



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:28 AM UTC

PDB ID : 3VKH / pdb_00003vkh
Title : X-ray structure of a functional full-length dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

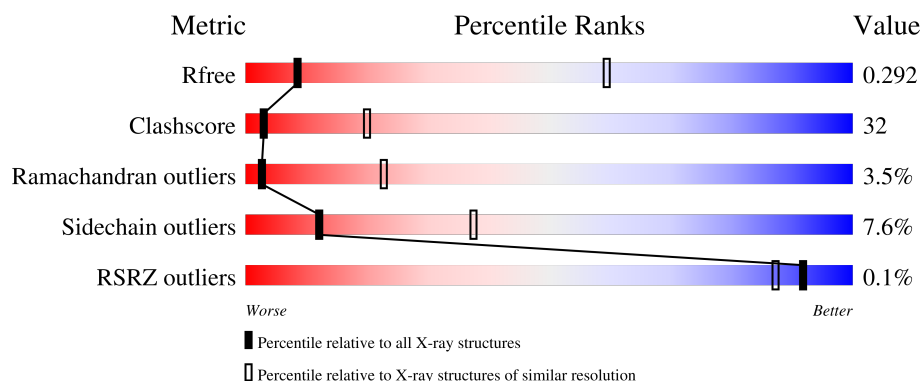
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3367	
1	B	3367	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 45974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	3042	Total	C	N	O	S	0	0	0
			23374	14951	3955	4368	100			
1	B	2908	Total	C	N	O	S	0	0	0
			22384	14307	3792	4190	95			

There are 48 discrepancies between the modelled and reference sequences:

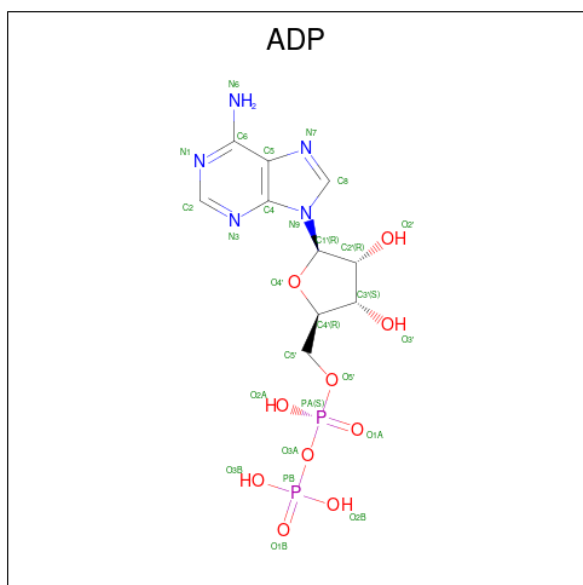
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	expression tag	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036
B	1364	MET	-	expression tag	UNP P34036

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1365	THR	-	expression tag	UNP P34036
B	1366	ARG	-	expression tag	UNP P34036
B	1367	HIS	-	expression tag	UNP P34036
B	1368	HIS	-	expression tag	UNP P34036
B	1369	HIS	-	expression tag	UNP P34036
B	1370	HIS	-	expression tag	UNP P34036
B	1371	HIS	-	expression tag	UNP P34036
B	1372	HIS	-	expression tag	UNP P34036
B	1373	GLY	-	expression tag	UNP P34036
B	1374	GLY	-	expression tag	UNP P34036
B	1375	GLY	-	expression tag	UNP P34036
B	1376	ASP	-	expression tag	UNP P34036
B	1377	TYR	-	expression tag	UNP P34036
B	1378	LYS	-	expression tag	UNP P34036
B	1379	ASP	-	expression tag	UNP P34036
B	1380	ASP	-	expression tag	UNP P34036
B	1381	ASP	-	expression tag	UNP P34036
B	1382	ASP	-	expression tag	UNP P34036
B	1383	LYS	-	expression tag	UNP P34036
B	1384	GLY	-	expression tag	UNP P34036
B	1385	GLY	-	expression tag	UNP P34036
B	1386	GLY	-	expression tag	UNP P34036
B	1387	LYS	-	expression tag	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

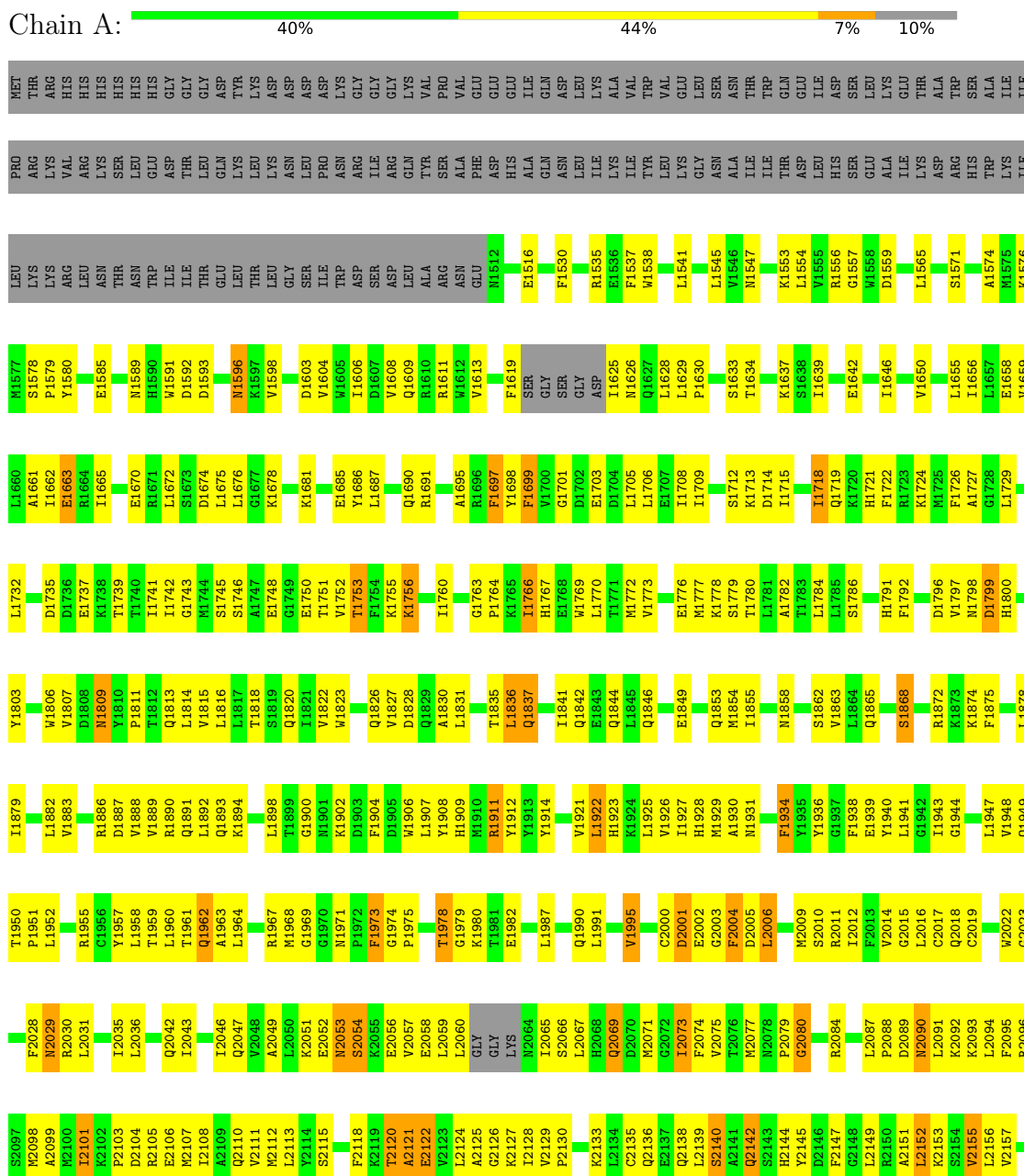


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots

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

- Molecule 1: Dynein heavy chain, cytoplasmic



L3216	F3145	C3064	L2988	L2912	L2842	V2773	V2697	Y2615	F2538	I1E	L2387	Q2315	H2248	K2163
M3217	T3146	K3065	V2989	F2913	L2842	R2774	S2698	S2616	S2539	THR	L2387	L2316	L2249	P2169
A3218	E3066	E3066	L2990	Q2914	R2943	T2775	L2899	S2617	L2540	SER	V2391	T2323	T2250	GLN
P3220	I3147	E3067	F2991	Q2914	S2844	S2776	M2700	S2618	M2541	PRO	R2392	T2324	T2251	LEU
P3221	P3149	K3068	E2992	L2917	F2945	T2779	F2701	L2619	N2542	I1E	M2394	F2332	T2252	PRO
	A3150	I3069	E2993	V2918	A2846	T2779	A2704	D2620		THR	F2395	V2327	W2255	PRO
	S3151	C3070	V2994	L2995	D2847	Q2780	T2705		V2546	THR	F2396	W2328	W2256	THR
R3224	F3152	D3075	T2998	E2922	N2848	T2781	T2706	W2624	V2547	SER	E2396	D2329	V2257	I1E
D3225	D3153	E3074	K2923	K2923	L2849	K2782	T2705	S2625	V2548	PRO	E2397	D2329	W2257	THR
A3226	F3154	S3075			L2850	L2783	P2707	L2626	L2549	PRO	Q2398	F2332	D2176	
S3229	H3155	S3076	T2926	T2926	D2851	D2784	E2708	W2627	E2550	THR	D2399	F2332	I2258	
S3230	H3156	S3077	I2930	I2930	A2852	K2785	L2709	K2628	Y2551	THR	L2400	T2335	I2259	
	R3157	V3077			L2853	L2786	L2710	N2629	N2552	THR	F2401	T2335	Q2260	
	S3158	V3078			V2854	Q2787	L2711	K2630	Q2553	SER	Y2402	T2335	Q2261	
		L3079	V2933	V2933	E2855	F2788	K2712	VAL	L2554	SER	A2403	T2338	L2262	
		G3010	A2934	A2934	F2856	V2789	T2713	PRO		SER		R2338	H2263	
		A3012	L2935	L2935	Y2857	F2714	T2714	SER	M2560	ARG	T2408	I2340	Q2264	
		L3013	K2936	K2936	Y2858	D2790	D2715	V2634	S2561	THR	S2409	D2341	I2265	
		F3083	H2937	H2937	E2859	C2792	H2716		P2562	THR	R2410	N2342	I2266	
		L3015	F2938	F2938		N2793			E2563		R2411	N2343		
		G3016	P2939	P2939	R2863	P2794	Y2720		N2564		G2412	E2346		
		V3017	S2940	S2940	F2864	P2795	E2727		Q2565		M2413			
		R3086	V2941	V2941	Y2872	T2796	T2728				W2414			
		M3087	N2942	N2942	L2873	D2797	W2729		T2570	SER	W2415	K2349	M2273	
		L3090	L2943	L2943	L2873	D2797	W2729		R2572	THR		R2350	M2274	
		G3021	D2944	D2944	A2870	Q2799	L2730			THR		H2351	W2275	
		R3022	A2945	A2945	H2871	R2800	P2732			THR		W2352		
		E3095	P2948	P2948	L2863	P2795	E2727			THR		W2352		
		V3024	L2948	L2948	F2864	P2795	E2727			THR		W2352		
		L3025	N2941	N2941	L2864	P2795	E2727			THR		W2352		
		R3026	S2949	S2949	L2864	P2795	E2727			THR		W2352		
		S3027	L2950	L2950	L2864	P2795	E2727			THR		W2352		
		F3028	T2951	T2951	L2864	P2795	E2727			THR		W2352		
		L3032	S2953	S2953	L2864	P2795	E2727			THR		W2352		
		M3033	N2954	N2954	L2864	P2795	E2727			THR		W2352		
		G3034	L2956	L2956	L2864	P2795	E2727			THR		W2352		
		L3035	T2957	T2957	L2864	P2795	E2727			THR		W2352		
		S3036	Q2961	Q2961	L2864	P2795	E2727			THR		W2352		
		L3037	P2962	P2962	L2864	P2795	E2727			THR		W2352		
		F3038	S2966	S2966	L2864	P2795	E2727			THR		W2352		
		T3039	I3040	I3040	L2864	P2795	E2727			THR		W2352		
		K3041	D2967	D2967	L2864	P2795	E2727			THR		W2352		
		V3042	L2968	L2968	L2864	P2795	E2727			THR		W2352		
		N3043	E2970	E2970	L2864	P2795	E2727			THR		W2352		
		S3048	Y2971	Y2971	L2864	P2795	E2727			THR		W2352		
		F3051	Q2972	Q2972	L2864	P2795	E2727			THR		W2352		
		D3052	R2975	R2975	L2864	P2795	E2727			THR		W2352		
		L3055	L2976	L2976	L2864	P2795	E2727			THR		W2352		
		V3137	Q2977	Q2977	L2864	P2795	E2727			THR		W2352		
		R3138	R2978	R2978	L2864	P2795	E2727			THR		W2352		
		L3058	F2979	F2979	L2864	P2795	E2727			THR		W2352		
		L3059	L2980	L2980	L2864	P2795	E2727			THR		W2352		
		K3060	Y2980	Y2980	L2864	P2795	E2727			THR		W2352		
		L3141	D2985	D2985	L2864	P2795	E2727			THR		W2352		
		H3142	A3061	A3061	L2864	P2795	E2727			THR		W2352		
		L3143	A3062	A3062	L2864	P2795	E2727			THR		W2352		
		V3144	G3063	G3063	L2864	P2795	E2727			THR		W2352		
					L2911	L2839	F2772			THR		A2386		





F4252	I4162	K4087	Q4016	N3927	L3835	LYS	P3672	T3583	SER	GLU	LYS	Y3254	A3159	E3066
I4253	G4163	S4091	L4020	F3928	A3841	GLY	L3673	T3584	GLU	PRO	ALA	V3255	T3160	E3067
G4254		R4092	I4021	N3929	S3842	ARG	V3674	M3584	ILE	ASN	GLY	P3256	K3068	
I4255	G4167	R4093	C4022	L3930	G3843	ARG	D3675	S3586	ASP	PHE	PRO	P3257	P3162	I3069
P4256		V4094	L4023	D3932	N3844	ILE	P3677	T3587	ARG	THR	ILE	H3259	L3164	I3072
A4257	A4171	L4095	R4024	D3935	I3845	LEU		F3165	ILE	SER	ILE	Y3260	K3166	
R4258		Q4025	Q4025	D3936	I3846	ILE		V3589	LYS	ILE	GLU	F3263	N3166	V3078
R4259	T4183	V4097	Q4026	F3928	D3847	ARG		M3682	PRO	ILE	ALA	L3170	L3079	E3080
M4260	V4185	S4098	V4027	R3939	D3848	LEU		E3683	LEU	ASN	GLN	L3170	E3080	L3080
Q4263		F4101	P4028	L3940	D3849	GLY		F3684	ARG	TYR	GLY	D3171	S3081	S3081
P4264		V4102	S4029	Y3941	S3850	ASP		A3595	GLU	ASP	ALA	V3267	V3172	S3082
A4265	K4188	V4102	F4030	Y3942	V3851	GLN		M3686	VAL	THR	VAL	F3173	F3083	F3083
E4266	M4189		S4031	L3943	I3852	ASP		F3598	VAL	LYS	SER	I3271	G3174	L3084
R4267	I4190	V4105	R4032	L3943	I3852	VAL		N3687	GLU	LYS	THR	K3272	E3175	E3085
A4270	H4191	F4106	L4033	F3947	K3859	ASP		Y3601	GLN	MET	ILE	K3273	R3086	R3086
F4271	L4192	G4107	V4034	F3948	T3872	PHE		A3590	LEU	THR	LYS	K3274	L3181	M3087
L4272	K4193	F4108	P4035	R3949	I3865	SER		C3603	GLU	THR	LYS	K3274	L3181	M3087
F4273	P4194	D4109	H4036	S3949	A3866	P3758		C3603	ASN	THR	LYS	G3288	F3182	N3088
L4274	L4197	F4110		V3955	L3867	S3759		F3604	ALA	PRO	LYS	L3289	V3184	L3090
		N4111	S4041	T3958	K3868	F3760		F3605	ALA	LYS	HIS	K3290	G3185	L3091
		N4112	S4042	L3959	V3869	M3761		Q3607	ASN	ARG	ASP	K3291	S3186	A3092
		T4113	A4043	T3958	V3869	K3696		K3608	GLU	GLU	GLY	L3292	E3187	G3093
			D4043	L3960	T3872	L3764		F3609	LEU	ALA	ILE	R3293		
F4277			R4044	L3960	T3872	L3764		F3609	LEU	ALA	ILE	D3294	L3192	G3094
A4279	M4118		F4045	N3961	F3765	F3765		S3698	K3512	ILE	LYS	T3295	E3095	
I4280	A4119	L4280	Q4046	D3962	K3877	P3766		F3699	THR	THR	SER	T3295	E3095	VAL
S4206	L4120		F4047	K3963	K3877	R3767		L3700	L3525	LYS	LEU	V3299	E3195	PRO
S4208	I4121		Q4282	K3964	E3878	D3701		D3701	L3525	LYS	LEU	V3299	N3196	GLY
P4209	V4122		D4051	L3965	I3879	P3769		S3702	Y3536	TYR	LYS	L3002	F3199	PHE
	F4123		Q4052	T3966	S3880	T3770		S3703	L3539	LEU	PRO	L3002	F3199	PHE
R4284	K4124		V4053	F3967	E3881	F3704		A3711	L3540	GLU	PRO	L3002	F3199	PHE
L4285	E4125				V3882	H3772		M3705	L3540	ASP	PRO	L3006	P3202	GLY
										ASP	PRO	L3006	P3202	GLY
										GLY	VAL	L3313	K3212	E3103
										PHE	LYS	D3314	GLY	E3104
										ASP	ALA	V3315	ASN	F3105
										TYR	ALA	K3316	ASN	F3105
										GLU	MET	Q3322	LEU	M3109
										THR	GLU	Q3322	K3217	R3118
										VAL	ALA	Q3338	A3218	ASN
										ASN	VAL	S3551	I3219	GLY
										ARG	CYS	P3220	P3220	LEU
										ALA	LEU	R3342	F3221	ILE
										SER	MET	Q3345	S3222	LEU
										LYS	LEU	Q3345	H3223	ASP
										ALA	GLY	V3350	S3125	S3125
										CYS	GLY	V3350	V3228	
										GLY	LYS	E3329	S3229	
										PRO	LYS	E3354	S3230	L3129
										VAL	LEU	L3231	L3231	S3135
										LEU	GLU	V3232	V3232	Q3136
										LYS	TRP	L3234	V3234	R3137
										ALA	ALA	V3235	R3138	R3138
										ASP	ASP	H3235	R3139	R3139
										ILE	ILE	Q3236	Q3236	N3140
										ALA	ARG	TYR	T3237	F3145
										THR	LYS	ASP	I3238	F3145
										GLN	LYS	ASP	ASP	LEU
										TYR	ILE	R3248	R3248	S3151
										TYR	TYR	F3274	F3274	

M4693	ILE	E4549	THR	L4399	D4327
	SER	W4550	ILE	P4400	K4328
	SER	K4551	THR	E4401	F4329
	GLU	W4552	GLU	I4402	L4329
	GLY	Y4553	TRP	S4403	P4330
	GLY	S4554	THR	T4404	W4331
	ALA	W4555	LYS	P4405	L4332
	S4636	W4556	LEU	I4406	A4333
	N4637	E4557	LEU	W4407	K4334
	V4638	T4558	PRO	L4408	R4335
F4701	V4639		LYS	G4409	T4336
	M4642	L4561	PRO	L4410	L4337
	L4643		LEU	P4411	L4338
	A4644	F4568	LYS	E4412	G4339
	E4645	R4571	GLN	M4413	S4340
	G4646	M4572	LEU	A4414	T4341
	A647	Q4573	LYS	E4415	T4342
	W4648	Q4574	ARG		Y4343
	W4649	L4575	THR	K4422	G4344
	N4650		THR	A4423	G4345
Y4717		S4581	GLN	R4424	R4346
	Q4653	SER	ASN	K4425	
		ASP	ILE	M4426	M4349
	T4657	TYR	L4492	L4427	E4350
	D4658	SER	P4494	A4428	P4351
	T4659	SER	SER	D4429	D4352
	L4660	ILE	F4499	L4430	
	S4661	Q4588	F4500	Q4431	L4355
	T4662	W4589	R4501	K4432	L4356
	P4663	W4590	L4502	M4433	Y4357
S4725		L4591	E4503	Q4434	F4358
	W4714	L4664	L4503		P4359
	W4715	S4665	G4592	L4360	L4360
	Y4717		C4593	E4437	E4361
	Q4718		G4593	GLU	Q4362
				ASP	L4363
	W4721		W4596	GLY	F4364
	S4722		P4597	GLU	T4365
	L4723		I4601	ASP	
	S4724		T4604	GLN	F4369
S4729		T4604	L4523	VAL	M4370
		K4674	ILE	SER	P4371
		D4673	SER	GLY	D4372
		D4675	GLY	SER	F4373
		ASP	ASN	ASN	P4374
		PRO	ILE	LYS	
		PHE	W4529	LYS	P4377
		ASN	S4530	GLU	S4378
		ASN	T4531	SER	I4379
		E4617	R4535	SER	G4380
ILE		M4618	SER	L4381	
		SER		S4456	T4388
		L4621	S4540		R4389
		K4622	T4541	E4459	A4390
		A4623	S4542		H4391
		S4624	K4543	A4464	
		SER	G4544	K4465	
		P4689	L4545	LEU	I4396
		V4690	L4545	ARG	F4397
		Y4691	GLY	ALA	A4398

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.79 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.3 (48.79-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.292 0.220 , 0.292	Depositor DCC
R_{free} test set	4469 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 128.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.28	0/23866	0.75	10/32482 (0.0%)
1	B	0.27	0/22846	0.73	4/31076 (0.0%)
All	All	0.27	0/46712	0.74	14/63558 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1737	GLU	N-CA-C	-6.59	105.21	113.18
1	A	3671	TYR	CA-C-N	6.24	126.27	119.90
1	A	3671	TYR	C-N-CA	6.24	126.27	119.90
1	A	3371	PRO	N-CA-CB	6.12	109.68	103.25
1	A	4005	ILE	CA-C-N	5.85	125.05	118.97
1	A	4005	ILE	C-N-CA	5.85	125.05	118.97
1	B	3078	VAL	N-CA-C	5.62	112.22	106.21
1	A	2838	LEU	N-CA-C	-5.52	106.31	113.16
1	B	3671	TYR	CA-C-N	5.44	125.38	119.78
1	B	3671	TYR	C-N-CA	5.44	125.38	119.78
1	A	3634	VAL	CB-CA-C	-5.28	108.69	113.70
1	A	4240	ASN	CA-C-N	5.25	125.79	120.38
1	A	4240	ASN	C-N-CA	5.25	125.79	120.38
1	A	2746	ILE	N-CA-C	5.00	117.34	111.09

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23374	0	22545	1654	0
1	B	22384	0	21550	1231	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2881	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 32.

