684	ASP
1	C	4689	THR
1	C	4694	ASP
1	C	4695	ASP
1	C	4697	VAL
1	C	4698	LYS
1	C	4704	LEU
1	C	4707	ASN
1	C	4708	THR
1	C	4710	SER
1	C	4717	ASP
1	C	4720	VAL
1	C	4722	ARG
1	C	4725	LEU
1	C	4731	ILE
1	C	4736	ARG
1	C	4737	ILE
1	C	4743	MET
1	C	4747	SER
1	C	4748	LEU
1	C	4773	VAL
1	C	4774	LYS
1	C	4788	SER
1	C	4813	LEU
1	C	4818	MET
1	C	4820	VAL

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Mol	Chain	Res	Type
1	C	4821	LYS
1	C	4822	THR
1	C	4823	LEU
1	C	4836	GLN
1	C	4839	MET
1	C	4844	LEU
1	C	4861	LYS
1	C	4866	SER
1	C	4871	GLU
1	C	4874	MET
1	C	4875	LYS
1	C	4879	MET
1	C	4880	MET
1	C	4882	CYS
1	C	4889	VAL
1	C	4914	VAL
1	C	4953	ASP
1	C	4957	LYS
1	C	4965	SER
1	C	4966	ASP
1	C	4971	THR
1	C	4980	LEU
1	C	4985	LEU
1	C	4989	MET
1	C	4992	LEU
1	C	4997	ASN
1	C	5000	GLU
1	C	5001	THR
1	C	5013	MET
1	C	5015	GLN
1	C	5027	CYS
1	C	5034	ASP
1	C	5035	GLN
1	D	846	LEU
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	4180	ARG
1	D	4181	ILE

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Mol	Chain	Res	Type
1	D	4196	GLU
1	D	4198	SER
1	D	4199	GLU
1	D	4200	THR
1	D	4202	ARG
1	D	4207	MET
1	D	4211	LYS
1	D	4213	SER
1	D	4221	VAL
1	D	4223	ASN
1	D	4227	GLU
1	D	4231	MET
1	D	4232	GLU
1	D	4543	GLU
1	D	4544	LEU
1	D	4545	GLU
1	D	4548	ARG
1	D	4549	VAL
1	D	4550	LYS
1	D	4552	LEU
1	D	4555	LEU
1	D	4557	ARG
1	D	4569	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4584	ASP
1	D	4585	SER
1	D	4587	PRO
1	D	4627	MET
1	D	4628	VAL
1	D	4634	GLU
1	D	4635	SER
1	D	4641	PRO
1	D	4647	SER
1	D	4651	THR
1	D	4658	ILE
1	D	4662	ASN
1	D	4665	LYS
1	D	4666	VAL
1	D	4675	LYS
1	D	4676	GLU
1	D	4681	LEU

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Mol	Chain	Res	Type
1	D	4684	ASP
1	D	4689	THR
1	D	4694	ASP
1	D	4695	ASP
1	D	4697	VAL
1	D	4698	LYS
1	D	4704	LEU
1	D	4707	ASN
1	D	4708	THR
1	D	4710	SER
1	D	4717	ASP
1	D	4720	VAL
1	D	4722	ARG
1	D	4725	LEU
1	D	4731	ILE
1	D	4736	ARG
1	D	4737	ILE
1	D	4743	MET
1	D	4747	SER
1	D	4748	LEU
1	D	4773	VAL
1	D	4774	LYS
1	D	4788	SER
1	D	4813	LEU
1	D	4818	MET
1	D	4820	VAL
1	D	4821	LYS
1	D	4822	THR
1	D	4823	LEU
1	D	4836	GLN
1	D	4839	MET
1	D	4844	LEU
1	D	4861	LYS
1	D	4866	SER
1	D	4871	GLU
1	D	4874	MET
1	D	4875	LYS
1	D	4879	MET
1	D	4880	MET
1	D	4882	CYS
1	D	4889	VAL
1	D	4914	VAL

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Mol	Chain	Res	Type
1	D	4953	ASP
1	D	4957	LYS
1	D	4965	SER
1	D	4966	ASP
1	D	4971	THR
1	D	4980	LEU
1	D	4985	LEU
1	D	4989	MET
1	D	4992	LEU
1	D	4997	ASN
1	D	5000	GLU
1	D	5001	THR
1	D	5013	MET
1	D	5015	GLN
1	D	5027	CYS
1	D	5034	ASP
1	D	5035	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	203	ASN
1	A	241	GLN
1	A	579	GLN
1	A	597	HIS
1	A	624	ASN
1	A	634	GLN
1	A	838	HIS
1	A	866	HIS
1	A	1058	GLN
1	A	1084	GLN
1	A	1158	ASN
1	A	1229	ASN
1	A	1281	ASN
1	A	1298	HIS
1	A	1463	ASN
1	A	1586	ASN
1	A	1590	GLN
1	A	1611	HIS
1	A	1719	HIS
1	A	1760	HIS

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Mol	Chain	Res	Type
1	A	1953	HIS
1	A	2260	ASN
1	A	2444	GLN
1	A	2734	ASN
1	A	2744	ASN
1	A	2763	HIS
1	A	2877	GLN
1	A	2881	ASN
1	A	2892	GLN
1	A	2933	ASN
1	A	3180	ASN
1	A	3313	ASN
1	A	3343	GLN
1	A	3378	GLN
1	A	3683	GLN
1	A	3766	GLN
1	A	3895	HIS
1	A	3914	ASN
1	A	4216	GLN
1	A	4558	ASN
1	A	4714	ASN
1	A	4728	HIS
1	A	4864	ASN
1	B	23	GLN
1	B	203	ASN
1	B	241	GLN
1	B	579	GLN
1	B	624	ASN
1	B	634	GLN
1	B	838	HIS
1	B	866	HIS
1	B	1058	GLN
1	B	1084	GLN
1	B	1158	ASN
1	B	1229	ASN
1	B	1298	HIS
1	B	1463	ASN
1	B	1511	HIS
1	B	1586	ASN
1	B	1590	GLN
1	B	1611	HIS
1	B	1719	HIS

