



Full wwPDB EM Validation Report ⓘ

Jul 20, 2026 – 04:42 pm BST

PDB ID : 9S1H / pdb_00009s1h
EMDB ID : EMD-54454
Title : Apo-state RyR1 with ACP in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-18
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:

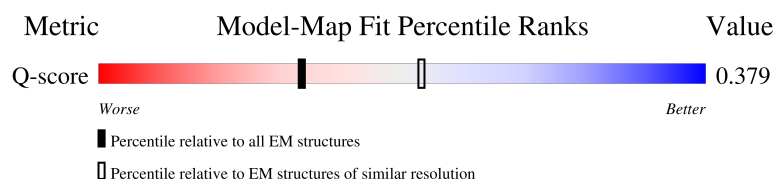
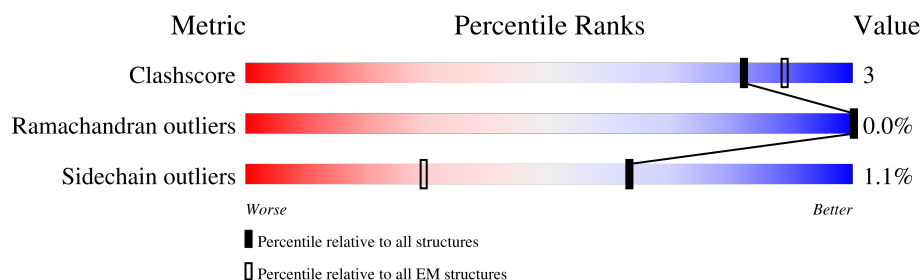
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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	20% 81% 6% 13%
1	B	5037	20% 81% 6% 13%
1	C	5037	20% 81% 6% 13%
1	D	5037	20% 81% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	90% 8% ..
2	F	108	90% 8% ..
2	G	108	90% 8% ..
2	H	108	90% 8% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 286116 atoms, of which 142308 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
			69822	22323	34734	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	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).

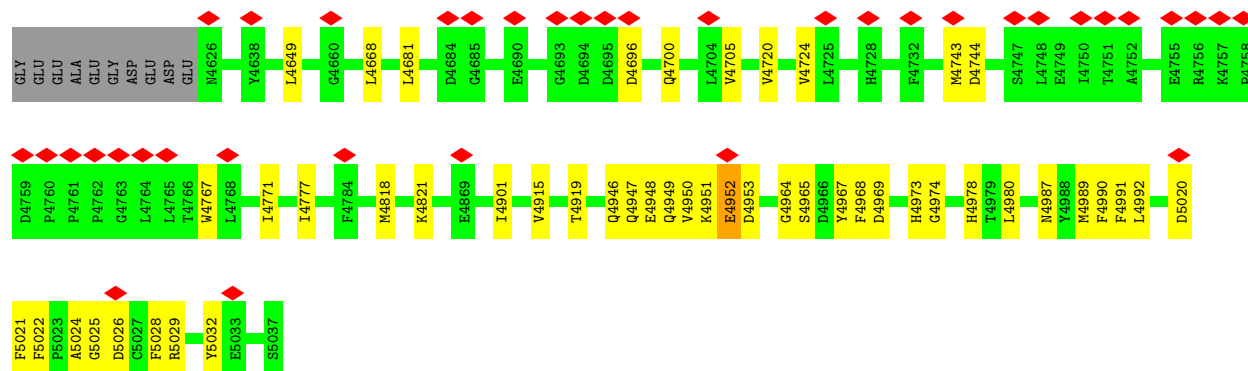
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- # ACP

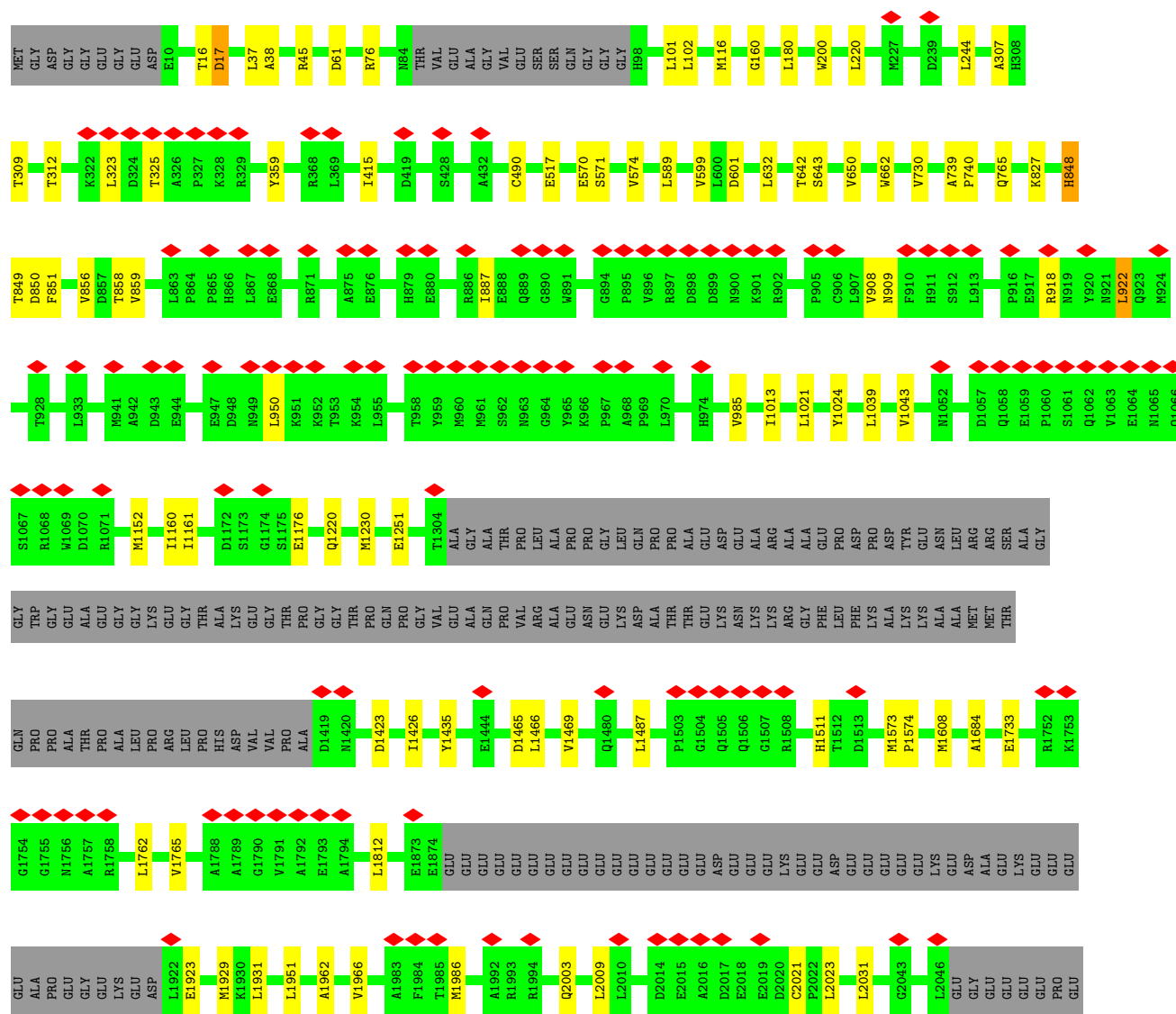
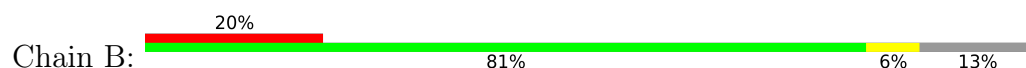
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
4	B	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
4	C	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
4	D	1	Total 45	C 11	H 14	N 5	O 12	P 3	0





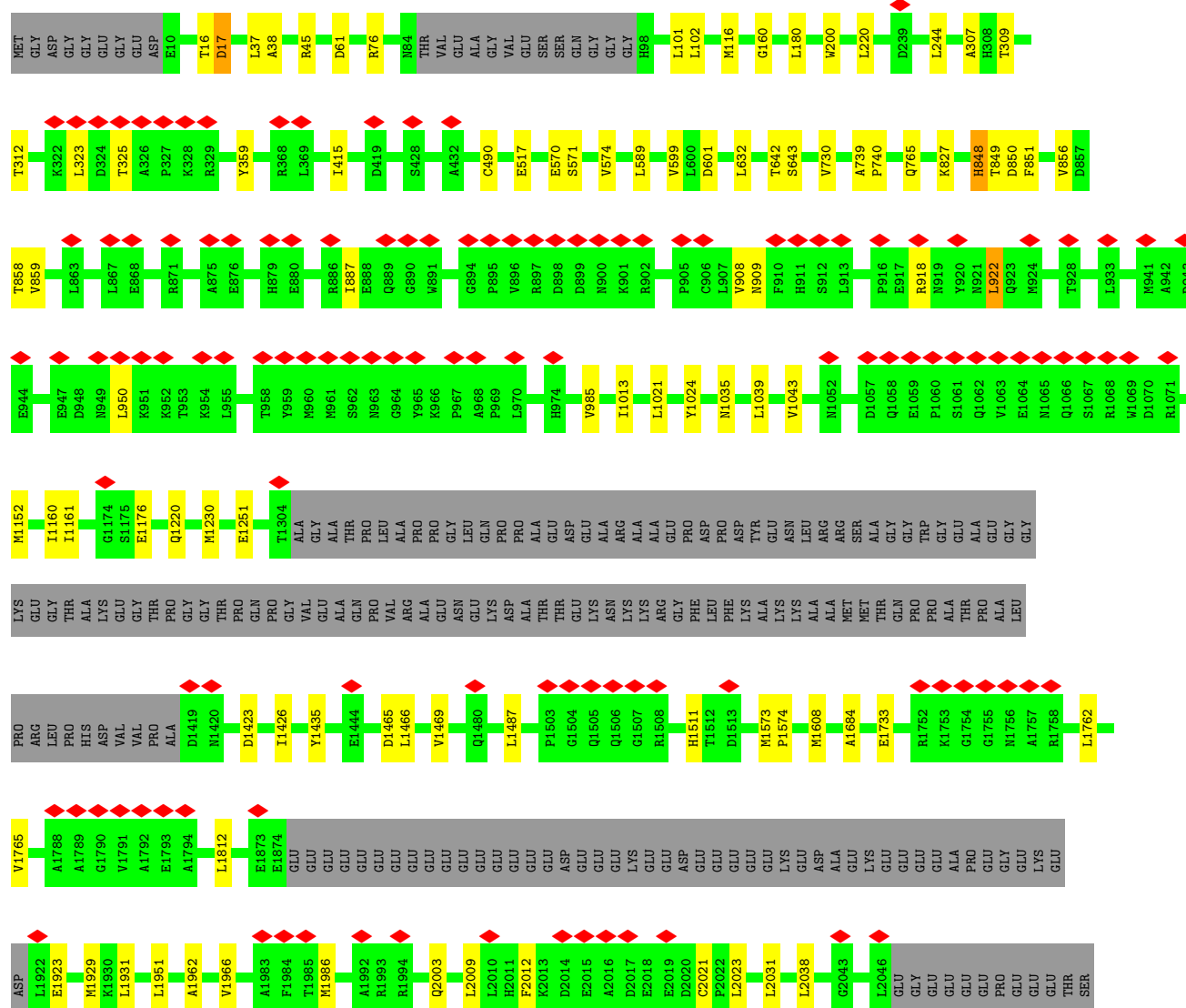


• Molecule 1: Ryanodine receptor 1



A3195	A3196	L3197	A3198	A3199	A3200	M3201	P3202	A3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	Q3151	F3152	G3153	D3154	A3155	V3156	L3157	L3158	G3159	D3160	T3161	Q3162	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	K3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	G3191	E3192	C3193	L3194
N3066	A3072	R3073	S3074	L3075	D3076	A3077	R3078	M3081	K3082	S3083	E3086	T3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	G3117	N3180	T3181	Y3182	V3183	E3184	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	Y3131	
T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	A3155	V3156	L3157	L3158	G3159	D3160	T3161	Q3162	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	K3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	Y3131	
Q2993	E2994	F2997	F2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	Q3008	Y3009	T3010	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	H3029	A3030	K3031	K3034	I3039	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3063	V3064	S3065					
N3066	A3072	R3073	S3074	L3075	D3076	A3077	R3078	M3081	K3082	S3083	E3086	T3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	G3117	N3180	T3181	Y3182	V3183	E3184	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	Y3131	
T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	A3155	V3156	L3157	L3158	G3159	D3160	T3161	Q3162	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	K3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	Y3131	
A3195	A3196	L3197	A3198	A3199	A3200	M3201	P3202	A3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	Q3151	F3152	G3153	D3154	A3155	V3156	L3157	L3158	G3159	D3160	T3161	Q3162	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	K3178	K3179	N3180	M3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	L3248	M3250	A3251	D3252	G3254
V2210	G2217	G2218	E2219	T2220	K2221	E2222	M2228	G2264	L2265	G2266	M2267	C2310	P2311	M2312	L2313	L2314	G2317	Y2318	P2319	D2320	L2376	P2390	A2391	R2392	D2393	G2394	P2395	G2396	V2397	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PRO	GLY	GLU	P2410	P2411	E2412	E2413	N2414	R2415	M2440	H2441										
GLU	GLU	THR	SER	LEU	SER	ARG	ARG	SER	LEU	LEU	VAL	LYS	LYS	LYS	GLU	GLU	LYS	PRO	GLU	GLU	LEU	PRO	ALA	GLU	E2088	K2089	K2090	M2101	D2109	V2110	V2111	V2117	M2120	D2129	G2130	L2131	G2132	E2133	L2155	M2170	M2178	M2198															



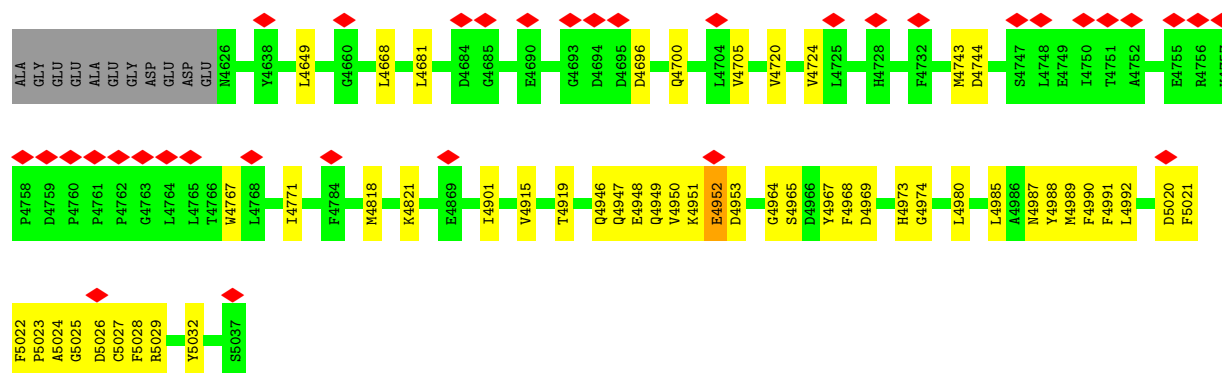


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F3144	Q3145	H3146	I3147	Q3148	Q3149	H3150	Q3151	F3152	G3153	F3154	D3155	F3156	I3157	L3158	D3159	F3160	V3161	Q3162	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181	Y3182	R3183	E3184	K3185	L3186	R3187	P3188	A3189	D3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	F3202	G3260	R3262	Y3263			
R3078	K3081	K3082	S3083	E3086	I3087	V3088	K3089	A3090	G3091	L3092	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	T3103	E3104	K3105	N3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	L3128	L3129	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	F3202	G3260	R3262	Y3263				
L3002	L3003	P3004	L3005	Q3008	Y3009	F3010	T3011	N3012	H3013	C3014	L3015	F3016	F3017	L3018	S3019	T3020	F3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	K3034	I3039	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3063	V3064	V3065	N3066	A3072	R3073	S3074	L3075	D3076	A3077									
T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	Q2961	L2964	R2965	W2966	M2967	D2968	S2970	Q2971	E2972	F2973	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	F2997	F2998	A2999	K3000	I3001								
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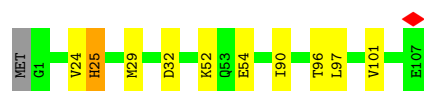




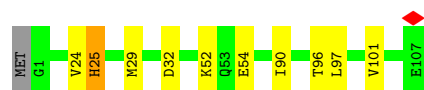
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LYS	ASP	ARG	R4202	ALA	ARG	ALA	R4202	S4009	E3736	L3603	T3538	D3473	L3405	Q3343	P3282
ALA	ALA	ALA	Q4204	GLY	GLY	GLY	Q4204	L4012	GLY	H3605	R3539	K3475	Y3406	P3344	R3283
PRO	PRO	GLY	E4212	ALA	ALA	ALA	E4212	D4046	GLY	L3606	Y3540	S3476	A3407	I3345	W3285
SER	PRO	ALA	R4215	ALA	ALA	ALA	R4215	T4058	GLY	E3642	A3541	K3477	L3408	Y3346	E3286
PRO	THR	GLY	Q4216	THR	GLY	GLY	Q4216	D4046	GLY	E3607	L3542	M3478	L3411	S3347	R3287
GLU	GLU	ALA	F4217	ALA	ALA	ALA	F4217	T4058	GLY	Q3608	K3543	M3479	L3412	R3348	G3288
ALA	ALA	ALA	I4218	ALA	ALA	ALA	I4218	K4069	GLY	L3609	D3544	A3479	I3413	R3350	P3289
PRO	PRO	GLY	F4219	ALA	ALA	ALA	F4219	D4070	GLY	E3610	T3545	L3414	R3414	P3351	E3290
ILE	GLY	ALA	V4220	ALA	ALA	ALA	V4220	V4071	GLY	H3611	D3546	Y3415	R3415	A3291	A3291
LEU	ALA	THR	V4221	THR	GLY	GLY	V4221	V4072	GLY	P3612	E3547	V3416	P3292	E3352	P3292
LYS	ALA	ALA	M4222	ALA	GLY	GLY	M4222	E4075	GLY	Y3613	E3548	D3417	L3353	L3353	P3293
ALA	ALA	ALA	V4223	ALA	ALA	ALA	V4223	E4075	GLY	K3614	V3549	N3418	L3354	H3355	P3294
ARG	ARG	ARG	E4224	LEU	LEU	LEU	E4224	V3749	GLY	S3615	R3550	A3418	H3422	A3356	A3295
LEU	ALA	ALA	G4225	ALA	ALA	ALA	G4225	E3750	GLY	K3616	E3551	GLY	P3296	S3357	L3296
ALA	ALA	ALA	Q4226	ALA	ALA	ALA	Q4226	V3751	GLY	A3617	F3552	SER	W3423	F3358	P3297
ASP	ALA	ALA	E4227	ALA	ALA	ALA	E4227	S3752	GLY	K3618	L3553	GLY	A3423	A3357	A3298
ALA	ALA	ALA	A4228	ALA	ALA	ALA	A4228	V3794	GLY	A3619	F3554	GLY	E3426	F3358	A3298
GLY	GLY	GLY	E4229	ALA	ALA	ALA	E4229	V3794	GLY	W3620	Q3554	GLY	P3427	A3362	G3299
GLY	GLY	GLY	F4230	ALA	ALA	ALA	F4230	L3835	GLY	H3621	N3555	ARG	A3300	R3364	A3300
GLY	GLY	GLY	V4234	ALA	ALA	ALA	V4234	V3841	GLY	L3622	N3556	THR	P3301	L3365	P3301
GLY	GLY	GLY	S4235	ALA	ALA	ALA	S4235	V3841	GLY	L3623	L3557	LYS	P3302	R3366	P3302
VAL	VAL	VAL	F4236	LEU	LEU	LEU	F4236	L3844	GLY	L3624	H3558	LYS	P3303	K3367	P3303
VAL	VAL	VAL	F4237	LEU	LEU	LEU	F4237	L3844	GLY	S3625	L3559	LYS	C3304	R3368	C3304
PRO	ALA	ALA	D4240	ALA	ALA	ALA	D4240	S4115	GLY	K3626	Q3560	GLY	T3305	A3369	T3305
GLY	GLY	GLY	E4244	ALA	ALA	ALA	E4244	E4116	GLY	Q3627	G3500	GLY	A3306	A3306	A3306
PRO	PRO	PRO	A4248	ALA	ALA	ALA	A4248	M4120	GLY	R3628	G3501	GLY	V3307	A3307	V3307
GLY	GLY	GLY	E4253	ALA	ALA	ALA	E4253	E4121	GLY	R3629	D3502	GLY	T3308	V3372	T3308
GLY	GLY	GLY	P4254	ALA	ALA	ALA	P4254	M4122	GLY	R3630	E3503	GLY	S3309	V3373	S3309
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	M4123	GLY	R3631	V3505	GLY	D3310	A3374	D3310
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	M4124	GLY	A3632	Q3506	GLY	H3311	E3376	H3311
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A4129	GLY	V3633	T3507	GLY	L3312	E3376	L3312
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	H4153	GLY	A3634	S3508	GLY	N3313	E3377	N3313
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	H4153	GLY	C3635	L3509	GLY	S3314	Q3378	S3314
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	L4178	GLY	L3663	I3510	GLY	L3315	L3379	L3315
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	G4179	GLY	T3664	V3511	GLY	L3316	R3380	L3316
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	R4180	GLY	E3665	A3512	GLY	G3317	G3317	G3317
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	L4181	GLY	E3665	L3579	GLY	N3318	L3381	N3318
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	L4182	GLY	D3666	P3580	GLY	E3382	L3319	I3319
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	L4183	GLY	H3667	Q3581	GLY	A3383	I3320	L3320
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	M4184	GLY	E3667	K3452	GLY	K3384	R3321	L3320
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	E4185	GLY	G3681	R3453	GLY	A3385	I3322	I3322
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A4186	GLY	E3682	E3454	GLY	A3386	T3322	T3322
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A4186	GLY	Q3683	E3455	GLY	A3387	N3325	N3325
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	R4189	GLY	E3684	Q3456	GLY	A3388	N3326	N3326
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	L4190	GLY	E3684	N3457	GLY	E3389	L3327	L3327
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	E4191	GLY	E3685	V3459	GLY	E3390	G3328	G3328
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	R4192	GLY	E3686	V3460	GLY	E3391	I3329	I3329
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	E4192	GLY	E3687	Q3461	GLY	E3392	D3330	D3330
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	E4196	GLY	E3688	N3465	GLY	E3393	A3331	A3331
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	L4197	GLY	E3688	D3466	GLY	E3394	A3332	A3332
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	F9951	GLY	E3689	N3466	GLY	E3395	T3333	T3333
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3689	N3467	GLY	E3396	W3334	W3334
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3690	M3467	GLY	E3397	K3335	K3335
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3691	S3468	GLY	E3398	K3336	K3336
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3691	F3469	GLY	E3399	R3337	R3337
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3692		GLY	E3400	L3338	L3338
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3692		GLY	L3401	A3339	A3339
GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	A3997	GLY	E3692		GLY	C3402	V3340	V3340