All (2881) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00
1:A:3373:ILE:HD13	1:A:3373:ILE:H	1.29	0.98
1:A:3673:LEU:HB2	1:A:3781:VAL:HG11	1.45	0.97
1:B:1959:THR:HG22	1:B:4341:THR:HA	1.46	0.96
1:B:1554:LEU:HB3	1:B:1609:GLN:HE22	1.29	0.95
1:B:4251:THR:HG23	1:B:4303:LEU:HD21	1.46	0.95
1:B:1928:HIS:CD2	1:B:1933:THR:HG22	2.02	0.95
1:A:4375:LEU:HD11	1:A:4383:VAL:HG23	1.48	0.95
1:B:3673:LEU:HB2	1:B:3781:VAL:HG11	1.44	0.95
1:A:2262:LEU:HD11	1:A:2274:MET:HE3	1.46	0.95
1:A:3425:LYS:HD2	1:A:3428:GLU:HG3	1.49	0.94
1:B:2533:VAL:HB	1:B:2581:LEU:HD22	1.51	0.93
1:B:1655:LEU:HB2	1:B:1658:GLU:HB2	1.45	0.93
1:B:4574:GLN:HE22	1:B:4590:TRP:H	1.15	0.93
1:B:4121:ILE:HA	1:B:4125:GLU:HG3	1.48	0.93
1:B:1972:PRO:HG2	1:B:2076:THR:HG22	1.52	0.92
1:A:4270:ILE:HA	1:A:4273:LEU:HD12	1.52	0.90
1:B:1789:LEU:HD23	1:B:1818:THR:HG23	1.50	0.90
1:A:2250:VAL:HB	1:A:2425:MET:HE3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3837:ALA:HB1	1:A:3850:SER:HB3	1.53	0.89
1:A:1639:ILE:HG23	1:A:1672:LEU:HD22	1.53	0.89
1:A:2313:LYS:HE3	1:A:2366:ASN:HD21	1.36	0.89
1:A:3018:SER:HB2	1:A:3256:THR:HG21	1.52	0.89
1:A:4495:LEU:H	1:A:4495:LEU:HD12	1.38	0.89
1:B:3930:LEU:HB3	1:B:3939:ARG:HH21	1.37	0.89
1:A:2200:ASN:HD22	1:A:2228:LEU:HD13	1.36	0.88
1:B:1813:GLN:HE22	1:B:1940:TYR:HA	1.37	0.88
1:B:2603:THR:HG22	1:B:2604:PRO:HD2	1.54	0.88
1:A:1690:GLN:HE22	1:A:1766:ILE:HG21	1.38	0.88
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.56	0.88
1:A:4046:GLN:HE22	1:A:4057:ILE:H	1.19	0.88
1:A:2447:GLN:HA	1:A:2450:ASN:HD22	1.39	0.88
1:B:4270:ILE:HG22	1:B:4310:ILE:HD13	1.55	0.88
1:B:1524:GLU:HG2	1:B:1580:TYR:HB3	1.57	0.87
1:A:3552:LYS:HA	1:A:3555:ASN:HD22	1.40	0.87
1:A:2570:THR:HG21	1:A:2603:THR:HG21	1.57	0.86
1:A:2274:MET:HE1	1:A:2286:TRP:HB3	1.56	0.86
1:B:2582:GLY:HA2	1:B:2585:MET:HE3	1.56	0.86
1:A:2914:GLN:HB2	1:A:2926:THR:HG21	1.56	0.86
1:B:2381:ASN:HD21	1:B:2383:GLU:HB2	1.40	0.86
1:A:2200:ASN:HB2	1:A:2228:LEU:HD22	1.56	0.86
1:B:4604:THR:HG23	1:B:4671:TRP:HE1	1.40	0.86
1:A:4621:LEU:HD21	1:A:4669:LEU:HD23	1.55	0.86
1:B:3271:ILE:HG13	1:B:3592:VAL:HG11	1.57	0.86
1:A:4389:ARG:HH12	1:A:4393:MET:HE2	1.42	0.85
1:A:2293:ILE:HG22	1:A:2350:ARG:HH22	1.41	0.85
1:B:4109:ASP:HA	1:B:4112:ASN:ND2	1.92	0.85
1:A:4686:LEU:HD21	1:A:4721:VAL:HG11	1.59	0.85
1:A:3809:THR:HA	1:A:3812:LYS:HE2	1.59	0.84
1:A:2560:MET:HG3	1:A:2561:SER:H	1.42	0.84
1:A:4251:THR:HG23	1:A:4303:LEU:HD21	1.58	0.84
1:B:2525:ILE:HD11	1:B:2815:LEU:HB2	1.58	0.84
1:A:3696:LYS:HZ2	1:A:4206:SER:HB3	1.44	0.83
1:A:4648:VAL:HG12	1:A:4662:THR:HG21	1.60	0.83
1:B:2841:ASN:ND2	1:B:2842:LEU:H	1.75	0.83
1:A:2910:LEU:HD23	1:A:2930:ILE:HD12	1.59	0.83
1:B:3930:LEU:HD11	1:B:3943:LEU:HD21	1.59	0.83
1:B:4548:LYS:HD2	1:B:4549:GLU:N	1.93	0.83
1:A:3718:LEU:HG	1:A:3719:LEU:H	1.42	0.83
1:B:4402:ILE:H	1:B:4402:ILE:HD12	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4109:ASP:HA	1:A:4112:ASN:ND2	1.95	0.82
1:A:4190:ILE:HG12	1:A:4219:SER:HB3	1.61	0.82
1:A:3981:ASN:HD22	1:A:4076:ILE:HB	1.44	0.82
1:B:3785:ASN:HD21	1:B:3787:THR:HG23	1.43	0.82
1:B:2250:VAL:HB	1:B:2425:MET:HG3	1.60	0.82
1:B:1926:VAL:HG22	1:B:1935:TYR:CE2	2.15	0.82
1:A:3652:LEU:HD12	1:A:3653:PRO:HD2	1.62	0.82
1:B:1781:LEU:HG	1:B:1814:LEU:HD11	1.61	0.81
1:A:2651:VAL:HG13	1:A:2652:ASP:H	1.44	0.81
1:B:4657:THR:HG22	1:B:4659:ILE:H	1.45	0.81
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	1.61	0.81
1:A:4185:VAL:HG12	1:A:4186:LEU:H	1.44	0.81
1:B:2129:VAL:HG22	1:B:2130:PRO:HD3	1.62	0.81
1:B:4335:ARG:HH21	1:B:4365:THR:HG22	1.46	0.81
1:A:2371:LEU:CB	1:A:2410:ARG:HG3	2.10	0.81
1:A:3238:ILE:HG12	1:A:3601:TYR:CD2	2.16	0.81
1:A:3700:LEU:HD22	1:A:3701:ASP:H	1.43	0.80
1:A:3789:THR:HB	1:A:3790:PRO:HD2	1.63	0.80
1:A:2140:SER:HB2	1:A:2142:GLN:HE22	1.45	0.80
1:A:2857:TYR:HA	1:A:2913:PHE:HE1	1.46	0.80
1:A:4353:MET:HE3	1:A:4356:LEU:HD23	1.63	0.80
1:A:2370:LEU:HD21	1:A:2387:LEU:HD13	1.64	0.80
1:A:4654:LEU:HD11	1:A:4705:LEU:HB2	1.64	0.80
1:B:1660:LEU:HA	1:B:1665:ILE:HD11	1.63	0.80
1:A:2236:LEU:HD21	1:A:2293:ILE:HD13	1.63	0.80
1:A:3694:ILE:HG12	1:A:3717:PRO:HB2	1.63	0.80
1:A:4654:LEU:HD13	1:A:4686:LEU:HD23	1.62	0.79
1:A:2110:GLN:HG3	1:A:2122:GLU:HA	1.64	0.79
1:B:3607:GLN:HG2	1:B:3657:LEU:HD22	1.65	0.79
1:B:4270:ILE:HD11	1:B:4329:ILE:HD13	1.65	0.79
1:A:4086:MET:HG3	1:A:4093:ARG:HB2	1.65	0.79
1:A:4349:ASN:HD21	1:A:4351:PHE:HB2	1.46	0.79
1:A:2300:LYS:O	1:A:2349:LYS:HB2	1.81	0.79
1:B:4189:ASN:H	1:B:4218:THR:HG22	1.47	0.79
1:B:3844:ASN:O	1:B:3848:ASP:HB3	1.81	0.79
1:A:2283:THR:HA	1:A:2286:TRP:HE1	1.48	0.78
1:A:2706:THR:HB	1:A:2707:PRO:HD2	1.65	0.78
1:A:2886:LEU:O	1:A:2890:ILE:HG12	1.84	0.78
1:B:2106:GLU:OE1	1:B:2129:VAL:HG21	1.82	0.78
1:B:4264:PRO:HB3	1:B:4323:ASN:HA	1.64	0.78
1:A:3673:LEU:HB2	1:A:3781:VAL:CG1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2657:VAL:HG13	1:B:2687:THR:HG23	1.64	0.78
1:B:3338:GLN:HG2	1:B:3525:LEU:HD13	1.65	0.78
1:A:1823:TRP:O	1:A:1827:VAL:HG23	1.84	0.78
1:A:2204:ILE:HA	1:A:2207:LEU:HD12	1.65	0.78
1:A:2705:THR:HA	1:A:2709:LEU:HD12	1.66	0.78
1:A:1796:ASP:HB3	1:A:1799:ASP:HB3	1.65	0.77
1:A:4575:LEU:H	1:A:4575:LEU:HD12	1.49	0.77
1:B:2578:MET:HB3	1:B:2597:ILE:HD12	1.65	0.77
1:B:4332:ILE:HD12	1:B:4332:ILE:H	1.48	0.77
1:B:4121:ILE:O	1:B:4125:GLU:HB2	1.85	0.77
1:B:3219:ILE:CB	1:B:3220:PRO:HD3	2.15	0.77
1:A:2766:MET:HB3	1:A:2783:LEU:HD11	1.67	0.76
1:A:4318:SER:HA	1:A:4321:ARG:HH21	1.50	0.76
1:A:3058:LEU:HD21	1:A:3141:LEU:HD11	1.67	0.76
1:A:3384:LYS:HD3	1:A:3386:LYS:HD3	1.66	0.76
1:B:3230:SER:HA	1:B:3620:ARG:HE	1.51	0.76
1:B:3313:LEU:HD13	1:B:3550:SER:HA	1.65	0.76
1:A:2505:TYR:O	1:A:2512:VAL:HG23	1.85	0.76
1:A:1959:THR:HA	1:A:4341:THR:OG1	1.85	0.76
1:B:3671:TYR:O	1:B:3781:VAL:HG13	1.86	0.76
1:B:4046:GLN:HG3	1:B:4047:PHE:N	2.00	0.76
1:B:4531:THR:O	1:B:4535:ARG:HG3	1.86	0.76
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.84	0.76
1:B:4067:ALA:HB1	1:B:4073:GLN:HG3	1.65	0.76
1:B:3639:SER:HB3	1:B:3663:ILE:HD11	1.68	0.76
1:A:1813:GLN:HE22	1:A:1940:TYR:HA	1.50	0.75
1:A:3927:ASN:HB3	1:A:3930:LEU:HB2	1.68	0.75
1:B:1822:VAL:HG22	1:B:1826:GLN:HE21	1.50	0.75
1:A:3731:ASN:HD22	1:A:3731:ASN:H	1.35	0.75
1:A:4122:VAL:HG21	1:A:4216:PHE:CZ	2.20	0.75
1:B:4011:LEU:HD11	1:B:4041:SER:HB2	1.68	0.75
1:A:2273:MET:HB2	1:A:2395:PHE:HB2	1.68	0.75
1:B:3027:ARG:HA	1:B:3037:ILE:HD11	1.68	0.75
1:B:3966:THR:HG22	1:B:4426:MET:HG3	1.68	0.75
1:B:2426:ILE:H	1:B:2426:ILE:HD12	1.51	0.75
1:A:3358:GLN:HA	1:A:3361:LYS:HE2	1.69	0.75
1:A:3443:MET:HG3	1:A:3449:ARG:HG3	1.68	0.75
1:A:3039:THR:HG22	1:A:3040:ILE:H	1.50	0.75
1:A:4622:HIS:HE2	1:A:4678:ILE:HG21	1.50	0.75
1:A:4648:VAL:HG13	1:A:4657:THR:HG21	1.68	0.75
1:B:3766:THR:HG22	1:B:3768:ASP:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3035:LEU:HD22	1:B:3068:LYS:HB3	1.68	0.75
1:A:2106:GLU:H	1:A:2106:GLU:CD	1.95	0.75
1:A:2586:GLY:HA2	1:A:2815:LEU:HD13	1.67	0.75
1:B:1950:THR:HB	1:B:1951:PRO:HD2	1.68	0.75
1:A:3015:ILE:HD13	1:A:3147:MET:HG3	1.68	0.74
1:B:2315:GLN:HB3	1:B:2775:THR:HG21	1.69	0.74
1:A:2397:VAL:HG21	1:A:2400:LEU:HD21	1.68	0.74
1:B:2638:THR:HG21	1:B:2838:LEU:HD21	1.68	0.74
1:A:1547:ASN:HA	1:A:1553:LYS:HG2	1.70	0.74
1:B:1476:ILE:HG23	1:B:1480:HIS:HB2	1.68	0.74
1:A:2105:ARG:HG2	1:A:2105:ARG:HH11	1.53	0.74
1:A:3774:THR:HB	1:A:3775:PRO:HD2	1.70	0.73
1:A:4122:VAL:HG21	1:A:4216:PHE:HZ	1.53	0.73
1:B:4278:HIS:HD2	1:B:4343:TYR:OH	1.71	0.73
1:A:2309:LYS:HE2	1:A:2756:THR:HG21	1.68	0.73
1:A:4053:VAL:O	1:A:4053:VAL:HG12	1.86	0.73
1:A:3388:LEU:HD23	1:A:3473:ALA:HB1	1.68	0.73
1:A:2793:ASN:HD22	1:A:2793:ASN:N	1.85	0.73
1:A:3725:ASN:HD22	1:A:3725:ASN:H	1.35	0.73
1:A:3281:GLU:HB3	1:A:3581:PHE:HE1	1.54	0.73
1:A:1886:ARG:HG3	1:A:1887:ASP:N	2.04	0.73
1:B:3700:LEU:HD13	1:B:3701:ASP:N	2.04	0.73
1:A:3202:PRO:HD2	1:A:3624:VAL:O	1.88	0.73
1:B:3602:ILE:HG23	1:B:3610:ARG:HG2	1.70	0.73
1:A:2675:PRO:HD2	1:A:2816:VAL:O	1.88	0.73
1:A:3453:THR:HA	1:A:3457:LEU:HB2	1.70	0.73
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	2.04	0.73
1:B:2572:ARG:HG2	1:B:2617:VAL:HG11	1.69	0.73
1:B:4157:TYR:HB3	1:B:4184:TRP:HB2	1.71	0.73
1:A:2080:GLY:HA3	1:A:2084:ARG:O	1.89	0.73
1:B:3789:THR:HB	1:B:3790:PRO:HD2	1.70	0.73
1:B:4189:ASN:N	1:B:4189:ASN:HD22	1.85	0.73
1:A:3475:GLY:O	1:A:3478:VAL:HG12	1.88	0.73
1:A:4024:ARG:HD3	1:A:4034:VAL:HG21	1.71	0.73
1:B:3584:GLN:O	1:B:3588:VAL:HG23	1.87	0.73
1:B:2514:LYS:HE2	1:B:2600:ILE:HD11	1.71	0.72
1:A:1655:LEU:HB2	1:A:1658:GLU:HB2	1.69	0.72
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	1.70	0.72
1:A:3281:GLU:HB3	1:A:3581:PHE:CE1	2.24	0.72
1:A:3724:GLU:OE2	1:A:3766:THR:HG23	1.88	0.72
1:B:4136:SER:HB3	1:B:4238:TYR:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1899:THR:HB	1:B:1903:ASP:HB2	1.72	0.72
1:B:2938:PHE:O	1:B:2941:VAL:HG12	1.88	0.72
1:B:4005:ILE:HD13	1:B:4020:LEU:HD23	1.70	0.72
1:A:2042:GLN:HE21	1:A:2059:LEU:HD11	1.54	0.72
1:B:2841:ASN:HD22	1:B:2842:LEU:H	1.37	0.72
1:A:1763:GLY:N	1:A:1764:PRO:HD3	2.04	0.72
1:A:2587:LEU:HG	1:A:2817:ASP:HB2	1.72	0.71
1:A:2626:LEU:H	1:A:2626:LEU:HD12	1.55	0.71
1:A:3700:LEU:HD13	1:A:3701:ASP:N	2.04	0.71
1:B:3292:LEU:HD13	1:B:3571:ARG:HA	1.72	0.71
1:B:4601:ILE:O	1:B:4604:THR:HG22	1.90	0.71
1:A:2042:GLN:NE2	1:A:2059:LEU:HD11	2.06	0.71
1:A:1742:ILE:HG22	1:A:1753:THR:HG22	1.71	0.71
1:A:3555:ASN:HB3	1:A:3559:ARG:NH1	2.04	0.71
1:A:4347:ILE:HG21	1:A:4353:MET:HG2	1.72	0.71
1:B:2839:LEU:HD13	1:B:2842:LEU:HD12	1.70	0.71
1:B:4506:GLY:O	1:B:4510:VAL:HG23	1.91	0.71
1:A:2371:LEU:HB3	1:A:2410:ARG:HG3	1.71	0.71
1:B:3700:LEU:HD22	1:B:3701:ASP:H	1.54	0.71
1:A:1807:VAL:HG13	1:A:1815:VAL:HG11	1.73	0.71
1:A:2208:VAL:HA	1:A:2415:TRP:CD1	2.24	0.71
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.06	0.71
1:B:3674:VAL:HG22	1:B:3784:VAL:HB	1.71	0.71
1:A:4242:PRO:HA	1:A:4286:ARG:NH1	2.01	0.71
1:A:4553:TYR:HD1	1:A:4553:TYR:H	1.38	0.71
1:B:3234:ILE:HG23	1:B:3617:TRP:NE1	2.06	0.71
1:A:2258:LYS:HA	1:A:2261:GLN:HG3	1.71	0.71
1:A:3859:LYS:O	1:A:3862:THR:HG22	1.90	0.71
1:A:4533:TYR:O	1:A:4537:LEU:HG	1.90	0.71
1:B:4157:TYR:CB	1:B:4184:TRP:HB2	2.21	0.71
1:A:3037:ILE:HD13	1:A:3037:ILE:H	1.56	0.71
1:A:4591:LEU:HD21	1:A:4601:ILE:HD11	1.72	0.71
1:A:1798:ASN:HA	1:A:1854:MET:HE1	1.71	0.71
1:A:2942:ASN:O	1:A:2944:ASP:N	2.24	0.71
1:A:4029:SER:HB2	1:A:4081:ARG:HH12	1.56	0.71
1:B:4703:ILE:HD12	1:B:4705:LEU:HD21	1.71	0.71
1:B:2282:LYS:HA	1:B:2416:PHE:CD1	2.26	0.71
1:A:4494:PRO:HG2	1:A:4607:SER:HA	1.73	0.70
1:B:2124:LEU:HD22	1:B:2195:LEU:HD22	1.71	0.70
1:B:4574:GLN:HE22	1:B:4590:TRP:N	1.89	0.70
1:B:1823:TRP:CD1	1:B:1885:GLN:HB3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1879:ILE:O	1:A:1883:VAL:HG23	1.91	0.70
1:A:2006:LEU:HD23	1:A:2035:ILE:HG23	1.73	0.70
1:A:2371:LEU:HB2	1:A:2410:ARG:HG3	1.71	0.70
1:A:4540:SER:HB2	1:A:4545:ILE:O	1.91	0.70
1:B:1879:ILE:O	1:B:1883:VAL:HG23	1.91	0.70
1:B:3238:ILE:CG2	1:B:3255:VAL:HG11	2.20	0.70
1:A:2113:LEU:HD21	1:A:2156:LEU:HD22	1.74	0.70
1:A:2788:PHE:O	1:A:2789:VAL:HG23	1.90	0.70
1:A:3153:ASP:HA	1:A:3156:ASN:ND2	2.06	0.70
1:A:3677:PRO:HG3	1:A:3787:THR:HG22	1.72	0.70
1:A:4095:LEU:HD11	1:A:4422:LYS:HB3	1.73	0.70
1:A:4649:TRP:HA	1:A:4649:TRP:CE3	2.27	0.70
1:A:2954:ASN:H	1:A:2954:ASN:HD22	1.39	0.70
1:A:2308:PRO:HD2	1:A:2357:GLY:HA3	1.74	0.70
1:A:4179:ALA:HB1	1:A:4209:PRO:HB3	1.73	0.70
1:A:4186:LEU:C	1:A:4187:LEU:HD12	2.17	0.70
1:A:3380:VAL:HG11	1:A:3435:ILE:HG21	1.72	0.70
1:A:3812:LYS:O	1:A:3816:LEU:HB3	1.91	0.70
1:A:4054:GLY:O	1:A:4055:GLU:C	2.34	0.70
1:B:1928:HIS:NE2	1:B:1933:THR:HG22	2.06	0.70
1:A:3331:GLN:HE22	1:A:3533:LYS:HG3	1.56	0.69
1:A:4086:MET:CG	1:A:4093:ARG:HB2	2.21	0.69
1:B:2850:THR:O	1:B:2854:VAL:HG23	1.90	0.69
1:A:2120:THR:O	1:A:2121:ALA:C	2.33	0.69
1:A:3433:THR:HG22	1:A:3437:ASN:ND2	2.06	0.69
1:B:1687:LEU:HD21	1:B:1706:LEU:HD23	1.74	0.69
1:B:2540:LEU:HD23	1:B:2576:SER:HA	1.72	0.69
1:A:1846:GLN:HA	1:A:1893:GLN:NE2	2.08	0.69
1:A:2127:LYS:C	1:A:2130:PRO:HD2	2.17	0.69
1:A:4128:SER:HB2	1:A:4213:PHE:HB3	1.74	0.69
1:B:1739:THR:HB	1:B:1761:ALA:HB2	1.74	0.69
1:B:3700:LEU:H	1:B:3700:LEU:HD12	1.58	0.69
1:B:2235:GLN:NE2	1:B:2296:VAL:HG13	2.06	0.69
1:A:3912:SER:HB3	1:A:4231:ARG:HG2	1.75	0.69
1:B:1846:GLN:O	1:B:1850:GLN:HG2	1.92	0.69
1:B:3238:ILE:HG12	1:B:3601:TYR:CG	2.28	0.69
1:A:2028:PHE:HB3	1:A:2075:VAL:HG13	1.72	0.69
1:B:1534:VAL:HG13	1:B:1568:HIS:HD2	1.58	0.69
1:B:3238:ILE:HG21	1:B:3255:VAL:HG11	1.73	0.69
1:B:3256:THR:HB	1:B:3257:PRO:HD2	1.74	0.69
1:B:3768:ASP:HB3	1:B:3771:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1746:SER:OG	1:A:1750:GLU:HB3	1.93	0.69
1:A:2202:THR:HG22	1:A:2265:ILE:HG12	1.74	0.69
1:B:2200:ASN:HB2	1:B:2228:LEU:HD22	1.75	0.69
1:B:2282:LYS:HA	1:B:2416:PHE:HD1	1.57	0.69
1:A:4623:ALA:HB2	1:A:4703:ILE:HD11	1.75	0.69
1:A:1770:LEU:O	1:A:1773:VAL:HG22	1.93	0.69
1:B:4005:ILE:CD1	1:B:4020:LEU:HD23	2.24	0.68
1:A:2748:LEU:HD21	1:A:2800:ARG:NH1	2.09	0.68
1:B:3724:GLU:OE2	1:B:3766:THR:HG23	1.93	0.68
1:B:4362:GLN:HB2	1:B:4714:GLN:NE2	2.08	0.68
1:B:2865:THR:H	1:B:2868:ILE:HD12	1.58	0.68
1:B:4574:GLN:NE2	1:B:4590:TRP:H	1.87	0.68
1:A:1886:ARG:NH1	1:A:1890:ARG:HH22	1.91	0.68
1:B:3652:LEU:HD12	1:B:3653:PRO:HD2	1.74	0.68
1:A:2266:LEU:HD21	1:A:2394:MET:HE3	1.76	0.68
1:A:3210:GLU:HG3	1:A:3211:ILE:H	1.57	0.68
1:B:1545:LEU:HD12	1:B:1545:LEU:H	1.57	0.68
1:B:3043:ASN:ND2	1:B:3046:TYR:HB2	2.07	0.68
1:A:1554:LEU:HB3	1:A:1609:GLN:HE21	1.59	0.68
1:A:2010:SER:HB3	1:A:2060:LEU:HD21	1.75	0.68
1:B:1743:GLY:HA2	1:B:1754:PHE:CD1	2.29	0.68
1:A:3603:GLY:HA2	1:A:3664:MET:HE1	1.76	0.68
1:B:2320:LEU:O	1:B:2320:LEU:HD23	1.93	0.68
1:A:4200:LEU:HD22	1:A:4204:LEU:HD11	1.75	0.68
1:A:1715:ILE:HD11	1:A:1760:ILE:HD13	1.74	0.68
1:A:1931:ASN:OD1	1:A:1962:GLN:NE2	2.25	0.68
1:A:2293:ILE:CG2	1:A:2350:ARG:HH22	2.07	0.68
1:B:2400:LEU:HD13	1:B:2408:ILE:HD11	1.76	0.68
1:A:2029:ASN:HB3	1:A:2077:MET:HE2	1.75	0.67
1:A:2306:MET:HE2	1:A:2355:PHE:HE1	1.59	0.67
1:A:1846:GLN:HA	1:A:1893:GLN:HE22	1.59	0.67
1:A:2742:PHE:HA	1:A:2789:VAL:O	1.94	0.67
1:A:3961:ASN:O	1:A:3964:LYS:HB2	1.94	0.67
1:A:2699:LEU:HD11	1:A:2713:THR:HG21	1.77	0.67
1:A:3013:LEU:HD12	1:A:3145:PHE:HB3	1.74	0.67
1:B:2231:ILE:HG21	1:B:2264:GLN:NE2	2.09	0.67
1:A:2212:ILE:HG22	1:A:2213:PRO:HD3	1.77	0.67
1:B:4251:THR:HG23	1:B:4303:LEU:CD2	2.23	0.67
1:A:3563:LEU:HD11	1:A:3851:VAL:HG22	1.77	0.67
1:B:2793:ASN:HB3	1:B:2794:PRO:HD2	1.76	0.67
1:A:1963:ALA:HB1	1:A:2096:ARG:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2447:GLN:HE22	1:A:2492:LEU:HD23	1.58	0.67
1:A:3397:PRO:HG2	1:A:3419:TRP:CZ2	2.29	0.67
1:B:4189:ASN:H	1:B:4218:THR:CG2	2.08	0.67
1:B:2815:LEU:HD23	1:B:2816:VAL:N	2.09	0.67
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.30	0.67
1:B:4189:ASN:H	1:B:4189:ASN:HD22	1.40	0.67
1:A:4210:HIS:ND1	1:A:4211:PRO:HD2	2.09	0.67
1:A:4259:ARG:HD3	1:A:4271:TYR:OH	1.95	0.67
1:B:4086:MET:HE3	1:B:4097:TYR:CE2	2.29	0.67
1:A:2014:VAL:HG13	1:A:2065:ILE:HG21	1.78	0.66
1:A:4548:LYS:HG3	1:A:4549:GLU:H	1.60	0.66
1:B:1719:GLN:HA	1:B:1722:PHE:CD2	2.29	0.66
1:B:3078:VAL:HG23	1:B:3083:PHE:HB2	1.76	0.66
1:B:3958:THR:HG23	1:B:4235:VAL:HB	1.76	0.66
1:A:2912:LEU:C	1:A:2913:PHE:HD2	2.04	0.66
1:B:2297:ASP:O	1:B:2299:ILE:HG13	1.94	0.66
1:B:2361:PRO:HD3	1:B:2402:TYR:O	1.96	0.66
1:A:2595:LYS:HE3	1:A:2611:PRO:HG3	1.75	0.66
1:A:4270:ILE:HD13	1:A:4314:VAL:HG21	1.78	0.66
1:B:2423:THR:HG23	1:B:2530:ARG:HD2	1.76	0.66
1:B:2766:MET:HB3	1:B:2783:LEU:HD11	1.75	0.66
1:A:2108:ILE:O	1:A:2112:MET:HB2	1.96	0.66
1:A:3875:VAL:O	1:A:3879:ILE:HG12	1.95	0.66
1:A:3925:ASN:HD22	1:A:3925:ASN:N	1.93	0.66
1:A:4086:MET:HE3	1:A:4097:TYR:CE2	2.30	0.66
1:B:2861:GLN:HG3	1:B:2874:TYR:HB2	1.75	0.66
1:A:2090:ASN:C	1:A:2090:ASN:HD22	2.02	0.66
1:A:3245:LEU:HD12	1:A:3249:GLN:HB2	1.78	0.66
1:A:2124:LEU:HD22	1:A:2195:LEU:HD22	1.78	0.66
1:A:2125:ALA:HA	1:A:2128:ILE:HG22	1.78	0.66
1:B:2113:LEU:HD21	1:B:2156:LEU:HD22	1.78	0.66
1:A:2315:GLN:HB3	1:A:2775:THR:HG21	1.76	0.66
1:A:2910:LEU:CD2	1:A:2930:ILE:HD12	2.25	0.66
1:A:3309:LYS:O	1:A:3313:LEU:HG	1.96	0.66
1:B:1769:TRP:O	1:B:1773:VAL:HG23	1.96	0.66
1:B:2984:LEU:HD22	1:B:2986:VAL:HG22	1.78	0.66
1:A:3989:ASP:O	1:A:3993:LYS:HB2	1.96	0.66
1:B:1885:GLN:O	1:B:1889:VAL:HG23	1.96	0.66
1:B:3785:ASN:ND2	1:B:3787:THR:HG23	2.11	0.66
1:A:3410:LEU:HD22	1:A:3452:ILE:HD11	1.78	0.65
1:A:3647:TRP:HB3	1:A:3652:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4230:LEU:H	1:A:4230:LEU:HD12	1.61	0.65
1:A:2289:TYR:O	1:A:2293:ILE:HG12	1.95	0.65
1:A:3285:LEU:HD13	1:A:3578:SER:HA	1.78	0.65
1:A:2535:ASN:HD22	1:A:2668:ARG:HH12	1.45	0.65
1:A:3271:ILE:HG13	1:A:3592:VAL:HG11	1.78	0.65
1:B:1901:ASN:H	1:B:1901:ASN:HD22	1.43	0.65
1:B:2498:CYS:HA	1:B:2501:ILE:HD12	1.77	0.65
1:B:3639:SER:HB3	1:B:3663:ILE:CD1	2.25	0.65
1:A:2552:ASN:HD21	1:A:2560:MET:HB2	1.59	0.65
1:A:3700:LEU:CD2	1:A:3701:ASP:H	2.09	0.65
1:B:2359:VAL:HG13	1:B:2364:VAL:HG21	1.79	0.65
1:B:3813:ARG:O	1:B:3817:LEU:HD13	1.97	0.65
1:A:2272:VAL:HB	1:A:2394:MET:HE3	1.78	0.65
1:A:2408:ILE:O	1:A:2409:SER:C	2.38	0.65
1:A:2975:ARG:HE	1:A:2975:ARG:HA	1.61	0.65
1:B:2339:ILE:HA	1:B:2346:GLU:HG2	1.76	0.65
1:A:1537:PHE:O	1:A:1541:LEU:HB2	1.97	0.65
1:A:1746:SER:HG	1:A:1750:GLU:HB3	1.62	0.65
1:A:2948:ARG:HG2	1:A:2948:ARG:HH11	1.62	0.65
1:A:3015:ILE:HG22	1:A:3149:PRO:HG3	1.77	0.65
1:A:3242:ASN:OD1	1:A:3253:ASN:HB3	1.96	0.65
1:A:4024:ARG:HG3	1:A:4031:SER:HA	1.78	0.65
1:A:4622:HIS:ND1	1:A:4623:ALA:N	2.45	0.65
1:A:3255:VAL:HA	1:A:3259:HIS:HD2	1.61	0.65
1:B:1920:ASN:HD22	1:B:1921:VAL:H	1.44	0.65
1:B:3949:SER:HA	1:B:4110:PHE:HE1	1.62	0.65
1:A:1748:GLU:HG2	1:A:1943:ILE:HB	1.79	0.65
1:A:2305:VAL:HG21	1:A:2769:LYS:HE2	1.79	0.65
1:A:4553:TYR:HB3	1:A:4595:LEU:HD23	1.79	0.65
1:A:4649:TRP:HA	1:A:4649:TRP:HE3	1.60	0.65
1:B:3109:MET:HB3	1:B:3129:LEU:HD23	1.79	0.65
1:B:4389:ARG:HG2	1:B:4389:ARG:HH11	1.62	0.65
1:A:2129:VAL:HB	1:A:2130:PRO:HD3	1.78	0.64
1:A:2968:LEU:O	1:A:2972:VAL:HG23	1.97	0.64
1:A:3270:LEU:HB2	1:A:3592:VAL:HG13	1.77	0.64
1:A:4221:ILE:H	1:A:4221:ILE:HD12	1.62	0.64
1:B:1931:ASN:HB2	1:B:4312:TYR:CZ	2.32	0.64
1:B:3063:GLY:HA2	1:B:3136:GLN:HB3	1.78	0.64
1:B:4063:ILE:HD12	1:B:4063:ILE:H	1.62	0.64
1:A:2704:ALA:HB3	1:A:3085:GLU:HG3	1.77	0.64
1:B:4288:ILE:HG23	1:B:4292:TRP:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2606:PRO:HD3	1:A:2624:TRP:CD1	2.32	0.64
1:A:3700:LEU:H	1:A:3700:LEU:HD12	1.62	0.64
1:A:1921:VAL:HG23	1:A:1922:LEU:HD22	1.79	0.64
1:A:2525:ILE:HG13	1:A:2584:SER:O	1.98	0.64
1:A:2578:MET:HE1	1:A:2613:LEU:HA	1.78	0.64
1:A:2651:VAL:HG13	1:A:2652:ASP:N	2.12	0.64
1:A:3387:HIS:CB	1:A:3473:ALA:HB2	2.27	0.64
1:B:1811:PRO:O	1:B:1815:VAL:HG23	1.98	0.64
1:B:2866:PRO:HG3	1:B:2873:ILE:HG22	1.78	0.64
1:A:1811:PRO:HD2	1:A:1814:LEU:HD12	1.78	0.64
1:A:3528:SER:O	1:A:3531:THR:HG22	1.98	0.64
1:B:4188:LYS:HA	1:B:4218:THR:HG22	1.80	0.64
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.80	0.64
1:A:4349:ASN:HD22	1:A:4352:ASP:N	1.95	0.64
1:A:2199:ILE:O	1:A:2203:MET:HB2	1.98	0.64
1:A:2273:MET:CB	1:A:2395:PHE:HB2	2.27	0.64
1:A:2506:PHE:CD1	1:A:2512:VAL:HG21	2.33	0.64
1:A:4050:LYS:O	1:A:4052:GLN:N	2.30	0.64
1:B:3991:LEU:O	1:B:4427:ILE:HD12	1.98	0.64
1:A:1545:LEU:HB3	1:A:1553:LYS:HE2	1.80	0.64
1:A:2979:PHE:CE2	1:A:3028:PHE:HA	2.33	0.64
1:A:3897:TYR:HE1	1:A:3913:LEU:HA	1.63	0.64
1:A:4296:PHE:CE2	1:A:4347:ILE:HD13	2.33	0.64
1:B:3299:VAL:HG11	1:B:3564:LEU:HG	1.78	0.64
1:A:3114:GLU:HG2	1:A:3118:ARG:NH1	2.13	0.64
1:A:4693:ASN:HD22	1:A:4693:ASN:N	1.95	0.64
1:B:1554:LEU:HD12	1:B:2323:THR:HG22	1.79	0.64
1:B:1694:PHE:HB3	1:B:1697:PHE:CD2	2.33	0.64
1:B:4548:LYS:HD2	1:B:4549:GLU:H	1.59	0.64
1:A:1611:ARG:HH11	1:A:1611:ARG:HG3	1.62	0.64
1:A:2051:LYS:O	1:A:2051:LYS:HD3	1.96	0.64
1:A:2163:LYS:HB2	1:A:2194:VAL:HG11	1.79	0.64
1:A:2207:LEU:HD13	1:A:2215:ILE:HG21	1.79	0.64
1:A:3293:ARG:HH11	1:A:3293:ARG:HG3	1.63	0.64
1:A:3785:ASN:HD22	1:A:3786:PHE:N	1.95	0.64
1:A:3804:THR:O	1:A:3807:PRO:HD3	1.98	0.64
1:A:4362:GLN:HG3	1:A:4714:GLN:OE1	1.97	0.64
1:B:1557:GLY:O	1:B:1561:LEU:HD23	1.98	0.64
1:B:4351:PHE:CE2	1:B:4689:PRO:HG3	2.32	0.64
1:A:2490:ALA:O	1:A:2494:VAL:HG23	1.97	0.63
1:A:4296:PHE:CE2	1:A:4347:ILE:HA	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4396:ILE:O	1:A:4399:LEU:HB2	1.98	0.63
1:B:3043:ASN:HD22	1:B:3046:TYR:HB2	1.63	0.63
1:B:3087:MET:CE	1:B:3090:LEU:HD23	2.28	0.63
1:A:3387:HIS:HB3	1:A:3473:ALA:HB2	1.80	0.63
1:A:3965:LEU:HG	1:A:4426:MET:HE3	1.79	0.63
1:B:4607:SER:O	1:B:4611:LEU:HG	1.98	0.63
1:A:1811:PRO:O	1:A:1815:VAL:HG23	1.98	0.63
1:A:3416:LYS:HE3	1:A:3418:GLU:HB3	1.80	0.63
1:A:3696:LYS:NZ	1:A:4206:SER:HB3	2.13	0.63
1:A:3711:ALA:HA	1:A:3716:CYS:SG	2.39	0.63
1:A:4277:PHE:HB2	1:A:4363:LEU:HD12	1.79	0.63
1:B:1525:ILE:HA	1:B:1528:GLU:HB3	1.80	0.63
1:B:1607:ASP:O	1:B:1611:ARG:HG2	1.97	0.63
1:B:1780:THR:HG22	1:B:1784:LEU:HD12	1.80	0.63
1:B:3563:LEU:HD11	1:B:3845:ILE:HD11	1.79	0.63
1:A:3985:GLU:O	1:A:3989:ASP:HB2	1.97	0.63
1:A:4571:ARG:HA	1:A:4590:TRP:HZ3	1.63	0.63
1:A:2995:LEU:HA	1:A:2998:ILE:HD11	1.80	0.63
1:B:1523:GLY:HA3	1:B:1580:TYR:CE2	2.33	0.63
1:B:3238:ILE:HD11	1:B:3617:TRP:HZ2	1.63	0.63
1:A:2938:PHE:HB3	1:A:2941:VAL:HG23	1.80	0.63
1:A:2972:VAL:O	1:A:2976:LEU:HB2	1.98	0.63
1:A:3482:THR:O	1:A:3486:TYR:HB2	1.99	0.63
1:A:3994:GLY:HA3	1:A:4087:LYS:CE	2.29	0.63
1:A:4310:ILE:O	1:A:4314:VAL:HB	1.99	0.63
1:A:2995:LEU:HD23	1:A:2998:ILE:HD11	1.80	0.63
1:A:3063:GLY:HA2	1:A:3136:GLN:HB3	1.81	0.63
1:B:3841:ALA:O	1:B:3842:SER:CB	2.35	0.63
1:A:2000:CYS:SG	1:A:2031:LEU:HD11	2.37	0.63
1:A:3255:VAL:HA	1:A:3259:HIS:CD2	2.33	0.63
1:A:3445:THR:HG23	1:A:3449:ARG:NH1	2.14	0.63
1:A:4269:ARG:CZ	1:A:4383:VAL:HG11	2.29	0.63
1:B:1592:ASP:O	1:B:1596:ASN:HB2	1.99	0.63
1:B:3035:LEU:CD2	1:B:3068:LYS:HB3	2.28	0.63
1:B:4133:LEU:HD23	1:B:4230:LEU:HD23	1.79	0.63
1:A:3969:LEU:HD12	1:A:4426:MET:HE2	1.79	0.63
1:B:2711:LEU:HD12	1:B:2714:PHE:HD2	1.63	0.63
1:B:2751:THR:HB	1:B:2756:THR:H	1.63	0.63
1:A:1777:MET:HE3	1:A:1939:GLU:HA	1.81	0.62
1:A:3300:LYS:HA	1:A:3564:LEU:HD11	1.81	0.62
1:A:3647:TRP:CH2	1:A:3663:ILE:HD12	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3725:ASN:H	1:A:3725:ASN:ND2	1.96	0.62
1:A:4049:GLY:O	1:A:4050:LYS:O	2.17	0.62
1:B:2841:ASN:HD22	1:B:2841:ASN:N	1.97	0.62
1:A:1922:LEU:HD13	1:A:1938:PHE:HD1	1.63	0.62
1:B:3865:ILE:O	1:B:3869:VAL:HG23	1.98	0.62
1:B:4194:PRO:O	1:B:4197:LEU:HB2	1.99	0.62
1:A:2247:ARG:HB2	1:A:2249:LEU:HG	1.81	0.62
1:A:2542:ASN:O	1:A:2546:VAL:HG23	1.99	0.62
1:A:3599:LEU:HD11	1:A:3638:LEU:HD13	1.80	0.62
1:B:2877:ARG:HB3	1:B:2881:ARG:HH12	1.63	0.62
1:A:1695:ALA:HB1	1:A:2019:CYS:SG	2.39	0.62
1:A:2205:PRO:HG2	1:A:2265:ILE:HD11	1.81	0.62
1:A:1743:GLY:HA3	1:A:1753:THR:HA	1.81	0.62
1:A:1975:PRO:HD2	1:A:2101:ILE:HA	1.80	0.62
1:A:2546:VAL:HA	1:A:2549:ILE:HD12	1.80	0.62
1:A:2793:ASN:N	1:A:2793:ASN:ND2	2.44	0.62
1:B:2080:GLY:HA2	1:B:2086:ASN:ND2	2.14	0.62
1:A:1927:ILE:HD13	1:A:1991:LEU:HD22	1.79	0.62
1:A:3011:HIS:ND1	1:A:3143:VAL:HG23	2.15	0.62
1:B:2277:PRO:HA	1:B:2398:GLN:HG3	1.81	0.62
1:B:3844:ASN:O	1:B:3848:ASP:CB	2.47	0.62
1:B:2584:SER:HB3	1:B:2813:ILE:HB	1.82	0.62
1:A:1957:TYR:CD2	1:A:1987:LEU:HD13	2.35	0.62
1:A:2645:ASP:O	1:A:2647:VAL:HG23	1.98	0.62
1:A:3557:VAL:O	1:A:3561:ILE:HG13	2.00	0.62
1:A:3686:MET:HE2	1:A:3696:LYS:HD2	1.81	0.62
1:B:2199:ILE:HG23	1:B:2203:MET:HG3	1.81	0.62
1:B:2206:LYS:HB3	1:B:2413:MET:HB3	1.81	0.62
1:A:2053:ASN:O	1:A:2054:SER:C	2.42	0.62
1:A:3408:VAL:HG11	1:A:3477:LEU:HG	1.82	0.62
1:A:3452:ILE:HG21	1:A:3485:THR:HG21	1.82	0.62
1:A:3634:VAL:HB	1:A:3635:PRO:HD3	1.82	0.62
1:A:3812:LYS:HB3	1:A:3875:VAL:HG22	1.81	0.62
1:A:4389:ARG:HG2	1:A:4389:ARG:HH11	1.65	0.62
1:A:3566:ASN:HB3	1:A:3855:LEU:HD22	1.82	0.62
1:A:4568:PHE:O	1:A:4572:MET:HG2	2.00	0.62
1:B:1726:PHE:CD2	1:B:1729:LEU:HD22	2.35	0.62
1:B:4410:LEU:HD22	1:B:4411:PRO:HD2	1.81	0.62
1:A:1967:ARG:HH22	1:A:2069:GLN:HG3	1.63	0.61
1:A:2151:ALA:O	1:A:2155:VAL:HG12	1.99	0.61
1:A:4402:ILE:H	1:A:4402:ILE:HD12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2357:GLY:O	1:A:2397:VAL:HG12	2.00	0.61
1:A:2954:ASN:H	1:A:2954:ASN:ND2	1.97	0.61
1:A:3445:THR:N	1:A:3446:PRO:HD2	2.16	0.61
1:B:2275:VAL:HG13	1:B:2397:VAL:HG13	1.82	0.61
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.35	0.61
1:A:4050:LYS:O	1:A:4051:ASP:C	2.42	0.61
1:B:2212:ILE:N	1:B:2213:PRO:HD2	2.15	0.61
1:A:2121:ALA:O	1:A:2122:GLU:C	2.43	0.61
1:A:2239:LYS:HA	1:A:2239:LYS:HE3	1.81	0.61
1:A:2243:ILE:HD12	1:A:2292:ALA:HB2	1.82	0.61
1:A:2670:LEU:HG	1:A:2789:VAL:HG22	1.83	0.61
1:A:2989:VAL:HG13	1:A:3187:GLU:CD	2.25	0.61
1:A:3271:ILE:O	1:A:3275:ARG:HB2	2.00	0.61
1:B:2208:VAL:HG23	1:B:2211:ASP:HB2	1.81	0.61
1:B:2704:ALA:HB2	1:B:3085:GLU:OE2	1.98	0.61
1:B:3664:MET:O	1:B:3668:PHE:HB3	1.99	0.61
1:B:4402:ILE:HD12	1:B:4402:ILE:N	2.14	0.61
1:A:3260:TYR:O	1:A:3264:ILE:HG12	2.01	0.61
1:A:3731:ASN:HD22	1:A:3731:ASN:N	1.97	0.61
1:A:4432:LYS:C	1:A:4434:GLN:H	2.08	0.61
1:A:2258:LYS:HD3	1:A:2261:GLN:HG3	1.83	0.61
1:A:2272:VAL:O	1:A:2394:MET:HA	2.00	0.61
1:A:2274:MET:CE	1:A:2286:TRP:HB3	2.30	0.61
1:A:2791:ALA:O	1:A:2792:CYS:HB3	2.00	0.61
1:A:2869:GLN:HB3	1:A:2872:TYR:CD1	2.36	0.61
1:A:4329:ILE:HD12	1:A:4331:TRP:CZ2	2.35	0.61
1:B:2140:SER:O	1:B:2142:GLN:HG2	1.99	0.61
1:B:3673:LEU:HB2	1:B:3781:VAL:CG1	2.26	0.61
1:A:2948:ARG:HD3	1:A:2950:ILE:HG13	1.82	0.61
1:A:4076:ILE:HD11	1:A:4104:SER:O	2.00	0.61
1:A:4589:VAL:HG12	1:A:4638:ASN:O	2.01	0.61
1:A:2088:PRO:HB2	1:A:2090:ASN:ND2	2.15	0.61
1:A:3474:CYS:HA	1:A:3477:LEU:HD22	1.83	0.61
1:A:4600:TYR:O	1:A:4604:THR:HG23	2.01	0.61
1:B:2305:VAL:HG22	1:B:2354:ILE:HB	1.83	0.61
1:B:2732:PRO:HG3	1:B:2739:LEU:HB2	1.83	0.61
1:A:3587:THR:HB	1:A:3628:PHE:HA	1.82	0.61
1:B:2586:GLY:HA2	1:B:2815:LEU:HD13	1.81	0.61
1:B:3291:LYS:HD2	1:B:3835:LEU:HG	1.81	0.61
1:B:4189:ASN:N	1:B:4218:THR:HG22	2.14	0.61
1:A:2190:TYR:O	1:A:2194:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2985:ASP:O	1:A:2987:PRO:HD3	2.01	0.61
1:A:4624:SER:HB2	1:A:4668:THR:HB	1.83	0.61
1:B:2578:MET:HE3	1:B:2579:TRP:NE1	2.16	0.61
1:B:3650:ASN:OD1	1:B:3688:GLN:HA	2.00	0.61
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.01	0.60
1:A:3385:LYS:O	1:A:3389:ASP:HB2	2.00	0.60
1:A:4396:ILE:HA	1:A:4399:LEU:HD12	1.83	0.60
1:A:4503:ILE:HG23	1:A:4575:LEU:HB3	1.82	0.60
1:B:2869:GLN:HB2	1:B:2872:TYR:CG	2.36	0.60
1:B:4135:CYS:HA	1:B:4219:SER:O	2.00	0.60
1:A:1687:LEU:HD22	1:A:1705:LEU:HD23	1.83	0.60
1:A:3137:VAL:HG13	1:A:3141:LEU:HD23	1.82	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:HE2	1.83	0.60
1:A:4590:TRP:CE3	1:A:4593:GLY:HA3	2.36	0.60
1:B:3559:ARG:NE	1:B:3846:LEU:O	2.35	0.60
1:A:3239:GLY:O	1:A:3243:ILE:HG13	2.00	0.60
1:A:4536:SER:HB2	1:A:4548:LYS:NZ	2.16	0.60
1:A:4636:SER:HB3	1:A:4670:THR:HA	1.83	0.60
1:A:2144:HIS:HB2	1:A:2413:MET:SD	2.40	0.60
1:A:2903:ARG:NH2	1:A:2950:ILE:HA	2.16	0.60
1:B:2231:ILE:HG21	1:B:2264:GLN:HE22	1.64	0.60
1:B:2364:VAL:HB	1:B:2407:THR:HG21	1.82	0.60
1:B:3219:ILE:O	1:B:3221:PRO:HD3	2.00	0.60
1:A:2118:PHE:CE1	1:A:2163:LYS:HD2	2.37	0.60
1:A:2309:LYS:HG3	1:A:2358:ASP:HB2	1.84	0.60
1:A:3345:GLN:O	1:A:3349:ASP:HB2	2.01	0.60
1:A:4690:VAL:O	1:A:4700:LEU:HB2	2.01	0.60
1:A:1763:GLY:H	1:A:1764:PRO:HD3	1.65	0.60
1:A:2532:ARG:HG3	1:A:2808:LEU:O	2.01	0.60
1:A:2917:LEU:HD12	1:A:2923:LYS:HA	1.84	0.60
1:A:3075:GLU:O	1:A:3078:VAL:HG12	2.01	0.60
1:A:3562:ALA:O	1:A:3566:ASN:HB2	2.02	0.60
1:A:3718:LEU:HD23	1:A:3762:ILE:HG13	1.84	0.60
1:A:4092:ASP:OD2	1:A:4093:ARG:HG2	2.01	0.60
1:A:4182:GLY:HA3	1:A:4212:SER:OG	2.02	0.60
1:B:1820:GLN:HE22	1:B:1990:GLN:NE2	1.99	0.60
1:B:2976:LEU:HD12	1:B:2990:LEU:HD11	1.84	0.60
1:B:3813:ARG:HB3	1:B:3879:ILE:HD13	1.83	0.60
1:A:2176:ASP:N	1:A:2179:SER:HG	1.99	0.60
1:A:3598:PHE:CD2	1:A:3634:VAL:HG11	2.36	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:NZ	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4503:ILE:HA	1:A:4575:LEU:HD23	1.84	0.60
1:B:1752:VAL:HG22	1:B:1811:PRO:HG3	1.84	0.60
1:B:1908:TYR:CE1	1:B:1958:LEU:HD22	2.37	0.60
1:A:2239:LYS:HD3	1:A:2295:GLN:NE2	2.16	0.60
1:A:2730:LEU:HD23	1:A:2783:LEU:HD23	1.83	0.60
1:A:4574:GLN:NE2	1:A:4590:TRP:HB3	2.17	0.60
1:B:2129:VAL:HG22	1:B:2130:PRO:CD	2.30	0.60
1:B:2522:ARG:HD3	1:B:2585:MET:SD	2.42	0.60
1:B:4153:LEU:HB2	1:B:4155:LYS:HG2	1.83	0.60
1:B:4541:ILE:HA	1:B:4561:LEU:HD11	1.83	0.60
1:A:1769:TRP:HA	1:A:1772:MET:HE3	1.84	0.60
1:A:1921:VAL:HG23	1:A:1922:LEU:CD2	2.32	0.60
1:A:3040:ILE:HG22	1:A:3042:VAL:HG13	1.82	0.60
1:A:3368:LYS:C	1:A:3374:ILE:HD11	2.26	0.60
1:A:3803:LYS:HE3	1:A:3810:HIS:NE2	2.17	0.60
1:B:1608:VAL:HG21	1:B:1669:MET:HG3	1.83	0.60
1:B:3559:ARG:O	1:B:3563:LEU:HB2	2.02	0.60
1:B:4060:GLU:O	1:B:4064:VAL:HG23	2.02	0.60
1:A:2091:LEU:HD22	1:A:2095:PHE:CE1	2.37	0.60
1:A:2439:PHE:H	1:A:2495:GLN:HE22	1.48	0.60
1:A:3262:ASP:HB2	1:A:3670:ARG:HE	1.67	0.60
1:A:1604:VAL:HG11	1:A:1670:GLU:HA	1.84	0.59
1:A:3922:ASN:HD22	1:A:3922:ASN:N	2.00	0.59
1:A:4004:THR:OG1	1:A:4006:PRO:HD3	2.01	0.59
1:B:3017:VAL:HG13	1:B:3174:GLY:O	2.02	0.59
1:A:4691:TYR:CD2	1:A:4696:ARG:HG2	2.36	0.59
1:B:1948:VAL:O	1:B:1950:THR:HG23	2.02	0.59
1:B:3671:TYR:HD2	1:B:3734:LEU:HA	1.67	0.59
1:B:4499:PHE:O	1:B:4503:ILE:HB	2.01	0.59
1:A:2864:PHE:HB3	1:A:2872:TYR:CD2	2.38	0.59
1:A:3785:ASN:HD22	1:A:3786:PHE:H	1.49	0.59
1:A:4644:LEU:HD12	1:A:4723:ILE:HG12	1.85	0.59
1:B:2000:CYS:C	1:B:2002:GLU:H	2.10	0.59
1:B:2494:VAL:HG11	1:B:2548:VAL:HB	1.84	0.59
1:A:2273:MET:SD	1:A:2408:ILE:HG22	2.42	0.59
1:A:3923:LEU:HD22	1:A:3947:ILE:HG12	1.83	0.59
1:A:4217:MET:HE1	1:A:4229:LEU:HD11	1.83	0.59
1:A:4545:ILE:O	1:A:4561:LEU:HD21	2.02	0.59
1:A:4715:ASN:O	1:A:4719:ARG:HB2	2.02	0.59
1:B:2377:LEU:O	1:B:2384:ARG:HA	2.02	0.59
1:B:2616:SER:HB3	1:B:2627:TRP:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3673:LEU:HD22	1:B:3783:PHE:HE1	1.66	0.59
1:B:4124:LYS:O	1:B:4125:GLU:HG2	2.01	0.59
1:B:4131:PRO:HD2	1:B:4232:MET:O	2.03	0.59
1:B:4137:VAL:HB	1:B:4138:PRO:HD2	1.85	0.59
1:A:3672:PRO:HA	1:A:3782:THR:HG23	1.84	0.59
1:A:4190:ILE:HB	1:A:4197:LEU:HD11	1.83	0.59
1:A:4371:PRO:HA	1:A:4385:GLU:OE1	2.03	0.59
1:B:1612:TRP:O	1:B:1616:GLU:HB2	2.02	0.59
1:B:2000:CYS:HB3	1:B:2031:LEU:HD13	1.83	0.59
1:A:2528:PHE:CE1	1:A:2533:VAL:HG11	2.38	0.59
1:A:2581:LEU:O	1:A:2585:MET:HE3	2.01	0.59
1:A:3730:LEU:HD11	1:A:3762:ILE:CD1	2.33	0.59
1:A:3731:ASN:HB2	1:A:3732:PRO:HD3	1.84	0.59
1:A:4157:TYR:OH	1:A:4186:LEU:HD22	2.03	0.59
1:A:4597:PRO:HB2	1:A:4700:LEU:HD21	1.85	0.59
1:B:3024:VAL:HG11	2:B:9010:ADP:H3'	1.83	0.59
1:B:3809:THR:HG21	1:B:3882:VAL:HG11	1.84	0.59
1:B:3897:TYR:HE1	1:B:3913:LEU:HA	1.67	0.59
1:B:4273:LEU:HD13	1:B:4363:LEU:O	2.02	0.59
1:A:2293:ILE:HG22	1:A:2350:ARG:NH2	2.12	0.59
1:A:2648:ILE:HG21	1:A:2827:ILE:HA	1.84	0.59
1:A:2938:PHE:HB3	1:A:2941:VAL:CG2	2.33	0.59
1:A:3924:LEU:HD23	1:A:3943:LEU:CD2	2.32	0.59
1:A:3951:THR:O	1:A:3955:VAL:HG23	2.02	0.59
1:B:1625:ILE:HD12	1:B:1628:LEU:HB2	1.83	0.59
1:B:2863:ARG:O	1:B:2863:ARG:HD3	2.02	0.59
1:A:3190:ARG:HA	1:A:3224:ARG:HH12	1.66	0.59
1:A:4494:PRO:HD3	1:A:4610:GLN:HE22	1.67	0.59
1:B:1546:VAL:HG22	1:B:1556:ARG:CZ	2.33	0.59
1:B:4207:LEU:O	1:B:4209:PRO:HD3	2.02	0.59
1:B:4424:ARG:NH2	1:B:4558:THR:HG21	2.17	0.59
1:A:2250:VAL:HB	1:A:2425:MET:CE	2.31	0.59
1:A:2863:ARG:HD2	1:A:2864:PHE:CE1	2.36	0.59
1:A:3313:LEU:HD13	1:A:3550:SER:OG	2.03	0.59
1:A:4136:SER:O	1:A:4221:ILE:HD12	2.03	0.59
1:B:1477:LYS:H	1:B:1480:HIS:HD2	1.50	0.59
1:B:2273:MET:HG2	1:B:2395:PHE:HB2	1.84	0.59
1:B:2598:GLN:HG2	1:B:2612:LEU:HD23	1.85	0.59
1:B:4332:ILE:O	1:B:4336:THR:HG23	2.02	0.59
1:A:1538:TRP:HZ3	1:A:1656:ILE:HD13	1.68	0.59
1:A:1978:THR:CG2	1:A:2103:PRO:HD3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2598:GLN:CG	1:A:2612:LEU:HB2	2.33	0.59
1:A:2991:PHE:HE1	1:A:2993:GLU:HB2	1.67	0.59
1:A:4572:MET:HA	1:A:4575:LEU:HD13	1.85	0.59
1:B:3788:VAL:HG11	1:B:3913:LEU:HD22	1.85	0.59
1:A:1763:GLY:N	1:A:1764:PRO:CD	2.65	0.58
1:A:1797:VAL:CG1	1:A:1855:ILE:HD11	2.33	0.58
1:A:1973:PHE:CE1	1:A:2099:ALA:HA	2.38	0.58
1:A:2278:SER:HA	1:A:2806:ARG:HH11	1.68	0.58
1:A:4066:GLN:NE2	1:A:4081:ARG:HD3	2.18	0.58
1:B:3233:TYR:CD2	1:B:3620:ARG:HG3	2.38	0.58
1:B:4109:ASP:HA	1:B:4112:ASN:HD22	1.67	0.58
1:A:1735:ASP:OD2	1:A:1737:GLU:HB2	2.03	0.58
1:B:2375:LYS:HB3	1:B:2387:LEU:HB3	1.84	0.58
1:B:4349:ASN:HB3	1:B:4352:ASP:OD2	2.03	0.58
1:B:4351:PHE:CD2	1:B:4689:PRO:HG3	2.38	0.58
1:A:2043:ILE:HG23	1:A:2073:ILE:HD12	1.84	0.58
1:A:3331:GLN:NE2	1:A:3533:LYS:HG3	2.18	0.58
1:A:3723:VAL:HG12	1:A:3766:THR:OG1	2.03	0.58
1:A:4193:ALA:O	1:A:4197:LEU:HD23	2.03	0.58
1:B:3027:ARG:HG2	1:B:3037:ILE:HD12	1.85	0.58
1:B:3170:LEU:HD21	1:B:3172:TRP:HE3	1.67	0.58
1:B:4030:PHE:HD1	1:B:4033:LEU:HD22	1.68	0.58
1:A:2153:LYS:O	1:A:2157:VAL:HG23	2.03	0.58
1:A:3830:LEU:HB3	1:A:3858:LEU:HD13	1.86	0.58
1:A:4251:THR:HG23	1:A:4303:LEU:CD2	2.30	0.58
1:A:4349:ASN:HD22	1:A:4352:ASP:H	1.51	0.58
1:A:4368:ALA:HA	1:A:4373:PHE:CE1	2.38	0.58
1:B:1901:ASN:HD22	1:B:1901:ASN:N	2.01	0.58
1:B:2166:CYS:HA	1:B:2190:TYR:OH	2.03	0.58
1:B:3182:PHE:O	1:B:3186:SER:HB2	2.03	0.58
1:A:2087:LEU:HB2	1:A:2092:LYS:HG3	1.86	0.58
1:A:2361:PRO:HD3	1:A:2402:TYR:O	2.03	0.58
1:A:3803:LYS:HG3	1:A:3810:HIS:CD2	2.39	0.58
1:A:4003:GLU:HG3	1:B:2842:LEU:CD2	2.34	0.58
1:A:4032:LYS:HG3	1:A:4069:LEU:HD11	1.83	0.58
1:B:1884:HIS:O	1:B:1888:VAL:HG23	2.03	0.58
