



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:30 AM UTC

PDB ID : 8UXM / pdb_00008uxm
EMDB ID : EMD-42769
Title : Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium and calmodulin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.56 Å(reported)
Based on initial model : 7UA5

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

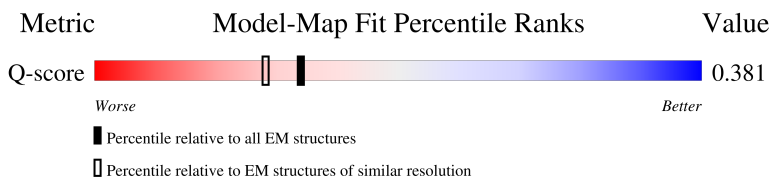
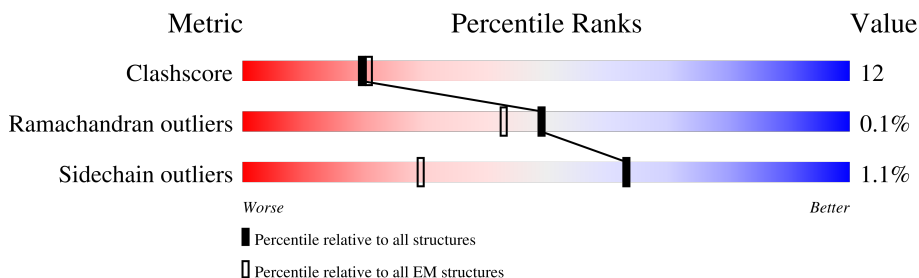
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.56 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12750 (3.06 - 4.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	149	
1	J	149	
1	K	149	
1	L	149	

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Mol	Chain	Length	Quality of chain
2	A	4967	10% 62% 23% • 15%
2	B	4967	10% 62% 22% • 15%
2	C	4967	10% 63% 22% • 15%
2	D	4967	10% 62% 22% • 15%
3	E	108	• 81% 17% ••
3	F	108	• 81% 18% ••
3	G	108	81% 18% ••
3	H	108	81% 17% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 143464 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	J	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	L	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	K	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	B	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	C	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	D	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

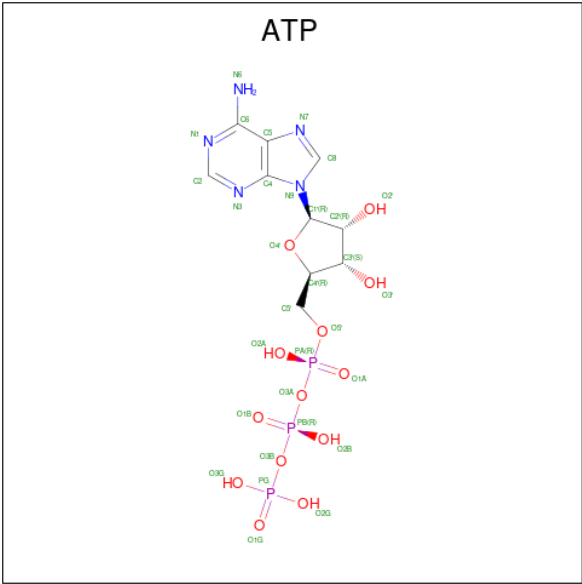
Mol	Chain	Residues	Atoms		AltConf
4	I	4	Total	Ca	0
			4	4	
4	A	1	Total	Ca	0
			1	1	
4	J	4	Total	Ca	0
			4	4	
4	L	4	Total	Ca	0
			4	4	
4	K	4	Total	Ca	0
			4	4	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

(labeled as "Ligand of Interest" by depositor).

