



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 08:21 pm BST

PDB ID : 9S5F / pdb_00009s5f
EMDB ID : EMD-54597
Title : Apo-state RyR1 in the native membrane solved by StA
Authors : Mikirtumov, V.
Deposited on : 2025-07-31
Resolution : 4.00 Å(reported)
Based on initial model : 7tzc

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:

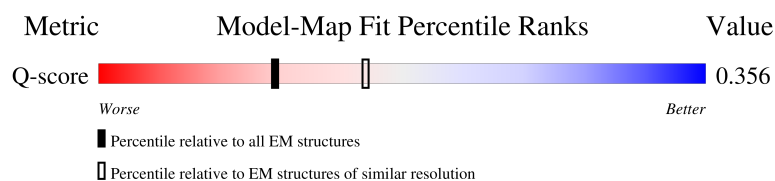
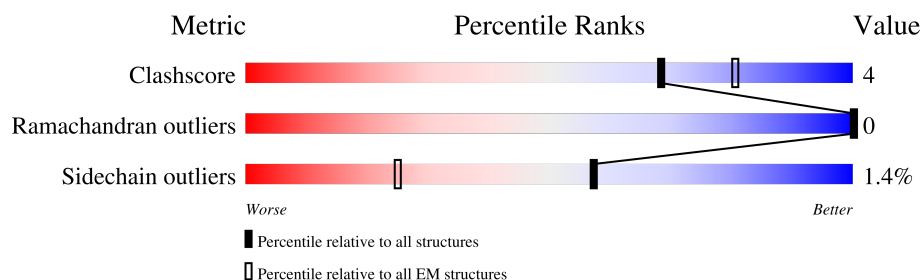
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

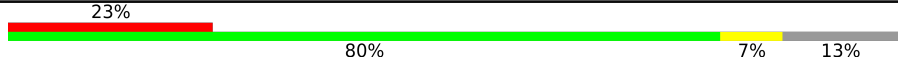
The reported resolution of this entry is 4.00 Å.

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	7587 (3.50 - 4.50)

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	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	108	 10% 83% 16%
2	F	108	 9% 82% 17%
2	G	108	 10% 84% 15%
2	H	108	 10% 86% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 285960 atoms, of which 142276 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	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

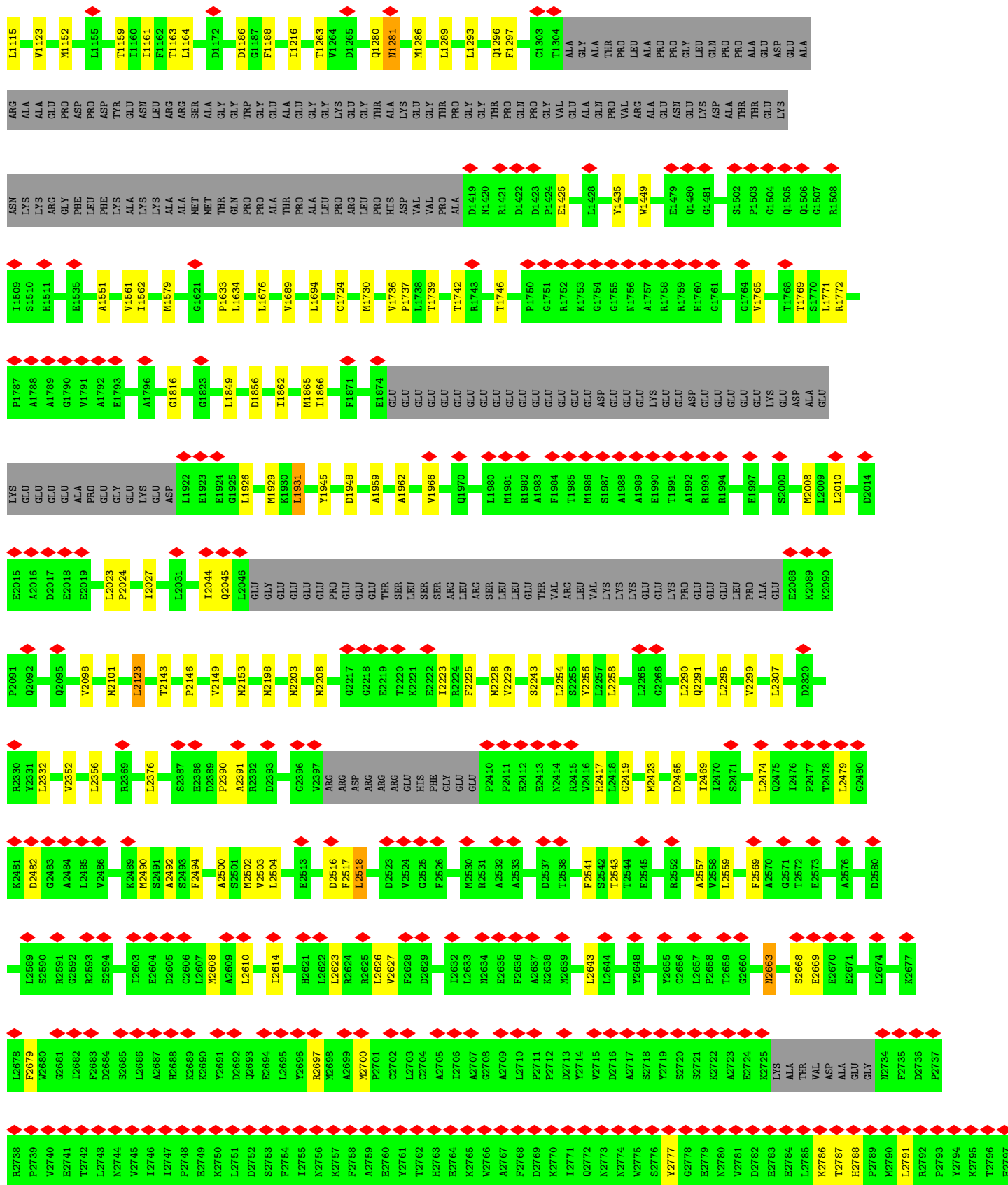
Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

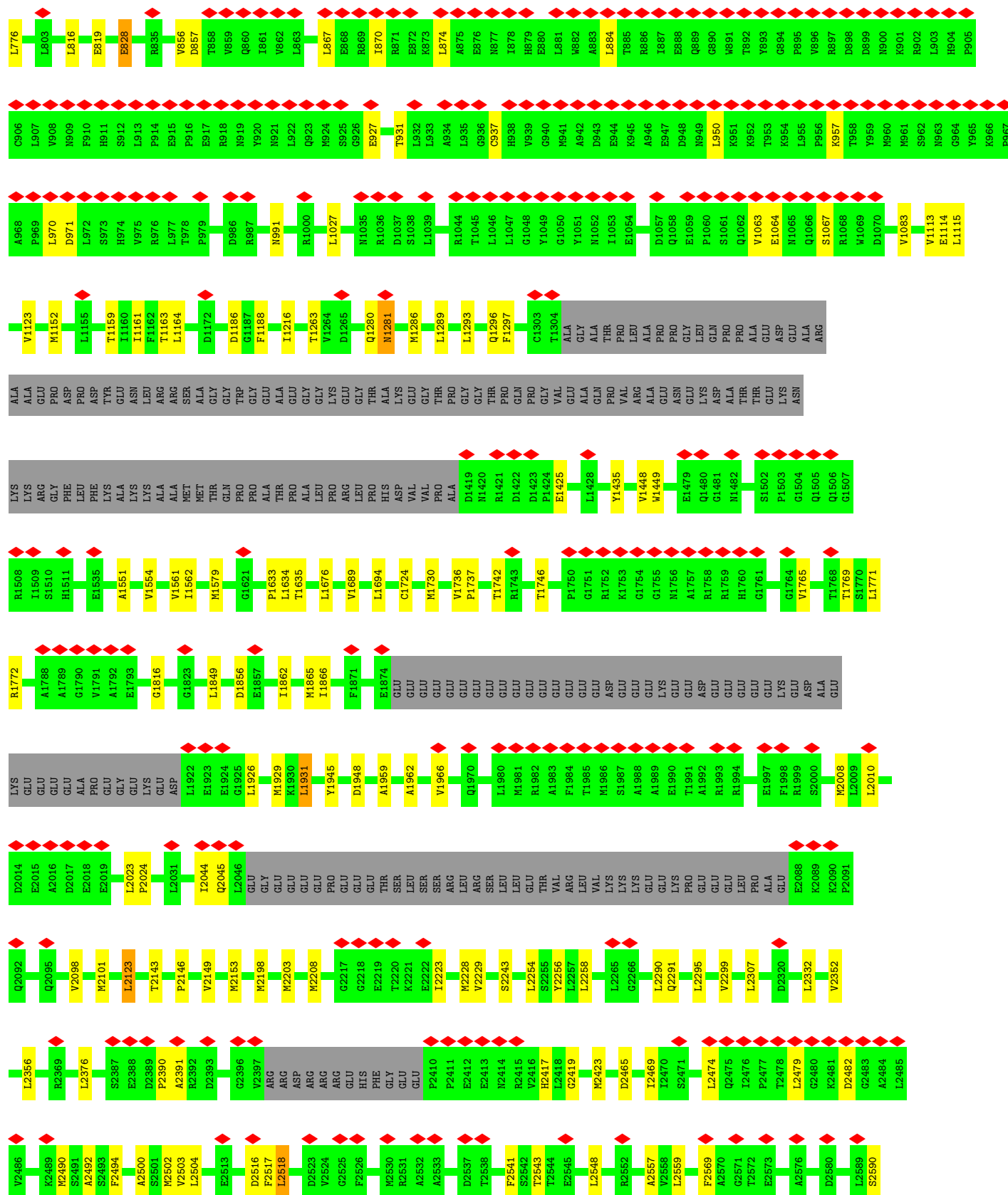
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	



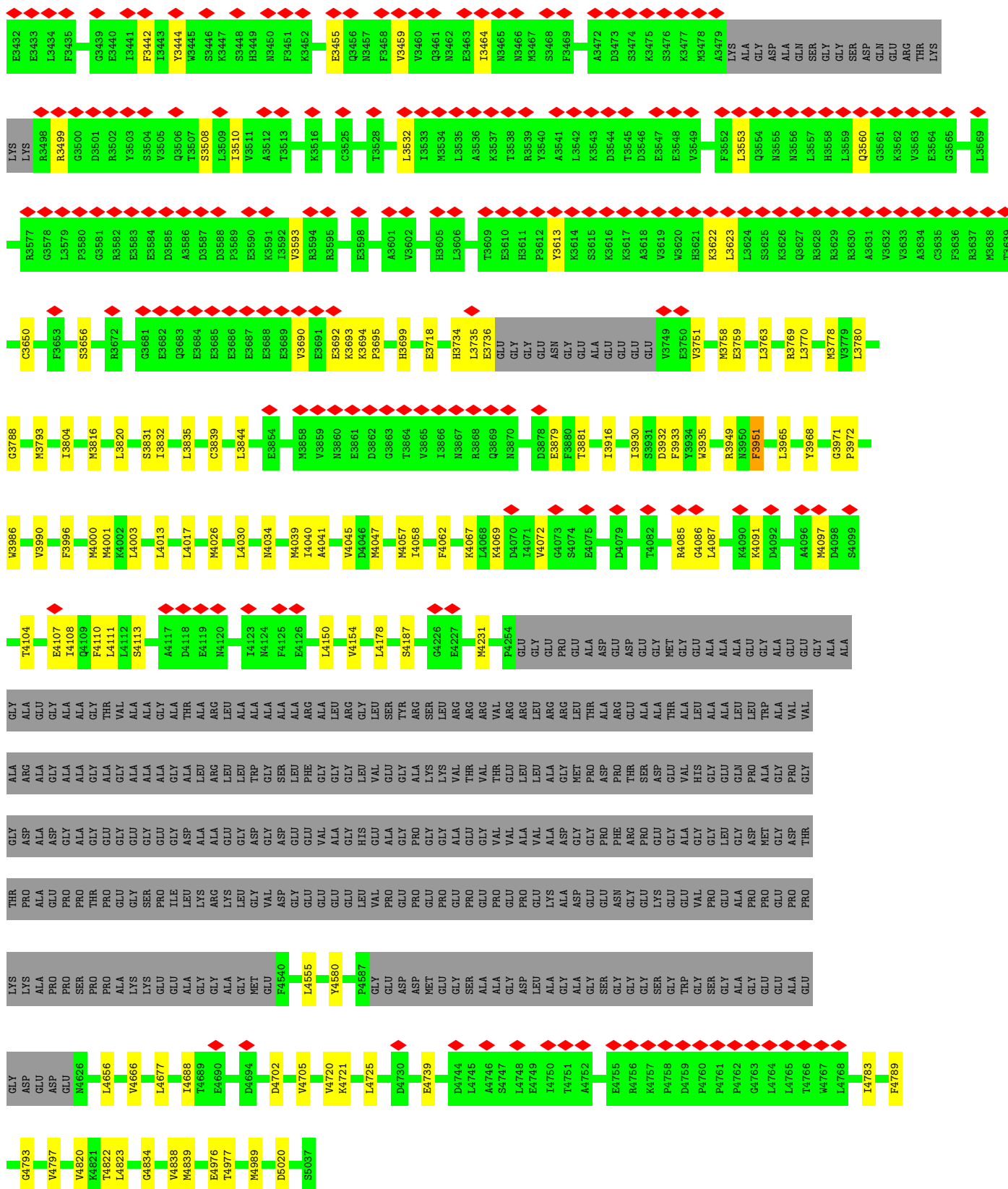
V3990	G3788	S3656	F3580	G3500	G3439	R3368	T3305	I3243	T3181	GLN	V3050	V2986
M4001	M3793	R3672	G3581	D3501	G3440	A3369	A3306	P3244	Y3182	ALA	R3051	E2987
L4002	I3804	R3672	E3582	R3502	E3441	G3370	V3307	V3245	V3183	ARG	L3056	K2988
L4003	I3804	F3442	E3583	Y3503	F3442	K3371	T3308	V3246	E3184	THR	F3057	S2989
L4013	M3816	I3443	E3584	S3504	I3443	V3372	S3309	D3247	K3185	GLN	L3056	H2990
L4017	L3820	Y3444	D3585	V3505	Y3444	A3374	D3310	K3248	L3186	VAL	F3057	H2991
L4017	L3820	G3681	A3586	Q3506	S3446	E3375	H3311	L3249	R3187		G3058	E2992
L3832	L3832	E3682	D3587	S3507	S3446	E3376	L3312	M3250	F3188		T3059	Q2993
L3835	Q3683	Q3683	D3588	T3508	K3447	E3377	S3313	A3251	A3189		D3060	E2994
M4026	Q3684	L3509	P3589	I3510	S3448	E3377	S3314	D3252	F3188		A3061	I2995
L4030	E3685	L3510	E3590	V3511	H3449	Q3378	L3315	I3253	L3190		P3062	I2996
M4034	E3686	A3512	K3591	A3512	M3450	L3379	L3316	I3253	G3191		V3065	F2997
M4039	E3687	T3513	F3592	T3513	F3451	R3380	I3319	L3256	Y3131		L3068	F2998
L4040	E3688	K3516	R3594	K3516	K3452	L3381	L3320	A3257	T3130		H3069	E2999
A4041	R3595	C3525	R3595	C3525	E3455	E3382	R3321	E3258	T3133		L3070	K3000
M4045	E3598	T3528	E3598	T3528	Q3456	A3383	T3322	S3259	V3134		L3071	I3001
M4047	A3601	L3532	A3601	L3532	F3458	K3384	V3324	G3260	A3135		A3072	L3002
D3861	V3602	L3535	V3602	L3535	V3459	A3385	T3325	A3261	L3136		R3073	L3003
G3863	H3605	M3534	H3605	M3534	V3460	E3386	N3326	R3262	L3137		S3074	P3004
T3864	L3606	L3536	L3606	L3536	Q3461	A3387	N3327	R3264	P3138		L3075	L3005
L3865	T3609	K3537	T3609	K3537	K3466	E3388	G3328	E3265	V3139		D3076	I3006
L3866	E3610	R3538	E3610	R3538	Q3467	A3389	T3329	H3268	T3141		A3077	F3010
N3867	H3611	Y3540	H3611	Y3540	K3467	E3391	D3330	I3270	T3142		R3078	T3011
R3868	P3612	A3541	P3612	A3541	S3468	L3392	K3331	E3271	L3143		T3079	N3012
Q3869	Y3613	L3542	Y3613	L3542	F3469	E3397	K3336	P3275	F3144		V3080	H3013
N3870	K3614	K3543	K3870	K3543	A3472	E3397	L3338	M3276	Q3145		M3081	C3014
D3878	S3615	D3544	D3878	D3544	D3473	F3398	L3338	L3277	L3015		K3082	L3015
F3880	K3616	T3545	F3880	T3545	A3473	S3399	A3339	C3278	Y3016		G3084	F3017
T3881	K3617	D3546	T3881	D3546	S3474	V3400	V3340	S3279	L3018		P3085	L3018
I3916	A3618	E3547	I3916	E3547	K3475	L3401	F3341	Y3280	S3019		E3086	S3019
I3930	V3619	K3476	I3930	K3476	S3477	C3402	A3342	L3281	T3020		V3087	T3020
S3931	H3620	M3478	S3931	M3478	K3477	R3403	Q3343	P3282	F3021		V3088	F3021
D3932	H3621	A3479	D3932	A3479	M3478	D3404	P3344	L3282	A3022		K3089	A3022
W3935	K3622	L3623	W3935	L3623	A3479	L3405	P3345	R3283	V3024		G3091	K3023
Y3936	L3624	S3625	Y3936	L3624	LYS	Y3406	V3346	W3284	L3025		L3092	L3025
R3949	S3625	Q3554	R3949	Q3554	ALA	A3407	V3346	W3284	G3026		F3095	G3026
N3950	K3626	N3555	N3950	N3555	GLY	L3408	S3347	E3286	S3027		F3096	S3027
F3951	Q3627	N3556	F3951	N3556	ASP	L3408	R3348	R3287	G3028		A3099	G3028
L3965	R3628	L3557	L3965	L3557	ALA	Y3409	A3349	G3288	G3029		S3100	G3029
L3965	R3629	H3558	L3965	H3558	GLN	P3410	R3350	P3289	H3030		E3101	H3030
Y3968	R3630	L3559	Y3968	L3559	SER	L3411	P3351	E3290	S3032		D3102	S3032
G3971	A3631	Q3560	G3971	Q3560	GLY	L3412	E3352	A3291	H3033		I3103	H3033
P3972	V3632	G3561	P3972	G3561	GLY	L3413	E3352	P3292	E3037		I3103	E3037
W3986	A3634	K3562	W3986	K3562	THR	R3414	L3353	P3293	K3038		I3104	K3038
	F3635	V3563		V3563	LYS	Y3415	H3357	P3294	I3039		K3105	I3039
	F3636	G3564		G3564	LYS	Y3416	T3359	A3295	T3040		M3106	T3040
	F3637	G3565		G3565	LYS	L3424	T3361	R3299	S3041		V3107	S3041
	K3638	L3569		L3569	LYS	N3428	R3364	A3300	L3042		R3110	L3042
	T3639	R3577		R3577	LYS	A3429	L3366	E3237	F3043		R3111	F3043
	C3650	G3578		G3578	LYS	N3430	R3366	P3301	C3044		L3112	C3044
	F3653	L3579		L3579	LYS	L3434	R3367	P3302	K3045		K3114	K3045
						F3435		C3304	A3048		V3115	A3048
									L3049		S3116	L3049



[illegible]