1:B:3620:ARG:HG2	1:B:3620:ARG:HH11	1.69	0.58
1:A:1950:THR:HB	1:A:1951:PRO:HD2	1.84	0.58
1:A:2212:ILE:N	1:A:2213:PRO:HD2	2.18	0.58
1:A:3218:ALA:O	1:A:3219:ILE:C	2.47	0.58
1:B:1821:ILE:HG21	1:B:1914:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2338:ARG:HD2	1:B:2346:GLU:OE1	2.04	0.58
1:A:1849:GLU:HG3	1:A:1893:GLN:OE1	2.03	0.58
1:B:1719:GLN:HA	1:B:1722:PHE:CE2	2.38	0.58
1:B:2766:MET:HE2	1:B:2783:LEU:HD11	1.84	0.58
1:B:2997:HIS:O	1:B:3001:ILE:HG13	2.03	0.58
1:B:3013:LEU:HD22	1:B:3164:LEU:HD12	1.85	0.58
1:B:4388:THR:HG23	1:B:4391:HIS:HD2	1.68	0.58
1:A:3615:ARG:O	1:A:3619:ILE:HG13	2.03	0.58
1:A:4572:MET:HA	1:A:4575:LEU:CD1	2.34	0.58
1:A:4596:ASN:HD22	1:A:4596:ASN:C	2.11	0.58
1:B:1855:ILE:HG22	1:B:1859:LEU:HD12	1.85	0.58
1:B:3923:LEU:HD22	1:B:3947:ILE:HG23	1.85	0.58
1:A:1863:VAL:HG21	1:A:2115:SER:O	2.04	0.58
1:A:2135:CYS:HB3	1:A:2147:PHE:CZ	2.38	0.58
1:B:1748:GLU:HB3	1:B:1943:ILE:HD12	1.85	0.58
1:B:4671:TRP:C	1:B:4672:LYS:HG2	2.29	0.58
1:A:1995:VAL:HA	1:A:2022:TRP:HB2	1.84	0.58
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.29	0.58
1:B:1643:PHE:CE2	1:B:1647:LEU:HD11	2.39	0.58
1:B:1926:VAL:HG12	1:B:1928:HIS:CD2	2.39	0.58
1:B:3192:LEU:HD11	1:B:3268:VAL:HA	1.84	0.58
1:B:3263:PHE:O	1:B:3267:VAL:HG23	2.03	0.58
1:B:4648:VAL:HA	1:B:4662:THR:HG21	1.85	0.58
1:A:2838:LEU:O	1:A:2839:LEU:HD23	2.04	0.57
1:A:3255:VAL:O	1:A:3255:VAL:HG13	2.03	0.57
1:A:3337:LYS:HA	1:A:3341:ALA:HB3	1.86	0.57
1:A:3595:ALA:HB1	1:A:3638:LEU:HD11	1.85	0.57
1:A:4559:ILE:O	1:A:4559:ILE:HG23	2.04	0.57
1:B:1813:GLN:NE2	1:B:1941:LEU:H	2.02	0.57
1:B:1939:GLU:O	1:B:1941:LEU:HG	2.03	0.57
1:B:2863:ARG:HG3	1:B:2925:TRP:CE2	2.39	0.57
1:B:3785:ASN:HD21	1:B:3787:THR:CG2	2.16	0.57
1:A:1982:GLU:HG3	2:A:9001:ADP:H3'	1.86	0.57
1:A:3274:LYS:O	1:A:3278:LEU:HD23	2.04	0.57
1:A:3487:TYR:O	1:A:3490:ILE:HG12	2.04	0.57
1:A:4284:ARG:HG3	1:A:4408:LEU:HB3	1.86	0.57
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.03	0.57
1:B:4189:ASN:N	1:B:4189:ASN:ND2	2.53	0.57
1:A:2739:LEU:HD23	1:A:2740:VAL:N	2.19	0.57
1:B:2869:GLN:HB2	1:B:2872:TYR:CD2	2.39	0.57
1:B:3674:VAL:HG13	1:B:3786:PHE:HD2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3897:TYR:CE1	1:B:3913:LEU:HA	2.38	0.57
1:B:4255:ILE:HD11	1:B:4307:LEU:HD11	1.85	0.57
1:A:2560:MET:HG3	1:A:2561:SER:N	2.16	0.57
1:A:2839:LEU:HD11	1:A:2890:ILE:HD12	1.85	0.57
1:A:2853:MET:HE3	1:A:2882:TRP:CG	2.38	0.57
1:A:3668:PHE:CD1	1:A:3672:PRO:HD3	2.39	0.57
1:A:4277:PHE:HB2	1:A:4363:LEU:CD1	2.34	0.57
1:B:1888:VAL:O	1:B:1892:LEU:HD12	2.04	0.57
1:B:2533:VAL:HB	1:B:2581:LEU:CD2	2.30	0.57
1:A:2297:ASP:C	1:A:2299:ILE:H	2.12	0.57
1:A:3909:TYR:OH	1:A:3960:LEU:HG	2.04	0.57
1:A:4313:TRP:HB3	1:A:4330:PRO:HG2	1.86	0.57
1:B:1687:LEU:HD21	1:B:1706:LEU:CD2	2.33	0.57
1:B:1889:VAL:HA	1:B:1892:LEU:HD13	1.86	0.57
1:B:2219:LEU:CD1	1:B:2228:LEU:HD11	2.35	0.57
1:B:2235:GLN:HE22	1:B:2296:VAL:HG13	1.68	0.57
1:B:2417:SER:O	1:B:2420:ILE:HG12	2.03	0.57
1:B:4379:ILE:O	1:B:4379:ILE:HG13	2.05	0.57
1:A:2195:LEU:O	1:A:2199:ILE:HG12	2.04	0.57
1:A:2252:LYS:O	1:A:2256:VAL:HG23	2.05	0.57
1:A:2873:ILE:H	1:A:2873:ILE:HD12	1.68	0.57
1:A:3863:THR:O	1:A:3867:LEU:HB3	2.04	0.57
1:B:2835:LEU:HD11	1:B:2890:ILE:HD12	1.85	0.57
1:B:2841:ASN:HD22	1:B:2842:LEU:N	2.02	0.57
1:B:3638:LEU:HD12	1:B:3663:ILE:HG21	1.86	0.57
1:B:4318:SER:HB3	1:B:4324:ILE:HD11	1.85	0.57
1:A:2274:MET:HE1	1:A:2286:TRP:CD1	2.40	0.57
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.40	0.57
1:A:4288:ILE:HG23	1:A:4292:TRP:O	2.04	0.57
1:A:4639:VAL:HB	1:A:4642:MET:HE2	1.87	0.57
1:B:2270:HIS:HA	1:B:2392:ARG:HH11	1.70	0.57
1:B:1591:TRP:O	1:B:1595:LEU:HB2	2.05	0.57
1:A:1718:ILE:HG22	1:A:1722:PHE:CE2	2.40	0.57
1:A:2836:MET:HE1	1:A:2901:LEU:HD22	1.87	0.57
1:A:3439:ASP:C	1:A:3441:LYS:H	2.13	0.57
1:A:4245:LYS:HD2	1:A:4399:LEU:O	2.04	0.57
1:B:2540:LEU:HD12	1:B:2662:ALA:HB3	1.85	0.57
1:B:3017:VAL:HG11	1:B:3175:GLU:CD	2.30	0.57
1:B:3238:ILE:HG12	1:B:3601:TYR:CD2	2.40	0.57
1:B:3793:LEU:HD23	1:B:3894:SER:HA	1.86	0.57
1:A:1681:LYS:O	1:A:1685:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:THR:HG22	1:A:2103:PRO:HD3	1.87	0.57
1:A:2689:ARG:C	1:A:2691:PHE:H	2.12	0.57
1:A:4006:PRO:C	1:A:4008:LEU:H	2.11	0.57
1:A:4415:GLU:HA	1:A:4415:GLU:OE2	2.05	0.57
1:B:2586:GLY:HA2	1:B:2815:LEU:CD1	2.34	0.57
1:B:3912:SER:HB3	1:B:4231:ARG:HG2	1.86	0.57
1:B:4313:TRP:HB3	1:B:4330:PRO:HG2	1.87	0.57
1:A:2139:LEU:O	1:A:2140:SER:C	2.48	0.56
1:A:3266:GLN:HE21	1:A:3270:LEU:CD2	2.18	0.56
1:A:3291:LYS:HG3	1:A:3835:LEU:HD22	1.86	0.56
1:A:3439:ASP:HB3	1:A:3442:LYS:HG2	1.87	0.56
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.69	0.56
1:A:4132:LEU:HD23	1:A:4236:PHE:HE2	1.70	0.56
1:A:4375:LEU:HD11	1:A:4383:VAL:CG2	2.30	0.56
1:B:1537:PHE:O	1:B:1541:LEU:HB2	2.05	0.56
1:B:3274:LYS:HE3	1:B:3637:PHE:CE2	2.39	0.56
1:B:3614:MET:O	1:B:3618:MET:HG3	2.04	0.56
1:B:4043:ASP:HB3	1:B:4059:PRO:HB3	1.87	0.56
1:B:4543:LYS:HD2	1:B:4545:ILE:HD13	1.87	0.56
1:A:1927:ILE:HD13	1:A:1991:LEU:CD2	2.35	0.56
1:A:1978:THR:HG21	1:A:2101:ILE:O	2.05	0.56
1:A:2003:GLY:O	1:A:2004:PHE:C	2.49	0.56
1:A:4132:LEU:HD13	1:A:4216:PHE:CE1	2.40	0.56
1:B:2252:LYS:HD3	1:B:2425:MET:HE1	1.88	0.56
1:B:2704:ALA:HB2	1:B:3085:GLU:CD	2.29	0.56
1:B:4407:TRP:CD1	1:B:4407:TRP:H	2.23	0.56
1:B:4618:ASN:HD22	1:B:4618:ASN:N	2.02	0.56
1:A:2560:MET:CE	1:A:2564:ASN:HD22	2.18	0.56
1:A:2675:PRO:HG2	1:A:2678:SER:HB3	1.88	0.56
1:A:2979:PHE:HE2	1:A:3028:PHE:HA	1.70	0.56
1:A:3195:GLU:OE1	1:A:3224:ARG:HB2	2.04	0.56
1:A:3299:VAL:HG21	1:A:3563:LEU:HD23	1.87	0.56
1:A:3567:LEU:CD2	1:A:3855:LEU:HD11	2.36	0.56
1:A:3698:SER:C	1:A:3700:LEU:H	2.13	0.56
1:A:3813:ARG:HB2	1:A:3813:ARG:CZ	2.34	0.56
1:A:3813:ARG:HB3	1:A:3879:ILE:HD11	1.88	0.56
1:B:1531:LEU:HD13	1:B:1587:GLU:OE2	2.05	0.56
1:B:1554:LEU:HB3	1:B:1609:GLN:NE2	2.09	0.56
1:B:1956:CYS:SG	1:B:1983:THR:HG21	2.45	0.56
1:B:2815:LEU:HD23	1:B:2815:LEU:C	2.31	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:GLN:HB3	1:A:2230:PRO:HD2	1.86	0.56
1:A:2274:MET:HE1	1:A:2286:TRP:CB	2.33	0.56
1:A:2806:ARG:HH12	2:A:9002:ADP:PB	2.28	0.56
1:A:3584:GLN:O	1:A:3588:VAL:HG23	2.06	0.56
1:A:3598:PHE:HA	1:A:3602:ILE:HG12	1.88	0.56
1:A:3682:MET:SD	1:A:3696:LYS:HE2	2.46	0.56
1:A:4277:PHE:O	1:A:4281:ILE:HG12	2.06	0.56
1:B:2660:LEU:HD21	1:B:2672:LEU:HD21	1.87	0.56
1:B:4213:PHE:CZ	1:B:4215:LEU:HB2	2.40	0.56
1:A:1752:VAL:HG22	1:A:1811:PRO:HG3	1.86	0.56
1:A:1947:LEU:HD11	1:A:1982:GLU:HB3	1.87	0.56
1:A:4117:ASP:OD1	1:A:4119:ALA:HB3	2.06	0.56
1:B:1998:PHE:CD1	1:B:2009:MET:HE1	2.41	0.56
1:B:2144:HIS:HB3	1:B:2400:LEU:HD12	1.86	0.56
1:B:2739:LEU:HB3	1:B:2786:ILE:HG12	1.87	0.56
1:A:2087:LEU:O	1:A:2092:LYS:HD2	2.06	0.56
1:A:1948:VAL:O	1:A:1950:THR:HG23	2.06	0.56
1:A:2262:LEU:CD1	1:A:2274:MET:HE3	2.29	0.56
1:A:2284:THR:O	1:A:2288:VAL:HG23	2.06	0.56
1:A:4534:LEU:HA	1:A:4537:LEU:HD12	1.88	0.56
1:B:2560:MET:HG3	1:B:2564:ASN:HB2	1.88	0.56
1:B:2670:LEU:HD11	1:B:2789:VAL:HG13	1.88	0.56
1:B:3843:GLY:C	1:B:3845:ILE:H	2.13	0.56
1:A:2954:ASN:ND2	1:A:2954:ASN:N	2.53	0.56
1:A:3445:THR:HA	1:A:3449:ARG:HD3	1.87	0.56
1:A:3848:ASP:HB3	1:A:3851:VAL:HG12	1.88	0.56
1:A:3887:ASN:HB3	1:A:3888:PRO:HD3	1.88	0.56
1:B:2841:ASN:ND2	1:B:2842:LEU:N	2.52	0.56
1:B:3043:ASN:HD22	1:B:3043:ASN:H	1.54	0.56
1:B:3758:PRO:HG2	1:B:3759:SER:H	1.71	0.56
1:B:3902:GLU:C	1:B:3904:SER:H	2.13	0.56
1:A:1687:LEU:HD21	1:A:1706:LEU:HD23	1.88	0.56
1:A:1862:SER:O	1:A:1865:GLN:HG2	2.06	0.56
1:A:2748:LEU:N	1:A:2749:PRO:CD	2.69	0.56
1:A:2798:ALA:C	1:A:2800:ARG:H	2.14	0.56
1:A:2906:ALA:O	1:A:2910:LEU:HG	2.05	0.56
1:A:2941:VAL:HG12	1:A:2942:ASN:N	2.20	0.56
1:A:3376:ALA:O	1:A:3380:VAL:HG23	2.06	0.56
1:A:3813:ARG:HH22	1:A:3817:LEU:CD1	2.18	0.56
1:A:4622:HIS:HE2	1:A:4678:ILE:CG2	2.16	0.56
1:B:1479:ARG:CZ	1:B:1479:ARG:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:TYR:O	1:B:2084:ARG:HD2	2.06	0.56
1:B:2163:LYS:HB2	1:B:2194:VAL:HG11	1.87	0.56
1:A:2381:ASN:OD1	1:A:2383:GLU:HB2	2.06	0.56
1:A:3404:ALA:HA	1:A:3462:PHE:HE1	1.71	0.56
1:A:4589:VAL:HG12	1:A:4639:VAL:HA	1.88	0.56
1:B:2276:GLY:O	1:B:2398:GLN:HA	2.06	0.56
1:B:3729:VAL:O	1:B:3729:VAL:HG22	2.05	0.56
1:A:1957:TYR:O	1:A:1961:THR:HG23	2.07	0.55
1:A:3292:LEU:HD22	1:A:3567:LEU:HD22	1.89	0.55
1:B:3908:LEU:HD22	1:B:4221:ILE:HG23	1.87	0.55
1:B:4147:ASP:HA	1:B:4157:TYR:OH	2.06	0.55
1:B:4190:ILE:HG12	1:B:4219:SER:HB2	1.86	0.55
1:B:4217:MET:HE1	1:B:4229:LEU:HD11	1.87	0.55
1:B:4389:ARG:HG2	1:B:4389:ARG:NH1	2.21	0.55
1:B:4535:ARG:HG2	1:B:4535:ARG:HH11	1.71	0.55
1:A:1800:HIS:HB2	1:A:1858:ASN:HD22	1.71	0.55
1:A:2910:LEU:HD23	1:A:2930:ILE:CD1	2.33	0.55
1:A:3673:LEU:HD13	1:A:3783:PHE:CE1	2.40	0.55
1:A:4005:ILE:HG22	1:A:4008:LEU:HB2	1.87	0.55
1:B:2829:GLY:HA2	1:B:2850:THR:OG1	2.06	0.55
1:B:3700:LEU:CD2	1:B:3701:ASP:H	2.18	0.55
1:B:4388:THR:O	1:B:4391:HIS:HB2	2.07	0.55
1:A:1699:PHE:HE1	1:A:2015:GLY:HA3	1.71	0.55
1:A:1926:VAL:HG12	1:A:1928:HIS:CD2	2.41	0.55
1:A:2615:TYR:HD1	1:A:2624:TRP:HB3	1.72	0.55
1:A:2650:THR:H	1:A:2653:THR:HB	1.71	0.55
1:A:2991:PHE:CE1	1:A:2993:GLU:HB2	2.40	0.55
1:A:3032:MET:C	1:A:3034:GLY:H	2.15	0.55
1:A:4590:TRP:CD2	1:A:4593:GLY:HA3	2.42	0.55
1:B:2101:ILE:O	1:B:2103:PRO:HD3	2.07	0.55
1:B:2440:ASP:OD1	1:B:2441:PRO:HD2	2.06	0.55
1:B:2603:THR:O	1:B:2605:VAL:HG13	2.06	0.55
1:A:3066:GLU:HG2	1:A:3136:GLN:HE21	1.71	0.55
1:A:3419:TRP:CE3	1:A:3422:ILE:HD11	2.42	0.55
1:B:2369:SER:HA	1:B:2372:ASP:OD2	2.07	0.55
1:B:2921:GLU:CD	1:B:2921:GLU:H	2.13	0.55
1:A:1625:ILE:HG23	1:A:1626:ASN:H	1.70	0.55
1:A:2606:PRO:HG2	1:A:2615:TYR:CE1	2.42	0.55
1:A:3555:ASN:HB3	1:A:3559:ARG:HH11	1.71	0.55
1:B:1578:SER:C	1:B:1580:TYR:H	2.14	0.55
1:B:2774:ARG:HB2	1:B:2781:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1763:GLY:H	1:A:1764:PRO:CD	2.19	0.55
1:A:1875:PHE:O	1:A:1879:ILE:HG12	2.07	0.55
1:A:2275:VAL:HB	1:A:2413:MET:HE2	1.88	0.55
1:A:3471:SER:HB3	1:A:3474:CYS:SG	2.47	0.55
1:A:3930:LEU:HG	1:A:3939:ARG:NH1	2.21	0.55
1:A:3991:LEU:O	1:A:3991:LEU:HD12	2.07	0.55
1:A:4094:VAL:HB	1:A:4423:ALA:HB1	1.88	0.55
1:B:1872:ARG:HH12	1:B:2164:ARG:HD3	1.71	0.55
1:A:1608:VAL:HG13	1:A:1676:LEU:CD1	2.37	0.55
1:A:1797:VAL:HG13	1:A:1855:ILE:HD11	1.89	0.55
1:A:2765:GLN:O	1:A:2769:LYS:HB2	2.07	0.55
1:A:3453:THR:O	1:A:3458:GLU:HG2	2.06	0.55
1:A:4319:LYS:H	1:A:4321:ARG:NH2	2.04	0.55
1:B:1555:VAL:HG23	1:B:1609:GLN:HE21	1.70	0.55
1:B:3018:SER:O	1:B:3256:THR:HB	2.06	0.55
1:B:3306:LEU:HD22	1:B:3553:VAL:HG13	1.89	0.55
1:B:4132:LEU:HD13	1:B:4216:PHE:CE1	2.42	0.55
1:B:4624:SER:HB2	1:B:4668:THR:HB	1.87	0.55
1:B:4644:LEU:HG	1:B:4664:ILE:HD11	1.88	0.55
1:B:4685:LYS:HE2	1:B:4706:PRO:HD3	1.88	0.55
1:A:2446:GLN:O	1:A:2450:ASN:HB3	2.07	0.55
1:A:4028:PRO:C	1:A:4030:PHE:H	2.15	0.55
1:A:4571:ARG:O	1:A:4574:GLN:HB3	2.07	0.55
1:A:1907:LEU:HA	1:A:1911:ARG:NH1	2.21	0.55
1:A:2439:PHE:H	1:A:2495:GLN:NE2	2.05	0.55
1:A:3647:TRP:HH2	1:A:3663:ILE:HD12	1.71	0.55
1:A:4052:GLN:C	1:A:4054:GLY:H	2.14	0.55
1:A:4389:ARG:NH1	1:A:4393:MET:HE2	2.18	0.55
1:B:2612:LEU:HD11	1:B:2624:TRP:CH2	2.42	0.55
1:B:2779:THR:O	1:B:2781:ILE:HD12	2.06	0.55
1:B:2863:ARG:HD2	1:B:2864:PHE:CE1	2.42	0.55
1:B:2918:VAL:HG13	1:B:3172:TRP:NE1	2.22	0.55
1:B:4095:LEU:HD11	1:B:4422:LYS:CB	2.37	0.55
1:A:3965:LEU:HG	1:A:4426:MET:CE	2.37	0.55
1:A:4495:LEU:H	1:A:4495:LEU:CD1	2.16	0.55
1:B:3691:ASP:C	1:B:3693:LYS:H	2.15	0.55
1:B:4024:ARG:HA	1:B:4030:PHE:O	2.07	0.55
1:A:1755:LYS:HG2	1:A:1780:THR:HG23	1.89	0.54
1:A:2648:ILE:HD13	1:A:2831:PHE:CZ	2.42	0.54
1:A:3253:ASN:HB2	1:A:3604:PHE:CE2	2.42	0.54
1:A:3373:ILE:H	1:A:3373:ILE:CD1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4068:GLN:C	1:A:4070:SER:H	2.15	0.54
1:B:2898:LEU:O	1:B:2902:VAL:HG23	2.06	0.54
1:B:4101:PHE:O	1:B:4105:VAL:HG23	2.07	0.54
1:B:4571:ARG:HD3	1:B:4593:GLY:O	2.06	0.54
1:A:1908:TYR:CE1	1:A:1958:LEU:HD13	2.42	0.54
1:A:2196:LEU:HD21	1:A:2219:LEU:HD22	1.89	0.54
1:A:2204:ILE:N	1:A:2205:PRO:CD	2.69	0.54
1:A:2275:VAL:HG13	1:A:2415:TRP:CE3	2.42	0.54
1:A:3266:GLN:HE21	1:A:3270:LEU:HD21	1.71	0.54
1:A:3390:GLU:O	1:A:3394:LEU:HG	2.07	0.54
1:A:4413:ASN:ND2	1:A:4660:LEU:HG	2.22	0.54
1:B:1694:PHE:CE1	1:B:1770:LEU:HD13	2.42	0.54
1:B:2832:ASN:HA	1:B:2835:LEU:HB3	1.89	0.54
1:B:3652:LEU:HB2	1:B:3684:PHE:CD1	2.43	0.54
1:A:1890:ARG:O	1:A:1894:LYS:HG3	2.07	0.54
1:A:2431:LEU:HD11	1:A:2506:PHE:CD2	2.42	0.54
1:A:3647:TRP:HB3	1:A:3652:LEU:CD2	2.37	0.54
1:A:3830:LEU:HB3	1:A:3858:LEU:CD1	2.37	0.54
1:B:2200:ASN:HA	1:B:2204:ILE:HG12	1.89	0.54
1:B:2968:LEU:O	1:B:2972:VAL:HG23	2.07	0.54
1:A:3086:ARG:HH11	1:A:3096:VAL:CG1	2.20	0.54
1:A:4319:LYS:N	1:A:4321:ARG:NH2	2.55	0.54
1:B:2283:THR:HA	1:B:2286:TRP:NE1	2.22	0.54
1:B:2331:LEU:HD21	1:B:2773:TRP:CD1	2.43	0.54
1:B:4013:SER:H	1:B:4016:GLN:HE21	1.54	0.54
1:B:4596:ASN:C	1:B:4596:ASN:HD22	2.15	0.54
1:A:1691:ARG:HD3	1:A:1698:TYR:CD1	2.41	0.54
1:A:3336:ILE:O	1:A:3340:ASP:HB3	2.08	0.54
1:A:3700:LEU:CG	1:A:3701:ASP:H	2.20	0.54
1:A:4121:ILE:O	1:A:4126:VAL:HG12	2.06	0.54
1:A:4553:TYR:N	1:A:4553:TYR:CD1	2.75	0.54
1:B:1548:TYR:CD1	1:B:1549:GLN:HG2	2.43	0.54
1:B:1655:LEU:H	1:B:1655:LEU:HD22	1.72	0.54
1:B:2024:CYS:HA	1:B:2074:PHE:O	2.06	0.54
1:B:2498:CYS:SG	1:B:2569:ILE:HG13	2.47	0.54
1:B:2803:LEU:HD12	1:B:2808:LEU:HD21	1.90	0.54
1:B:2990:LEU:HD23	1:B:2994:VAL:HG11	1.90	0.54
1:B:4323:ASN:N	1:B:4323:ASN:ND2	2.54	0.54
1:A:1951:PRO:HG2	1:A:2104:ASP:OD1	2.08	0.54
1:A:2014:VAL:HG22	1:A:2065:ILE:HD13	1.90	0.54
1:A:2766:MET:HB3	1:A:2783:LEU:CD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3602:ILE:O	1:A:3604:PHE:N	2.40	0.54
1:A:4122:VAL:HG23	1:A:4214:ARG:HD2	1.89	0.54
1:B:1782:ALA:HA	1:B:1938:PHE:CE1	2.42	0.54
1:B:2603:THR:CG2	1:B:2604:PRO:HD2	2.31	0.54
1:B:2874:TYR:OH	1:B:2916:ARG:HD2	2.08	0.54
1:A:2121:ALA:O	1:A:2124:LEU:N	2.41	0.54
1:A:3398:PRO:C	1:A:3400:PRO:HD2	2.33	0.54
1:A:3423:ARG:O	1:A:3426:ILE:HG22	2.07	0.54
1:A:4254:GLY:O	1:A:4256:PRO:HD3	2.07	0.54
1:B:2516:LEU:HD12	1:B:2581:LEU:HD13	1.90	0.54
1:B:2519:ALA:HB2	1:B:2593:PHE:CZ	2.43	0.54
1:B:4080:PHE:HB2	1:B:4101:PHE:CE1	2.43	0.54
1:A:2031:LEU:HD23	1:A:2035:ILE:HG22	1.89	0.54
1:A:2751:THR:HB	1:A:2755:GLY:HA2	1.90	0.54
1:A:3217:MET:O	1:A:3218:ALA:C	2.50	0.54
1:A:3263:PHE:O	1:A:3267:VAL:HG23	2.07	0.54
1:A:3399:THR:N	1:A:3400:PRO:HD2	2.23	0.54
1:A:4013:SER:H	1:A:4016:GLN:HB3	1.73	0.54
1:A:4348:ASP:OD2	1:A:4349:ASN:N	2.40	0.54
1:B:2641:VAL:HG12	1:B:2642:ALA:N	2.23	0.54
1:B:4058:ILE:HD12	1:B:4082:LYS:HG2	1.89	0.54
1:A:1724:LYS:HD3	1:A:2382:GLY:O	2.07	0.54
1:A:2447:GLN:HE22	1:A:2492:LEU:CD2	2.21	0.54
1:A:3043:ASN:HD22	1:A:3043:ASN:N	2.05	0.54
1:A:4547:PRO:HB2	1:A:4550:TRP:CE3	2.43	0.54
1:B:1975:PRO:HD2	1:B:2100:MET:O	2.07	0.54
1:B:1982:GLU:OE1	1:B:1982:GLU:HA	2.08	0.54
1:B:2500:ALA:HA	1:B:2503:SER:OG	2.08	0.54
1:B:2636:VAL:HG21	1:B:2648:ILE:HD11	1.89	0.54
1:B:2929:LYS:O	1:B:2933:VAL:HG23	2.07	0.54
1:B:4336:THR:O	1:B:4340:SER:HB3	2.08	0.54
1:A:1822:VAL:HG12	1:A:1826:GLN:OE1	2.07	0.54
1:A:2128:ILE:HG13	1:A:2152:LEU:HD21	1.90	0.54
1:A:2819:PRO:HD2	1:A:2876:PRO:HG2	1.89	0.54
1:A:3109:MET:O	1:A:3112:CYS:HB2	2.08	0.54
1:A:3373:ILE:HD13	1:A:3373:ILE:N	2.12	0.54
1:A:3760:PHE:CG	1:A:3761:MET:N	2.75	0.54
1:A:3827:LEU:O	1:A:3831:GLU:HG3	2.08	0.54
1:A:4295:PHE:C	1:A:4295:PHE:CD2	2.86	0.54
1:A:4318:SER:CA	1:A:4321:ARG:HH21	2.19	0.54
1:B:2653:THR:O	1:B:2657:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3255:VAL:HA	1:B:3259:HIS:CD2	2.43	0.54
1:B:3677:PRO:CD	1:B:3787:THR:HG22	2.38	0.54
1:B:4257:ALA:HB2	1:B:4389:ARG:HD3	1.90	0.54
1:A:2653:THR:O	1:A:2657:VAL:HG23	2.07	0.53
1:A:4518:ALA:C	1:A:4520:LEU:H	2.15	0.53
1:B:1910:MET:CA	1:B:1929:MET:HG3	2.39	0.53
1:B:4639:VAL:O	1:B:4666:ILE:HD12	2.08	0.53
1:A:2969:ARG:HG3	1:A:2970:GLU:N	2.23	0.53
1:A:3698:SER:HB2	1:A:3721:GLN:HB2	1.90	0.53
1:A:4375:LEU:CD1	1:A:4383:VAL:HG23	2.32	0.53
1:A:4553:TYR:HD1	1:A:4553:TYR:N	2.05	0.53
1:B:1581:TYR:O	1:B:1585:GLU:HB2	2.08	0.53
1:B:1646:ILE:O	1:B:1650:VAL:HG23	2.08	0.53
1:B:1831:LEU:HD13	1:B:1900:GLY:O	2.07	0.53
1:B:2863:ARG:HG3	1:B:2925:TRP:CZ2	2.44	0.53
1:B:3342:ARG:O	1:B:3345:GLN:HB3	2.07	0.53
1:A:2825:THR:O	1:A:2829:GLY:HA3	2.08	0.53
1:A:3418:GLU:O	1:A:3422:ILE:HG23	2.08	0.53
1:A:4012:LEU:HD12	1:A:4012:LEU:N	2.23	0.53
1:B:1655:LEU:HB2	1:B:1658:GLU:CB	2.31	0.53
1:B:1920:ASN:HD22	1:B:1921:VAL:N	2.06	0.53
1:B:2050:LEU:HG	1:B:2067:LEU:HD21	1.89	0.53
1:A:1699:PHE:N	1:A:1699:PHE:HD1	2.06	0.53
1:A:1803:TYR:HE1	1:A:1855:ILE:HD13	1.74	0.53
1:A:1827:VAL:O	1:A:1831:LEU:HG	2.08	0.53
1:A:3150:ALA:O	1:A:3151:SER:C	2.51	0.53
1:A:4376:VAL:HG12	1:A:4379:ILE:HG22	1.90	0.53
1:B:2118:PHE:CE1	1:B:2163:LYS:HG3	2.44	0.53
1:B:2309:LYS:CE	1:B:2756:THR:HG21	2.39	0.53
1:B:3677:PRO:HG3	1:B:3787:THR:HG22	1.89	0.53
1:B:3700:LEU:HD13	1:B:3701:ASP:H	1.71	0.53
1:B:4263:GLN:HA	1:B:4264:PRO:C	2.34	0.53
1:A:1650:VAL:HG13	1:A:1659:VAL:HG11	1.91	0.53
1:A:2704:ALA:O	1:A:2706:THR:HG23	2.08	0.53
1:A:2994:VAL:O	1:A:2998:ILE:HG12	2.08	0.53
1:B:2841:ASN:ND2	1:B:2841:ASN:N	2.54	0.53
1:A:1974:GLY:C	1:A:2079:PRO:HD3	2.34	0.53
1:A:2016:LEU:HD21	1:A:2023:GLY:HA3	1.89	0.53
1:A:2088:PRO:C	1:A:2090:ASN:H	2.16	0.53
1:A:2341:ASP:O	1:A:2343:VAL:N	2.40	0.53
1:A:2752:ASP:C	1:A:2754:TYR:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2515:VAL:HG11	1:B:2577:LEU:HD13	1.90	0.53
1:B:2540:LEU:HD12	1:B:2662:ALA:CB	2.39	0.53
1:B:3067:GLU:O	1:B:3069:ILE:HG13	2.08	0.53
1:B:3109:MET:O	1:B:3129:LEU:HD21	2.09	0.53
1:B:4098:SER:O	1:B:4102:VAL:HG23	2.09	0.53
1:A:1709:ILE:HA	1:A:1766:ILE:HG12	1.90	0.53
1:A:1820:GLN:HB3	1:A:1912:TYR:CD2	2.44	0.53
1:A:2397:VAL:HG21	1:A:2400:LEU:CD2	2.38	0.53
1:A:2745:GLU:HB3	1:A:2748:LEU:HD12	1.91	0.53
1:B:1948:VAL:O	1:B:1950:THR:N	2.41	0.53
1:B:4260:MET:HG3	1:B:4271:TYR:CD1	2.43	0.53
1:B:4693:ASN:H	1:B:4693:ASN:ND2	2.06	0.53
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.73	0.53
1:A:3371:PRO:O	1:A:3372:ALA:C	2.52	0.53
1:A:3700:LEU:HD13	1:A:3701:ASP:H	1.73	0.53
1:A:3924:LEU:C	1:A:3925:ASN:HD22	2.15	0.53
1:A:4036:HIS:HD2	1:A:4044:TRP:HE1	1.56	0.53
1:B:1541:LEU:HD23	1:B:1656:ILE:HG21	1.91	0.53
1:B:1558:TRP:CZ3	1:B:1606:ILE:HB	2.44	0.53
1:B:1932:ALA:HB1	1:B:1934:PHE:CE2	2.44	0.53
1:B:2621:ASP:C	1:B:2623:ASN:H	2.16	0.53
1:B:4278:HIS:CD2	1:B:4303:LEU:HB2	2.44	0.53
1:B:4597:PRO:HG2	1:B:4692:LEU:HD13	1.90	0.53
1:A:2701:PHE:CG	1:A:2705:THR:HG21	2.43	0.53
1:A:3821:GLY:O	1:A:3825:VAL:HG23	2.08	0.53
1:A:4207:LEU:O	1:A:4209:PRO:HD3	2.08	0.53
1:B:2280:GLY:O	1:B:2420:ILE:HD11	2.08	0.53
1:B:2497:GLU:O	1:B:2501:ILE:HG13	2.08	0.53
1:B:4360:LEU:C	1:B:4362:GLN:H	2.17	0.53
1:A:1538:TRP:CH2	1:A:1565:LEU:HG	2.44	0.53
1:A:2142:GLN:HE21	1:A:2208:VAL:HG11	1.75	0.53
1:A:2359:VAL:CG2	1:A:2397:VAL:HG11	2.38	0.53
1:A:3802:LEU:CD2	1:A:3882:VAL:HG12	2.39	0.53
1:A:3809:THR:HG22	1:A:3812:LYS:HZ1	1.74	0.53
1:A:4122:VAL:O	1:A:4122:VAL:HG22	2.08	0.53
1:A:4188:LYS:HA	1:A:4218:THR:HB	1.90	0.53
1:B:1538:TRP:HZ3	1:B:1656:ILE:HD13	1.73	0.53
1:B:3895:ARG:HH12	1:B:3977:LYS:HG2	1.73	0.53
1:B:4070:SER:O	1:B:4071:ASN:C	2.52	0.53
1:A:2598:GLN:HG2	1:A:2612:LEU:HD22	1.90	0.52
1:A:3956:THR:OG1	1:A:3964:LYS:HE3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2017:CYS:HB3	1:A:2067:LEU:HD12	1.90	0.52
1:A:3555:ASN:O	1:A:3559:ARG:HD3	2.09	0.52
1:A:3776:ASP:O	1:A:3780:ARG:HG2	2.09	0.52
1:A:3927:ASN:HB3	1:A:3930:LEU:CB	2.39	0.52
1:B:1525:ILE:HG13	1:B:1529:GLU:HG2	1.91	0.52
1:B:1612:TRP:CZ2	1:B:1644:ILE:HD11	2.44	0.52
1:B:1863:VAL:HG21	1:B:2115:SER:O	2.09	0.52
1:B:2205:PRO:HA	1:B:2261:GLN:OE1	2.09	0.52
1:B:2661:HIS:O	1:B:2665:SER:HB3	2.09	0.52
1:B:2818:PHE:HD1	1:B:2876:PRO:HD3	1.74	0.52
1:A:2142:GLN:HE21	1:A:2208:VAL:CG1	2.22	0.52
1:A:2431:LEU:HD21	1:A:2506:PHE:CE2	2.44	0.52
1:A:2578:MET:CE	1:A:2613:LEU:HA	2.39	0.52
1:A:3233:TYR:O	1:A:3237:THR:HG23	2.10	0.52
1:A:3878:GLU:O	1:A:3882:VAL:HG23	2.10	0.52
1:A:4693:ASN:N	1:A:4693:ASN:ND2	2.57	0.52
1:B:1659:VAL:C	1:B:1661:ALA:H	2.18	0.52
1:B:3023:SER:HB2	2:B:9010:ADP:O1A	2.09	0.52
1:B:3059:LEU:HD23	1:B:3137:VAL:HG11	1.92	0.52
1:B:4118:MET:O	1:B:4122:VAL:HG22	2.08	0.52
1:A:2956:LEU:HD21	1:A:2971:TYR:CG	2.44	0.52
1:A:4335:ARG:HD3	1:A:4360:LEU:C	2.35	0.52
1:B:2838:LEU:O	1:B:2840:PRO:HD3	2.10	0.52
1:A:2560:MET:HE1	1:A:2564:ASN:HD22	1.75	0.52
1:A:4048:PHE:HD1	1:A:4048:PHE:H	1.58	0.52
1:B:1930:ALA:HB2	1:B:1958:LEU:HD11	1.91	0.52
1:B:2036:LEU:HD23	1:B:2040:SER:HB3	1.90	0.52
1:B:2532:ARG:HG2	1:B:2532:ARG:HH11	1.74	0.52
1:B:3082:SER:HA	1:B:3085:GLU:OE1	2.09	0.52
1:B:3681:ALA:HB2	1:B:3786:PHE:CG	2.45	0.52
1:A:1690:GLN:HE22	1:A:1766:ILE:CG2	2.17	0.52
1:A:2258:LYS:HE3	1:A:2415:TRP:O	2.10	0.52
1:A:2857:TYR:HA	1:A:2913:PHE:CE1	2.36	0.52
1:A:3225:ASP:O	1:A:3229:SER:HB3	2.08	0.52
1:A:3415:LYS:O	1:A:3417:LEU:HD12	2.09	0.52
1:A:3804:THR:C	1:A:3806:ARG:H	2.18	0.52
1:A:4103:CYS:SG	1:A:4108:GLU:HA	2.50	0.52
1:A:4371:PRO:O	1:A:4372:ASP:HB2	2.09	0.52
1:B:2144:HIS:HB3	1:B:2400:LEU:CD1	2.40	0.52
1:B:2754:TYR:O	1:B:2755:GLY:C	2.52	0.52
1:B:2907:HIS:HA	1:B:2910:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4323:ASN:N	1:B:4323:ASN:HD22	2.06	0.52
1:A:1628:LEU:C	1:A:1630:PRO:HD3	2.35	0.52
1:A:2142:GLN:HG2	1:A:2208:VAL:HG11	1.91	0.52
1:A:2531:LEU:HD12	1:A:2809:ARG:HD2	1.91	0.52
1:A:2708:GLU:O	1:A:2711:LEU:HB2	2.10	0.52
1:A:2793:ASN:HD22	1:A:2793:ASN:H	1.57	0.52
1:A:4413:ASN:HD21	1:A:4660:LEU:HG	1.74	0.52
1:B:1600:SER:O	1:B:1604:VAL:HG23	2.10	0.52
1:B:2282:LYS:HB2	1:B:2282:LYS:NZ	2.25	0.52
1:B:2578:MET:HE3	1:B:2579:TRP:HE1	1.74	0.52
1:B:2748:LEU:N	1:B:2749:PRO:CD	2.73	0.52
1:B:4156:GLN:O	1:B:4183:THR:HB	2.10	0.52
1:A:1629:LEU:HD11	1:A:1686:TYR:CD2	2.44	0.52
1:A:2105:ARG:HG2	1:A:2105:ARG:NH1	2.23	0.52
1:A:2528:PHE:HE1	1:A:2533:VAL:HG11	1.73	0.52
1:A:3373:ILE:HG12	1:A:3374:ILE:H	1.74	0.52
1:A:3653:PRO:HB2	1:A:3658:CYS:SG	2.50	0.52
1:A:4288:ILE:CG2	1:A:4289:PRO:HA	2.40	0.52
1:B:1565:LEU:HD23	1:B:1595:LEU:CD1	2.39	0.52
1:B:1873:LYS:HB3	1:B:1943:ILE:HG21	1.90	0.52
1:B:2231:ILE:HD11	1:B:2260:LEU:HG	1.91	0.52
1:B:2354:ILE:HG12	1:B:2394:MET:HE3	1.90	0.52
1:B:2506:PHE:CE1	1:B:2512:VAL:HG21	2.43	0.52
1:B:2531:LEU:HD13	1:B:2809:ARG:NH2	2.24	0.52
1:B:3233:TYR:O	1:B:3237:THR:HG23	2.09	0.52
1:B:4270:ILE:CG2	1:B:4310:ILE:HD13	2.34	0.52
1:A:2408:ILE:O	1:A:2410:ARG:N	2.43	0.52
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.09	0.52
1:A:3370:GLU:O	1:A:3371:PRO:C	2.51	0.52
1:A:3924:LEU:HD23	1:A:3943:LEU:HD21	1.91	0.52
1:A:3988:TRP:NE1	1:A:3992:LEU:HD11	2.25	0.52
1:B:2741:VAL:HB	1:B:2788:PHE:CD2	2.44	0.52
1:B:2836:MET:HE2	1:B:2836:MET:HA	1.91	0.52
1:B:2906:ALA:O	1:B:2909:ALA:HB3	2.10	0.52
1:B:4157:TYR:HB2	1:B:4184:TRP:HB2	1.92	0.52
1:A:1964:LEU:HD12	1:A:2074:PHE:HZ	1.75	0.52
1:A:2641:VAL:HG12	1:A:2831:PHE:HB3	1.92	0.52
1:A:3813:ARG:HG3	1:A:3814:SER:N	2.24	0.52
1:A:4033:LEU:HD13	1:A:4062:TRP:CE2	2.45	0.52
1:B:2282:LYS:HB2	1:B:2282:LYS:HZ2	1.75	0.52
1:B:4423:ALA:O	1:B:4427:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4673:ASP:C	1:B:4675:ASP:H	2.18	0.52
1:A:1715:ILE:HD11	1:A:1760:ILE:HG21	1.92	0.51
1:A:1927:ILE:C	1:A:1928:HIS:HD2	2.18	0.51
1:A:2561:SER:OG	1:A:2564:ASN:HB3	2.09	0.51
1:B:1957:TYR:O	1:B:1961:THR:HG23	2.10	0.51
1:B:2556:SER:C	1:B:2558:PHE:H	2.17	0.51
1:B:2820:SER:OG	1:B:2823:SER:HB2	2.09	0.51
1:B:2910:LEU:O	1:B:2914:GLN:HB3	2.10	0.51
1:B:3563:LEU:HD11	1:B:3845:ILE:CD1	2.40	0.51
1:B:3603:GLY:H	1:B:3664:MET:HE1	1.73	0.51
1:B:3843:GLY:O	1:B:3845:ILE:N	2.35	0.51
1:A:2582:GLY:HA2	1:A:2585:MET:HE3	1.92	0.51
1:A:2898:LEU:CD1	1:A:2941:VAL:HG22	2.40	0.51
1:A:4213:PHE:CZ	1:A:4215:LEU:HB2	2.45	0.51
1:A:4269:ARG:HG2	1:A:4369:PHE:CE1	2.45	0.51
1:A:4295:PHE:C	1:A:4295:PHE:HD2	2.18	0.51
1:B:1817:LEU:O	1:B:1821:ILE:HG13	2.10	0.51
1:B:2764:ARG:HD2	1:B:2806:ARG:O	2.10	0.51
1:B:3601:TYR:O	1:B:3602:ILE:C	2.53	0.51
1:B:4690:VAL:HG21	1:B:4701:PHE:CE1	2.45	0.51
1:A:2271:GLY:O	1:A:2411:CYS:HA	2.10	0.51
1:A:2535:ASN:ND2	1:A:2668:ARG:HH12	2.08	0.51
1:A:3567:LEU:HD23	1:A:3855:LEU:HD11	1.92	0.51
1:A:4136:SER:O	1:A:4220:GLU:HA	2.10	0.51
1:B:1937:GLY:HA3	1:B:1992:GLY:O	2.10	0.51
1:B:1975:PRO:HG2	1:B:1978:THR:HG21	1.91	0.51
1:B:2549:ILE:O	1:B:2553:GLN:HB2	2.09	0.51
1:B:3595:ALA:O	1:B:3598:PHE:HB3	2.11	0.51
1:B:3682:MET:SD	1:B:3696:LYS:HE2	2.49	0.51
1:B:3930:LEU:O	1:B:3931:VAL:C	2.53	0.51
1:B:4157:TYR:HB2	1:B:4184:TRP:C	2.35	0.51
1:B:4671:TRP:O	1:B:4672:LYS:HG2	2.11	0.51
1:B:4690:VAL:HG11	1:B:4701:PHE:CZ	2.44	0.51
1:A:1904:PHE:C	1:A:1906:TRP:H	2.17	0.51
1:A:1959:THR:HG21	1:A:2098:MET:HB2	1.92	0.51
1:A:2144:HIS:O	1:A:2413:MET:HG2	2.10	0.51
1:A:2732:PRO:CG	1:A:2739:LEU:HB2	2.40	0.51
1:A:2918:VAL:HG13	1:A:3172:TRP:NE1	2.26	0.51
1:A:3366:LEU:HD12	1:A:3366:LEU:O	2.10	0.51
1:A:3730:LEU:HD13	1:A:3734:LEU:HD21	1.91	0.51
1:A:3969:LEU:HD12	1:A:4426:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2311:ILE:HB	1:B:2315:GLN:HE21	1.76	0.51
1:B:4592:GLY:HA3	1:B:4725:SER:O	2.10	0.51
1:B:4636:SER:HA	1:B:4670:THR:HG22	1.91	0.51
1:A:1611:ARG:HG3	1:A:1611:ARG:NH1	2.23	0.51
1:A:2370:LEU:HD12	1:A:2377:LEU:CB	2.41	0.51
1:A:2586:GLY:HA2	1:A:2815:LEU:CD1	2.37	0.51
1:A:3114:GLU:HG2	1:A:3118:ARG:HH12	1.74	0.51
1:A:3353:LYS:O	1:A:3357:VAL:HG23	2.10	0.51
1:A:3452:ILE:CG2	1:A:3485:THR:HG21	2.39	0.51
1:A:3670:ARG:O	1:A:3782:THR:HG22	2.10	0.51
1:A:3768:ASP:HB3	1:A:3771:ALA:HB2	1.93	0.51
1:A:4025:GLN:HG3	1:B:2899:GLU:OE2	2.10	0.51
1:A:4067:ALA:C	1:A:4073:GLN:HE21	2.19	0.51
1:A:4240:ASN:OD1	1:A:4240:ASN:N	2.38	0.51
1:B:1920:ASN:ND2	1:B:1921:VAL:H	2.09	0.51
1:B:2238:LYS:HA	1:B:2241:GLN:HE21	1.74	0.51
1:A:1625:ILE:HG23	1:A:1626:ASN:OD1	2.11	0.51
1:A:2738:TRP:CE2	1:A:2785:LYS:HG2	2.46	0.51
1:A:3283:LEU:C	1:A:3283:LEU:HD23	2.36	0.51
1:A:3975:SER:C	1:A:3977:LYS:H	2.18	0.51
1:A:4200:LEU:HD22	1:A:4204:LEU:CD1	2.41	0.51
1:B:1662:ILE:HB	1:B:1665:ILE:CG2	2.40	0.51
1:B:1971:ASN:O	1:B:2097:SER:HA	2.11	0.51
1:B:3889:MET:CE	1:B:3943:LEU:HB3	2.41	0.51
1:B:4086:MET:HG3	1:B:4097:TYR:CD2	2.45	0.51
1:B:4222:HIS:CG	1:B:4223:PRO:HD2	2.45	0.51
1:B:4340:SER:HB2	1:B:4357:TYR:OH	2.10	0.51
1:B:2638:THR:O	1:B:2641:VAL:HG23	2.10	0.51
1:B:2937:HIS:C	1:B:2939:PRO:HD3	2.35	0.51
1:B:3306:LEU:HD13	1:B:3557:VAL:HG22	1.92	0.51
1:B:4596:ASN:C	1:B:4596:ASN:ND2	2.68	0.51
1:A:2732:PRO:HG3	1:A:2739:LEU:HB2	1.93	0.51
1:A:3289:LEU:HD13	1:A:3293:ARG:NH2	2.25	0.51
1:A:3721:GLN:NE2	1:A:4205:HIS:NE2	2.58	0.51
1:A:3733:VAL:C	1:A:3735:ASN:H	2.19	0.51
1:A:4384:PRO:HB3	1:A:4395:TRP:CD1	2.45	0.51
1:B:1556:ARG:HG2	1:B:1557:GLY:N	2.25	0.51
1:B:2127:LYS:C	1:B:2130:PRO:HD2	2.35	0.51
1:B:2219:LEU:HD13	1:B:2228:LEU:HD11	1.93	0.51
1:B:2643:SER:HB3	1:B:2646:VAL:HG23	1.93	0.51
1:B:2801:VAL:HG12	1:B:2802:GLN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2877:ARG:HB3	1:B:2881:ARG:NH1	2.26	0.51
1:B:2931:ASP:O	1:B:2935:LEU:HG	2.11	0.51
1:B:3063:GLY:HA2	1:B:3136:GLN:CB	2.41	0.51
1:B:3566:ASN:ND2	1:B:3859:LYS:NZ	2.59	0.51
1:B:4121:ILE:HA	1:B:4125:GLU:CG	2.32	0.51
1:B:4550:TRP:O	1:B:4552:TRP:N	2.40	0.51
1:A:1713:LYS:O	1:A:1715:ILE:N	2.44	0.51
1:A:2138:GLN:NE2	1:A:2218:LEU:HD21	2.26	0.51
1:A:2327:TRP:CZ3	1:A:2380:PRO:HD2	2.46	0.51
1:A:2540:LEU:HD23	1:A:2662:ALA:HB3	1.92	0.51
1:A:2619:ILE:HG13	1:A:2619:ILE:O	2.11	0.51
1:A:3933:LYS:HZ3	1:A:3933:LYS:HB3	1.76	0.51
1:A:4299:ASN:OD1	1:A:4301:ALA:HB3	2.11	0.51
1:A:4428:ASN:O	1:A:4432:LYS:HG2	2.10	0.51
1:B:1520:ALA:HA	1:B:1580:TYR:CE1	2.46	0.51
1:B:1639:ILE:HG21	1:B:1676:LEU:HG	1.93	0.51
1:B:2283:THR:HA	1:B:2286:TRP:HE1	1.76	0.51
1:B:2542:ASN:O	1:B:2546:VAL:HG23	2.10	0.51
1:B:2849:LEU:HD21	1:B:2886:LEU:HD13	1.93	0.51
1:B:2968:LEU:CD2	1:B:2999:LEU:HD11	2.41	0.51
1:B:3219:ILE:CB	1:B:3220:PRO:CD	2.89	0.51
1:A:2009:MET:HA	1:A:2009:MET:HE3	1.93	0.51
1:A:2204:ILE:HG13	1:A:2205:PRO:HD3	1.92	0.51
1:A:3425:LYS:HA	1:A:3428:GLU:CG	2.41	0.51
1:A:4222:HIS:ND1	1:A:4223:PRO:HD2	2.26	0.51
1:B:1823:TRP:O	1:B:1827:VAL:HG23	2.10	0.51
1:B:1892:LEU:HA	1:B:1895:CYS:SG	2.51	0.51
1:B:2199:ILE:O	1:B:2203:MET:HB2	2.11	0.51
1:B:3583:THR:O	1:B:3587:THR:HG23	2.11	0.51
1:B:3618:MET:HB3	1:B:3628:PHE:CZ	2.46	0.51
1:B:3790:PRO:HA	1:B:3898:PHE:CE2	2.46	0.51
1:A:2582:GLY:O	1:A:2585:MET:HB2	2.11	0.50
1:A:2839:LEU:HD22	1:A:2896:CYS:HB3	1.93	0.50
1:A:3116:ALA:HB1	1:A:3121:LEU:O	2.12	0.50
1:B:1527:LEU:HD22	1:B:1575:MET:HB2	1.92	0.50
1:B:1573:SER:HA	1:B:1576:LYS:HE2	1.93	0.50
1:B:1687:LEU:HD11	1:B:1706:LEU:HD21	1.93	0.50
1:B:3993:LYS:O	1:B:3994:GLY:C	2.54	0.50
1:B:4288:ILE:HG23	1:B:4289:PRO:HA	1.92	0.50
1:B:4644:LEU:HD13	1:B:4647:ALA:HB3	1.92	0.50
1:A:1776:GLU:HA	1:A:1779:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1963:ALA:HB1	1:A:2096:ARG:CG	2.41	0.50
1:A:2212:ILE:N	1:A:2213:PRO:CD	2.75	0.50
1:A:2856:PHE:CE1	1:A:2930:ILE:HG12	2.46	0.50
1:A:3923:LEU:HD11	1:A:3943:LEU:HA	1.94	0.50
1:B:1479:ARG:O	1:B:1483:ILE:HG13	2.11	0.50
1:B:1534:VAL:HG13	1:B:1568:HIS:CD2	2.42	0.50
1:B:2075:VAL:CG1	1:B:2077:MET:HE3	2.41	0.50
1:B:2729:VAL:HG12	1:B:2782:LYS:HB3	1.94	0.50
1:B:3038:TYR:CD2	1:B:3058:LEU:HD13	2.46	0.50
1:B:4267:ARG:NH2	1:B:4315:ASP:OD1	2.43	0.50
1:A:1719:GLN:HA	1:A:1722:PHE:CD2	2.46	0.50
1:A:3011:HIS:C	1:A:3168:CYS:HB3	2.36	0.50
1:A:4285:LEU:O	1:A:4288:ILE:HG13	2.10	0.50
1:A:4596:ASN:C	1:A:4596:ASN:ND2	2.69	0.50
1:B:1951:PRO:HG2	1:B:2104:ASP:OD2	2.10	0.50
1:B:4170:LEU:HD12	1:B:4171:ALA:N	2.26	0.50
1:B:4686:LEU:HD12	1:B:4687:SER:N	2.27	0.50
1:A:2049:ALA:O	1:A:2054:SER:HB3	2.12	0.50
1:A:2586:GLY:O	1:A:2590:ARG:HB2	2.10	0.50
1:A:3067:GLU:O	1:A:3069:ILE:HD12	2.12	0.50
1:A:4044:TRP:CE3	1:A:4048:PHE:HE1	2.29	0.50
1:A:4122:VAL:HA	1:A:4126:VAL:HG11	1.91	0.50
1:A:4326:PRO:HB3	1:A:4369:PHE:CD2	2.46	0.50
1:B:1907:LEU:HA	1:B:1911:ARG:NH1	2.26	0.50
1:B:1967:ARG:HG2	1:B:1967:ARG:HH11	1.75	0.50
1:B:2135:CYS:HB3	1:B:2139:LEU:HD12	1.92	0.50
1:B:2142:GLN:HB2	1:B:2145:TYR:CD1	2.46	0.50
1:A:2533:VAL:HB	1:A:2581:LEU:HA	1.94	0.50
1:A:2954:ASN:HD22	1:A:2954:ASN:N	2.02	0.50
1:A:3380:VAL:HG11	1:A:3435:ILE:CG2	2.41	0.50
1:A:3834:LEU:HA	1:A:3854:THR:HG21	1.93	0.50
1:A:4118:MET:HB3	1:A:4149:LEU:HD22	1.94	0.50
1:B:2865:THR:N	1:B:2868:ILE:HD12	2.26	0.50
1:A:2720:TYR:HE1	1:A:2781:ILE:HG21	1.76	0.50
1:A:3190:ARG:C	1:A:3192:LEU:H	2.20	0.50
1:A:3814:SER:C	1:A:3818:LYS:HD3	2.37	0.50
1:B:1862:SER:O	1:B:1867:LEU:HD21	2.12	0.50
1:B:1926:VAL:HG22	1:B:1935:TYR:HE2	1.75	0.50
1:B:2367:LEU:HD12	1:B:2367:LEU:N	2.26	0.50
1:B:4111:LEU:N	1:B:4111:LEU:HD12	2.26	0.50
1:A:1971:ASN:ND2	1:A:2087:LEU:HD11	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2090:ASN:C	1:A:2090:ASN:ND2	2.70	0.50
1:A:2197:ASN:O	1:A:2201:ASP:HB2	2.12	0.50
1:A:2627:TRP:O	1:A:2629:ASN:N	2.45	0.50
1:A:2913:PHE:N	1:A:2913:PHE:CD2	2.79	0.50
1:A:4388:THR:O	1:A:4391:HIS:HB2	2.12	0.50
1:B:1662:ILE:HB	1:B:1665:ILE:HG23	1.93	0.50
1:B:2723:THR:CG2	1:B:2727:GLU:HB2	2.42	0.50
1:B:4020:LEU:HD11	1:B:4033:LEU:HG	1.93	0.50
1:A:4668:THR:C	1:A:4669:LEU:HD12	2.37	0.50
1:B:2918:VAL:HG22	1:B:3172:TRP:CD2	2.47	0.50
1:B:3087:MET:HE2	1:B:3087:MET:HA	1.93	0.50
1:B:3105:PHE:O	1:B:3109:MET:HG3	2.12	0.50
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.94	0.50
1:A:1889:VAL:HA	1:A:1892:LEU:HD12	1.94	0.50
1:A:3410:LEU:HA	1:A:3414:GLY:O	2.12	0.50
1:A:3433:THR:HG22	1:A:3437:ASN:HD22	1.75	0.50
1:A:3583:THR:O	1:A:3587:THR:HG23	2.11	0.50
1:A:3977:LYS:O	1:A:3979:THR:HG23	2.12	0.50
1:A:4078:SER:HA	1:A:4081:ARG:HD2	1.94	0.50
1:A:4185:VAL:HG12	1:A:4186:LEU:N	2.19	0.50
1:B:2714:PHE:CE2	1:B:2766:MET:HE1	2.47	0.50
1:B:2989:VAL:HG13	1:B:3187:GLU:OE2	2.12	0.50
1:B:4644:LEU:O	1:B:4661:SER:HB2	2.11	0.50
1:A:1926:VAL:HG12	1:A:1928:HIS:NE2	2.26	0.49
1:A:3992:LEU:HD22	1:A:4430:LEU:CB	2.41	0.49
1:A:4278:HIS:CD2	1:A:4343:TYR:OH	2.64	0.49
1:B:1522:GLN:O	1:B:1525:ILE:HG22	2.11	0.49
1:B:1781:LEU:O	1:B:1814:LEU:HD21	2.12	0.49
1:B:2504:GLN:HA	1:B:2507:GLU:OE2	2.12	0.49
1:B:2976:LEU:HD11	1:B:2990:LEU:HD21	1.94	0.49
1:B:3061:ARG:HB3	1:B:3067:GLU:OE2	2.12	0.49
1:B:3181:LEU:CB	1:B:3232:VAL:HG13	2.42	0.49
1:B:4132:LEU:HD13	1:B:4216:PHE:CZ	2.47	0.49
1:B:4259:ARG:NH2	1:B:4307:LEU:HB3	2.27	0.49
1:B:4339:GLY:HA3	1:B:4360:LEU:HD11	1.93	0.49
1:A:2511:LEU:HD11	1:A:2574:LEU:HD21	1.94	0.49
1:A:3011:HIS:CE1	1:A:3143:VAL:HG23	2.47	0.49
1:A:3051:PHE:CZ	1:A:3087:MET:HE3	2.47	0.49
1:A:3059:LEU:HD21	1:A:3090:LEU:HD13	1.94	0.49
1:A:3337:LYS:CB	1:A:3525:LEU:HD13	2.24	0.49
1:A:3602:ILE:O	1:A:3603:GLY:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3919:ILE:HG21	1:A:3951:THR:HA	1.94	0.49
1:A:4055:GLU:HG3	1:A:4093:ARG:NH1	2.27	0.49
1:B:1494:ILE:HA	1:B:1497:LEU:HD12	1.93	0.49
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.94	0.49
1:B:3935:ASP:O	1:B:3939:ARG:HG3	2.12	0.49
1:B:4060:GLU:HA	1:B:4063:ILE:HD13	1.94	0.49
1:B:4402:ILE:H	1:B:4402:ILE:CD1	2.21	0.49
1:B:4642:MET:HG2	1:B:4725:SER:HA	1.94	0.49
1:A:1739:THR:O	1:A:1760:ILE:HG12	2.12	0.49
1:A:2018:GLN:HE21	1:A:2066:SER:HB3	1.77	0.49
1:A:2057:VAL:HG22	1:A:2058:GLU:H	1.78	0.49
1:A:2133:LYS:O	1:A:2133:LYS:HD3	2.12	0.49
1:A:2526:MET:O	1:A:2527:ASP:C	2.55	0.49
1:A:2869:GLN:HG2	1:A:2871:HIS:CE1	2.47	0.49
1:A:3192:LEU:O	1:A:3224:ARG:NH2	2.46	0.49
1:A:3723:VAL:HG23	1:A:3764:LEU:HD22	1.94	0.49
1:A:4365:THR:HB	1:A:4366:PRO:HD2	1.93	0.49
1:A:4574:GLN:HE22	1:A:4590:TRP:H	1.60	0.49
1:B:3135:SER:HA	1:B:3138:ARG:HG2	1.95	0.49
1:B:3700:LEU:CG	1:B:3701:ASP:H	2.23	0.49