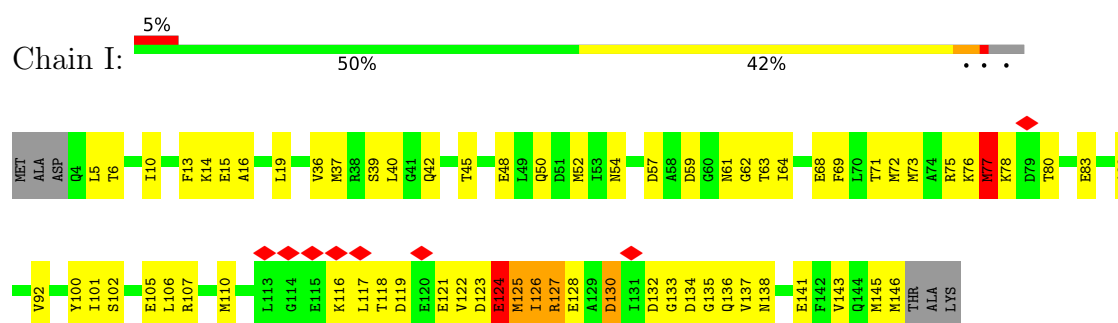


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

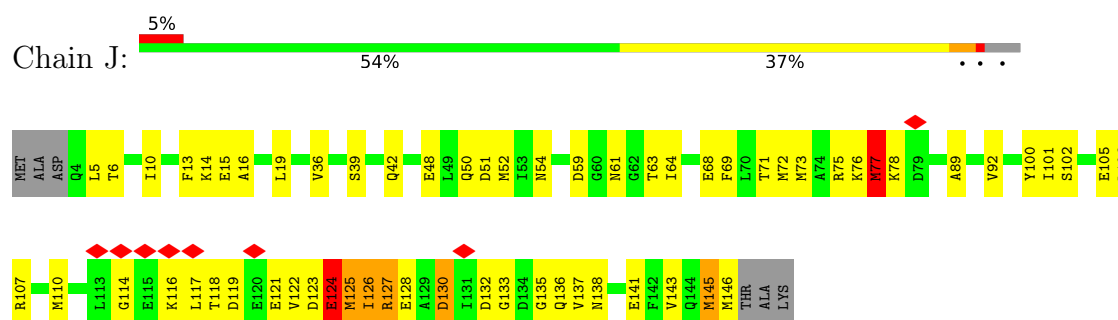
3 Residue-property plots [i](#)

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

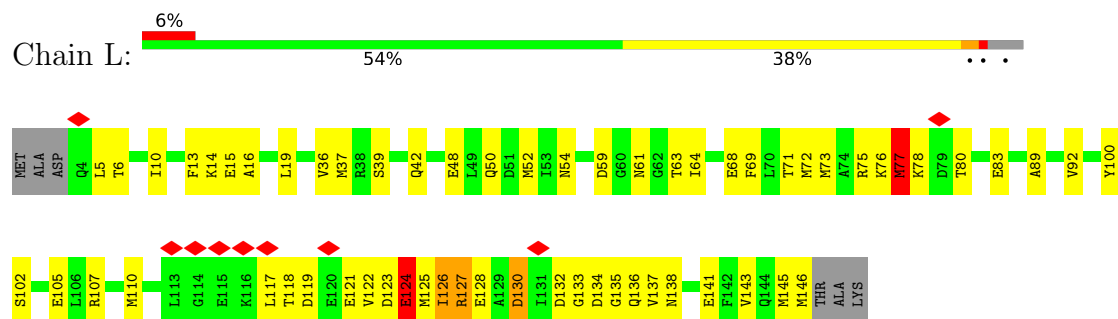
• Molecule 1: Calmodulin-1



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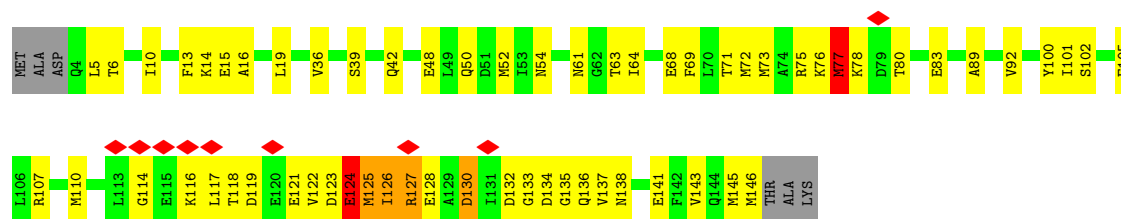