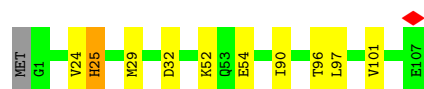
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



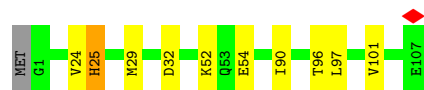
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- 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	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	27861	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 ($e^-/\text{\AA}^2$)	59.9	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.429	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.046	Depositor
Map value standard deviation	0.265	Depositor
Recommended contour level	0.977	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, 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	0.43	23/35885 (0.1%)	0.56	109/48603 (0.2%)
1	B	0.43	23/35885 (0.1%)	0.56	108/48603 (0.2%)
1	C	0.43	23/35885 (0.1%)	0.56	107/48603 (0.2%)
1	D	0.43	24/35885 (0.1%)	0.56	123/48603 (0.3%)
2	E	0.30	1/851 (0.1%)	0.46	2/1146 (0.2%)
2	F	0.30	1/851 (0.1%)	0.46	2/1146 (0.2%)
2	G	0.31	1/851 (0.1%)	0.46	2/1146 (0.2%)
2	H	0.30	1/851 (0.1%)	0.46	2/1146 (0.2%)
All	All	0.42	97/146944 (0.1%)	0.56	455/198996 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	5

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4973	HIS	CE1-NE2	-8.83	1.23	1.32
1	C	4973	HIS	CE1-NE2	-8.83	1.23	1.32
1	A	4973	HIS	CE1-NE2	-8.78	1.23	1.32
1	D	4973	HIS	CE1-NE2	-8.75	1.23	1.32
1	B	4192	ARG	CZ-NH2	-8.33	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4202	ARG	CZ-NH2	-8.29	1.22	1.33
1	C	4192	ARG	CZ-NH2	-8.29	1.22	1.33
1	B	5029	ARG	CZ-NH2	-8.26	1.22	1.33
1	D	4192	ARG	CZ-NH2	-8.25	1.22	1.33
1	B	4202	ARG	CZ-NH2	-8.24	1.22	1.33
1	D	4180	ARG	CZ-NH2	-8.23	1.22	1.33
1	D	5029	ARG	CZ-NH2	-8.23	1.22	1.33
1	B	4180	ARG	CZ-NH2	-8.22	1.22	1.33
1	C	4180	ARG	CZ-NH2	-8.21	1.22	1.33
1	A	4180	ARG	CZ-NH2	-8.21	1.22	1.33
1	C	4202	ARG	CZ-NH2	-8.20	1.22	1.33
1	A	4192	ARG	CZ-NH2	-8.20	1.22	1.33
1	A	5029	ARG	CZ-NH2	-8.20	1.22	1.33
1	C	5029	ARG	CZ-NH2	-8.20	1.22	1.33
1	A	4202	ARG	CZ-NH2	-8.19	1.22	1.33
1	A	4973	HIS	CD2-NE2	-8.05	1.28	1.37
1	B	4973	HIS	CD2-NE2	-8.04	1.29	1.37
1	D	4973	HIS	CD2-NE2	-8.03	1.29	1.37
1	C	4973	HIS	CD2-NE2	-7.96	1.29	1.37
1	B	4228	ALA	CA-CB	-7.22	1.42	1.53
1	A	4228	ALA	CA-CB	-7.21	1.42	1.53
1	B	4203	ALA	CA-CB	-7.17	1.42	1.53
1	C	4203	ALA	CA-CB	-7.17	1.42	1.53
1	A	4203	ALA	CA-CB	-7.11	1.42	1.53
1	C	4228	ALA	CA-CB	-7.07	1.42	1.53
1	D	4228	ALA	CA-CB	-7.07	1.42	1.53
1	D	4203	ALA	CA-CB	-7.04	1.42	1.53
1	B	5024	ALA	CA-CB	-6.96	1.41	1.53
1	C	5024	ALA	CA-CB	-6.96	1.41	1.53
1	A	5024	ALA	CA-CB	-6.86	1.41	1.53
1	D	5024	ALA	CA-CB	-6.81	1.42	1.53
1	B	4202	ARG	CZ-NH1	-6.77	1.23	1.32
1	C	4192	ARG	CZ-NH1	-6.69	1.23	1.32
1	D	4180	ARG	CZ-NH1	-6.69	1.23	1.32
1	C	4202	ARG	CZ-NH1	-6.68	1.23	1.32
1	D	4202	ARG	CZ-NH1	-6.68	1.23	1.32
1	D	5029	ARG	CZ-NH1	-6.67	1.23	1.32
1	A	4180	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	4192	ARG	CZ-NH1	-6.66	1.23	1.32
1	C	5029	ARG	CZ-NH1	-6.65	1.23	1.32
1	B	4180	ARG	CZ-NH1	-6.64	1.23	1.32
1	A	4202	ARG	CZ-NH1	-6.63	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4192	ARG	CZ-NH1	-6.63	1.23	1.32
1	D	4192	ARG	CZ-NH1	-6.63	1.23	1.32
1	A	5029	ARG	CZ-NH1	-6.62	1.23	1.32
1	B	5029	ARG	CZ-NH1	-6.62	1.23	1.32
1	C	4180	ARG	CZ-NH1	-6.61	1.23	1.32
1	B	4974	GLY	N-CA	-6.20	1.38	1.45
1	C	4974	GLY	N-CA	-6.20	1.38	1.45
1	A	4974	GLY	N-CA	-6.19	1.38	1.45
1	B	4179	GLY	CA-C	-6.19	1.47	1.52
1	D	4974	GLY	N-CA	-6.16	1.38	1.45
1	D	4179	GLY	N-CA	-6.15	1.38	1.46
1	A	4179	GLY	CA-C	-6.13	1.47	1.52
1	C	4179	GLY	CA-C	-6.09	1.47	1.52
1	C	4179	GLY	N-CA	-6.01	1.38	1.46
1	D	4179	GLY	CA-C	-6.01	1.48	1.52
1	B	4179	GLY	N-CA	-5.96	1.38	1.46
1	A	4179	GLY	N-CA	-5.92	1.38	1.46
1	B	4964	GLY	N-CA	-5.87	1.37	1.45
1	D	4964	GLY	N-CA	-5.82	1.37	1.45
1	C	4964	GLY	N-CA	-5.80	1.37	1.45
1	A	4964	GLY	N-CA	-5.80	1.37	1.45
1	D	4225	GLY	N-CA	-5.67	1.37	1.45
1	B	4202	ARG	CD-NE	-5.64	1.38	1.46
1	C	4202	ARG	CD-NE	-5.64	1.38	1.46
1	C	4225	GLY	N-CA	-5.64	1.37	1.45
1	A	4225	GLY	N-CA	-5.63	1.37	1.45
1	B	4225	GLY	N-CA	-5.59	1.37	1.45
1	D	4202	ARG	CD-NE	-5.59	1.38	1.46
1	A	4202	ARG	CD-NE	-5.58	1.38	1.46
1	B	5029	ARG	CD-NE	-5.53	1.38	1.46
1	C	4180	ARG	CD-NE	-5.53	1.38	1.46
1	A	5029	ARG	CD-NE	-5.51	1.38	1.46
1	D	4180	ARG	CD-NE	-5.51	1.38	1.46
1	D	5029	ARG	CD-NE	-5.51	1.38	1.46
1	B	4180	ARG	CD-NE	-5.50	1.38	1.46
1	C	5029	ARG	CD-NE	-5.46	1.38	1.46
1	A	4180	ARG	CD-NE	-5.45	1.38	1.46
1	C	5025	GLY	N-CA	-5.34	1.37	1.45
1	B	5025	GLY	N-CA	-5.25	1.37	1.45
1	D	5025	GLY	N-CA	-5.25	1.37	1.45
1	A	5025	GLY	N-CA	-5.22	1.38	1.45
1	B	4192	ARG	CD-NE	-5.21	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4192	ARG	CD-NE	-5.18	1.39	1.46
1	C	4192	ARG	CD-NE	-5.18	1.39	1.46
1	D	4192	ARG	CD-NE	-5.18	1.39	1.46
2	E	25	HIS	CE1-NE2	-5.15	1.27	1.32
2	G	25	HIS	CE1-NE2	-5.15	1.27	1.32
2	F	25	HIS	CE1-NE2	-5.13	1.27	1.32
1	D	5023	PRO	CA-CB	-5.06	1.46	1.53
2	H	25	HIS	CE1-NE2	-5.05	1.27	1.32