1:A:1887:ASP:O	1:A:1891:GLN:HG3	2.12	0.49
1:A:1973:PHE:C	1:A:1973:PHE:CD1	2.89	0.49
1:A:2029:ASN:HD22	1:A:2030:ARG:N	2.11	0.49
1:A:2302:GLU:HG2	1:A:2304:HIS:CE1	2.46	0.49
1:A:2374:ASN:O	1:A:2375:LYS:HB2	2.11	0.49
1:A:3338:GLN:HA	1:A:3342:ARG:CB	2.42	0.49
1:A:3725:ASN:ND2	1:A:3725:ASN:N	2.58	0.49
1:A:4075:THR:HG23	1:A:4076:ILE:N	2.27	0.49
1:A:4122:VAL:HA	1:A:4126:VAL:CG1	2.42	0.49
1:A:4244:VAL:HG23	1:A:4403:SER:CB	2.42	0.49
1:B:2774:ARG:C	1:B:2776:SER:H	2.20	0.49
1:B:3192:LEU:HD11	1:B:3268:VAL:HG22	1.94	0.49
1:A:1934:PHE:CD2	1:A:1934:PHE:N	2.81	0.49
1:A:2370:LEU:HD23	1:A:2387:LEU:HD22	1.95	0.49
1:A:3116:ALA:HB1	1:A:3123:LEU:HD12	1.94	0.49
1:A:3411:MET:HE1	1:A:3481:ALA:HB1	1.95	0.49
1:A:3947:ILE:CG2	1:A:3948:PHE:N	2.76	0.49
1:A:4455:SER:C	1:A:4457:SER:H	2.20	0.49
1:B:2021:ALA:O	1:B:2071:MET:HA	2.13	0.49
1:B:3316:LYS:HD2	1:B:3546:ILE:HD12	1.94	0.49
1:A:1629:LEU:N	1:A:1630:PRO:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1699:PHE:N	1:A:1699:PHE:CD1	2.77	0.49
1:A:1907:LEU:HA	1:A:1911:ARG:HH11	1.77	0.49
1:A:2029:ASN:HD22	1:A:2029:ASN:N	2.10	0.49
1:A:3655:ASP:O	1:A:3659:ILE:HG13	2.13	0.49
1:A:3674:VAL:HG13	1:A:3786:PHE:HD2	1.78	0.49
1:B:2315:GLN:HB3	1:B:2775:THR:CG2	2.41	0.49
1:B:2832:ASN:HD22	1:B:2835:LEU:HD23	1.77	0.49
1:B:2839:LEU:HD22	1:B:2896:CYS:HB3	1.95	0.49
1:B:4012:LEU:N	1:B:4012:LEU:HD23	2.27	0.49
1:B:4313:TRP:HB3	1:B:4330:PRO:CG	2.42	0.49
1:A:2272:VAL:HA	1:A:2412:GLY:H	1.77	0.49
1:A:2848:ASN:HB3	1:A:2938:PHE:HE1	1.77	0.49
1:A:3039:THR:HG22	1:A:3040:ILE:N	2.24	0.49
1:B:2612:LEU:HD11	1:B:2624:TRP:CZ3	2.48	0.49
1:B:4167:GLY:HA2	1:B:4170:LEU:HD11	1.93	0.49
1:A:2948:ARG:HG2	1:A:2948:ARG:NH1	2.28	0.49
1:A:3262:ASP:CB	1:A:3670:ARG:HE	2.25	0.49
1:A:3997:ASN:HD21	1:A:4001:ILE:HD11	1.77	0.49
1:A:4068:GLN:N	1:A:4073:GLN:HE21	2.11	0.49
1:A:4072:GLN:OE1	1:A:4077:VAL:HG21	2.11	0.49
1:B:2000:CYS:CB	1:B:2031:LEU:HD13	2.42	0.49
1:B:2517:GLU:O	1:B:2521:GLN:HG2	2.13	0.49
1:B:2677:GLY:HA3	1:B:2875:SER:OG	2.12	0.49
1:B:3991:LEU:HG	1:B:3992:LEU:HD23	1.94	0.49
1:B:4109:ASP:HA	1:B:4112:ASN:HD21	1.72	0.49
1:A:2208:VAL:HG22	1:A:2211:ASP:HB2	1.95	0.49
1:A:2610:ILE:HD12	1:A:2615:TYR:OH	2.13	0.49
1:A:3069:ILE:O	1:A:3141:LEU:O	2.30	0.49
1:A:3981:ASN:HD22	1:A:4076:ILE:CB	2.20	0.49
1:A:4054:GLY:O	1:A:4055:GLU:O	2.30	0.49
1:A:4230:LEU:HB3	1:A:4235:VAL:HG21	1.94	0.49
1:A:4536:SER:HB2	1:A:4548:LYS:HZ1	1.77	0.49
1:A:4548:LYS:O	1:A:4550:TRP:N	2.46	0.49
1:A:4596:ASN:ND2	1:A:4599:ALA:H	2.11	0.49
1:B:2723:THR:OG1	1:B:2724:PRO:HD2	2.13	0.49
1:B:4618:ASN:ND2	1:B:4618:ASN:H	2.11	0.49
1:A:1565:LEU:HD11	1:A:1598:VAL:HG12	1.94	0.49
1:A:1603:ASP:O	1:A:1606:ILE:HG22	2.13	0.49
1:A:1639:ILE:HG21	1:A:1676:LEU:HG	1.94	0.49
1:A:1800:HIS:HB2	1:A:1858:ASN:ND2	2.28	0.49
1:A:3180:ALA:O	1:A:3184:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3370:GLU:O	1:A:3372:ALA:N	2.46	0.49
1:A:3410:LEU:HD23	1:A:3410:LEU:C	2.38	0.49
1:A:3689:TYR:CB	1:A:3694:ILE:HD11	2.21	0.49
1:A:4402:ILE:HD12	1:A:4402:ILE:N	2.26	0.49
1:B:1823:TRP:NE1	1:B:1885:GLN:HB3	2.27	0.49
1:B:1934:PHE:CD2	1:B:1934:PHE:N	2.81	0.49
1:B:1959:THR:HG21	1:B:2098:MET:SD	2.53	0.49
1:B:2241:GLN:HA	1:B:2244:ALA:HB3	1.93	0.49
1:B:2502:ILE:HD13	1:B:2541:MET:HE2	1.95	0.49
1:B:2655:ARG:O	1:B:2659:VAL:HG23	2.13	0.49
1:B:3929:ASN:HB3	1:B:3942:TYR:CD1	2.47	0.49
1:B:4693:ASN:HD22	1:B:4693:ASN:N	2.09	0.49
1:A:1820:GLN:HE22	1:A:1990:GLN:HE22	1.60	0.48
1:A:2572:ARG:O	1:A:2575:TYR:HB3	2.12	0.48
1:A:2991:PHE:O	1:A:2992:ASN:C	2.55	0.48
1:A:3017:VAL:HG22	1:A:3018:SER:N	2.27	0.48
1:A:3048:SER:HB2	1:A:3080:GLU:OE1	2.13	0.48
1:A:3457:LEU:HD11	1:A:3482:THR:HA	1.95	0.48
1:A:3598:PHE:O	1:A:3602:ILE:HB	2.11	0.48
1:B:1926:VAL:HG12	1:B:1928:HIS:NE2	2.28	0.48
1:B:2616:SER:HB3	1:B:2627:TRP:CD2	2.47	0.48
1:B:3164:LEU:C	1:B:3166:ASN:H	2.22	0.48
1:B:3540:ILE:O	1:B:3544:GLU:HG3	2.13	0.48
1:A:2376:LEU:HD12	1:A:2385:LEU:C	2.38	0.48
1:A:2720:TYR:CE1	1:A:2781:ILE:HG21	2.48	0.48
1:A:3238:ILE:HG12	1:A:3601:TYR:HD2	1.69	0.48
1:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.95	0.48
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	1.95	0.48
1:A:4083:ILE:HD11	1:A:4098:SER:HA	1.94	0.48
1:A:4589:VAL:CG1	1:A:4639:VAL:HA	2.43	0.48
1:B:1813:GLN:NE2	1:B:1940:TYR:HA	2.17	0.48
1:B:1934:PHE:HB3	1:B:1993:ARG:HH22	1.78	0.48
1:B:2125:ALA:C	1:B:2127:LYS:H	2.21	0.48
1:B:2229:GLN:O	1:B:2230:PRO:O	2.30	0.48
1:B:2276:GLY:O	1:B:2282:LYS:HE2	2.13	0.48
1:B:2968:LEU:HG	1:B:2995:LEU:HD22	1.95	0.48
1:B:3295:THR:O	1:B:3299:VAL:HG23	2.12	0.48
1:B:4192:LEU:C	1:B:4194:PRO:HD3	2.38	0.48
1:B:4201:GLU:HG2	1:B:4232:MET:HE3	1.95	0.48
1:B:4513:ILE:HD12	1:B:4568:PHE:CE2	2.47	0.48
1:A:2941:VAL:CG1	1:A:2942:ASN:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3007:GLN:NE2	1:A:3008:PRO:HD2	2.29	0.48
1:A:4133:LEU:HD21	1:A:4225:LEU:HD13	1.94	0.48
1:A:4604:THR:OG1	1:A:4671:TRP:HZ3	1.96	0.48
1:B:2604:PRO:O	1:B:2624:TRP:NE1	2.46	0.48
1:B:2720:TYR:CE1	1:B:2730:LEU:HD13	2.48	0.48
1:B:3965:LEU:HG	1:B:4426:MET:HE1	1.95	0.48
1:B:4306:ALA:HB1	1:B:4338:LEU:HD13	1.94	0.48
1:A:3145:PHE:CE2	1:A:3164:LEU:HD21	2.48	0.48
1:A:3920:PHE:O	1:A:3923:LEU:HB3	2.13	0.48
1:A:4133:LEU:HA	1:A:4217:MET:HB2	1.94	0.48
1:A:4335:ARG:HD3	1:A:4361:GLU:HA	1.96	0.48
1:B:1910:MET:HA	1:B:1929:MET:HG3	1.95	0.48
1:B:2080:GLY:HA3	1:B:2084:ARG:O	2.13	0.48
1:B:2782:LYS:HB2	1:B:2782:LYS:NZ	2.28	0.48
1:B:3673:LEU:HD13	1:B:3783:PHE:CE1	2.48	0.48
1:A:2273:MET:HG3	1:A:2413:MET:CE	2.44	0.48
1:A:2893:MET:HE3	1:A:2896:CYS:HB2	1.96	0.48
1:A:3042:VAL:HB	1:A:3079:LEU:HD11	1.96	0.48
1:A:3154:PHE:C	1:A:3156:ASN:H	2.21	0.48
1:A:3289:LEU:HD13	1:A:3293:ARG:HH22	1.77	0.48
1:A:3411:MET:HE1	1:A:3481:ALA:CB	2.43	0.48
1:A:3425:LYS:HA	1:A:3428:GLU:HG2	1.95	0.48
1:A:4047:PHE:HD2	1:A:4048:PHE:CD1	2.32	0.48
1:A:4190:ILE:HB	1:A:4197:LEU:HD21	1.94	0.48
1:A:4684:SER:O	1:A:4707:TYR:CE2	2.67	0.48
1:B:2025:PHE:HB2	1:B:2075:VAL:HG22	1.94	0.48
1:B:2641:VAL:CG2	1:B:2887:LEU:HD22	2.43	0.48
1:B:2774:ARG:HB2	1:B:2781:ILE:HD13	1.94	0.48
1:B:3677:PRO:HG3	1:B:3769:PRO:HB3	1.94	0.48
1:B:4024:ARG:HG3	1:B:4031:SER:O	2.14	0.48
1:A:2204:ILE:CG1	1:A:2205:PRO:HD3	2.44	0.48
1:A:2526:MET:HE1	1:A:2803:LEU:HD12	1.94	0.48
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.95	0.48
1:A:2952:TYR:CE1	1:A:2962:PRO:HG3	2.48	0.48
1:A:3238:ILE:N	1:A:3238:ILE:HD12	2.28	0.48
1:A:3408:VAL:HG11	1:A:3477:LEU:CG	2.43	0.48
1:A:3487:TYR:O	1:A:3489:GLU:N	2.47	0.48
1:A:3664:MET:O	1:A:3668:PHE:HB3	2.13	0.48
1:A:4029:SER:CB	1:A:4081:ARG:HH12	2.25	0.48
1:A:4384:PRO:HB3	1:A:4395:TRP:CG	2.48	0.48
1:B:2964:ASN:HD21	1:B:2967:ASP:CG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3196:ASN:ND2	1:B:3199:TYR:HB2	2.28	0.48
1:B:3911:PHE:CZ	1:B:3955:VAL:HG13	2.49	0.48
1:B:3990:PHE:CE2	1:B:4023:LEU:HD13	2.48	0.48
1:B:4410:LEU:CD2	1:B:4411:PRO:HD2	2.43	0.48
1:B:4653:GLN:OE1	1:B:4708:ASP:HA	2.14	0.48
1:A:1960:LEU:O	1:A:1964:LEU:N	2.39	0.48
1:A:1973:PHE:HE1	1:A:2099:ALA:CB	2.27	0.48
1:A:3323:LYS:HE3	1:A:3539:LEU:HG	1.95	0.48
1:A:3865:ILE:HA	1:A:3869:VAL:HG23	1.94	0.48
1:A:3891:LEU:HD21	1:A:3895:ARG:NH2	2.28	0.48
1:B:1525:ILE:HD12	1:B:1528:GLU:HB3	1.96	0.48
1:B:1694:PHE:CE1	1:B:1770:LEU:HB3	2.48	0.48
1:B:3011:HIS:ND1	1:B:3091:LEU:HD22	2.28	0.48
1:B:3677:PRO:HB3	1:B:3769:PRO:HD3	1.94	0.48
1:B:3887:ASN:N	1:B:3888:PRO:CD	2.77	0.48
1:B:4400:PRO:HG2	1:B:4407:TRP:CH2	2.49	0.48
1:B:4540:SER:HB2	1:B:4545:ILE:O	2.13	0.48
1:A:1974:GLY:CA	1:A:2079:PRO:HD3	2.44	0.48
1:A:2306:MET:HE2	1:A:2355:PHE:CE1	2.45	0.48
1:A:3863:THR:O	1:A:3863:THR:HG22	2.12	0.48
1:A:3987:GLU:HG3	1:A:4027:VAL:CG1	2.44	0.48
1:A:4184:TRP:N	1:A:4184:TRP:CD1	2.82	0.48
1:A:4406:ILE:HB	1:A:4412:GLU:OE2	2.14	0.48
1:A:4591:LEU:CD2	1:A:4601:ILE:HD11	2.42	0.48
1:B:2084:ARG:HG2	1:B:2084:ARG:HH11	1.79	0.48
1:B:2381:ASN:ND2	1:B:2381:ASN:C	2.71	0.48
1:B:3955:VAL:HG12	1:B:3959:LEU:HG	1.96	0.48
1:A:1701:GLY:HA2	1:A:2011:ARG:NH1	2.29	0.48
1:A:1800:HIS:CB	1:A:1858:ASN:HD22	2.26	0.48
1:A:3397:PRO:HG2	1:A:3419:TRP:CE2	2.48	0.48
1:A:3473:ALA:O	1:A:3476:PRO:HD2	2.13	0.48
1:A:3686:MET:HE1	1:A:3696:LYS:HB2	1.95	0.48
1:A:4132:LEU:HB2	1:A:4216:PHE:HD1	1.79	0.48
1:A:4655:THR:HG22	1:A:4708:ASP:HB2	1.96	0.48
1:B:1962:GLN:HB3	1:B:4341:THR:HG21	1.96	0.48
1:B:3273:GLU:OE1	1:B:3667:ARG:NH2	2.47	0.48
1:B:3585:MET:HA	1:B:3588:VAL:HG23	1.96	0.48
1:B:3635:PRO:C	1:B:3637:PHE:H	2.21	0.48
1:B:3638:LEU:HB2	1:B:3663:ILE:HD12	1.96	0.48
1:B:3731:ASN:HB2	1:B:3732:PRO:HD3	1.94	0.48
1:B:4407:TRP:CD1	1:B:4407:TRP:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:ARG:HA	1:A:1591:TRP:CZ2	2.49	0.48
1:A:2208:VAL:HA	1:A:2415:TRP:HD1	1.74	0.48
1:A:2299:ILE:CG2	1:A:2349:LYS:HA	2.44	0.48
1:A:2375:LYS:HG2	1:A:2387:LEU:HD23	1.95	0.48
1:A:2704:ALA:HB3	1:A:3085:GLU:CG	2.44	0.48
1:A:3145:PHE:CD1	1:A:3164:LEU:HD11	2.48	0.48
1:A:3695:THR:HG21	1:A:3707:ASN:OD1	2.14	0.48
1:A:4201:GLU:HG3	1:A:4228:ASN:HB2	1.94	0.48
1:A:4432:LYS:C	1:A:4434:GLN:N	2.72	0.48
1:B:2532:ARG:HG2	1:B:2532:ARG:NH1	2.29	0.48
1:B:3232:VAL:O	1:B:3236:GLN:HG3	2.14	0.48
1:B:3350:VAL:HG12	1:B:3354:GLU:OE2	2.13	0.48
1:B:3902:GLU:C	1:B:3904:SER:N	2.71	0.48
1:B:4083:ILE:CD1	1:B:4098:SER:HA	2.44	0.48
1:B:4288:ILE:CG2	1:B:4289:PRO:HA	2.44	0.48
1:A:3078:VAL:O	1:A:3078:VAL:HG13	2.13	0.47
1:A:3699:PHE:CZ	1:A:3726:ILE:HG13	2.49	0.47
1:A:3859:LYS:C	1:A:3859:LYS:HD3	2.39	0.47
1:A:4048:PHE:CD1	1:A:4048:PHE:N	2.82	0.47
1:A:4296:PHE:CZ	1:A:4347:ILE:HD13	2.49	0.47
1:B:2071:MET:HE3	1:B:2071:MET:HB2	1.81	0.47
1:B:2397:VAL:HG22	1:B:2398:GLN:N	2.29	0.47
1:B:2613:LEU:HD22	1:B:2655:ARG:NH1	2.29	0.47
1:B:2886:LEU:HD23	1:B:2904:LEU:CD2	2.44	0.47
1:B:3065:LYS:O	1:B:3066:GLU:C	2.57	0.47
1:B:3960:LEU:HD23	1:B:4237:SER:HB2	1.96	0.47
1:A:2128:ILE:HG23	1:A:2129:VAL:N	2.29	0.47
1:A:2207:LEU:CD1	1:A:2215:ILE:HG21	2.43	0.47
1:A:2497:GLU:O	1:A:2501:ILE:HG13	2.13	0.47
1:A:2645:ASP:O	1:A:2646:VAL:C	2.57	0.47
1:A:2813:ILE:HG22	1:A:2814:LEU:N	2.28	0.47
1:A:3074:ASP:H	1:A:3077:ASN:HD22	1.62	0.47
1:A:3408:VAL:HG23	1:A:3409:CYS:H	1.80	0.47
1:A:3903:LEU:HD23	1:A:4433:MET:SD	2.54	0.47
1:A:3930:LEU:HD11	1:A:3939:ARG:HG2	1.95	0.47
1:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.96	0.47
1:A:4268:SER:OG	1:A:4387:THR:HA	2.14	0.47
1:B:1568:HIS:O	1:B:1572:ILE:HG13	2.14	0.47
1:B:1910:MET:HB2	1:B:1929:MET:HG3	1.95	0.47
1:B:2212:ILE:N	1:B:2213:PRO:CD	2.77	0.47
1:B:2918:VAL:HG22	1:B:3172:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4568:PHE:O	1:B:4572:MET:HG2	2.14	0.47
1:A:1639:ILE:CD1	1:A:1675:LEU:HB3	2.44	0.47
1:A:1892:LEU:C	1:A:1894:LYS:H	2.22	0.47
1:A:1934:PHE:HE1	1:A:1964:LEU:HD22	1.78	0.47
1:A:2313:LYS:CE	1:A:2366:ASN:HD21	2.17	0.47
1:A:3781:VAL:HG12	1:A:3782:THR:N	2.29	0.47
1:A:3897:TYR:CE1	1:A:3913:LEU:HA	2.47	0.47
1:A:3997:ASN:O	1:A:3999:THR:N	2.47	0.47
1:A:3997:ASN:ND2	1:A:4001:ILE:HD11	2.27	0.47
1:A:4708:ASP:C	1:A:4710:SER:H	2.22	0.47
1:B:1628:LEU:HD13	1:B:1709:ILE:HG22	1.95	0.47
1:B:3013:LEU:HG	1:B:3013:LEU:O	2.13	0.47
1:A:2211:ASP:C	1:A:2213:PRO:HD2	2.38	0.47
1:A:2368:ASN:HB3	1:A:2410:ARG:NH1	2.29	0.47
1:A:2598:GLN:HG3	1:A:2612:LEU:HB2	1.96	0.47
1:A:2616:SER:OG	1:A:2617:VAL:N	2.47	0.47
1:A:2832:ASN:CG	1:A:2849:LEU:HD23	2.39	0.47
1:A:3219:ILE:CB	1:A:3220:PRO:CD	2.93	0.47
1:A:3338:GLN:HG3	1:A:3529:ILE:HD12	1.96	0.47
1:A:3480:TRP:HE1	1:A:3484:GLN:HE21	1.62	0.47
1:A:3862:THR:C	1:A:3864:GLU:H	2.22	0.47
1:B:1591:TRP:HA	1:B:1591:TRP:CE3	2.49	0.47
1:B:1811:PRO:HB2	1:B:1814:LEU:HD12	1.95	0.47
1:B:1971:ASN:HA	1:B:2075:VAL:O	2.14	0.47
1:B:2107:MET:HE3	1:B:2107:MET:HB2	1.85	0.47
1:B:2309:LYS:O	1:B:2758:ARG:HD2	2.14	0.47
1:B:2363:TRP:CH2	1:B:2395:PHE:HE1	2.32	0.47
1:B:2427:PHE:O	1:B:2431:LEU:HG	2.14	0.47
1:B:2595:LYS:HE3	1:B:2611:PRO:HG3	1.96	0.47
1:A:1592:ASP:O	1:A:1596:ASN:HB2	2.14	0.47
1:A:2010:SER:O	1:A:2060:LEU:HD11	2.14	0.47
1:A:2282:LYS:HB2	2:A:9002:ADP:O3B	2.15	0.47
1:A:3648:HIS:CE1	1:A:3654:SER:HA	2.49	0.47
1:A:3661:ASN:HA	1:A:3664:MET:HE2	1.96	0.47
1:A:3730:LEU:CD2	1:A:3733:VAL:HB	2.44	0.47
1:A:4200:LEU:HD22	1:A:4204:LEU:CG	2.45	0.47
1:A:4313:TRP:HB3	1:A:4330:PRO:CG	2.45	0.47
1:A:4572:MET:HA	1:A:4572:MET:HE2	1.96	0.47
1:B:1603:ASP:O	1:B:1606:ILE:HG22	2.15	0.47
1:B:1920:ASN:ND2	1:B:1921:VAL:N	2.62	0.47
1:B:3605:PHE:HB3	1:B:3609:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3962:ASP:C	1:B:3964:LYS:H	2.23	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:CG2	2.45	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:HG23	1.96	0.47
1:A:2204:ILE:HA	1:A:2207:LEU:CD1	2.42	0.47
1:A:2250:VAL:HG21	1:A:2425:MET:HA	1.97	0.47
1:A:2362:GLU:C	1:A:2364:VAL:H	2.22	0.47
1:A:3794:GLN:HG3	1:A:3891:LEU:HA	1.96	0.47
1:A:4257:ALA:C	1:A:4259:ARG:H	2.21	0.47
1:A:4326:PRO:HB3	1:A:4369:PHE:HD2	1.79	0.47
1:B:1766:ILE:HG23	1:B:1767:HIS:N	2.30	0.47
1:B:2532:ARG:CZ	1:B:2813:ILE:HD12	2.45	0.47
1:B:2667:HIS:HA	1:B:2787:GLN:OE1	2.14	0.47
1:B:4618:ASN:HD22	1:B:4618:ASN:H	1.60	0.47
1:A:2051:LYS:HD3	1:A:2051:LYS:C	2.39	0.47
1:A:2088:PRO:HB2	1:A:2090:ASN:HD21	1.80	0.47
1:A:2196:LEU:HA	1:A:2199:ILE:HG12	1.97	0.47
1:A:2273:MET:HB3	1:A:2395:PHE:CD1	2.50	0.47
1:A:2870:ALA:C	1:A:2872:TYR:H	2.21	0.47
1:A:2990:LEU:HD23	1:A:2994:VAL:HG11	1.97	0.47
1:A:3032:MET:O	1:A:3034:GLY:N	2.47	0.47
1:A:3036:SER:N	1:A:3068:LYS:O	2.48	0.47
1:A:3051:PHE:HZ	1:A:3087:MET:HE3	1.80	0.47
1:A:3074:ASP:H	1:A:3077:ASN:ND2	2.13	0.47
1:A:3156:ASN:C	1:A:3158:SER:H	2.21	0.47
1:A:4043:ASP:OD2	1:A:4043:ASP:N	2.45	0.47
1:A:4109:ASP:O	1:A:4112:ASN:HB2	2.15	0.47
1:A:4344:GLY:HA2	1:A:4347:ILE:HG13	1.95	0.47
1:A:4430:LEU:O	1:A:4434:GLN:HB2	2.15	0.47
1:A:4690:VAL:HG21	1:A:4701:PHE:CE1	2.50	0.47
1:B:1505:SER:O	1:B:1506:ASP:C	2.57	0.47
1:B:1547:ASN:HD21	1:B:1550:ARG:H	1.63	0.47
1:B:1611:ARG:O	1:B:1615:LEU:HD23	2.14	0.47
1:B:1782:ALA:HB2	1:B:1922:LEU:HD23	1.96	0.47
1:B:2125:ALA:O	1:B:2129:VAL:HG13	2.14	0.47
1:B:2231:ILE:HG12	1:B:2260:LEU:HD23	1.96	0.47
1:B:2335:THR:O	1:B:2339:ILE:HG13	2.14	0.47
1:B:2512:VAL:HA	1:B:2515:VAL:HG12	1.95	0.47
1:B:2540:LEU:HB3	1:B:2576:SER:OG	2.14	0.47
1:B:2578:MET:HE3	1:B:2579:TRP:CD1	2.50	0.47
1:B:2676:PRO:HG3	1:B:2873:ILE:HD12	1.96	0.47
1:B:2882:TRP:CZ2	1:B:2909:ALA:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3650:ASN:O	1:B:3651:SER:HB2	2.15	0.47
1:B:3698:SER:HB3	1:B:3700:LEU:CD1	2.44	0.47
1:B:4059:PRO:O	1:B:4063:ILE:HD12	2.15	0.47
1:B:4119:ALA:HA	1:B:4149:LEU:HD11	1.96	0.47
1:B:4359:PHE:O	1:B:4362:GLN:HB3	2.15	0.47
1:B:4429:ASP:O	1:B:4433:MET:HG3	2.15	0.47
1:A:2127:LYS:HB3	1:A:2222:VAL:HG13	1.97	0.47
1:A:2641:VAL:O	1:A:2646:VAL:HG11	2.15	0.47
1:A:2766:MET:CB	1:A:2783:LEU:HD11	2.42	0.47
1:A:3563:LEU:O	1:A:3567:LEU:HG	2.14	0.47
1:A:3988:TRP:O	1:A:3992:LEU:HG	2.14	0.47
1:A:4162:ILE:HG13	1:A:4187:LEU:HD23	1.97	0.47
1:A:4244:VAL:HG23	1:A:4403:SER:HB3	1.96	0.47
1:A:4269:ARG:HA	1:A:4392:PHE:CZ	2.50	0.47
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.49	0.47
1:B:3043:ASN:HD22	1:B:3043:ASN:N	2.10	0.47
1:B:3160:THR:C	1:B:3162:PRO:HD3	2.40	0.47
1:B:3849:ASP:HA	1:B:3852:ILE:HG22	1.97	0.47
1:A:1868:SER:O	1:A:1872:ARG:HB2	2.15	0.47
1:A:2370:LEU:CD2	1:A:2387:LEU:HD22	2.45	0.47
1:A:2573:LEU:HD23	1:A:2573:LEU:C	2.40	0.47
1:A:3776:ASP:HB3	1:A:3780:ARG:HH12	1.80	0.47
1:B:2252:LYS:HE2	1:B:2254:GLU:HG2	1.96	0.47
1:B:2587:LEU:HD12	1:B:2817:ASP:HB3	1.96	0.47
1:B:4005:ILE:HG21	1:B:4008:LEU:HD12	1.96	0.47
1:A:1792:PHE:C	1:A:1792:PHE:CD2	2.92	0.47
1:A:2316:LEU:HD23	1:A:2363:TRP:HB2	1.97	0.47
1:A:2424:GLN:HG3	1:A:2508:PRO:HG3	1.97	0.47
1:A:2905:TRP:CZ3	1:A:2934:ALA:HB2	2.50	0.47
1:A:4376:VAL:HB	1:A:4381:LEU:HB2	1.97	0.47
1:B:2309:LYS:HE2	1:B:2756:THR:HG21	1.96	0.47
1:B:2660:LEU:O	1:B:2664:LEU:HB2	2.15	0.47
1:B:2669:PRO:HG2	1:B:2810:HIS:O	2.14	0.47
1:B:2701:PHE:CE2	1:B:2759:VAL:HG11	2.50	0.47
1:B:2890:ILE:HA	1:B:2893:MET:HE3	1.97	0.47
1:B:3677:PRO:CG	1:B:3787:THR:HG22	2.45	0.47
1:B:4136:SER:O	1:B:4220:GLU:HA	2.15	0.47
1:B:4650:ASN:O	1:B:4653:GLN:HG3	2.15	0.47
1:A:2065:ILE:HG22	1:A:2066:SER:N	2.30	0.46
1:A:2222:VAL:C	1:A:2224:PRO:HD3	2.40	0.46
1:A:2651:VAL:CG1	1:A:2652:ASP:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3040:ILE:HG22	1:A:3040:ILE:O	2.14	0.46
1:A:3270:LEU:CB	1:A:3592:VAL:HG13	2.44	0.46
1:A:3285:LEU:HD22	1:A:3578:SER:HB2	1.97	0.46
1:A:3452:ILE:O	1:A:3457:LEU:HD23	2.15	0.46
1:A:3614:MET:HG3	1:A:3618:MET:HE2	1.97	0.46
1:A:3639:SER:HB2	1:A:3643:GLU:OE1	2.15	0.46
1:A:4099:HIS:ND1	1:A:4111:LEU:HD12	2.30	0.46
1:A:4537:LEU:HD23	1:A:4548:LYS:HE3	1.97	0.46
1:A:4599:ALA:O	1:A:4602:THR:HG22	2.15	0.46
1:B:1576:LYS:HG2	1:B:1585:GLU:OE2	2.14	0.46
1:B:1642:GLU:O	1:B:1646:ILE:HG12	2.16	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CZ	2.49	0.46
1:B:2270:HIS:HB3	1:B:2392:ARG:NH1	2.29	0.46
1:B:2556:SER:C	1:B:2558:PHE:N	2.73	0.46
1:B:2774:ARG:HG2	1:B:2776:SER:OG	2.15	0.46
1:B:3973:ILE:HG13	1:B:3988:TRP:CZ3	2.50	0.46
1:A:1886:ARG:CZ	1:A:1890:ARG:HH22	2.28	0.46
1:A:1969:GLY:N	1:A:2047:GLN:NE2	2.64	0.46
1:A:2101:ILE:HD13	1:A:2101:ILE:N	2.30	0.46
1:A:3889:MET:SD	1:A:3889:MET:C	2.99	0.46
1:B:1555:VAL:H	1:B:1609:GLN:NE2	2.12	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CE2	2.50	0.46
1:B:2532:ARG:HG3	1:B:2808:LEU:O	2.14	0.46
1:B:3027:ARG:HA	1:B:3037:ILE:CD1	2.43	0.46
1:B:4128:SER:HB2	1:B:4213:PHE:HB3	1.96	0.46
1:B:4604:THR:HG23	1:B:4671:TRP:NE1	2.21	0.46
1:A:1809:ASN:HD22	1:A:1809:ASN:HA	1.60	0.46
1:A:1904:PHE:C	1:A:1906:TRP:N	2.71	0.46
1:A:2415:TRP:CE3	1:A:2415:TRP:HA	2.51	0.46
1:A:2720:TYR:CE1	1:A:2730:LEU:HD13	2.50	0.46
1:A:2842:LEU:HD11	1:A:2897:THR:C	2.40	0.46
1:A:2956:LEU:HD21	1:A:2971:TYR:CD2	2.50	0.46
1:A:3021:GLY:O	1:A:3025:LEU:HB2	2.14	0.46
1:A:3900:MET:HE3	1:A:3955:VAL:HG22	1.97	0.46
1:A:4070:SER:C	1:A:4072:GLN:N	2.72	0.46
1:A:4220:GLU:O	1:A:4222:HIS:N	2.49	0.46
1:B:1601:LEU:HA	1:B:1666:GLN:OE1	2.16	0.46
1:B:2684:LEU:HD13	1:B:2684:LEU:C	2.40	0.46
1:B:4030:PHE:HE1	1:B:4085:LEU:HG	1.80	0.46
1:B:4190:ILE:HG12	1:B:4219:SER:CB	2.44	0.46
1:A:1630:PRO:O	1:A:1634:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2492:LEU:HG	1:A:2496:LYS:NZ	2.31	0.46
1:A:2882:TRP:CZ2	1:A:2905:TRP:NE1	2.83	0.46
1:A:2903:ARG:HB2	1:A:2945:ALA:O	2.15	0.46
1:A:3219:ILE:CB	1:A:3220:PRO:HD3	2.46	0.46
1:A:3808:ASP:CG	1:A:3809:THR:N	2.73	0.46
1:A:4087:LYS:O	1:A:4087:LYS:HG2	2.15	0.46
1:A:4589:VAL:HG22	1:A:4590:TRP:N	2.29	0.46
1:B:2191:GLU:HA	1:B:2194:VAL:HG23	1.98	0.46
1:B:2223:PHE:C	1:B:2225:GLY:H	2.23	0.46
1:B:2529:THR:OG1	1:B:2532:ARG:HB2	2.15	0.46
1:B:3288:GLY:HA3	1:B:3574:TRP:CZ3	2.49	0.46
1:B:3773:PHE:HB3	1:B:3777:LEU:HD23	1.98	0.46
1:A:1948:VAL:O	1:A:1950:THR:N	2.49	0.46
1:A:1973:PHE:C	1:A:1973:PHE:HD1	2.23	0.46
1:A:2257:GLU:O	1:A:2261:GLN:HG2	2.16	0.46
1:A:2856:PHE:CZ	1:A:2930:ILE:HG12	2.49	0.46
1:A:3324:LEU:HD12	1:A:3539:LEU:CD2	2.46	0.46
1:A:3994:GLY:O	1:A:3995:GLY:C	2.58	0.46
1:A:3998:LEU:O	1:A:3998:LEU:HD13	2.15	0.46
1:B:1555:VAL:H	1:B:1609:GLN:HE22	1.64	0.46
1:B:1846:GLN:O	1:B:1849:GLU:HB3	2.16	0.46
1:B:2907:HIS:HB2	1:B:2950:ILE:HG21	1.96	0.46
1:A:1786:SER:HB2	1:A:1914:TYR:OH	2.16	0.46
1:A:1979:GLY:O	1:A:1980:LYS:C	2.58	0.46
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	1.98	0.46
1:A:2376:LEU:HA	1:A:2385:LEU:O	2.15	0.46
1:A:2435:SER:HB3	1:A:2496:LYS:HG2	1.97	0.46
1:A:2832:ASN:ND2	1:A:2883:ASP:OD2	2.49	0.46
1:A:3007:GLN:O	1:A:3142:HIS:HE1	1.99	0.46
1:A:3113:LYS:HG3	1:A:3123:LEU:O	2.15	0.46
1:A:3387:HIS:HB2	1:A:3473:ALA:HB2	1.95	0.46
1:A:3725:ASN:HD22	1:A:3725:ASN:N	1.99	0.46
1:A:4044:TRP:HE3	1:A:4048:PHE:HE1	1.62	0.46
1:A:4044:TRP:CE2	1:A:4059:PRO:HG3	2.51	0.46
1:B:1799:ASP:OD1	1:B:1801:SER:HB3	2.15	0.46
1:B:2748:LEU:HD11	1:B:3162:PRO:HG2	1.97	0.46
1:B:3602:ILE:O	1:B:3603:GLY:C	2.59	0.46
1:B:3891:LEU:HD21	1:B:3895:ARG:NH2	2.31	0.46
1:B:4296:PHE:HB3	1:B:4346:ARG:HD2	1.98	0.46
1:A:2243:ILE:HG21	1:A:2288:VAL:HG13	1.96	0.46
1:A:3830:LEU:HD12	1:A:3858:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3990:PHE:HD2	1:A:4084:LEU:HD22	1.81	0.46
1:A:4318:SER:HA	1:A:4321:ARG:NH2	2.23	0.46
1:B:1962:GLN:CB	1:B:4341:THR:HG21	2.46	0.46
1:B:2532:ARG:NH1	1:B:2813:ILE:HD12	2.31	0.46
1:B:2749:PRO:O	1:B:2757:GLN:HG2	2.16	0.46
1:B:2841:ASN:ND2	1:B:2842:LEU:HG	2.31	0.46
1:B:3788:VAL:HG11	1:B:3913:LEU:CD2	2.46	0.46
1:B:4006:PRO:C	1:B:4008:LEU:H	2.24	0.46
1:B:4020:LEU:HG	1:B:4034:VAL:HG22	1.98	0.46
1:B:4068:GLN:C	1:B:4070:SER:H	2.24	0.46
1:B:4222:HIS:ND1	1:B:4223:PRO:HD2	2.31	0.46
1:B:4281:ILE:HG13	1:B:4282:GLN:N	2.31	0.46
1:B:4645:GLU:HG3	1:B:4722:SER:OG	2.15	0.46
1:A:2052:GLU:C	1:A:2053:ASN:CG	2.83	0.46
1:A:2059:LEU:HG	1:A:2060:LEU:HG	1.97	0.46
1:A:2205:PRO:HG3	1:A:2261:GLN:OE1	2.16	0.46
1:A:2360:ASP:HB2	1:A:2361:PRO:HD2	1.96	0.46
1:A:2443:GLU:OE2	1:A:2489:PRO:HB2	2.15	0.46
1:A:2603:THR:HG22	1:A:2604:PRO:HD2	1.97	0.46
1:A:2829:GLY:HA2	1:A:2850:THR:OG1	2.16	0.46
1:A:3443:MET:HE1	1:A:3485:THR:HG22	1.98	0.46
1:A:3819:ILE:C	1:A:3821:GLY:H	2.23	0.46
1:A:4022:CYS:O	1:A:4026:GLN:HB2	2.16	0.46
1:A:4681:ASN:ND2	1:A:4685:LYS:HE3	2.30	0.46
1:A:4719:ARG:HH11	1:A:4719:ARG:HG3	1.81	0.46
1:B:2670:LEU:C	1:B:2670:LEU:HD12	2.41	0.46
1:B:3705:MET:HE1	1:B:3708:LEU:HD23	1.98	0.46
1:B:4597:PRO:HG2	1:B:4692:LEU:CD1	2.46	0.46
1:A:1530:PHE:CZ	1:A:1571:SER:HB2	2.51	0.46
1:A:1745:SER:OG	1:A:1751:THR:HG22	2.16	0.46
1:A:4395:TRP:CZ3	1:A:4399:LEU:HD11	2.51	0.46
1:B:1683:LEU:HD12	1:B:1683:LEU:O	2.16	0.46
1:B:2363:TRP:C	1:B:2365:GLU:H	2.24	0.46
1:B:3715:GLY:HA3	1:B:3758:PRO:HG2	1.98	0.46
1:B:4284:ARG:NH2	1:B:4355:LEU:HD21	2.31	0.46
1:B:4331:TRP:CZ2	1:B:4369:PHE:HE2	2.34	0.46
1:A:1662:ILE:HG22	1:A:1663:GLU:N	2.32	0.46
1:A:1911:ARG:H	1:A:1911:ARG:HD3	1.81	0.46
1:A:2000:CYS:O	1:A:2001:ASP:C	2.58	0.46
1:A:2641:VAL:O	1:A:2643:SER:N	2.49	0.46
1:A:2864:PHE:HB3	1:A:2872:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2952:TYR:CZ	1:A:2962:PRO:HG3	2.51	0.46
1:A:3017:VAL:HG21	1:A:3257:PRO:HD3	1.98	0.46
1:A:4263:GLN:NE2	1:A:4322:SER:HA	2.30	0.46
1:A:4278:HIS:HD2	1:A:4343:TYR:OH	1.99	0.46
1:A:4402:ILE:H	1:A:4402:ILE:CD1	2.28	0.46
1:B:2044:GLN:O	1:B:2048:VAL:HG23	2.16	0.46
1:B:3789:THR:H	1:B:3792:SER:HB3	1.81	0.46
1:B:4095:LEU:HD11	1:B:4422:LYS:HB3	1.97	0.46
1:B:4274:LEU:HD11	1:B:4306:ALA:HB1	1.98	0.46
1:B:4400:PRO:HG2	1:B:4407:TRP:HH2	1.81	0.46
1:A:1642:GLU:O	1:A:1646:ILE:HG13	2.16	0.45
1:A:2249:LEU:HB3	2:A:9002:ADP:N6	2.30	0.45
1:A:2338:ARG:HH11	1:A:2338:ARG:HG2	1.81	0.45
1:A:2851:ASP:HB3	1:A:2937:HIS:CE1	2.51	0.45
1:A:2980:TYR:OH	1:A:2987:PRO:HA	2.15	0.45
1:A:4726:TRP:CH2	1:A:4728:SER:HB2	2.51	0.45
1:B:1534:VAL:HG22	1:B:1568:HIS:CD2	2.50	0.45
1:B:1604:VAL:O	1:B:1608:VAL:HG23	2.16	0.45
1:B:1985:LYS:HD3	1:B:1997:VAL:HG21	1.98	0.45
1:B:2275:VAL:HG11	1:B:2400:LEU:HG	1.97	0.45
1:B:2492:LEU:O	1:B:2493:LYS:C	2.59	0.45
1:B:2873:ILE:O	1:B:2873:ILE:HG13	2.14	0.45
1:B:3912:SER:HB3	1:B:4231:ARG:CG	2.45	0.45
1:B:4122:VAL:HG11	1:B:4216:PHE:HZ	1.81	0.45
1:B:4434:GLN:HE21	1:B:4434:GLN:HB3	1.55	0.45
1:B:4574:GLN:NE2	1:B:4590:TRP:HB3	2.31	0.45
1:A:3015:ILE:CG2	1:A:3149:PRO:HG3	2.45	0.45
1:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.16	0.45
1:A:3271:ILE:HG12	1:A:3592:VAL:HG21	1.97	0.45
1:A:3551:SER:O	1:A:3554:LYS:HB2	2.16	0.45
1:A:4039:GLN:HB3	1:A:4040:ASN:H	1.57	0.45
1:A:4309:SER:O	1:A:4312:TYR:HB3	2.16	0.45
1:B:1931:ASN:HD21	1:B:1962:GLN:HE22	1.64	0.45
1:B:2309:LYS:HZ3	1:B:2756:THR:HG21	1.77	0.45
1:B:2331:LEU:HD21	1:B:2773:TRP:CG	2.51	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:O	2.16	0.45
1:B:4379:ILE:HG23	1:B:4381:LEU:HG	1.98	0.45
1:A:3481:ALA:O	1:A:3485:THR:HG23	2.16	0.45
1:A:3698:SER:C	1:A:3700:LEU:HD12	2.41	0.45
1:A:3798:LEU:O	1:A:3802:LEU:HG	2.17	0.45
1:A:4026:GLN:HB3	1:A:4027:VAL:H	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4281:ILE:HG13	1:A:4282:GLN:N	2.31	0.45
1:A:4337:ILE:O	1:A:4341:THR:HG22	2.16	0.45
1:A:4653:GLN:O	1:A:4655:THR:HG23	2.17	0.45
1:B:2745:GLU:HG2	1:B:2748:LEU:HD11	1.98	0.45
1:B:3017:VAL:HG13	1:B:3174:GLY:C	2.41	0.45
1:B:4431:GLN:O	1:B:4431:GLN:HG2	2.16	0.45
1:A:2274:MET:HE1	1:A:2286:TRP:CG	2.52	0.45
1:A:2323:THR:O	1:A:2324:THR:HG23	2.16	0.45
1:A:2398:GLN:NE2	1:A:2806:ARG:HG2	2.31	0.45
1:A:2738:TRP:CZ3	1:A:2785:LYS:HA	2.51	0.45
1:A:2845:PHE:O	1:A:2848:ASN:HB2	2.16	0.45
1:A:2896:CYS:SG	1:A:2897:THR:N	2.90	0.45
1:A:2935:LEU:HD23	1:A:2935:LEU:C	2.41	0.45
1:A:2976:LEU:HD12	1:A:3028:PHE:CE1	2.51	0.45
1:A:3792:SER:OG	1:A:3793:LEU:N	2.50	0.45
1:A:3893:CYS:HB3	1:A:3916:PHE:HZ	1.81	0.45
1:A:3997:ASN:O	1:A:3998:LEU:C	2.60	0.45
1:B:2381:ASN:C	1:B:2381:ASN:HD22	2.25	0.45
1:B:2849:LEU:HD13	1:B:2901:LEU:HD11	1.99	0.45
1:B:3015:ILE:HD12	1:B:3170:LEU:HD11	1.98	0.45
1:B:3306:LEU:HD13	1:B:3557:VAL:CG2	2.46	0.45
1:B:3536:TYR:O	1:B:3540:ILE:HD13	2.16	0.45
1:B:3990:PHE:HD2	1:B:4084:LEU:HD22	1.82	0.45
1:B:4335:ARG:NH2	1:B:4365:THR:HG22	2.22	0.45
1:A:3075:GLU:C	1:A:3077:ASN:H	2.23	0.45
1:A:3459:ASP:HB3	1:A:3462:PHE:CB	2.47	0.45
1:A:3549:GLU:O	1:A:3553:VAL:HG23	2.17	0.45
1:A:3686:MET:CE	1:A:3696:LYS:HB2	2.46	0.45
1:A:3727:ASP:C	1:A:3729:VAL:H	2.25	0.45
1:A:4279:ALA:O	1:A:4283:GLU:HB2	2.17	0.45
1:A:4349:ASN:O	1:A:4352:ASP:HB2	2.16	0.45
1:A:4648:VAL:HG23	1:A:4655:THR:OG1	2.16	0.45
1:B:2630:LYS:CB	1:B:2654:THR:HG21	2.47	0.45
1:B:3218:ALA:O	1:B:3219:ILE:C	2.60	0.45
1:B:3930:LEU:HD22	1:B:3939:ARG:HE	1.81	0.45
1:B:4012:LEU:HA	1:B:4016:GLN:NE2	2.31	0.45
1:A:1726:PHE:HB2	1:A:1729:LEU:HB3	1.98	0.45
1:A:1784:LEU:HB3	1:A:1814:LEU:HD13	1.99	0.45
1:A:1842:GLN:OE1	1:A:1893:GLN:HG2	2.17	0.45
1:A:1964:LEU:HD12	1:A:2074:PHE:CZ	2.51	0.45
1:A:1968:MET:HB3	1:A:2094:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2603:THR:CB	1:A:2604:PRO:HD2	2.46	0.45
1:A:3350:VAL:HG12	1:A:3350:VAL:O	2.15	0.45
1:A:3897:TYR:HD2	1:A:3898:PHE:CD2	2.34	0.45
1:A:3919:ILE:HD13	1:A:3951:THR:HA	1.98	0.45
1:B:2209:ALA:C	1:B:2211:ASP:H	2.25	0.45
1:B:2819:PRO:HB2	1:B:2824:LEU:CD2	2.46	0.45
1:B:3673:LEU:HD22	1:B:3783:PHE:CE1	2.48	0.45
1:B:4404:THR:HB	1:B:4405:PRO:HD2	1.99	0.45
1:B:4693:ASN:ND2	1:B:4693:ASN:N	2.64	0.45
1:B:4714:GLN:O	1:B:4718:GLN:HG3	2.16	0.45
1:A:1907:LEU:HD22	1:A:1911:ARG:NH1	2.31	0.45
1:A:2124:LEU:HD22	1:A:2195:LEU:CD2	2.46	0.45
1:A:2435:SER:CB	1:A:2496:LYS:HG2	2.47	0.45
1:A:2529:THR:O	1:A:2530:ARG:C	2.60	0.45
1:A:3022:LYS:HA	1:A:3173:PHE:CE1	2.52	0.45
1:A:3234:ILE:O	1:A:3238:ILE:HD13	2.17	0.45
1:A:3388:LEU:CD2	1:A:3473:ALA:HB1	2.44	0.45
1:A:3463:ASP:O	1:A:3467:VAL:HG23	2.17	0.45
1:A:4249:LEU:O	1:A:4253:ILE:HG13	2.17	0.45
1:B:2825:THR:HG23	1:B:2854:VAL:HG21	1.98	0.45
1:B:3004:VAL:O	1:B:3010:GLY:HA3	2.17	0.45
1:B:3542:GLU:O	1:B:3546:ILE:HG12	2.16	0.45
1:B:3696:LYS:HG3	1:B:3719:LEU:HD23	1.99	0.45
1:B:4666:ILE:HG13	1:B:4667:ALA:N	2.32	0.45
1:A:1800:HIS:CD2	1:A:1858:ASN:HB3	2.52	0.45
1:A:1922:LEU:HD13	1:A:1938:PHE:CD1	2.48	0.45
1:A:2902:VAL:HG21	1:A:2941:VAL:CG2	2.47	0.45
1:A:3670:ARG:C	1:A:3782:THR:HG22	2.42	0.45
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.52	0.45
1:A:4329:ILE:HB	1:A:4331:TRP:CE2	2.51	0.45
1:A:4384:PRO:HG2	1:A:4392:PHE:CD1	2.51	0.45
1:B:1618:ILE:HD13	1:B:1683:LEU:HD21	1.99	0.45
1:B:1740:THR:HG22	1:B:1759:SER:HA	1.98	0.45
1:B:2091:LEU:HD22	1:B:2095:PHE:CE2	2.51	0.45
1:B:3990:PHE:CZ	1:B:4023:LEU:HD13	2.52	0.45
1:B:4197:LEU:HB3	1:B:4226:PRO:HG2	1.98	0.45
1:B:4618:ASN:N	1:B:4618:ASN:ND2	2.65	0.45
1:A:1925:LEU:HD23	1:A:1936:TYR:HB2	1.98	0.45
1:A:2052:GLU:O	1:A:2053:ASN:CB	2.64	0.45
1:A:2140:SER:HB2	1:A:2211:ASP:OD2	2.15	0.45
1:A:2196:LEU:HA	1:A:2199:ILE:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2269:ASN:C	1:A:2271:GLY:H	2.24	0.45
1:A:2937:HIS:C	1:A:2939:PRO:HD3	2.42	0.45
1:A:3145:PHE:CG	1:A:3164:LEU:HD11	2.52	0.45
1:A:3218:ALA:O	1:A:3220:PRO:N	2.49	0.45
1:A:3639:SER:OG	1:A:3663:ILE:HD11	2.17	0.45
1:A:4032:LYS:HE2	1:A:4032:LYS:HA	1.97	0.45
1:A:4046:GLN:NE2	1:A:4057:ILE:HG22	2.32	0.45
1:A:4311:ASP:O	1:A:4315:ASP:HB3	2.17	0.45
1:A:4347:ILE:CG2	1:A:4353:MET:HG2	2.43	0.45
1:B:2204:ILE:N	1:B:2205:PRO:CD	2.80	0.45
1:B:2211:ASP:C	1:B:2213:PRO:HD2	2.42	0.45
1:B:2270:HIS:HB3	1:B:2392:ARG:HH11	1.82	0.45
1:B:3254:TYR:CD2	1:B:3775:PRO:HA	2.52	0.45
1:B:3992:LEU:HD12	1:B:4434:GLN:NE2	2.31	0.45
1:B:4095:LEU:HD11	1:B:4422:LYS:HB2	1.99	0.45
1:B:4621:LEU:HG	1:B:4622:HIS:H	1.82	0.45
1:B:4657:THR:HG22	1:B:4658:ASP:N	2.32	0.45
1:A:3027:ARG:HH11	1:A:3027:ARG:HB2	1.81	0.45
1:A:3540:ILE:HD12	1:A:3540:ILE:N	2.32	0.45
1:A:3542:GLU:O	1:A:3546:ILE:HG13	2.17	0.45
1:A:3813:ARG:HA	1:A:3875:VAL:HG11	1.99	0.45
1:A:3903:LEU:HD13	1:A:3959:LEU:HD21	1.99	0.45
1:A:3908:LEU:HD21	1:A:4237:SER:OG	2.16	0.45
1:A:3912:SER:HB3	1:A:4231:ARG:CG	2.45	0.45
1:A:4116:LEU:HB3	1:A:4117:ASP:H	1.52	0.45
1:B:1548:TYR:HD2	1:B:1554:LEU:HD11	1.82	0.45
1:B:1764:PRO:HB2	1:B:1768:GLU:CB	2.47	0.45
1:B:2641:VAL:HG13	1:B:2831:PHE:HB3	1.98	0.45
1:B:2998:ILE:CG2	1:B:3025:LEU:HD22	2.47	0.45
1:B:3078:VAL:O	1:B:3078:VAL:HG13	2.16	0.45
1:B:4197:LEU:HD13	1:B:4226:PRO:HD3	1.99	0.45
1:B:4220:GLU:O	1:B:4222:HIS:N	2.50	0.45
1:B:4253:ILE:O	1:B:4253:ILE:HG22	2.17	0.45
1:B:4343:TYR:C	1:B:4345:GLY:H	2.25	0.45
1:A:1958:LEU:O	1:A:1962:GLN:HB2	2.16	0.44
1:A:2730:LEU:HD22	1:A:2772:PHE:CZ	2.52	0.44
1:A:3682:MET:CE	1:A:3721:GLN:HE21	2.31	0.44
1:A:3776:ASP:HB3	1:A:3780:ARG:NH1	2.31	0.44
1:A:3825:VAL:HA	1:A:3828:ARG:HD3	1.99	0.44
1:A:4076:ILE:HD12	1:A:4105:VAL:HG22	1.99	0.44
1:A:4117:ASP:C	1:A:4119:ALA:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1629:LEU:HD22	1:B:1632:GLU:HG2	1.98	0.44
1:B:1748:GLU:CD	1:B:1944:GLY:H	2.25	0.44
1:B:1869:ALA:HA	1:B:1872:ARG:HB3	1.99	0.44
1:B:2381:ASN:ND2	1:B:2383:GLU:HB2	2.20	0.44
1:B:2705:THR:HG22	1:B:2759:VAL:HG21	1.98	0.44
1:B:3067:GLU:C	1:B:3140:ASN:HD22	2.25	0.44
1:A:1609:GLN:O	1:A:1613:VAL:HG23	2.17	0.44
1:A:1748:GLU:HB3	1:A:1943:ILE:HD12	1.99	0.44
1:A:2142:GLN:NE2	1:A:2208:VAL:HG21	2.32	0.44
1:A:2302:GLU:HG2	1:A:2304:HIS:HE1	1.81	0.44
1:A:2359:VAL:HG11	1:A:2400:LEU:HD22	1.99	0.44
1:A:2433:THR:HG23	1:A:2437:GLU:HG3	1.99	0.44
1:A:2898:LEU:O	1:A:2898:LEU:HD13	2.17	0.44
1:A:3408:VAL:HG23	1:A:3409:CYS:N	2.32	0.44
1:A:3490:ILE:O	1:A:3490:ILE:HG13	2.18	0.44
1:A:3974:ILE:O	1:A:3977:LYS:HB2	2.17	0.44
1:A:4121:ILE:HG22	1:A:4122:VAL:N	2.32	0.44
1:A:4131:PRO:C	1:A:4132:LEU:HD12	2.42	0.44
1:B:1822:VAL:HG13	1:B:1823:TRP:N	2.31	0.44
1:B:2263:HIS:HB2	1:B:2289:TYR:CE1	2.52	0.44
1:B:2560:MET:HE1	1:B:2619:ILE:O	2.17	0.44
1:B:2955:TRP:HZ2	1:B:3002:ASP:OD1	2.00	0.44
1:B:3088:ASN:OD1	1:B:3163:ALA:HB3	2.17	0.44
1:B:3233:TYR:CG	1:B:3620:ARG:HG3	2.52	0.44
1:B:3848:ASP:C	1:B:3850:SER:H	2.25	0.44
1:B:3965:LEU:CG	1:B:4426:MET:HE1	2.45	0.44
1:A:2016:LEU:HD21	1:A:2023:GLY:CA	2.47	0.44
1:A:2056:GLU:O	1:A:2056:GLU:HG3	2.17	0.44
1:A:2340:ILE:HD11	1:A:2386:ALA:O	2.17	0.44
1:A:2502:ILE:HD12	1:A:2506:PHE:HE2	1.82	0.44
1:A:3055:LEU:O	1:A:3059:LEU:HD23	2.17	0.44
1:A:3361:LYS:HE2	1:A:3361:LYS:HB3	1.84	0.44
1:A:3809:THR:HG22	1:A:3812:LYS:NZ	2.32	0.44
1:A:4691:TYR:HA	1:A:4699:LEU:HA	1.99	0.44
1:B:2621:ASP:C	1:B:2623:ASN:N	2.75	0.44
1:B:2660:LEU:HD21	1:B:2672:LEU:CD2	2.48	0.44
1:B:4266:GLU:HG3	1:B:4369:PHE:CE1	2.52	0.44
1:B:4686:LEU:HD12	1:B:4687:SER:H	1.83	0.44
1:A:2046:ILE:HD11	1:A:2059:LEU:HD22	2.00	0.44
1:A:2269:ASN:C	1:A:2271:GLY:N	2.74	0.44
1:A:2399:ASP:O	1:A:2400:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2641:VAL:HG21	1:A:2887:LEU:HD13	1.99	0.44
1:A:2742:PHE:HD1	1:A:2789:VAL:HG12	1.83	0.44
1:A:2902:VAL:HG22	1:A:2938:PHE:CD2	2.53	0.44
1:A:3439:ASP:C	1:A:3441:LYS:N	2.75	0.44
1:A:3670:ARG:NH1	1:A:3781:VAL:O	2.51	0.44
1:A:3675:ILE:O	1:A:3675:ILE:HG22	2.17	0.44
1:A:3731:ASN:H	1:A:3731:ASN:ND2	2.09	0.44
1:A:3805:GLU:HB3	1:A:3886:TYR:OH	2.17	0.44
1:A:3838:LEU:C	1:A:3840:GLN:H	2.26	0.44
1:A:4680:ASN:C	1:A:4682:SER:H	2.26	0.44
1:B:1640:ASN:ND2	1:B:1644:ILE:HG12	2.32	0.44
1:B:3011:HIS:CE1	1:B:3091:LEU:HA	2.53	0.44
1:B:3316:LYS:HD2	1:B:3546:ILE:CD1	2.47	0.44
1:B:3601:TYR:O	1:B:3603:GLY:N	2.50	0.44
1:B:3958:THR:CG2	1:B:4235:VAL:HB	2.47	0.44
1:B:4087:LYS:HG2	1:B:4087:LYS:O	2.17	0.44
1:B:4244:VAL:HG23	1:B:4403:SER:OG	2.18	0.44
1:B:4405:PRO:HD3	1:B:4415:GLU:HG2	1.98	0.44
1:B:4693:ASN:H	1:B:4693:ASN:HD22	1.64	0.44
1:A:1719:GLN:OE1	1:A:1732:LEU:N	2.50	0.44
1:A:2200:ASN:O	1:A:2204:ILE:HG12	2.18	0.44
1:A:2200:ASN:ND2	1:A:2228:LEU:HD13	2.18	0.44
1:A:2339:ILE:HG21	1:A:2391:VAL:CG2	2.48	0.44
1:A:3274:LYS:HD3	1:A:3274:LYS:HA	1.77	0.44
1:A:3293:ARG:HG3	1:A:3293:ARG:NH1	2.27	0.44
1:A:3338:GLN:NE2	1:A:3525:LEU:HB2	2.32	0.44
1:A:3727:ASP:CB	1:A:3729:VAL:HG12	2.48	0.44
1:A:3902:GLU:O	1:A:3905:GLN:HG2	2.17	0.44
1:A:4513:ILE:HA	1:A:4550:TRP:HE1	1.82	0.44
1:A:4673:ASP:O	1:A:4677:PRO:HD2	2.18	0.44
1:B:1828:ASP:OD2	1:B:1901:ASN:HB2	2.17	0.44
1:B:2301:SER:HA	1:B:2350:ARG:O	2.18	0.44
1:B:2886:LEU:O	1:B:2890:ILE:HG13	2.18	0.44
1:B:2976:LEU:CD1	1:B:2990:LEU:HD11	2.48	0.44
1:B:3602:ILE:HG23	1:B:3610:ARG:CG	2.43	0.44
1:A:1628:LEU:HD23	1:A:1628:LEU:O	2.18	0.44
1:A:2125:ALA:HA	1:A:2128:ILE:CG2	2.46	0.44
1:A:2152:LEU:O	1:A:2152:LEU:HD13	2.18	0.44
1:A:2360:ASP:C	1:A:2362:GLU:H	2.26	0.44
1:A:4075:THR:HG23	1:A:4076:ILE:H	1.82	0.44
1:A:4296:PHE:HE2	1:A:4347:ILE:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2986:VAL:O	1:B:2988:LEU:HG	2.17	0.44
1:B:3966:THR:N	1:B:4426:MET:HE2	2.33	0.44