• Molecule 1: Calmodulin-1

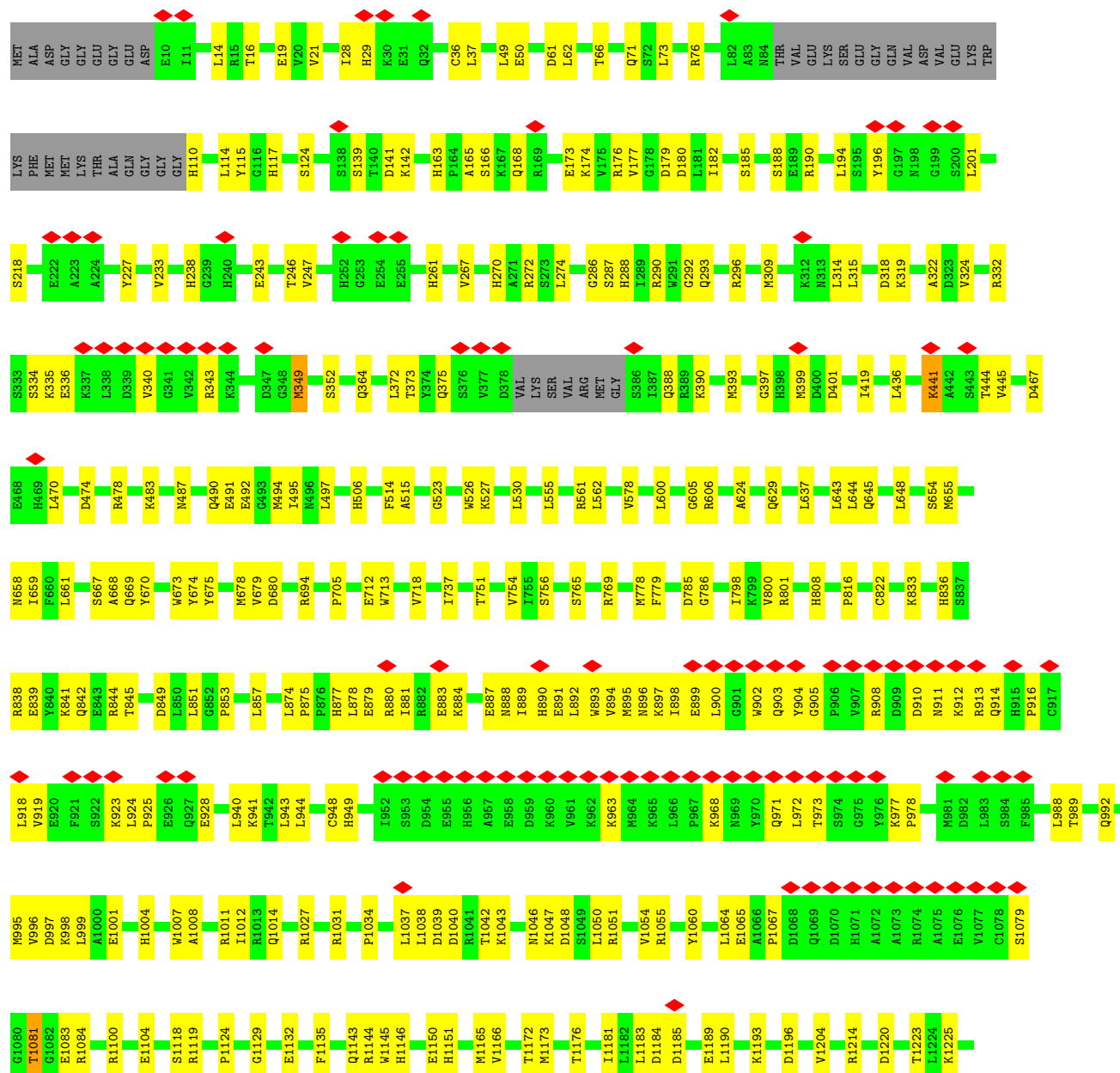