All (455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4220	ASP	CA-CB-CG	7.78	120.38	112.60
1	B	4220	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	4220	ASP	CA-CB-CG	7.70	120.30	112.60
1	C	4220	ASP	CA-CB-CG	7.70	120.30	112.60
1	D	4969	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	4969	ASP	CA-CB-CG	7.32	119.92	112.60
1	C	4969	ASP	CA-CB-CG	7.32	119.92	112.60
1	B	4969	ASP	CA-CB-CG	7.32	119.92	112.60
1	D	5022	PHE	CA-CB-CG	7.27	121.07	113.80
1	A	5022	PHE	CA-CB-CG	7.25	121.05	113.80
1	C	5022	PHE	CA-CB-CG	7.21	121.01	113.80
1	D	4201	ASN	CA-CB-CG	7.20	119.80	112.60
1	B	5022	PHE	CA-CB-CG	7.18	120.98	113.80
1	A	4201	ASN	CA-CB-CG	7.16	119.76	112.60
1	B	4201	ASN	CA-CB-CG	7.16	119.76	112.60
1	C	4201	ASN	CA-CB-CG	7.16	119.75	112.60
1	D	5026	ASP	CA-CB-CG	7.12	119.72	112.60
1	C	5026	ASP	CA-CB-CG	7.10	119.70	112.60
1	D	4953	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	5026	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	5026	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	4953	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	4953	ASP	CA-CB-CG	7.05	119.65	112.60
1	D	4223	ASN	CA-CB-CG	7.05	119.65	112.60
1	A	4223	ASN	CA-CB-CG	7.01	119.61	112.60
1	C	4953	ASP	CA-CB-CG	7.01	119.61	112.60
1	B	4223	ASN	CA-CB-CG	6.99	119.59	112.60
1	C	4223	ASN	CA-CB-CG	6.99	119.59	112.60
1	D	4968	PHE	CA-CB-CG	6.99	120.79	113.80
1	D	4987	ASN	CA-CB-CG	6.90	119.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4968	PHE	CA-CB-CG	6.88	120.68	113.80
1	B	4968	PHE	CA-CB-CG	6.87	120.67	113.80
1	C	4968	PHE	CA-CB-CG	6.85	120.65	113.80
1	A	4987	ASN	CA-CB-CG	6.79	119.39	112.60
1	B	4987	ASN	CA-CB-CG	6.75	119.35	112.60
1	C	4987	ASN	CA-CB-CG	6.75	119.35	112.60
1	D	4219	PHE	CA-CB-CG	6.63	120.43	113.80
1	D	4178	LEU	CA-C-N	6.60	129.20	122.80
1	D	4178	LEU	C-N-CA	6.60	129.20	122.80
1	A	4219	PHE	CA-CB-CG	6.55	120.35	113.80
1	C	4219	PHE	CA-CB-CG	6.54	120.34	113.80
1	D	4990	PHE	CA-CB-CG	6.49	120.29	113.80
1	C	4178	LEU	CA-C-N	6.48	129.09	122.80
1	C	4178	LEU	C-N-CA	6.48	129.09	122.80
1	A	4178	LEU	CA-C-N	6.48	129.09	122.80
1	A	4178	LEU	C-N-CA	6.48	129.09	122.80
1	C	4973	HIS	CA-CB-CG	6.48	120.28	113.80
1	A	4973	HIS	CA-CB-CG	6.48	120.28	113.80
1	B	4219	PHE	CA-CB-CG	6.48	120.28	113.80
1	D	4973	HIS	CA-CB-CG	6.48	120.28	113.80
1	D	4234	PHE	CA-CB-CG	6.45	120.25	113.80
1	B	4178	LEU	CA-C-N	6.45	129.05	122.80
1	B	4178	LEU	C-N-CA	6.45	129.05	122.80
2	H	25	HIS	ND1-CG-CD2	-6.42	99.68	106.10
2	F	25	HIS	ND1-CG-CD2	-6.41	99.69	106.10
1	B	4234	PHE	CA-CB-CG	6.41	120.21	113.80
1	B	4973	HIS	CA-CB-CG	6.40	120.20	113.80
2	E	25	HIS	ND1-CG-CD2	-6.40	99.70	106.10
1	B	4990	PHE	CA-CB-CG	6.40	120.20	113.80
2	G	25	HIS	ND1-CG-CD2	-6.40	99.70	106.10
1	A	4234	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	4990	PHE	CA-CB-CG	6.39	120.19	113.80
1	D	4991	PHE	CA-CB-CG	6.38	120.18	113.80
1	C	4234	PHE	CA-CB-CG	6.37	120.17	113.80
1	C	4990	PHE	CA-CB-CG	6.37	120.17	113.80
1	B	4991	PHE	CA-CB-CG	6.35	120.15	113.80
1	D	5028	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	4991	PHE	CA-CB-CG	6.30	120.10	113.80
1	C	4991	PHE	CA-CB-CG	6.29	120.09	113.80
1	B	5028	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	5028	PHE	CA-CB-CG	6.27	120.07	113.80
1	C	5028	PHE	CA-CB-CG	6.27	120.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4237	PHE	CA-CB-CG	6.08	119.88	113.80
1	B	4237	PHE	CA-CB-CG	6.07	119.87	113.80
1	D	4196	GLU	CA-C-N	6.07	131.09	123.14
1	D	4196	GLU	C-N-CA	6.07	131.09	123.14
1	C	4196	GLU	CA-C-N	6.05	131.07	123.14
1	C	4196	GLU	C-N-CA	6.05	131.07	123.14
1	C	4237	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	4196	GLU	CA-C-N	6.03	131.04	123.14
1	A	4196	GLU	C-N-CA	6.03	131.04	123.14
1	D	4237	PHE	CA-CB-CG	6.03	119.83	113.80
1	D	4192	ARG	CD-NE-CZ	6.02	132.82	124.40
1	B	4196	GLU	CA-C-N	6.01	131.01	123.14
1	B	4196	GLU	C-N-CA	6.01	131.01	123.14
1	C	4192	ARG	CD-NE-CZ	5.99	132.79	124.40
1	A	4192	ARG	CD-NE-CZ	5.97	132.76	124.40
1	B	4192	ARG	CD-NE-CZ	5.97	132.75	124.40
1	D	4217	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	4217	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	4217	PHE	CA-CB-CG	5.77	119.57	113.80
1	C	4217	PHE	CA-CB-CG	5.77	119.57	113.80
1	D	4191	GLU	CA-C-N	5.77	130.96	123.00
1	D	4191	GLU	C-N-CA	5.77	130.96	123.00
1	A	4191	GLU	CA-C-N	5.76	130.95	123.00
1	A	4191	GLU	C-N-CA	5.76	130.95	123.00
1	C	4191	GLU	CA-C-N	5.74	130.93	123.00
1	C	4191	GLU	C-N-CA	5.74	130.93	123.00
1	B	4191	GLU	CA-C-N	5.74	130.92	123.00
1	B	4191	GLU	C-N-CA	5.74	130.92	123.00
1	D	4222	VAL	CA-C-N	5.67	129.40	120.89
1	D	4222	VAL	C-N-CA	5.67	129.40	120.89
1	A	4222	VAL	CA-C-N	5.66	129.38	120.89
1	A	4222	VAL	C-N-CA	5.66	129.38	120.89
1	C	4222	VAL	CA-C-N	5.65	129.36	120.89
1	C	4222	VAL	C-N-CA	5.65	129.36	120.89
1	D	4180	ARG	CA-C-N	5.64	130.70	122.69
1	D	4180	ARG	C-N-CA	5.64	130.70	122.69
1	A	4180	ARG	CA-C-N	5.62	130.67	122.69
1	A	4180	ARG	C-N-CA	5.62	130.67	122.69
1	C	4180	ARG	CA-C-N	5.62	130.67	122.69
1	C	4180	ARG	C-N-CA	5.62	130.67	122.69
1	B	4180	ARG	CA-C-N	5.62	130.67	122.69
1	B	4180	ARG	C-N-CA	5.62	130.67	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4222	VAL	CA-C-N	5.59	129.28	120.89
1	B	4222	VAL	C-N-CA	5.59	129.28	120.89
1	D	4220	ASP	CA-C-N	5.55	127.55	120.56
1	D	4220	ASP	C-N-CA	5.55	127.55	120.56
1	A	4220	ASP	CA-C-N	5.53	127.52	120.56
1	A	4220	ASP	C-N-CA	5.53	127.52	120.56
1	D	4219	PHE	CA-C-N	5.52	127.61	120.44
1	D	4219	PHE	C-N-CA	5.52	127.61	120.44
1	D	4182	GLU	CA-C-N	5.50	130.51	123.03
1	D	4182	GLU	C-N-CA	5.50	130.51	123.03
1	A	4219	PHE	CA-C-N	5.49	127.58	120.44
1	A	4219	PHE	C-N-CA	5.49	127.58	120.44
1	D	4217	PHE	CA-C-N	5.48	127.46	120.56
1	D	4217	PHE	C-N-CA	5.48	127.46	120.56
1	A	4182	GLU	CA-C-N	5.47	130.47	123.03
1	A	4182	GLU	C-N-CA	5.47	130.47	123.03
1	B	4220	ASP	CA-C-N	5.47	127.45	120.56
1	B	4220	ASP	C-N-CA	5.47	127.45	120.56
1	C	4220	ASP	CA-C-N	5.47	127.45	120.56
1	C	4220	ASP	C-N-CA	5.47	127.45	120.56
1	B	4182	GLU	CA-C-N	5.46	130.46	123.03
1	B	4182	GLU	C-N-CA	5.46	130.46	123.03
1	C	4182	GLU	CA-C-N	5.45	130.44	123.03
1	C	4182	GLU	C-N-CA	5.45	130.44	123.03
1	B	4219	PHE	CA-C-N	5.43	127.50	120.44
1	B	4219	PHE	C-N-CA	5.43	127.50	120.44
1	C	4219	PHE	CA-C-N	5.43	127.50	120.44
1	C	4219	PHE	C-N-CA	5.43	127.50	120.44
1	B	4217	PHE	CA-C-N	5.42	127.38	120.56
1	B	4217	PHE	C-N-CA	5.42	127.38	120.56
1	A	4217	PHE	CA-C-N	5.41	127.38	120.56
1	A	4217	PHE	C-N-CA	5.41	127.38	120.56
1	C	4217	PHE	CA-C-N	5.38	127.34	120.56
1	C	4217	PHE	C-N-CA	5.38	127.34	120.56
1	D	4216	GLN	CA-C-N	5.38	127.43	120.44
1	D	4216	GLN	C-N-CA	5.38	127.43	120.44
1	A	4181	ILE	CA-C-N	5.37	130.99	122.94
1	A	4181	ILE	C-N-CA	5.37	130.99	122.94
1	D	4234	PHE	CA-C-N	5.36	127.31	120.56
1	D	4234	PHE	C-N-CA	5.36	127.31	120.56
1	D	4181	ILE	CA-C-N	5.34	130.96	122.94
1	D	4181	ILE	C-N-CA	5.34	130.96	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4216	GLN	CA-C-N	5.34	127.38	120.44
1	A	4216	GLN	C-N-CA	5.34	127.38	120.44
2	H	25	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
1	D	4946	GLN	CA-C-N	5.33	127.37	120.44
1	D	4946	GLN	C-N-CA	5.33	127.37	120.44
1	B	4181	ILE	CA-C-N	5.32	130.92	122.94
1	B	4181	ILE	C-N-CA	5.32	130.92	122.94
1	C	4181	ILE	CA-C-N	5.32	130.91	122.94
1	C	4181	ILE	C-N-CA	5.32	130.91	122.94
1	A	4234	PHE	CA-C-N	5.31	127.25	120.56
1	A	4234	PHE	C-N-CA	5.31	127.25	120.56
2	F	25	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	A	4946	GLN	CA-C-N	5.30	127.34	120.44
1	A	4946	GLN	C-N-CA	5.30	127.34	120.44
1	C	4946	GLN	CA-C-N	5.30	127.34	120.44
1	C	4946	GLN	C-N-CA	5.30	127.34	120.44
1	D	4244	GLU	CA-C-N	5.30	127.65	120.44
1	D	4244	GLU	C-N-CA	5.30	127.65	120.44
1	C	4216	GLN	CA-C-N	5.30	127.33	120.44
1	C	4216	GLN	C-N-CA	5.30	127.33	120.44
2	G	25	HIS	CE1-NE2-CD2	-5.29	103.70	109.00
1	A	4244	GLU	CA-C-N	5.29	127.64	120.44
1	A	4244	GLU	C-N-CA	5.29	127.64	120.44
1	D	4967	TYR	N-CA-CB	5.28	117.66	110.01
1	D	4234	PHE	N-CA-CB	5.28	117.66	110.01
1	D	4218	ILE	CA-C-N	5.27	127.29	120.44
1	D	4218	ILE	C-N-CA	5.27	127.29	120.44
1	A	4218	ILE	CA-C-N	5.27	127.29	120.44
1	A	4218	ILE	C-N-CA	5.27	127.29	120.44
1	B	4234	PHE	N-CA-CB	5.27	117.65	110.01
2	E	25	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	B	4216	GLN	CA-C-N	5.25	127.27	120.44
1	B	4216	GLN	C-N-CA	5.25	127.27	120.44
1	B	4234	PHE	CA-C-N	5.25	127.18	120.56
1	B	4234	PHE	C-N-CA	5.25	127.18	120.56
1	C	4218	ILE	CA-C-N	5.25	127.27	120.44
1	C	4218	ILE	C-N-CA	5.25	127.27	120.44
1	C	4234	PHE	CA-C-N	5.25	127.18	120.56
1	C	4234	PHE	C-N-CA	5.25	127.18	120.56
1	A	4234	PHE	N-CA-CB	5.25	117.62	110.01
1	C	4244	GLU	CA-C-N	5.25	127.58	120.44
1	C	4244	GLU	C-N-CA	5.25	127.58	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4967	TYR	N-CA-CB	5.25	117.62	110.01
1	B	4946	GLN	CA-C-N	5.25	127.26	120.44
1	B	4946	GLN	C-N-CA	5.25	127.26	120.44
1	D	5028	PHE	CA-C-N	5.24	127.30	120.28
1	D	5028	PHE	C-N-CA	5.24	127.30	120.28
1	C	4234	PHE	N-CA-CB	5.24	117.60	110.01
1	A	4967	TYR	N-CA-CB	5.23	117.60	110.01
1	B	4218	ILE	CA-C-N	5.22	127.23	120.44
1	B	4218	ILE	C-N-CA	5.22	127.23	120.44
1	C	5028	PHE	CA-C-N	5.22	127.28	120.28
1	C	5028	PHE	C-N-CA	5.22	127.28	120.28
1	A	5028	PHE	CA-C-N	5.22	127.27	120.28
1	A	5028	PHE	C-N-CA	5.22	127.27	120.28
1	A	4967	TYR	CA-C-N	5.22	127.27	120.28
1	A	4967	TYR	C-N-CA	5.22	127.27	120.28
1	A	4989	MET	CA-C-N	5.22	127.27	120.28
1	A	4989	MET	C-N-CA	5.22	127.27	120.28
1	B	4967	TYR	N-CA-CB	5.21	117.57	110.01
1	A	4951	LYS	CA-C-N	5.21	127.21	120.44
1	A	4951	LYS	C-N-CA	5.21	127.21	120.44
1	B	4948	GLU	CA-C-N	5.20	127.20	120.44
1	B	4948	GLU	C-N-CA	5.20	127.20	120.44
1	C	4948	GLU	CA-C-N	5.20	127.20	120.44
1	C	4948	GLU	C-N-CA	5.20	127.20	120.44
1	D	4967	TYR	CA-C-N	5.20	127.25	120.28
1	D	4967	TYR	C-N-CA	5.20	127.25	120.28
1	B	4244	GLU	CA-C-N	5.20	127.50	120.44
1	B	4244	GLU	C-N-CA	5.20	127.50	120.44
1	A	4948	GLU	CA-C-N	5.19	127.19	120.44
1	A	4948	GLU	C-N-CA	5.19	127.19	120.44
1	D	4990	PHE	CA-C-N	5.19	127.18	120.44
1	D	4990	PHE	C-N-CA	5.19	127.18	120.44
1	B	4951	LYS	CA-C-N	5.18	127.18	120.44
1	B	4951	LYS	C-N-CA	5.18	127.18	120.44
1	D	4202	ARG	N-CA-CB	5.18	117.53	110.01
1	A	4237	PHE	N-CA-CB	5.18	117.52	110.01
1	D	4202	ARG	CA-C-N	5.17	127.17	120.44
1	D	4202	ARG	C-N-CA	5.17	127.17	120.44
1	D	4216	GLN	N-CA-CB	5.17	117.57	110.07
1	D	4948	GLU	CA-C-N	5.17	127.17	120.44
1	D	4948	GLU	C-N-CA	5.17	127.17	120.44
1	A	4216	GLN	N-CA-CB	5.17	117.57	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5021	PHE	CA-C-N	5.17	127.83	120.49
1	A	5021	PHE	C-N-CA	5.17	127.83	120.49
1	D	4991	PHE	N-CA-CB	5.17	117.51	110.01
1	D	5021	PHE	CA-C-N	5.17	127.83	120.49
1	D	5021	PHE	C-N-CA	5.17	127.83	120.49
1	B	5028	PHE	CA-C-N	5.17	127.20	120.28
1	B	5028	PHE	C-N-CA	5.17	127.20	120.28
1	B	4967	TYR	CA-C-N	5.17	127.20	120.28
1	B	4967	TYR	C-N-CA	5.17	127.20	120.28
1	D	4951	LYS	CA-C-N	5.17	127.15	120.44
1	D	4951	LYS	C-N-CA	5.17	127.15	120.44
1	D	4989	MET	CA-C-N	5.16	127.20	120.28
1	D	4989	MET	C-N-CA	5.16	127.20	120.28
1	D	4952	GLU	CA-C-N	5.16	127.20	120.28
1	D	4952	GLU	C-N-CA	5.16	127.20	120.28
1	D	4965	SER	CA-C-N	5.16	127.15	120.44
1	D	4965	SER	C-N-CA	5.16	127.15	120.44
1	A	4952	GLU	CA-C-N	5.16	127.19	120.28
1	A	4952	GLU	C-N-CA	5.16	127.19	120.28
1	B	4216	GLN	N-CA-CB	5.16	117.55	110.07
1	C	4237	PHE	N-CA-CB	5.16	117.49	110.01
1	B	4965	SER	CA-C-N	5.16	127.14	120.44
1	B	4965	SER	C-N-CA	5.16	127.14	120.44
1	B	4237	PHE	N-CA-CB	5.15	117.48	110.01
1	C	4952	GLU	CA-C-N	5.15	127.18	120.28
1	C	4952	GLU	C-N-CA	5.15	127.18	120.28
1	A	4237	PHE	CA-C-N	5.15	127.18	120.28
1	A	4237	PHE	C-N-CA	5.15	127.18	120.28
1	A	4965	SER	CA-C-N	5.15	127.13	120.44
1	A	4965	SER	C-N-CA	5.15	127.13	120.44
1	C	4216	GLN	N-CA-CB	5.14	117.53	110.07
1	D	4237	PHE	N-CA-CB	5.14	117.47	110.01
1	C	4967	TYR	CA-C-N	5.14	127.17	120.28
1	C	4967	TYR	C-N-CA	5.14	127.17	120.28
1	D	4240	ASP	CA-C-N	5.14	127.17	120.28
1	D	4240	ASP	C-N-CA	5.14	127.17	120.28
1	A	4198	SER	CA-C-N	5.14	127.17	120.28
1	A	4198	SER	C-N-CA	5.14	127.17	120.28
1	B	4198	SER	CA-C-N	5.13	127.16	120.28
1	B	4198	SER	C-N-CA	5.13	127.16	120.28
1	D	4212	GLU	CA-C-N	5.13	127.42	120.38
1	D	4212	GLU	C-N-CA	5.13	127.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4992	LEU	CA-C-N	5.13	127.11	120.44
1	B	4992	LEU	C-N-CA	5.13	127.11	120.44
1	C	4951	LYS	CA-C-N	5.13	127.11	120.44
1	C	4951	LYS	C-N-CA	5.13	127.11	120.44
1	C	4990	PHE	CA-C-N	5.13	127.11	120.44
1	C	4990	PHE	C-N-CA	5.13	127.11	120.44
1	D	4992	LEU	CA-C-N	5.13	127.11	120.44
1	D	4992	LEU	C-N-CA	5.13	127.11	120.44
1	C	4237	PHE	CA-C-N	5.13	127.15	120.28
1	C	4237	PHE	C-N-CA	5.13	127.15	120.28
1	D	4237	PHE	CA-C-N	5.13	127.15	120.28
1	D	4237	PHE	C-N-CA	5.13	127.15	120.28
1	B	4991	PHE	N-CA-CB	5.13	117.45	110.01
1	A	4204	GLN	CA-C-N	5.13	127.66	120.28
1	A	4204	GLN	C-N-CA	5.13	127.66	120.28
1	D	4947	GLN	CA-C-N	5.13	127.15	120.28
1	D	4947	GLN	C-N-CA	5.13	127.15	120.28
1	B	5021	PHE	CA-C-N	5.12	127.77	120.49
1	B	5021	PHE	C-N-CA	5.12	127.77	120.49
1	C	4992	LEU	CA-C-N	5.12	127.10	120.44
1	C	4992	LEU	C-N-CA	5.12	127.10	120.44
1	D	4198	SER	CA-C-N	5.12	127.14	120.28
1	D	4198	SER	C-N-CA	5.12	127.14	120.28
1	D	4951	LYS	N-CA-CB	5.12	117.44	110.01
1	C	5021	PHE	CA-C-N	5.12	127.76	120.49
1	C	5021	PHE	C-N-CA	5.12	127.76	120.49
1	A	4202	ARG	CA-C-N	5.12	127.09	120.44
1	A	4202	ARG	C-N-CA	5.12	127.09	120.44
1	A	4990	PHE	CA-C-N	5.12	127.09	120.44
1	A	4990	PHE	C-N-CA	5.12	127.09	120.44
1	B	4989	MET	CA-C-N	5.12	127.13	120.28
1	B	4989	MET	C-N-CA	5.12	127.13	120.28
1	C	4198	SER	CA-C-N	5.12	127.14	120.28
1	C	4198	SER	C-N-CA	5.12	127.14	120.28
1	C	4989	MET	CA-C-N	5.12	127.13	120.28
1	C	4989	MET	C-N-CA	5.12	127.13	120.28
1	B	4204	GLN	CA-C-N	5.11	127.64	120.28
1	B	4204	GLN	C-N-CA	5.11	127.64	120.28
1	A	4991	PHE	N-CA-CB	5.11	117.42	110.01
1	B	4952	GLU	CA-C-N	5.11	127.13	120.28
1	B	4952	GLU	C-N-CA	5.11	127.13	120.28
1	D	4204	GLN	CA-C-N	5.11	127.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4204	GLN	C-N-CA	5.11	127.64	120.28
1	C	4965	SER	CA-C-N	5.11	127.08	120.44
1	C	4965	SER	C-N-CA	5.11	127.08	120.44
1	C	4991	PHE	N-CA-CB	5.11	117.41	110.01
1	D	4221	VAL	CA-C-N	5.11	127.45	120.46
1	D	4221	VAL	C-N-CA	5.11	127.45	120.46
1	D	4203	ALA	CA-C-N	5.10	127.07	120.44
1	D	4203	ALA	C-N-CA	5.10	127.07	120.44
1	A	4202	ARG	N-CA-CB	5.10	117.41	110.01
1	C	4202	ARG	N-CA-CB	5.10	117.40	110.01
1	B	4240	ASP	CA-C-N	5.10	127.11	120.28
1	B	4240	ASP	C-N-CA	5.10	127.11	120.28
1	A	4992	LEU	CA-C-N	5.09	127.06	120.44
1	A	4992	LEU	C-N-CA	5.09	127.06	120.44
1	B	4226	GLY	CA-C-N	5.09	127.11	120.28
1	B	4226	GLY	C-N-CA	5.09	127.11	120.28
1	A	4240	ASP	CA-C-N	5.09	127.10	120.28
1	A	4240	ASP	C-N-CA	5.09	127.10	120.28
1	C	4978	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
1	D	5020	ASP	CA-C-N	5.09	128.04	120.31
1	D	5020	ASP	C-N-CA	5.09	128.04	120.31
1	B	4202	ARG	CA-C-N	5.09	127.05	120.44
1	B	4202	ARG	C-N-CA	5.09	127.05	120.44
1	C	4202	ARG	CA-C-N	5.09	127.05	120.44
1	C	4202	ARG	C-N-CA	5.09	127.05	120.44
1	D	4950	VAL	CA-C-N	5.08	127.05	120.44
1	D	4950	VAL	C-N-CA	5.08	127.05	120.44
1	C	4227	GLU	CA-C-N	5.08	127.05	120.44
1	C	4227	GLU	C-N-CA	5.08	127.05	120.44
1	B	4990	PHE	CA-C-N	5.08	127.04	120.44
1	B	4990	PHE	C-N-CA	5.08	127.04	120.44
1	C	4221	VAL	CA-C-N	5.08	127.42	120.46
1	C	4221	VAL	C-N-CA	5.08	127.42	120.46
1	C	4240	ASP	CA-C-N	5.08	127.08	120.28
1	C	4240	ASP	C-N-CA	5.08	127.08	120.28
1	C	4204	GLN	CA-C-N	5.08	127.59	120.28
1	C	4204	GLN	C-N-CA	5.08	127.59	120.28
1	B	4202	ARG	N-CA-CB	5.08	117.37	110.01
1	A	4221	VAL	CA-C-N	5.07	127.41	120.46
1	A	4221	VAL	C-N-CA	5.07	127.41	120.46
1	A	4951	LYS	N-CA-CB	5.07	117.37	110.01
1	D	4190	ILE	CA-C-N	5.07	130.53	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4190	ILE	C-N-CA	5.07	130.53	122.62
1	A	4950	VAL	CA-C-N	5.07	127.03	120.44
1	A	4950	VAL	C-N-CA	5.07	127.03	120.44
1	A	5020	ASP	CA-C-N	5.07	128.01	120.31
1	A	5020	ASP	C-N-CA	5.07	128.01	120.31
1	D	4201	ASN	CA-C-N	5.07	127.03	120.44
1	D	4201	ASN	C-N-CA	5.07	127.03	120.44
1	C	4203	ALA	CA-C-N	5.07	127.03	120.44
1	C	4203	ALA	C-N-CA	5.07	127.03	120.44
1	C	4950	VAL	CA-C-N	5.06	127.02	120.44
1	C	4950	VAL	C-N-CA	5.06	127.02	120.44
1	C	4226	GLY	CA-C-N	5.06	127.06	120.28
1	C	4226	GLY	C-N-CA	5.06	127.06	120.28
1	D	4189	ARG	CA-C-N	5.06	127.36	120.63
1	D	4189	ARG	C-N-CA	5.06	127.36	120.63
1	A	4190	ILE	CA-C-N	5.06	130.51	122.62
1	A	4190	ILE	C-N-CA	5.06	130.51	122.62
1	C	4951	LYS	N-CA-CB	5.06	117.34	110.01
1	B	4947	GLN	CA-C-N	5.06	127.06	120.28
1	B	4947	GLN	C-N-CA	5.06	127.06	120.28
1	D	4226	GLY	CA-C-N	5.06	127.06	120.28
1	D	4226	GLY	C-N-CA	5.06	127.06	120.28
1	A	4226	GLY	CA-C-N	5.05	127.05	120.28
1	A	4226	GLY	C-N-CA	5.05	127.05	120.28
1	A	4947	GLN	CA-C-N	5.05	127.05	120.28
1	A	4947	GLN	C-N-CA	5.05	127.05	120.28
1	D	4200	THR	CA-C-N	5.05	127.05	120.28
1	D	4200	THR	C-N-CA	5.05	127.05	120.28
1	B	4212	GLU	CA-C-N	5.05	127.30	120.38
1	B	4212	GLU	C-N-CA	5.05	127.30	120.38
1	C	4212	GLU	CA-C-N	5.04	127.29	120.38
1	C	4212	GLU	C-N-CA	5.04	127.29	120.38
1	C	4236	SER	CA-C-N	5.04	127.00	120.44
1	C	4236	SER	C-N-CA	5.04	127.00	120.44
1	D	4991	PHE	CA-C-N	5.04	127.00	120.44
1	D	4991	PHE	C-N-CA	5.04	127.00	120.44
1	A	4212	GLU	CA-C-N	5.04	127.29	120.38
1	A	4212	GLU	C-N-CA	5.04	127.29	120.38
1	B	4189	ARG	CA-C-N	5.04	127.34	120.63
1	B	4189	ARG	C-N-CA	5.04	127.34	120.63
1	A	4189	ARG	CA-C-N	5.04	127.33	120.63
1	A	4189	ARG	C-N-CA	5.04	127.33	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4950	VAL	CA-C-N	5.04	126.99	120.44
1	B	4950	VAL	C-N-CA	5.04	126.99	120.44
1	B	5020	ASP	CA-C-N	5.04	127.97	120.31
1	B	5020	ASP	C-N-CA	5.04	127.97	120.31
1	C	5020	ASP	CA-C-N	5.04	127.97	120.31
1	C	5020	ASP	C-N-CA	5.04	127.97	120.31
1	D	4227	GLU	CA-C-N	5.04	126.99	120.44
1	D	4227	GLU	C-N-CA	5.04	126.99	120.44
1	A	4203	ALA	CA-C-N	5.04	126.99	120.44
1	A	4203	ALA	C-N-CA	5.04	126.99	120.44
1	B	4951	LYS	N-CA-CB	5.04	117.31	110.01
1	D	4236	SER	CA-C-N	5.04	126.99	120.44
1	D	4236	SER	C-N-CA	5.04	126.99	120.44
1	C	4189	ARG	CA-C-N	5.03	127.33	120.63
1	C	4189	ARG	C-N-CA	5.03	127.33	120.63
1	C	4947	GLN	CA-C-N	5.03	127.02	120.28
1	C	4947	GLN	C-N-CA	5.03	127.02	120.28
1	B	4203	ALA	CA-C-N	5.03	126.98	120.44
1	B	4203	ALA	C-N-CA	5.03	126.98	120.44
1	C	4949	GLN	N-CA-CB	5.03	117.30	110.01
1	B	4237	PHE	CA-C-N	5.03	127.02	120.28
1	B	4237	PHE	C-N-CA	5.03	127.02	120.28
1	B	4221	VAL	CA-C-N	5.03	127.35	120.46
1	B	4221	VAL	C-N-CA	5.03	127.35	120.46
1	A	4236	SER	CA-C-N	5.03	126.97	120.44
1	A	4236	SER	C-N-CA	5.03	126.97	120.44
1	B	4988	TYR	CA-C-N	5.02	127.32	120.54
1	B	4988	TYR	C-N-CA	5.02	127.32	120.54
1	D	4949	GLN	N-CA-CB	5.02	117.29	110.01
1	D	4199	GLU	CA-C-N	5.02	126.97	120.44
1	D	4199	GLU	C-N-CA	5.02	126.97	120.44
1	A	4949	GLN	N-CA-CB	5.01	117.28	110.01
1	A	4978	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	D	5027	CYS	CA-C-N	5.01	127.25	120.38
1	D	5027	CYS	C-N-CA	5.01	127.25	120.38
1	D	4221	VAL	N-CA-CB	5.01	116.42	110.55
1	B	5027	CYS	CA-C-N	5.01	127.24	120.38
1	B	5027	CYS	C-N-CA	5.01	127.24	120.38
1	B	4991	PHE	CA-C-N	5.01	126.95	120.44
1	B	4991	PHE	C-N-CA	5.01	126.95	120.44
1	A	4991	PHE	CA-C-N	5.01	126.95	120.44
1	A	4991	PHE	C-N-CA	5.01	126.95	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4987	ASN	CA-C-N	5.01	126.95	120.44
1	D	4987	ASN	C-N-CA	5.01	126.95	120.44
1	B	4949	GLN	N-CA-CB	5.00	117.27	110.01
1	D	4988	TYR	CA-C-N	5.00	127.29	120.54
1	D	4988	TYR	C-N-CA	5.00	127.29	120.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4215	ARG	Sidechain
2	E	25	HIS	Sidechain
2	F	25	HIS	Sidechain
2	G	25	HIS	Sidechain
2	H	25	HIS	Sidechain

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	35088	34734	34715	173	0
1	B	35088	34734	34715	183	0
1	C	35088	34734	34715	182	0
1	D	35088	34734	34715	177	0
2	E	832	829	831	5	0
2	F	832	829	831	6	0
2	G	832	829	831	5	0
2	H	832	829	831	5	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
4	A	31	14	14	0	0
4	B	31	14	14	0	0
4	C	31	14	14	1	0
4	D	31	14	14	1	0
All	All	143808	142308	142240	723	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 3.