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Mol	Chain	Res	Type
1	B	1760	HIS
1	B	1953	HIS
1	B	2260	ASN
1	B	2444	GLN
1	B	2734	ASN
1	B	2744	ASN
1	B	2763	HIS
1	B	2877	GLN
1	B	2881	ASN
1	B	2933	ASN
1	B	3180	ASN
1	B	3313	ASN
1	B	3343	GLN
1	B	3683	GLN
1	B	3766	GLN
1	B	3895	HIS
1	B	3897	ASN
1	B	3914	ASN
1	B	4216	GLN
1	B	4547	GLN
1	B	4558	ASN
1	B	4714	ASN
1	B	4728	HIS
1	B	4864	ASN
1	C	23	GLN
1	C	203	ASN
1	C	241	GLN
1	C	579	GLN
1	C	597	HIS
1	C	624	ASN
1	C	634	GLN
1	C	838	HIS
1	C	877	ASN
1	C	904	HIS
1	C	1084	GLN
1	C	1158	ASN
1	C	1229	ASN
1	C	1281	ASN
1	C	1298	HIS
1	C	1463	ASN
1	C	1511	HIS
1	C	1586	ASN

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Mol	Chain	Res	Type
1	C	1590	GLN
1	C	1611	HIS
1	C	1719	HIS
1	C	1760	HIS
1	C	1953	HIS
1	C	2260	ASN
1	C	2444	GLN
1	C	2734	ASN
1	C	2744	ASN
1	C	2763	HIS
1	C	2877	GLN
1	C	2881	ASN
1	C	2933	ASN
1	C	3180	ASN
1	C	3313	ASN
1	C	3343	GLN
1	C	3683	GLN
1	C	3766	GLN
1	C	3895	HIS
1	C	3914	ASN
1	C	4216	GLN
1	C	4558	ASN
1	C	4714	ASN
1	C	4728	HIS
1	C	4864	ASN
1	D	23	GLN
1	D	203	ASN
1	D	241	GLN
1	D	579	GLN
1	D	624	ASN
1	D	634	GLN
1	D	838	HIS
1	D	1058	GLN
1	D	1158	ASN
1	D	1229	ASN
1	D	1281	ASN
1	D	1298	HIS
1	D	1463	ASN
1	D	1511	HIS
1	D	1586	ASN
1	D	1590	GLN
1	D	1611	HIS

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Mol	Chain	Res	Type
1	D	1719	HIS
1	D	1760	HIS
1	D	1953	HIS
1	D	2127	GLN
1	D	2260	ASN
1	D	2444	GLN
1	D	2734	ASN
1	D	2744	ASN
1	D	2763	HIS
1	D	2877	GLN
1	D	2881	ASN
1	D	2892	GLN
1	D	2933	ASN
1	D	3007	ASN
1	D	3180	ASN
1	D	3313	ASN
1	D	3343	GLN
1	D	3378	GLN
1	D	3683	GLN
1	D	3766	GLN
1	D	3895	HIS
1	D	3897	ASN
1	D	3914	ASN
1	D	4216	GLN
1	D	4547	GLN
1	D	4558	ASN
1	D	4714	ASN
1	D	4728	HIS
1	D	4864	ASN
2	E	53	GLN
2	E	87	HIS
2	E	94	ASN
2	F	53	GLN
2	F	87	HIS
2	F	94	ASN
2	G	53	GLN
2	G	87	HIS
2	H	53	GLN
2	H	87	HIS
2	H	94	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

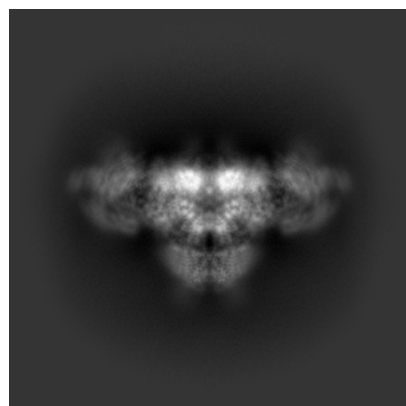
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40422. These allow visual inspection of the internal detail of the map and identification of artifacts.

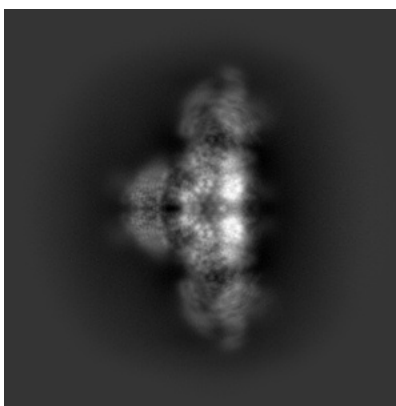
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