1:B:4265:ALA:H	1:B:4323:ASN:HB3	1.83	0.44
1:B:4304:ARG:HA	1:B:4307:LEU:HD12	1.99	0.44
1:B:4330:PRO:O	1:B:4333:ALA:HB3	2.17	0.44
1:B:4432:LYS:C	1:B:4434:GLN:H	2.25	0.44
1:A:1674:ASP:OD1	1:A:1678:LYS:HE2	2.17	0.44
1:A:2056:GLU:HB2	1:A:2065:ILE:O	2.18	0.44
1:A:3065:LYS:O	1:A:3066:GLU:C	2.60	0.44
1:A:3521:THR:O	1:A:3525:LEU:HD12	2.18	0.44
1:A:4260:MET:HE3	1:A:4271:TYR:CB	2.48	0.44
1:B:1530:PHE:CZ	1:B:1571:SER:HB2	2.53	0.44
1:B:2694:PHE:HA	1:B:2738:TRP:O	2.18	0.44
1:B:3013:LEU:HD13	1:B:3145:PHE:HB3	2.00	0.44
1:B:3715:GLY:HA2	1:B:3760:PHE:HB2	2.00	0.44
1:B:4252:PHE:C	1:B:4254:GLY:N	2.76	0.44
1:B:4374:PRO:HB3	1:B:4377:PRO:HG3	1.98	0.44
1:B:4686:LEU:HD22	1:B:4716:TRP:HB3	2.00	0.44
1:A:1535:ARG:HA	1:A:1591:TRP:HZ2	1.83	0.44
1:A:1695:ALA:CB	1:A:2019:CYS:SG	3.06	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HA	1.81	0.44
1:A:2289:TYR:CE1	1:A:2293:ILE:HD11	2.53	0.44
1:A:2903:ARG:HD2	1:A:2945:ALA:O	2.18	0.44
1:A:2926:THR:O	1:A:2930:ILE:HG13	2.18	0.44
1:A:3205:PHE:CE2	1:A:3221:PRO:HB3	2.52	0.44
1:A:3812:LYS:HB3	1:A:3875:VAL:CG2	2.47	0.44
1:A:3813:ARG:HH22	1:A:3817:LEU:HD13	1.83	0.44
1:A:3869:VAL:O	1:A:3869:VAL:HG12	2.18	0.44
1:A:4090:HIS:C	1:A:4092:ASP:H	2.24	0.44
1:B:1506:ASP:C	1:B:1508:ALA:H	2.26	0.44
1:B:1831:LEU:HB3	1:B:1900:GLY:C	2.43	0.44
1:B:2612:LEU:O	1:B:2612:LEU:HD13	2.18	0.44
1:B:2766:MET:HB3	1:B:2783:LEU:CD1	2.43	0.44
1:B:2828:TYR:HE1	1:B:2880:SER:HA	1.83	0.44
1:B:3552:LYS:HB2	1:B:3552:LYS:NZ	2.33	0.44
1:B:3553:VAL:O	1:B:3557:VAL:HG23	2.18	0.44
1:B:3872:THR:O	1:B:3876:MET:HG2	2.18	0.44
1:B:4289:PRO:HB2	1:B:4696:ARG:HD2	2.00	0.44
1:B:4689:PRO:HD2	1:B:4721:VAL:O	2.18	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HB2	1.83	0.44
1:A:2125:ALA:C	1:A:2127:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2361:PRO:HD2	1:A:2754:TYR:CE1	2.53	0.44
1:A:2903:ARG:HH22	1:A:2950:ILE:HA	1.82	0.44
1:A:2913:PHE:HD2	1:A:2913:PHE:N	2.15	0.44
1:A:2942:ASN:O	1:A:2943:LEU:C	2.61	0.44
1:A:3190:ARG:HA	1:A:3224:ARG:NH1	2.32	0.44
1:A:3700:LEU:CD1	1:A:3701:ASP:H	2.31	0.44
1:B:1721:HIS:CB	1:B:1725:MET:HE2	2.48	0.44
1:B:1869:ALA:O	1:B:1872:ARG:HB3	2.17	0.44
1:B:2112:MET:O	1:B:2116:GLN:HG2	2.17	0.44
1:B:2839:LEU:CD2	1:B:2896:CYS:HB3	2.48	0.44
1:B:2965:ARG:HG3	1:B:2965:ARG:HH11	1.82	0.44
1:B:3903:LEU:HD11	1:B:3967:PHE:CD1	2.53	0.44
1:A:1591:TRP:HA	1:A:1591:TRP:CE3	2.53	0.43
1:A:1756:LYS:HB2	1:A:1756:LYS:NZ	2.32	0.43
1:A:2091:LEU:HD22	1:A:2095:PHE:HE1	1.80	0.43
1:A:2249:LEU:HD22	2:A:9002:ADP:C5	2.53	0.43
1:A:2255:TRP:CH2	1:A:2259:ILE:HD11	2.53	0.43
1:A:2617:VAL:HG13	1:A:2617:VAL:O	2.18	0.43
1:A:3585:MET:HA	1:A:3588:VAL:HG23	2.00	0.43
1:A:3652:LEU:HD12	1:A:3653:PRO:CD	2.41	0.43
1:A:4690:VAL:HG11	1:A:4701:PHE:CE2	2.53	0.43
1:B:2426:ILE:H	1:B:2426:ILE:CD1	2.27	0.43
1:B:2714:PHE:HE1	1:B:2741:VAL:HG21	1.83	0.43
1:B:2902:VAL:HG21	1:B:2941:VAL:HG21	2.00	0.43
1:B:3038:TYR:HE2	1:B:3058:LEU:HD22	1.82	0.43
1:B:3046:TYR:CE1	1:B:3050:ASP:HB2	2.53	0.43
1:B:3961:ASN:HA	1:B:3964:LYS:HE2	2.00	0.43
1:A:2547:ASN:O	1:A:2551:TYR:HB2	2.17	0.43
1:A:2714:PHE:C	1:A:2716:HIS:H	2.26	0.43
1:A:3462:PHE:CE2	1:A:3478:VAL:HG23	2.53	0.43
1:A:4055:GLU:O	1:A:4056:PRO:C	2.61	0.43
1:B:1674:ASP:O	1:B:1678:LYS:HG3	2.18	0.43
1:B:2265:ILE:HD12	1:B:2414:VAL:HG22	1.99	0.43
1:B:2522:ARG:NH1	1:B:2593:PHE:HD1	2.16	0.43
1:B:4024:ARG:O	1:B:4024:ARG:HG2	2.17	0.43
1:B:4153:LEU:HB2	1:B:4155:LYS:CG	2.46	0.43
1:B:4691:TYR:HA	1:B:4698:GLU:O	2.18	0.43
1:A:1755:LYS:HA	1:A:1755:LYS:HD2	1.80	0.43
1:A:1922:LEU:CD1	1:A:1938:PHE:HD1	2.31	0.43
1:A:1958:LEU:HD23	1:A:4341:THR:HB	1.99	0.43
1:A:2053:ASN:N	1:A:2053:ASN:ND2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2400:LEU:HB3	1:A:2403:ALA:HB3	2.00	0.43
1:A:2408:ILE:HG13	1:A:2409:SER:H	1.83	0.43
1:A:3019:GLY:HA2	2:A:9004:ADP:H5'2	2.00	0.43
1:A:3470:ALA:O	1:A:3471:SER:HB2	2.17	0.43
1:A:4091:SER:O	1:A:4420:SER:HA	2.18	0.43
1:A:4319:LYS:O	1:A:4321:ARG:NH1	2.52	0.43
1:B:1497:LEU:HD22	1:B:1501:SER:HB2	1.99	0.43
1:B:2404:THR:C	1:B:2406:ALA:H	2.26	0.43
1:B:2665:SER:C	1:B:2667:HIS:H	2.25	0.43
1:B:2714:PHE:HE2	1:B:2766:MET:HE1	1.83	0.43
1:B:2773:TRP:CZ3	1:B:2780:TRP:HB2	2.53	0.43
1:B:3686:MET:HA	1:B:3694:ILE:HG21	2.00	0.43
1:B:4225:LEU:HD23	1:B:4230:LEU:HD21	2.00	0.43
1:A:1604:VAL:O	1:A:1608:VAL:HG23	2.18	0.43
1:A:1835:THR:O	1:A:1836:LEU:CB	2.67	0.43
1:A:2233:MET:O	1:A:2234:ASP:C	2.61	0.43
1:A:2359:VAL:HB	1:A:2397:VAL:HG11	2.00	0.43
1:A:3062:ALA:HB2	1:A:3069:ILE:HD13	1.99	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CD2	2.53	0.43
1:A:3808:ASP:C	1:A:3810:HIS:H	2.26	0.43
1:A:3960:LEU:O	1:A:3961:ASN:C	2.59	0.43
1:A:3990:PHE:CE2	1:A:4023:LEU:HG	2.54	0.43
1:A:4052:GLN:O	1:A:4054:GLY:N	2.43	0.43
1:B:1831:LEU:HA	1:B:1841:ILE:HG23	1.99	0.43
1:B:1975:PRO:HG2	1:B:1978:THR:CG2	2.48	0.43
1:B:3041:LYS:N	1:B:3041:LYS:HD2	2.33	0.43
1:B:3192:LEU:HD22	1:B:3271:ILE:HG21	2.00	0.43
1:B:3634:VAL:HB	1:B:3635:PRO:HD3	1.99	0.43
1:B:4012:LEU:HD11	1:B:4020:LEU:HD22	2.01	0.43
1:B:4022:CYS:HB3	1:B:4026:GLN:HE21	1.84	0.43
1:A:1828:ASP:C	1:A:1830:ALA:N	2.77	0.43
1:A:1830:ALA:O	1:A:1841:ILE:HG23	2.18	0.43
1:A:3096:VAL:HB	1:A:3099:LEU:HB2	2.00	0.43
1:A:3445:THR:HA	1:A:3449:ARG:HB2	2.00	0.43
1:A:4052:GLN:C	1:A:4054:GLY:N	2.77	0.43
1:A:4132:LEU:HB2	1:A:4216:PHE:CD1	2.52	0.43
1:B:1639:ILE:HG23	1:B:1672:LEU:HD22	2.01	0.43
1:B:1956:CYS:HB2	1:B:2100:MET:HE3	2.00	0.43
1:B:2352:TRP:CD1	1:B:2392:ARG:HB2	2.54	0.43
1:B:3234:ILE:HG23	1:B:3617:TRP:CD1	2.54	0.43
1:B:3289:LEU:HA	1:B:3292:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4574:GLN:HE22	1:B:4590:TRP:HB3	1.82	0.43
1:A:1836:LEU:O	1:A:1837:GLN:C	2.62	0.43
1:A:1955:ARG:NH1	1:A:1955:ARG:HB2	2.33	0.43
1:A:2012:ILE:HG22	1:A:2016:LEU:CD1	2.49	0.43
1:A:2057:VAL:HG22	1:A:2058:GLU:N	2.34	0.43
1:A:2200:ASN:ND2	1:A:2228:LEU:HB3	2.33	0.43
1:A:2842:LEU:C	1:A:2844:SER:H	2.26	0.43
1:A:3015:ILE:HG21	1:A:3172:TRP:CH2	2.54	0.43
1:A:3078:VAL:O	1:A:3078:VAL:HG22	2.19	0.43
1:A:3357:VAL:O	1:A:3357:VAL:HG12	2.18	0.43
1:A:3638:LEU:HD22	1:A:3667:ARG:HD3	2.01	0.43
1:A:4066:GLN:HE22	1:A:4081:ARG:HD3	1.81	0.43
1:A:4337:ILE:HG22	1:A:4338:LEU:HD12	1.99	0.43
1:B:1653:ALA:HB1	1:B:1658:GLU:HG2	2.01	0.43
1:B:1744:MET:SD	1:B:1777:MET:HG3	2.59	0.43
1:B:2882:TRP:O	1:B:2886:LEU:HG	2.18	0.43
1:B:3160:THR:O	1:B:3162:PRO:HD3	2.18	0.43
1:B:3181:LEU:HB3	1:B:3232:VAL:HG13	2.00	0.43
1:B:3993:LYS:HG3	1:B:4431:GLN:HG3	1.99	0.43
1:B:4357:TYR:O	1:B:4358:SER:C	2.62	0.43
1:B:4407:TRP:H	1:B:4407:TRP:HD1	1.64	0.43
1:B:4728:SER:OG	1:B:4729:ASP:N	2.51	0.43
1:A:1906:TRP:CZ2	1:A:1911:ARG:HG2	2.54	0.43
1:A:2145:TYR:OH	1:A:2207:LEU:HA	2.18	0.43
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.54	0.43
1:A:2270:HIS:ND1	1:A:2270:HIS:N	2.66	0.43
1:A:2678:SER:HB2	1:A:2817:ASP:O	2.18	0.43
1:A:2748:LEU:HD21	1:A:2800:ARG:CZ	2.48	0.43
1:A:3414:GLY:C	1:A:3416:LYS:H	2.27	0.43
1:A:3451:ALA:O	1:A:3455:GLY:N	2.51	0.43
1:A:4046:GLN:CD	1:A:4057:ILE:HG22	2.44	0.43
1:A:4070:SER:C	1:A:4072:GLN:H	2.27	0.43
1:A:4179:ALA:HA	1:A:4213:PHE:CD1	2.53	0.43
1:A:4280:ILE:HG21	1:A:4359:PHE:CE1	2.53	0.43
1:A:4288:ILE:HG23	1:A:4289:PRO:HA	2.01	0.43
1:A:4389:ARG:HG2	1:A:4389:ARG:NH1	2.32	0.43
1:A:4648:VAL:HG13	1:A:4657:THR:CG2	2.44	0.43
1:B:1546:VAL:O	1:B:1553:LYS:HA	2.19	0.43
1:B:1766:ILE:HD12	1:B:1769:TRP:HE1	1.84	0.43
1:B:2229:GLN:O	1:B:2230:PRO:C	2.61	0.43
1:B:2968:LEU:HD22	1:B:2999:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3238:ILE:HD11	1:B:3617:TRP:CZ2	2.48	0.43
1:B:4293:THR:HG23	1:B:4352:ASP:OD1	2.19	0.43
1:A:1658:GLU:O	1:A:1661:ALA:HB3	2.19	0.43
1:A:2088:PRO:C	1:A:2090:ASN:N	2.75	0.43
1:A:2290:LEU:HD23	1:A:2301:SER:O	2.19	0.43
1:A:2304:HIS:N	1:A:2352:TRP:O	2.51	0.43
1:A:2327:TRP:CZ2	1:A:2379:LEU:HD22	2.54	0.43
1:A:2842:LEU:C	1:A:2844:SER:N	2.77	0.43
1:A:3197:PRO:HG2	1:A:3198:GLN:OE1	2.18	0.43
1:A:3324:LEU:HD12	1:A:3539:LEU:HD23	2.00	0.43
1:A:3416:LYS:HE3	1:A:3418:GLU:CB	2.48	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CG	2.54	0.43
1:A:4260:MET:HE3	1:A:4271:TYR:HB2	2.01	0.43
1:A:4379:ILE:HG23	1:A:4381:LEU:HD13	2.00	0.43
1:A:4673:ASP:C	1:A:4677:PRO:HG2	2.44	0.43
1:B:1606:ILE:HG23	1:B:1607:ASP:N	2.33	0.43
1:B:1777:MET:HE3	1:B:1939:GLU:HA	2.01	0.43
1:B:1780:THR:HG22	1:B:1784:LEU:CD1	2.48	0.43
1:B:2088:PRO:O	1:B:2089:ASP:C	2.62	0.43
1:B:2404:THR:C	1:B:2406:ALA:N	2.77	0.43
1:B:2582:GLY:CA	1:B:2585:MET:HE3	2.38	0.43
1:B:2840:PRO:O	1:B:2843:ARG:HB2	2.19	0.43
1:B:3139:ARG:HG3	1:B:3139:ARG:HH11	1.84	0.43
1:B:3289:LEU:O	1:B:3293:ARG:HG3	2.19	0.43
1:B:3725:ASN:ND2	1:B:3725:ASN:N	2.67	0.43
1:B:4028:PRO:O	1:B:4031:SER:N	2.52	0.43
1:B:4058:ILE:CD1	1:B:4082:LYS:HG2	2.48	0.43
1:B:4331:TRP:HZ2	1:B:4369:PHE:CE2	2.37	0.43
1:A:1578:SER:HA	1:A:1579:PRO:HD3	1.92	0.43
1:A:2269:ASN:O	1:A:2272:VAL:HG23	2.19	0.43
1:A:2650:THR:OG1	1:A:2651:VAL:N	2.50	0.43
1:A:2774:ARG:CZ	1:A:2781:ILE:HD11	2.48	0.43
1:A:2957:THR:HB	1:A:2961:GLN:CD	2.44	0.43
1:A:3588:VAL:O	1:A:3592:VAL:HG23	2.18	0.43
1:A:3902:GLU:HB3	1:A:4433:MET:HG2	2.00	0.43
1:A:4565:ILE:HG22	1:A:4566:SER:N	2.34	0.43
1:B:2304:HIS:NE2	1:B:2351:HIS:HD2	2.17	0.43
1:B:2339:ILE:HG21	1:B:2391:VAL:CG2	2.49	0.43
1:B:2836:MET:HE1	1:B:2839:LEU:HD12	2.01	0.43
1:B:3202:PRO:HG3	1:B:3623:SER:O	2.19	0.43
1:B:3272:ASN:HD22	1:B:3272:ASN:HA	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3620:ARG:HG2	1:B:3620:ARG:NH1	2.34	0.43
1:B:3895:ARG:NH1	1:B:3977:LYS:HG2	2.34	0.43
1:B:4023:LEU:O	1:B:4027:VAL:HB	2.18	0.43
1:B:4079:ASN:O	1:B:4082:LYS:HB2	2.18	0.43
1:B:4185:VAL:O	1:B:4215:LEU:HD12	2.19	0.43
1:B:4282:GLN:O	1:B:4285:LEU:HB2	2.19	0.43
1:B:4639:VAL:C	1:B:4666:ILE:HD12	2.44	0.43
1:A:1927:ILE:O	1:A:1928:HIS:HD2	2.01	0.43
1:A:2273:MET:HG3	1:A:2413:MET:HE1	2.01	0.43
1:A:3078:VAL:C	1:A:3080:GLU:H	2.27	0.43
1:A:3391:ILE:HD11	1:A:3471:SER:OG	2.19	0.43
1:A:3953:ASN:O	1:A:3956:THR:HG22	2.19	0.43
1:A:4171:ALA:O	1:A:4172:GLU:C	2.62	0.43
1:A:4335:ARG:HG2	1:A:4360:LEU:HG	2.01	0.43
1:A:4659:ILE:N	1:A:4659:ILE:HD12	2.34	0.43
1:B:4075:THR:HG23	1:B:4076:ILE:N	2.34	0.43
1:B:4324:ILE:H	1:B:4324:ILE:HG13	1.52	0.43
1:B:4617:GLU:HG2	1:B:4618:ASN:N	2.34	0.43
1:B:4638:ASN:HB3	1:B:4666:ILE:HD11	2.00	0.43
1:A:1963:ALA:HA	1:A:2096:ARG:HH11	1.83	0.42
1:A:1967:ARG:NH1	1:A:2053:ASN:HA	2.34	0.42
1:A:3443:MET:O	1:A:3444:MET:C	2.61	0.42
1:A:3716:CYS:H	1:A:3760:PHE:HB2	1.84	0.42
1:A:4024:ARG:HA	1:A:4030:PHE:O	2.19	0.42
1:A:4354:ARG:HD3	1:A:4717:TYR:CD2	2.53	0.42
1:A:4692:LEU:HD13	1:A:4698:GLU:CD	2.44	0.42
1:B:2196:LEU:HD11	1:B:2223:PHE:CD2	2.54	0.42
1:B:2271:GLY:HA2	1:B:2393:VAL:O	2.19	0.42
1:B:2368:ASN:O	1:B:2410:ARG:NH1	2.52	0.42
1:B:2849:LEU:CD1	1:B:2901:LEU:HD11	2.49	0.42
1:B:3722:ASP:HA	1:B:3724:GLU:OE1	2.19	0.42
1:B:3723:VAL:HG23	1:B:3764:LEU:HD22	2.01	0.42
1:B:4006:PRO:C	1:B:4008:LEU:N	2.76	0.42
1:A:1554:LEU:HD22	1:A:1609:GLN:HG3	2.00	0.42
1:A:1907:LEU:HD22	1:A:1911:ARG:CZ	2.49	0.42
1:A:2560:MET:CG	1:A:2565:GLN:HB2	2.49	0.42
1:A:2819:PRO:O	1:A:2820:SER:C	2.61	0.42
1:A:3782:THR:HG23	1:A:3782:THR:O	2.18	0.42
1:A:3992:LEU:CD1	1:A:4434:GLN:HG3	2.48	0.42
1:A:4358:SER:O	1:A:4362:GLN:HB2	2.19	0.42
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2109:ALA:HA	1:B:2156:LEU:CD1	2.49	0.42
1:B:2423:THR:HA	1:B:2426:ILE:HD13	2.00	0.42
1:B:2723:THR:C	1:B:2725:SER:H	2.27	0.42
1:B:2886:LEU:HD23	1:B:2904:LEU:HD22	2.01	0.42
1:B:2991:PHE:CE1	1:B:2993:GLU:HB2	2.54	0.42
1:B:3234:ILE:HG23	1:B:3617:TRP:CE2	2.54	0.42
1:B:3598:PHE:CD2	1:B:3634:VAL:HG11	2.55	0.42
1:B:3647:TRP:HB3	1:B:3652:LEU:CD2	2.49	0.42
1:B:3676:ASP:CB	1:B:3681:ALA:HB3	2.49	0.42
1:B:4086:MET:HE3	1:B:4097:TYR:CZ	2.55	0.42
1:B:4396:ILE:C	1:B:4398:ALA:N	2.77	0.42
1:B:4673:ASP:OD1	1:B:4674:LYS:N	2.52	0.42
1:A:1816:LEU:HD23	1:A:1878:LEU:CD1	2.49	0.42
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	2.02	0.42
1:A:2525:ILE:HD12	1:A:2526:MET:N	2.33	0.42
1:A:3067:GLU:HG2	1:A:3068:LYS:N	2.34	0.42
1:A:3096:VAL:HB	1:A:3099:LEU:HD22	2.01	0.42
1:A:3416:LYS:C	1:A:3417:LEU:HD12	2.45	0.42
1:A:3718:LEU:HG	1:A:3719:LEU:N	2.21	0.42
1:A:4000:SER:O	1:B:2940:SER:HB3	2.19	0.42
1:B:1960:LEU:HD13	1:B:2074:PHE:CE1	2.54	0.42
1:B:2017:CYS:SG	1:B:2046:ILE:HD13	2.59	0.42
1:B:2129:VAL:N	1:B:2130:PRO:CD	2.82	0.42
1:B:2669:PRO:HA	1:B:2788:PHE:O	2.19	0.42
1:B:3030:ALA:HB3	1:B:3037:ILE:HD11	2.00	0.42
1:B:3078:VAL:O	1:B:3078:VAL:HG22	2.18	0.42
1:B:3675:ILE:O	1:B:3675:ILE:HG22	2.19	0.42
1:B:3698:SER:HB3	1:B:3700:LEU:HD12	2.00	0.42
1:B:4396:ILE:C	1:B:4398:ALA:H	2.26	0.42
1:A:1639:ILE:HG12	1:A:1675:LEU:HD23	2.01	0.42
1:A:1732:LEU:HD13	1:A:1741:ILE:HD12	2.01	0.42
1:A:1752:VAL:CG2	1:A:1811:PRO:HG3	2.48	0.42
1:A:1816:LEU:O	1:A:1820:GLN:HG3	2.19	0.42
1:A:1927:ILE:C	1:A:1928:HIS:CD2	2.97	0.42
1:A:1973:PHE:HD1	1:A:1973:PHE:O	2.02	0.42
1:A:2142:GLN:HB2	1:A:2145:TYR:CD1	2.54	0.42
1:A:2615:TYR:CD2	1:A:2615:TYR:N	2.87	0.42
1:A:2819:PRO:HB2	1:A:2824:LEU:CD2	2.50	0.42
1:A:3018:SER:O	1:A:3257:PRO:HD2	2.18	0.42
1:A:3156:ASN:C	1:A:3158:SER:N	2.77	0.42
1:A:3209:ALA:CB	1:A:3221:PRO:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3700:LEU:CD1	1:A:3701:ASP:N	2.80	0.42
1:A:3819:ILE:C	1:A:3821:GLY:N	2.77	0.42
1:A:3993:LYS:O	1:A:3995:GLY:N	2.53	0.42
1:A:4109:ASP:CA	1:A:4112:ASN:HD22	2.11	0.42
1:A:4134:LEU:HD23	1:A:4236:PHE:HB2	2.01	0.42
1:A:4168:PHE:O	1:A:4172:GLU:HG3	2.19	0.42
1:A:4203:LYS:O	1:A:4204:LEU:C	2.62	0.42
1:A:4289:PRO:HA	1:A:4292:TRP:O	2.20	0.42
1:B:1811:PRO:HB2	1:B:1814:LEU:CD1	2.49	0.42
1:B:2272:VAL:HG12	1:B:2273:MET:N	2.34	0.42
1:B:2591:GLU:HA	1:B:2613:LEU:HD12	2.01	0.42
1:B:3039:THR:HG22	1:B:3072:ILE:HB	2.01	0.42
1:B:3057:MET:O	1:B:3061:ARG:HG3	2.19	0.42
1:B:3181:LEU:HB2	1:B:3232:VAL:HG13	2.01	0.42
1:B:3960:LEU:CD2	1:B:4237:SER:HB2	2.50	0.42
1:A:1708:ILE:HD11	1:A:1721:HIS:HB3	2.01	0.42
1:A:1967:ARG:CB	1:A:2051:LYS:HA	2.50	0.42
1:A:2408:ILE:O	1:A:2411:CYS:HB2	2.20	0.42
1:A:2502:ILE:CG2	1:A:2573:LEU:HD12	2.48	0.42
1:A:2534:LEU:HB3	1:A:2538:PHE:CE2	2.55	0.42
1:A:2587:LEU:CG	1:A:2817:ASP:HB2	2.45	0.42
1:A:2627:TRP:C	1:A:2629:ASN:N	2.78	0.42
1:A:2905:TRP:HZ3	1:A:2934:ALA:HB2	1.83	0.42
1:A:3192:LEU:HD11	1:A:3271:ILE:HG22	2.01	0.42
1:A:3262:ASP:OD2	1:A:3670:ARG:NE	2.52	0.42
1:A:3536:TYR:O	1:A:3540:ILE:HD13	2.20	0.42
1:A:4373:PHE:CD1	1:A:4374:PRO:HD2	2.54	0.42
1:B:2112:MET:SD	1:B:2153:LYS:HG2	2.59	0.42
1:B:2528:PHE:HE1	1:B:2533:VAL:HG11	1.85	0.42
1:B:2682:MET:HE2	1:B:2682:MET:HB3	1.93	0.42
1:B:2706:THR:HA	1:B:2759:VAL:HG22	2.01	0.42
1:B:3084:LEU:O	1:B:3087:MET:N	2.52	0.42
1:B:3598:PHE:O	1:B:3602:ILE:HB	2.20	0.42
1:B:3727:ASP:C	1:B:3729:VAL:H	2.28	0.42
1:A:1766:ILE:HG23	1:A:1767:HIS:N	2.35	0.42
1:A:2091:LEU:C	1:A:2093:LYS:H	2.27	0.42
1:A:2297:ASP:C	1:A:2299:ILE:N	2.78	0.42
1:A:2370:LEU:HD23	1:A:2370:LEU:O	2.19	0.42
1:A:2415:TRP:HA	1:A:2415:TRP:HE3	1.83	0.42
1:A:2910:LEU:HB3	1:A:2911:ARG:HH12	1.85	0.42
1:A:3009:GLN:HG2	1:A:3138:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3061:ARG:O	1:A:3067:GLU:HB3	2.18	0.42
1:A:3108:LEU:HD11	1:A:3133:PHE:CZ	2.54	0.42
1:A:3915:ALA:O	1:A:3918:ASP:HB2	2.19	0.42
1:A:3954:ARG:O	1:A:3954:ARG:HD3	2.19	0.42
1:A:4128:SER:CB	1:A:4213:PHE:HB3	2.48	0.42
1:A:4178:ALA:HA	1:A:4183:THR:OG1	2.20	0.42
1:B:1598:VAL:HG22	1:B:1660:LEU:HD22	2.01	0.42
1:B:1914:TYR:CZ	1:B:1924:LYS:HB3	2.54	0.42
1:B:2230:PRO:HB3	1:B:2237:ARG:HH22	1.84	0.42
1:B:2327:TRP:CH2	1:B:2380:PRO:HD2	2.55	0.42
1:B:2610:ILE:HD12	1:B:2615:TYR:OH	2.20	0.42
1:B:3043:ASN:ND2	1:B:3043:ASN:N	2.68	0.42
1:B:3702:SER:C	1:B:3704:PHE:N	2.77	0.42
1:A:2126:GLY:O	1:A:2130:PRO:HG2	2.19	0.42
1:A:2269:ASN:O	1:A:2271:GLY:N	2.53	0.42
1:A:2270:HIS:HB2	1:A:2392:ARG:HD2	2.02	0.42
1:A:2426:ILE:CD1	1:A:2530:ARG:HD3	2.50	0.42
1:A:2552:ASN:C	1:A:2554:LEU:H	2.28	0.42
1:A:2701:PHE:HB2	1:A:2745:GLU:O	2.20	0.42
1:A:3457:LEU:HD12	1:A:3486:TYR:CE1	2.55	0.42
1:A:3868:LYS:C	1:A:3870:GLU:N	2.77	0.42
1:B:2290:LEU:HD22	1:B:2352:TRP:CZ3	2.55	0.42
1:B:2588:VAL:HG23	1:B:2589:GLU:N	2.34	0.42
1:B:2773:TRP:CH2	1:B:2780:TRP:HB2	2.54	0.42
1:B:3061:ARG:O	1:B:3067:GLU:HB3	2.19	0.42
1:B:3990:PHE:CD2	1:B:4084:LEU:HD22	2.55	0.42
1:B:4107:GLY:C	1:B:4109:ASP:H	2.27	0.42
1:A:1791:HIS:HD2	1:A:1806:TRP:HD1	1.66	0.42
1:A:1952:LEU:HD22	1:A:2103:PRO:HA	2.01	0.42
1:A:2057:VAL:HB	1:A:2067:LEU:HD13	2.01	0.42
1:A:2106:GLU:CD	1:A:2106:GLU:N	2.69	0.42
1:A:2561:SER:HA	1:A:2562:PRO:HD3	1.95	0.42
1:A:2849:LEU:HA	1:A:2938:PHE:HZ	1.85	0.42
1:A:3268:VAL:HG13	1:A:3269:LEU:N	2.35	0.42
1:A:3602:ILE:HG22	1:A:3603:GLY:N	2.34	0.42
1:A:4313:TRP:CD1	1:A:4334:VAL:HG22	2.55	0.42
1:B:1608:VAL:HG13	1:B:1676:LEU:CD1	2.50	0.42
1:B:1907:LEU:HD22	1:B:1911:ARG:NH2	2.34	0.42
1:B:2084:ARG:CZ	1:B:4295:PHE:CD2	3.03	0.42
1:B:2222:VAL:C	1:B:2224:PRO:HD3	2.44	0.42
1:B:2513:HIS:O	1:B:2517:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2528:PHE:CE1	1:B:2533:VAL:HG11	2.54	0.42
1:B:2650:THR:C	1:B:2652:ASP:N	2.76	0.42
1:B:2825:THR:CG2	1:B:2854:VAL:HG21	2.50	0.42
1:B:3259:HIS:NE2	1:B:3779:SER:HA	2.34	0.42
1:B:4036:HIS:CD2	1:B:4044:TRP:HE1	2.38	0.42
1:B:4280:ILE:HG23	1:B:4408:LEU:HA	2.01	0.42
1:B:4284:ARG:CG	1:B:4408:LEU:HB3	2.49	0.42
1:A:1578:SER:C	1:A:1580:TYR:H	2.27	0.42
1:A:2585:MET:O	1:A:2815:LEU:HD13	2.19	0.42
1:A:2798:ALA:C	1:A:2800:ARG:N	2.78	0.42
1:A:3224:ARG:HB2	1:A:3224:ARG:HE	1.73	0.42
1:A:3449:ARG:NH1	1:A:3449:ARG:HB3	2.35	0.42
1:B:1659:VAL:C	1:B:1661:ALA:N	2.75	0.42
1:B:2540:LEU:HB3	1:B:2576:SER:CB	2.49	0.42
1:B:2856:PHE:HE2	1:B:2913:PHE:CD2	2.37	0.42
1:B:2989:VAL:HG21	1:B:3184:VAL:HA	2.02	0.42
1:B:3039:THR:CG2	1:B:3072:ILE:HB	2.50	0.42
1:B:3235:HIS:CE1	1:B:3260:TYR:HB2	2.55	0.42
1:B:3256:THR:CG2	1:B:3779:SER:HB3	2.50	0.42
1:B:3976:VAL:O	1:B:3979:THR:HG23	2.20	0.42
1:A:1556:ARG:HG2	1:A:1557:GLY:N	2.35	0.42
1:A:1746:SER:HB3	1:A:1940:TYR:CZ	2.55	0.42
1:A:1818:THR:O	1:A:1822:VAL:HG23	2.20	0.42
1:A:1929:MET:O	1:A:1930:ALA:HB3	2.20	0.42
1:A:1973:PHE:HE1	1:A:2099:ALA:CA	2.33	0.42
1:A:2833:ARG:HA	1:A:2846:ALA:HB1	2.02	0.42
1:A:3148:ASN:HA	1:A:3149:PRO:HD3	1.93	0.42
1:A:3315:VAL:O	1:A:3319:GLN:HB2	2.19	0.42
1:A:4065:ALA:O	1:A:4069:LEU:HB2	2.20	0.42
1:A:4354:ARG:HD2	1:A:4354:ARG:C	2.44	0.42
1:A:4418:LEU:HD11	1:A:4422:LYS:HZ3	1.84	0.42
1:A:4575:LEU:H	1:A:4575:LEU:CD1	2.26	0.42
1:B:1615:LEU:HD13	1:B:1618:ILE:HD12	2.01	0.42
1:B:1952:LEU:HA	1:B:1955:ARG:NH2	2.35	0.42
1:B:3017:VAL:HG11	1:B:3175:GLU:HA	2.01	0.42
1:B:3698:SER:C	1:B:3700:LEU:H	2.27	0.42
1:B:4070:SER:O	1:B:4072:GLN:N	2.53	0.42
1:B:4434:GLN:O	1:B:4434:GLN:HG2	2.19	0.42
1:A:2140:SER:HB2	1:A:2142:GLN:NE2	2.23	0.41
1:A:2204:ILE:HG13	1:A:2205:PRO:CD	2.50	0.41
1:A:2898:LEU:HD11	1:A:2941:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4370:ASN:N	1:A:4370:ASN:HD22	2.16	0.41
1:B:1565:LEU:HD23	1:B:1595:LEU:HD12	2.00	0.41
1:B:1721:HIS:C	1:B:1725:MET:HE2	2.45	0.41
1:B:2272:VAL:O	1:B:2394:MET:HA	2.20	0.41
1:B:2292:ALA:O	1:B:2296:VAL:HG23	2.20	0.41
1:B:2370:LEU:HD12	1:B:2377:LEU:HB2	2.02	0.41
1:B:2579:TRP:HZ2	1:B:2655:ARG:HD2	1.84	0.41
1:B:3923:LEU:HD22	1:B:3947:ILE:CG2	2.47	0.41
1:B:4191:HIS:CD2	1:B:4220:GLU:HG2	2.54	0.41
1:A:1574:ALA:C	1:A:1576:LYS:H	2.27	0.41
1:A:1831:LEU:HA	1:A:1841:ILE:HG12	2.02	0.41
1:A:2258:LYS:HA	1:A:2261:GLN:CG	2.44	0.41
1:A:2370:LEU:HA	1:A:2375:LYS:HA	2.02	0.41
1:A:2745:GLU:CB	1:A:2748:LEU:HD12	2.50	0.41
1:A:2783:LEU:HD22	1:A:2786:ILE:HB	2.01	0.41
1:A:3256:THR:HB	1:A:3257:PRO:HD2	2.01	0.41
1:A:3570:GLU:CD	1:A:3858:LEU:HD23	2.44	0.41
1:A:3696:LYS:HZ3	1:A:3721:GLN:CD	2.28	0.41
1:A:3990:PHE:O	1:A:3994:GLY:HA2	2.20	0.41
1:A:4337:ILE:O	1:A:4341:THR:CG2	2.68	0.41
1:A:4623:ALA:HB2	1:A:4703:ILE:CD1	2.48	0.41
1:A:4684:SER:O	1:A:4707:TYR:HE2	2.02	0.41
1:B:1785:LEU:HB2	1:B:1814:LEU:HD23	2.00	0.41
1:B:1960:LEU:HD13	1:B:2074:PHE:HE1	1.85	0.41
1:B:2815:LEU:C	1:B:2815:LEU:CD2	2.93	0.41
1:B:2955:TRP:HZ2	1:B:3002:ASP:CG	2.27	0.41
1:B:3573:ARG:HG2	1:B:3573:ARG:HH11	1.84	0.41
1:B:3700:LEU:CD1	1:B:3701:ASP:H	2.30	0.41
1:B:3877:GLN:O	1:B:3881:GLU:HB2	2.20	0.41
1:B:4068:GLN:C	1:B:4070:SER:N	2.77	0.41
1:B:4277:PHE:HZ	1:B:4356:LEU:HD21	1.84	0.41
1:A:1625:ILE:HG23	1:A:1626:ASN:N	2.33	0.41
1:A:1719:GLN:HA	1:A:1722:PHE:CE2	2.56	0.41
1:A:1900:GLY:C	1:A:1902:LYS:H	2.28	0.41
1:A:1959:THR:O	1:A:1963:ALA:CB	2.69	0.41
1:A:2293:ILE:C	1:A:2295:GLN:H	2.27	0.41
1:A:2893:MET:O	1:A:2895:GLY:N	2.46	0.41
1:A:3148:ASN:OD1	1:A:3150:ALA:N	2.45	0.41
1:A:3206:ILE:HA	1:A:3221:PRO:HG2	2.03	0.41
1:A:4006:PRO:C	1:A:4008:LEU:N	2.77	0.41
1:A:4278:HIS:O	1:A:4282:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1590:HIS:NE2	1:B:1594:ARG:NH1	2.68	0.41
1:B:1663:GLU:O	1:B:1664:ARG:C	2.63	0.41
1:B:1872:ARG:NH2	1:B:2164:ARG:NE	2.68	0.41
1:B:2208:VAL:HG12	1:B:2415:TRP:NE1	2.36	0.41
1:B:2231:ILE:CG2	1:B:2264:GLN:HE22	2.31	0.41
1:B:2578:MET:O	1:B:2582:GLY:HA3	2.19	0.41
1:B:2670:LEU:HD12	1:B:2670:LEU:O	2.20	0.41
1:B:3563:LEU:CD1	1:B:3845:ILE:HD11	2.49	0.41
1:B:3566:ASN:HD21	1:B:3859:LYS:HZ2	1.69	0.41
1:B:3886:TYR:CE2	1:B:3940:LEU:HD23	2.56	0.41
1:B:3910:GLN:HB3	1:B:4231:ARG:HD3	2.03	0.41
1:B:3960:LEU:HB3	1:B:4239:GLU:OE2	2.21	0.41
1:B:4201:GLU:HG3	1:B:4228:ASN:HB2	2.03	0.41
1:B:4284:ARG:HG2	1:B:4408:LEU:HB3	2.02	0.41
1:A:1697:PHE:CD2	1:A:1705:LEU:HD11	2.55	0.41
1:A:1701:GLY:HA2	1:A:2011:ARG:CZ	2.50	0.41
1:A:2127:LYS:O	1:A:2130:PRO:HD2	2.20	0.41
1:A:2376:LEU:HD12	1:A:2386:ALA:N	2.35	0.41
1:A:2586:GLY:CA	1:A:2815:LEU:HD13	2.43	0.41
1:A:2612:LEU:O	1:A:2612:LEU:HD12	2.21	0.41
1:A:2749:PRO:HG2	1:A:2759:VAL:HG11	2.01	0.41
1:A:2774:ARG:HH21	1:A:2779:THR:HB	1.85	0.41
1:A:2868:ILE:HG21	1:A:2922:GLU:OE2	2.21	0.41
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	2.01	0.41
1:A:3164:LEU:HD12	1:A:3164:LEU:HA	1.81	0.41
1:A:3553:VAL:O	1:A:3557:VAL:HG23	2.21	0.41
1:A:3652:LEU:HD21	1:A:3662:ALA:HB2	2.02	0.41
1:A:4012:LEU:HD12	1:A:4012:LEU:H	1.84	0.41
1:A:4270:ILE:HG22	1:A:4310:ILE:HD13	2.01	0.41
1:A:4314:VAL:O	1:A:4314:VAL:CG1	2.68	0.41
1:A:4349:ASN:ND2	1:A:4352:ASP:N	2.65	0.41
1:A:4648:VAL:CG1	1:A:4662:THR:HG21	2.41	0.41
1:A:4692:LEU:HD12	1:A:4700:LEU:HD21	2.02	0.41
1:B:2036:LEU:HD23	1:B:2036:LEU:O	2.20	0.41
1:B:2235:GLN:CD	1:B:2296:VAL:HG13	2.45	0.41
1:B:4377:PRO:O	1:B:4378:SER:C	2.63	0.41
1:A:1782:ALA:HA	1:A:1938:PHE:CZ	2.55	0.41
1:A:2204:ILE:CA	1:A:2207:LEU:HD12	2.44	0.41
1:A:2376:LEU:HD21	1:A:2384:ARG:HB3	2.02	0.41
1:A:2606:PRO:HG2	1:A:2615:TYR:CD1	2.56	0.41
1:A:2832:ASN:HA	1:A:2835:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2853:MET:HE3	1:A:2882:TRP:CD2	2.55	0.41
1:A:3071:PHE:HE2	1:A:3087:MET:HE1	1.84	0.41
1:A:3145:PHE:CD2	1:A:3147:MET:HE3	2.55	0.41
1:A:4012:LEU:HD21	1:A:4020:LEU:HD22	2.02	0.41
1:A:4283:GLU:OE2	1:A:4286:ARG:NH1	2.54	0.41
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	2.01	0.41
1:A:4401:GLU:HB2	1:A:4402:ILE:HD12	2.01	0.41
1:B:1493:ILE:O	1:B:1497:LEU:HG	2.21	0.41
1:B:1817:LEU:HD11	1:B:1936:TYR:CD2	2.55	0.41
1:B:2441:PRO:C	1:B:2443:GLU:H	2.28	0.41
1:B:3606:ASP:O	1:B:3610:ARG:HG3	2.21	0.41
1:B:4553:TYR:O	1:B:4555:VAL:HG22	2.20	0.41
1:A:1766:ILE:HG23	1:A:1767:HIS:H	1.84	0.41
1:A:1888:VAL:HG22	1:A:1909:HIS:CE1	2.56	0.41
1:A:2275:VAL:HG23	1:A:2397:VAL:HG23	2.03	0.41
1:A:2579:TRP:HZ2	1:A:2655:ARG:HD2	1.85	0.41
1:A:2694:PHE:CD2	1:A:2738:TRP:HB2	2.56	0.41
1:A:2748:LEU:CD2	1:A:2800:ARG:HD3	2.51	0.41
1:A:3145:PHE:CE2	1:A:3147:MET:HE3	2.55	0.41
1:A:3439:ASP:OD2	1:A:3442:LYS:HE2	2.21	0.41
1:A:3571:ARG:HB3	1:A:3571:ARG:NH1	2.35	0.41
1:A:4001:ILE:HB	1:A:4018:LYS:HD3	2.02	0.41
1:A:4006:PRO:O	1:A:4008:LEU:N	2.52	0.41
1:A:4240:ASN:HA	1:A:4241:PRO:HD2	1.89	0.41
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.67	0.41
1:A:4278:HIS:HD2	1:A:4343:TYR:CE1	2.39	0.41
1:A:4389:ARG:HH12	1:A:4393:MET:CE	2.24	0.41
1:A:4535:ARG:HH11	1:A:4535:ARG:HG2	1.84	0.41
1:A:4537:LEU:CD2	1:A:4548:LYS:HE3	2.50	0.41
1:A:4670:THR:HG22	1:A:4671:TRP:N	2.36	0.41
1:B:1820:GLN:HE22	1:B:1990:GLN:CD	2.27	0.41
1:B:1910:MET:CB	1:B:1929:MET:HG3	2.50	0.41
1:B:2711:LEU:HD12	1:B:2711:LEU:HA	1.89	0.41
1:B:2907:HIS:C	1:B:2909:ALA:N	2.77	0.41
1:B:3730:LEU:O	1:B:3731:ASN:C	2.62	0.41
1:B:3843:GLY:C	1:B:3845:ILE:N	2.76	0.41
1:B:4184:TRP:NE1	1:B:4214:ARG:HB2	2.35	0.41
1:B:4371:PRO:O	1:B:4372:ASP:HB2	2.20	0.41
1:A:2057:VAL:HG13	1:A:2059:LEU:H	1.86	0.41
1:A:2615:TYR:N	1:A:2615:TYR:HD2	2.18	0.41
1:A:2696:VAL:HG22	1:A:2697:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2855:GLU:OE2	1:A:2933:VAL:HG22	2.21	0.41
1:A:3903:LEU:C	1:A:3905:GLN:N	2.77	0.41
1:B:1483:ILE:HG22	1:B:1517:VAL:HG22	2.02	0.41
1:B:1497:LEU:HB3	1:B:1501:SER:CB	2.51	0.41
1:B:1500:GLY:O	1:B:1504:ASP:N	2.50	0.41
1:B:2239:LYS:O	1:B:2243:ILE:HG13	2.21	0.41
1:B:2278:SER:H	1:B:2398:GLN:NE2	2.17	0.41
1:B:2400:LEU:HD13	1:B:2408:ILE:CD1	2.48	0.41
1:B:2853:MET:HA	1:B:2882:TRP:CZ3	2.56	0.41
1:B:3567:LEU:HD23	1:B:3567:LEU:HA	1.94	0.41
1:B:3903:LEU:O	1:B:3909:TYR:HB2	2.21	0.41
1:B:4023:LEU:HG	1:B:4030:PHE:CD1	2.56	0.41
1:B:4509:LEU:HD23	1:B:4568:PHE:CE1	2.55	0.41
1:B:4535:ARG:HG2	1:B:4535:ARG:NH1	2.34	0.41
1:B:4644:LEU:HD23	1:B:4723:ILE:HG12	2.02	0.41
1:A:2028:PHE:CB	1:A:2075:VAL:HG13	2.44	0.41
1:A:2579:TRP:CE3	1:A:2659:VAL:HG21	2.56	0.41
1:A:2794:PRO:C	1:A:2796:THR:H	2.29	0.41
1:A:2989:VAL:HG13	1:A:3187:GLU:OE2	2.20	0.41
1:A:3567:LEU:HD23	1:A:3567:LEU:HA	1.91	0.41
1:A:3603:GLY:HA2	1:A:3664:MET:CE	2.48	0.41
1:A:3652:LEU:HB2	1:A:3684:PHE:CD1	2.55	0.41
1:A:4033:LEU:HD13	1:A:4062:TRP:CZ2	2.55	0.41
1:A:4426:MET:O	1:A:4430:LEU:HG	2.21	0.41
1:B:2628:LYS:C	1:B:2630:LYS:H	2.28	0.41
1:B:3258:ARG:HD2	1:B:3779:SER:HB2	2.01	0.41
1:B:3700:LEU:O	1:B:3701:ASP:C	2.63	0.41
1:B:3781:VAL:HG12	1:B:3782:THR:N	2.34	0.41
1:B:3930:LEU:O	1:B:3932:ASP:N	2.54	0.41
1:A:1712:SER:HB3	1:A:1766:ILE:HB	2.03	0.41
1:A:1726:PHE:CD2	1:A:1729:LEU:HD22	2.55	0.41
1:A:1756:LYS:HB3	1:A:1776:GLU:CD	2.46	0.41
1:A:1886:ARG:HG3	1:A:1887:ASP:H	1.81	0.41
1:A:2598:GLN:CD	1:A:2612:LEU:HB2	2.46	0.41
1:A:2848:ASN:HB3	1:A:2938:PHE:CE1	2.55	0.41
1:A:2890:ILE:HD13	1:A:2893:MET:CE	2.51	0.41
1:A:3078:VAL:HG23	1:A:3083:PHE:HB2	2.02	0.41
1:A:3093:GLY:O	1:A:3095:GLU:N	2.54	0.41
1:A:3230:SER:HA	1:A:3620:ARG:HE	1.86	0.41
1:A:3597:ALA:O	1:A:3601:TYR:HD1	2.04	0.41
1:A:3733:VAL:C	1:A:3735:ASN:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3844:ASN:O	1:A:3848:ASP:HB2	2.20	0.41
1:A:4024:ARG:CG	1:A:4031:SER:HA	2.49	0.41
1:A:4028:PRO:C	1:A:4030:PHE:N	2.79	0.41
1:A:4060:GLU:O	1:A:4064:VAL:HG23	2.21	0.41
1:A:4068:GLN:C	1:A:4070:SER:N	2.76	0.41
1:A:4592:GLY:CA	1:A:4725:SER:HB2	2.50	0.41
1:A:4678:ILE:O	1:A:4678:ILE:HG22	2.19	0.41
1:B:1734:LEU:HA	1:B:1742:ILE:HG12	2.03	0.41
1:B:1739:THR:O	1:B:1760:ILE:N	2.54	0.41
1:B:1831:LEU:HB3	1:B:1900:GLY:HA2	2.02	0.41
1:B:1844:GLN:O	1:B:1847:SER:HB2	2.21	0.41
1:B:2029:ASN:N	1:B:2029:ASN:HD22	2.18	0.41
1:B:2084:ARG:HG2	1:B:2084:ARG:NH1	2.36	0.41
1:B:2151:ALA:O	1:B:2154:SER:N	2.52	0.41
1:B:2236:LEU:O	1:B:2240:ILE:HG13	2.21	0.41
1:B:2270:HIS:CA	1:B:2392:ARG:HH11	2.33	0.41
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.43	0.41
1:B:2607:ALA:C	1:B:2609:THR:H	2.29	0.41
1:B:2887:LEU:O	1:B:2891:GLN:HG3	2.21	0.41
1:B:3087:MET:HE1	1:B:3090:LEU:HD23	2.02	0.41
1:B:3228:VAL:HA	1:B:3231:LEU:HD12	2.03	0.41
1:B:3539:LEU:HD12	1:B:3539:LEU:HA	1.92	0.41
1:B:3571:ARG:O	1:B:3575:GLU:HG3	2.19	0.41
1:B:3647:TRP:HB3	1:B:3652:LEU:HD22	2.02	0.41
1:B:3717:PRO:HG3	1:B:3761:MET:HE3	2.02	0.41
1:B:4022:CYS:HB3	1:B:4026:GLN:NE2	2.36	0.41
1:B:4056:PRO:HD2	1:B:4093:ARG:NH2	2.36	0.41
1:B:4094:VAL:HB	1:B:4423:ALA:HB1	2.02	0.41
1:B:4141:ASP:OD2	1:B:4143:SER:HB2	2.21	0.41
1:B:4145:LYS:HE2	1:B:4238:TYR:CE1	2.55	0.41
1:B:4157:TYR:HB2	1:B:4184:TRP:CB	2.50	0.41
1:B:4277:PHE:HB2	1:B:4363:LEU:HD12	2.03	0.41
1:B:4306:ALA:HA	1:B:4338:LEU:HD22	2.03	0.41
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.36	0.41
1:B:4503:ILE:HD11	1:B:4575:LEU:O	2.21	0.41
1:B:4509:LEU:O	1:B:4513:ILE:HG13	2.20	0.41
1:B:4649:TRP:CE3	1:B:4649:TRP:HA	2.55	0.41
1:A:1939:GLU:O	1:A:1941:LEU:HG	2.21	0.41
1:A:2332:PHE:HA	1:A:2335:THR:OG1	2.20	0.41
1:A:2359:VAL:HG23	1:A:2397:VAL:HG11	2.03	0.41
1:A:2550:GLU:HA	1:A:2553:GLN:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2618:SER:C	1:A:2620:ASP:N	2.79	0.41
1:A:3606:ASP:O	1:A:3610:ARG:HG3	2.21	0.41
1:A:4033:LEU:O	1:A:4034:VAL:C	2.64	0.41
1:A:4063:ILE:HD13	1:A:4082:LYS:NZ	2.36	0.41
1:A:4122:VAL:HB	1:A:4132:LEU:CD2	2.51	0.41
1:A:4606:GLN:HA	1:A:4609:SER:OG	2.21	0.41
1:B:1909:HIS:O	1:B:1911:ARG:HD3	2.22	0.41
1:B:1947:LEU:HD21	1:B:1982:GLU:CG	2.51	0.41
1:B:2260:LEU:O	1:B:2263:HIS:HB3	2.21	0.41
1:B:2370:LEU:C	1:B:2370:LEU:HD23	2.46	0.41
1:B:3015:ILE:O	1:B:3173:PHE:N	2.51	0.41
1:B:3685:LEU:O	1:B:3689:TYR:HB2	2.20	0.41
1:B:4162:ILE:HG22	1:B:4163:GLY:N	2.35	0.41
1:B:4711:THR:OG1	1:B:4716:TRP:NE1	2.54	0.41
1:A:1633:SER:O	1:A:1637:LYS:HG2	2.21	0.40
1:A:2439:PHE:HZ	1:A:2542:ASN:OD1	2.03	0.40
1:A:2877:ARG:HD2	1:A:2881:ARG:NH2	2.36	0.40
1:A:3022:LYS:HB2	1:A:3022:LYS:NZ	2.36	0.40
1:A:3025:LEU:HD23	1:A:3025:LEU:HA	1.86	0.40
1:A:3199:TYR:OH	1:A:3226:ALA:HB2	2.21	0.40
1:A:3237:THR:OG1	1:A:3238:ILE:HD12	2.21	0.40
1:A:3488:SER:C	1:A:3490:ILE:H	2.29	0.40
1:A:3720:VAL:HG21	1:A:3762:ILE:HD11	2.03	0.40
1:A:4086:MET:HG2	1:A:4093:ARG:HB2	1.99	0.40
1:A:4647:ALA:HA	1:A:4657:THR:HG22	2.02	0.40
1:A:4664:ILE:O	1:A:4665:SER:C	2.63	0.40
1:B:2120:THR:HB	1:B:2124:LEU:HG	2.03	0.40
1:B:2754:TYR:O	1:B:2756:THR:HG22	2.21	0.40
1:B:2914:GLN:O	1:B:2915:ASP:C	2.64	0.40
1:B:3046:TYR:CZ	1:B:3050:ASP:HB2	2.55	0.40
1:B:3222:SER:O	1:B:3223:HIS:C	2.64	0.40
1:B:3234:ILE:O	1:B:3238:ILE:HD13	2.21	0.40
1:B:3976:VAL:HG13	1:B:4105:VAL:HG11	2.01	0.40
1:B:4499:PHE:HA	1:B:4502:GLU:HB2	2.03	0.40
1:A:2005:ASP:OD1	1:A:2006:LEU:N	2.55	0.40
1:A:2212:ILE:O	1:A:2215:ILE:HG22	2.22	0.40
1:A:2489:PRO:O	1:A:2490:ALA:C	2.64	0.40
1:A:3225:ASP:O	1:A:3229:SER:CB	2.69	0.40
1:A:3698:SER:O	1:A:3704:PHE:HB2	2.22	0.40
1:A:4413:ASN:O	1:A:4414:ALA:C	2.64	0.40
1:B:1546:VAL:HG12	1:B:1547:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1820:GLN:NE2	1:B:1990:GLN:NE2	2.66	0.40
1:B:1928:HIS:CG	1:B:1933:THR:HG22	2.52	0.40
1:B:2630:LYS:O	1:B:2631:VAL:C	2.64	0.40
1:B:4083:ILE:HD11	1:B:4098:SER:HA	2.03	0.40
1:B:4264:PRO:HA	1:B:4322:SER:O	2.21	0.40
1:B:4493:ASP:OD1	1:B:4494:PRO:HD2	2.21	0.40
1:A:1619:PHE:C	1:A:1626:ASN:HD21	2.30	0.40
1:A:1726:PHE:CB	1:A:1729:LEU:HB3	2.51	0.40
1:A:2793:ASN:HB3	1:A:2794:PRO:HD2	2.04	0.40
1:A:2986:VAL:O	1:A:2988:LEU:HG	2.20	0.40
1:A:2995:LEU:CD2	1:A:2998:ILE:HD11	2.48	0.40
1:A:3256:THR:HB	1:A:3257:PRO:CD	2.51	0.40
1:A:3414:GLY:C	1:A:3416:LYS:N	2.79	0.40
1:A:4130:SER:HA	1:A:4131:PRO:HD3	1.88	0.40
1:A:4189:ASN:HA	1:A:4191:HIS:CD2	2.57	0.40
1:A:4245:LYS:HE2	1:A:4249:LEU:HD11	2.03	0.40
1:A:4418:LEU:HD11	1:A:4422:LYS:NZ	2.36	0.40
1:B:1578:SER:C	1:B:1580:TYR:N	2.78	0.40
1:B:1696:ARG:HH21	1:B:1726:PHE:HA	1.86	0.40
1:B:2379:LEU:HD12	1:B:2383:GLU:HG2	2.03	0.40
1:B:2946:LEU:O	1:B:2947:LYS:C	2.64	0.40
1:B:3084:LEU:O	1:B:3085:GLU:C	2.65	0.40
1:B:3256:THR:N	1:B:3259:HIS:HD2	2.19	0.40
1:B:3700:LEU:CD1	1:B:3701:ASP:N	2.80	0.40
1:B:4252:PHE:C	1:B:4254:GLY:H	2.27	0.40
1:B:4402:ILE:N	1:B:4402:ILE:CD1	2.81	0.40
1:B:4403:SER:HB2	1:B:4407:TRP:CD2	2.56	0.40
1:B:4428:ASN:O	1:B:4432:LYS:HG3	2.21	0.40
1:B:4703:ILE:CD1	1:B:4705:LEU:HD21	2.45	0.40
1:A:1853:GLN:HE22	1:A:1886:ARG:HH11	1.68	0.40
1:A:1898:LEU:HD23	1:A:1898:LEU:HA	1.89	0.40
1:A:2536:SER:HB2	1:A:2580:GLY:O	2.21	0.40
1:A:3947:ILE:O	1:A:3947:ILE:HD13	2.21	0.40
1:A:4247:ASN:HD21	1:A:4282:GLN:NE2	2.19	0.40
1:B:1867:LEU:H	1:B:1867:LEU:HD12	1.86	0.40
1:B:2029:ASN:HD22	1:B:2030:ARG:N	2.20	0.40
1:B:2135:CYS:O	1:B:2139:LEU:HB2	2.21	0.40
1:B:2258:LYS:HD3	1:B:2261:GLN:OE1	2.21	0.40
1:B:2688:LEU:HD13	1:B:2696:VAL:HB	2.04	0.40
1:B:3002:ASP:HA	1:B:3029:VAL:HG11	2.04	0.40
1:A:1778:LYS:HB3	1:A:1922:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1831:LEU:HD22	1:A:1898:LEU:HD13	2.04	0.40
1:A:2036:LEU:HD12	1:A:2036:LEU:O	2.21	0.40
1:A:2236:LEU:HD21	1:A:2293:ILE:CD1	2.44	0.40
1:A:2591:GLU:OE1	1:A:2611:PRO:HG2	2.22	0.40
1:A:2710:LEU:HD23	1:A:2762:PHE:CE2	2.57	0.40
1:A:3066:GLU:HG2	1:A:3136:GLN:NE2	2.36	0.40
1:A:3296:GLU:HG3	1:A:3567:LEU:HD13	2.04	0.40
1:A:3459:ASP:HA	1:A:3460:PRO:HD3	1.97	0.40
1:A:3845:ILE:H	1:A:3845:ILE:HG13	1.57	0.40
1:A:3868:LYS:C	1:A:3870:GLU:H	2.29	0.40
1:A:4057:ILE:HD12	1:A:4057:ILE:HA	1.96	0.40
1:A:4252:PHE:C	1:A:4254:GLY:N	2.79	0.40
1:A:4263:GLN:HA	1:A:4264:PRO:C	2.46	0.40
1:A:4284:ARG:CG	1:A:4408:LEU:HB3	2.49	0.40
1:B:1813:GLN:HE22	1:B:1941:LEU:H	1.69	0.40
1:B:1906:TRP:CZ2	1:B:1911:ARG:HG2	2.57	0.40
1:B:1928:HIS:NE2	1:B:1933:THR:CG2	2.81	0.40
1:B:2081:TYR:O	1:B:2082:ALA:HB3	2.21	0.40
1:B:2270:HIS:CB	1:B:2392:ARG:HH11	2.34	0.40
1:B:2309:LYS:HG3	1:B:2358:ASP:HB2	2.02	0.40
1:B:2420:ILE:HG13	1:B:2421:LEU:N	2.36	0.40
1:B:2519:ALA:HB2	1:B:2593:PHE:CE1	2.57	0.40
1:B:2580:GLY:C	1:B:2581:LEU:HD23	2.46	0.40
1:B:2645:ASP:OD2	1:B:2645:ASP:N	2.54	0.40
1:B:2745:GLU:HG2	1:B:2748:LEU:CD1	2.51	0.40
1:B:2799:GLY:HA3	1:B:3159:ALA:HB1	2.04	0.40
1:B:3271:ILE:HA	1:B:3592:VAL:HG21	2.03	0.40
1:B:3728:PRO:C	1:B:3730:LEU:H	2.29	0.40
1:B:3927:ASN:HB3	1:B:3930:LEU:HD12	2.02	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 X-ray entries followed by that with respect to entries of similar resolution.