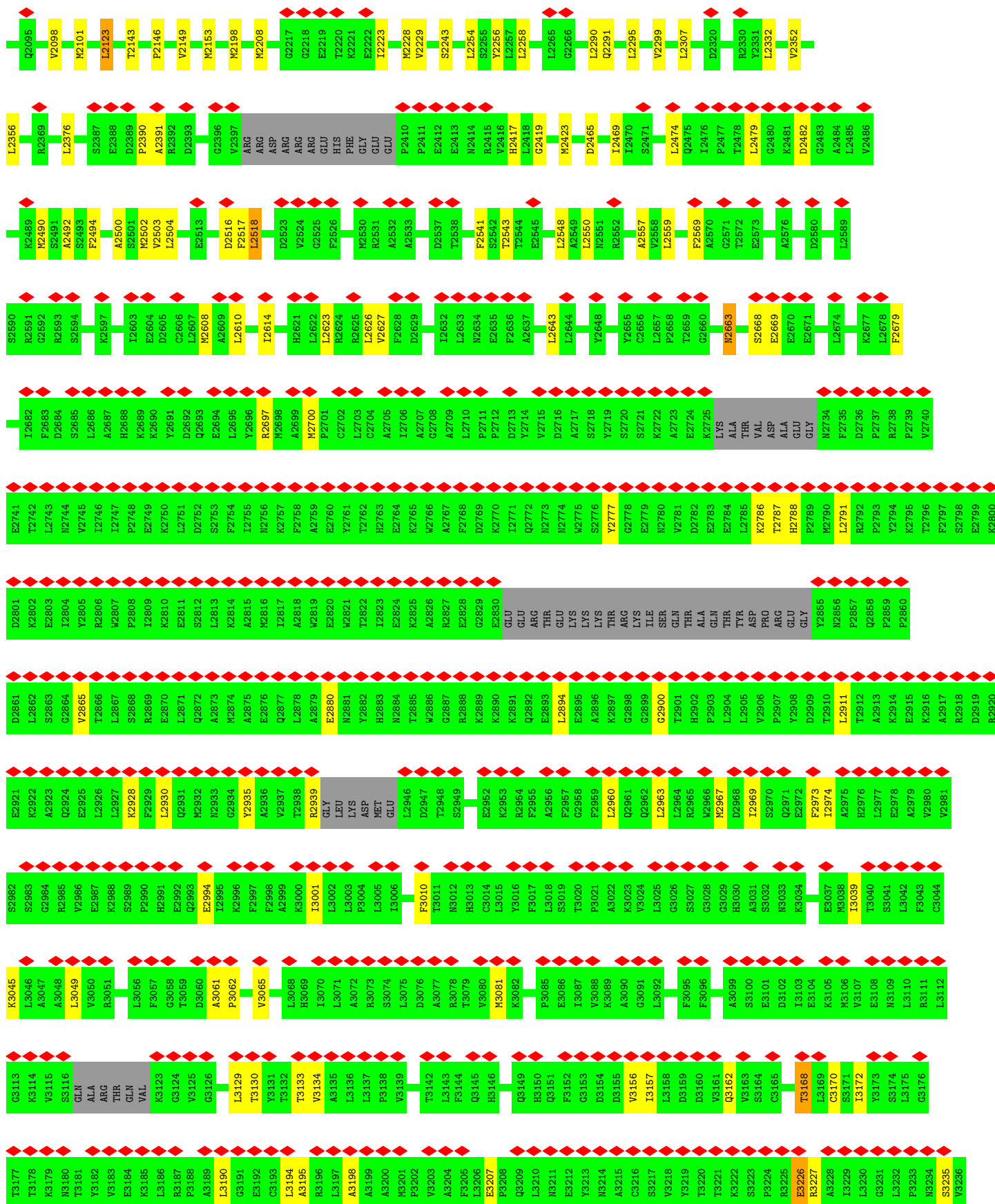


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P3301	P3302	P3303	C3304	T3305	A3306	V3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316											I3319	L3320	R3321	I3322	I3323	V3324	N3325	N3326	L3327	G3328	I3329	D3330	E3331	A3332	L3333	W3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	A3349	P3350	P3351	E3352	L3353	L3354											H3357	F3358	I3359	P3360	T3361																																					
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L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126											L3129	T3130	Y3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	T3142	L3143	F3144	Q3145	H3146											Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	V3161	Q3162	V3163	S3164	C3165											T3168	L3169	C3170	S3171	I3172	Y3173	S3174																											
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L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126											L3129	T3130	Y3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	T3142	L3143	F3144	Q3145	H3146											Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	V3161	Q3162	V3163	S3164	C3165											T3168	L3169	C3170	S3171	I3172	Y3173	S3174																											
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P3301	P3302	P3303	C3304	T3305	A3306	V3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316											I3319	L3320	R3321	I3322	I3323	V3324	N3325	N3326	L3327	G3328	I3329	D3330	E3331	A3332	L3333	W3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	A3349	P3350	P3351	E3352	L3353	L3354											H3357	F3358	I3359	P3360	T3361																																					
R3364	L3365	R3366	K3367	R3368	A3369	G3370	K3371	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3405	A3406	A3407	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	Y3415	V3416	L3424	N3428	A3429	N3430	A3431																																																									

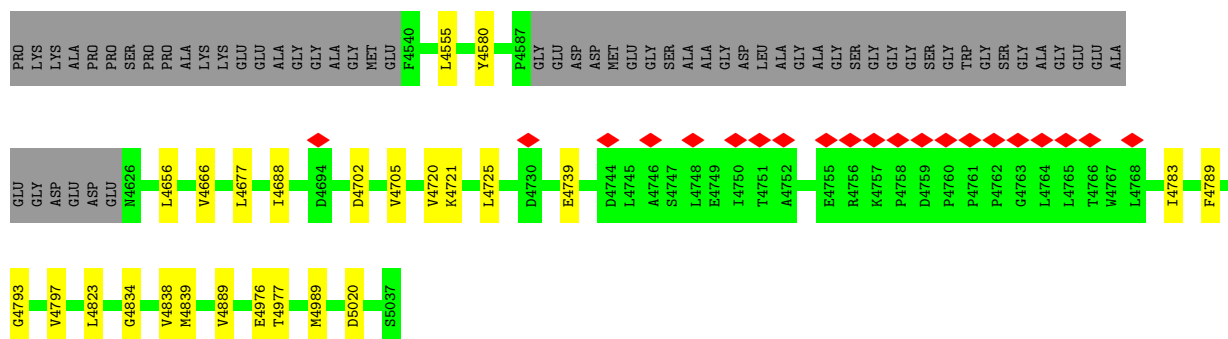


- Molecule 1: Ryanodine receptor 1

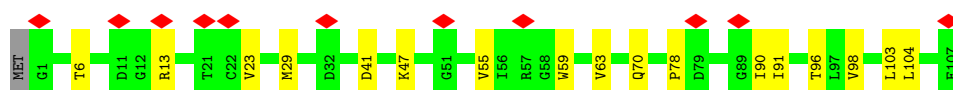
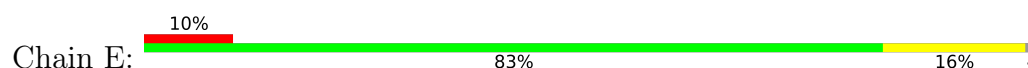




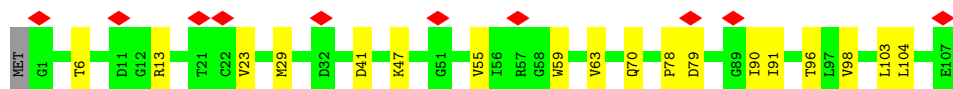
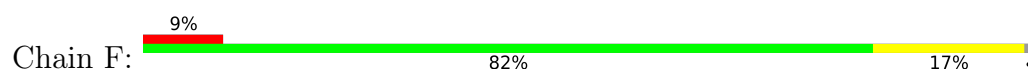
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PRO	PRO	ASP	ALA	ARG	ALA	PRO	PRO	E4107	F9996	T3804	S3656	L3579	R3499	L3434	L3365	P3303	E3238
PRO	PRO	ASP	ALA	GLY	ALA	PRO	PRO	M4109	M4000	M3816	K3679	G3581	D3501	G3439	R3367	T3305	M3239
PRO	PRO	GLY	ALA	ALA	ALA	PRO	PRO	F4110	M4001	L3820	A3680	G3582	R3502	E3440	R3368	A3306	C3241
PRO	PRO	GLY	ALA	THR	GLY	PRO	PRO	L4111	K4002	L3820	A3681	E3583	R3503	E3441	R3369	A3307	C3242
GLU	GLU	GLY	ALA	VAL	VAL	PRO	PRO	L4112	L4003	S3831	G3682	E3584	S3504	I3441	G3370	S3308	I3243
GLY	GLY	GLY	ALA	VAL	VAL	PRO	PRO	S4113	L4013	T3832	E3683	D3585	R3505	F4442	R3371	S3309	F3244
SER	SER	ALA	ALA	ALA	ALA	PRO	PRO	L4117	L4017	L3835	Q3683	D3587	R3506	I3443	R3372	D3310	V3245
PRO	PRO	GLY	ALA	GLY	GLY	PRO	PRO	L4118	L4017	L3835	Q3684	D3588	R3507	Y3444	L3246	H3311	L3246
ILE	ILE	GLY	GLY	ALA	ALA	PRO	PRO	E4119	M4026	C3839	E3685	F3588	L3508	W3445	D3247	L3312	D3247
LYS	LYS	ASP	ALA	THR	ALA	PRO	PRO	M4120	M4026	L3844	E3686	F3589	I3510	S3446	R3248	N3313	R3248
ARG	ARG	ALA	ALA	ALA	ALA	PRO	PRO	L4123	L4030	L3844	E3687	E3590	V3511	S3447	R3249	S3314	L3249
LYS	LYS	ALA	ARG	ARG	ALA	PRO	PRO	E4126	L4030	L3844	E3688	K3591	A3512	H3448	R3250	L3315	K3250
GLY	GLY	ALA	ALA	ALA	ALA	PRO	PRO	M4034	M4034	F3854	E3689	V3593	T3513	R3451	K3251	L3316	K3251
GLY	GLY	ALA	ALA	ALA	ALA	PRO	PRO	M4039	M4039	M3858	V3690	K3594	K3516	R3380	L3253	I3319	I3252
VAL	VAL	GLY	GLY	ALA	ALA	PRO	PRO	A4041	A4041	R3859	E3691	R3595	C3525	L3381	L3256	L3320	L3256
GLY	GLY	ASP	ALA	ALA	ALA	PRO	PRO	V4045	V4045	M3860	E3692	E3598	G3528	E3382	A3257	R3321	L3256
GLY	GLY	VAL	PHE	ARG	ALA	PRO	PRO	D4046	D4046	E3861	K3693	E3598	E3456	E3383	E3258	I3322	A3257
ALA	ALA	GLY	GLY	ALA	ALA	PRO	PRO	M4047	M4047	D3862	K3694	V3598	Q3456	E3384	S3259	V3324	E3258
GLY	GLY	ALA	GLY	ALA	ALA	PRO	PRO	Y4177	Y4177	G3863	P3695	E3598	V3459	K3385	S3260	N3325	G3260
VAL	VAL	GLY	VAL	ALA	ALA	PRO	PRO	L4178	L4058	T3864	H3699	V3602	L3532	E3386	A3261	N3326	G3260
GLY	GLY	VAL	GLY	ALA	ALA	PRO	PRO	S4187	S4187	V3865	E3718	L3606	L3532	E3387	R3262	L3327	A3261
PRO	PRO	PRO	ALA	ALA	ALA	PRO	PRO	F4082	F4082	I3866	E3718	L3606	L3532	E3388	R3262	G3328	R3262
GLY	GLY	GLY	LYS	SER	ALA	PRO	PRO	K4087	K4087	R3867	H3734	T3609	T3633	E3388	R3263	G3329	R3263
PRO	PRO	GLY	LYS	ALA	ALA	PRO	PRO	L4088	L4088	R3868	L3735	E3610	M3534	E3389	T3264	D3330	T3264
PRO	PRO	GLY	VAL	ALA	ALA	PRO	PRO	K4089	K4089	Q3869	E3736	H3611	A3536	E3390	R3265	E3331	R3265
PRO	PRO	VAL	THR	ALA	ALA	PRO	PRO	D4070	D4070	N3870	GLY	P3612	R3539	L3392	R3266	D3332	R3266
VAL	VAL	VAL	THR	ALA	ALA	PRO	PRO	V4072	V4072	D3878	GLY	K3614	A3541	L3393	R3267	A3332	R3267
VAL	VAL	VAL	THR	ALA	ALA	PRO	PRO	G4073	G4073	E3879	ASN	K3614	L3542	L3394	R3268	A3333	R3268
LYS	LYS	ALA	ALA	ALA	ALA	PRO	PRO	S4074	S4074	F3880	GLY	K3615	R3542	R3395	R3269	I3270	R3269
ALA	ALA	ALA	ALA	ALA	ALA	PRO	PRO	E4075	E4075	T3881	ALA	K3616	R3544	D3396	R3271	I3272	R3271
ASP	ASP	GLY	MET	LEU	LEU	PRO	PRO	D4079	D4079	I3916	ALA	K3617	D3544	E3397	R3272	I3273	R3272
GLY	GLY	GLY	PRO	THR	THR	PRO	PRO	Y4080	Y4080	T3930	GLY	K3618	T3545	F3398	L3274	L3274	L3274
PRO	PRO	PHE	ASP	ALA	ALA	PRO	PRO	V4081	V4081	S3931	GLY	A3618	R3546	S3399	F3275	F3275	F3275
GLY	GLY	THR	THR	GLY	GLY	PRO	PRO	T4082	T4082	D3932	GLY	V3619	E3547	R3401	R3276	R3276	R3276
LYS	LYS	SER	SER	ALA	ALA	PRO	PRO	Y3934	Y3934	F3933	GLY	W3620	E3547	L3401	L3277	L3277	L3277
GLY	GLY	ASP	ASP	ALA	ALA	PRO	PRO	MET	MET	T3935	V3749	H3621	E3548	A3342	C3278	C3278	C3278
THR	THR	THR	THR	THR	THR	PRO	PRO	R4085	R4085	Y3936	V3751	K3622	R3549	Q3343	R3402	R3402	R3402
ALA	ALA	ALA	ALA	ALA	ALA	PRO	PRO	G4086	G4086	R3949	M3758	L3623	F3552	D3404	R3403	R3403	R3403
VAL	VAL	ALA	VAL	ALA	ALA	PRO	PRO	L4087	L4087	E3759	L3553	L3624	L3553	L3405	R3404	I3345	R3283
GLY	GLY	GLY	HIS	LEU	LEU	PRO	PRO	K4090	K4090	K3950	GLY	S3625	Q3554	Y3406	V3346	V3346	V3284
GLY	GLY	GLY	GLY	ALA	ALA	PRO	PRO	F3951	F3951	L3763	ASP	K3626	N3555	A3407	S3347	S3347	W3284
ALA	ALA	ALA	GLN	LEU	LEU	PRO	PRO	L3965	L3965	R3769	N3556	Q3627	N3556	L3408	R3348	R3348	W3285
PRO	PRO	ASP	PRO	LEU	LEU	PRO	PRO	D4092	D4092	L3770	R3628	R3628	L3557	L3409	A3349	A3349	E3286
PRO	PRO	MET	ALA	THR	THR	PRO	PRO	M4096	M4096	M3778	R3629	R3629	H3558	Y3409	R3350	R3350	R3287
GLY	GLY	GLY	GLY	ALA	ALA	PRO	PRO	A4097	A4097	V3779	R3630	R3630	L3559	P3410	R3351	P3351	E3290
ASP	ASP	ASP	GLY	GLY	GLY	PRO	PRO	D4098	D4098	L3780	Q3560	V3632	Q3561	L3411	A3291	A3291	A3291
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO	S4099	S4099	G3788	K3562	V3633	K3562	L3412	P3292	P3292	P3292
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO				V3563	V3633	V3563	L3413	F3293	F3293	F3293
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO				E3564	V3633	E3564	R3414	P3294	P3294	P3294
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO				G3565	V3633	G3565	V3415	A3295	A3295	A3295
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO				L3569	V3633	L3569	THR	L3296	L3296	L3296
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO				R3577	V3633	R3577	LYS	F3297	F3297	F3297
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO					T3639		LYS	A3300	A3300	A3300
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO							LYS	F3301	F3301	F3301
PRO	PRO	ASP	PRO	ALA	ALA	PRO	PRO							LYS	E3432	E3432	E3432



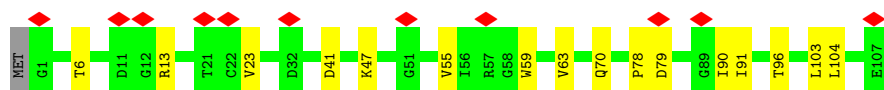
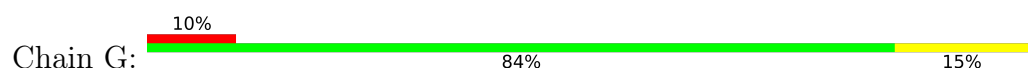
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



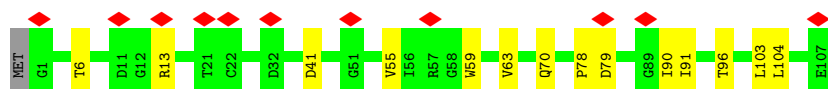
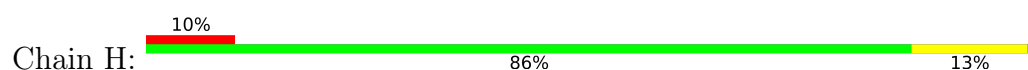
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of subtomograms used	13726	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 ($e^-/\text{\AA}^2$)	132	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	64000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	5.530	Depositor
Minimum map value	0.000	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.181	Depositor
Recommended contour level	0.779	Depositor
Map size (Å)	409.80002, 409.80002, 409.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/35885	0.27	0/48603
1	B	0.10	0/35885	0.27	0/48603
1	C	0.10	0/35885	0.27	0/48603
1	D	0.10	0/35885	0.27	0/48603
2	E	0.14	0/851	0.32	0/1146
2	F	0.13	0/851	0.31	0/1146
2	G	0.13	0/851	0.31	0/1146
2	H	0.13	0/851	0.31	0/1146
All	All	0.10	0/146944	0.27	0/198996

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35088	34740	34715	258	0
1	B	35088	34740	34715	261	0
1	C	35088	34740	34715	262	0
1	D	35088	34740	34715	265	0
2	E	832	829	831	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	832	829	831	12	0
2	G	832	829	831	11	0
2	H	832	829	831	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	143684	142276	142184	1070	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 4.