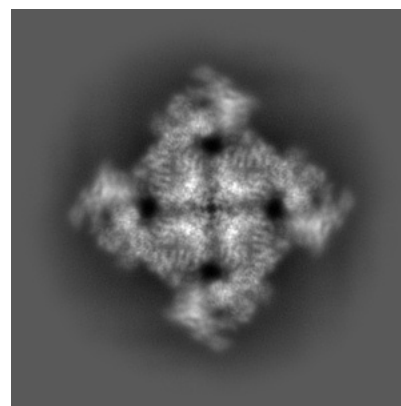
6.1.1 Primary map



X

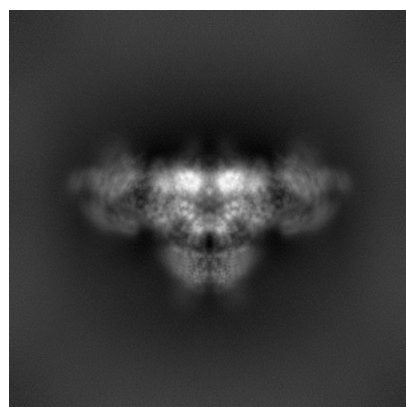


Y

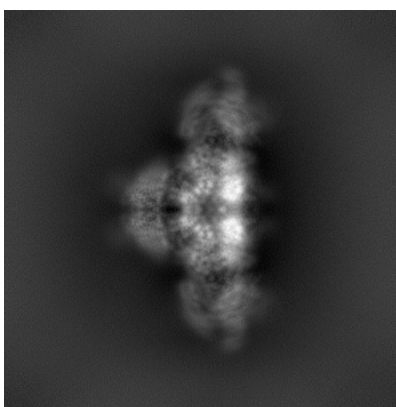


Z

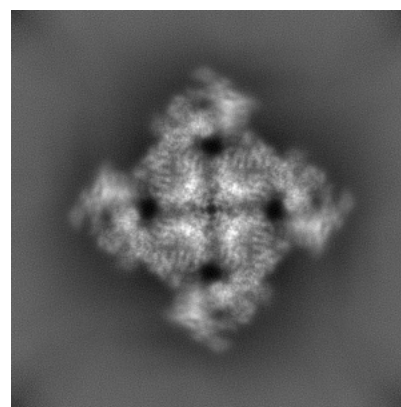
6.1.2 Raw map



X



Y

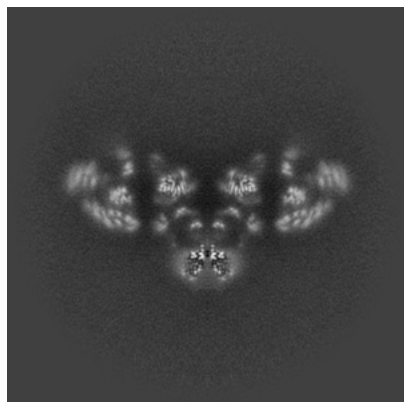


Z

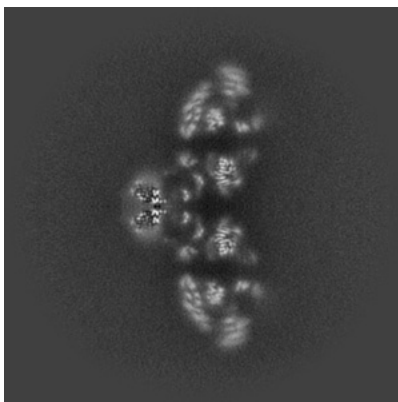
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

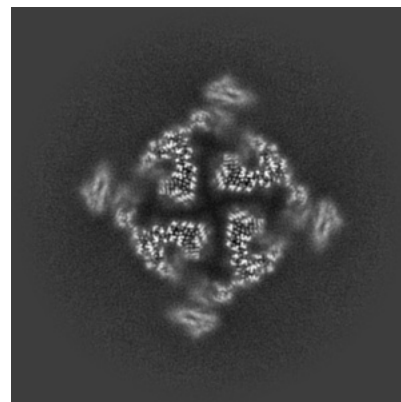
6.2.1 Primary map



X Index: 200

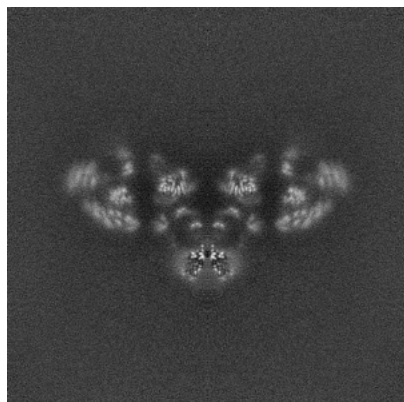


Y Index: 200

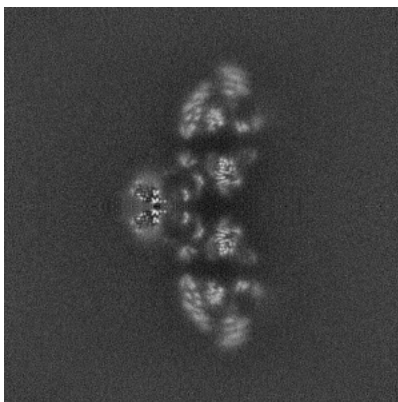


Z Index: 200

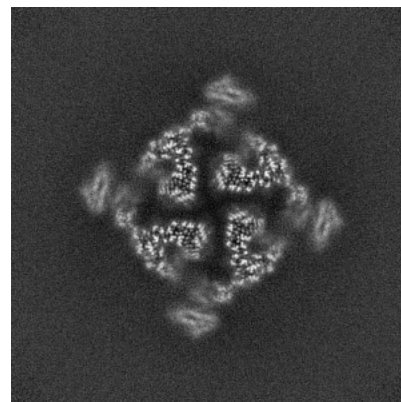
6.2.2 Raw map



X Index: 200



Y Index: 200

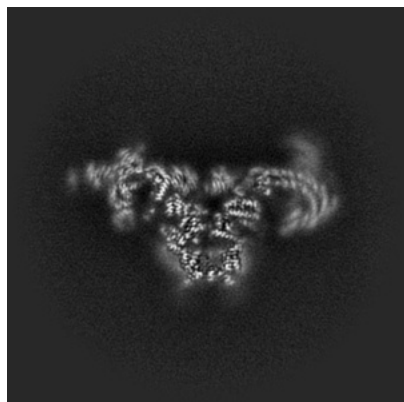


Z Index: 200

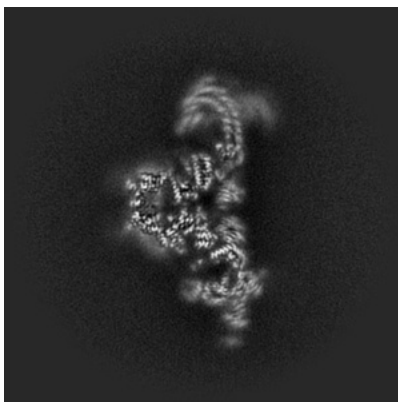
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