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	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	2	18
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	5	30
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	3	23

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1836	LEU
1	A	2121	ALA
1	A	2409	SER
1	A	2560	MET
1	A	2617	VAL
1	A	2641	VAL
1	A	2646	VAL
1	A	2943	LEU
1	A	2992	ASN
1	A	3033	ASN
1	A	3219	ILE
1	A	3370	GLU
1	A	3371	PRO
1	A	3372	ALA
1	A	3603	GLY
1	A	4050	LYS
1	A	4051	ASP
1	A	4117	ASP
1	A	4121	ILE
1	A	4207	LEU
1	A	4548	LYS
1	A	4549	GLU
1	A	4660	LEU
1	B	1949	GLN
1	B	1975	PRO
1	B	1980	LYS
1	B	2071	MET
1	B	3602	ILE
1	B	3931	VAL
1	B	4207	LEU
1	A	1714	ASP
1	A	1949	GLN
1	A	2004	PHE
1	A	2080	GLY
1	A	2101	ILE

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Mol	Chain	Res	Type
1	A	2342	ASN
1	A	2527	ASP
1	A	2530	ARG
1	A	2628	LYS
1	A	2642	ALA
1	A	2645	ASP
1	A	2727	GLU
1	A	2776	SER
1	A	2789	VAL
1	A	2792	CYS
1	A	3218	ALA
1	A	3430	ASN
1	A	3440	THR
1	A	3488	SER
1	A	3715	GLY
1	A	3719	LEU
1	A	3841	ALA
1	A	3926	ASN
1	A	3994	GLY
1	A	3998	LEU
1	A	4000	SER
1	A	4014	THR
1	A	4053	VAL
1	A	4116	LEU
1	A	4123	GLU
1	A	4125	GLU
1	A	4158	LYS
1	A	4221	ILE
1	A	4342	ILE
1	A	4594	LEU
1	A	4666	ILE
1	A	4672	LYS
1	A	4709	GLN
1	B	1919	GLU
1	B	2141	ALA
1	B	2230	PRO
1	B	2384	ARG
1	B	2600	ILE
1	B	2641	VAL
1	B	2755	GLY
1	B	2775	THR
1	B	3092	ALA