All (723) 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:B:589:LEU:HD22	1:B:599:VAL:HG21	1.66	0.76
1:D:589:LEU:HD22	1:D:599:VAL:HG21	1.66	0.76
1:C:589:LEU:HD22	1:C:599:VAL:HG21	1.66	0.76
1:A:589:LEU:HD22	1:A:599:VAL:HG21	1.66	0.75
1:B:2675:THR:HG21	1:B:2710:LEU:HD21	1.69	0.74
1:C:2675:THR:HG21	1:C:2710:LEU:HD21	1.69	0.73
1:A:76:ARG:NH1	1:B:3844:LEU:HD11	2.03	0.73
1:D:2675:THR:HG21	1:D:2710:LEU:HD21	1.69	0.73
1:A:2675:THR:HG21	1:A:2710:LEU:HD21	1.69	0.73
1:B:76:ARG:NH1	1:C:3844:LEU:HD11	2.05	0.71
1:C:76:ARG:NH1	1:D:3844:LEU:HD11	2.06	0.71
1:A:3844:LEU:HD11	1:D:76:ARG:NH1	2.08	0.69
1:B:1220:GLN:HB3	1:C:3522:LEU:HD22	1.76	0.67
1:A:1220:GLN:HB3	1:B:3522:LEU:HD22	1.75	0.67
1:A:2586:VAL:HG13	1:A:2607:LEU:HD12	1.80	0.64
1:C:1220:GLN:HB3	1:D:3522:LEU:HD22	1.79	0.64
1:B:2586:VAL:HG13	1:B:2607:LEU:HD12	1.80	0.64
1:B:3169:LEU:HD11	1:B:3205:PHE:CE2	2.33	0.64
1:C:3169:LEU:HD11	1:C:3205:PHE:CE2	2.33	0.64
1:D:2526:PHE:CD2	1:D:2558:VAL:HG13	2.33	0.64
1:D:3169:LEU:HD11	1:D:3205:PHE:CE2	2.33	0.64
1:C:2526:PHE:CD2	1:C:2558:VAL:HG13	2.33	0.63
1:C:2586:VAL:HG13	1:C:2607:LEU:HD12	1.80	0.63
1:B:323:LEU:O	1:B:325:THR:HG23	1.99	0.63
1:B:2526:PHE:CD2	1:B:2558:VAL:HG13	2.33	0.63
1:A:2526:PHE:CD2	1:A:2558:VAL:HG13	2.33	0.63
1:A:2550:LEU:O	1:A:2554:LEU:HD12	1.99	0.62
1:B:2550:LEU:O	1:B:2554:LEU:HD12	1.99	0.62
1:A:3169:LEU:HD11	1:A:3205:PHE:CE2	2.33	0.62
1:C:2550:LEU:O	1:C:2554:LEU:HD12	1.99	0.62
1:D:2586:VAL:HG13	1:D:2607:LEU:HD12	1.80	0.62
1:D:2550:LEU:O	1:D:2554:LEU:HD12	1.99	0.62
1:B:1230:MET:HE3	1:B:1230:MET:HA	1.82	0.62
1:C:323:LEU:O	1:C:325:THR:HG23	1.99	0.62
1:A:323:LEU:O	1:A:325:THR:HG23	1.99	0.62
1:A:1230:MET:HE3	1:A:1230:MET:HA	1.82	0.62
1:D:323:LEU:O	1:D:325:THR:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1230:MET:HE3	1:D:1230:MET:HA	1.82	0.61
1:C:571:SER:OG	1:C:574:VAL:HG23	2.01	0.61
1:C:1230:MET:HE3	1:C:1230:MET:HA	1.82	0.61
1:A:3522:LEU:HD22	1:D:1220:GLN:HB3	1.81	0.60
1:D:571:SER:OG	1:D:574:VAL:HG23	2.01	0.60
1:A:2700:MET:HE3	1:A:2701:PRO:HD3	1.84	0.60
1:C:2675:THR:CG2	1:C:2710:LEU:HD21	2.32	0.60
1:B:571:SER:OG	1:B:574:VAL:HG23	2.01	0.60
1:C:2700:MET:HE3	1:C:2701:PRO:HD3	1.84	0.60
1:D:2700:MET:HE3	1:D:2701:PRO:HD3	1.84	0.60
1:B:2700:MET:HE3	1:B:2701:PRO:HD3	1.84	0.59
1:D:4915:VAL:O	1:D:4919:THR:HG23	2.02	0.59
1:A:571:SER:OG	1:A:574:VAL:HG23	2.01	0.59
1:B:2675:THR:CG2	1:B:2710:LEU:HD21	2.32	0.59
1:A:2031:LEU:HD12	1:A:2031:LEU:O	2.03	0.59
1:A:2675:THR:CG2	1:A:2710:LEU:HD21	2.32	0.59
1:A:3018:LEU:HD21	1:A:3150:HIS:NE2	2.18	0.59
1:C:3018:LEU:HD21	1:C:3150:HIS:NE2	2.18	0.59
1:A:4915:VAL:O	1:A:4919:THR:HG23	2.03	0.59
1:A:2619:LEU:CD1	1:A:2622:LEU:HD23	2.33	0.58
1:B:2619:LEU:CD1	1:B:2622:LEU:HD23	2.33	0.58
1:B:4915:VAL:O	1:B:4919:THR:HG23	2.03	0.58
1:D:2031:LEU:HD12	1:D:2031:LEU:O	2.03	0.58
1:D:2619:LEU:CD1	1:D:2622:LEU:HD23	2.33	0.58
1:B:2031:LEU:HD12	1:B:2031:LEU:O	2.03	0.58
1:D:3018:LEU:HD21	1:D:3150:HIS:NE2	2.18	0.58
1:C:2031:LEU:O	1:C:2031:LEU:HD12	2.03	0.58
1:C:4915:VAL:O	1:C:4919:THR:HG23	2.03	0.58
1:D:2675:THR:CG2	1:D:2710:LEU:HD21	2.32	0.58
1:B:3018:LEU:HD21	1:B:3150:HIS:NE2	2.18	0.58
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.85	0.58
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.85	0.58
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.85	0.58
1:C:2619:LEU:CD1	1:C:2622:LEU:HD23	2.33	0.58
1:A:2619:LEU:HD11	1:A:2622:LEU:HD23	1.87	0.57
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.85	0.57
1:C:1160:ILE:C	1:C:1161:ILE:HD12	2.29	0.57
1:B:589:LEU:HD22	1:B:599:VAL:CG2	2.35	0.57
1:D:2619:LEU:HD11	1:D:2622:LEU:HD23	1.87	0.57
1:D:1160:ILE:C	1:D:1161:ILE:HD12	2.29	0.57
1:A:1160:ILE:C	1:A:1161:ILE:HD12	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1160:ILE:C	1:B:1161:ILE:HD12	2.29	0.56
1:D:589:LEU:HD22	1:D:599:VAL:CG2	2.35	0.56
1:B:2619:LEU:HD11	1:B:2622:LEU:HD23	1.87	0.56
1:C:37:LEU:HD23	1:C:38:ALA:N	2.21	0.56
1:B:37:LEU:HD23	1:B:38:ALA:N	2.21	0.56
1:A:37:LEU:HD23	1:A:38:ALA:N	2.21	0.56
1:A:589:LEU:HD22	1:A:599:VAL:CG2	2.35	0.56
1:C:2619:LEU:HD11	1:C:2622:LEU:HD23	1.86	0.56
1:C:2170:MET:CE	1:C:2228:MET:HE1	2.36	0.55
1:D:37:LEU:HD23	1:D:38:ALA:N	2.21	0.55
1:B:4097:MET:HE2	1:B:4097:MET:HA	1.89	0.55
1:D:2170:MET:CE	1:D:2228:MET:HE1	2.36	0.55
1:B:1684:ALA:HB1	2:F:90:ILE:HD11	1.88	0.55
1:C:1962:ALA:O	1:C:1966:VAL:HG12	2.06	0.55
1:B:2170:MET:CE	1:B:2228:MET:HE1	2.36	0.55
1:A:1962:ALA:O	1:A:1966:VAL:HG12	2.06	0.55
1:A:2170:MET:CE	1:A:2228:MET:HE1	2.36	0.55
1:A:517:GLU:C	1:A:517:GLU:OE1	2.50	0.55
1:A:4097:MET:HA	1:A:4097:MET:HE2	1.89	0.55
1:B:1962:ALA:O	1:B:1966:VAL:HG12	2.06	0.55
1:D:4097:MET:HE2	1:D:4097:MET:HA	1.89	0.54
1:B:517:GLU:C	1:B:517:GLU:OE1	2.50	0.54
1:B:3005:LEU:HD23	1:B:3005:LEU:O	2.08	0.54
1:C:589:LEU:HD22	1:C:599:VAL:CG2	2.35	0.54
1:D:517:GLU:C	1:D:517:GLU:OE1	2.50	0.54
1:D:1962:ALA:O	1:D:1966:VAL:HG12	2.06	0.54
1:C:4097:MET:HA	1:C:4097:MET:HE2	1.89	0.54
1:B:3178:THR:HG22	1:B:3180:ASN:H	1.73	0.54
1:C:517:GLU:OE1	1:C:517:GLU:C	2.50	0.54
1:D:2639:MET:HE3	1:D:2640:PRO:HD3	1.90	0.54
1:C:1684:ALA:HB1	2:G:90:ILE:HD11	1.89	0.53
1:A:1684:ALA:HB1	2:E:90:ILE:HD11	1.90	0.53
1:C:2639:MET:HE3	1:C:2640:PRO:HD3	1.91	0.53
1:A:3005:LEU:O	1:A:3005:LEU:HD23	2.08	0.53
1:A:3540:TYR:CE1	1:A:3549:VAL:HG11	2.44	0.53
1:C:3005:LEU:O	1:C:3005:LEU:HD23	2.08	0.53
1:A:2639:MET:HE3	1:A:2640:PRO:HD3	1.91	0.53
1:A:3178:THR:HG22	1:A:3180:ASN:H	1.73	0.53
1:B:2178:MET:SD	1:B:2228:MET:HE2	2.49	0.53
1:C:3178:THR:HG22	1:C:3180:ASN:H	1.73	0.53
1:C:4681:LEU:HD23	1:C:4681:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2639:MET:HE3	1:B:2640:PRO:HD3	1.91	0.53
1:C:2178:MET:SD	1:C:2228:MET:HE2	2.49	0.53
1:C:3540:TYR:CE1	1:C:3549:VAL:HG11	2.44	0.53
1:D:3540:TYR:CE1	1:D:3549:VAL:HG11	2.44	0.53
1:A:4681:LEU:HD23	1:A:4681:LEU:O	2.09	0.52
1:C:3794:VAL:HG21	1:C:3835:LEU:HD11	1.91	0.52
1:D:4980:LEU:O	1:D:4980:LEU:HD12	2.09	0.52
1:B:4980:LEU:HD12	1:B:4980:LEU:O	2.09	0.52
1:D:3005:LEU:HD23	1:D:3005:LEU:O	2.08	0.52
1:A:2178:MET:SD	1:A:2228:MET:HE2	2.49	0.52
1:C:2131:LEU:O	1:C:2131:LEU:HD12	2.09	0.52
1:C:3540:TYR:HE1	1:C:3549:VAL:HG11	1.75	0.52
1:D:3178:THR:HG22	1:D:3180:ASN:H	1.73	0.52
1:B:3794:VAL:HG21	1:B:3835:LEU:HD11	1.91	0.52
1:D:2131:LEU:HD12	1:D:2131:LEU:O	2.10	0.52
1:D:2523:ASP:OD1	1:D:2524:VAL:HG13	2.10	0.52
1:D:3794:VAL:HG21	1:D:3835:LEU:HD11	1.91	0.52
1:B:3540:TYR:CE1	1:B:3549:VAL:HG11	2.44	0.52
1:C:37:LEU:HD23	1:C:38:ALA:H	1.75	0.52
1:B:2131:LEU:HD12	1:B:2131:LEU:O	2.10	0.52
1:D:4681:LEU:O	1:D:4681:LEU:HD23	2.09	0.52
1:B:2009:LEU:CD2	1:B:2023:LEU:HD11	2.40	0.52
1:C:2523:ASP:OD1	1:C:2524:VAL:HG13	2.10	0.52
1:B:4681:LEU:O	1:B:4681:LEU:HD23	2.09	0.52
1:C:3997:ALA:HB2	1:C:4058:ILE:HD11	1.92	0.52
1:D:101:LEU:C	1:D:102:LEU:HD12	2.35	0.52
1:D:3540:TYR:HE1	1:D:3549:VAL:HG11	1.75	0.52
1:A:3540:TYR:HE1	1:A:3549:VAL:HG11	1.75	0.51
1:A:4980:LEU:HD12	1:A:4980:LEU:O	2.09	0.51
1:C:4980:LEU:HD12	1:C:4980:LEU:O	2.09	0.51
1:D:4069:LYS:O	1:D:4072:VAL:HG22	2.10	0.51
1:A:4069:LYS:O	1:A:4072:VAL:HG22	2.10	0.51
1:B:3540:TYR:HE1	1:B:3549:VAL:HG11	1.75	0.51
1:A:2131:LEU:O	1:A:2131:LEU:HD12	2.09	0.51
1:B:2618:MET:HA	1:B:2618:MET:HE2	1.93	0.51
1:B:4569:LEU:HD21	1:B:4649:LEU:HD22	1.93	0.51
1:D:2009:LEU:CD2	1:D:2023:LEU:HD11	2.40	0.51
1:D:2178:MET:SD	1:D:2228:MET:HE2	2.49	0.51
1:A:2523:ASP:OD1	1:A:2524:VAL:HG13	2.10	0.51
1:A:3794:VAL:HG21	1:A:3835:LEU:HD11	1.92	0.51
1:C:2618:MET:HE2	1:C:2618:MET:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:C	1:B:102:LEU:HD12	2.36	0.51
1:A:2009:LEU:CD2	1:A:2023:LEU:HD11	2.40	0.51
1:B:2523:ASP:OD1	1:B:2524:VAL:HG13	2.10	0.51
1:C:2009:LEU:CD2	1:C:2023:LEU:HD11	2.40	0.51
1:A:2618:MET:HE2	1:A:2618:MET:HA	1.93	0.51
1:A:3997:ALA:HB2	1:A:4058:ILE:HD11	1.92	0.51
1:C:4069:LYS:O	1:C:4072:VAL:HG22	2.10	0.51
1:B:3997:ALA:HB2	1:B:4058:ILE:HD11	1.92	0.51
1:D:37:LEU:HD23	1:D:38:ALA:H	1.75	0.51
2:E:96:THR:C	2:E:97:LEU:HD12	2.36	0.50
1:A:4700:GLN:HA	1:A:4700:GLN:OE1	2.12	0.50
1:D:4569:LEU:HD21	1:D:4649:LEU:HD22	1.93	0.50
1:D:4700:GLN:OE1	1:D:4700:GLN:HA	2.12	0.50
1:A:37:LEU:HD23	1:A:38:ALA:H	1.75	0.50
1:A:101:LEU:C	1:A:102:LEU:HD12	2.35	0.50
1:C:101:LEU:C	1:C:102:LEU:HD12	2.36	0.50
1:D:2003:GLN:C	1:D:2003:GLN:OE1	2.55	0.50
1:D:2618:MET:HA	1:D:2618:MET:HE2	1.93	0.50
1:C:4569:LEU:HD21	1:C:4649:LEU:HD22	1.93	0.50
1:B:4069:LYS:O	1:B:4072:VAL:HG22	2.10	0.50
2:F:96:THR:C	2:F:97:LEU:HD12	2.37	0.50
1:A:2003:GLN:C	1:A:2003:GLN:OE1	2.55	0.50
1:A:4569:LEU:HD21	1:A:4649:LEU:HD22	1.93	0.50
1:B:37:LEU:HD23	1:B:38:ALA:H	1.75	0.50
1:D:3194:LEU:HD21	1:D:3276:MET:SD	2.52	0.50
2:G:96:THR:C	2:G:97:LEU:HD12	2.36	0.50
1:B:2003:GLN:OE1	1:B:2003:GLN:C	2.55	0.50
1:D:3103:ILE:HD13	1:D:3168:THR:HG23	1.94	0.50
1:B:985:VAL:HG22	1:B:1043:VAL:HG21	1.94	0.49
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.94	0.49
1:D:570:GLU:OE1	1:D:570:GLU:HA	2.12	0.49
1:D:3997:ALA:HB2	1:D:4058:ILE:HD11	1.92	0.49
1:A:2101:MET:HA	1:A:2101:MET:HE2	1.94	0.49
1:C:570:GLU:HA	1:C:570:GLU:OE1	2.13	0.49
1:D:2021:CYS:SG	1:D:2023:LEU:HD13	2.53	0.49
1:C:985:VAL:HG22	1:C:1043:VAL:HG21	1.94	0.49
1:C:2021:CYS:SG	1:C:2023:LEU:HD13	2.53	0.49
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.94	0.49
2:H:96:THR:C	2:H:97:LEU:HD12	2.36	0.49
1:A:1465:ASP:OD1	1:A:1465:ASP:C	2.55	0.49
1:A:3194:LEU:HD21	1:A:3276:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1465:ASP:OD1	1:B:1465:ASP:C	2.55	0.49
1:B:3194:LEU:HD21	1:B:3276:MET:SD	2.52	0.49
1:C:2003:GLN:C	1:C:2003:GLN:OE1	2.55	0.49
1:D:1465:ASP:OD1	1:D:1465:ASP:C	2.55	0.49
1:B:570:GLU:OE1	1:B:570:GLU:HA	2.13	0.49
1:A:570:GLU:OE1	1:A:570:GLU:HA	2.13	0.49
1:C:1465:ASP:C	1:C:1465:ASP:OD1	2.55	0.49
1:C:3194:LEU:HD21	1:C:3276:MET:SD	2.52	0.49
1:A:2021:CYS:SG	1:A:2023:LEU:HD13	2.53	0.49
1:B:2021:CYS:SG	1:B:2023:LEU:HD13	2.53	0.49
1:C:4700:GLN:HA	1:C:4700:GLN:OE1	2.12	0.49
1:A:985:VAL:HG22	1:A:1043:VAL:HG21	1.94	0.49
1:C:3343:GLN:O	1:C:3346:VAL:HG12	2.13	0.49
1:D:985:VAL:HG22	1:D:1043:VAL:HG21	1.94	0.49
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.94	0.49
1:D:3343:GLN:O	1:D:3346:VAL:HG12	2.13	0.49
1:D:4075:GLU:N	1:D:4075:GLU:OE1	2.46	0.49
1:A:3103:ILE:HD13	1:A:3168:THR:HG23	1.94	0.48
1:C:4075:GLU:OE1	1:C:4075:GLU:N	2.46	0.48
1:D:4012:LEU:HD23	1:D:4012:LEU:O	2.13	0.48
1:B:3343:GLN:O	1:B:3346:VAL:HG12	2.13	0.48
1:B:4075:GLU:N	1:B:4075:GLU:OE1	2.46	0.48
1:D:1487:LEU:HD12	1:D:1487:LEU:N	2.29	0.48
1:D:3547:GLU:N	1:D:3547:GLU:OE1	2.46	0.48
1:A:1487:LEU:HD12	1:A:1487:LEU:N	2.29	0.48
1:B:3103:ILE:HD13	1:B:3168:THR:HG23	1.94	0.48
1:D:848:HIS:CE1	1:D:849:THR:HG23	2.49	0.48
1:D:2101:MET:HA	1:D:2101:MET:HE2	1.94	0.48
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.94	0.48
1:A:3547:GLU:OE1	1:A:3547:GLU:N	2.46	0.48
1:B:3547:GLU:N	1:B:3547:GLU:OE1	2.46	0.48
1:C:4012:LEU:O	1:C:4012:LEU:HD23	2.13	0.48
1:A:848:HIS:CE1	1:A:849:THR:HG23	2.49	0.48
1:B:3665:GLU:OE1	1:B:3665:GLU:HA	2.14	0.48
1:C:3103:ILE:HD13	1:C:3168:THR:HG23	1.94	0.48
1:C:3547:GLU:N	1:C:3547:GLU:OE1	2.46	0.48
1:D:2170:MET:HE2	1:D:2228:MET:HE1	1.96	0.48
1:A:2867:LEU:HD21	1:A:2871:LEU:HB3	1.95	0.48
1:A:3343:GLN:O	1:A:3346:VAL:HG12	2.13	0.48
1:A:3665:GLU:HA	1:A:3665:GLU:OE1	2.14	0.48
1:A:4075:GLU:N	1:A:4075:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2867:LEU:HD21	1:B:2871:LEU:HB3	1.95	0.48
1:C:1487:LEU:HD12	1:C:1487:LEU:N	2.28	0.48
1:C:2858:GLN:N	1:C:2859:PRO:CD	2.77	0.48
1:C:3665:GLU:OE1	1:C:3665:GLU:HA	2.14	0.48
1:D:1684:ALA:HB1	2:H:90:ILE:HD11	1.96	0.48
1:B:2101:MET:HE2	1:B:2101:MET:HA	1.95	0.48
1:B:4700:GLN:OE1	1:B:4700:GLN:HA	2.12	0.48
1:C:2101:MET:HE2	1:C:2101:MET:HA	1.95	0.48
1:D:2858:GLN:N	1:D:2859:PRO:CD	2.77	0.48
1:A:2170:MET:HE2	1:A:2228:MET:HE1	1.96	0.48
1:A:2858:GLN:N	1:A:2859:PRO:CD	2.77	0.47
1:C:848:HIS:CE1	1:C:849:THR:HG23	2.49	0.47
1:B:2858:GLN:N	1:B:2859:PRO:CD	2.77	0.47
1:D:2867:LEU:HD21	1:D:2871:LEU:HB3	1.95	0.47
1:A:4681:LEU:CD2	1:A:4724:VAL:HG11	2.45	0.47
1:A:4012:LEU:O	1:A:4012:LEU:HD23	2.13	0.47
2:G:24:VAL:CG2	2:G:101:VAL:HG13	2.45	0.47
1:B:3346:VAL:HG11	1:B:3414:ARG:HB2	1.97	0.47
1:D:3665:GLU:HA	1:D:3665:GLU:OE1	2.14	0.47
1:B:1487:LEU:N	1:B:1487:LEU:HD12	2.29	0.47
2:E:24:VAL:CG2	2:E:101:VAL:HG13	2.45	0.47
1:A:2518:LEU:HD23	1:A:2518:LEU:O	2.15	0.47
1:A:3522:LEU:C	1:A:3522:LEU:HD23	2.40	0.47
1:B:848:HIS:CE1	1:B:849:THR:HG23	2.49	0.47
1:B:3522:LEU:HD23	1:B:3522:LEU:C	2.40	0.47
1:B:4568:PHE:CD1	1:B:4568:PHE:C	2.93	0.47
1:B:4681:LEU:CD2	1:B:4724:VAL:HG11	2.45	0.47
1:C:2867:LEU:HD21	1:C:2871:LEU:HB3	1.95	0.47
1:C:3140:LEU:HD11	1:C:3144:PHE:CE2	2.50	0.47
1:C:3239:MET:SD	1:C:3239:MET:N	2.88	0.47
1:D:3239:MET:SD	1:D:3239:MET:N	2.88	0.47
1:C:3346:VAL:HG11	1:C:3414:ARG:HB2	1.97	0.47
1:B:3239:MET:SD	1:B:3239:MET:N	2.88	0.47
1:B:4012:LEU:HD23	1:B:4012:LEU:O	2.13	0.47
1:C:2643:LEU:HD12	1:C:2643:LEU:O	2.15	0.47
1:D:2643:LEU:HD12	1:D:2643:LEU:O	2.15	0.47
1:D:3103:ILE:HD13	1:D:3168:THR:CG2	2.45	0.47
1:A:2643:LEU:HD12	1:A:2643:LEU:O	2.15	0.46
1:A:3346:VAL:HG11	1:A:3414:ARG:HB2	1.97	0.46
1:D:3522:LEU:HD23	1:D:3522:LEU:C	2.40	0.46
1:A:3239:MET:SD	1:A:3239:MET:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3573:MET:HE3	1:A:3573:MET:HA	1.98	0.46
1:A:3727:ASP:OD1	1:A:3727:ASP:C	2.58	0.46
1:B:3103:ILE:HD13	1:B:3168:THR:CG2	2.45	0.46
1:C:2518:LEU:HD23	1:C:2518:LEU:O	2.15	0.46
1:C:3522:LEU:C	1:C:3522:LEU:HD23	2.40	0.46
1:D:859:VAL:HG12	1:D:859:VAL:O	2.15	0.46
1:B:3105:LYS:HZ3	1:B:3125:VAL:HG22	1.81	0.46
1:B:4212:GLU:OE1	1:B:4212:GLU:C	2.59	0.46
1:C:3103:ILE:HD13	1:C:3168:THR:CG2	2.45	0.46
1:D:4681:LEU:CD2	1:D:4724:VAL:HG11	2.45	0.46
1:B:3573:MET:HE3	1:B:3573:MET:HA	1.98	0.46
1:B:3727:ASP:C	1:B:3727:ASP:OD1	2.58	0.46
1:C:3727:ASP:OD1	1:C:3727:ASP:C	2.58	0.46
1:C:4212:GLU:C	1:C:4212:GLU:OE1	2.59	0.46
1:C:4681:LEU:CD2	1:C:4724:VAL:HG11	2.45	0.46
2:F:24:VAL:CG2	2:F:101:VAL:HG13	2.45	0.46
2:H:24:VAL:CG2	2:H:101:VAL:HG13	2.45	0.46
1:B:3140:LEU:HD11	1:B:3144:PHE:CE2	2.50	0.46
1:D:4568:PHE:CD1	1:D:4568:PHE:C	2.93	0.46
1:A:859:VAL:O	1:A:859:VAL:HG12	2.15	0.46
1:D:3346:VAL:HG11	1:D:3414:ARG:HB2	1.97	0.46
1:B:3577:ARG:HA	1:B:3577:ARG:NH2	2.31	0.46
1:C:2170:MET:HE2	1:C:2228:MET:HE1	1.96	0.46
1:C:4568:PHE:CD1	1:C:4568:PHE:C	2.93	0.46
1:D:3573:MET:HE3	1:D:3573:MET:HA	1.98	0.46
1:D:4116:GLU:O	1:D:4123:ILE:HD12	2.16	0.46
1:D:4767:TRP:CD1	1:D:4771:ILE:HD11	2.51	0.46
1:A:4116:GLU:O	1:A:4123:ILE:HD12	2.16	0.46
1:B:4116:GLU:O	1:B:4123:ILE:HD12	2.16	0.46
1:C:4116:GLU:O	1:C:4123:ILE:HD12	2.16	0.46
2:G:32:ASP:C	2:G:32:ASP:OD1	2.59	0.46
1:A:3140:LEU:HD11	1:A:3144:PHE:CE2	2.50	0.46
1:A:4212:GLU:C	1:A:4212:GLU:OE1	2.59	0.46
1:B:859:VAL:HG12	1:B:859:VAL:O	2.15	0.46
1:B:2170:MET:HE2	1:B:2228:MET:HE1	1.96	0.46
1:B:2518:LEU:O	1:B:2518:LEU:HD23	2.15	0.46
1:C:859:VAL:HG12	1:C:859:VAL:O	2.15	0.46
1:C:3573:MET:HE3	1:C:3573:MET:HA	1.98	0.46
1:C:3577:ARG:HA	1:C:3577:ARG:NH2	2.31	0.46
1:D:2518:LEU:HD23	1:D:2518:LEU:O	2.15	0.46
1:D:3140:LEU:HD11	1:D:3144:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3727:ASP:OD1	1:D:3727:ASP:C	2.58	0.46
1:A:3103:ILE:HD13	1:A:3168:THR:CG2	2.45	0.46
1:A:4568:PHE:CD1	1:A:4568:PHE:C	2.93	0.46
1:D:4212:GLU:OE1	1:D:4212:GLU:C	2.59	0.46
2:H:32:ASP:C	2:H:32:ASP:OD1	2.59	0.46
1:A:2997:PHE:CD1	1:A:2997:PHE:C	2.95	0.45
1:A:3577:ARG:HA	1:A:3577:ARG:NH2	2.31	0.45
1:D:3577:ARG:HA	1:D:3577:ARG:NH2	2.31	0.45
1:D:589:LEU:C	1:D:589:LEU:HD23	2.42	0.45
1:B:2643:LEU:O	1:B:2643:LEU:HD12	2.16	0.45
1:B:4767:TRP:CD1	1:B:4771:ILE:HD11	2.51	0.45
1:C:589:LEU:HD23	1:C:589:LEU:C	2.42	0.45
1:D:908:VAL:HG23	1:D:909:ASN:H	1.82	0.45
1:D:2310:CYS:O	1:D:2314:LEU:HD22	2.16	0.45
1:A:2440:MET:HA	1:A:2440:MET:HE2	1.98	0.45
1:A:589:LEU:C	1:A:589:LEU:HD23	2.42	0.45
1:C:2524:VAL:HG23	1:C:2525:GLY:N	2.32	0.45
1:B:2858:GLN:O	1:B:2859:PRO:C	2.60	0.45
1:D:3060:ASP:OD1	1:D:3060:ASP:O	2.35	0.45
2:F:32:ASP:OD1	2:F:32:ASP:C	2.59	0.45
1:B:589:LEU:C	1:B:589:LEU:HD23	2.42	0.45
1:B:849:THR:O	1:B:851:PHE:N	2.50	0.45
1:C:908:VAL:HG23	1:C:909:ASN:H	1.82	0.45
1:C:4767:TRP:CD1	1:C:4771:ILE:HD11	2.51	0.45
1:D:2440:MET:HA	1:D:2440:MET:HE2	1.98	0.45
1:A:2310:CYS:O	1:A:2314:LEU:HD22	2.16	0.45
1:C:849:THR:O	1:C:851:PHE:N	2.50	0.45
1:A:908:VAL:HG23	1:A:909:ASN:H	1.82	0.45
1:A:3103:ILE:O	1:A:3107:VAL:HG13	2.17	0.45
1:D:2524:VAL:HG23	1:D:2525:GLY:N	2.32	0.45
1:D:3103:ILE:O	1:D:3107:VAL:HG13	2.17	0.45
1:A:739:ALA:HB1	1:A:740:PRO:CD	2.47	0.45
1:B:4743:MET:HE3	1:B:4744:ASP:H	1.82	0.45
1:C:739:ALA:HB1	1:C:740:PRO:CD	2.47	0.45
1:C:3103:ILE:O	1:C:3107:VAL:HG13	2.17	0.45
1:C:3456:GLN:O	1:C:3460:VAL:HG22	2.17	0.45
1:D:849:THR:O	1:D:851:PHE:N	2.50	0.45
1:B:3103:ILE:O	1:B:3107:VAL:HG13	2.17	0.44
1:C:2310:CYS:O	1:C:2314:LEU:HD22	2.16	0.44
1:C:2314:LEU:HD22	1:C:2314:LEU:H	1.82	0.44