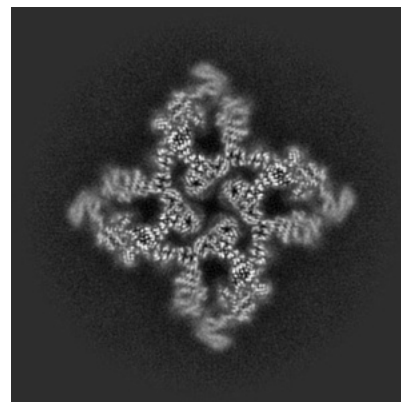
6.3.1 Primary map



X Index: 218

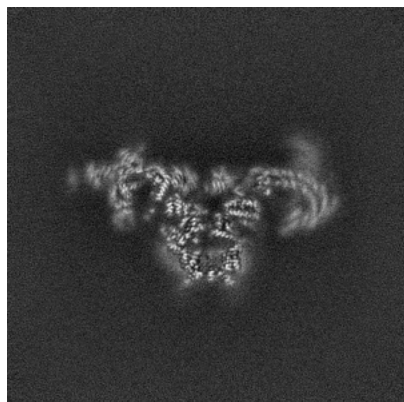


Y Index: 182

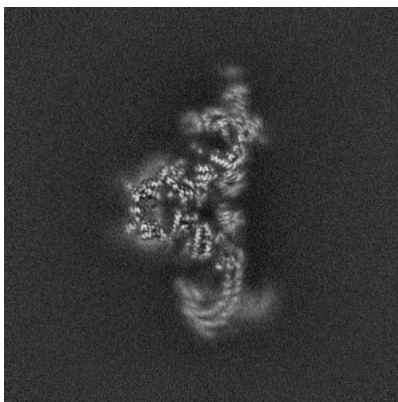


Z Index: 225

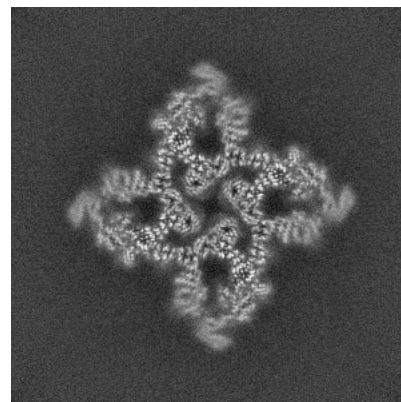
6.3.2 Raw map



X Index: 218



Y Index: 218

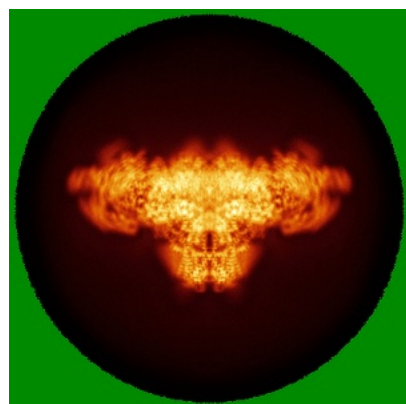


Z Index: 225

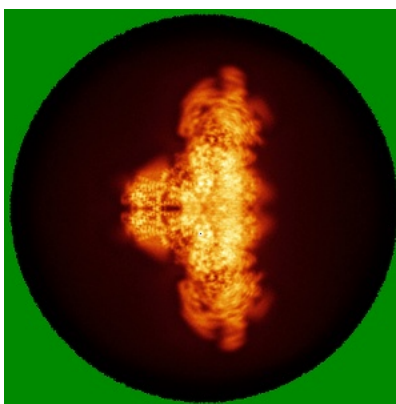
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

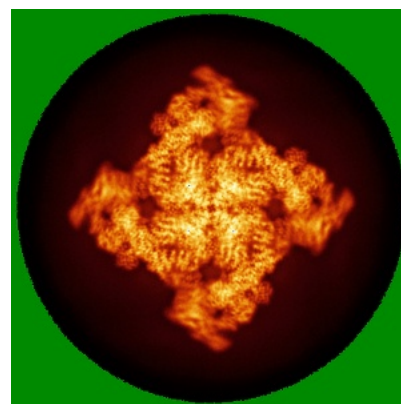
6.4.1 Primary map



X

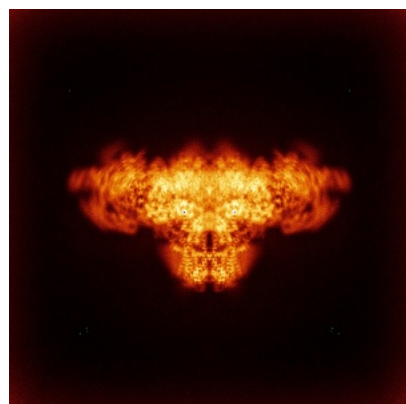


Y

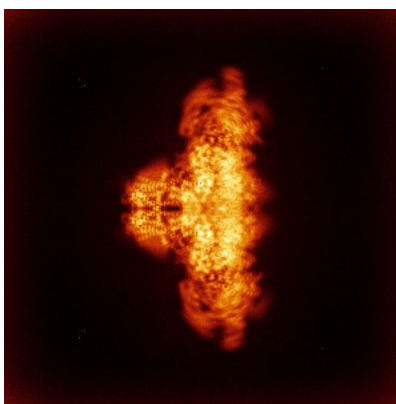


Z

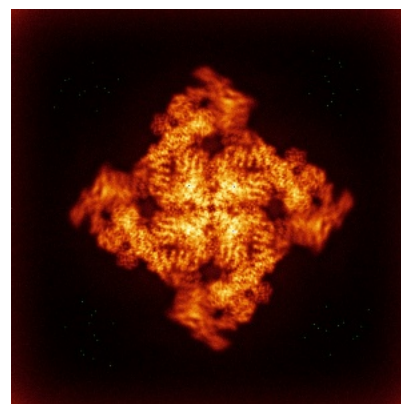
6.4.2 Raw map



X



Y

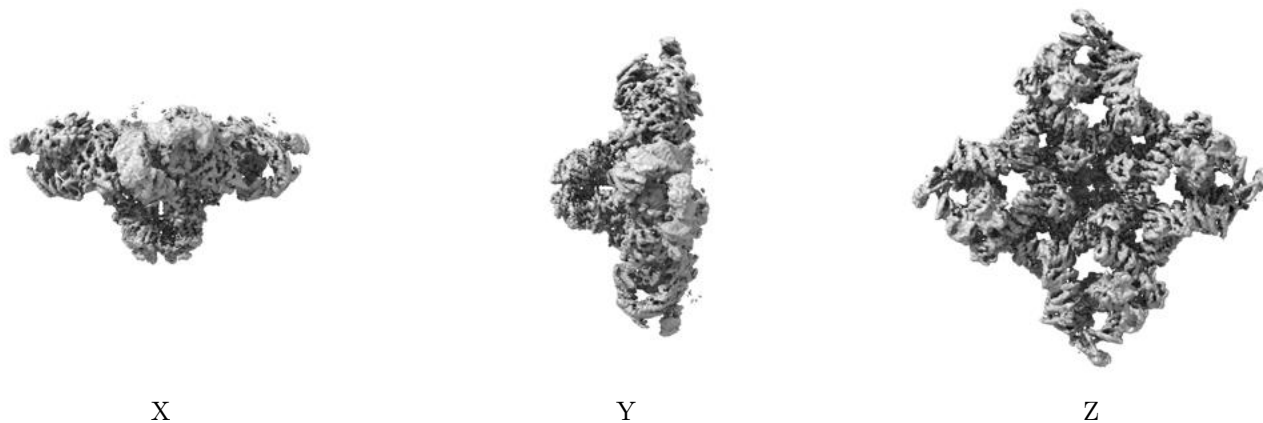


Z

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.