All (1070) 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:D:2503:VAL:HG11	1:D:2557:ALA:HB1	1.62	0.81
1:B:2503:VAL:HG11	1:B:2557:ALA:HB1	1.61	0.81
1:C:2503:VAL:HG11	1:C:2557:ALA:HB1	1.62	0.80
1:A:2503:VAL:HG11	1:A:2557:ALA:HB1	1.61	0.80
1:D:2307:LEU:O	1:D:2307:LEU:HD23	1.83	0.78
1:A:2307:LEU:HD23	1:A:2307:LEU:O	1.83	0.78
1:C:2307:LEU:HD23	1:C:2307:LEU:O	1.83	0.77
1:B:2307:LEU:O	1:B:2307:LEU:HD23	1.84	0.77
1:D:2610:LEU:HD22	1:D:2614:ILE:HD11	1.69	0.75
1:A:2610:LEU:HD22	1:A:2614:ILE:HD11	1.69	0.74
1:C:2610:LEU:HD22	1:C:2614:ILE:HD11	1.69	0.74
1:B:2610:LEU:HD22	1:B:2614:ILE:HD11	1.69	0.74
1:A:4001:MET:HG3	1:A:4057:MET:HE2	1.70	0.73
1:B:4001:MET:HG3	1:B:4057:MET:HE2	1.70	0.73
1:B:334:MET:HE3	1:B:334:MET:HA	1.71	0.73
1:A:334:MET:HE3	1:A:334:MET:HA	1.71	0.73
1:C:4001:MET:HG3	1:C:4057:MET:HE2	1.70	0.72
1:D:4001:MET:HG3	1:D:4057:MET:HE2	1.70	0.72
1:D:2518:LEU:HD21	1:D:2569:PHE:HE2	1.55	0.71
1:C:334:MET:HE3	1:C:334:MET:HA	1.70	0.71
1:A:2518:LEU:HD21	1:A:2569:PHE:HE2	1.55	0.71
1:D:3010:PHE:CZ	1:D:3039:ILE:HD12	2.26	0.71
1:D:334:MET:HA	1:D:334:MET:HE3	1.70	0.71
1:A:3010:PHE:CZ	1:A:3039:ILE:HD12	2.26	0.71
1:C:2518:LEU:HD21	1:C:2569:PHE:HE2	1.55	0.71
1:B:3010:PHE:CZ	1:B:3039:ILE:HD12	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3010:PHE:CZ	1:C:3039:ILE:HD12	2.26	0.70
1:C:4555:LEU:HD11	1:C:4656:LEU:HD12	1.73	0.70
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.74	0.70
1:B:2518:LEU:HD21	1:B:2569:PHE:HE2	1.55	0.70
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.74	0.70
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.74	0.70
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.74	0.69
2:H:90:ILE:HG22	2:H:91:ILE:HG13	1.75	0.69
2:F:90:ILE:HG22	2:F:91:ILE:HG13	1.74	0.69
1:A:4555:LEU:HD11	1:A:4656:LEU:HD12	1.73	0.69
1:D:4555:LEU:HD11	1:D:4656:LEU:HD12	1.73	0.69
2:G:90:ILE:HG22	2:G:91:ILE:HG13	1.74	0.69
1:B:4555:LEU:HD11	1:B:4656:LEU:HD12	1.73	0.68
2:E:90:ILE:HG22	2:E:91:ILE:HG13	1.74	0.68
1:A:2543:THR:HG22	1:A:2543:THR:O	1.95	0.66
1:C:2543:THR:HG22	1:C:2543:THR:O	1.95	0.66
1:A:2098:VAL:HG13	1:A:2123:LEU:HD21	1.78	0.66
1:A:3168:THR:O	1:A:3172:ILE:HD12	1.96	0.66
1:B:2543:THR:O	1:B:2543:THR:HG22	1.95	0.65
1:C:3168:THR:O	1:C:3172:ILE:HD12	1.96	0.65
1:D:2543:THR:HG22	1:D:2543:THR:O	1.95	0.65
1:C:3133:THR:HG23	1:C:3134:VAL:HG23	1.79	0.65
1:D:3168:THR:O	1:D:3172:ILE:HD12	1.96	0.65
1:B:3133:THR:HG23	1:B:3134:VAL:HG23	1.79	0.65
1:B:3168:THR:O	1:B:3172:ILE:HD12	1.96	0.65
1:B:2098:VAL:HG13	1:B:2123:LEU:HD21	1.78	0.65
1:C:2098:VAL:HG13	1:C:2123:LEU:HD21	1.78	0.64
1:A:3133:THR:HG23	1:A:3134:VAL:HG23	1.79	0.64
1:D:3133:THR:HG23	1:D:3134:VAL:HG23	1.79	0.64
1:A:3780:LEU:HD13	1:A:3820:LEU:CD2	2.29	0.63
1:D:2098:VAL:HG13	1:D:2123:LEU:HD21	1.78	0.63
1:D:4041:ALA:O	1:D:4045:VAL:HG23	1.99	0.63
1:B:3780:LEU:HD13	1:B:3820:LEU:CD2	2.29	0.63
1:A:4041:ALA:O	1:A:4045:VAL:HG23	1.99	0.63
1:B:4041:ALA:O	1:B:4045:VAL:HG23	1.99	0.63
1:C:4041:ALA:O	1:C:4045:VAL:HG23	1.99	0.62
1:D:3780:LEU:HD13	1:D:3820:LEU:CD2	2.29	0.62
1:B:2010:LEU:HD12	1:B:3656:SER:HB3	1.82	0.62
1:D:2010:LEU:HD12	1:D:3656:SER:HB3	1.82	0.62
1:A:2010:LEU:HD12	1:A:3656:SER:HB3	1.82	0.62
1:C:3780:LEU:HD13	1:C:3820:LEU:CD2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HG21	1:B:202:MET:CE	2.30	0.61
1:A:20:VAL:HG21	1:A:202:MET:CE	2.31	0.61
1:C:2010:LEU:HD12	1:C:3656:SER:HB3	1.82	0.61
1:C:2623:LEU:O	1:C:2627:VAL:HG23	2.01	0.61
1:D:3455:GLU:O	1:D:3459:VAL:HG23	2.01	0.61
1:D:4069:LYS:O	1:D:4072:VAL:HG22	2.01	0.61
1:A:4069:LYS:O	1:A:4072:VAL:HG22	2.01	0.61
1:B:3455:GLU:O	1:B:3459:VAL:HG23	2.01	0.61
1:D:20:VAL:HG21	1:D:202:MET:CE	2.31	0.61
1:B:970:LEU:HD23	1:B:971:ASP:N	2.16	0.60
1:C:20:VAL:HG21	1:C:202:MET:CE	2.31	0.60
1:C:970:LEU:HD23	1:C:971:ASP:N	2.16	0.60
1:A:2098:VAL:CG1	1:A:2123:LEU:HD21	2.32	0.60
1:C:2098:VAL:CG1	1:C:2123:LEU:HD21	2.32	0.60
1:A:3455:GLU:O	1:A:3459:VAL:HG23	2.01	0.60
1:A:4231:MET:HE3	1:A:4231:MET:HA	1.84	0.60
1:B:2098:VAL:CG1	1:B:2123:LEU:HD21	2.32	0.60
1:C:4069:LYS:O	1:C:4072:VAL:HG22	2.01	0.60
1:D:2623:LEU:O	1:D:2627:VAL:HG23	2.01	0.60
1:B:2623:LEU:O	1:B:2627:VAL:HG23	2.01	0.60
1:B:4069:LYS:O	1:B:4072:VAL:HG22	2.01	0.60
1:A:970:LEU:HD23	1:A:971:ASP:N	2.16	0.60
1:B:3247:ASP:O	1:B:3250:MET:HE3	2.01	0.60
1:D:2098:VAL:CG1	1:D:2123:LEU:HD21	2.32	0.60
1:C:3247:ASP:O	1:C:3250:MET:HE3	2.01	0.60
1:D:4231:MET:HE3	1:D:4231:MET:HA	1.84	0.60
1:C:3455:GLU:O	1:C:3459:VAL:HG23	2.01	0.60
1:D:970:LEU:HD23	1:D:971:ASP:N	2.16	0.60
1:A:2623:LEU:O	1:A:2627:VAL:HG23	2.01	0.59
1:D:3247:ASP:O	1:D:3250:MET:HE3	2.01	0.59
1:C:4231:MET:HE3	1:C:4231:MET:HA	1.84	0.59
1:B:1293:LEU:HB2	1:B:1579:MET:HE2	1.84	0.59
1:B:4231:MET:HA	1:B:4231:MET:HE3	1.84	0.59
1:D:3553:LEU:HB3	1:D:3593:VAL:HG12	1.84	0.59
1:A:3247:ASP:O	1:A:3250:MET:HE3	2.01	0.59
1:A:3357:HIS:O	1:A:3361:THR:HG23	2.03	0.59
1:A:3553:LEU:HB3	1:A:3593:VAL:HG12	1.85	0.59
1:A:2352:VAL:O	1:A:2356:LEU:HD22	2.03	0.59
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.03	0.59
1:A:1293:LEU:HB2	1:A:1579:MET:HE2	1.84	0.59
1:C:2352:VAL:O	1:C:2356:LEU:HD22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1772:ARG:C	1:D:2153:MET:HE1	2.28	0.59
1:D:2352:VAL:O	1:D:2356:LEU:HD22	2.03	0.59
1:D:3357:HIS:O	1:D:3361:THR:HG23	2.03	0.58
1:C:1772:ARG:C	1:C:2153:MET:HE1	2.28	0.58
1:A:2474:LEU:HD22	1:A:2494:PHE:CE1	2.39	0.58
1:A:3081:MET:HE2	1:A:3156:VAL:O	2.04	0.58
1:C:2490:MET:HE2	1:C:2490:MET:N	2.19	0.58
1:B:1772:ARG:C	1:B:2153:MET:HE1	2.28	0.58
1:B:2352:VAL:O	1:B:2356:LEU:HD22	2.03	0.58
1:D:2474:LEU:HD22	1:D:2494:PHE:CE1	2.39	0.58
1:A:2490:MET:N	1:A:2490:MET:HE2	2.19	0.58
1:D:2490:MET:N	1:D:2490:MET:HE2	2.19	0.58
1:B:1737:PRO:O	1:B:1742:THR:HG21	2.04	0.58
1:B:3081:MET:HE2	1:B:3156:VAL:O	2.04	0.58
1:C:1293:LEU:HB2	1:C:1579:MET:HE2	1.84	0.58
1:C:1737:PRO:O	1:C:1742:THR:HG21	2.04	0.58
1:B:4104:THR:O	1:B:4108:ILE:HD12	2.04	0.57
1:C:2474:LEU:HD22	1:C:2494:PHE:CE1	2.39	0.57
1:D:4104:THR:O	1:D:4108:ILE:HD12	2.04	0.57
1:A:1772:ARG:C	1:A:2153:MET:HE1	2.28	0.57
1:B:2474:LEU:HD22	1:B:2494:PHE:CE1	2.39	0.57
1:C:3553:LEU:HB3	1:C:3593:VAL:HG12	1.84	0.57
1:B:2490:MET:N	1:B:2490:MET:HE2	2.19	0.57
1:B:3553:LEU:HB3	1:B:3593:VAL:HG12	1.84	0.57
1:D:1293:LEU:HB2	1:D:1579:MET:HE2	1.84	0.57
1:A:4104:THR:O	1:A:4108:ILE:HD12	2.04	0.57
1:D:3081:MET:HE2	1:D:3156:VAL:O	2.04	0.57
1:C:144:GLU:OE2	1:C:174:VAL:HG12	2.04	0.57
1:C:3081:MET:HE2	1:C:3156:VAL:O	2.04	0.57
1:C:3357:HIS:O	1:C:3361:THR:HG23	2.03	0.57
1:A:1730:MET:HE3	1:A:1730:MET:HA	1.87	0.57
1:C:4104:THR:O	1:C:4108:ILE:HD12	2.04	0.57
1:A:196:MET:HE2	1:A:196:MET:N	2.20	0.56
1:D:1737:PRO:O	1:D:1742:THR:HG21	2.04	0.56
1:B:20:VAL:HG21	1:B:202:MET:HE3	1.87	0.56
1:A:3780:LEU:HD11	1:A:3816:MET:SD	2.46	0.56
1:B:144:GLU:OE2	1:B:174:VAL:HG12	2.04	0.56
1:C:20:VAL:HG21	1:C:202:MET:HE3	1.87	0.56
1:C:196:MET:HE2	1:C:196:MET:N	2.21	0.56
1:C:3780:LEU:HD11	1:C:3816:MET:SD	2.46	0.56
1:D:1730:MET:HE3	1:D:1730:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD23	1:A:78:LEU:C	2.30	0.56
1:B:78:LEU:C	1:B:78:LEU:HD23	2.30	0.56
1:D:144:GLU:OE2	1:D:174:VAL:HG12	2.04	0.56
1:B:3780:LEU:HD11	1:B:3816:MET:SD	2.46	0.56
1:A:144:GLU:OE2	1:A:174:VAL:HG12	2.04	0.56
1:D:196:MET:HE2	1:D:196:MET:N	2.21	0.56
1:A:1737:PRO:O	1:A:1742:THR:HG21	2.04	0.56
1:A:2223:ILE:HG23	1:A:2223:ILE:O	2.06	0.56
1:C:1730:MET:HA	1:C:1730:MET:HE3	1.87	0.56
1:B:196:MET:N	1:B:196:MET:HE2	2.20	0.56
1:C:78:LEU:HD23	1:C:78:LEU:C	2.30	0.56
1:B:2223:ILE:HG23	1:B:2223:ILE:O	2.06	0.56
1:D:78:LEU:C	1:D:78:LEU:HD23	2.30	0.55
1:A:20:VAL:HG21	1:A:202:MET:HE3	1.87	0.55
1:A:1962:ALA:O	1:A:1966:VAL:HG23	2.06	0.55
1:C:3373:VAL:HG11	1:C:3444:TYR:HB3	1.87	0.55
1:A:2008:MET:HE2	1:A:2008:MET:N	2.22	0.55
2:F:78:PRO:HD3	2:F:96:THR:HG22	1.88	0.55
1:B:2008:MET:HE2	1:B:2008:MET:N	2.22	0.55
1:C:4086:GLY:C	1:C:4087:LEU:HD12	2.31	0.55
1:D:20:VAL:HG21	1:D:202:MET:HE3	1.87	0.55
1:D:4086:GLY:C	1:D:4087:LEU:HD12	2.31	0.55
1:A:3373:VAL:HG11	1:A:3444:TYR:HB3	1.87	0.55
1:B:1730:MET:HE3	1:B:1730:MET:HA	1.87	0.55
1:B:4705:VAL:HG22	1:B:4705:VAL:O	2.07	0.55
1:C:819:GLU:N	1:C:819:GLU:OE1	2.40	0.55
1:C:1962:ALA:O	1:C:1966:VAL:HG23	2.06	0.55
1:C:2008:MET:N	1:C:2008:MET:HE2	2.22	0.55
1:D:3780:LEU:HD11	1:D:3816:MET:SD	2.46	0.55
1:D:2223:ILE:O	1:D:2223:ILE:HG23	2.06	0.55
1:A:1926:LEU:O	1:A:1931:LEU:HD21	2.07	0.55
1:C:2223:ILE:HG23	1:C:2223:ILE:O	2.06	0.55
1:D:819:GLU:N	1:D:819:GLU:OE1	2.40	0.55
1:D:2008:MET:HE2	1:D:2008:MET:N	2.22	0.55
2:E:78:PRO:HD3	2:E:96:THR:HG22	1.88	0.55
1:B:1962:ALA:O	1:B:1966:VAL:HG23	2.06	0.55
1:B:4086:GLY:C	1:B:4087:LEU:HD12	2.31	0.55
1:A:819:GLU:N	1:A:819:GLU:OE1	2.40	0.55
1:A:2500:ALA:O	1:A:2503:VAL:HG12	2.07	0.55
1:B:819:GLU:N	1:B:819:GLU:OE1	2.40	0.55
1:B:3373:VAL:HG11	1:B:3444:TYR:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4705:VAL:O	1:C:4705:VAL:HG22	2.07	0.55
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.88	0.55
1:A:2894:LEU:HD21	1:A:2900:GLY:O	2.07	0.54
1:B:2894:LEU:HD21	1:B:2900:GLY:O	2.07	0.54
1:C:2894:LEU:HD21	1:C:2900:GLY:O	2.07	0.54
1:D:2500:ALA:O	1:D:2503:VAL:HG12	2.07	0.54
1:D:2643:LEU:HD23	1:D:2643:LEU:C	2.32	0.54
2:G:78:PRO:HD3	2:G:96:THR:HG22	1.88	0.54
1:C:1926:LEU:O	1:C:1931:LEU:HD21	2.07	0.54
1:A:4705:VAL:O	1:A:4705:VAL:HG22	2.07	0.54
1:D:4705:VAL:HG22	1:D:4705:VAL:O	2.07	0.54
1:A:2295:LEU:O	1:A:2299:VAL:HG23	2.08	0.54
1:A:4086:GLY:C	1:A:4087:LEU:HD12	2.31	0.54
1:B:1926:LEU:O	1:B:1931:LEU:HD21	2.07	0.54
1:C:2500:ALA:O	1:C:2503:VAL:HG12	2.07	0.54
1:C:2643:LEU:C	1:C:2643:LEU:HD23	2.32	0.54
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.89	0.54
1:D:1926:LEU:O	1:D:1931:LEU:HD21	2.07	0.54
1:D:1962:ALA:O	1:D:1966:VAL:HG23	2.06	0.54
1:D:3373:VAL:HG11	1:D:3444:TYR:HB3	1.87	0.54
1:A:2417:HIS:CD2	1:A:2492:ALA:HB2	2.43	0.54
1:B:2608:MET:HE3	1:B:2608:MET:O	2.08	0.54
1:C:2608:MET:HE3	1:C:2608:MET:O	2.08	0.54
1:D:1931:LEU:H	1:D:1931:LEU:HD22	1.73	0.54
1:B:2417:HIS:CD2	1:B:2492:ALA:HB2	2.43	0.54
1:D:2894:LEU:HD21	1:D:2900:GLY:O	2.07	0.54
1:A:2643:LEU:C	1:A:2643:LEU:HD23	2.32	0.53
1:B:2643:LEU:C	1:B:2643:LEU:HD23	2.32	0.53
1:C:2417:HIS:CD2	1:C:2492:ALA:HB2	2.43	0.53
1:D:2608:MET:HE3	1:D:2608:MET:O	2.08	0.53
1:A:2290:LEU:HD23	1:A:2291:GLN:N	2.23	0.53
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.90	0.53
1:B:2290:LEU:HD23	1:B:2291:GLN:N	2.23	0.53
1:D:2295:LEU:O	1:D:2299:VAL:HG23	2.08	0.53
1:B:927:GLU:O	1:B:931:THR:HG23	2.08	0.53
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.89	0.53
1:A:4839:MET:HE1	1:B:4823:LEU:HB2	1.91	0.53
1:B:3293:PRO:N	1:B:3294:PRO:CD	2.72	0.53
1:C:3293:PRO:N	1:C:3294:PRO:CD	2.72	0.53
1:B:3788:GLY:O	1:B:3835:LEU:HD23	2.08	0.53
1:C:1931:LEU:HD22	1:C:1931:LEU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3198:ALA:HB2	1:C:3276:MET:HE1	1.91	0.53
1:A:1931:LEU:H	1:A:1931:LEU:HD22	1.73	0.53
1:B:2500:ALA:O	1:B:2503:VAL:HG12	2.07	0.53
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.89	0.53
1:B:3198:ALA:HB2	1:B:3276:MET:HE1	1.91	0.53
1:B:4839:MET:HE1	1:C:4823:LEU:HB2	1.91	0.53
1:D:927:GLU:O	1:D:931:THR:HG23	2.08	0.53
1:D:2417:HIS:CD2	1:D:2492:ALA:HB2	2.43	0.53
1:A:1736:VAL:HG23	1:A:1736:VAL:O	2.09	0.53
1:A:3198:ALA:HB2	1:A:3276:MET:HE1	1.91	0.53
1:B:2295:LEU:O	1:B:2299:VAL:HG23	2.08	0.53
1:C:1736:VAL:O	1:C:1736:VAL:HG23	2.09	0.53
1:C:2295:LEU:O	1:C:2299:VAL:HG23	2.08	0.53
2:E:90:ILE:HG22	2:E:91:ILE:CG1	2.39	0.53
2:H:90:ILE:HG22	2:H:91:ILE:CG1	2.39	0.53
1:A:927:GLU:O	1:A:931:THR:HG23	2.08	0.53
1:B:1931:LEU:HD22	1:B:1931:LEU:H	1.73	0.53
1:A:2608:MET:HE3	1:A:2608:MET:O	2.08	0.53
1:C:2290:LEU:HD23	1:C:2291:GLN:N	2.23	0.53
1:D:3198:ALA:HB2	1:D:3276:MET:HE1	1.91	0.53
1:D:3788:GLY:O	1:D:3835:LEU:HD23	2.09	0.53
2:G:90:ILE:HG22	2:G:91:ILE:CG1	2.39	0.53
1:C:927:GLU:O	1:C:931:THR:HG23	2.08	0.52
1:D:1862:ILE:HG22	1:D:1866:ILE:HD11	1.91	0.52
1:A:1115:LEU:HD21	1:A:1123:VAL:HG11	1.91	0.52
1:A:2569:PHE:CE1	1:A:2610:LEU:HD21	2.45	0.52
1:B:2208:MET:C	1:B:2208:MET:HE2	2.35	0.52
1:C:1115:LEU:HD21	1:C:1123:VAL:HG11	1.91	0.52
1:D:3293:PRO:N	1:D:3294:PRO:CD	2.72	0.52
1:D:2290:LEU:HD23	1:D:2291:GLN:N	2.23	0.52
1:B:3769:ARG:C	1:B:3770:LEU:HD12	2.35	0.52
1:C:3788:GLY:O	1:C:3835:LEU:HD23	2.09	0.52
1:D:3341:PHE:HD1	1:D:3341:PHE:O	1.93	0.52
1:A:2208:MET:C	1:A:2208:MET:HE2	2.35	0.52
1:A:3780:LEU:HD13	1:A:3820:LEU:HD21	1.92	0.52
1:B:2569:PHE:CE1	1:B:2610:LEU:HD21	2.45	0.52
1:C:3341:PHE:HD1	1:C:3341:PHE:O	1.93	0.52
1:A:3293:PRO:N	1:A:3294:PRO:CD	2.72	0.52
1:A:3788:GLY:O	1:A:3835:LEU:HD23	2.08	0.52
1:C:3195:ALA:HB1	1:C:3341:PHE:HZ	1.75	0.52
1:C:4989:MET:HA	1:C:4989:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2208:MET:C	1:D:2208:MET:HE2	2.35	0.52
1:D:3769:ARG:C	1:D:3770:LEU:HD12	2.35	0.52
1:C:1063:VAL:HG13	1:C:1064:GLU:H	1.74	0.52
1:C:1862:ILE:HG22	1:C:1866:ILE:HD11	1.91	0.52
1:A:1063:VAL:HG13	1:A:1064:GLU:N	2.25	0.52
1:A:3172:ILE:HD13	1:A:3194:LEU:HD21	1.92	0.52
1:B:1063:VAL:HG13	1:B:1064:GLU:H	1.74	0.52
1:B:1063:VAL:HG13	1:B:1064:GLU:N	2.25	0.52
1:D:2569:PHE:CE1	1:D:2610:LEU:HD21	2.45	0.52
1:D:3195:ALA:HB1	1:D:3341:PHE:HZ	1.75	0.52
1:A:3769:ARG:C	1:A:3770:LEU:HD12	2.35	0.52
1:B:1736:VAL:HG23	1:B:1736:VAL:O	2.09	0.52
1:B:1862:ILE:HG22	1:B:1866:ILE:HD11	1.91	0.52
1:C:2569:PHE:CE1	1:C:2610:LEU:HD21	2.45	0.52
1:C:3832:ILE:HA	1:C:3835:LEU:HD12	1.92	0.52
1:D:3832:ILE:HA	1:D:3835:LEU:HD12	1.92	0.52
1:A:3832:ILE:HA	1:A:3835:LEU:HD12	1.92	0.52
1:B:3780:LEU:HD13	1:B:3820:LEU:HD21	1.92	0.52
1:B:3832:ILE:HA	1:B:3835:LEU:HD12	1.92	0.52
1:A:4677:LEU:HD12	1:A:4702:ASP:OD2	2.10	0.51
1:D:1063:VAL:HG13	1:D:1064:GLU:N	2.25	0.51
1:D:1063:VAL:HG13	1:D:1064:GLU:H	1.75	0.51
1:D:3172:ILE:HD13	1:D:3194:LEU:HD21	1.92	0.51
1:D:4677:LEU:HD12	1:D:4702:ASP:OD2	2.10	0.51
1:A:1063:VAL:HG13	1:A:1064:GLU:H	1.75	0.51
1:B:3172:ILE:HD13	1:B:3194:LEU:HD21	1.92	0.51
1:B:4677:LEU:HD12	1:B:4702:ASP:OD2	2.10	0.51
1:C:3168:THR:HG22	1:C:3172:ILE:HD11	1.92	0.51
1:C:3769:ARG:C	1:C:3770:LEU:HD12	2.35	0.51
2:F:90:ILE:HG22	2:F:91:ILE:CG1	2.39	0.51
1:A:3341:PHE:HD1	1:A:3341:PHE:O	1.93	0.51
1:C:1063:VAL:HG13	1:C:1064:GLU:N	2.25	0.51
1:C:4677:LEU:HD12	1:C:4702:ASP:OD2	2.10	0.51
1:A:1862:ILE:HG22	1:A:1866:ILE:HD11	1.91	0.51
1:B:3195:ALA:HB1	1:B:3341:PHE:HZ	1.75	0.51
1:D:1115:LEU:HD21	1:D:1123:VAL:HG11	1.91	0.51
1:D:1687:SER:HB3	2:H:90:ILE:HD11	1.93	0.51
1:D:1736:VAL:HG23	1:D:1736:VAL:O	2.09	0.51
1:D:4989:MET:HE2	1:D:4989:MET:HA	1.92	0.51
1:A:1929:MET:HB3	1:A:1931:LEU:HD11	1.92	0.51
1:C:1216:ILE:HD12	1:D:3424:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3172:ILE:HD13	1:C:3194:LEU:HD21	1.92	0.51
1:B:3341:PHE:HD1	1:B:3341:PHE:O	1.93	0.51
1:C:2208:MET:HE2	1:C:2208:MET:C	2.35	0.51
1:C:3780:LEU:HD13	1:C:3820:LEU:HD21	1.92	0.51
1:A:4677:LEU:C	1:A:4677:LEU:HD23	2.36	0.51
1:A:4989:MET:HA	1:A:4989:MET:HE2	1.92	0.51
1:C:1929:MET:HB3	1:C:1931:LEU:HD11	1.93	0.51
1:B:4989:MET:HE2	1:B:4989:MET:HA	1.91	0.50
1:C:1115:LEU:CD2	1:C:1123:VAL:HG11	2.41	0.50
1:D:1115:LEU:CD2	1:D:1123:VAL:HG11	2.41	0.50
1:D:3780:LEU:HD13	1:D:3820:LEU:HD21	1.92	0.50
1:B:1115:LEU:HD21	1:B:1123:VAL:HG11	1.91	0.50
1:C:4839:MET:HE1	1:D:4823:LEU:HB2	1.94	0.50
1:B:3168:THR:HG22	1:B:3172:ILE:HD11	1.92	0.50
1:D:3168:THR:HG22	1:D:3172:ILE:HD11	1.92	0.50
1:A:196:MET:HE2	1:A:196:MET:H	1.77	0.50
1:A:857:ASP:OD2	1:A:857:ASP:C	2.55	0.50
1:B:4677:LEU:C	1:B:4677:LEU:HD23	2.36	0.50
1:C:196:MET:HE2	1:C:196:MET:H	1.77	0.50
1:C:857:ASP:OD2	1:C:857:ASP:C	2.55	0.50
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.94	0.50
1:A:3195:ALA:HB1	1:A:3341:PHE:HZ	1.75	0.50
1:B:1929:MET:HB3	1:B:1931:LEU:HD11	1.93	0.50
1:D:1929:MET:HB3	1:D:1931:LEU:HD11	1.93	0.50
1:D:4085:ARG:HB2	1:D:4087:LEU:HD13	1.93	0.50
1:B:749:ASP:OD2	1:B:749:ASP:C	2.55	0.50
1:B:4030:LEU:HB3	1:B:4040:ILE:HD11	1.94	0.50
1:C:749:ASP:C	1:C:749:ASP:OD2	2.55	0.50
1:A:3168:THR:HG22	1:A:3172:ILE:HD11	1.92	0.50
1:B:1115:LEU:CD2	1:B:1123:VAL:HG11	2.41	0.50
1:B:4666:VAL:HG22	1:B:4783:ILE:HD13	1.94	0.50
1:C:4666:VAL:HG22	1:C:4783:ILE:HD13	1.94	0.50
1:C:4677:LEU:HD23	1:C:4677:LEU:C	2.36	0.50
1:D:774:ASP:C	1:D:774:ASP:OD1	2.55	0.50
1:A:749:ASP:C	1:A:749:ASP:OD2	2.55	0.49
1:A:774:ASP:C	1:A:774:ASP:OD1	2.55	0.49
1:B:857:ASP:C	1:B:857:ASP:OD2	2.55	0.49
1:A:1115:LEU:CD2	1:A:1123:VAL:HG11	2.41	0.49
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.94	0.49
1:A:4823:LEU:HB2	1:D:4839:MET:HE1	1.94	0.49
1:B:774:ASP:OD1	1:B:774:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:857:ASP:C	1:D:857:ASP:OD2	2.55	0.49
1:D:4677:LEU:C	1:D:4677:LEU:HD23	2.36	0.49
1:B:1771:LEU:HB3	1:B:2153:MET:HE2	1.94	0.49