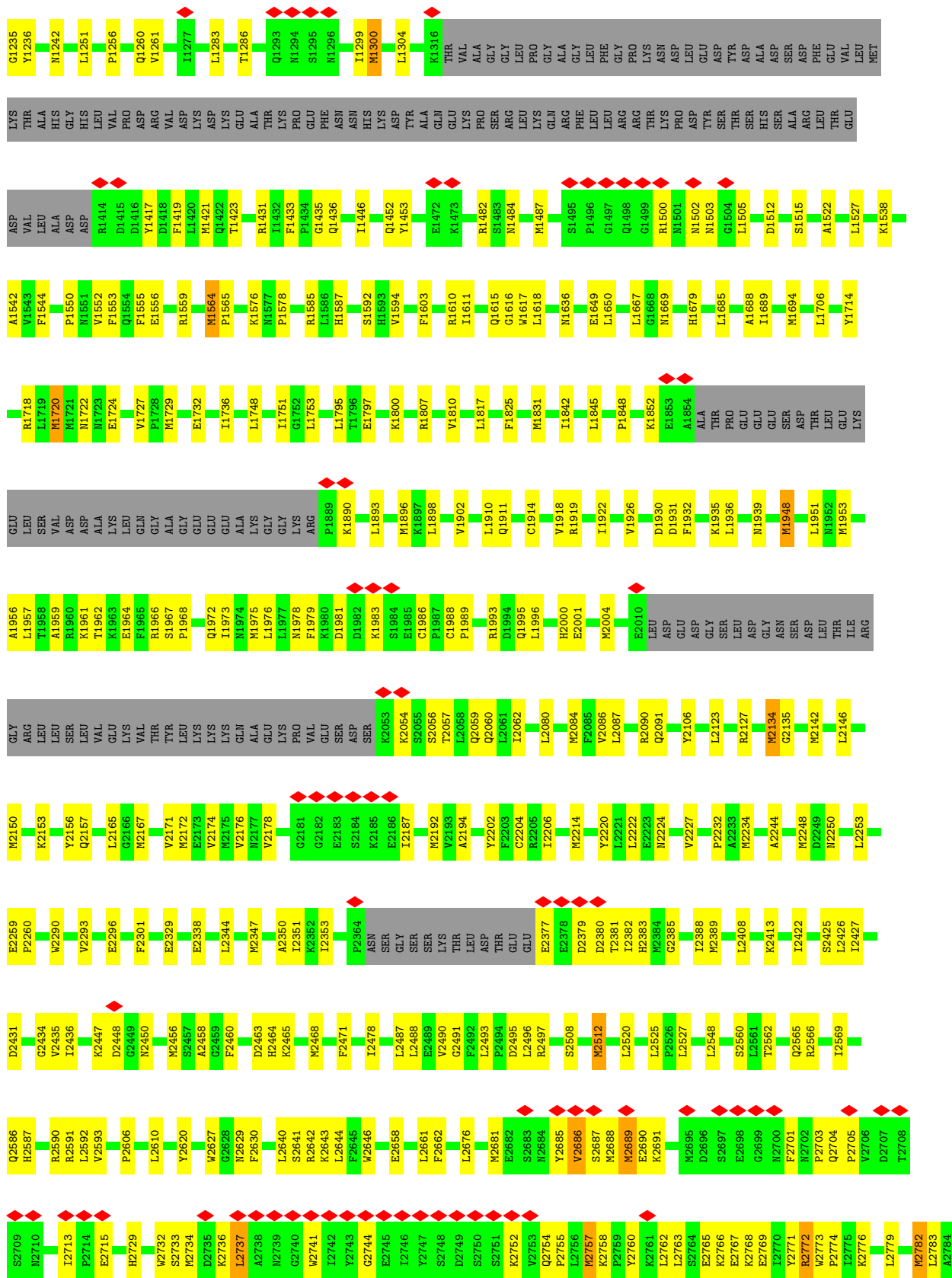
• Molecule 1: Calmodulin-1