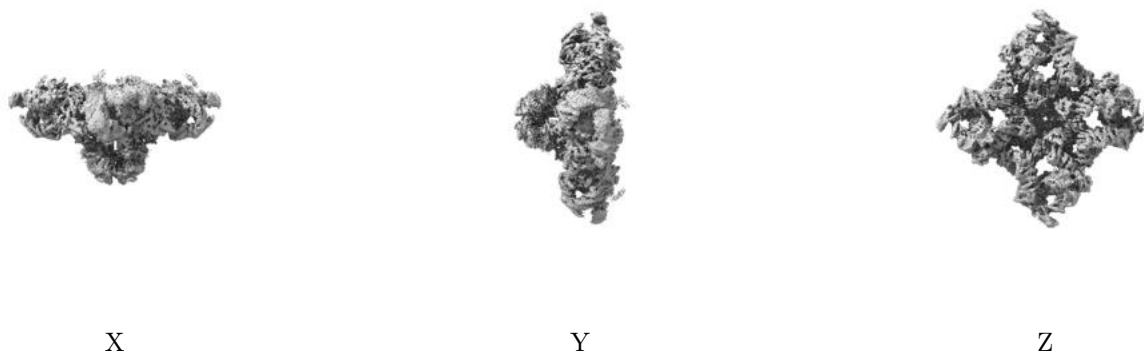
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.428. 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.

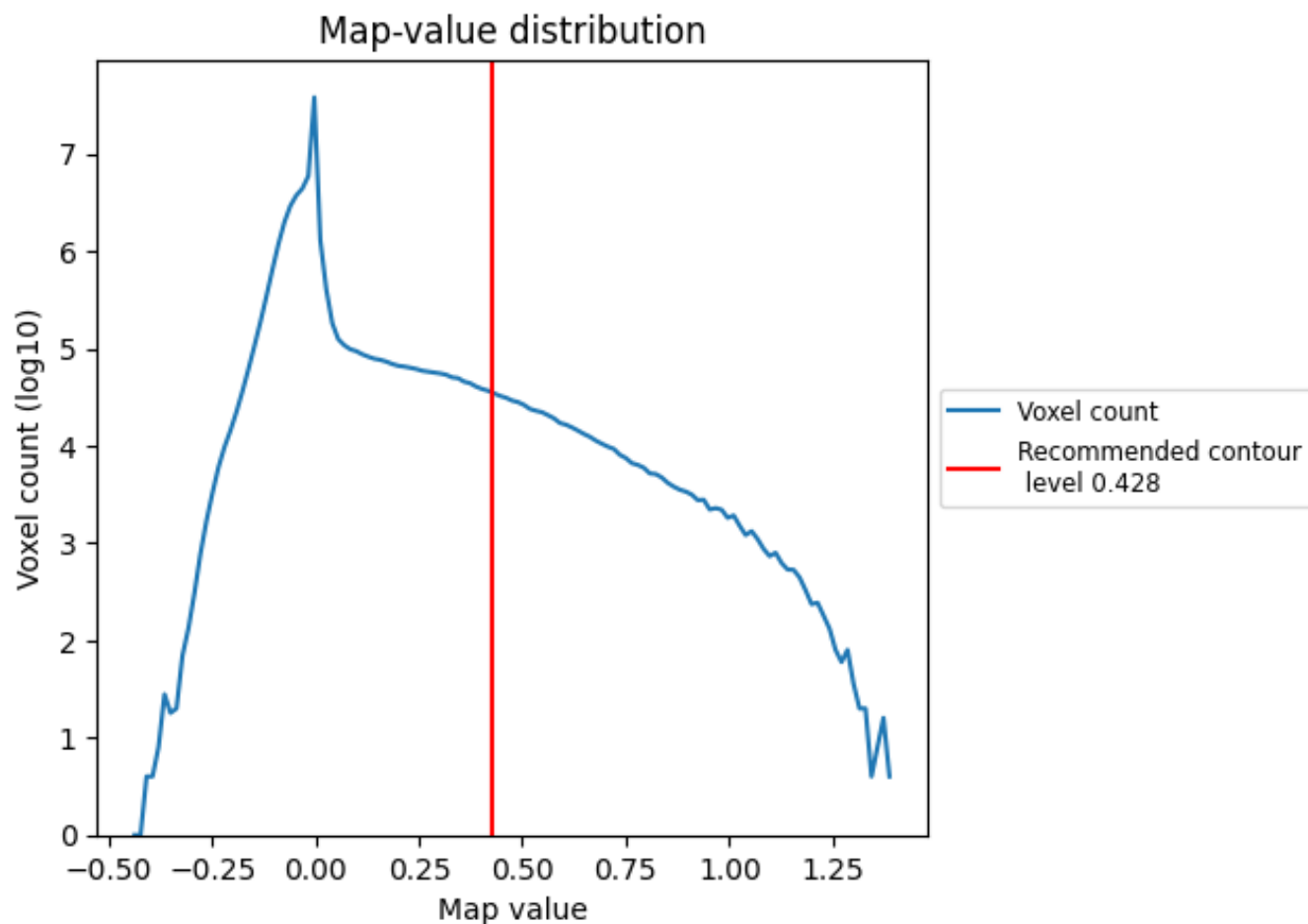
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