1:B:2440:MET:HE2	1:B:2440:MET:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3456:GLN:O	1:B:3460:VAL:HG22	2.17	0.44
1:D:2314:LEU:HD22	1:D:2314:LEU:H	1.82	0.44
1:B:2310:CYS:O	1:B:2314:LEU:HD22	2.16	0.44
1:B:2678:LEU:CD2	1:B:2706:ILE:HD13	2.48	0.44
1:C:2178:MET:HE1	1:C:2210:VAL:HG11	2.00	0.44
1:C:4743:MET:HE3	1:C:4744:ASP:H	1.82	0.44
1:D:3456:GLN:O	1:D:3460:VAL:HG22	2.17	0.44
1:A:2314:LEU:HD22	1:A:2314:LEU:H	1.82	0.44
1:B:918:ARG:O	1:B:922:LEU:HD23	2.17	0.44
1:B:2997:PHE:CD1	1:B:2997:PHE:C	2.95	0.44
1:A:918:ARG:O	1:A:922:LEU:HD23	2.17	0.44
1:A:2178:MET:HE1	1:A:2210:VAL:HG11	2.00	0.44
1:A:3456:GLN:O	1:A:3460:VAL:HG22	2.17	0.44
1:A:4743:MET:HE3	1:A:4744:ASP:H	1.82	0.44
1:A:4767:TRP:CD1	1:A:4771:ILE:HD11	2.51	0.44
1:B:3060:ASP:OD1	1:B:3060:ASP:O	2.35	0.44
1:B:3165:CYS:SG	1:B:3197:LEU:HD21	2.58	0.44
1:C:4705:VAL:O	1:C:4705:VAL:HG22	2.18	0.44
2:E:32:ASP:C	2:E:32:ASP:OD1	2.59	0.44
1:A:849:THR:O	1:A:851:PHE:N	2.50	0.44
1:D:2678:LEU:CD2	1:D:2706:ILE:HD13	2.48	0.44
1:D:2997:PHE:CD1	1:D:2997:PHE:C	2.95	0.44
1:D:3169:LEU:HD11	1:D:3205:PHE:CD2	2.52	0.44
1:A:2858:GLN:O	1:A:2859:PRO:C	2.60	0.44
1:A:4568:PHE:HD1	1:A:4569:LEU:HD12	1.83	0.44
1:B:908:VAL:HG23	1:B:909:ASN:H	1.82	0.44
1:B:2524:VAL:HG23	1:B:2525:GLY:N	2.32	0.44
1:B:2588:ARG:O	1:B:2588:ARG:NE	2.51	0.44
1:B:4705:VAL:HG22	1:B:4705:VAL:O	2.18	0.44
1:C:2440:MET:HE2	1:C:2440:MET:HA	1.98	0.44
1:C:3169:LEU:HD11	1:C:3205:PHE:CD2	2.52	0.44
1:D:1466:LEU:O	1:D:1469:VAL:HG12	2.18	0.44
1:D:4705:VAL:HG22	1:D:4705:VAL:O	2.18	0.44
1:A:3018:LEU:HD21	1:A:3150:HIS:CE1	2.53	0.44
1:A:3018:LEU:HD12	1:A:3018:LEU:O	2.18	0.44
1:A:3169:LEU:HD11	1:A:3205:PHE:CD2	2.52	0.44
1:B:2178:MET:HE1	1:B:2210:VAL:HG11	2.00	0.44
1:B:3018:LEU:HD21	1:B:3150:HIS:CE1	2.53	0.44
1:B:3169:LEU:HD11	1:B:3205:PHE:CD2	2.52	0.44
1:B:4568:PHE:HD1	1:B:4569:LEU:HD12	1.83	0.44
1:C:2678:LEU:CD2	1:C:2706:ILE:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2997:PHE:CD1	1:C:2997:PHE:C	2.95	0.44
1:C:3018:LEU:HD21	1:C:3150:HIS:CE1	2.53	0.44
1:C:3060:ASP:OD1	1:C:3060:ASP:O	2.35	0.44
1:C:4668:LEU:C	1:C:4668:LEU:HD23	2.43	0.44
1:A:2524:VAL:HG23	1:A:2525:GLY:N	2.32	0.44
1:A:3060:ASP:OD1	1:A:3060:ASP:O	2.35	0.44
1:D:3018:LEU:HD21	1:D:3150:HIS:CE1	2.53	0.44
1:D:3844:LEU:H	1:D:3844:LEU:HD23	1.83	0.44
1:D:4568:PHE:HD1	1:D:4569:LEU:HD12	1.83	0.44
1:D:4720:VAL:O	1:D:4724:VAL:HG23	2.18	0.44
1:A:2678:LEU:CD2	1:A:2706:ILE:HD13	2.48	0.43
1:A:3165:CYS:SG	1:A:3197:LEU:HD21	2.58	0.43
1:B:739:ALA:HB1	1:B:740:PRO:CD	2.47	0.43
1:B:2314:LEU:HD22	1:B:2314:LEU:H	1.82	0.43
1:B:2390:PRO:O	1:B:2391:ALA:HB3	2.18	0.43
1:C:918:ARG:O	1:C:922:LEU:HD23	2.17	0.43
1:D:4668:LEU:HD23	1:D:4668:LEU:C	2.43	0.43
1:C:4568:PHE:HD1	1:C:4569:LEU:HD12	1.83	0.43
1:D:739:ALA:HB1	1:D:740:PRO:CD	2.47	0.43
1:A:1466:LEU:O	1:A:1469:VAL:HG12	2.18	0.43
1:A:2390:PRO:O	1:A:2391:ALA:HB3	2.18	0.43
1:C:2390:PRO:O	1:C:2391:ALA:HB3	2.19	0.43
1:D:2178:MET:HE1	1:D:2210:VAL:HG11	2.00	0.43
1:A:2588:ARG:O	1:A:2588:ARG:NE	2.51	0.43
1:A:3844:LEU:HD23	1:A:3844:LEU:H	1.83	0.43
1:A:4705:VAL:O	1:A:4705:VAL:HG22	2.18	0.43
1:B:3018:LEU:HD12	1:B:3018:LEU:O	2.18	0.43
1:D:918:ARG:O	1:D:922:LEU:HD23	2.17	0.43
1:D:3015:LEU:HD22	1:D:3015:LEU:H	1.84	0.43
1:D:4743:MET:HE3	1:D:4744:ASP:H	1.82	0.43
1:A:856:VAL:O	1:A:858:THR:HG23	2.18	0.43
1:B:1024:TYR:CD1	1:B:1024:TYR:C	2.96	0.43
1:B:2751:LEU:HD23	1:B:2751:LEU:H	1.84	0.43
1:B:3621:HIS:O	1:B:3622:LYS:HG3	2.19	0.43
1:C:1466:LEU:O	1:C:1469:VAL:HG12	2.18	0.43
1:C:2858:GLN:O	1:C:2859:PRO:C	2.60	0.43
1:C:3165:CYS:SG	1:C:3197:LEU:HD21	2.58	0.43
1:C:3621:HIS:O	1:C:3622:LYS:HG3	2.19	0.43
1:D:1024:TYR:CD1	1:D:1024:TYR:C	2.96	0.43
1:D:3165:CYS:SG	1:D:3197:LEU:HD21	2.58	0.43
1:D:3621:HIS:O	1:D:3622:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:VAL:O	1:B:858:THR:HG23	2.18	0.43
1:C:3453:ARG:HB2	1:C:3453:ARG:NH2	2.34	0.43
1:A:4720:VAL:O	1:A:4724:VAL:HG23	2.18	0.43
1:B:3015:LEU:H	1:B:3015:LEU:HD22	1.83	0.43
1:B:4668:LEU:C	1:B:4668:LEU:HD23	2.43	0.43
1:C:856:VAL:O	1:C:858:THR:HG23	2.18	0.43
1:C:2376:LEU:HD12	1:C:2376:LEU:O	2.19	0.43
1:D:1013:ILE:HD12	1:D:1013:ILE:H	1.84	0.43
1:D:2390:PRO:O	1:D:2391:ALA:HB3	2.19	0.43
1:A:1024:TYR:CD1	1:A:1024:TYR:C	2.96	0.43
1:A:3015:LEU:HD22	1:A:3015:LEU:H	1.84	0.43
1:B:1573:MET:SD	1:B:1574:PRO:HD2	2.59	0.43
1:D:2858:GLN:O	1:D:2859:PRO:C	2.60	0.43
1:A:102:LEU:HD23	1:A:160:GLY:O	2.19	0.43
1:B:1684:ALA:CB	2:F:90:ILE:HD11	2.49	0.43
1:C:3015:LEU:HD22	1:C:3015:LEU:H	1.84	0.43
1:C:3018:LEU:HD12	1:C:3018:LEU:O	2.18	0.43
1:A:589:LEU:HD23	1:A:589:LEU:O	2.19	0.43
1:A:730:VAL:HG23	1:A:765:GLN:O	2.19	0.43
1:A:1573:MET:SD	1:A:1574:PRO:HD2	2.59	0.43
1:A:3453:ARG:NH2	1:A:3453:ARG:HB2	2.34	0.43
1:B:589:LEU:HD23	1:B:589:LEU:O	2.19	0.43
1:C:1024:TYR:CD1	1:C:1024:TYR:C	2.96	0.43
1:C:1423:ASP:HB3	1:C:1426:ILE:HG22	2.01	0.43
1:C:2997:PHE:C	1:C:2997:PHE:HD1	2.27	0.43
1:C:3844:LEU:HD23	1:C:3844:LEU:H	1.83	0.43
1:C:4720:VAL:O	1:C:4724:VAL:HG23	2.18	0.43
1:D:856:VAL:O	1:D:858:THR:HG23	2.18	0.43
1:D:2376:LEU:HD12	1:D:2376:LEU:O	2.19	0.43
1:D:2751:LEU:H	1:D:2751:LEU:HD23	1.84	0.43
1:D:2997:PHE:C	1:D:2997:PHE:HD1	2.27	0.43
1:A:642:THR:HG22	1:A:643:SER:N	2.34	0.42
1:A:739:ALA:HB1	1:A:740:PRO:HD2	2.01	0.42
1:B:2376:LEU:HD12	1:B:2376:LEU:O	2.19	0.42
1:B:3453:ARG:NH2	1:B:3453:ARG:HB2	2.34	0.42
1:B:3457:ASN:HA	1:B:3460:VAL:HG22	2.01	0.42
1:D:2588:ARG:O	1:D:2588:ARG:NE	2.51	0.42
1:B:102:LEU:HD12	1:B:102:LEU:N	2.34	0.42
1:B:102:LEU:HD23	1:B:160:GLY:O	2.18	0.42
1:B:739:ALA:HB1	1:B:740:PRO:HD2	2.01	0.42
1:B:1466:LEU:O	1:B:1469:VAL:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4720:VAL:O	1:B:4724:VAL:HG23	2.18	0.42
1:D:1176:GLU:C	1:D:1176:GLU:OE1	2.62	0.42
1:A:1013:ILE:H	1:A:1013:ILE:HD12	1.84	0.42
1:A:3457:ASN:HA	1:A:3460:VAL:HG22	2.01	0.42
1:A:3906:GLN:H	1:A:3912:THR:HG23	1.85	0.42
1:B:1013:ILE:HD12	1:B:1013:ILE:H	1.84	0.42
1:D:589:LEU:HD23	1:D:589:LEU:O	2.19	0.42
1:D:642:THR:HG22	1:D:643:SER:N	2.34	0.42
1:D:1423:ASP:HB3	1:D:1426:ILE:HG22	2.01	0.42
1:D:3018:LEU:HD12	1:D:3018:LEU:O	2.18	0.42
1:D:3453:ARG:NH2	1:D:3453:ARG:HB2	2.34	0.42
1:D:3906:GLN:H	1:D:3912:THR:HG23	1.84	0.42
1:A:2376:LEU:O	1:A:2376:LEU:HD12	2.19	0.42
1:A:2751:LEU:H	1:A:2751:LEU:HD23	1.84	0.42
1:A:4668:LEU:HD23	1:A:4668:LEU:C	2.43	0.42
1:B:16:THR:C	1:B:17:ASP:OD1	2.63	0.42
1:B:730:VAL:HG23	1:B:765:GLN:O	2.19	0.42
1:C:1573:MET:SD	1:C:1574:PRO:HD2	2.59	0.42
1:D:102:LEU:HD23	1:D:160:GLY:O	2.18	0.42
1:B:3696:ASP:OD1	1:B:3696:ASP:C	2.63	0.42
1:B:3844:LEU:HD23	1:B:3844:LEU:H	1.83	0.42
1:C:1176:GLU:C	1:C:1176:GLU:OE1	2.62	0.42
2:H:52:LYS:HB2	2:H:54:GLU:OE1	2.19	0.42
1:A:1251:GLU:HG3	1:A:1251:GLU:O	2.20	0.42
1:A:3050:VAL:HG22	1:A:3050:VAL:O	2.20	0.42
1:A:3621:HIS:O	1:A:3622:LYS:HG3	2.19	0.42
1:B:309:THR:O	1:B:309:THR:HG22	2.20	0.42
1:B:3050:VAL:O	1:B:3050:VAL:HG22	2.20	0.42
1:B:3937:TYR:CD2	1:B:3943:ILE:HG22	2.55	0.42
1:C:102:LEU:HD23	1:C:160:GLY:O	2.19	0.42
1:C:589:LEU:HD23	1:C:589:LEU:O	2.19	0.42
1:C:642:THR:HG22	1:C:643:SER:N	2.34	0.42
1:C:1013:ILE:HD12	1:C:1013:ILE:H	1.84	0.42
1:C:3457:ASN:HA	1:C:3460:VAL:HG22	2.01	0.42
2:G:52:LYS:HB2	2:G:54:GLU:OE1	2.19	0.42
1:B:2886:TRP:CD1	1:B:2886:TRP:C	2.98	0.42
1:C:2412:GLU:O	1:C:2413:GLU:HB3	2.20	0.42
1:C:3133:THR:HG23	1:C:3134:VAL:HG23	2.02	0.42
1:D:2412:GLU:O	1:D:2413:GLU:HB3	2.20	0.42
1:D:2619:LEU:HD12	1:D:2622:LEU:HD23	2.02	0.42
1:D:2886:TRP:CD1	1:D:2886:TRP:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4818:MET:SD	1:D:4818:MET:C	3.03	0.42
1:A:102:LEU:HD12	1:A:102:LEU:N	2.34	0.42
1:A:1176:GLU:C	1:A:1176:GLU:OE1	2.62	0.42
1:A:3696:ASP:OD1	1:A:3696:ASP:C	2.63	0.42
1:B:4184:MET:HE1	1:B:4189:ARG:C	2.45	0.42
1:C:61:ASP:OD1	1:C:61:ASP:C	2.63	0.42
1:C:2444:GLN:HA	1:C:2444:GLN:OE1	2.20	0.42
1:C:3696:ASP:OD1	1:C:3696:ASP:C	2.62	0.42
1:C:3906:GLN:H	1:C:3912:THR:HG23	1.85	0.42
1:D:1762:LEU:HB2	1:D:1765:VAL:HG11	2.02	0.42
1:A:61:ASP:OD1	1:A:61:ASP:C	2.63	0.42
1:B:2412:GLU:O	1:B:2413:GLU:HB3	2.20	0.42
1:B:3906:GLN:H	1:B:3912:THR:HG23	1.85	0.42
1:C:730:VAL:HG23	1:C:765:GLN:O	2.19	0.42
1:C:3050:VAL:O	1:C:3050:VAL:HG22	2.20	0.42
1:C:4818:MET:SD	1:C:4818:MET:C	3.03	0.42
1:D:1573:MET:SD	1:D:1574:PRO:HD2	2.59	0.42
1:D:2444:GLN:HA	1:D:2444:GLN:OE1	2.20	0.42
1:D:3227:ARG:HH21	1:D:3227:ARG:HB3	1.85	0.42
1:D:3457:ASN:HA	1:D:3460:VAL:HG22	2.01	0.42
1:A:1762:LEU:HB2	1:A:1765:VAL:HG11	2.02	0.42
1:A:2444:GLN:OE1	1:A:2444:GLN:HA	2.20	0.42
1:B:642:THR:HG22	1:B:643:SER:N	2.34	0.42
1:B:1951:LEU:HD22	1:B:2133:GLU:OE2	2.20	0.42
1:B:2444:GLN:OE1	1:B:2444:GLN:HA	2.20	0.42
1:B:4818:MET:SD	1:B:4818:MET:C	3.03	0.42
1:C:102:LEU:HD12	1:C:102:LEU:N	2.34	0.42
1:C:2751:LEU:HD23	1:C:2751:LEU:H	1.84	0.42
1:C:3937:TYR:CD2	1:C:3943:ILE:HG22	2.55	0.42
1:D:730:VAL:HG23	1:D:765:GLN:O	2.19	0.42
1:A:309:THR:O	1:A:309:THR:HG22	2.20	0.41
1:A:415:ILE:HD11	1:A:490:CYS:SG	2.60	0.41
1:A:1951:LEU:HD22	1:A:2133:GLU:OE2	2.20	0.41
1:A:2412:GLU:O	1:A:2413:GLU:HB3	2.20	0.41
1:A:2619:LEU:HD12	1:A:2622:LEU:HD23	2.02	0.41
1:A:4818:MET:SD	1:A:4818:MET:C	3.03	0.41
1:C:1762:LEU:HB2	1:C:1765:VAL:HG11	2.02	0.41
1:C:3227:ARG:HH21	1:C:3227:ARG:HB3	1.85	0.41
1:D:102:LEU:HD12	1:D:102:LEU:N	2.34	0.41
1:D:2672:LEU:HD12	1:D:2672:LEU:H	1.86	0.41
2:F:52:LYS:HB2	2:F:54:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:VAL:HG21	1:A:2117:VAL:HG22	2.02	0.41
1:B:415:ILE:HD11	1:B:490:CYS:SG	2.60	0.41
1:B:2111:VAL:HG21	1:B:2117:VAL:HG22	2.02	0.41
1:C:16:THR:C	1:C:17:ASP:OD1	2.63	0.41
1:C:309:THR:O	1:C:309:THR:HG22	2.20	0.41
1:C:2588:ARG:O	1:C:2588:ARG:NE	2.51	0.41
1:C:2886:TRP:CD1	1:C:2886:TRP:C	2.98	0.41
1:C:3844:LEU:H	1:C:3844:LEU:CD2	2.34	0.41
1:D:827:LYS:O	1:D:827:LYS:HG3	2.20	0.41
1:A:1423:ASP:HB3	1:A:1426:ILE:HG22	2.01	0.41
1:A:3227:ARG:HB3	1:A:3227:ARG:HH21	1.85	0.41
1:B:950:LEU:C	1:B:950:LEU:HD12	2.46	0.41
1:B:1423:ASP:HB3	1:B:1426:ILE:HG22	2.01	0.41
1:B:3227:ARG:HH21	1:B:3227:ARG:HB3	1.85	0.41
1:C:1951:LEU:HD22	1:C:2133:GLU:OE2	2.20	0.41
1:C:4696:ASP:OD1	1:C:4696:ASP:C	2.63	0.41
1:D:2997:PHE:CE1	1:D:3002:LEU:CD2	3.04	0.41
1:A:16:THR:C	1:A:17:ASP:OD1	2.63	0.41
1:A:2625:ARG:HD2	1:A:2625:ARG:N	2.36	0.41
1:A:2997:PHE:C	1:A:2997:PHE:HD1	2.27	0.41
1:A:2997:PHE:CE1	1:A:3002:LEU:CD2	3.04	0.41
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.03	0.41
1:C:739:ALA:HB1	1:C:740:PRO:HD2	2.01	0.41
1:C:2625:ARG:HD2	1:C:2625:ARG:N	2.36	0.41
1:C:3624:LEU:HD22	1:C:3855:GLY:O	2.21	0.41
1:D:16:THR:C	1:D:17:ASP:OD1	2.63	0.41
1:D:309:THR:O	1:D:309:THR:HG22	2.20	0.41
1:D:415:ILE:HD11	1:D:490:CYS:SG	2.60	0.41
1:D:739:ALA:HB1	1:D:740:PRO:HD2	2.01	0.41
1:D:950:LEU:C	1:D:950:LEU:HD12	2.46	0.41
1:D:1251:GLU:O	1:D:1251:GLU:HG3	2.20	0.41
1:D:3696:ASP:OD1	1:D:3696:ASP:C	2.63	0.41
1:A:2414:ASN:O	1:A:2415:ARG:C	2.63	0.41
1:A:3624:LEU:HD22	1:A:3855:GLY:O	2.21	0.41
1:B:1176:GLU:OE1	1:B:1176:GLU:C	2.62	0.41
1:B:2672:LEU:HD12	1:B:2672:LEU:H	1.86	0.41
1:B:3624:LEU:HD22	1:B:3855:GLY:O	2.21	0.41
1:C:180:LEU:HD23	1:C:200:TRP:CE2	2.56	0.41
1:C:415:ILE:HD11	1:C:490:CYS:SG	2.60	0.41
1:C:950:LEU:HD12	1:C:950:LEU:C	2.46	0.41
1:C:2997:PHE:CE1	1:C:3002:LEU:CD2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:LYS:HB2	2:E:54:GLU:OE1	2.19	0.41
1:A:950:LEU:HD12	1:A:950:LEU:C	2.46	0.41
1:B:2997:PHE:C	1:B:2997:PHE:HD1	2.27	0.41
1:B:4696:ASP:OD1	1:B:4696:ASP:C	2.64	0.41
1:D:2111:VAL:HG21	1:D:2117:VAL:HG22	2.02	0.41
1:D:2414:ASN:O	1:D:2415:ARG:C	2.63	0.41
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	2.03	0.41
1:A:3937:TYR:CD2	1:A:3943:ILE:HG22	2.55	0.41
1:B:61:ASP:OD1	1:B:61:ASP:C	2.63	0.41
1:B:1762:LEU:HB2	1:B:1765:VAL:HG11	2.02	0.41
1:B:2997:PHE:CE1	1:B:3002:LEU:CD2	3.04	0.41
1:D:1929:MET:HE3	1:D:1931:LEU:HD11	2.03	0.41
1:D:3937:TYR:CD2	1:D:3943:ILE:HG22	2.55	0.41
1:A:2886:TRP:CD1	1:A:2886:TRP:C	2.98	0.41
1:A:4115:SER:HB2	1:A:4123:ILE:HD11	2.03	0.41
1:B:632:LEU:HD23	1:B:632:LEU:N	2.36	0.41
1:B:1929:MET:HE3	1:B:1931:LEU:HD11	2.03	0.41
1:B:3133:THR:HG23	1:B:3134:VAL:HG23	2.02	0.41
1:C:2672:LEU:HD12	1:C:2672:LEU:H	1.86	0.41
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	2.02	0.41
1:D:61:ASP:OD1	1:D:61:ASP:C	2.63	0.41
1:D:2625:ARG:N	1:D:2625:ARG:HD2	2.36	0.41
1:A:180:LEU:HD23	1:A:200:TRP:CE2	2.56	0.41
1:A:827:LYS:O	1:A:827:LYS:HG3	2.20	0.41
1:A:1929:MET:HE3	1:A:1931:LEU:HD11	2.03	0.41
1:A:2672:LEU:HD12	1:A:2672:LEU:H	1.86	0.41
1:A:2684:ASP:O	1:A:2687:ALA:HB3	2.21	0.41
1:A:2959:PHE:CE1	1:A:2963:LEU:HD21	2.56	0.41
1:A:4184:MET:HE1	1:A:4189:ARG:C	2.45	0.41
1:A:4777:ILE:HD13	1:A:4777:ILE:N	2.36	0.41
1:B:650:VAL:HG11	1:B:662:TRP:NE1	2.36	0.41
1:B:2619:LEU:HD12	1:B:2622:LEU:HD23	2.02	0.41
1:B:2959:PHE:CE1	1:B:2963:LEU:HD21	2.56	0.41
1:B:4047:MET:HE3	1:B:4047:MET:HB3	1.99	0.41
1:B:4777:ILE:HD13	1:B:4777:ILE:N	2.36	0.41
1:C:827:LYS:O	1:C:827:LYS:HG3	2.20	0.41
1:C:1251:GLU:O	1:C:1251:GLU:HG3	2.20	0.41
1:C:2414:ASN:O	1:C:2415:ARG:C	2.63	0.41
1:C:3005:LEU:HD23	1:C:3005:LEU:C	2.46	0.41
1:C:3105:LYS:HZ3	1:C:3125:VAL:HG22	1.86	0.41
1:C:3723:MET:HE2	1:C:3723:MET:HB2	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4942:GLU:O	1:C:4946:GLN:HG3	2.21	0.41
1:D:650:VAL:HG11	1:D:662:TRP:NE1	2.36	0.41
1:D:3133:THR:HG23	1:D:3134:VAL:HG23	2.02	0.41
1:D:3624:LEU:HD22	1:D:3855:GLY:O	2.21	0.41
1:D:4115:SER:HB2	1:D:4123:ILE:HD11	2.03	0.41
1:B:2776:SER:O	1:B:2785:LEU:HD21	2.21	0.41
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	2.02	0.41
1:C:2111:VAL:HG21	1:C:2117:VAL:HG22	2.02	0.41
1:C:4115:SER:HB2	1:C:4123:ILE:HD11	2.03	0.41
1:D:1951:LEU:HD22	1:D:2133:GLU:OE2	2.20	0.41
1:D:3105:LYS:HZ3	1:D:3125:VAL:HG22	1.86	0.41
1:A:650:VAL:HG11	1:A:662:TRP:NE1	2.36	0.40
1:A:2606:CYS:O	1:A:2610:LEU:HD23	2.22	0.40
1:A:4696:ASP:OD1	1:A:4696:ASP:C	2.64	0.40
1:B:180:LEU:HD23	1:B:200:TRP:CE2	2.56	0.40
1:B:307:ALA:HB1	1:B:312:THR:HG21	2.04	0.40
1:B:2414:ASN:O	1:B:2415:ARG:C	2.63	0.40
1:B:2625:ARG:HD2	1:B:2625:ARG:N	2.36	0.40
1:C:3157:ILE:HG22	1:C:3162:GLN:CG	2.51	0.40
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.96	0.40
1:D:632:LEU:N	1:D:632:LEU:HD23	2.36	0.40
1:D:2684:ASP:O	1:D:2687:ALA:HB3	2.21	0.40
1:A:2624:ARG:O	1:A:2627:VAL:HG12	2.22	0.40
1:B:45:ARG:NE	1:B:116:MET:HE1	2.37	0.40
1:B:827:LYS:O	1:B:827:LYS:HG3	2.20	0.40
1:B:1251:GLU:O	1:B:1251:GLU:HG3	2.20	0.40
1:B:4942:GLU:O	1:B:4946:GLN:HG3	2.21	0.40
1:C:45:ARG:NE	1:C:116:MET:HE1	2.37	0.40
1:C:632:LEU:N	1:C:632:LEU:HD23	2.36	0.40
1:C:1929:MET:HE3	1:C:1931:LEU:HD11	2.03	0.40
1:C:2012:PHE:O	1:C:2012:PHE:CG	2.75	0.40
1:C:2155:LEU:HD21	1:C:2198:MET:HE1	2.04	0.40
1:C:4184:MET:HE1	1:C:4189:ARG:C	2.45	0.40
1:C:4985:LEU:H	4:C:5101:ACP:HN61	1.68	0.40
1:D:180:LEU:HD23	1:D:200:TRP:CE2	2.56	0.40
1:D:4184:MET:HE1	1:D:4189:ARG:C	2.45	0.40
1:D:4696:ASP:OD1	1:D:4696:ASP:C	2.64	0.40
1:A:2012:PHE:O	1:A:2012:PHE:CG	2.75	0.40
1:A:3133:THR:HG23	1:A:3134:VAL:HG23	2.02	0.40
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.36	0.40
1:B:1986:MET:HA	1:B:1986:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2624:ARG:O	1:B:2627:VAL:HG12	2.22	0.40
1:B:3005:LEU:HD23	1:B:3005:LEU:C	2.46	0.40
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.86	0.40
1:C:3140:LEU:HD11	1:C:3144:PHE:CZ	2.57	0.40
1:D:2606:CYS:O	1:D:2610:LEU:HD23	2.22	0.40
1:D:3050:VAL:HG22	1:D:3050:VAL:O	2.20	0.40
1:D:3844:LEU:H	1:D:3844:LEU:CD2	2.34	0.40
1:B:2155:LEU:HD21	1:B:2198:MET:HE1	2.04	0.40
1:B:2867:LEU:CD1	1:B:2927:LEU:HD21	2.52	0.40
1:B:3140:LEU:HD11	1:B:3144:PHE:CZ	2.57	0.40
1:B:3157:ILE:HG22	1:B:3162:GLN:CG	2.51	0.40
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.86	0.40
1:C:3346:VAL:HG11	1:C:3414:ARG:CB	2.51	0.40
1:D:45:ARG:NE	1:D:116:MET:HE1	2.37	0.40
1:D:2959:PHE:CE1	1:D:2963:LEU:HD21	2.56	0.40
1:D:3137:LEU:HB3	1:D:3138:PRO:HD3	2.04	0.40
1:A:632:LEU:N	1:A:632:LEU:HD23	2.36	0.40
1:A:3157:ILE:HG22	1:A:3162:GLN:CG	2.51	0.40
1:B:2684:ASP:O	1:B:2687:ALA:HB3	2.21	0.40
1:B:4115:SER:HB2	1:B:4123:ILE:HD11	2.03	0.40
1:C:307:ALA:HB1	1:C:312:THR:HG21	2.04	0.40
1:C:1931:LEU:H	1:C:1931:LEU:HD22	1.87	0.40
1:C:1986:MET:HA	1:C:1986:MET:HE3	2.03	0.40
1:C:2038:LEU:O	1:C:2038:LEU:HD23	2.22	0.40
1:C:2776:SER:O	1:C:2785:LEU:HD21	2.21	0.40
1:C:2867:LEU:CD1	1:C:2927:LEU:HD21	2.52	0.40
1:D:826:ILE:O	1:D:826:ILE:HG23	2.22	0.40
1:D:2867:LEU:CD1	1:D:2927:LEU:HD21	2.52	0.40
1:D:3346:VAL:HG11	1:D:3414:ARG:CB	2.52	0.40
1:D:4985:LEU:H	4:D:5102:ACP:HN61	1.68	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%)	4201 (96%)	173 (4%)	2 (0%)	100	100
1	B	4376/5037 (87%)	4200 (96%)	174 (4%)	2 (0%)	100	100
1	C	4376/5037 (87%)	4201 (96%)	173 (4%)	2 (0%)	100	100
1	D	4376/5037 (87%)	4201 (96%)	173 (4%)	2 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17924/20580 (87%)	17208 (96%)	708 (4%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	850	ASP
1	B	850	ASP
1	C	850	ASP
1	D	850	ASP
1	A	3623	LEU
1	B	3623	LEU
1	C	3623	LEU
1	D	3623	LEU