1:C:774:ASP:OD1	1:C:774:ASP:C	2.55	0.49
1:D:196:MET:HE2	1:D:196:MET:H	1.77	0.49
1:D:3338:LEU:HD12	1:D:3338:LEU:O	2.12	0.49
1:A:3338:LEU:HD12	1:A:3338:LEU:O	2.13	0.49
1:B:570:GLU:HA	1:B:570:GLU:OE2	2.13	0.49
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.95	0.49
1:C:4085:ARG:HB2	1:C:4087:LEU:HD13	1.93	0.49
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.95	0.49
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.95	0.49
1:A:1771:LEU:HB3	1:A:2153:MET:HE2	1.94	0.49
1:A:4030:LEU:HB3	1:A:4040:ILE:HD11	1.94	0.49
1:B:2479:LEU:HD13	1:B:2541:PHE:CZ	2.48	0.49
1:D:570:GLU:OE2	1:D:570:GLU:HA	2.13	0.49
1:A:570:GLU:OE2	1:A:570:GLU:HA	2.12	0.49
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.94	0.49
1:B:3793:MET:HE2	1:B:3793:MET:N	2.28	0.49
1:B:4085:ARG:HB2	1:B:4087:LEU:HD13	1.93	0.49
1:C:570:GLU:OE2	1:C:570:GLU:HA	2.13	0.49
1:D:4030:LEU:HB3	1:D:4040:ILE:HD11	1.94	0.49
1:C:1771:LEU:HB3	1:C:2153:MET:HE2	1.94	0.49
1:D:749:ASP:OD2	1:D:749:ASP:C	2.55	0.49
1:D:2479:LEU:HD13	1:D:2541:PHE:CZ	2.48	0.49
2:E:41:ASP:OD1	2:E:41:ASP:C	2.56	0.49
1:A:1929:MET:HG3	1:A:1929:MET:O	2.13	0.49
1:A:2479:LEU:HD13	1:A:2541:PHE:CZ	2.48	0.49
1:B:1633:PRO:O	1:B:1634:LEU:HD22	2.13	0.49
1:B:3338:LEU:HD12	1:B:3338:LEU:O	2.13	0.49
1:B:3718:GLU:HG2	1:B:3793:MET:HE3	1.95	0.49
1:A:3401:LEU:HD12	1:A:3405:LEU:HD13	1.95	0.49
1:A:4739:GLU:OE1	1:A:4739:GLU:HA	2.13	0.49
1:B:4739:GLU:HA	1:B:4739:GLU:OE1	2.13	0.49
1:C:2479:LEU:HD13	1:C:2541:PHE:CZ	2.48	0.49
1:C:3793:MET:N	1:C:3793:MET:HE2	2.28	0.49
1:C:4739:GLU:OE1	1:C:4739:GLU:HA	2.12	0.49
2:F:13:ARG:HD2	2:F:13:ARG:N	2.28	0.49
2:G:13:ARG:HD2	2:G:13:ARG:N	2.28	0.49
1:A:1633:PRO:O	1:A:1634:LEU:HD22	2.13	0.49
1:A:3718:GLU:HG2	1:A:3793:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.95	0.49
1:C:2679:PHE:C	1:C:2679:PHE:CD2	2.91	0.49
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.94	0.49
1:D:2679:PHE:C	1:D:2679:PHE:CD2	2.91	0.49
1:A:1765:VAL:HG13	1:A:1856:ASP:OD1	2.13	0.48
1:A:2198:MET:N	1:A:2198:MET:HE2	2.28	0.48
1:A:3793:MET:N	1:A:3793:MET:HE2	2.28	0.48
1:B:1929:MET:O	1:B:1929:MET:HG3	2.13	0.48
1:B:2679:PHE:C	1:B:2679:PHE:CD2	2.91	0.48
1:C:3986:TRP:O	1:C:3990:VAL:HG23	2.13	0.48
1:D:3793:MET:HE2	1:D:3793:MET:N	2.28	0.48
1:C:3338:LEU:O	1:C:3338:LEU:HD12	2.13	0.48
1:D:4666:VAL:HG22	1:D:4783:ILE:HD13	1.94	0.48
1:A:4085:ARG:HB2	1:A:4087:LEU:HD13	1.93	0.48
1:A:4666:VAL:HG22	1:A:4783:ILE:HD13	1.94	0.48
1:B:2143:THR:HG21	1:B:3650:CYS:SG	2.53	0.48
1:C:2143:THR:HG21	1:C:3650:CYS:SG	2.54	0.48
1:C:2198:MET:N	1:C:2198:MET:HE2	2.29	0.48
1:C:4030:LEU:HB3	1:C:4040:ILE:HD11	1.94	0.48
1:D:1929:MET:O	1:D:1929:MET:HG3	2.13	0.48
2:F:41:ASP:C	2:F:41:ASP:OD1	2.56	0.48
1:A:1736:VAL:HG21	1:A:1959:ALA:CB	2.44	0.48
1:A:2143:THR:HG21	1:A:3650:CYS:SG	2.53	0.48
1:B:1765:VAL:HG13	1:B:1856:ASP:OD1	2.13	0.48
1:B:3986:TRP:O	1:B:3990:VAL:HG23	2.13	0.48
2:G:41:ASP:C	2:G:41:ASP:OD1	2.56	0.48
1:C:1633:PRO:O	1:C:1634:LEU:HD22	2.13	0.48
1:D:1765:VAL:HG13	1:D:1856:ASP:OD1	2.13	0.48
1:D:2198:MET:HE2	1:D:2198:MET:N	2.28	0.48
1:D:3401:LEU:HD12	1:D:3405:LEU:HD13	1.95	0.48
1:C:1929:MET:HG3	1:C:1929:MET:O	2.13	0.48
1:D:1736:VAL:HG21	1:D:1959:ALA:CB	2.44	0.48
2:H:13:ARG:HD2	2:H:13:ARG:N	2.28	0.48
1:A:2679:PHE:C	1:A:2679:PHE:CD2	2.91	0.48
1:C:2663:ASN:O	1:C:2663:ASN:ND2	2.47	0.48
1:C:3459:VAL:HG13	1:C:3464:ILE:O	2.14	0.48
1:D:1771:LEU:HB3	1:D:2153:MET:HE2	1.94	0.48
1:D:4739:GLU:HA	1:D:4739:GLU:OE1	2.13	0.48
2:E:13:ARG:HD2	2:E:13:ARG:N	2.28	0.48
1:B:2663:ASN:O	1:B:2663:ASN:ND2	2.47	0.48
1:C:2626:LEU:HD12	1:C:2626:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2626:LEU:HD12	1:A:2626:LEU:N	2.29	0.48
1:B:2198:MET:HE2	1:B:2198:MET:N	2.28	0.48
1:D:2143:THR:HG21	1:D:3650:CYS:SG	2.54	0.48
2:H:59:TRP:O	2:H:63:VAL:HG12	2.14	0.48
1:B:1736:VAL:HG21	1:B:1959:ALA:CB	2.44	0.48
1:B:1931:LEU:HD22	1:B:1931:LEU:N	2.29	0.48
1:B:3751:VAL:O	1:B:3751:VAL:HG13	2.14	0.48
1:C:1281:ASN:OD1	1:C:1281:ASN:C	2.57	0.48
1:C:3718:GLU:HG2	1:C:3793:MET:HE3	1.95	0.48
1:C:3751:VAL:O	1:C:3751:VAL:HG13	2.14	0.48
1:D:1931:LEU:HD22	1:D:1931:LEU:N	2.29	0.48
1:D:3986:TRP:O	1:D:3990:VAL:HG23	2.13	0.48
2:E:59:TRP:O	2:E:63:VAL:HG12	2.14	0.48
1:A:700:GLU:N	1:A:700:GLU:OE1	2.47	0.47
1:A:3459:VAL:HG13	1:A:3464:ILE:O	2.14	0.47
1:A:3986:TRP:O	1:A:3990:VAL:HG23	2.13	0.47
1:B:1425:GLU:OE1	1:B:1425:GLU:N	2.47	0.47
1:D:2663:ASN:ND2	1:D:2663:ASN:O	2.47	0.47
1:D:3442:PHE:HA	1:D:3510:ILE:HD11	1.96	0.47
1:D:3459:VAL:HG13	1:D:3464:ILE:O	2.14	0.47
1:D:3718:GLU:HG2	1:D:3793:MET:HE3	1.95	0.47
1:A:3971:GLY:N	1:A:3972:PRO:HA	2.29	0.47
1:B:102:LEU:HD23	1:B:160:GLY:O	2.14	0.47
1:C:1736:VAL:HG21	1:C:1959:ALA:CB	2.44	0.47
1:C:1765:VAL:HG13	1:C:1856:ASP:OD1	2.13	0.47
1:C:3401:LEU:HD12	1:C:3405:LEU:HD13	1.95	0.47
1:D:1633:PRO:O	1:D:1634:LEU:HD22	2.13	0.47
1:D:2626:LEU:HD12	1:D:2626:LEU:N	2.29	0.47
2:H:41:ASP:OD1	2:H:41:ASP:C	2.56	0.47
1:A:2663:ASN:O	1:A:2663:ASN:ND2	2.47	0.47
1:A:3442:PHE:HA	1:A:3510:ILE:HD11	1.96	0.47
1:B:856:VAL:HG12	1:B:991:ASN:OD1	2.14	0.47
1:C:700:GLU:N	1:C:700:GLU:OE1	2.47	0.47
1:C:3442:PHE:HA	1:C:3510:ILE:HD11	1.96	0.47
1:D:856:VAL:HG12	1:D:991:ASN:OD1	2.14	0.47
1:D:1281:ASN:OD1	1:D:1281:ASN:C	2.57	0.47
2:G:59:TRP:O	2:G:63:VAL:HG12	2.14	0.47
1:A:1281:ASN:OD1	1:A:1281:ASN:C	2.57	0.47
1:B:1281:ASN:C	1:B:1281:ASN:OD1	2.57	0.47
1:B:3442:PHE:HA	1:B:3510:ILE:HD11	1.95	0.47
1:C:856:VAL:HG12	1:C:991:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:TRP:O	2:F:63:VAL:HG12	2.14	0.47
1:A:1216:ILE:HD12	1:B:3424:LEU:HD12	1.96	0.47
1:B:1816:GLY:HA2	1:B:1865:MET:HE1	1.97	0.47
1:B:3401:LEU:HD12	1:B:3405:LEU:HD13	1.95	0.47
1:B:4067:LYS:HD3	1:B:4067:LYS:C	2.40	0.47
1:C:102:LEU:HD23	1:C:160:GLY:O	2.14	0.47
1:C:1816:GLY:HA2	1:C:1865:MET:HE1	1.97	0.47
1:D:102:LEU:HD23	1:D:160:GLY:O	2.14	0.47
1:A:1425:GLU:N	1:A:1425:GLU:OE1	2.47	0.47
1:A:2788:HIS:O	1:A:2791:LEU:HD12	2.15	0.47
1:D:700:GLU:OE1	1:D:700:GLU:N	2.47	0.47
1:A:856:VAL:HG12	1:A:991:ASN:OD1	2.14	0.47
1:A:4067:LYS:HD3	1:A:4067:LYS:C	2.40	0.47
1:B:196:MET:HE2	1:B:196:MET:H	1.77	0.47
1:B:700:GLU:N	1:B:700:GLU:OE1	2.47	0.47
1:B:3971:GLY:N	1:B:3972:PRO:HA	2.29	0.47
1:C:1425:GLU:N	1:C:1425:GLU:OE1	2.47	0.47
1:C:4067:LYS:HD3	1:C:4067:LYS:C	2.40	0.47
1:B:2626:LEU:N	1:B:2626:LEU:HD12	2.29	0.47
1:B:3459:VAL:HG13	1:B:3464:ILE:O	2.14	0.47
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.29	0.47
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.29	0.47
1:D:4047:MET:SD	1:D:4047:MET:C	2.98	0.47
1:A:1931:LEU:HD22	1:A:1931:LEU:N	2.29	0.47
1:B:2788:HIS:O	1:B:2791:LEU:HD12	2.15	0.47
1:C:220:LEU:HD12	1:C:220:LEU:C	2.40	0.47
1:A:591:ASP:OD2	1:A:591:ASP:C	2.58	0.47
1:C:688:LEU:HD12	1:C:776:LEU:O	2.15	0.47
1:C:4154:VAL:HG12	1:C:4154:VAL:O	2.15	0.47
1:D:688:LEU:HD12	1:D:776:LEU:O	2.15	0.47
1:D:2788:HIS:O	1:D:2791:LEU:HD12	2.15	0.47
1:D:4067:LYS:HD3	1:D:4067:LYS:C	2.40	0.47
1:B:591:ASP:OD2	1:B:591:ASP:C	2.58	0.46
1:C:2788:HIS:O	1:C:2791:LEU:HD12	2.15	0.46
1:A:102:LEU:HD23	1:A:160:GLY:O	2.14	0.46
1:A:2967:MET:HE2	1:A:3045:LYS:CE	2.46	0.46
1:B:220:LEU:HD12	1:B:220:LEU:C	2.40	0.46
1:B:1216:ILE:HD12	1:C:3424:LEU:HD12	1.98	0.46
1:D:2967:MET:HE2	1:D:3045:LYS:CE	2.46	0.46
1:A:688:LEU:HD12	1:A:776:LEU:O	2.15	0.46
1:A:4047:MET:SD	1:A:4047:MET:C	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:LEU:HD12	1:B:874:LEU:O	2.16	0.46
1:B:4047:MET:SD	1:B:4047:MET:C	2.98	0.46
1:D:2969:ILE:HG23	1:D:2994:GLU:OE2	2.16	0.46
1:A:1816:GLY:HA2	1:A:1865:MET:HE1	1.97	0.46
1:A:2146:PRO:HA	1:A:2149:VAL:HG23	1.98	0.46
1:A:2969:ILE:HG23	1:A:2994:GLU:OE2	2.16	0.46
1:B:76:ARG:HD3	1:C:3935:TRP:HB2	1.97	0.46
1:C:2500:ALA:O	1:C:2504:LEU:HD12	2.15	0.46
1:C:3198:ALA:HB2	1:C:3276:MET:CE	2.46	0.46
1:C:4047:MET:SD	1:C:4047:MET:C	2.98	0.46
1:D:3770:LEU:HD12	1:D:3770:LEU:N	2.30	0.46
1:A:170:ILE:HD11	1:A:199:LEU:CD2	2.45	0.46
1:A:2930:LEU:HD22	1:A:2935:TYR:CB	2.46	0.46
1:A:3770:LEU:HD12	1:A:3770:LEU:N	2.30	0.46
1:B:170:ILE:HD11	1:B:199:LEU:CD2	2.45	0.46
1:C:1931:LEU:HD22	1:C:1931:LEU:N	2.29	0.46
1:C:2569:PHE:CD1	1:C:2610:LEU:HD21	2.51	0.46
1:D:220:LEU:C	1:D:220:LEU:HD12	2.40	0.46
1:D:1425:GLU:N	1:D:1425:GLU:OE1	2.47	0.46
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.98	0.46
1:A:2494:PHE:CD1	1:A:2494:PHE:C	2.94	0.46
1:A:4154:VAL:O	1:A:4154:VAL:HG12	2.15	0.46
1:C:874:LEU:O	1:C:874:LEU:HD12	2.16	0.46
1:C:2967:MET:HE2	1:C:3045:LYS:CE	2.46	0.46
1:D:591:ASP:OD2	1:D:591:ASP:C	2.58	0.46
1:D:3129:LEU:HD23	1:D:3130:THR:N	2.31	0.46
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.98	0.46
1:B:2500:ALA:O	1:B:2504:LEU:HD12	2.16	0.46
1:B:2969:ILE:HG23	1:B:2994:GLU:OE2	2.16	0.46
1:C:719:LEU:HD21	1:C:736:HIS:C	2.41	0.46
1:C:2930:LEU:HD22	1:C:2935:TYR:CB	2.46	0.46
1:D:2146:PRO:HA	1:D:2149:VAL:HG23	1.98	0.46
1:D:2930:LEU:HD22	1:D:2935:TYR:CB	2.46	0.46
1:A:3129:LEU:HD23	1:A:3130:THR:N	2.31	0.46
1:B:2569:PHE:CD1	1:B:2610:LEU:HD21	2.51	0.46
1:B:2967:MET:HE2	1:B:3045:LYS:CE	2.46	0.46
1:C:170:ILE:HD11	1:C:199:LEU:CD2	2.45	0.46
1:C:2146:PRO:HA	1:C:2149:VAL:HG23	1.98	0.46
1:D:719:LEU:HD21	1:D:736:HIS:C	2.41	0.46
1:D:874:LEU:HD12	1:D:874:LEU:O	2.16	0.46
1:D:2569:PHE:CD1	1:D:2610:LEU:HD21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3198:ALA:HB2	1:A:3276:MET:CE	2.46	0.46
1:C:2494:PHE:CD1	1:C:2494:PHE:C	2.94	0.46
1:D:1816:GLY:HA2	1:D:1865:MET:HE1	1.97	0.46
1:D:3198:ALA:HB2	1:D:3276:MET:CE	2.46	0.46
1:B:2146:PRO:HA	1:B:2149:VAL:HG23	1.98	0.46
1:C:2969:ILE:HG23	1:C:2994:GLU:OE2	2.16	0.46
1:C:3316:LEU:HD23	1:C:3316:LEU:C	2.41	0.46
1:D:3751:VAL:O	1:D:3751:VAL:HG13	2.14	0.46
1:D:4154:VAL:HG12	1:D:4154:VAL:O	2.15	0.46
1:A:719:LEU:HD21	1:A:736:HIS:C	2.41	0.45
1:A:3751:VAL:HG13	1:A:3751:VAL:O	2.14	0.45
1:B:688:LEU:HD12	1:B:776:LEU:O	2.15	0.45
1:B:3061:ALA:HB3	1:B:3062:PRO:HD3	1.99	0.45
1:B:3316:LEU:C	1:B:3316:LEU:HD23	2.42	0.45
1:B:3932:ASP:O	1:B:3932:ASP:OD2	2.35	0.45
1:A:220:LEU:C	1:A:220:LEU:HD12	2.40	0.45
1:B:2930:LEU:HD22	1:B:2935:TYR:CB	2.46	0.45
1:C:3770:LEU:HD12	1:C:3770:LEU:N	2.30	0.45
1:A:2500:ALA:O	1:A:2504:LEU:HD12	2.15	0.45
1:A:2569:PHE:CD1	1:A:2610:LEU:HD21	2.51	0.45
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.98	0.45
1:B:3770:LEU:HD12	1:B:3770:LEU:N	2.30	0.45
1:C:591:ASP:OD2	1:C:591:ASP:C	2.58	0.45
1:A:3061:ALA:HB3	1:A:3062:PRO:HD3	1.98	0.45
1:B:4154:VAL:O	1:B:4154:VAL:HG12	2.15	0.45
1:C:3129:LEU:HD23	1:C:3130:THR:N	2.31	0.45
1:D:2494:PHE:CD1	1:D:2494:PHE:C	2.94	0.45
1:B:719:LEU:HD21	1:B:736:HIS:C	2.41	0.45
1:C:3932:ASP:O	1:C:3932:ASP:OD2	2.35	0.45
1:D:170:ILE:HD11	1:D:199:LEU:CD2	2.45	0.45
1:A:3736:GLU:HG2	1:A:3763:LEU:HD21	1.99	0.45
1:B:3235:SER:O	1:B:3239:MET:SD	2.75	0.45
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.98	0.45
1:C:3690:VAL:HG22	1:C:3690:VAL:O	2.17	0.45
1:C:3736:GLU:HG2	1:C:3763:LEU:HD21	1.99	0.45
1:D:3690:VAL:HG22	1:D:3690:VAL:O	2.17	0.45
1:D:3736:GLU:HG2	1:D:3763:LEU:HD21	1.99	0.45
1:A:874:LEU:HD12	1:A:874:LEU:O	2.16	0.45
1:A:3316:LEU:C	1:A:3316:LEU:HD23	2.41	0.45
1:B:3695:PRO:HB2	1:B:3699:HIS:HB3	1.99	0.45
1:C:2973:PHE:CD1	1:C:2973:PHE:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3061:ALA:HB3	1:C:3062:PRO:HD3	1.99	0.45
1:C:3695:PRO:HB2	1:C:3699:HIS:HB3	1.99	0.45
1:D:3316:LEU:C	1:D:3316:LEU:HD23	2.41	0.45
1:A:1164:LEU:C	1:A:1164:LEU:HD23	2.42	0.45
1:C:76:ARG:HD3	1:D:3935:TRP:HB2	1.98	0.45
1:A:4793:GLY:O	1:A:4797:VAL:HG23	2.17	0.45
1:C:3235:SER:O	1:C:3239:MET:SD	2.75	0.45
1:C:4097:MET:SD	1:C:4111:LEU:HD12	2.57	0.45
1:D:2500:ALA:O	1:D:2504:LEU:HD12	2.16	0.45
1:C:578:ILE:HG21	1:C:583:ILE:HD11	1.99	0.45
1:D:4045:VAL:HG22	1:D:4150:LEU:HD23	1.99	0.45
2:E:104:LEU:N	2:E:104:LEU:HD23	2.32	0.45
2:H:104:LEU:N	2:H:104:LEU:HD23	2.32	0.45
1:A:688:LEU:HD11	1:A:775:GLY:HA3	2.00	0.44
1:A:1186:ASP:OD2	1:A:1186:ASP:N	2.50	0.44
1:A:3932:ASP:O	1:A:3932:ASP:OD2	2.35	0.44
1:B:1164:LEU:HD23	1:B:1164:LEU:C	2.42	0.44
1:B:2494:PHE:CD1	1:B:2494:PHE:C	2.94	0.44
1:D:578:ILE:HG21	1:D:583:ILE:HD11	1.99	0.44
1:A:1687:SER:HB3	2:E:90:ILE:HD11	1.99	0.44
1:A:4097:MET:SD	1:A:4111:LEU:HD12	2.57	0.44
1:B:2973:PHE:CD1	1:B:2973:PHE:C	2.95	0.44
1:C:4793:GLY:O	1:C:4797:VAL:HG23	2.18	0.44
1:D:688:LEU:HD11	1:D:775:GLY:HA3	1.99	0.44
1:B:75:VAL:HG23	1:B:76:ARG:N	2.33	0.44
1:B:578:ILE:HG21	1:B:583:ILE:HD11	1.99	0.44
1:B:3690:VAL:HG22	1:B:3690:VAL:O	2.17	0.44
1:B:3778:MET:SD	1:B:3778:MET:C	3.01	0.44
1:D:3235:SER:O	1:D:3239:MET:SD	2.75	0.44
1:D:3508:SER:OG	1:D:3510:ILE:HG22	2.18	0.44
1:D:3932:ASP:O	1:D:3932:ASP:OD2	2.35	0.44
2:F:104:LEU:N	2:F:104:LEU:HD23	2.32	0.44
1:A:3235:SER:O	1:A:3239:MET:SD	2.75	0.44
1:A:3690:VAL:HG22	1:A:3690:VAL:O	2.17	0.44
1:B:3129:LEU:HD23	1:B:3130:THR:N	2.31	0.44
1:C:3508:SER:OG	1:C:3510:ILE:HG22	2.18	0.44
1:C:4045:VAL:HG22	1:C:4150:LEU:HD23	2.00	0.44
1:D:2973:PHE:CD1	1:D:2973:PHE:C	2.95	0.44
1:D:3695:PRO:HB2	1:D:3699:HIS:HB3	1.99	0.44
1:D:5020:ASP:N	1:D:5020:ASP:OD2	2.51	0.44
1:A:2973:PHE:CD1	1:A:2973:PHE:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3695:PRO:HB2	1:A:3699:HIS:HB3	1.99	0.44
1:B:1186:ASP:OD2	1:B:1186:ASP:N	2.50	0.44
1:B:3198:ALA:HB2	1:B:3276:MET:CE	2.46	0.44
1:B:3736:GLU:HG2	1:B:3763:LEU:HD21	1.99	0.44
1:B:3780:LEU:HD21	1:B:3816:MET:HE1	2.00	0.44
1:C:688:LEU:HD11	1:C:775:GLY:HA3	1.99	0.44
1:C:1164:LEU:C	1:C:1164:LEU:HD23	2.42	0.44
1:C:1286:MET:HE1	1:C:1449:TRP:HZ3	1.83	0.44
1:C:5020:ASP:OD2	1:C:5020:ASP:N	2.51	0.44
1:D:3061:ALA:HB3	1:D:3062:PRO:HD3	1.98	0.44
1:D:3780:LEU:HD21	1:D:3816:MET:HE1	2.00	0.44
1:A:3778:MET:SD	1:A:3778:MET:C	3.01	0.44
1:A:3930:ILE:HD11	1:A:3951:PHE:CE1	2.53	0.44
1:D:345:LEU:HB3	1:D:387:ALA:HB1	2.00	0.44
1:D:3778:MET:SD	1:D:3778:MET:C	3.01	0.44
1:D:75:VAL:HG23	1:D:76:ARG:N	2.32	0.44
1:D:1286:MET:HE1	1:D:1449:TRP:HZ3	1.83	0.44
1:B:4097:MET:SD	1:B:4111:LEU:HD12	2.57	0.44
1:C:3778:MET:SD	1:C:3778:MET:C	3.01	0.44
1:D:1164:LEU:C	1:D:1164:LEU:HD23	2.42	0.44
1:D:2256:TYR:CD1	1:D:2256:TYR:C	2.96	0.44
2:G:104:LEU:HD23	2:G:104:LEU:N	2.32	0.44
1:C:4107:GLU:O	1:C:4111:LEU:HG	2.18	0.44
1:D:1186:ASP:OD2	1:D:1186:ASP:N	2.50	0.44
1:D:2777:TYR:HB2	1:D:2791:LEU:HD13	1.99	0.44
1:D:3930:ILE:HD11	1:D:3951:PHE:CE1	2.53	0.44
1:D:4097:MET:SD	1:D:4111:LEU:HD12	2.57	0.44
1:D:4793:GLY:O	1:D:4797:VAL:HG23	2.17	0.44
1:A:4045:VAL:HG22	1:A:4150:LEU:HD23	1.99	0.43
1:B:688:LEU:HD11	1:B:775:GLY:HA3	1.99	0.43
1:B:3693:LYS:O	1:B:3694:LYS:C	2.61	0.43
1:C:75:VAL:HG23	1:C:76:ARG:N	2.33	0.43
1:C:459:LEU:HD12	1:C:459:LEU:H	1.83	0.43
1:D:4039:MET:SD	1:D:4039:MET:C	3.01	0.43
1:A:3935:TRP:HB2	1:D:76:ARG:HD3	1.99	0.43
1:B:4107:GLU:O	1:B:4111:LEU:HG	2.18	0.43
1:B:4793:GLY:O	1:B:4797:VAL:HG23	2.17	0.43
1:C:1186:ASP:OD2	1:C:1186:ASP:N	2.50	0.43
1:C:3844:LEU:C	1:C:3844:LEU:HD12	2.43	0.43
1:C:3930:ILE:HD11	1:C:3951:PHE:CE1	2.53	0.43
1:A:613:ALA:HB2	1:A:1676:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3734:HIS:CG	1:A:3735:LEU:N	2.86	0.43
1:B:3734:HIS:CG	1:B:3735:LEU:N	2.86	0.43
1:B:3758:MET:SD	1:B:3758:MET:C	3.02	0.43
1:B:3930:ILE:HD11	1:B:3951:PHE:CE1	2.53	0.43
1:B:5020:ASP:OD2	1:B:5020:ASP:N	2.51	0.43
1:C:2490:MET:HE2	1:C:2490:MET:CA	2.49	0.43
1:C:2777:TYR:HB2	1:C:2791:LEU:HD13	1.99	0.43
1:C:4039:MET:SD	1:C:4039:MET:C	3.01	0.43
1:D:613:ALA:HB2	1:D:1676:LEU:HD12	2.01	0.43
1:D:3239:MET:SD	1:D:3239:MET:N	2.92	0.43
1:A:75:VAL:HG23	1:A:76:ARG:N	2.33	0.43
1:A:3693:LYS:O	1:A:3694:LYS:C	2.61	0.43
1:B:2332:LEU:N	1:B:2332:LEU:HD23	2.34	0.43
1:C:3239:MET:SD	1:C:3239:MET:N	2.92	0.43
1:C:3758:MET:SD	1:C:3758:MET:C	3.02	0.43
1:D:50:GLU:HA	1:D:50:GLU:OE1	2.19	0.43
1:D:3734:HIS:CG	1:D:3735:LEU:N	2.86	0.43
1:D:4178:LEU:HD23	1:D:4178:LEU:C	2.43	0.43
1:A:345:LEU:HB3	1:A:387:ALA:HB1	2.00	0.43
1:A:578:ILE:HG21	1:A:583:ILE:HD11	1.99	0.43
1:A:2256:TYR:C	1:A:2256:TYR:CD1	2.96	0.43
1:A:3758:MET:SD	1:A:3758:MET:C	3.02	0.43
1:B:459:LEU:H	1:B:459:LEU:HD12	1.83	0.43
1:D:459:LEU:HD12	1:D:459:LEU:H	1.83	0.43
1:A:459:LEU:HD12	1:A:459:LEU:H	1.83	0.43
1:A:2332:LEU:N	1:A:2332:LEU:HD23	2.34	0.43
1:A:2490:MET:HE2	1:A:2490:MET:CA	2.49	0.43
1:A:3195:ALA:CB	1:A:3341:PHE:HZ	2.32	0.43
1:A:4039:MET:SD	1:A:4039:MET:C	3.01	0.43
1:A:5020:ASP:OD2	1:A:5020:ASP:N	2.51	0.43
1:B:2256:TYR:CD1	1:B:2256:TYR:C	2.96	0.43
1:B:3844:LEU:HD12	1:B:3844:LEU:C	2.43	0.43
1:D:2490:MET:HE2	1:D:2490:MET:CA	2.49	0.43
1:D:3844:LEU:HD12	1:D:3844:LEU:C	2.43	0.43
1:D:4107:GLU:O	1:D:4111:LEU:HG	2.18	0.43
1:A:50:GLU:HA	1:A:50:GLU:OE1	2.19	0.43
1:A:3239:MET:SD	1:A:3239:MET:N	2.92	0.43
1:A:3844:LEU:C	1:A:3844:LEU:HD12	2.43	0.43
1:B:418:LEU:HD23	1:B:418:LEU:O	2.19	0.43
1:B:3239:MET:SD	1:B:3239:MET:N	2.92	0.43