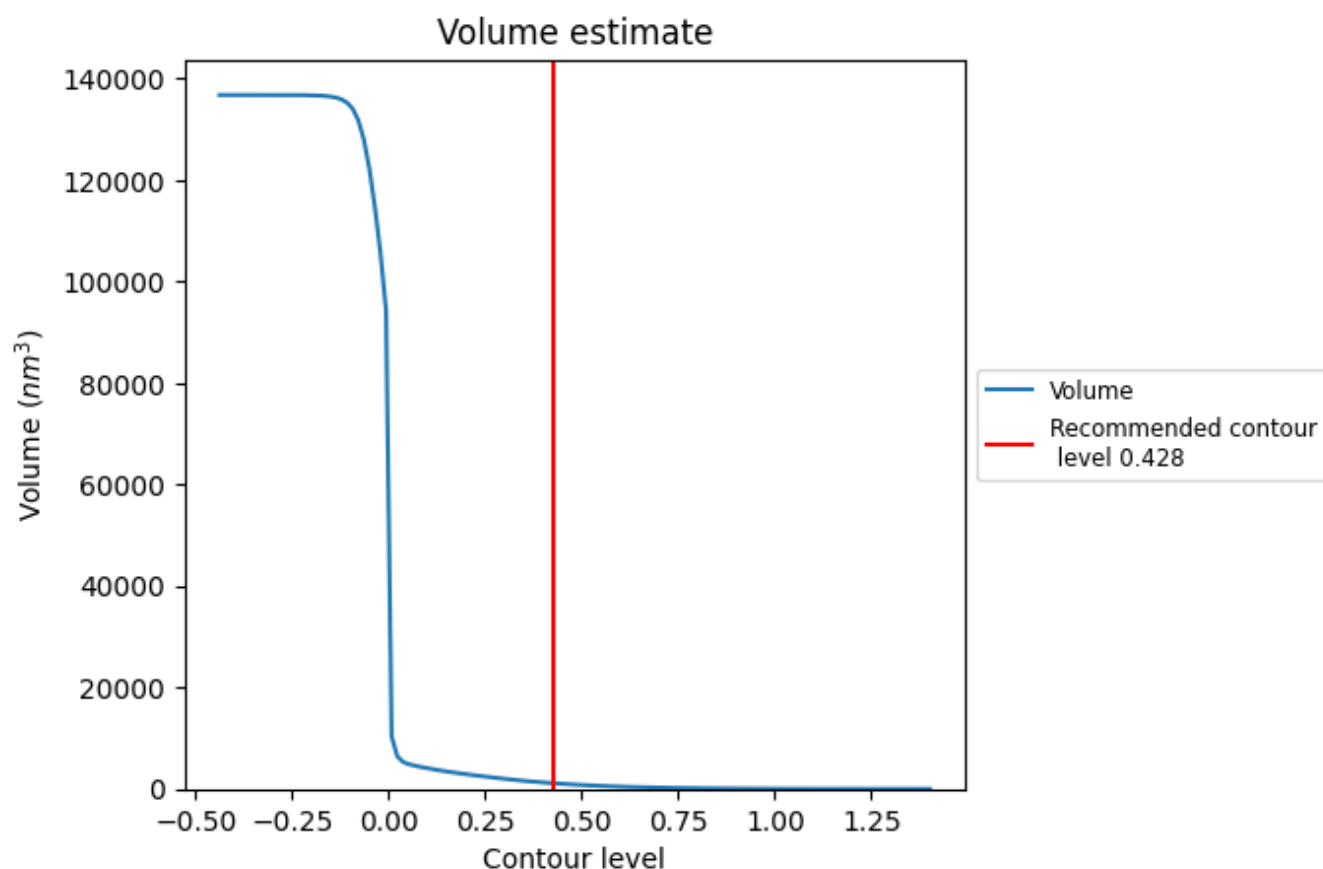
This section contains the results of statistical analysis of the map.

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.

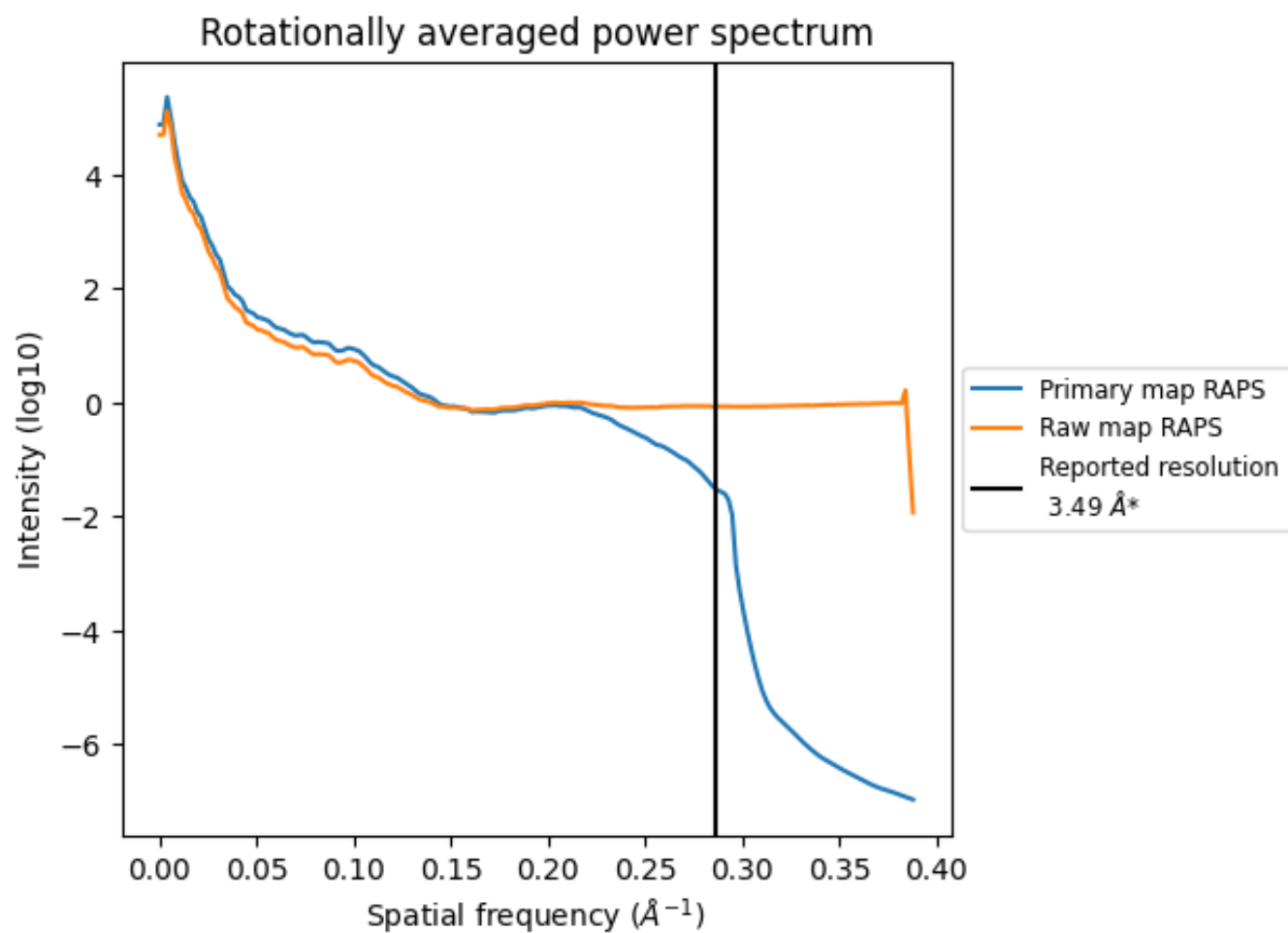
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1121 nm³; this corresponds to an approximate mass of 1013 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