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%)	3785 (99%)	42 (1%)	65	74
1	B	3827/4276 (90%)	3784 (99%)	43 (1%)	65	74
1	C	3827/4276 (90%)	3785 (99%)	42 (1%)	65	74
1	D	3827/4276 (90%)	3785 (99%)	42 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	15491 (99%)	173 (1%)	63	74

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	220	LEU
1	A	244	LEU
1	A	359	TYR
1	A	601	ASP
1	A	848	HIS
1	A	887	ILE
1	A	922	LEU
1	A	1021	LEU
1	A	1035	ASN
1	A	1039	LEU
1	A	1152	MET
1	A	1435	TYR
1	A	1511	HIS
1	A	1733	GLU
1	A	1812	LEU
1	A	1923	GLU
1	A	2120	MET
1	A	2441	HIS
1	A	2443	ILE
1	A	2522	LEU
1	A	2768	PHE
1	A	2777	TYR
1	A	2937	VAL
1	A	3305	THR
1	A	3663	LEU
1	A	3702	VAL
1	A	3752	SER
1	A	3841	VAL
1	A	3951	PHE
1	A	4046	ASP
1	A	4071	ILE

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Mol	Chain	Res	Type
1	A	4088	ILE
1	A	4153	HIS
1	A	4183	ILE
1	A	4212	GLU
1	A	4544	LEU
1	A	4580	TYR
1	A	4821	LYS
1	A	4901	ILE
1	A	4952	GLU
1	A	5032	TYR
1	B	17	ASP
1	B	220	LEU
1	B	244	LEU
1	B	359	TYR
1	B	601	ASP
1	B	848	HIS
1	B	887	ILE
1	B	922	LEU
1	B	1021	LEU
1	B	1039	LEU
1	B	1152	MET
1	B	1435	TYR
1	B	1511	HIS
1	B	1608	MET
1	B	1733	GLU
1	B	1812	LEU
1	B	1923	GLU
1	B	2120	MET
1	B	2441	HIS
1	B	2443	ILE
1	B	2522	LEU
1	B	2768	PHE
1	B	2777	TYR
1	B	2937	VAL
1	B	3305	THR
1	B	3663	LEU
1	B	3702	VAL
1	B	3752	SER
1	B	3841	VAL
1	B	3951	PHE
1	B	4046	ASP
1	B	4071	ILE

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Mol	Chain	Res	Type
1	B	4088	ILE
1	B	4153	HIS
1	B	4183	ILE
1	B	4212	GLU
1	B	4544	LEU
1	B	4580	TYR
1	B	4821	LYS
1	B	4852	THR
1	B	4901	ILE
1	B	4952	GLU
1	B	5032	TYR
1	C	17	ASP
1	C	220	LEU
1	C	244	LEU
1	C	359	TYR
1	C	601	ASP
1	C	848	HIS
1	C	887	ILE
1	C	922	LEU
1	C	1021	LEU
1	C	1035	ASN
1	C	1039	LEU
1	C	1152	MET
1	C	1435	TYR
1	C	1511	HIS
1	C	1608	MET
1	C	1733	GLU
1	C	1812	LEU
1	C	1923	GLU
1	C	2120	MET
1	C	2441	HIS
1	C	2443	ILE
1	C	2522	LEU
1	C	2768	PHE
1	C	2937	VAL
1	C	3305	THR
1	C	3663	LEU
1	C	3702	VAL
1	C	3752	SER
1	C	3841	VAL
1	C	3951	PHE
1	C	4046	ASP

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Mol	Chain	Res	Type
1	C	4071	ILE
1	C	4088	ILE
1	C	4153	HIS
1	C	4183	ILE
1	C	4212	GLU
1	C	4544	LEU
1	C	4580	TYR
1	C	4821	LYS
1	C	4901	ILE
1	C	4952	GLU
1	C	5032	TYR
1	D	17	ASP
1	D	220	LEU
1	D	244	LEU
1	D	359	TYR
1	D	601	ASP
1	D	848	HIS
1	D	887	ILE
1	D	922	LEU
1	D	1021	LEU
1	D	1039	LEU
1	D	1152	MET
1	D	1435	TYR
1	D	1511	HIS
1	D	1608	MET
1	D	1733	GLU
1	D	1812	LEU
1	D	1923	GLU
1	D	2120	MET
1	D	2441	HIS
1	D	2443	ILE
1	D	2522	LEU
1	D	2768	PHE
1	D	2777	TYR
1	D	2937	VAL
1	D	3305	THR
1	D	3663	LEU
1	D	3702	VAL
1	D	3752	SER
1	D	3841	VAL
1	D	3951	PHE
1	D	4046	ASP

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Mol	Chain	Res	Type
1	D	4071	ILE
1	D	4088	ILE
1	D	4153	HIS
1	D	4183	ILE
1	D	4212	GLU
1	D	4544	LEU
1	D	4580	TYR
1	D	4821	LYS
1	D	4901	ILE
1	D	4952	GLU
1	D	5032	TYR
2	E	29	MET
2	F	29	MET
2	G	29	MET
2	H	29	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	405	HIS
1	A	461	HIS
1	A	582	HIS
1	A	1545	ASN
1	A	1560	ASN
1	A	1611	HIS
1	A	1776	HIS
1	A	2284	ASN
1	A	2342	ASN
1	A	2688	HIS
1	A	2774	ASN
1	A	3313	ASN
1	A	3554	GLN
1	A	3927	GLN
1	A	3998	HIS
1	A	4153	HIS
1	A	4662	ASN
1	A	4753	HIS
1	A	4803	HIS
1	A	5003	HIS
1	B	98	HIS
1	B	405	HIS

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Mol	Chain	Res	Type
1	B	461	HIS
1	B	582	HIS
1	B	1231	GLN
1	B	1560	ASN
1	B	1611	HIS
1	B	1776	HIS
1	B	2032	GLN
1	B	2284	ASN
1	B	2342	ASN
1	B	2688	HIS
1	B	2774	ASN
1	B	2892	GLN
1	B	3313	ASN
1	B	3554	GLN
1	B	3927	GLN
1	B	3998	HIS
1	B	4153	HIS
1	B	4662	ASN
1	B	4803	HIS
1	B	4812	HIS
1	B	5003	HIS
1	C	98	HIS
1	C	226	HIS
1	C	405	HIS
1	C	461	HIS
1	C	582	HIS
1	C	681	HIS
1	C	1231	GLN
1	C	1545	ASN
1	C	1560	ASN
1	C	1611	HIS
1	C	1775	HIS
1	C	1776	HIS
1	C	2032	GLN
1	C	2284	ASN
1	C	2342	ASN
1	C	2688	HIS
1	C	2773	ASN
1	C	2774	ASN
1	C	3069	HIS
1	C	3313	ASN
1	C	3554	GLN