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Mol	Chain	Res	Type
1	B	3603	GLY
1	B	3842	SER
1	B	3844	ASN
1	B	4113	THR
1	B	4221	ILE
1	B	4297	GLU
1	B	4340	SER
1	B	4464	ALA
1	B	4551	LYS
1	A	1663	GLU
1	A	1697	PHE
1	A	1703	GLU
1	A	1727	ALA
1	A	1923	HIS
1	A	2001	ASP
1	A	2089	ASP
1	A	2140	SER
1	A	2282	LYS
1	A	2329	ASP
1	A	2374	ASN
1	A	2705	THR
1	A	2871	HIS
1	A	2990	LEU
1	A	3082	SER
1	A	3671	TYR
1	A	3693	LYS
1	A	3843	GLY
1	A	3933	LYS
1	A	4007	GLN
1	A	4055	GLU
1	A	4118	MET
1	A	4131	PRO
1	A	4163	GLY
1	A	4168	PHE
1	A	4318	SER
1	A	4401	GLU
1	A	4412	GLU
1	B	1663	GLU
1	B	2001	ASP
1	B	2527	ASP
1	B	2915	ASP
1	B	3080	GLU

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Mol	Chain	Res	Type
1	B	3094	GLY
1	B	3248	ARG
1	B	3692	LYS
1	B	4071	ASN
1	B	4692	LEU
1	A	1799	ASP
1	A	1837	GLN
1	A	2002	GLU
1	A	2054	SER
1	A	2122	GLU
1	A	2177	ALA
1	A	2270	HIS
1	A	2370	LEU
1	A	2653	THR
1	A	2690	ALA
1	A	2744	ASP
1	A	2891	GLN
1	A	3094	GLY
1	A	3166	ASN
1	A	3444	MET
1	A	3699	PHE
1	A	3907	HIS
1	A	4026	GLN
1	A	4029	SER
1	A	4259	ARG
1	A	4519	ASN
1	B	1506	ASP
1	B	2165	LYS
1	B	2308	PRO
1	B	2401	LYS
1	B	2749	PRO
1	B	2947	LYS
1	B	3932	ASP
1	B	4003	GLU
1	B	4051	ASP
1	B	4053	VAL
1	B	4189	ASN
1	B	4674	LYS
1	A	2363	TRP
1	A	2601	ALA
1	A	2987	PRO
1	A	3140	ASN

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Mol	Chain	Res	Type
1	A	3142	HIS
1	A	3471	SER
1	A	3712	LEU
1	A	3999	THR
1	A	4011	LEU
1	A	4169	GLU
1	A	4579	SER
1	A	4691	TYR
1	A	4712	SER
1	B	1498	THR
1	B	2069	GLN
1	B	2140	SER
1	B	2210	ASP
1	B	2558	PHE
1	B	3693	LYS
1	B	3849	ASP
1	B	3963	ASP
1	B	4412	GLU
1	A	1868	SER
1	A	1944	GLY
1	A	2966	SER
1	A	3164	LEU
1	A	3716	CYS
1	A	3845	ILE
1	B	1582	LYS
1	B	1630	PRO
1	B	1727	ALA
1	B	4459	GLU
1	B	4621	LEU
1	A	3395	PRO
1	A	3806	ARG
1	A	3976	VAL
1	B	4131	PRO
1	A	4056	PRO
1	B	3093	GLY
1	B	4556	PRO
1	A	2644	PRO
1	A	2755	GLY
1	A	3602	ILE
1	A	3677	PRO
1	B	1579	PRO
1	B	2380	PRO

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Mol	Chain	Res	Type
1	A	2208	VAL
1	B	4094	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	2457/3028 (81%)	2242 (91%)	215 (9%)	9	33
1	B	2353/3028 (78%)	2202 (94%)	151 (6%)	16	42
All	All	4810/6056 (79%)	4444 (92%)	366 (8%)	12	37

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1516	GLU
1	A	1559	ASP
1	A	1585	GLU
1	A	1589	ASN
1	A	1593	ASP
1	A	1596	ASN
1	A	1665	ILE
1	A	1699	PHE
1	A	1718	ILE
1	A	1753	THR
1	A	1756	LYS
1	A	1766	ILE
1	A	1809	ASN
1	A	1844	GLN
1	A	1874	LYS
1	A	1882	LEU
1	A	1911	ARG
1	A	1922	LEU
1	A	1934	PHE
1	A	1962	GLN
1	A	1973	PHE

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Mol	Chain	Res	Type
1	A	1978	THR
1	A	1995	VAL
1	A	2006	LEU
1	A	2029	ASN
1	A	2053	ASN
1	A	2069	GLN
1	A	2071	MET
1	A	2073	ILE
1	A	2090	ASN
1	A	2107	MET
1	A	2120	THR
1	A	2136	GLN
1	A	2142	GLN
1	A	2149	LEU
1	A	2152	LEU
1	A	2155	VAL
1	A	2191	GLU
1	A	2199	ILE
1	A	2203	MET
1	A	2239	LYS
1	A	2274	MET
1	A	2324	THR
1	A	2329	ASP
1	A	2346	GLU
1	A	2354	ILE
1	A	2359	VAL
1	A	2369	SER
1	A	2392	ARG
1	A	2408	ILE
1	A	2409	SER
1	A	2415	TRP
1	A	2421	LEU
1	A	2424	GLN
1	A	2435	SER
1	A	2442	GLN
1	A	2450	ASN
1	A	2511	LEU
1	A	2512	VAL
1	A	2529	THR
1	A	2572	ARG
1	A	2587	LEU
1	A	2603	THR

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Mol	Chain	Res	Type
1	A	2613	LEU
1	A	2615	TYR
1	A	2626	LEU
1	A	2641	VAL
1	A	2645	ASP
1	A	2650	THR
1	A	2683	THR
1	A	2685	THR
1	A	2694	PHE
1	A	2728	THR
1	A	2747	ASN
1	A	2761	THR
1	A	2775	THR
1	A	2793	ASN
1	A	2859	GLU
1	A	2873	ILE
1	A	2880	SER
1	A	2883	ASP
1	A	2897	THR
1	A	2926	THR
1	A	2930	ILE
1	A	2944	ASP
1	A	2954	ASN
1	A	2978	VAL
1	A	2998	ILE
1	A	3007	GLN
1	A	3022	LYS
1	A	3024	VAL
1	A	3026	SER
1	A	3027	ARG
1	A	3037	ILE
1	A	3043	ASN
1	A	3052	ASP
1	A	3084	LEU
1	A	3134	THR
1	A	3141	LEU
1	A	3143	VAL
1	A	3145	PHE
1	A	3158	SER
1	A	3168	CYS
1	A	3175	GLU
1	A	3179	GLU

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Mol	Chain	Res	Type
1	A	3186	SER
1	A	3195	GLU
1	A	3200	ILE
1	A	3204	VAL
1	A	3206	ILE
1	A	3216	LEU
1	A	3240	GLU
1	A	3269	LEU
1	A	3270	LEU
1	A	3271	ILE
1	A	3278	LEU
1	A	3324	LEU
1	A	3366	LEU
1	A	3373	ILE
1	A	3381	SER
1	A	3399	THR
1	A	3405	MET
1	A	3412	LEU
1	A	3415	LYS
1	A	3432	ILE
1	A	3457	LEU
1	A	3516	ASP
1	A	3522	ILE
1	A	3564	LEU
1	A	3566	ASN
1	A	3569	SER
1	A	3571	ARG
1	A	3583	THR
1	A	3584	GLN
1	A	3612	ASP
1	A	3623	SER
1	A	3630	SER
1	A	3663	ILE
1	A	3676	ASP
1	A	3678	SER
1	A	3691	ASP
1	A	3695	THR
1	A	3700	LEU
1	A	3707	ASN
1	A	3719	LEU
1	A	3720	VAL
1	A	3725	ASN

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Mol	Chain	Res	Type
1	A	3729	VAL
1	A	3730	LEU
1	A	3731	ASN
1	A	3759	SER
1	A	3760	PHE
1	A	3776	ASP
1	A	3791	SER
1	A	3806	ARG
1	A	3813	ARG
1	A	3817	LEU
1	A	3830	LEU
1	A	3865	ILE
1	A	3867	LEU
1	A	3922	ASN
1	A	3925	ASN
1	A	3947	ILE
1	A	3974	ILE
1	A	3998	LEU
1	A	4004	THR
1	A	4007	GLN
1	A	4023	LEU
1	A	4026	GLN
1	A	4034	VAL
1	A	4039	GLN
1	A	4040	ASN
1	A	4043	ASP
1	A	4048	PHE
1	A	4055	GLU
1	A	4069	LEU
1	A	4079	ASN
1	A	4091	SER
1	A	4100	SER
1	A	4134	LEU
1	A	4200	LEU
1	A	4206	SER
1	A	4225	LEU
1	A	4232	MET
1	A	4240	ASN
1	A	4259	ARG
1	A	4267	ARG
1	A	4282	GLN
1	A	4290	LEU

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Mol	Chain	Res	Type
1	A	4295	PHE
1	A	4337	ILE
1	A	4353	MET
1	A	4360	LEU
1	A	4362	GLN
1	A	4385	GLU
1	A	4388	THR
1	A	4404	THR
1	A	4428	ASN
1	A	4434	GLN
1	A	4495	LEU
1	A	4503	ILE
1	A	4550	TRP
1	A	4553	TYR
1	A	4565	ILE
1	A	4566	SER
1	A	4606	GLN
1	A	4610	GLN
1	A	4638	ASN
1	A	4649	TRP
1	A	4671	TRP
1	A	4692	LEU
1	A	4693	ASN
1	A	4694	GLU
1	A	4711	THR
1	A	4714	GLN
1	B	1479	ARG
1	B	1490	THR
1	B	1545	LEU
1	B	1555	VAL
1	B	1629	LEU
1	B	1658	GLU
1	B	1665	ILE
1	B	1712	SER
1	B	1734	LEU
1	B	1736	ASP
1	B	1742	ILE
1	B	1762	ASN
1	B	1781	LEU
1	B	1809	ASN
1	B	1828	ASP
1	B	1840	LYS

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Mol	Chain	Res	Type
1	B	1867	LEU
1	B	1882	LEU
1	B	1901	ASN
1	B	1941	LEU
1	B	1946	ARG
1	B	1968	MET
1	B	2029	ASN
1	B	2031	LEU
1	B	2071	MET
1	B	2075	VAL
1	B	2097	SER
1	B	2106	GLU
1	B	2129	VAL
1	B	2149	LEU
1	B	2166	CYS
1	B	2189	GLN
1	B	2194	VAL
1	B	2210	ASP
1	B	2215	ILE
1	B	2231	ILE
1	B	2235	GLN
1	B	2236	LEU
1	B	2239	LYS
1	B	2253	GLN
1	B	2254	GLU
1	B	2260	LEU
1	B	2275	VAL
1	B	2282	LYS
1	B	2290	LEU
1	B	2320	LEU
1	B	2368	ASN
1	B	2374	ASN
1	B	2381	ASN
1	B	2408	ILE
1	B	2414	VAL
1	B	2421	LEU
1	B	2423	THR
1	B	2425	MET
1	B	2504	GLN
1	B	2525	ILE
1	B	2540	LEU
1	B	2550	GLU

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Mol	Chain	Res	Type
1	B	2581	LEU
1	B	2587	LEU
1	B	2603	THR
1	B	2612	LEU
1	B	2613	LEU
1	B	2650	THR
1	B	2699	LEU
1	B	2745	GLU
1	B	2759	VAL
1	B	2782	LYS
1	B	2821	THR
1	B	2825	THR
1	B	2841	ASN
1	B	2883	ASP
1	B	2897	THR
1	B	2899	GLU
1	B	2927	ASP
1	B	2928	LYS
1	B	2929	LYS
1	B	2946	LEU
1	B	2966	SER
1	B	2977	LYS
1	B	2984	LEU
1	B	2996	ASP
1	B	3018	SER
1	B	3026	SER
1	B	3043	ASN
1	B	3050	ASP
1	B	3059	LEU
1	B	3087	MET
1	B	3140	ASN
1	B	3151	SER
1	B	3164	LEU
1	B	3195	GLU
1	B	3302	LEU
1	B	3315	VAL
1	B	3322	GLN
1	B	3539	LEU
1	B	3552	LYS
1	B	3560	SER
1	B	3563	LEU
1	B	3589	VAL

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Mol	Chain	Res	Type
1	B	3619	ILE
1	B	3623	SER
1	B	3634	VAL
1	B	3676	ASP
1	B	3700	LEU
1	B	3720	VAL
1	B	3725	ASN
1	B	3867	LEU
1	B	3947	ILE
1	B	3998	LEU
1	B	4005	ILE
1	B	4012	LEU
1	B	4029	SER
1	B	4046	GLN
1	B	4091	SER
1	B	4105	VAL
1	B	4157	TYR
1	B	4185	VAL
1	B	4189	ASN
1	B	4200	LEU
1	B	4206	SER
1	B	4218	THR
1	B	4219	SER
1	B	4231	ARG
1	B	4232	MET
1	B	4258	THR
1	B	4318	SER
1	B	4323	ASN
1	B	4324	ILE
1	B	4327	ASP
1	B	4334	VAL
1	B	4341	THR
1	B	4356	LEU
1	B	4379	ILE
1	B	4402	ILE
1	B	4413	ASN
1	B	4425	LYS
1	B	4434	GLN
1	B	4500	GLU
1	B	4503	ILE
1	B	4548	LYS
1	B	4555	VAL

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Mol	Chain	Res	Type
1	B	4558	THR
1	B	4573	GLN
1	B	4607	SER
1	B	4618	ASN
1	B	4644	LEU
1	B	4693	ASN
1	B	4698	GLU
1	B	4709	GLN
1	B	4715	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1549	GLN
1	A	1609	GLN
1	A	1640	ASN
1	A	1680	GLN
1	A	1690	GLN
1	A	1791	HIS
1	A	1809	ASN
1	A	1813	GLN
1	A	1844	GLN
1	A	1850	GLN
1	A	1853	GLN
1	A	1857	ASN
1	A	1858	ASN
1	A	1865	GLN
1	A	1877	HIS
1	A	1891	GLN
1	A	1909	HIS
1	A	1949	GLN
1	A	1971	ASN
1	A	1990	GLN
1	A	2018	GLN
1	A	2029	ASN
1	A	2042	GLN
1	A	2044	GLN
1	A	2047	GLN
1	A	2053	ASN
1	A	2086	ASN
1	A	2090	ASN

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Mol	Chain	Res	Type
1	A	2136	GLN
1	A	2138	GLN
1	A	2142	GLN
1	A	2167	GLN
1	A	2200	ASN
1	A	2269	ASN
1	A	2295	GLN
1	A	2351	HIS
1	A	2366	ASN
1	A	2368	ASN
1	A	2428	GLN
1	A	2429	ASN
1	A	2436	ASN
1	A	2447	GLN
1	A	2450	ASN
1	A	2495	GLN
1	A	2535	ASN
1	A	2552	ASN
1	A	2564	ASN
1	A	2565	GLN
1	A	2598	GLN
1	A	2656	HIS
1	A	2747	ASN
1	A	2778	HIS
1	A	2787	GLN
1	A	2793	ASN
1	A	2810	HIS
1	A	2826	GLN
1	A	2832	ASN
1	A	2869	GLN
1	A	2891	GLN
1	A	2907	HIS
1	A	2942	ASN
1	A	2954	ASN
1	A	2961	GLN
1	A	3007	GLN
1	A	3009	GLN
1	A	3033	ASN
1	A	3043	ASN
1	A	3077	ASN
1	A	3088	ASN
1	A	3119	ASN

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Mol	Chain	Res	Type
1	A	3156	ASN
1	A	3223	HIS
1	A	3253	ASN
1	A	3266	GLN
1	A	3277	GLN
1	A	3286	ASN
1	A	3310	ASN
1	A	3326	GLN
1	A	3331	GLN
1	A	3338	GLN
1	A	3377	GLN
1	A	3430	ASN
1	A	3437	ASN
1	A	3484	GLN
1	A	3555	ASN
1	A	3566	ASN
1	A	3607	GLN
1	A	3646	ASN
1	A	3687	ASN
1	A	3721	GLN
1	A	3725	ASN
1	A	3731	ASN
1	A	3785	ASN
1	A	3794	GLN
1	A	3820	GLN
1	A	3824	GLN
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3961	ASN
1	A	3981	ASN
1	A	4017	GLN
1	A	4046	GLN
1	A	4066	GLN
1	A	4073	GLN
1	A	4079	ASN
1	A	4112	ASN
1	A	4191	HIS
1	A	4210	HIS
1	A	4234	ASN
1	A	4250	HIS
1	A	4263	GLN

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Mol	Chain	Res	Type
1	A	4278	HIS
1	A	4282	GLN
1	A	4323	ASN
1	A	4349	ASN
1	A	4362	GLN
1	A	4370	ASN
1	A	4413	ASN
1	A	4428	ASN
1	A	4573	GLN
1	A	4574	GLN
1	A	4596	ASN
1	A	4610	GLN
1	A	4718	GLN
1	B	1480	HIS
1	B	1522	GLN
1	B	1547	ASN
1	B	1568	HIS
1	B	1589	ASN
1	B	1609	GLN
1	B	1626	ASN
1	B	1640	ASN
1	B	1690	GLN
1	B	1793	ASN
1	B	1798	ASN
1	B	1800	HIS
1	B	1813	GLN
1	B	1820	GLN
1	B	1826	GLN
1	B	1857	ASN
1	B	1865	GLN
1	B	1877	HIS
1	B	1891	GLN
1	B	1893	GLN
1	B	1901	ASN
1	B	1920	ASN
1	B	1931	ASN
1	B	1990	GLN
1	B	2029	ASN
1	B	2042	GLN
1	B	2044	GLN
1	B	2047	GLN
1	B	2053	ASN

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Mol	Chain	Res	Type
1	B	2110	GLN
1	B	2216	GLN
1	B	2235	GLN
1	B	2241	GLN
1	B	2264	GLN
1	B	2295	GLN
1	B	2315	GLN
1	B	2342	ASN
1	B	2351	HIS
1	B	2368	ASN
1	B	2381	ASN
1	B	2398	GLN
1	B	2429	ASN
1	B	2504	GLN
1	B	2542	ASN
1	B	2547	ASN
1	B	2564	ASN
1	B	2571	ASN
1	B	2667	HIS
1	B	2700	ASN
1	B	2765	GLN
1	B	2793	ASN
1	B	2832	ASN
1	B	2841	ASN
1	B	2861	GLN
1	B	2964	ASN
1	B	2992	ASN
1	B	3033	ASN
1	B	3043	ASN
1	B	3142	HIS
1	B	3196	ASN
1	B	3223	HIS
1	B	3235	HIS
1	B	3253	ASN
1	B	3259	HIS
1	B	3272	ASN
1	B	3322	GLN
1	B	3338	GLN
1	B	3555	ASN
1	B	3566	ASN
1	B	3577	GLN
1	B	3580	ASN

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Mol	Chain	Res	Type
1	B	3731	ASN
1	B	3785	ASN
1	B	3794	GLN
1	B	3799	HIS
1	B	3820	GLN
1	B	3887	ASN
1	B	3925	ASN
1	B	3926	ASN
1	B	3953	ASN
1	B	3981	ASN
1	B	4016	GLN
1	B	4026	GLN
1	B	4038	GLN
1	B	4152	GLN
1	B	4189	ASN
1	B	4199	GLN
1	B	4205	HIS
1	B	4263	GLN
1	B	4278	HIS
1	B	4323	ASN
1	B	4391	HIS
1	B	4434	GLN
1	B	4573	GLN
1	B	4574	GLN
1	B	4596	ASN
1	B	4618	ASN
1	B	4651	ASN
1	B	4693	ASN
1	B	4709	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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
2	ADP	B	9007	-	28,29,29	1.68	5 (17%)	43,45,45	1.93	11 (25%)
2	ADP	B	9008	-	28,29,29	1.67	5 (17%)	43,45,45	1.92	11 (25%)
2	ADP	A	9001	-	28,29,29	1.67	5 (17%)	43,45,45	1.92	10 (23%)
2	ADP	A	9003	-	28,29,29	1.69	5 (17%)	43,45,45	1.94	10 (23%)
2	ADP	B	9010	-	28,29,29	1.68	5 (17%)	43,45,45	1.94	12 (27%)
2	ADP	B	9009	-	28,29,29	1.68	5 (17%)	43,45,45	1.93	10 (23%)
2	ADP	A	9002	-	28,29,29	1.66	5 (17%)	43,45,45	1.91	11 (25%)
2	ADP	A	9004	-	28,29,29	1.68	5 (17%)	43,45,45	1.94	11 (25%)

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
2	ADP	B	9007	-	-	5/16/32/32	0/3/3/3
2	ADP	B	9008	-	-	3/16/32/32	0/3/3/3
2	ADP	A	9001	-	-	6/16/32/32	0/3/3/3
2	ADP	A	9003	-	-	6/16/32/32	0/3/3/3
2	ADP	B	9010	-	-	6/16/32/32	0/3/3/3
2	ADP	B	9009	-	-	6/16/32/32	0/3/3/3
2	ADP	A	9002	-	-	4/16/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/16/32/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	5.47	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9008	ADP	C5-C4	5.41	1.48	1.39
2	B	9009	ADP	C5-C4	5.38	1.48	1.39
2	A	9003	ADP	C5-C4	5.37	1.48	1.39
2	A	9004	ADP	C5-C4	5.35	1.48	1.39
2	B	9010	ADP	C5-C4	5.35	1.48	1.39
2	B	9007	ADP	C5-C4	5.34	1.48	1.39
2	A	9001	ADP	C5-C4	5.33	1.48	1.39
2	A	9003	ADP	C5-C6	3.29	1.50	1.41
2	B	9009	ADP	C5-C6	3.28	1.50	1.41
2	B	9008	ADP	C5-C6	3.28	1.50	1.41
2	B	9007	ADP	C5-C6	3.26	1.50	1.41
2	A	9002	ADP	C5-C6	3.26	1.50	1.41
2	A	9001	ADP	C5-C6	3.26	1.50	1.41
2	B	9010	ADP	C5-C6	3.25	1.50	1.41
2	A	9004	ADP	C5-C6	3.25	1.50	1.41
2	B	9010	ADP	PA-O3A	2.80	1.62	1.59
2	B	9007	ADP	PA-O3A	2.80	1.62	1.59
2	A	9004	ADP	PA-O3A	2.79	1.62	1.59
2	A	9003	ADP	PA-O3A	2.71	1.62	1.59
2	B	9009	ADP	PA-O3A	2.65	1.62	1.59
2	B	9008	ADP	PA-O3A	2.56	1.62	1.59
2	B	9009	ADP	C8-N7	2.54	1.36	1.31
2	A	9004	ADP	C8-N7	2.52	1.36	1.31
2	A	9001	ADP	PA-O3A	2.52	1.62	1.59
2	B	9007	ADP	C8-N7	2.52	1.36	1.31
2	A	9003	ADP	C8-N7	2.51	1.36	1.31
2	A	9001	ADP	C8-N7	2.50	1.36	1.31
2	A	9002	ADP	C5-N7	-2.49	1.34	1.39
2	B	9010	ADP	C8-N7	2.47	1.36	1.31
2	A	9003	ADP	C5-N7	-2.46	1.34	1.39
2	B	9010	ADP	C5-N7	-2.45	1.34	1.39
2	B	9007	ADP	C5-N7	-2.44	1.34	1.39
2	B	9008	ADP	C8-N7	2.43	1.36	1.31
2	A	9004	ADP	C5-N7	-2.41	1.34	1.39
2	A	9001	ADP	C5-N7	-2.41	1.34	1.39
2	B	9009	ADP	C5-N7	-2.39	1.34	1.39
2	A	9002	ADP	C8-N7	2.38	1.36	1.31
2	B	9008	ADP	C5-N7	-2.37	1.34	1.39
2	A	9002	ADP	PA-O3A	2.24	1.61	1.59

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9003	ADP	C5-C4-N3	-5.67	118.91	126.72
2	A	9002	ADP	C5-C4-N3	-5.67	118.91	126.72
2	B	9008	ADP	C5-C4-N3	-5.67	118.91	126.72
2	B	9009	ADP	C5-C4-N3	-5.62	118.98	126.72
2	B	9010	ADP	C5-C4-N3	-5.60	119.00	126.72
2	B	9007	ADP	C5-C4-N3	-5.60	119.00	126.72
2	A	9001	ADP	C5-C4-N3	-5.57	119.04	126.72
2	A	9004	ADP	C5-C4-N3	-5.57	119.05	126.72
2	A	9003	ADP	N3-C4-N9	4.63	135.04	127.17
2	B	9008	ADP	N3-C4-N9	4.60	135.00	127.17
2	A	9002	ADP	N3-C4-N9	4.59	134.97	127.17
2	B	9009	ADP	N3-C4-N9	4.58	134.95	127.17
2	B	9010	ADP	N3-C4-N9	4.57	134.93	127.17
2	B	9007	ADP	N3-C4-N9	4.54	134.88	127.17
2	A	9004	ADP	N3-C4-N9	4.53	134.87	127.17
2	A	9001	ADP	N3-C4-N9	4.51	134.84	127.17
2	A	9004	ADP	N3-C2-N1	-4.41	121.91	128.58
2	A	9003	ADP	N3-C2-N1	-4.38	121.96	128.58
2	B	9007	ADP	N3-C2-N1	-4.37	121.97	128.58
2	B	9010	ADP	N3-C2-N1	-4.35	122.00	128.58
2	A	9001	ADP	N3-C2-N1	-4.35	122.00	128.58
2	B	9009	ADP	N3-C2-N1	-4.33	122.03	128.58
2	A	9002	ADP	N3-C2-N1	-4.27	122.11	128.58
2	B	9008	ADP	N3-C2-N1	-4.26	122.14	128.58
2	A	9003	ADP	C2-N3-C4	4.12	121.89	111.83
2	A	9004	ADP	C2-N3-C4	4.09	121.82	111.83
2	B	9007	ADP	C2-N3-C4	4.08	121.80	111.83
2	B	9009	ADP	C2-N3-C4	4.07	121.78	111.83
2	B	9010	ADP	C2-N3-C4	4.07	121.77	111.83
2	A	9002	ADP	C2-N3-C4	4.06	121.75	111.83
2	B	9008	ADP	C2-N3-C4	4.05	121.73	111.83
2	A	9001	ADP	C2-N3-C4	4.05	121.71	111.83
2	B	9007	ADP	C4-C5-N7	-3.41	106.68	110.58
2	B	9010	ADP	C4-C5-N7	-3.41	106.69	110.58
2	A	9001	ADP	C4-C5-N7	-3.39	106.71	110.58
2	A	9004	ADP	C4-C5-N7	-3.39	106.71	110.58
2	A	9002	ADP	C4-C5-N7	-3.38	106.71	110.58
2	B	9009	ADP	C4-C5-N7	-3.38	106.71	110.58
2	A	9003	ADP	C4-C5-N7	-3.38	106.72	110.58
2	B	9008	ADP	C4-C5-N7	-3.38	106.72	110.58
2	A	9003	ADP	C5-N7-C8	2.82	107.88	103.45
2	B	9009	ADP	C5-N7-C8	2.77	107.81	103.45
2	A	9002	ADP	C5-N7-C8	2.77	107.80	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9007	ADP	C5-N7-C8	2.74	107.76	103.45
2	B	9010	ADP	C5-N7-C8	2.72	107.73	103.45
2	A	9004	ADP	C5-N7-C8	2.72	107.73	103.45
2	A	9001	ADP	C5-N7-C8	2.72	107.72	103.45
2	B	9008	ADP	C5-N7-C8	2.70	107.69	103.45
2	A	9003	ADP	C3'-C2'-C1'	2.69	106.55	101.46
2	A	9001	ADP	C3'-C2'-C1'	2.67	106.52	101.46
2	A	9004	ADP	C4-N9-C8	2.67	108.54	105.74
2	B	9009	ADP	C3'-C2'-C1'	2.66	106.50	101.46
2	B	9010	ADP	C4-N9-C8	2.64	108.51	105.74
2	B	9007	ADP	C3'-C2'-C1'	2.61	106.40	101.46
2	B	9008	ADP	C3'-C2'-C1'	2.59	106.36	101.46
2	B	9008	ADP	C4-N9-C8	2.57	108.44	105.74
2	A	9002	ADP	C3'-C2'-C1'	2.56	106.31	101.46
2	B	9010	ADP	C3'-C2'-C1'	2.56	106.31	101.46
2	A	9004	ADP	C3'-C2'-C1'	2.54	106.28	101.46
2	B	9007	ADP	C4-N9-C8	2.54	108.40	105.74
2	A	9001	ADP	C4-N9-C8	2.48	108.34	105.74
2	B	9009	ADP	C4-N9-C8	2.44	108.30	105.74
2	B	9007	ADP	C6-C5-N7	2.43	136.78	132.09
2	A	9004	ADP	C6-C5-N7	2.42	136.75	132.09
2	A	9002	ADP	C4-N9-C8	2.42	108.28	105.74
2	B	9010	ADP	C6-C5-N7	2.41	136.73	132.09
2	A	9003	ADP	C6-C5-N7	2.39	136.70	132.09
2	A	9004	ADP	C2-N1-C6	2.39	122.66	118.73
2	A	9003	ADP	C4-N9-C8	2.39	108.24	105.74
2	B	9009	ADP	C6-C5-N7	2.39	136.69	132.09
2	A	9001	ADP	C6-C5-N7	2.37	136.66	132.09
2	A	9002	ADP	C6-C5-N7	2.37	136.66	132.09
2	B	9008	ADP	C6-C5-N7	2.35	136.63	132.09
2	B	9007	ADP	C2-N1-C6	2.35	122.58	118.73
2	A	9001	ADP	C2-N1-C6	2.34	122.57	118.73
2	A	9003	ADP	C2-N1-C6	2.33	122.56	118.73
2	B	9010	ADP	C2-N1-C6	2.33	122.56	118.73
2	B	9009	ADP	C2-N1-C6	2.32	122.54	118.73
2	B	9008	ADP	C2-N1-C6	2.31	122.53	118.73
2	A	9002	ADP	C2-N1-C6	2.29	122.49	118.73
2	A	9004	ADP	N9-C8-N7	-2.11	110.94	113.94
2	B	9010	ADP	N9-C8-N7	-2.06	111.01	113.94
2	B	9007	ADP	N9-C8-N7	-2.04	111.04	113.94
2	B	9008	ADP	N9-C8-N7	-2.03	111.06	113.94
2	A	9002	ADP	N9-C8-N7	-2.01	111.09	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9010	ADP	C2'-C3'-C4'	2.00	106.47	102.61