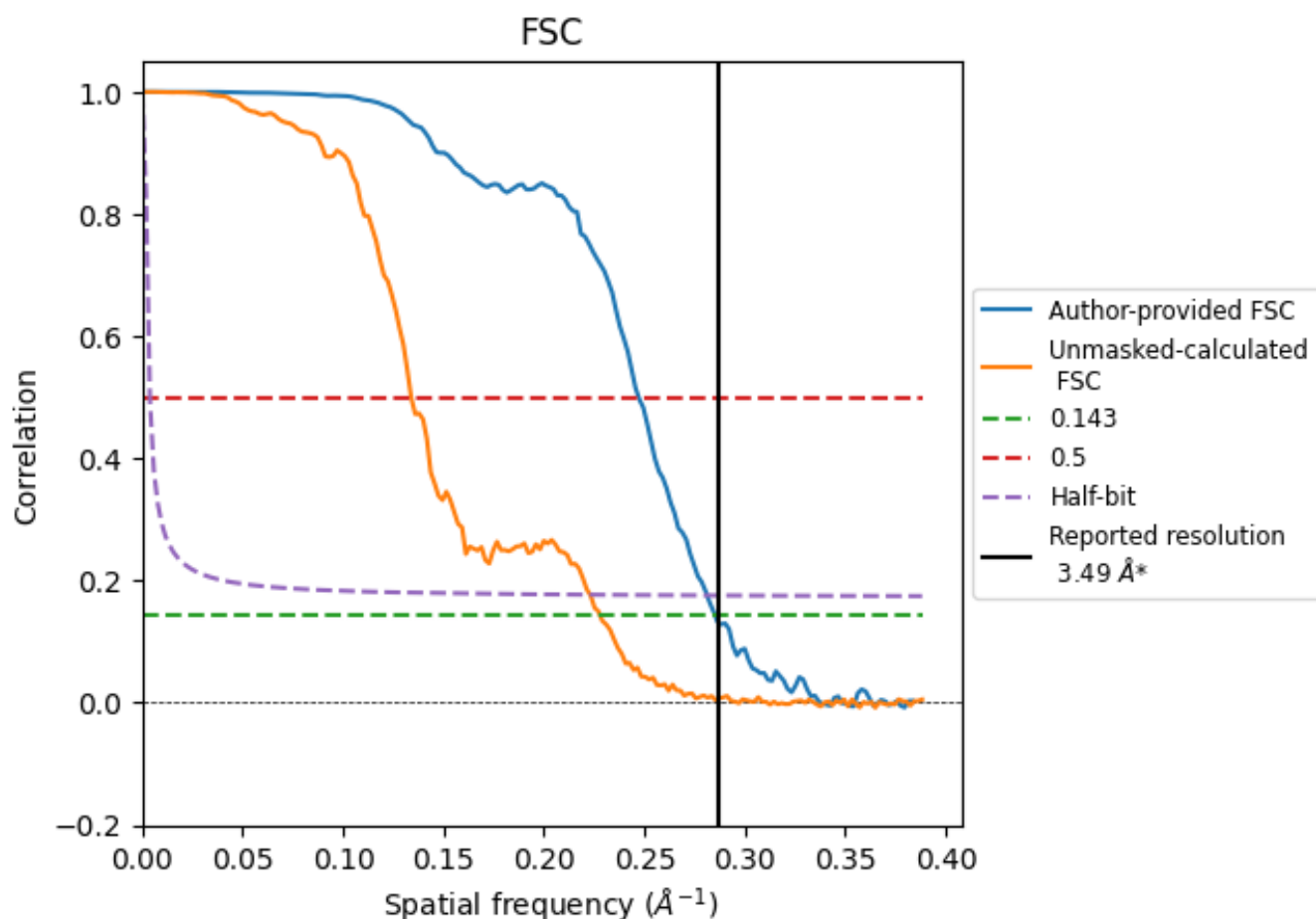


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

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 0.287 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

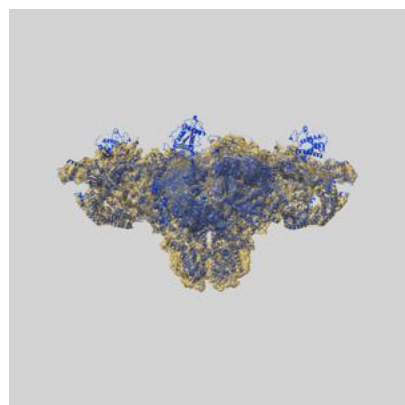
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.51	4.05	3.56
Unmasked-calculated*	4.39	7.47	4.48

*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 4.39 differs from the reported value 3.49 by more than 10 %

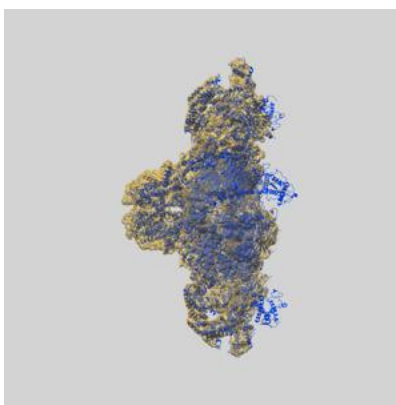
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40422 and PDB model 8SEN. Per-residue inclusion information can be found in section [3](#) on page [8](#).

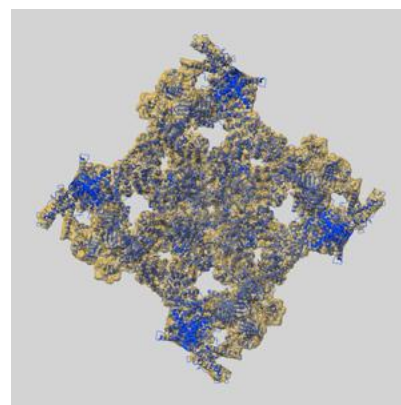
9.1 Map-model overlay [i](#)