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Mol	Chain	Res	Type
1	C	3927	GLN
1	C	3998	HIS
1	C	4153	HIS
1	C	4803	HIS
1	C	4812	HIS
1	C	4832	HIS
1	C	4833	ASN
1	C	4836	GLN
1	C	5003	HIS
1	D	98	HIS
1	D	405	HIS
1	D	461	HIS
1	D	582	HIS
1	D	1545	ASN
1	D	1560	ASN
1	D	1775	HIS
1	D	1776	HIS
1	D	2284	ASN
1	D	2342	ASN
1	D	2584	HIS
1	D	2774	ASN
1	D	2892	GLN
1	D	3313	ASN
1	D	3554	GLN
1	D	3927	GLN
1	D	3998	HIS
1	D	4153	HIS
1	D	4803	HIS
1	D	5003	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACP	D	5102	-	30,33,33	1.30	4 (13%)	45,52,52	1.35	7 (15%)
4	ACP	B	5102	-	30,33,33	1.30	4 (13%)	45,52,52	1.30	6 (13%)
4	ACP	A	5102	-	30,33,33	1.28	3 (10%)	45,52,52	1.34	8 (17%)
4	ACP	C	5101	-	30,33,33	1.30	4 (13%)	45,52,52	1.32	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	D	5102	-	-	6/19/38/38	0/3/3/3
4	ACP	B	5102	-	-	2/19/38/38	0/3/3/3
4	ACP	A	5102	-	-	9/19/38/38	0/3/3/3
4	ACP	C	5101	-	-	7/19/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5102	ACP	PB-O2B	-3.32	1.48	1.56
4	B	5102	ACP	PB-O2B	-3.26	1.48	1.56
4	C	5101	ACP	PB-O2B	-3.12	1.49	1.56
4	D	5102	ACP	PB-O2B	-3.07	1.49	1.56
4	B	5102	ACP	PG-O3G	-2.94	1.48	1.54
4	C	5101	ACP	PG-O3G	-2.79	1.48	1.54
4	D	5102	ACP	PG-O3G	-2.77	1.48	1.54
4	A	5102	ACP	PG-O2G	-2.74	1.48	1.54
4	D	5102	ACP	PG-O2G	-2.72	1.48	1.54
4	A	5102	ACP	PG-O3G	-2.71	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	ACP	PG-O2G	-2.63	1.48	1.54
4	C	5101	ACP	PG-O2G	-2.59	1.49	1.54
4	D	5102	ACP	C5-C4	-2.19	1.34	1.39
4	B	5102	ACP	C5-C4	-2.08	1.35	1.39
4	C	5101	ACP	C5-C4	-2.03	1.35	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5102	ACP	O1G-PG-C3B	3.48	118.74	111.24
4	A	5102	ACP	C5-C4-N3	-3.37	122.35	126.75
4	C	5101	ACP	O1G-PG-C3B	3.25	118.24	111.24
4	D	5102	ACP	PB-O3A-PA	-3.09	122.75	132.56
4	C	5101	ACP	C5-C4-N3	-3.09	122.72	126.75
4	B	5102	ACP	C5-C4-N3	-3.09	122.72	126.75
4	B	5102	ACP	O3G-PG-C3B	3.08	113.86	106.40
4	D	5102	ACP	C5-C4-N3	-2.95	122.91	126.75
4	C	5101	ACP	PB-O3A-PA	-2.93	123.27	132.56
4	A	5102	ACP	O1G-PG-C3B	2.89	117.48	111.24
4	D	5102	ACP	C4-C5-N7	2.84	114.08	110.62
4	C	5101	ACP	C4-C5-N7	2.81	114.03	110.62
4	B	5102	ACP	PB-O3A-PA	-2.74	123.87	132.56
4	A	5102	ACP	C4-C5-N7	2.64	113.84	110.62
4	A	5102	ACP	PB-O3A-PA	-2.54	124.49	132.56
4	B	5102	ACP	C4-C5-N7	2.48	113.64	110.62
4	B	5102	ACP	C2-N1-C6	-2.44	114.58	118.77
4	C	5101	ACP	C5-C6-N1	2.32	122.37	117.39
4	A	5102	ACP	N3-C4-N9	2.31	130.89	127.08
4	D	5102	ACP	C5-C6-N1	2.30	122.34	117.39
4	B	5102	ACP	C5-C6-N1	2.30	122.33	117.39
4	A	5102	ACP	C5-C6-N1	2.28	122.29	117.39
4	A	5102	ACP	O4'-C1'-C2'	-2.22	101.79	106.64
4	C	5101	ACP	N3-C4-N9	2.19	130.69	127.08
4	D	5102	ACP	C2-N1-C6	-2.18	115.02	118.77
4	A	5102	ACP	C2-N1-C6	-2.14	115.09	118.77
4	D	5102	ACP	N3-C4-N9	2.11	130.56	127.08
4	C	5101	ACP	C2-N1-C6	-2.10	115.17	118.77

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5102	ACP	PB-C3B-PG-O1G
4	A	5102	ACP	PB-C3B-PG-O2G
4	A	5102	ACP	PB-C3B-PG-O3G
4	A	5102	ACP	C4'-C5'-O5'-PA
4	C	5101	ACP	PB-C3B-PG-O1G
4	C	5101	ACP	PB-C3B-PG-O2G
4	C	5101	ACP	PB-C3B-PG-O3G
4	C	5101	ACP	PB-O3A-PA-O5'
4	D	5102	ACP	PB-C3B-PG-O1G
4	D	5102	ACP	PB-C3B-PG-O2G
4	D	5102	ACP	PB-C3B-PG-O3G
4	A	5102	ACP	C3'-C4'-C5'-O5'
4	A	5102	ACP	O4'-C4'-C5'-O5'
4	C	5101	ACP	C3'-C4'-C5'-O5'
4	D	5102	ACP	O4'-C4'-C5'-O5'
4	D	5102	ACP	C3'-C4'-C5'-O5'
4	C	5101	ACP	O4'-C4'-C5'-O5'
4	B	5102	ACP	O4'-C4'-C5'-O5'
4	C	5101	ACP	C4'-C5'-O5'-PA
4	D	5102	ACP	C4'-C5'-O5'-PA
4	B	5102	ACP	C3'-C4'-C5'-O5'
4	A	5102	ACP	C2'-C1'-N9-C8
4	A	5102	ACP	C5'-O5'-PA-O3A
4	A	5102	ACP	C5'-O5'-PA-O2A

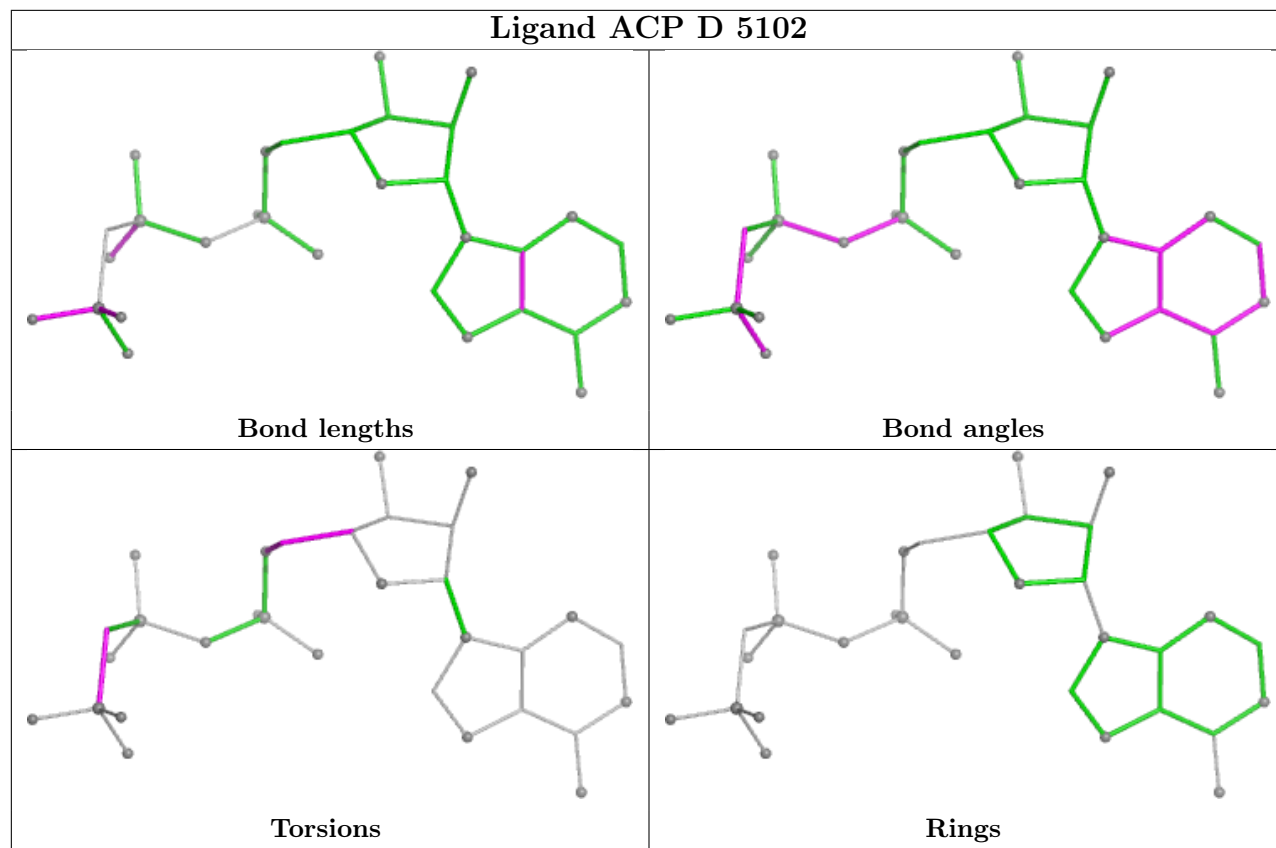
There are no ring outliers.

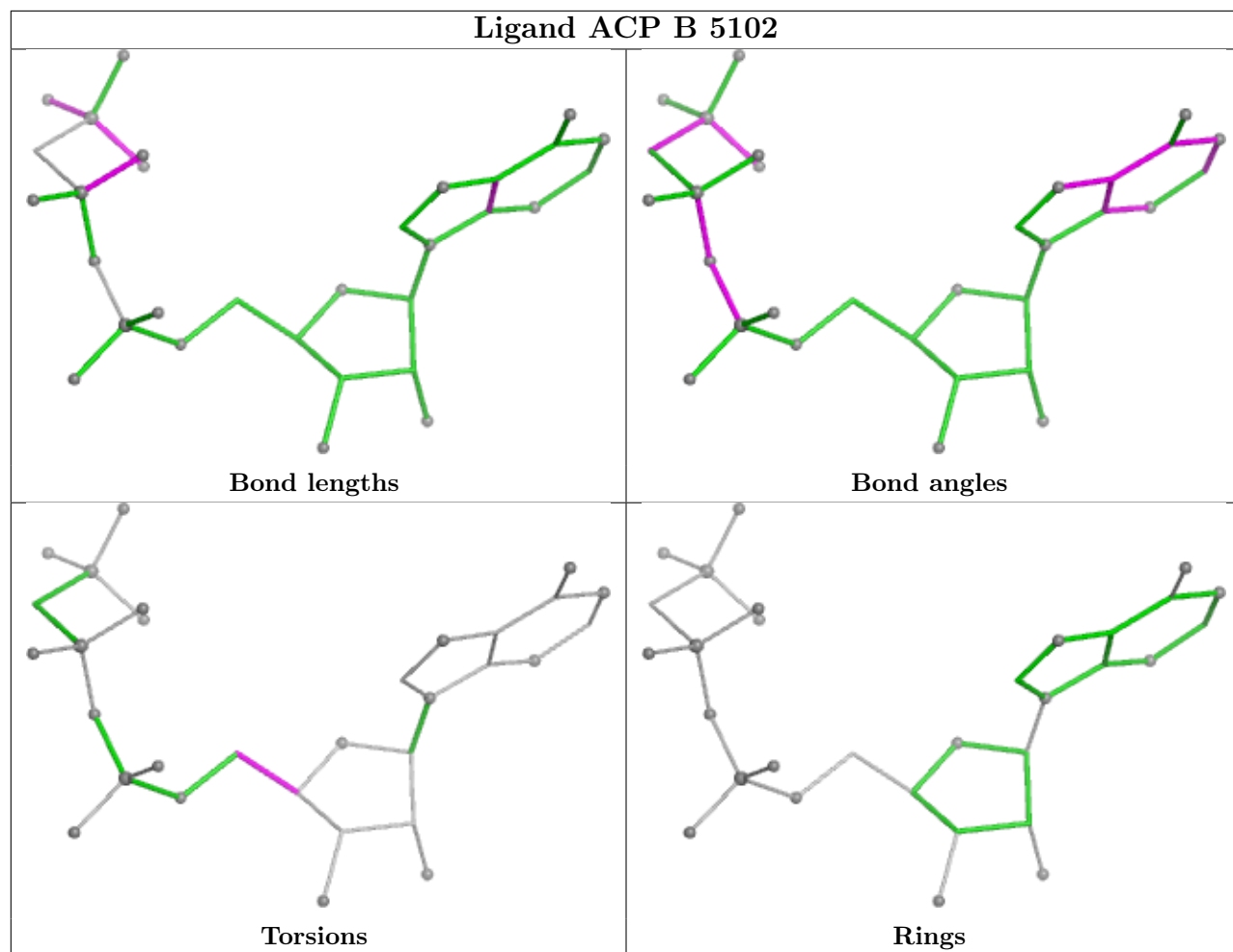
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5102	ACP	1	0
4	C	5101	ACP	1	0

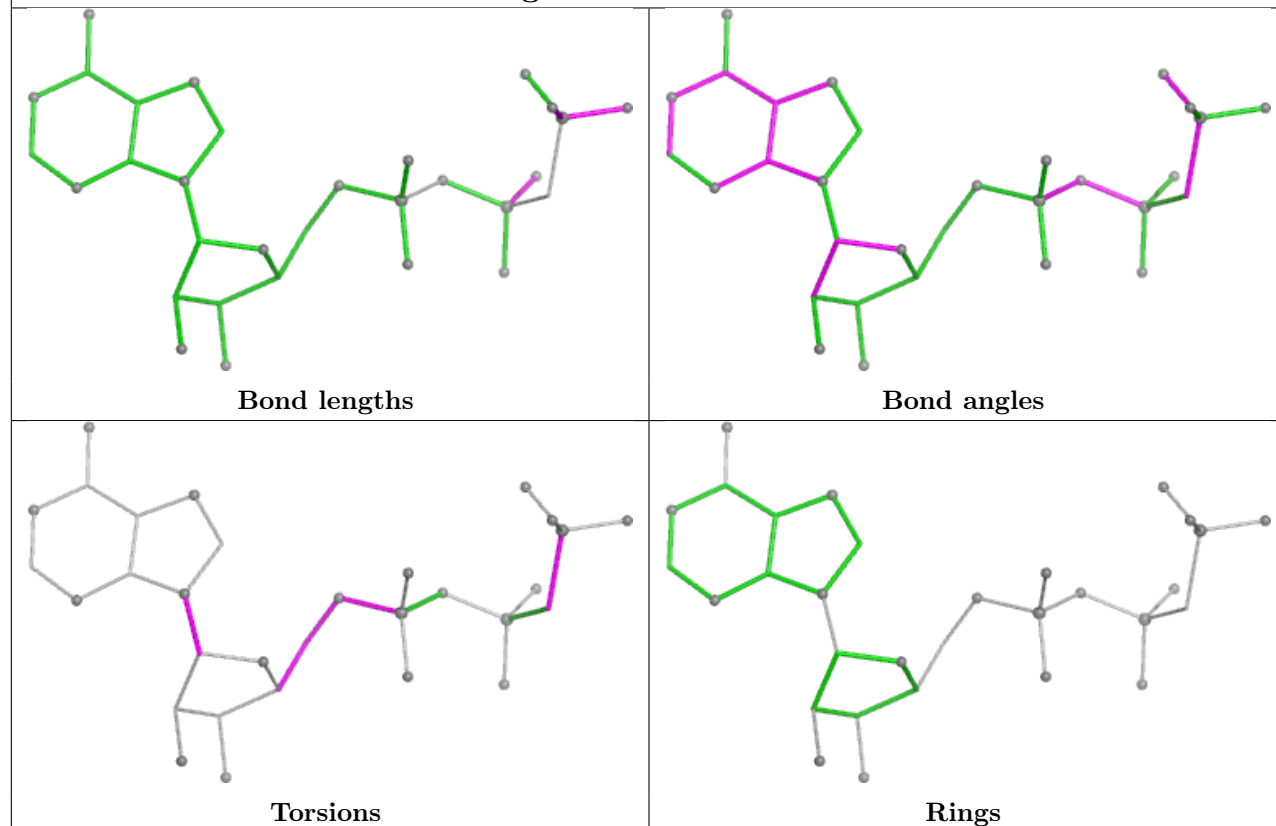
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

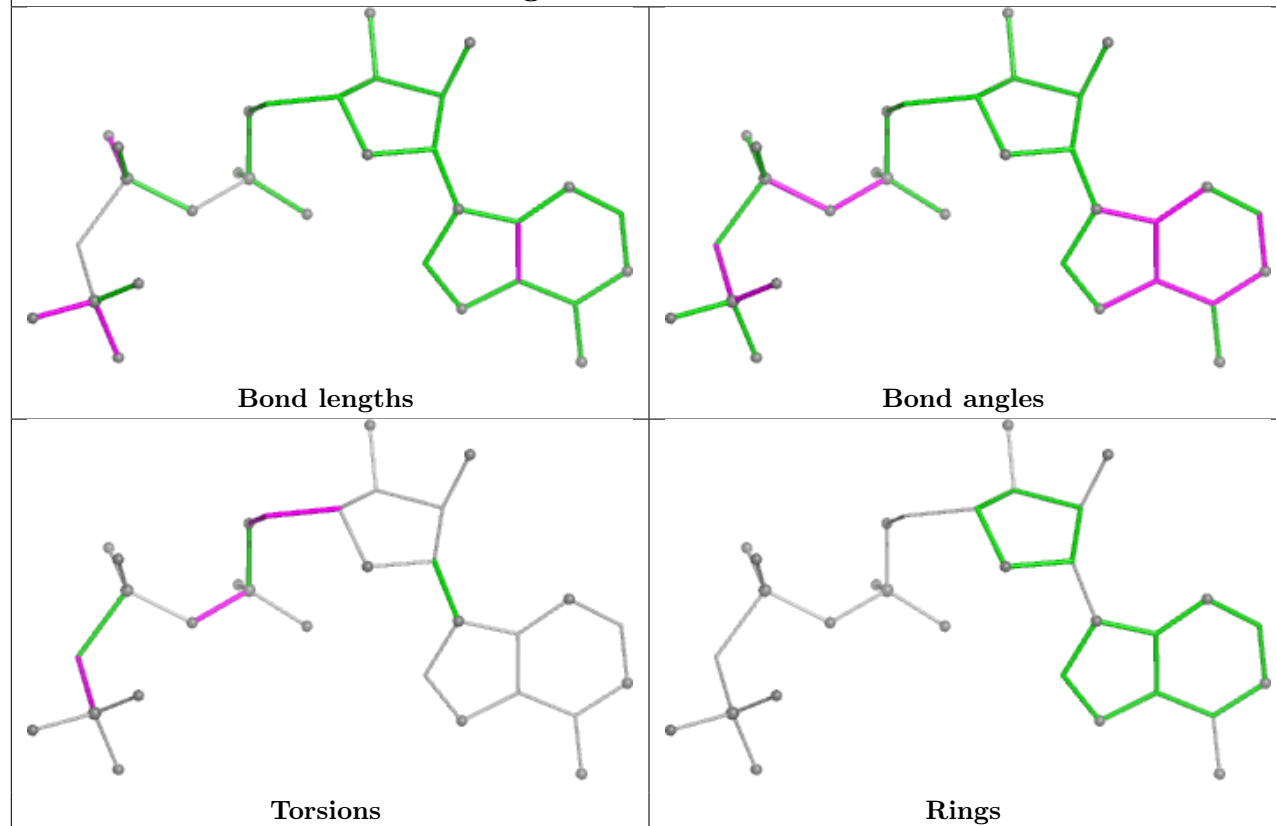




Ligand ACP A 5102



Ligand ACP C 5101



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.

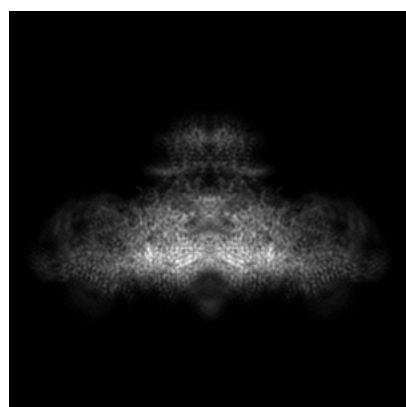
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54454. These allow visual inspection of the internal detail of the map and identification of artifacts.

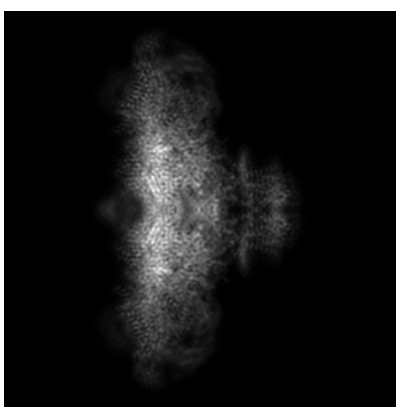
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

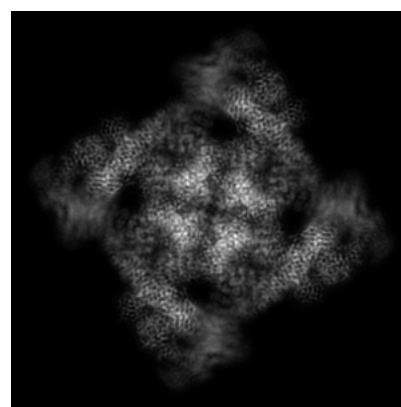
6.1.1 Primary map



X



Y

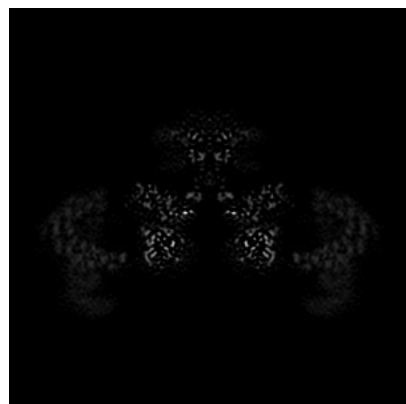


Z

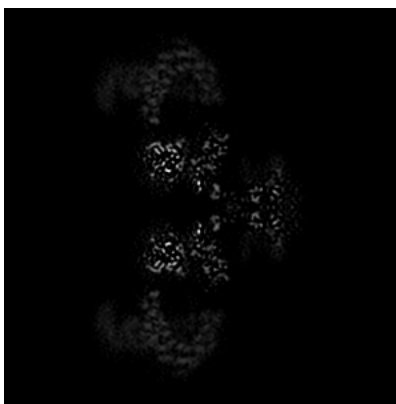
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

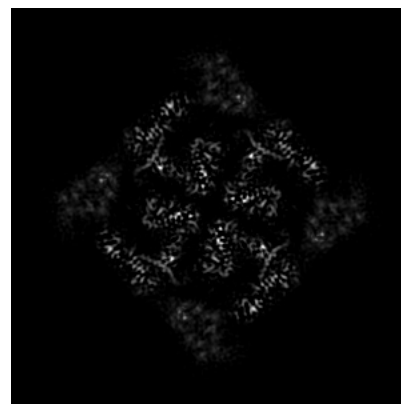
6.2.1 Primary map



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: 174



Y Index: 126

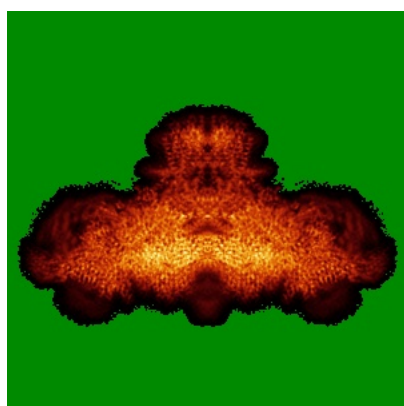


Z Index: 116

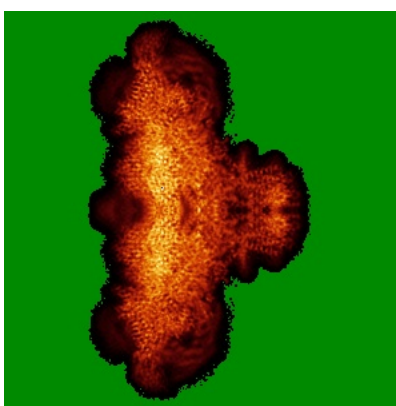
The images above show the largest variance slices of the map in three orthogonal directions.