1:B:3508:SER:OG	1:B:3510:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4178:LEU:C	1:C:4178:LEU:HD23	2.43	0.43
1:D:4834:GLY:O	1:D:4838:VAL:HG23	2.19	0.43
1:A:3508:SER:OG	1:A:3510:ILE:HG22	2.17	0.43
1:B:2490:MET:HE2	1:B:2490:MET:CA	2.49	0.43
1:B:3622:LYS:O	1:B:3623:LEU:C	2.62	0.43
1:B:4045:VAL:HG22	1:B:4150:LEU:HD23	1.99	0.43
1:C:345:LEU:HB3	1:C:387:ALA:HB1	2.00	0.43
1:C:3734:HIS:CG	1:C:3735:LEU:N	2.86	0.43
1:D:2974:ILE:HD13	1:D:3049:LEU:CD1	2.49	0.43
1:A:1286:MET:HE1	1:A:1449:TRP:HZ3	1.83	0.43
1:A:4178:LEU:HD23	1:A:4178:LEU:C	2.43	0.43
1:B:613:ALA:HB2	1:B:1676:LEU:HD12	2.00	0.43
1:B:1286:MET:HE1	1:B:1449:TRP:HZ3	1.83	0.43
1:B:4013:LEU:O	1:B:4017:LEU:HD23	2.18	0.43
1:C:368:ARG:CG	1:C:2307:LEU:HD22	2.49	0.43
1:C:613:ALA:HB2	1:C:1676:LEU:HD12	2.01	0.43
1:C:2256:TYR:CD1	1:C:2256:TYR:C	2.96	0.43
1:D:2332:LEU:N	1:D:2332:LEU:HD23	2.34	0.43
1:D:3780:LEU:HD21	1:D:3816:MET:SD	2.59	0.43
1:D:4001:MET:CG	1:D:4057:MET:HE2	2.46	0.43
2:E:6:THR:HG23	2:E:70:GLN:NE2	2.34	0.43
1:A:2974:ILE:HD13	1:A:3049:LEU:CD1	2.49	0.43
1:A:4013:LEU:O	1:A:4017:LEU:HD23	2.18	0.43
1:A:4107:GLU:O	1:A:4111:LEU:HG	2.18	0.43
1:B:4834:GLY:O	1:B:4838:VAL:HG23	2.19	0.43
1:B:4839:MET:HE1	1:C:4823:LEU:CB	2.49	0.43
1:C:3270:ILE:HD11	1:C:3338:LEU:HD22	2.01	0.43
1:D:2865:VAL:HG21	1:D:2928:LYS:HE2	2.01	0.43
1:A:418:LEU:O	1:A:418:LEU:HD23	2.19	0.42
1:A:2023:LEU:HD23	1:A:2024:PRO:HD2	2.01	0.42
1:A:2419:GLY:O	1:A:2423:MET:HG3	2.19	0.42
1:A:3780:LEU:HD21	1:A:3816:MET:HE1	2.00	0.42
1:B:368:ARG:CG	1:B:2307:LEU:HD22	2.49	0.42
1:B:459:LEU:HD12	1:B:459:LEU:N	2.34	0.42
1:B:4039:MET:SD	1:B:4039:MET:C	3.01	0.42
1:B:4178:LEU:C	1:B:4178:LEU:HD23	2.44	0.42
1:C:418:LEU:HD23	1:C:418:LEU:O	2.19	0.42
1:C:3693:LYS:O	1:C:3694:LYS:C	2.61	0.42
1:C:3780:LEU:HD21	1:C:3816:MET:HE1	2.00	0.42
1:C:3780:LEU:HD21	1:C:3816:MET:SD	2.59	0.42
1:D:2023:LEU:HD23	1:D:2024:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3758:MET:SD	1:D:3758:MET:C	3.02	0.42
1:D:4013:LEU:O	1:D:4017:LEU:HD23	2.18	0.42
2:G:6:THR:HG23	2:G:70:GLN:NE2	2.34	0.42
1:A:368:ARG:CG	1:A:2307:LEU:HD22	2.49	0.42
1:A:3424:LEU:HD12	1:D:1216:ILE:HD12	2.01	0.42
1:C:4013:LEU:O	1:C:4017:LEU:HD23	2.18	0.42
1:C:4834:GLY:O	1:C:4838:VAL:HG23	2.19	0.42
1:B:345:LEU:HB3	1:B:387:ALA:HB1	2.00	0.42
1:B:828:GLU:OE1	1:B:828:GLU:N	2.53	0.42
1:B:1296:GLN:OE1	1:B:1297:PHE:N	2.53	0.42
1:B:2777:TYR:HB2	1:B:2791:LEU:HD13	1.99	0.42
1:B:3195:ALA:CB	1:B:3341:PHE:HZ	2.32	0.42
1:B:3256:LEU:HD22	1:B:3261:ALA:HB3	2.01	0.42
1:C:2332:LEU:N	1:C:2332:LEU:HD23	2.34	0.42
1:C:2419:GLY:O	1:C:2423:MET:HG3	2.19	0.42
1:C:3010:PHE:CE1	1:C:3039:ILE:HD12	2.55	0.42
1:C:3622:LYS:O	1:C:3623:LEU:C	2.62	0.42
1:D:3759:GLU:O	1:D:3763:LEU:HD13	2.20	0.42
2:F:6:THR:HG23	2:F:70:GLN:NE2	2.34	0.42
2:H:6:THR:HG23	2:H:70:GLN:NE2	2.34	0.42
1:A:1280:GLN:O	1:A:1281:ASN:OD1	2.38	0.42
1:A:2777:TYR:HB2	1:A:2791:LEU:HD13	1.99	0.42
1:B:1280:GLN:O	1:B:1281:ASN:OD1	2.38	0.42
1:B:2668:SER:O	1:B:2669:GLU:HB3	2.20	0.42
1:B:4001:MET:CG	1:B:4057:MET:HE2	2.46	0.42
1:C:459:LEU:HD12	1:C:459:LEU:N	2.34	0.42
1:C:828:GLU:N	1:C:828:GLU:OE1	2.53	0.42
1:C:1280:GLN:O	1:C:1281:ASN:OD1	2.38	0.42
1:A:3172:ILE:HD12	1:A:3172:ILE:H	1.85	0.42
1:A:3622:LYS:O	1:A:3623:LEU:C	2.62	0.42
1:C:2865:VAL:HG21	1:C:2928:LYS:HE2	2.01	0.42
1:D:1113:VAL:HG12	1:D:1114:GLU:N	2.35	0.42
1:D:2390:PRO:O	1:D:2391:ALA:HB3	2.20	0.42
1:A:3780:LEU:HD21	1:A:3816:MET:SD	2.59	0.42
1:A:4834:GLY:O	1:A:4838:VAL:HG23	2.19	0.42
1:A:4839:MET:HE1	1:B:4823:LEU:CB	2.50	0.42
1:B:3010:PHE:CE1	1:B:3039:ILE:HD12	2.55	0.42
1:B:3172:ILE:HG23	1:B:3190:LEU:HD22	2.02	0.42
1:C:50:GLU:OE1	1:C:50:GLU:HA	2.19	0.42
1:D:828:GLU:OE1	1:D:828:GLU:N	2.52	0.42
1:D:3256:LEU:HD22	1:D:3261:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2376:LEU:CD2	1:A:2469:ILE:HD11	2.50	0.42
1:A:2465:ASP:O	1:A:2469:ILE:HD12	2.20	0.42
1:B:2465:ASP:O	1:B:2469:ILE:HD12	2.20	0.42
1:B:4058:ILE:HG22	1:B:4062:PHE:CE2	2.55	0.42
1:C:1083:VAL:HG22	1:C:1188:PHE:O	2.20	0.42
1:C:3172:ILE:HD12	1:C:3172:ILE:H	1.85	0.42
1:D:1108:GLU:OE2	1:D:1108:GLU:N	2.52	0.42
1:D:2419:GLY:O	1:D:2423:MET:HG3	2.19	0.42
2:F:103:LEU:N	2:F:103:LEU:HD12	2.34	0.42
1:A:2967:MET:HE2	1:A:3045:LYS:HD3	2.01	0.42
1:B:724:GLY:O	1:B:726:VAL:HG23	2.20	0.42
1:B:2376:LEU:CD2	1:B:2469:ILE:HD11	2.50	0.42
1:B:3759:GLU:O	1:B:3763:LEU:HD13	2.19	0.42
1:C:724:GLY:O	1:C:726:VAL:HG23	2.20	0.42
1:C:2376:LEU:CD2	1:C:2469:ILE:HD11	2.50	0.42
1:D:3010:PHE:CE1	1:D:3039:ILE:HD12	2.54	0.42
1:D:3693:LYS:O	1:D:3694:LYS:C	2.61	0.42
1:A:76:ARG:HD3	1:B:3935:TRP:HB2	2.01	0.42
1:A:2865:VAL:HG21	1:A:2928:LYS:HE2	2.01	0.42
1:A:3010:PHE:CE1	1:A:3039:ILE:HD12	2.54	0.42
1:A:3256:LEU:HD22	1:A:3261:ALA:HB3	2.01	0.42
1:A:4058:ILE:HG22	1:A:4062:PHE:CE2	2.55	0.42
1:B:334:MET:HA	1:B:334:MET:CE	2.47	0.42
1:B:2376:LEU:HD22	1:B:2469:ILE:HD11	2.01	0.42
1:C:2390:PRO:O	1:C:2391:ALA:HB3	2.20	0.42
1:C:3172:ILE:HG23	1:C:3190:LEU:HD22	2.02	0.42
1:C:3839:CYS:SG	1:C:3881:THR:HG23	2.60	0.42
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	2.02	0.42
1:D:2465:ASP:O	1:D:2469:ILE:HD12	2.20	0.42
1:D:2967:MET:HE2	1:D:3045:LYS:HD3	2.01	0.42
1:D:3195:ALA:CB	1:D:3341:PHE:HZ	2.32	0.42
1:D:3622:LYS:O	1:D:3623:LEU:C	2.62	0.42
1:D:4058:ILE:HG22	1:D:4062:PHE:CE2	2.55	0.42
2:E:103:LEU:HD12	2:E:103:LEU:N	2.35	0.42
1:A:165:VAL:HG13	1:A:204:PRO:HD3	2.02	0.42
1:A:2502:MET:HE2	1:A:2502:MET:HA	2.02	0.42
1:A:3312:LEU:N	1:A:3312:LEU:HD12	2.35	0.42
1:A:3759:GLU:O	1:A:3763:LEU:HD13	2.19	0.42
1:A:3916:ILE:HD12	1:A:3968:TYR:CD2	2.55	0.42
1:B:1152:MET:HE1	1:B:1161:ILE:HG22	2.02	0.42
1:B:2419:GLY:O	1:B:2423:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2023:LEU:HD23	1:C:2024:PRO:HD2	2.01	0.42
1:C:2668:SER:O	1:C:2669:GLU:HB3	2.20	0.42
1:C:2967:MET:HE2	1:C:3045:LYS:HD3	2.01	0.42
1:C:3195:ALA:CB	1:C:3341:PHE:HZ	2.32	0.42
1:D:368:ARG:CG	1:D:2307:LEU:HD22	2.49	0.42
1:D:418:LEU:O	1:D:418:LEU:HD23	2.19	0.42
1:D:2376:LEU:CD2	1:D:2469:ILE:HD11	2.50	0.42
1:D:3226:GLU:O	1:D:3227:ARG:HB2	2.20	0.42
1:D:3270:ILE:HD11	1:D:3338:LEU:HD22	2.01	0.42
1:D:3342:ALA:HB3	1:D:3411:LEU:HD21	2.02	0.42
1:D:3839:CYS:SG	1:D:3881:THR:HG23	2.60	0.42
1:D:3916:ILE:HD12	1:D:3968:TYR:CD2	2.55	0.42
1:A:459:LEU:HD12	1:A:459:LEU:N	2.34	0.41
1:A:828:GLU:N	1:A:828:GLU:OE1	2.53	0.41
1:A:3532:LEU:HD21	1:A:3560:GLN:HA	2.02	0.41
1:B:165:VAL:HG13	1:B:204:PRO:HD3	2.02	0.41
1:B:1083:VAL:HG22	1:B:1188:PHE:O	2.20	0.41
1:B:1113:VAL:HG12	1:B:1114:GLU:N	2.35	0.41
1:B:2023:LEU:HD23	1:B:2024:PRO:HD2	2.01	0.41
1:B:2390:PRO:O	1:B:2391:ALA:HB3	2.20	0.41
1:B:2974:ILE:HD13	1:B:3049:LEU:CD1	2.49	0.41
1:C:1113:VAL:HG12	1:C:1114:GLU:N	2.35	0.41
1:C:1296:GLN:OE1	1:C:1297:PHE:N	2.53	0.41
1:C:2376:LEU:HD22	1:C:2469:ILE:HD11	2.01	0.41
1:C:2502:MET:HE2	1:C:2502:MET:HA	2.02	0.41
1:C:3226:GLU:O	1:C:3227:ARG:HB2	2.20	0.41
1:C:3759:GLU:O	1:C:3763:LEU:HD13	2.19	0.41
1:D:459:LEU:HD12	1:D:459:LEU:N	2.34	0.41
1:D:1280:GLN:O	1:D:1281:ASN:OD1	2.38	0.41
2:G:103:LEU:HD12	2:G:103:LEU:N	2.35	0.41
2:H:103:LEU:N	2:H:103:LEU:HD12	2.34	0.41
1:A:2376:LEU:HD22	1:A:2469:ILE:HD11	2.01	0.41
1:A:3226:GLU:O	1:A:3227:ARG:HB2	2.20	0.41
1:B:2228:MET:HE1	1:B:2229:VAL:HG23	2.02	0.41
1:B:2502:MET:HA	1:B:2502:MET:HE2	2.02	0.41
1:B:3226:GLU:O	1:B:3227:ARG:HB2	2.20	0.41
1:B:3780:LEU:HD21	1:B:3816:MET:SD	2.59	0.41
1:C:165:VAL:HG13	1:C:204:PRO:HD3	2.02	0.41
1:C:2203:MET:HE2	1:C:2203:MET:HB3	1.94	0.41
1:C:3916:ILE:HD12	1:C:3968:TYR:CD2	2.55	0.41
1:D:2376:LEU:HD22	1:D:2469:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2502:MET:HE2	1:D:2502:MET:HA	2.02	0.41
1:D:3312:LEU:HD12	1:D:3312:LEU:N	2.35	0.41
1:A:724:GLY:O	1:A:726:VAL:HG23	2.20	0.41
1:B:2044:ILE:HG23	1:B:2045:GLN:N	2.35	0.41
1:B:3172:ILE:HD12	1:B:3172:ILE:H	1.85	0.41
1:B:4003:LEU:CB	1:B:4013:LEU:HD13	2.51	0.41
1:C:2465:ASP:O	1:C:2469:ILE:HD12	2.20	0.41
1:C:3256:LEU:HD22	1:C:3261:ALA:HB3	2.01	0.41
1:C:4003:LEU:CB	1:C:4013:LEU:HD13	2.50	0.41
1:D:2228:MET:HE1	1:D:2229:VAL:HG23	2.03	0.41
1:A:3270:ILE:HD11	1:A:3338:LEU:HD22	2.01	0.41
1:A:3613:TYR:O	1:A:3613:TYR:CD2	2.74	0.41
1:A:3839:CYS:SG	1:A:3881:THR:HG23	2.60	0.41
1:A:3936:TYR:HB2	1:D:76:ARG:HH21	1.86	0.41
1:B:50:GLU:OE1	1:B:50:GLU:HA	2.19	0.41
1:B:2865:VAL:HG21	1:B:2928:LYS:HE2	2.01	0.41
1:B:3270:ILE:HD11	1:B:3338:LEU:HD22	2.01	0.41
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	2.02	0.41
1:C:2786:LYS:O	1:C:2787:THR:HG23	2.20	0.41
1:C:4058:ILE:HG22	1:C:4062:PHE:CE2	2.55	0.41
1:C:4720:VAL:HG13	1:C:4721:LYS:N	2.35	0.41
1:D:165:VAL:HG13	1:D:204:PRO:HD3	2.02	0.41
1:D:1289:LEU:O	1:D:1551:ALA:HB1	2.21	0.41
1:D:3996:PHE:O	1:D:4000:MET:HG3	2.21	0.41
1:A:1083:VAL:HG22	1:A:1188:PHE:O	2.20	0.41
1:A:1113:VAL:HG12	1:A:1114:GLU:N	2.35	0.41
1:A:1152:MET:HE1	1:A:1161:ILE:HG22	2.02	0.41
1:A:1296:GLN:OE1	1:A:1297:PHE:N	2.53	0.41
1:A:3172:ILE:HG23	1:A:3190:LEU:HD22	2.02	0.41
1:B:1769:THR:O	1:B:1769:THR:HG22	2.20	0.41
1:B:2786:LYS:O	1:B:2787:THR:HG23	2.20	0.41
1:B:3312:LEU:N	1:B:3312:LEU:HD12	2.35	0.41
1:B:3996:PHE:O	1:B:4000:MET:HG3	2.21	0.41
1:C:76:ARG:HH21	1:D:3936:TYR:HB2	1.86	0.41
1:C:1769:THR:HG22	1:C:1769:THR:O	2.20	0.41
1:C:2228:MET:HE1	1:C:2229:VAL:HG23	2.02	0.41
1:D:2668:SER:O	1:D:2669:GLU:HB3	2.20	0.41
1:D:3172:ILE:HG23	1:D:3190:LEU:HD22	2.02	0.41
1:D:4003:LEU:HB3	1:D:4013:LEU:HD13	2.02	0.41
1:A:2786:LYS:O	1:A:2787:THR:HG23	2.20	0.41
1:A:3965:LEU:HD13	1:A:4026:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2203:MET:HE2	1:B:2203:MET:HB3	1.94	0.41
1:B:3816:MET:HE3	1:B:3816:MET:HB3	2.00	0.41
1:B:3916:ILE:HD12	1:B:3968:TYR:CD2	2.55	0.41
1:C:76:ARG:HH22	1:D:3933:PHE:CA	2.34	0.41
1:C:1152:MET:HE1	1:C:1161:ILE:HG22	2.02	0.41
1:C:1289:LEU:O	1:C:1551:ALA:HB1	2.21	0.41
1:C:3342:ALA:HB3	1:C:3411:LEU:HD21	2.02	0.41
1:D:724:GLY:O	1:D:726:VAL:HG23	2.20	0.41
1:D:1689:VAL:HG11	1:D:1694:LEU:HD21	2.03	0.41
1:D:1769:THR:O	1:D:1769:THR:HG22	2.20	0.41
1:D:3965:LEU:HD13	1:D:4026:MET:HE1	2.03	0.41
2:F:23:VAL:HG13	2:F:47:LYS:HZ2	1.86	0.41
2:G:79:ASP:OD2	2:G:79:ASP:C	2.64	0.41
1:A:1689:VAL:HG11	1:A:1694:LEU:HD21	2.03	0.41
1:A:2044:ILE:HG23	1:A:2045:GLN:N	2.35	0.41
1:A:4003:LEU:CB	1:A:4013:LEU:HD13	2.51	0.41
1:B:1689:VAL:HG11	1:B:1694:LEU:HD21	2.03	0.41
1:B:2967:MET:HE2	1:B:3045:LYS:HD3	2.01	0.41
1:B:4976:GLU:OE1	1:B:4977:THR:HG23	2.20	0.41
1:C:1689:VAL:HG11	1:C:1694:LEU:HD21	2.03	0.41
1:C:2044:ILE:HG23	1:C:2045:GLN:N	2.35	0.41
1:C:2974:ILE:HD13	1:C:3049:LEU:CD1	2.49	0.41
1:C:4688:ILE:N	1:C:4688:ILE:HD12	2.35	0.41
1:D:867:LEU:HA	1:D:870:ILE:HG22	2.03	0.41
1:D:1296:GLN:OE1	1:D:1297:PHE:N	2.53	0.41
1:D:3172:ILE:HD12	1:D:3172:ILE:H	1.85	0.41
1:D:3499:ARG:O	1:D:3499:ARG:HG3	2.21	0.41
1:A:2023:LEU:HD22	1:A:2027:ILE:HB	2.03	0.41
1:A:2225:PHE:O	1:A:2228:MET:SD	2.79	0.41
1:A:2228:MET:HE1	1:A:2229:VAL:HG23	2.03	0.41
1:A:4003:LEU:HB3	1:A:4013:LEU:HD13	2.03	0.41
1:B:816:LEU:N	1:B:816:LEU:HD22	2.36	0.41
1:B:3532:LEU:HD21	1:B:3560:GLN:HA	2.02	0.41
1:C:867:LEU:HA	1:C:870:ILE:HG22	2.03	0.41
1:C:2254:LEU:O	1:C:2258:LEU:HD23	2.21	0.41
1:C:3499:ARG:HG3	1:C:3499:ARG:O	2.21	0.41
1:D:816:LEU:N	1:D:816:LEU:HD22	2.36	0.41
1:D:2023:LEU:HD22	1:D:2027:ILE:HB	2.03	0.41
1:D:2101:MET:SD	1:D:2101:MET:C	3.04	0.41
1:D:4720:VAL:HG13	1:D:4721:LYS:N	2.35	0.41
1:D:4976:GLU:OE1	1:D:4977:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:VAL:HG13	2:E:47:LYS:HZ2	1.86	0.41
2:H:79:ASP:OD2	2:H:79:ASP:C	2.64	0.41
1:A:816:LEU:HD22	1:A:816:LEU:N	2.36	0.41
1:A:1289:LEU:O	1:A:1551:ALA:HB1	2.21	0.41
1:A:1849:LEU:HD11	1:A:1945:TYR:CE1	2.56	0.41
1:A:2101:MET:SD	1:A:2101:MET:C	3.04	0.41
1:A:3342:ALA:HB3	1:A:3411:LEU:HD21	2.02	0.41
1:A:4001:MET:CG	1:A:4057:MET:HE2	2.46	0.41
1:A:4720:VAL:HG13	1:A:4721:LYS:N	2.35	0.41
1:A:4976:GLU:OE1	1:A:4977:THR:HG23	2.20	0.41
1:B:168:ASP:C	1:B:169:LEU:HD22	2.46	0.41
1:B:456:SER:OG	1:B:457:GLU:N	2.54	0.41
1:B:2101:MET:SD	1:B:2101:MET:C	3.04	0.41
1:B:2225:PHE:O	1:B:2228:MET:SD	2.79	0.41
1:B:2254:LEU:O	1:B:2258:LEU:HD23	2.21	0.41
1:B:3499:ARG:O	1:B:3499:ARG:HG3	2.21	0.41
1:B:3613:TYR:O	1:B:3613:TYR:CD2	2.74	0.41
1:B:3839:CYS:SG	1:B:3881:THR:HG23	2.60	0.41
1:B:4720:VAL:HG13	1:B:4721:LYS:N	2.35	0.41
1:B:4820:VAL:HG12	1:B:4822:THR:H	1.86	0.41
1:C:2101:MET:C	1:C:2101:MET:SD	3.04	0.41
1:C:3312:LEU:N	1:C:3312:LEU:HD12	2.35	0.41
1:C:3409:TYR:N	1:C:3410:PRO:HD2	2.36	0.41
1:C:3613:TYR:O	1:C:3613:TYR:CD2	2.74	0.41
1:C:4976:GLU:OE1	1:C:4977:THR:HG23	2.20	0.41
1:D:334:MET:HA	1:D:334:MET:CE	2.47	0.41
1:D:456:SER:OG	1:D:457:GLU:N	2.54	0.41
1:D:1083:VAL:HG22	1:D:1188:PHE:O	2.20	0.41
1:D:1849:LEU:HD11	1:D:1945:TYR:CE1	2.56	0.41
1:D:2044:ILE:HG23	1:D:2045:GLN:N	2.35	0.41
1:D:4003:LEU:CB	1:D:4013:LEU:HD13	2.50	0.41
1:A:334:MET:HA	1:A:334:MET:CE	2.47	0.41
1:A:2668:SER:O	1:A:2669:GLU:HB3	2.20	0.41
1:B:2516:ASP:OD1	1:B:2517:PHE:N	2.54	0.41
1:B:4688:ILE:N	1:B:4688:ILE:HD12	2.35	0.41
1:B:4789:PHE:CD1	1:B:4789:PHE:C	2.99	0.41
1:C:1849:LEU:HD11	1:C:1945:TYR:CE1	2.56	0.41
1:C:4067:LYS:HD3	1:C:4067:LYS:O	2.21	0.41
1:C:4091:LYS:N	1:C:4091:LYS:HD3	2.36	0.41
1:D:2516:ASP:OD1	1:D:2517:PHE:N	2.54	0.41
1:D:2543:THR:HG23	1:D:2548:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3532:LEU:HD21	1:D:3560:GLN:HA	2.02	0.41
1:D:4067:LYS:HD3	1:D:4067:LYS:O	2.21	0.41
2:G:23:VAL:HG13	2:G:47:LYS:HZ2	1.86	0.41
1:A:3499:ARG:HG3	1:A:3499:ARG:O	2.21	0.40
1:A:3758:MET:HE3	1:A:3759:GLU:N	2.36	0.40
1:A:4688:ILE:HD12	1:A:4688:ILE:N	2.35	0.40
1:B:293:LEU:HD13	1:B:378:LEU:HD12	2.04	0.40
1:B:623:GLU:C	1:B:623:GLU:OE1	2.64	0.40
1:B:1289:LEU:O	1:B:1551:ALA:HB1	2.21	0.40
1:B:3965:LEU:HD13	1:B:4026:MET:HE1	2.03	0.40
1:B:4067:LYS:HD3	1:B:4067:LYS:O	2.21	0.40
1:C:816:LEU:N	1:C:816:LEU:HD22	2.36	0.40
1:D:3858:MET:SD	1:D:3859:VAL:N	2.94	0.40
1:D:4789:PHE:CD1	1:D:4789:PHE:C	2.99	0.40
2:E:29:MET:HB2	2:E:98:VAL:HG13	2.04	0.40
2:F:79:ASP:OD2	2:F:79:ASP:C	2.64	0.40
1:A:76:ARG:HH22	1:B:3933:PHE:CA	2.35	0.40
1:A:456:SER:OG	1:A:457:GLU:N	2.54	0.40
1:A:2390:PRO:O	1:A:2391:ALA:HB3	2.20	0.40
1:B:1849:LEU:HD11	1:B:1945:TYR:CE1	2.56	0.40
1:B:2663:ASN:ND2	1:B:2663:ASN:C	2.80	0.40
1:C:2516:ASP:OD1	1:C:2517:PHE:N	2.54	0.40
1:C:2543:THR:HG23	1:C:2548:LEU:HD11	2.03	0.40
1:C:3965:LEU:HD13	1:C:4026:MET:HE1	2.03	0.40
2:F:29:MET:HB2	2:F:98:VAL:HG13	2.04	0.40
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.02	0.40
1:A:3858:MET:SD	1:A:3859:VAL:N	2.94	0.40
1:B:2023:LEU:HD22	1:B:2027:ILE:HB	2.03	0.40
1:C:4003:LEU:HB3	1:C:4013:LEU:HD13	2.02	0.40
1:C:4839:MET:HE1	1:D:4823:LEU:CB	2.51	0.40
1:D:368:ARG:HG3	1:D:2307:LEU:HD22	2.03	0.40
1:D:2254:LEU:O	1:D:2258:LEU:HD23	2.21	0.40
1:D:2376:LEU:C	1:D:2376:LEU:HD23	2.47	0.40
1:D:2786:LYS:O	1:D:2787:THR:HG23	2.20	0.40
1:D:3613:TYR:O	1:D:3613:TYR:CD2	2.74	0.40
1:D:3758:MET:HE3	1:D:3759:GLU:N	2.36	0.40
1:A:50:GLU:OE1	1:A:50:GLU:CA	2.70	0.40
1:A:1769:THR:HG22	1:A:1769:THR:O	2.20	0.40
1:A:2590:SER:OG	1:A:2639:MET:HE1	2.22	0.40
1:B:76:ARG:HH22	1:C:3933:PHE:CA	2.34	0.40
1:B:3342:ALA:HB3	1:B:3411:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3943:ILE:HD12	1:B:3943:ILE:N	2.37	0.40
1:C:30:LYS:O	1:C:30:LYS:CG	2.70	0.40
1:C:168:ASP:C	1:C:169:LEU:HD22	2.46	0.40
1:C:456:SER:OG	1:C:457:GLU:N	2.54	0.40
1:C:3532:LEU:HD21	1:C:3560:GLN:HA	2.02	0.40
1:C:3996:PHE:O	1:C:4000:MET:HG3	2.21	0.40
1:C:4820:VAL:HG12	1:C:4822:THR:H	1.86	0.40
1:D:2550:LEU:HD12	1:D:2550:LEU:HA	1.97	0.40
1:D:4091:LYS:N	1:D:4091:LYS:HD3	2.36	0.40
1:D:4688:ILE:HD12	1:D:4688:ILE:N	2.35	0.40
1:A:2550:LEU:HD12	1:A:2550:LEU:HA	1.97	0.40
1:A:3281:LEU:HB2	1:A:3282:PRO:HD3	2.04	0.40
1:A:4564:PHE:CD1	1:A:4564:PHE:C	3.00	0.40
1:A:4789:PHE:CD1	1:A:4789:PHE:C	2.99	0.40
1:C:623:GLU:OE1	1:C:623:GLU:C	2.64	0.40
1:C:2590:SER:OG	1:C:2639:MET:HE1	2.22	0.40
1:C:4789:PHE:CD1	1:C:4789:PHE:C	2.99	0.40
1:D:623:GLU:C	1:D:623:GLU:OE1	2.64	0.40
1:D:4177:TYR:CD1	1:D:4177:TYR:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4376/5037 (87%)	4180 (96%)	196 (4%)	0	100	100
1	B	4376/5037 (87%)	4180 (96%)	196 (4%)	0	100	100
1	C	4376/5037 (87%)	4179 (96%)	197 (4%)	0	100	100
1	D	4376/5037 (87%)	4177 (96%)	199 (4%)	0	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17924/20580 (87%)	17124 (96%)	800 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	3827/4276 (90%)	3772 (99%)	55 (1%)	59	71
1	B	3827/4276 (90%)	3773 (99%)	54 (1%)	59	71
1	C	3827/4276 (90%)	3773 (99%)	54 (1%)	59	71
1	D	3827/4276 (90%)	3770 (98%)	57 (2%)	57	70
2	E	89/90 (99%)	88 (99%)	1 (1%)	65	74
2	F	89/90 (99%)	88 (99%)	1 (1%)	65	74
2	G	89/90 (99%)	88 (99%)	1 (1%)	65	74
2	H	89/90 (99%)	88 (99%)	1 (1%)	65	74
All	All	15664/17464 (90%)	15440 (99%)	224 (1%)	57	71