X



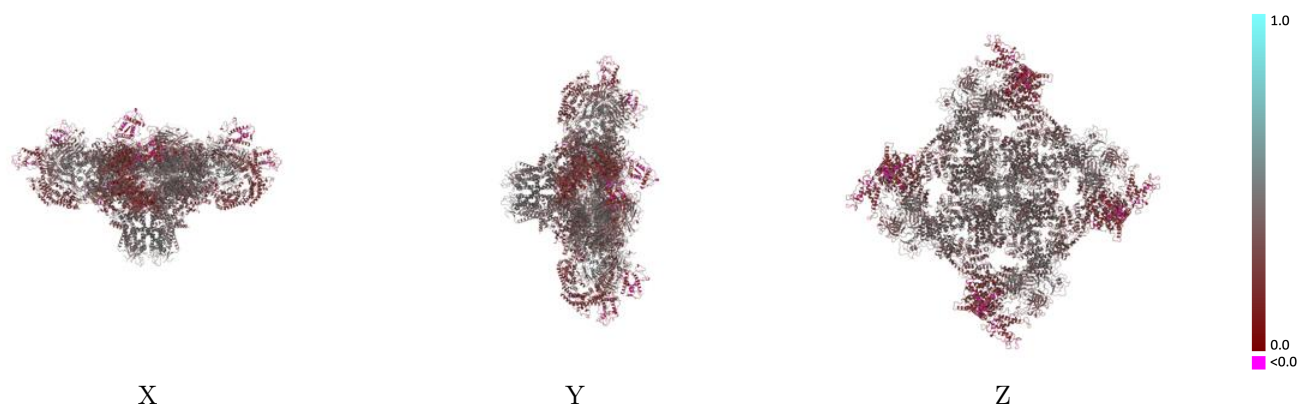
Y



Z

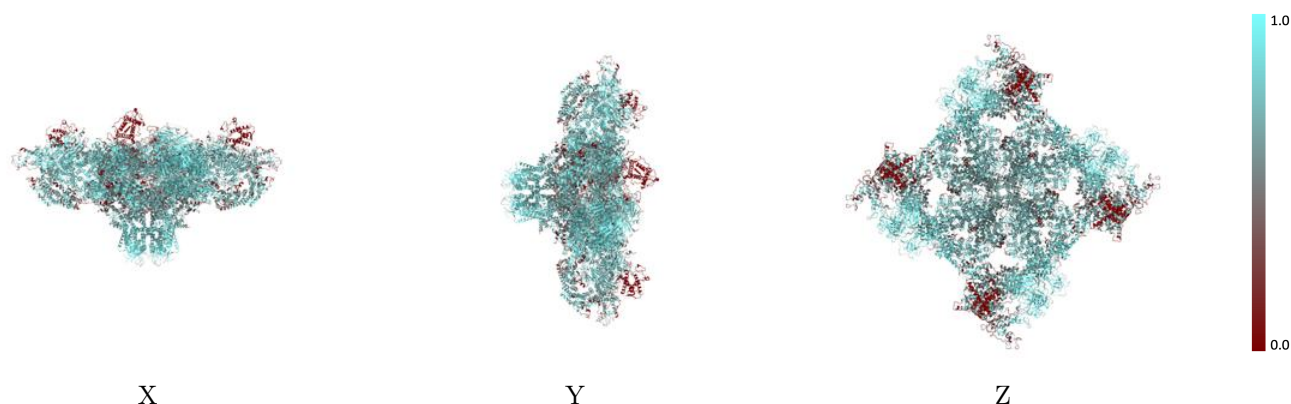
The images above show the 3D surface view of the map at the recommended contour level 0.428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



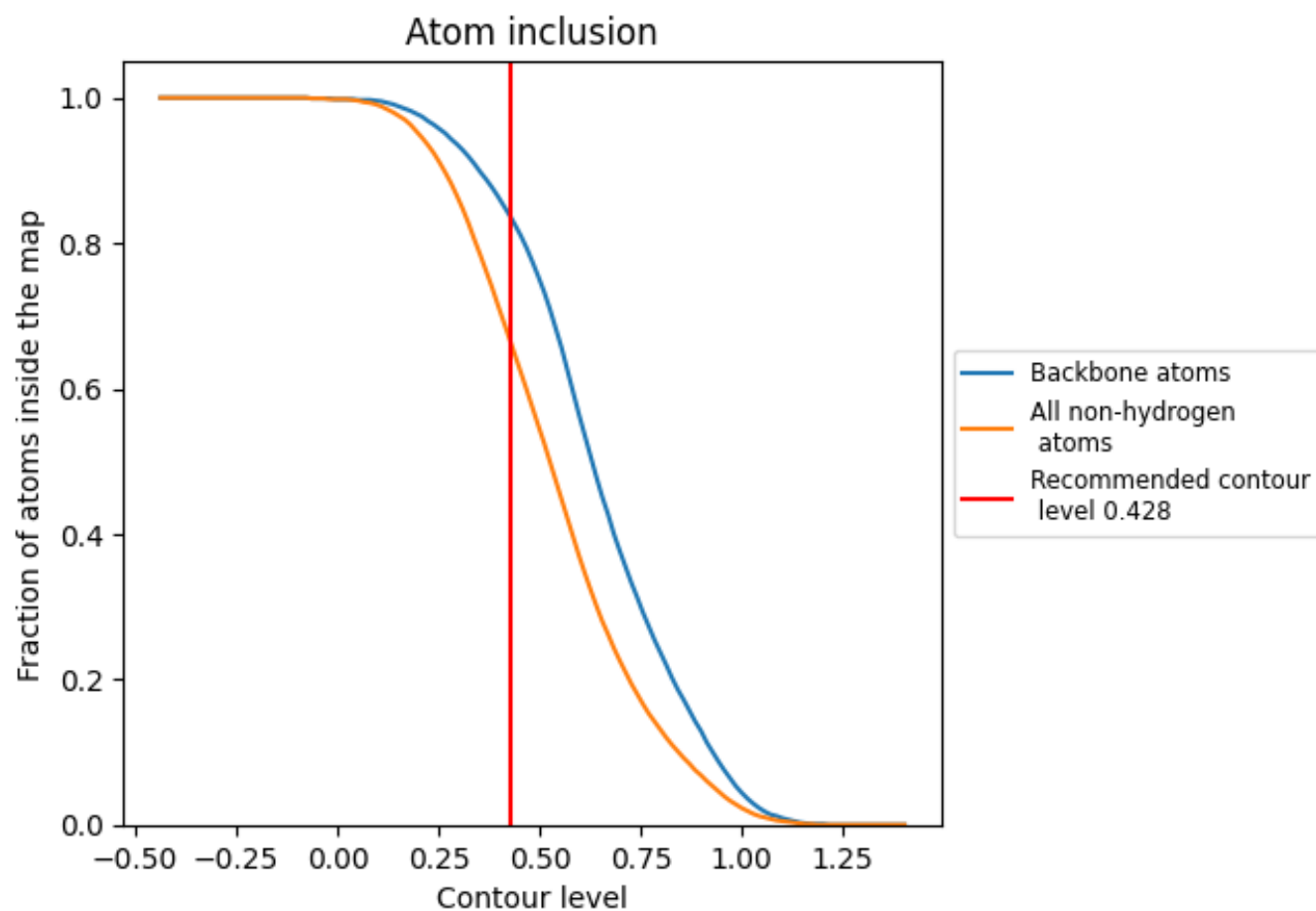
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.428).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (0.428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.3380
A	0.6600	0.3370
B	0.6600	0.3360
C	0.6600	0.3360
D	0.6600	0.3370
E	0.8210	0.4140
F	0.8210	0.4130
G	0.8210	0.4130
H	0.8210	0.4160

1.0

0.0

<0.0