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

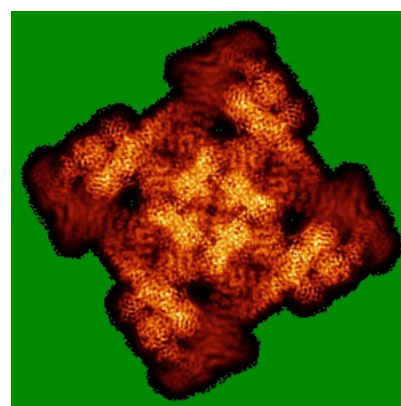
6.4.1 Primary map



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

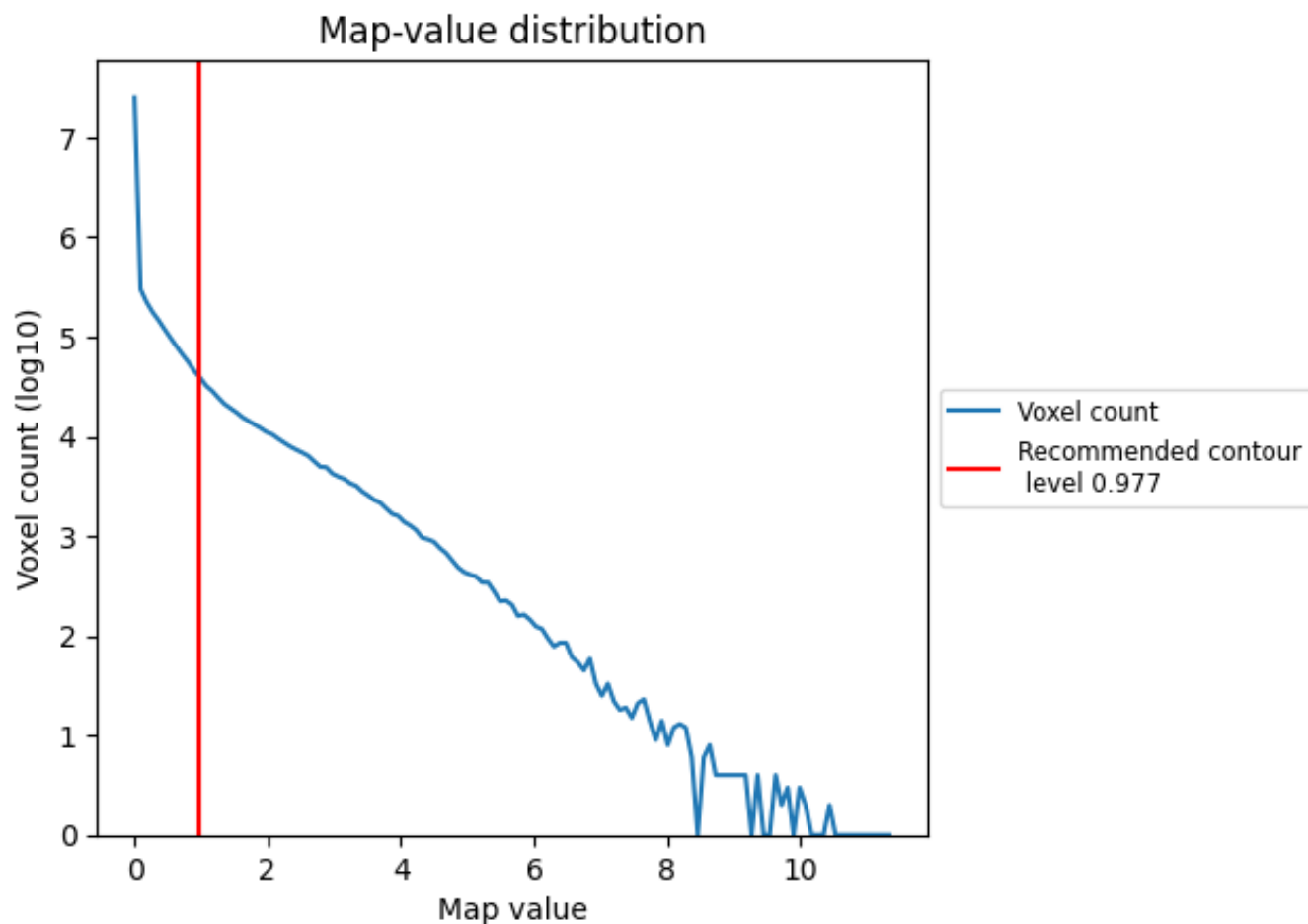
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

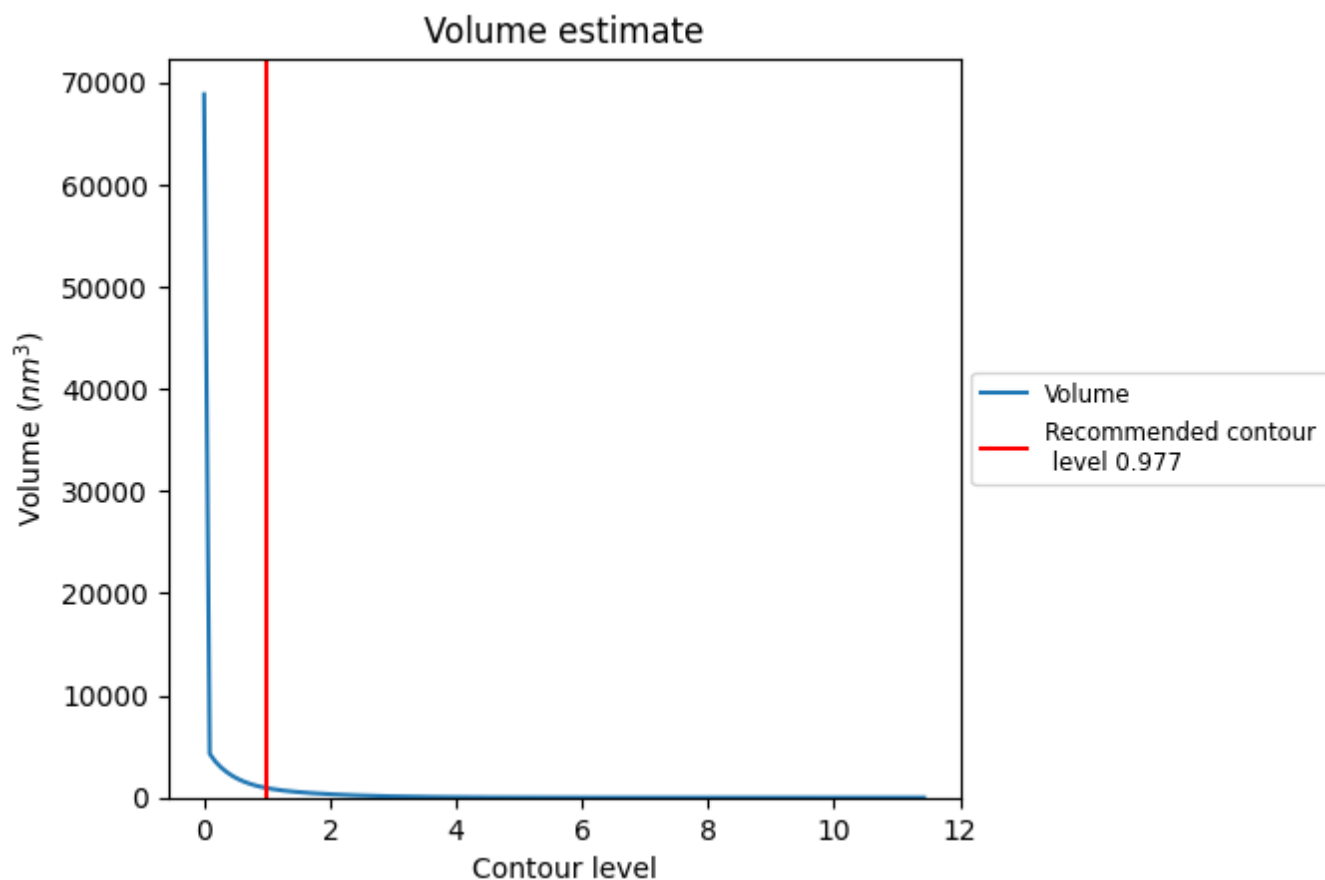
This section contains the results of statistical analysis of the map.

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.

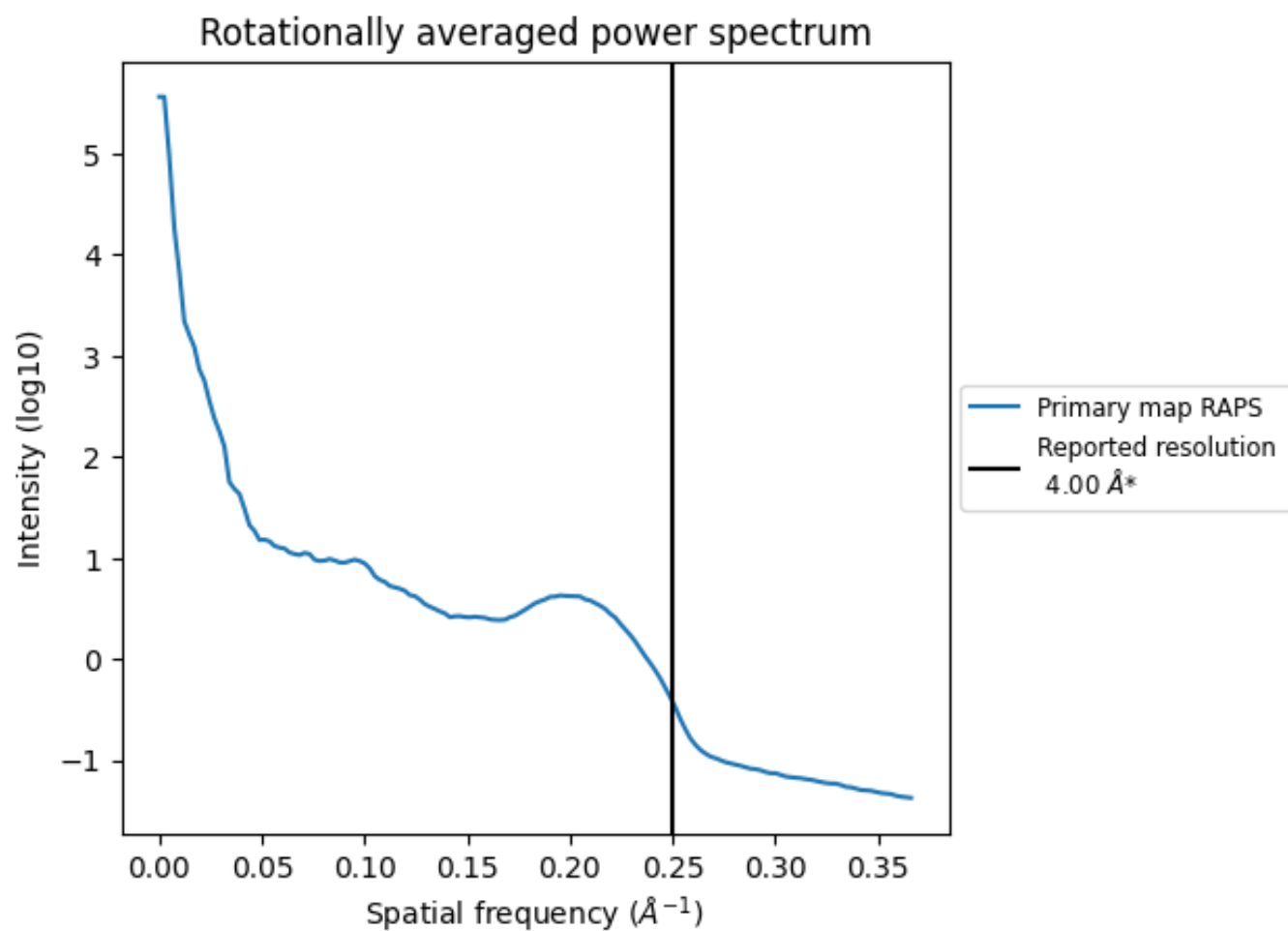
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 952 nm^3 ; this corresponds to an approximate mass of 860 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

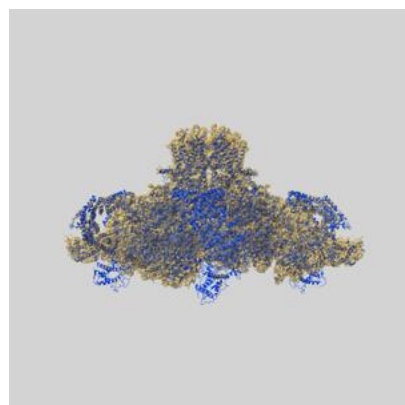
8 Fourier-Shell correlation ⓘ

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

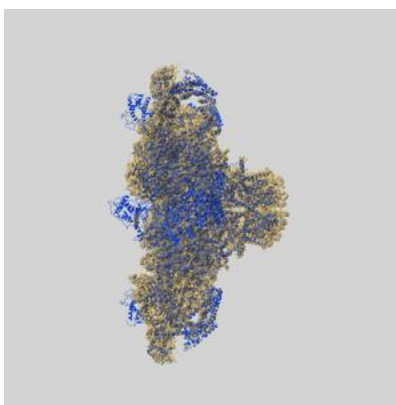
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54454 and PDB model 9S1H. Per-residue inclusion information can be found in section [3](#) on page [6](#).

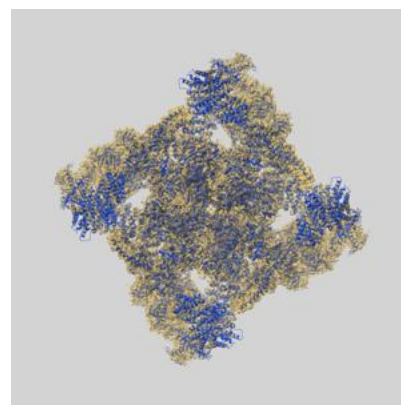
9.1 Map-model overlay [i](#)



X



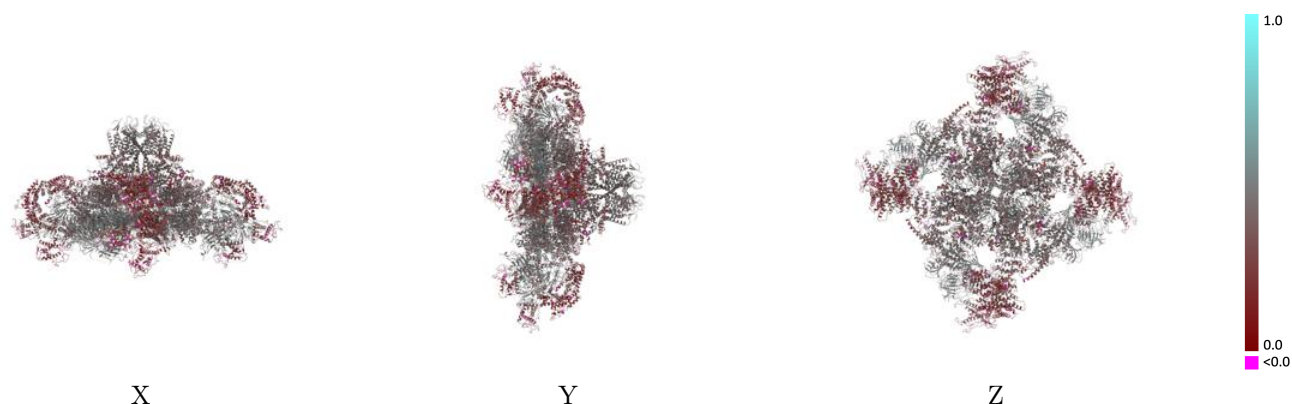
Y



Z

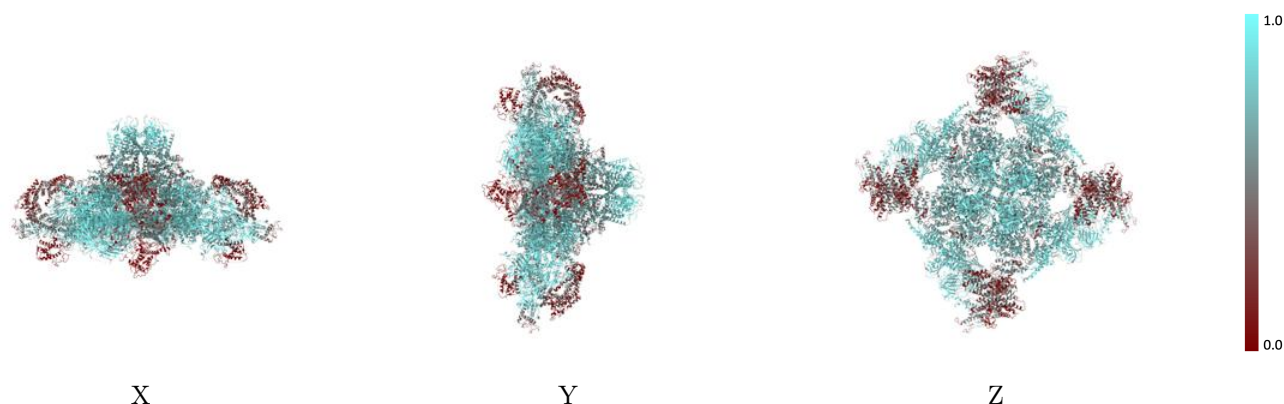
The images above show the 3D surface view of the map at the recommended contour level 0.977 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



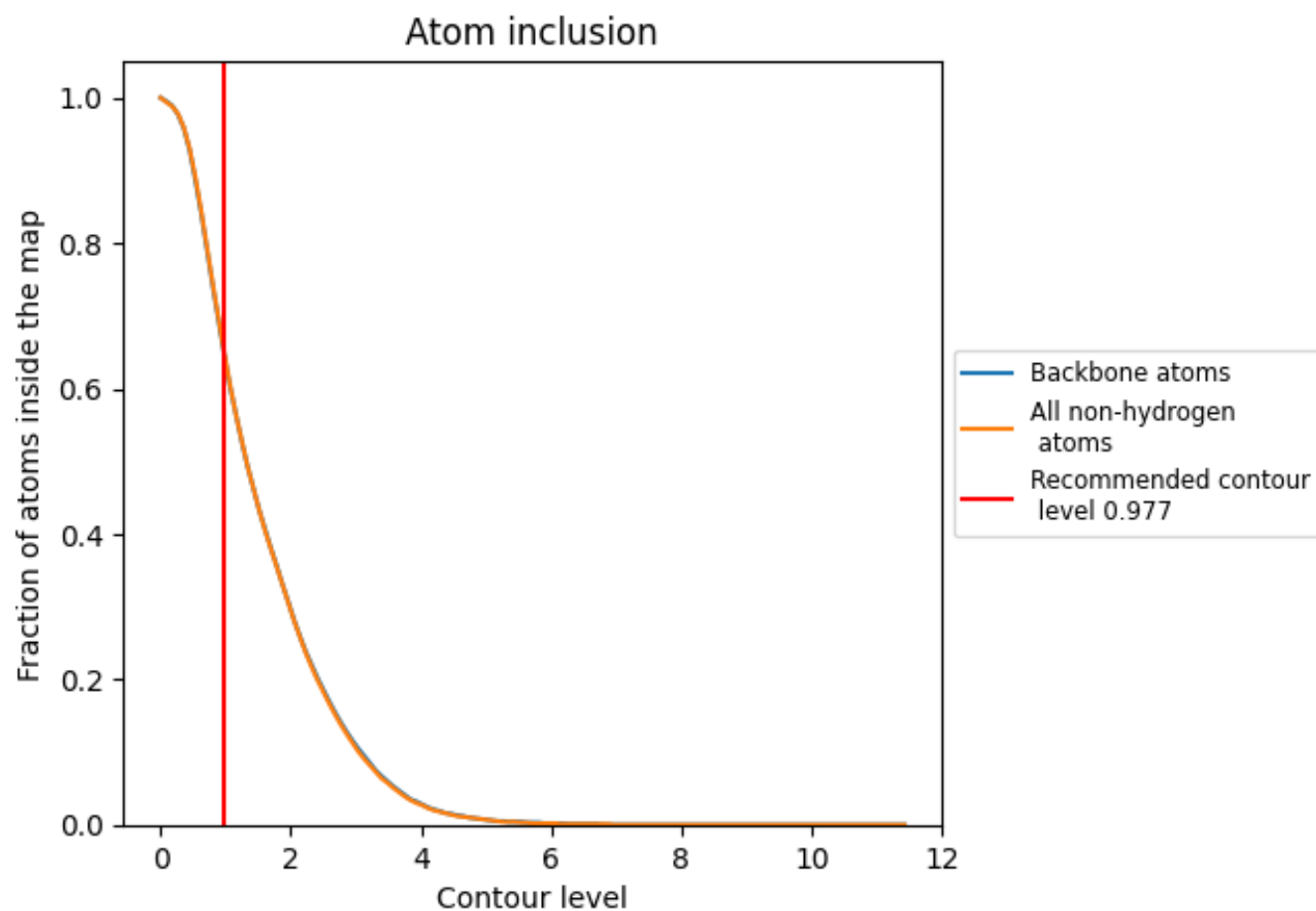
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.977).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.977) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.3790
A	0.6480	0.3770
B	0.6470	0.3780
C	0.6480	0.3770
D	0.6580	0.3750
E	0.8650	0.4620
F	0.8650	0.4630
G	0.8650	0.4660
H	0.8760	0.4590

1.0

0.0

<0.0