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	78	LEU
1	A	421	PHE
1	A	449	ILE
1	A	453	GLU
1	A	557	SER
1	A	710	ASP
1	A	714	TYR

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Mol	Chain	Res	Type
1	A	828	GLU
1	A	884	LEU
1	A	937	CYS
1	A	950	LEU
1	A	957	LYS
1	A	1027	LEU
1	A	1067	SER
1	A	1159	THR
1	A	1163	THR
1	A	1263	THR
1	A	1281	ASN
1	A	1435	TYR
1	A	1635	THR
1	A	1724	CYS
1	A	1746	THR
1	A	1931	LEU
1	A	1948	ASP
1	A	2123	LEU
1	A	2243	SER
1	A	2356	LEU
1	A	2482	ASP
1	A	2518	LEU
1	A	2559	LEU
1	A	2663	ASN
1	A	2697	ARG
1	A	2700	MET
1	A	2880	GLU
1	A	2911	LEU
1	A	2939	ARG
1	A	3001	ILE
1	A	3168	THR
1	A	3170	CYS
1	A	3226	GLU
1	A	3270	ILE
1	A	3359	ILE
1	A	3692	GLU
1	A	3804	ILE
1	A	3879	GLU
1	A	3949	ARG
1	A	3951	PHE
1	A	4034	ASN
1	A	4110	PHE