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	A	9001	ADP	C5'-O5'-PA-O3A
2	A	9003	ADP	C5'-O5'-PA-O1A
2	A	9003	ADP	C5'-O5'-PA-O2A
2	A	9003	ADP	C5'-O5'-PA-O3A
2	B	9007	ADP	C5'-O5'-PA-O3A
2	B	9009	ADP	C5'-O5'-PA-O1A
2	B	9009	ADP	C5'-O5'-PA-O2A
2	B	9009	ADP	C5'-O5'-PA-O3A
2	B	9010	ADP	C5'-O5'-PA-O2A
2	B	9010	ADP	C5'-O5'-PA-O3A
2	A	9001	ADP	PB-O3A-PA-O2A
2	A	9002	ADP	PB-O3A-PA-O2A
2	A	9003	ADP	PB-O3A-PA-O2A
2	A	9004	ADP	PB-O3A-PA-O2A
2	B	9007	ADP	PB-O3A-PA-O2A
2	B	9008	ADP	PB-O3A-PA-O2A
2	B	9009	ADP	PB-O3A-PA-O2A
2	B	9010	ADP	PB-O3A-PA-O2A
2	A	9002	ADP	C5'-O5'-PA-O1A
2	B	9007	ADP	C5'-O5'-PA-O1A
2	B	9010	ADP	C5'-O5'-PA-O1A
2	A	9002	ADP	O4'-C4'-C5'-O5'
2	A	9001	ADP	O4'-C4'-C5'-O5'
2	B	9008	ADP	O4'-C4'-C5'-O5'
2	A	9004	ADP	PB-O3A-PA-O1A
2	B	9010	ADP	PB-O3A-PA-O1A
2	A	9003	ADP	O4'-C4'-C5'-O5'
2	A	9004	ADP	O4'-C4'-C5'-O5'
2	B	9007	ADP	O4'-C4'-C5'-O5'
2	B	9009	ADP	O4'-C4'-C5'-O5'
2	B	9010	ADP	O4'-C4'-C5'-O5'
2	A	9001	ADP	PB-O3A-PA-O1A
2	A	9002	ADP	PB-O3A-PA-O1A
2	A	9003	ADP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	9007	ADP	PB-O3A-PA-O1A
2	B	9008	ADP	PB-O3A-PA-O1A
2	B	9009	ADP	PB-O3A-PA-O1A

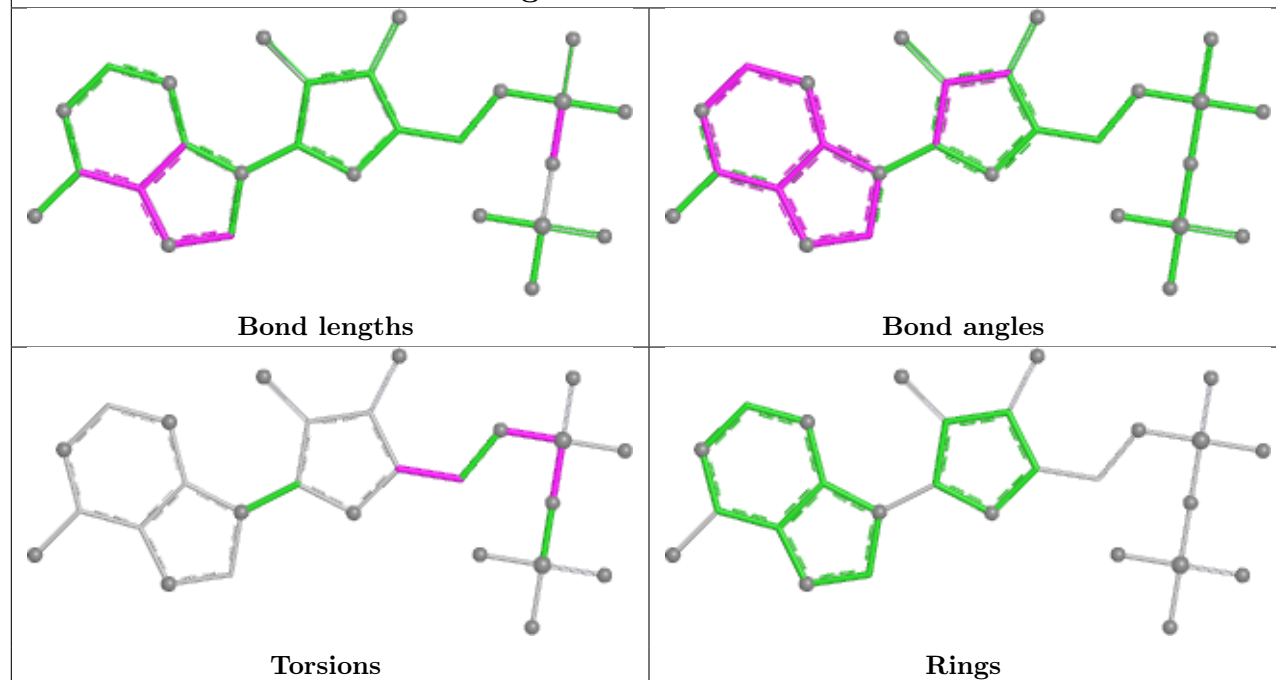
There are no ring outliers.

5 monomers are involved in 10 short contacts:

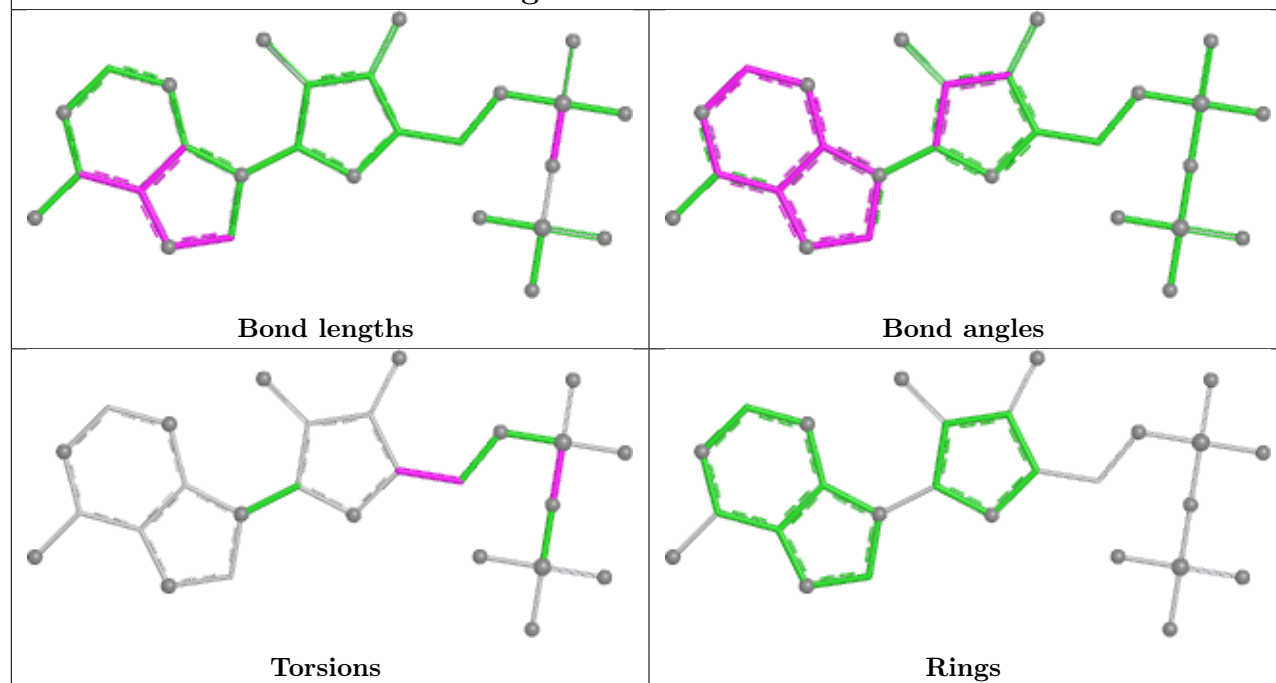
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	B	9010	ADP	2	0
2	B	9009	ADP	1	0
2	A	9002	ADP	4	0
2	A	9004	ADP	2	0

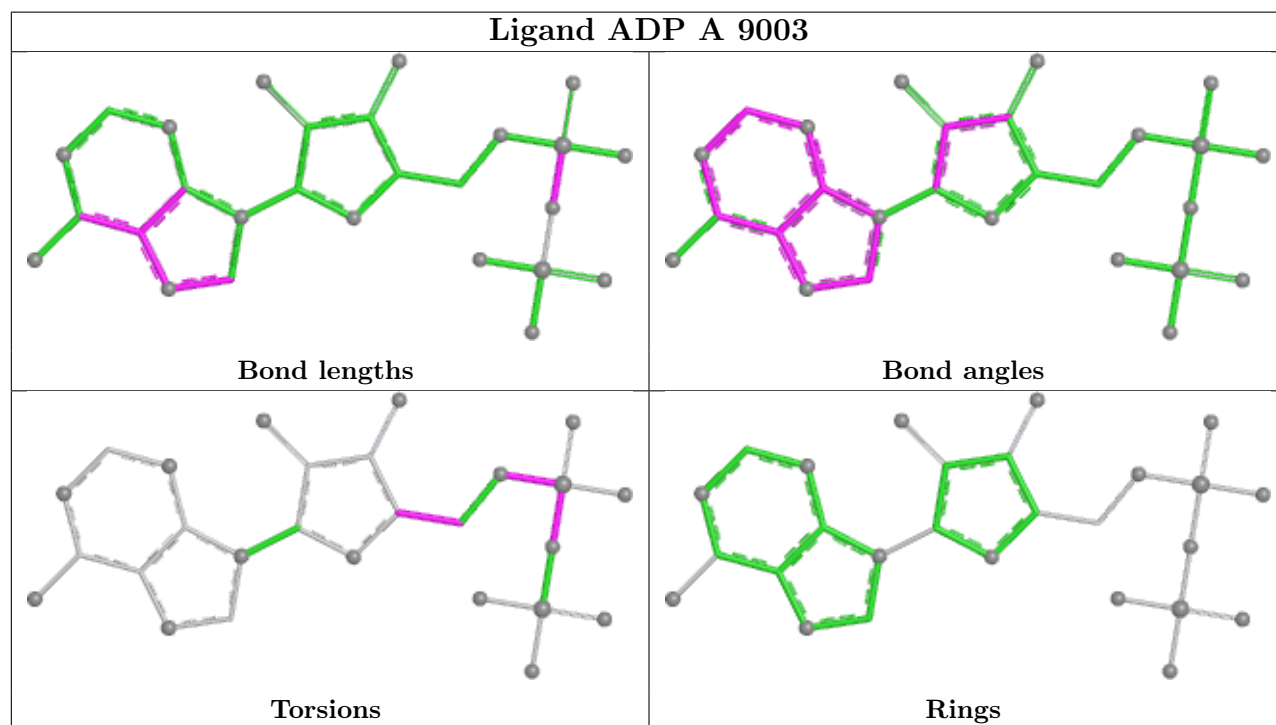
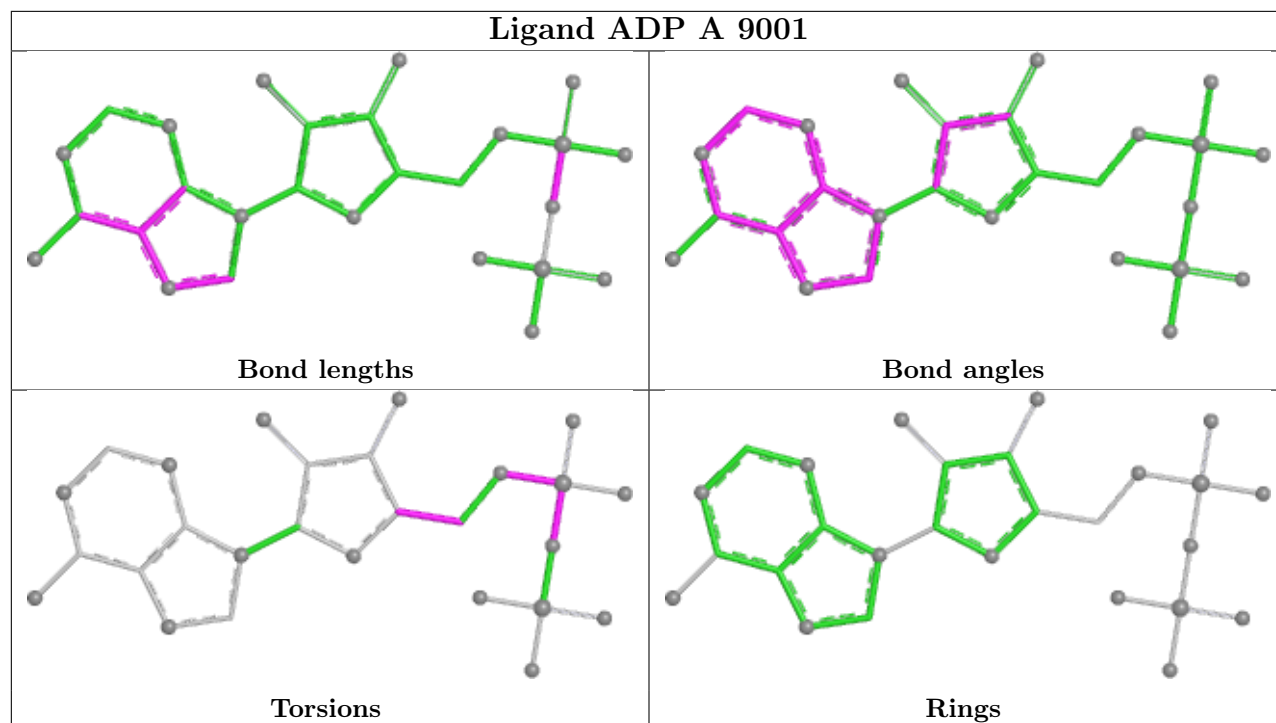
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

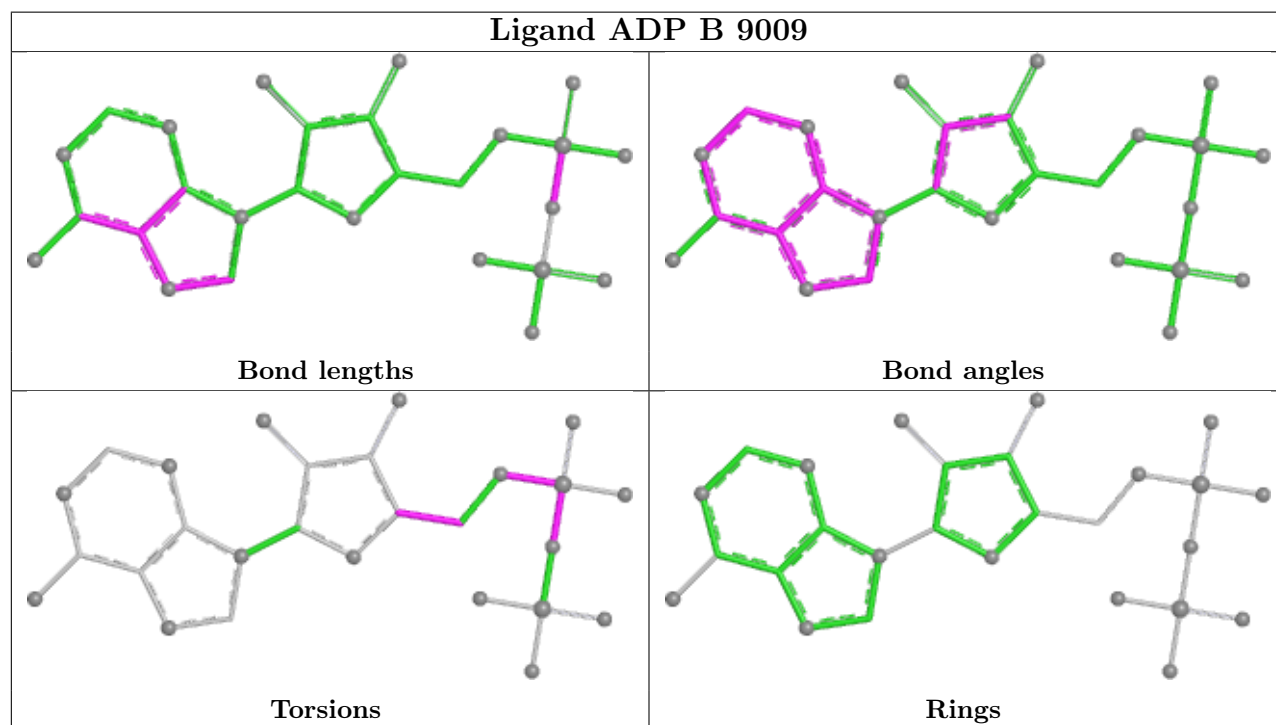
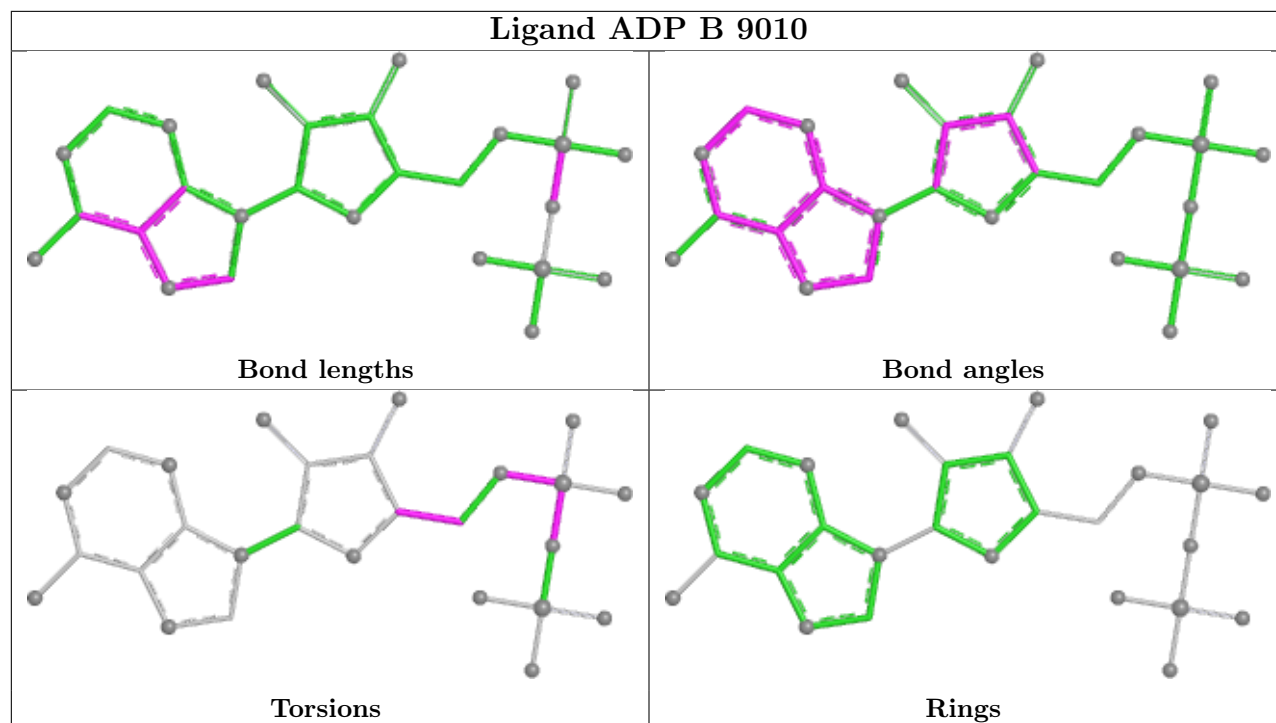
Ligand ADP B 9007

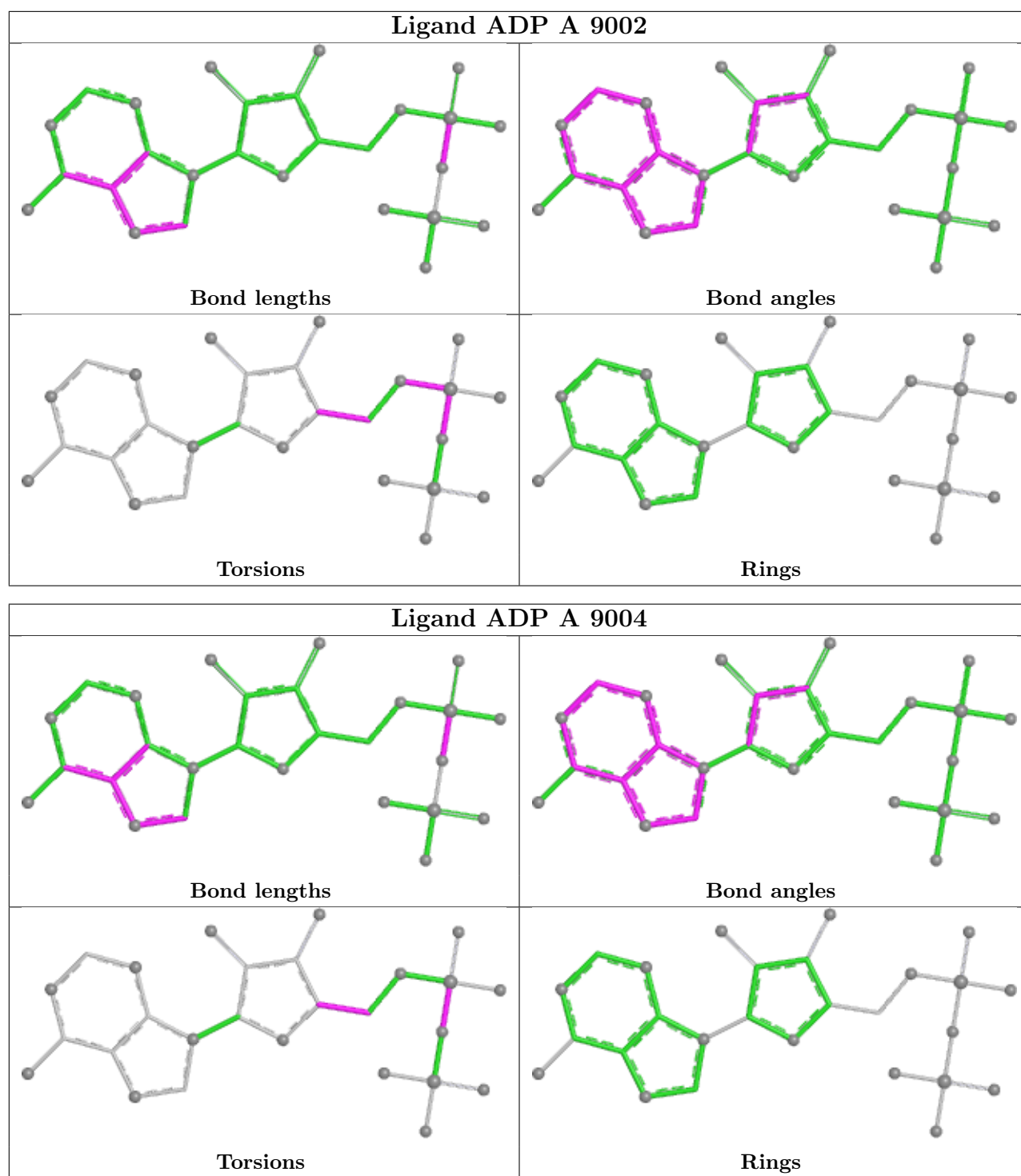


Ligand ADP B 9008









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	3042/3367 (90%)	-0.48	2 (0%) 92 87	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.46	6 (0%) 91 81	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.47	8 (0%) 92 87	64, 133, 209, 335	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4550	TRP	2.8
1	B	3094	GLY	2.7
1	B	3727	ASP	2.6
1	B	3095	GLU	2.5
1	B	3708	LEU	2.5
1	A	4122	VAL	2.2
1	B	2101	ILE	2.2
1	B	2280	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

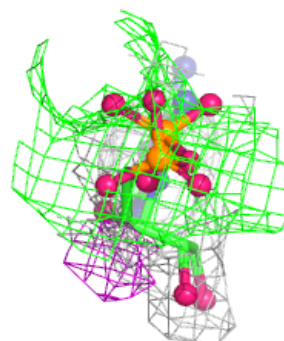
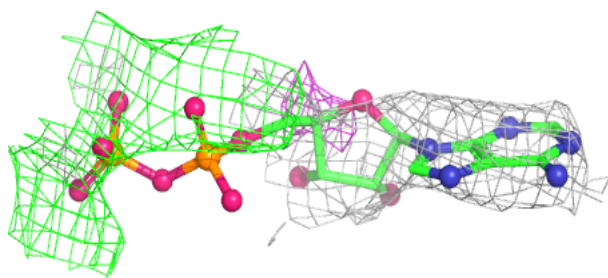
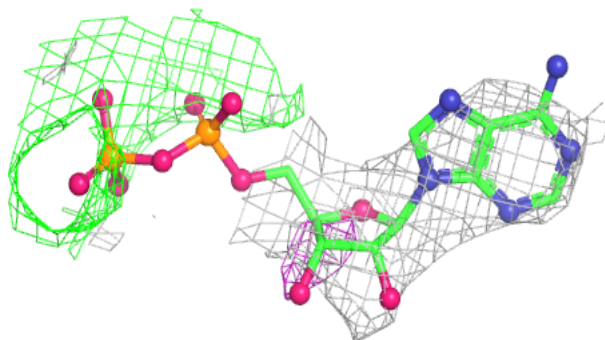
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	B	9008	27/27	0.88	0.12	129,129,129,129	0
2	ADP	A	9004	27/27	0.93	0.09	129,129,129,129	0
2	ADP	B	9010	27/27	0.93	0.09	129,129,129,129	0
2	ADP	A	9001	27/27	0.94	0.12	129,129,129,129	0
2	ADP	A	9002	27/27	0.95	0.10	129,129,129,129	0
2	ADP	A	9003	27/27	0.96	0.09	129,129,129,129	0
2	ADP	B	9007	27/27	0.96	0.10	129,129,129,129	0
2	ADP	B	9009	27/27	0.97	0.08	129,129,129,129	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

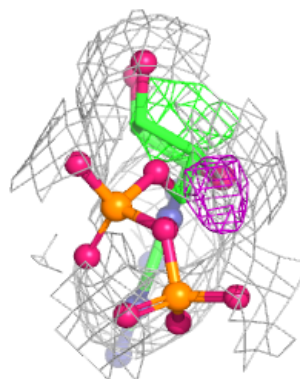
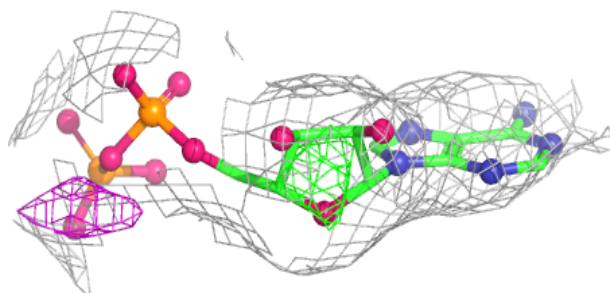
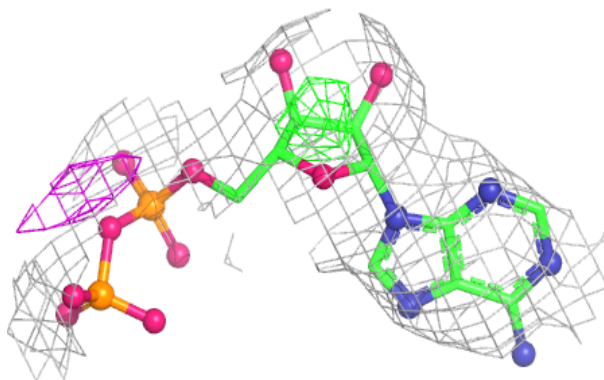
Electron density around ADP B 9008:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

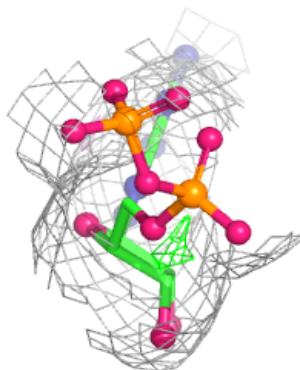
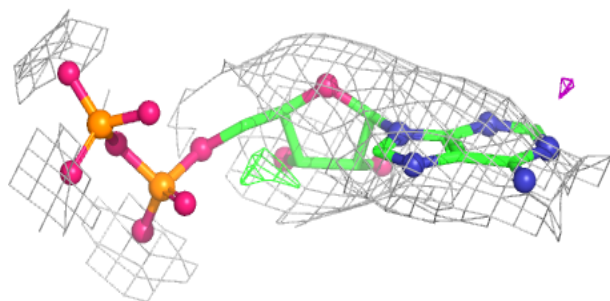
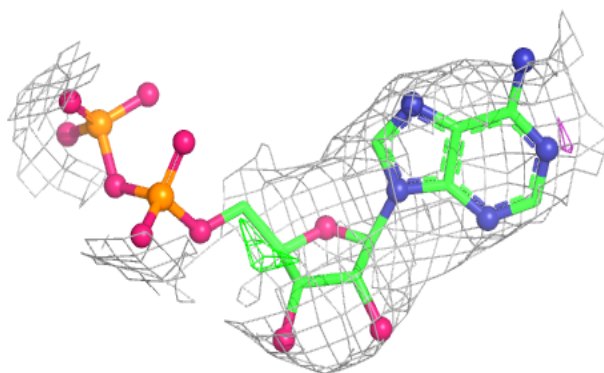


Electron density around ADP A 9004:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

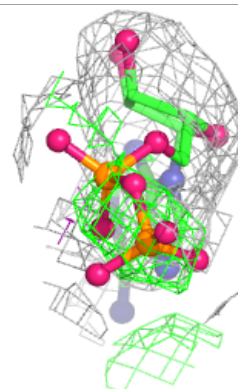
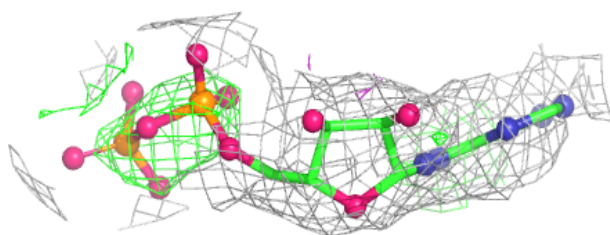
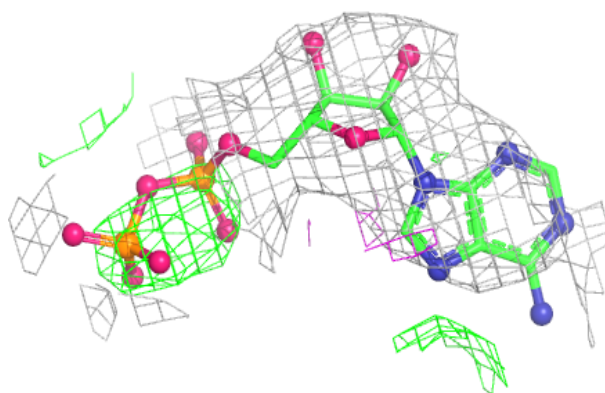
**Electron density around ADP B 9010:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

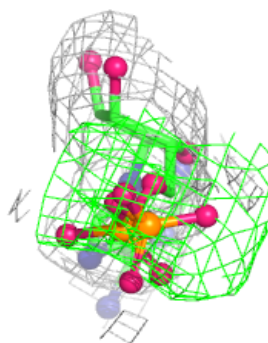
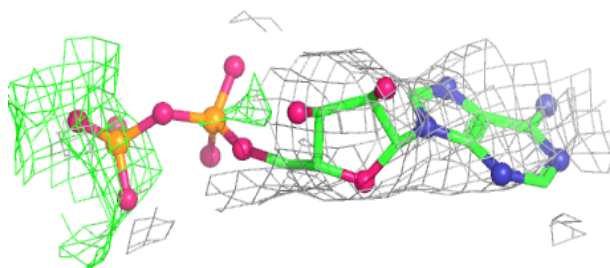
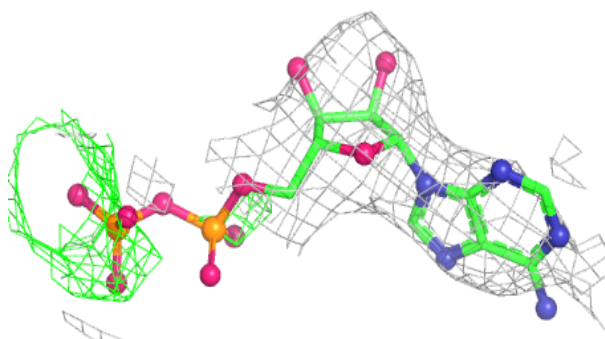


Electron density around ADP A 9001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

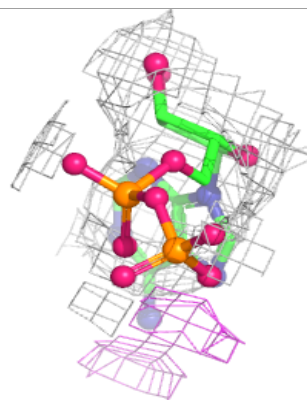
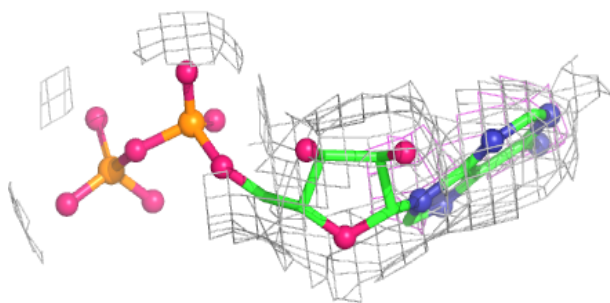
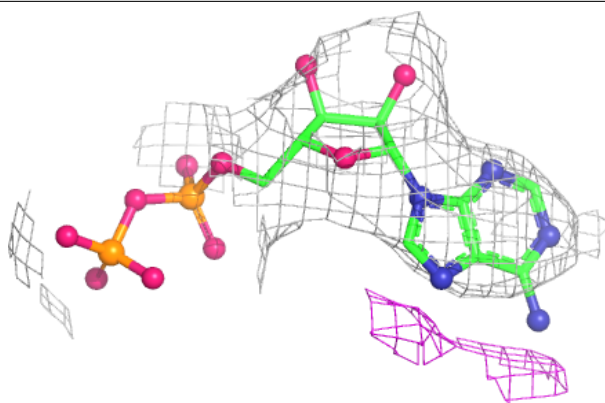
**Electron density around ADP A 9002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

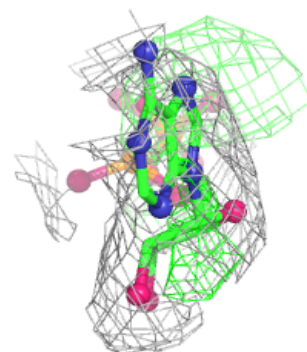
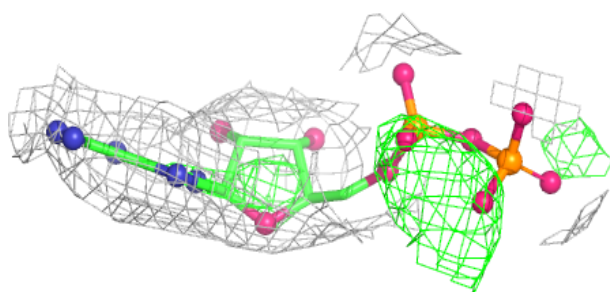
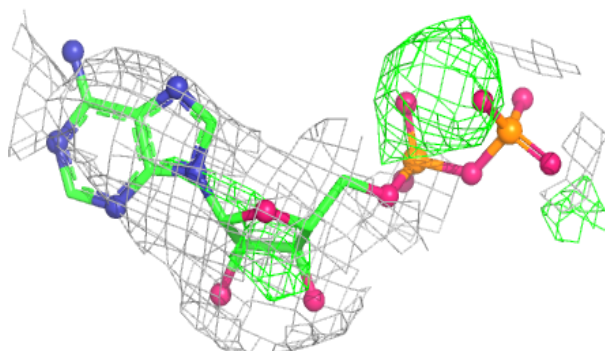


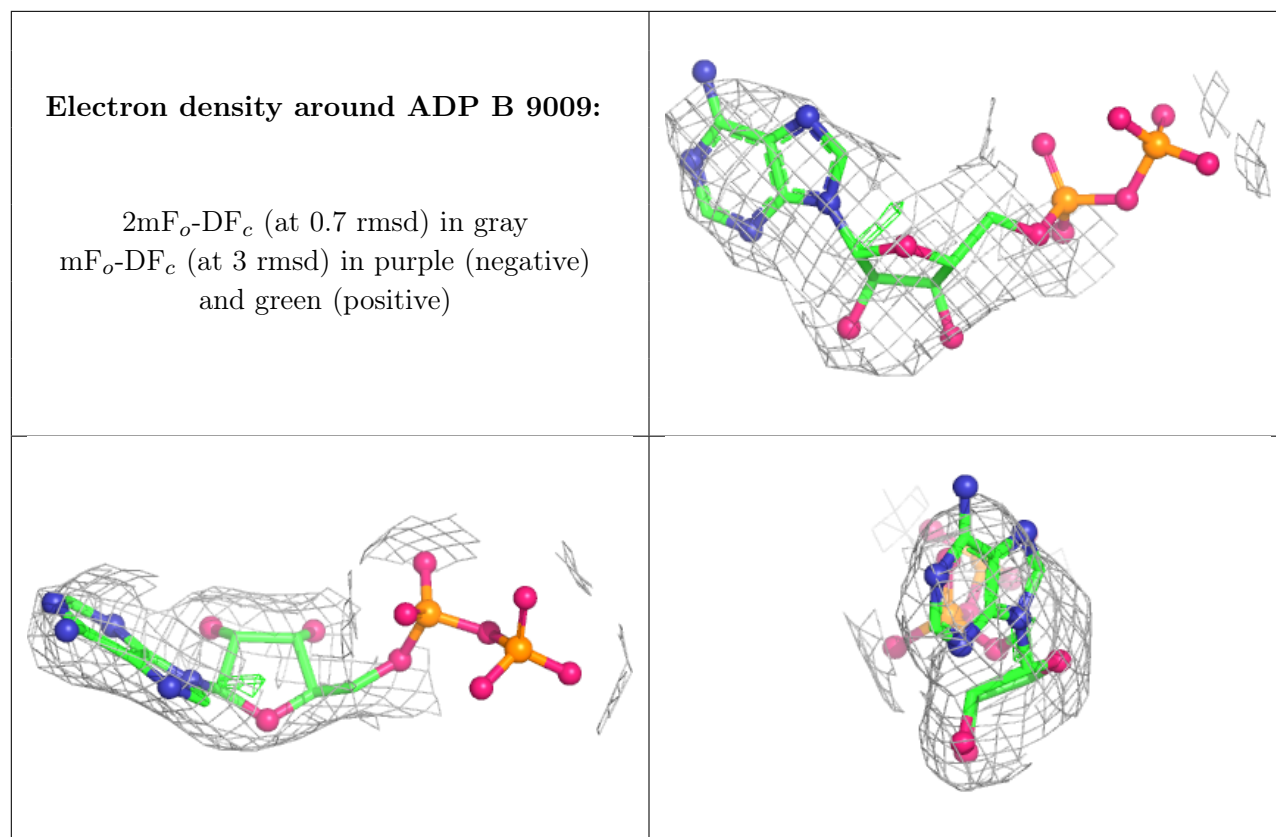
Electron density around ADP A 9003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 9007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.