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Mol	Chain	Res	Type
1	A	4113	SER
1	A	4162	ASN
1	A	4187	SER
1	A	4580	TYR
1	A	4725	LEU
1	B	17	ASP
1	B	78	LEU
1	B	421	PHE
1	B	449	ILE
1	B	453	GLU
1	B	557	SER
1	B	710	ASP
1	B	714	TYR
1	B	828	GLU
1	B	884	LEU
1	B	937	CYS
1	B	950	LEU
1	B	957	LYS
1	B	1027	LEU
1	B	1067	SER
1	B	1159	THR
1	B	1163	THR
1	B	1263	THR
1	B	1281	ASN
1	B	1435	TYR
1	B	1724	CYS
1	B	1739	THR
1	B	1746	THR
1	B	1931	LEU
1	B	1948	ASP
1	B	2123	LEU
1	B	2243	SER
1	B	2482	ASP
1	B	2518	LEU
1	B	2559	LEU
1	B	2663	ASN
1	B	2697	ARG
1	B	2700	MET
1	B	2880	GLU
1	B	2911	LEU
1	B	2939	ARG
1	B	3001	ILE

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Mol	Chain	Res	Type
1	B	3168	THR
1	B	3170	CYS
1	B	3226	GLU
1	B	3270	ILE
1	B	3359	ILE
1	B	3692	GLU
1	B	3804	ILE
1	B	3831	SER
1	B	3879	GLU
1	B	3949	ARG
1	B	3951	PHE
1	B	4034	ASN
1	B	4110	PHE
1	B	4113	SER
1	B	4187	SER
1	B	4580	TYR
1	B	4725	LEU
1	C	17	ASP
1	C	78	LEU
1	C	421	PHE
1	C	449	ILE
1	C	453	GLU
1	C	557	SER
1	C	710	ASP
1	C	714	TYR
1	C	828	GLU
1	C	884	LEU
1	C	937	CYS
1	C	950	LEU
1	C	957	LYS
1	C	1027	LEU
1	C	1067	SER
1	C	1159	THR
1	C	1163	THR
1	C	1263	THR
1	C	1281	ASN
1	C	1435	TYR
1	C	1635	THR
1	C	1724	CYS
1	C	1746	THR
1	C	1931	LEU
1	C	1948	ASP

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Mol	Chain	Res	Type
1	C	2123	LEU
1	C	2243	SER
1	C	2482	ASP
1	C	2518	LEU
1	C	2559	LEU
1	C	2663	ASN
1	C	2697	ARG
1	C	2700	MET
1	C	2880	GLU
1	C	2911	LEU
1	C	2939	ARG
1	C	3001	ILE
1	C	3168	THR
1	C	3170	CYS
1	C	3226	GLU
1	C	3270	ILE
1	C	3359	ILE
1	C	3692	GLU
1	C	3804	ILE
1	C	3831	SER
1	C	3879	GLU
1	C	3949	ARG
1	C	3951	PHE
1	C	4034	ASN
1	C	4110	PHE
1	C	4113	SER
1	C	4187	SER
1	C	4580	TYR
1	C	4725	LEU
1	D	17	ASP
1	D	78	LEU
1	D	421	PHE
1	D	449	ILE
1	D	453	GLU
1	D	557	SER
1	D	710	ASP
1	D	714	TYR
1	D	828	GLU
1	D	884	LEU
1	D	937	CYS
1	D	950	LEU
1	D	957	LYS

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Mol	Chain	Res	Type
1	D	1027	LEU
1	D	1067	SER
1	D	1159	THR
1	D	1163	THR
1	D	1263	THR
1	D	1281	ASN
1	D	1435	TYR
1	D	1635	THR
1	D	1724	CYS
1	D	1739	THR
1	D	1746	THR
1	D	1931	LEU
1	D	1948	ASP
1	D	2123	LEU
1	D	2243	SER
1	D	2482	ASP
1	D	2518	LEU
1	D	2559	LEU
1	D	2663	ASN
1	D	2697	ARG
1	D	2700	MET
1	D	2880	GLU
1	D	2911	LEU
1	D	2939	ARG
1	D	3001	ILE
1	D	3168	THR
1	D	3170	CYS
1	D	3207	GLU
1	D	3226	GLU
1	D	3270	ILE
1	D	3359	ILE
1	D	3692	GLU
1	D	3804	ILE
1	D	3831	SER
1	D	3879	GLU
1	D	3949	ARG
1	D	3951	PHE
1	D	4034	ASN
1	D	4110	PHE
1	D	4113	SER
1	D	4187	SER
1	D	4580	TYR

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Mol	Chain	Res	Type
1	D	4725	LEU
1	D	4889	VAL
2	E	55	VAL
2	F	55	VAL
2	G	55	VAL
2	H	55	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	226	HIS
1	A	582	HIS
1	A	797	HIS
1	A	1420	ASN
1	A	1511	HIS
1	A	1611	HIS
1	A	1941	ASN
1	A	1970	GLN
1	A	2007	ASN
1	A	2245	GLN
1	A	2291	GLN
1	A	2308	GLN
1	A	2417	HIS
1	A	2487	GLN
1	A	2574	HIS
1	A	2584	HIS
1	A	2646	ASN
1	A	2774	ASN
1	A	2892	GLN
1	A	3069	HIS
1	A	3109	ASN
1	A	3430	ASN
1	A	3994	HIS
1	A	3998	HIS
1	A	4156	HIS
1	A	4547	GLN
1	A	4805	ASN
1	A	4812	HIS
1	A	4832	HIS
1	B	57	ASN
1	B	226	HIS

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Mol	Chain	Res	Type
1	B	284	HIS
1	B	797	HIS
1	B	1511	HIS
1	B	1611	HIS
1	B	1970	GLN
1	B	2007	ASN
1	B	2245	GLN
1	B	2308	GLN
1	B	2417	HIS
1	B	2487	GLN
1	B	2574	HIS
1	B	2584	HIS
1	B	2646	ASN
1	B	2774	ASN
1	B	3069	HIS
1	B	3430	ASN
1	B	3994	HIS
1	B	3998	HIS
1	B	4156	HIS
1	B	4547	GLN
1	B	4805	ASN
1	B	4832	HIS
1	B	4836	GLN
1	C	57	ASN
1	C	226	HIS
1	C	582	HIS
1	C	797	HIS
1	C	1280	GLN
1	C	1511	HIS
1	C	1611	HIS
1	C	1970	GLN
1	C	2007	ASN
1	C	2308	GLN
1	C	2417	HIS
1	C	2487	GLN
1	C	2574	HIS
1	C	2584	HIS
1	C	2646	ASN
1	C	2774	ASN
1	C	2892	GLN
1	C	3052	HIS
1	C	3069	HIS

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Mol	Chain	Res	Type
1	C	3430	ASN
1	C	3457	ASN
1	C	3994	HIS
1	C	3998	HIS
1	C	4156	HIS
1	C	4547	GLN
1	C	4812	HIS
1	C	4832	HIS
1	C	4836	GLN
1	D	57	ASN
1	D	226	HIS
1	D	797	HIS
1	D	1420	ASN
1	D	1511	HIS
1	D	1611	HIS
1	D	1941	ASN
1	D	1970	GLN
1	D	2007	ASN
1	D	2245	GLN
1	D	2417	HIS
1	D	2487	GLN
1	D	2574	HIS
1	D	2584	HIS
1	D	2646	ASN
1	D	2774	ASN
1	D	2892	GLN
1	D	3052	HIS
1	D	3069	HIS
1	D	3109	ASN
1	D	3430	ASN
1	D	3457	ASN
1	D	3994	HIS
1	D	3998	HIS
1	D	4156	HIS
1	D	4547	GLN
1	D	4832	HIS
1	D	4836	GLN

5.3.3 RNA ⓘ

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.

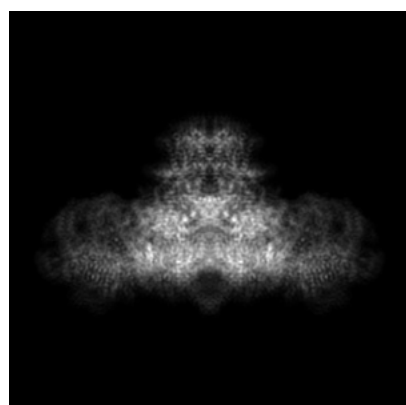
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54597. These allow visual inspection of the internal detail of the map and identification of artifacts.

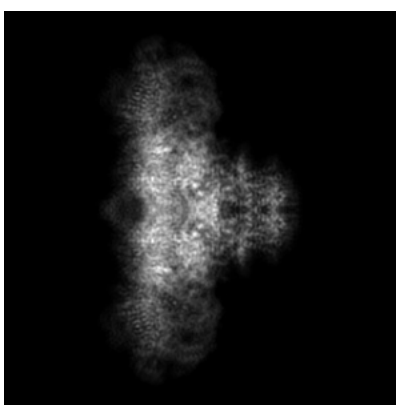
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

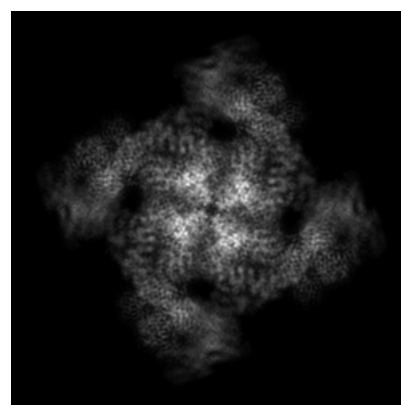
6.1.1 Primary map



X



Y



Z

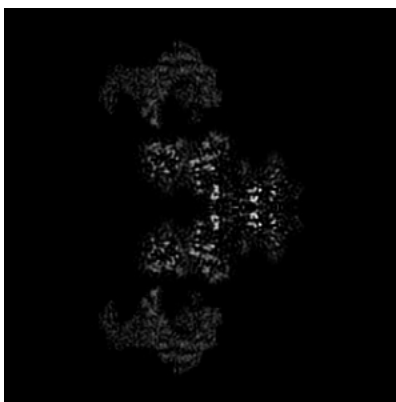
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

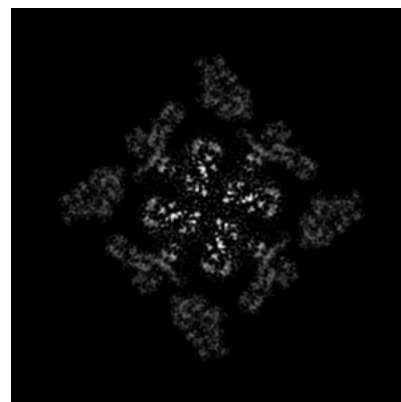
6.2.1 Primary map



X Index: 150



Y Index: 150

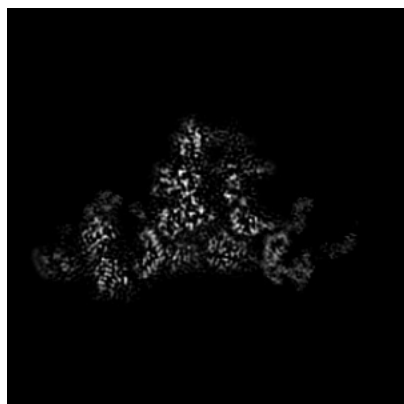


Z Index: 150

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: 127



Y Index: 127

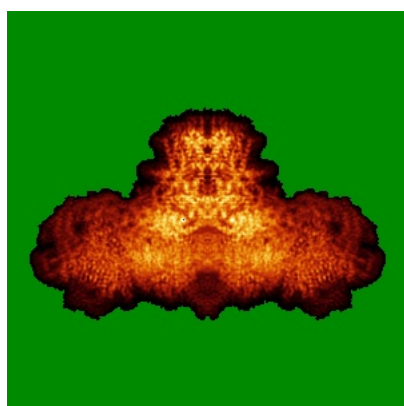


Z Index: 114

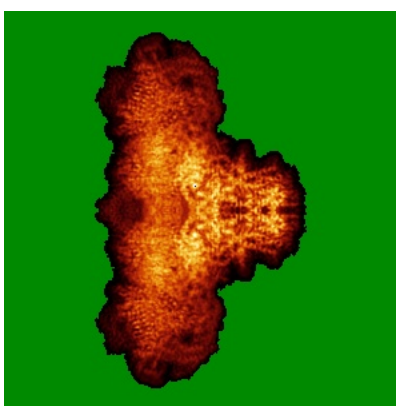
The images above show the largest variance slices of the map in three orthogonal directions.

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

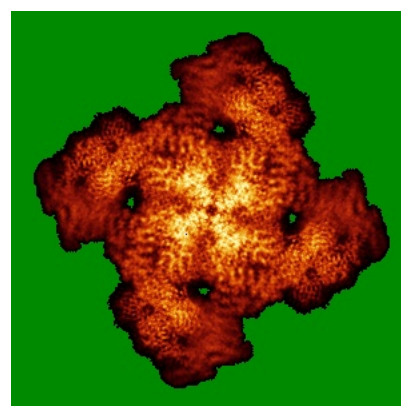
6.4.1 Primary map



X



Y



Z

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 0.779. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

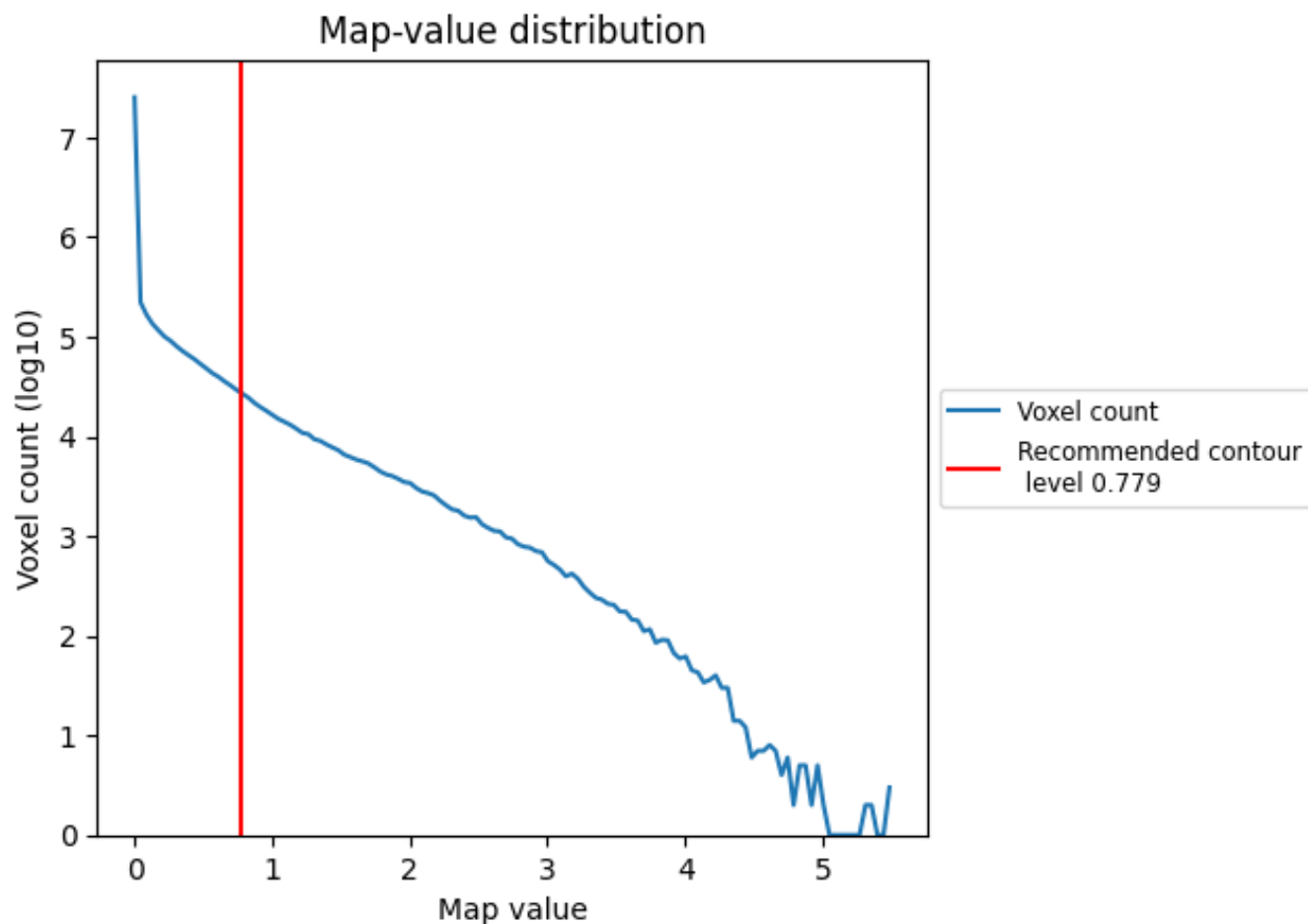
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

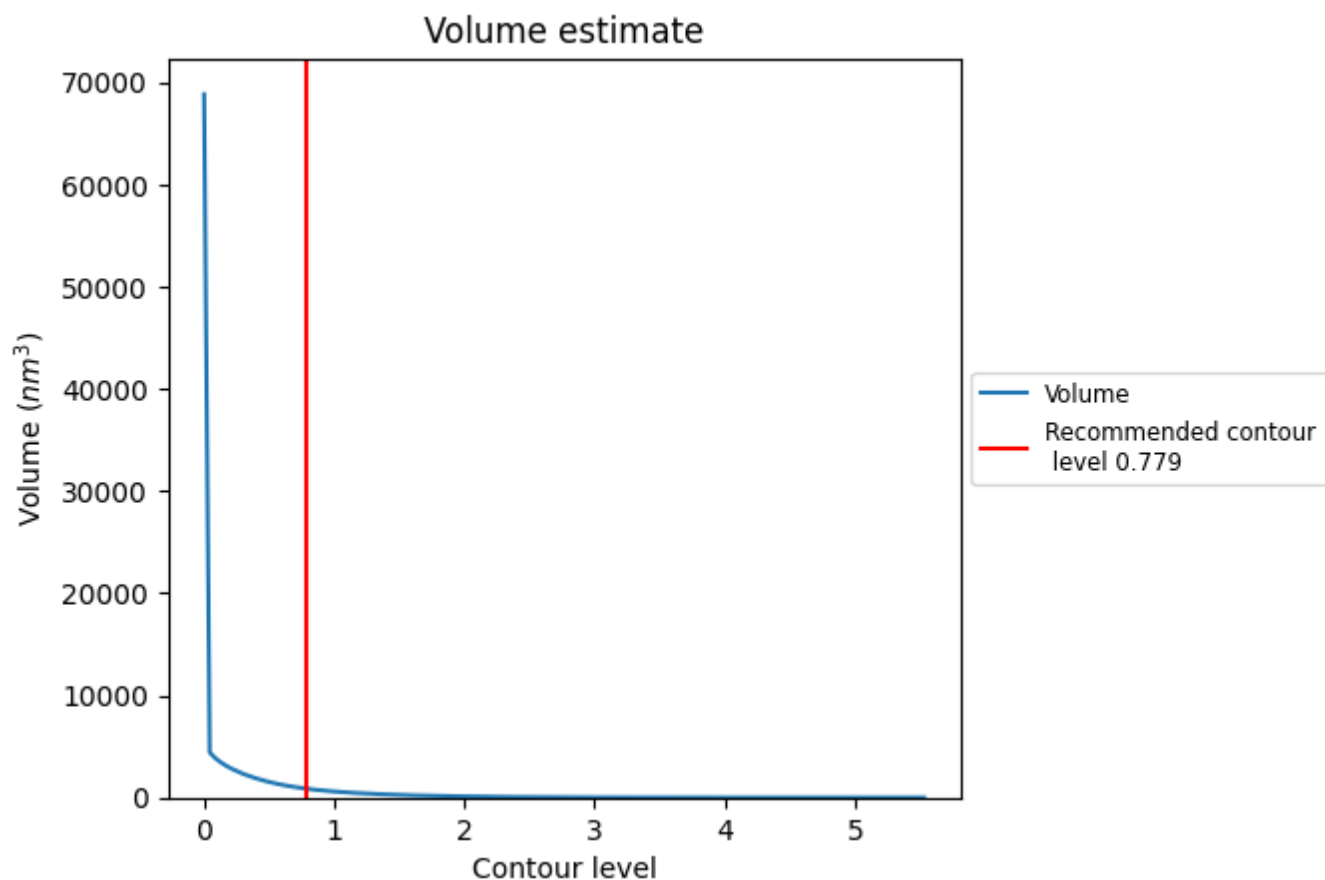
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

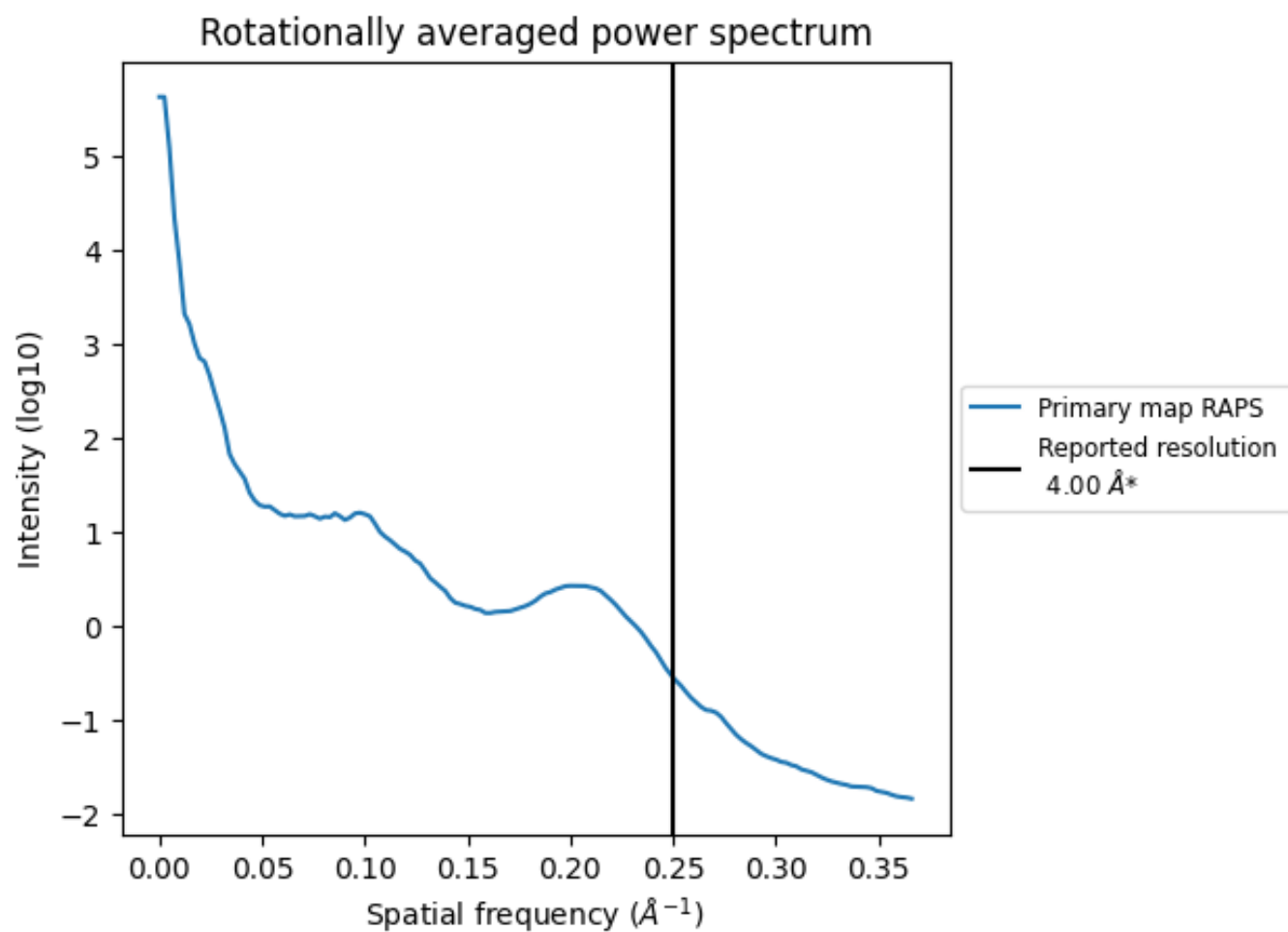
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880 nm³; this corresponds to an approximate mass of 794 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 0.250 Å⁻¹

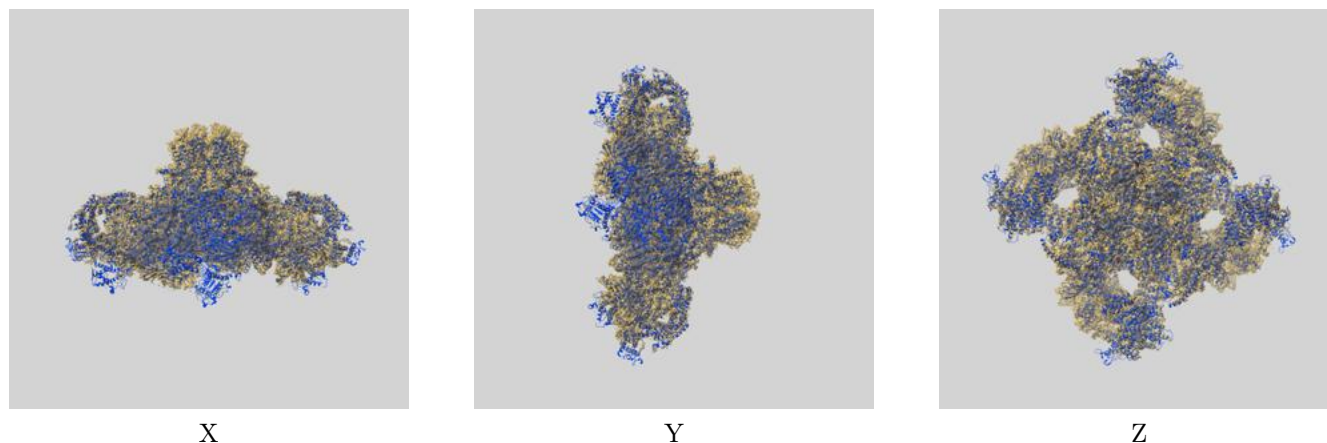
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

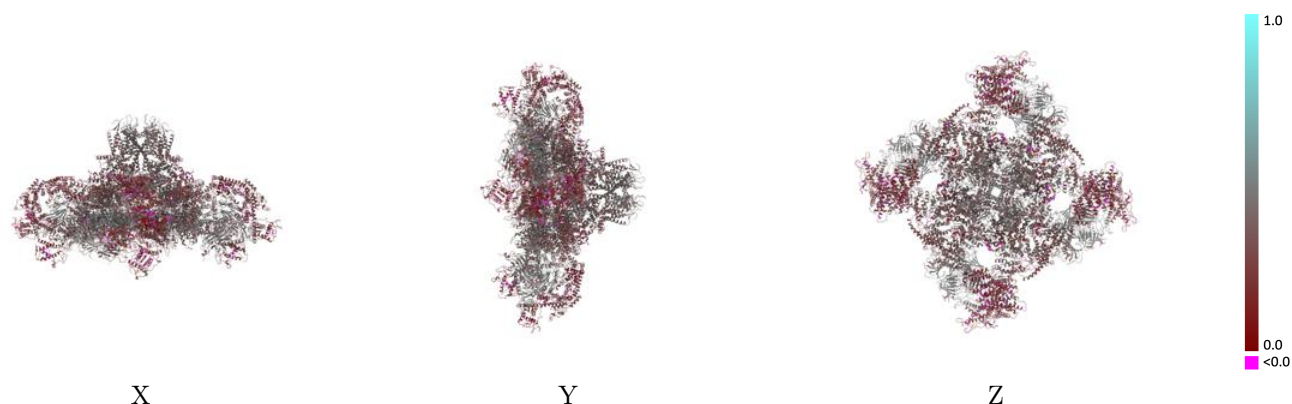
This section contains information regarding the fit between EMDB map EMD-54597 and PDB model 9S5F. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



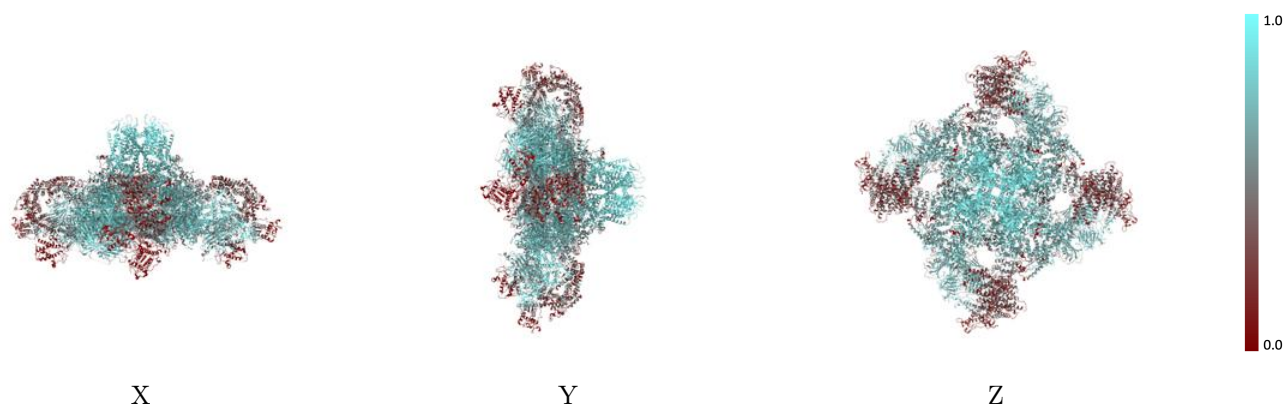
The images above show the 3D surface view of the map at the recommended contour level 0.779 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



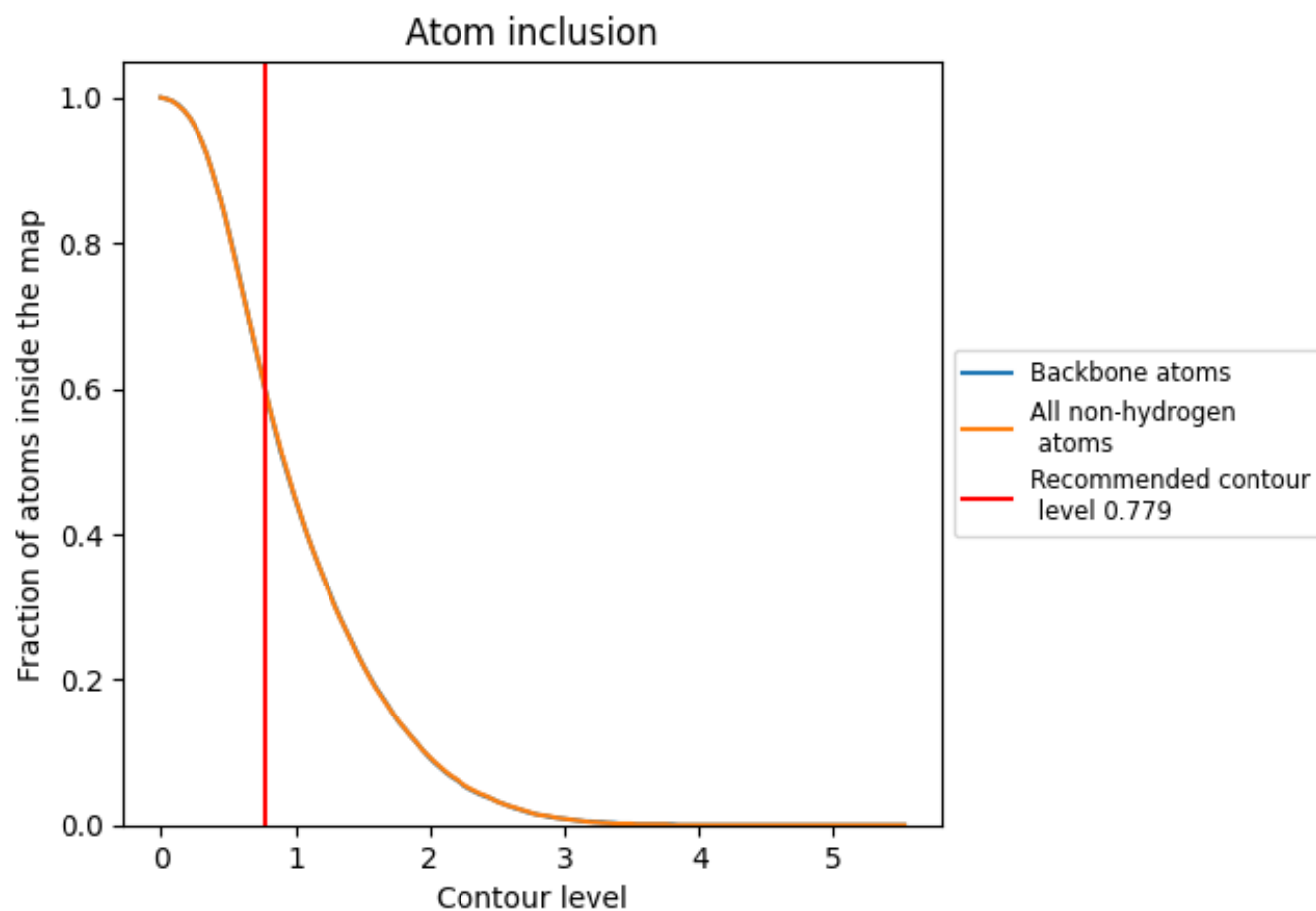
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.779).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.779) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5970	0.3560
A	0.6030	0.3540
B	0.6030	0.3540
C	0.6030	0.3540
D	0.6050	0.3540
E	0.6590	0.4340
F	0.6630	0.4370
G	0.6580	0.4380
H	0.6530	0.4350

1.0

0.0

<0.0