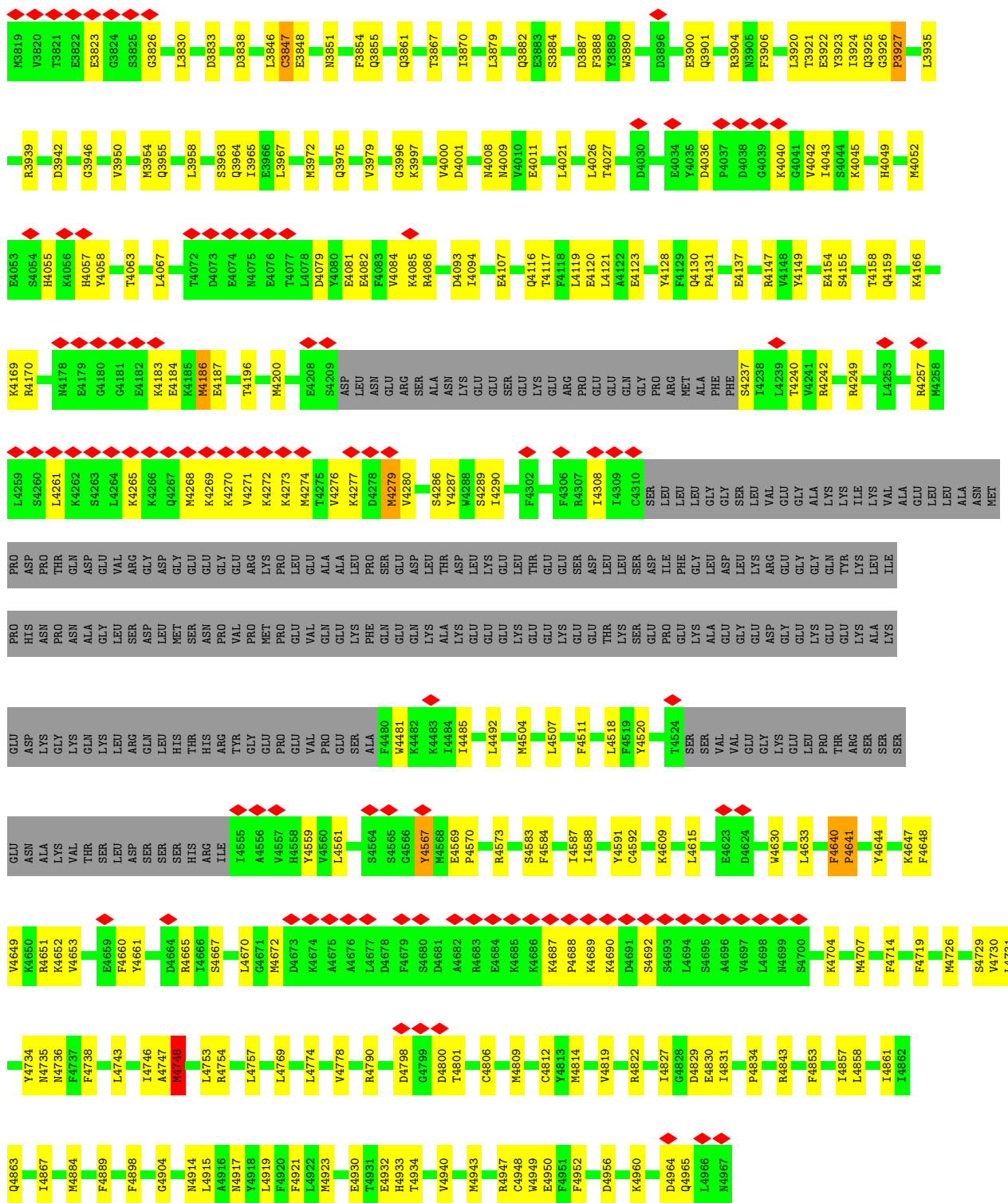


Molecule 2: Ryanodine receptor 2



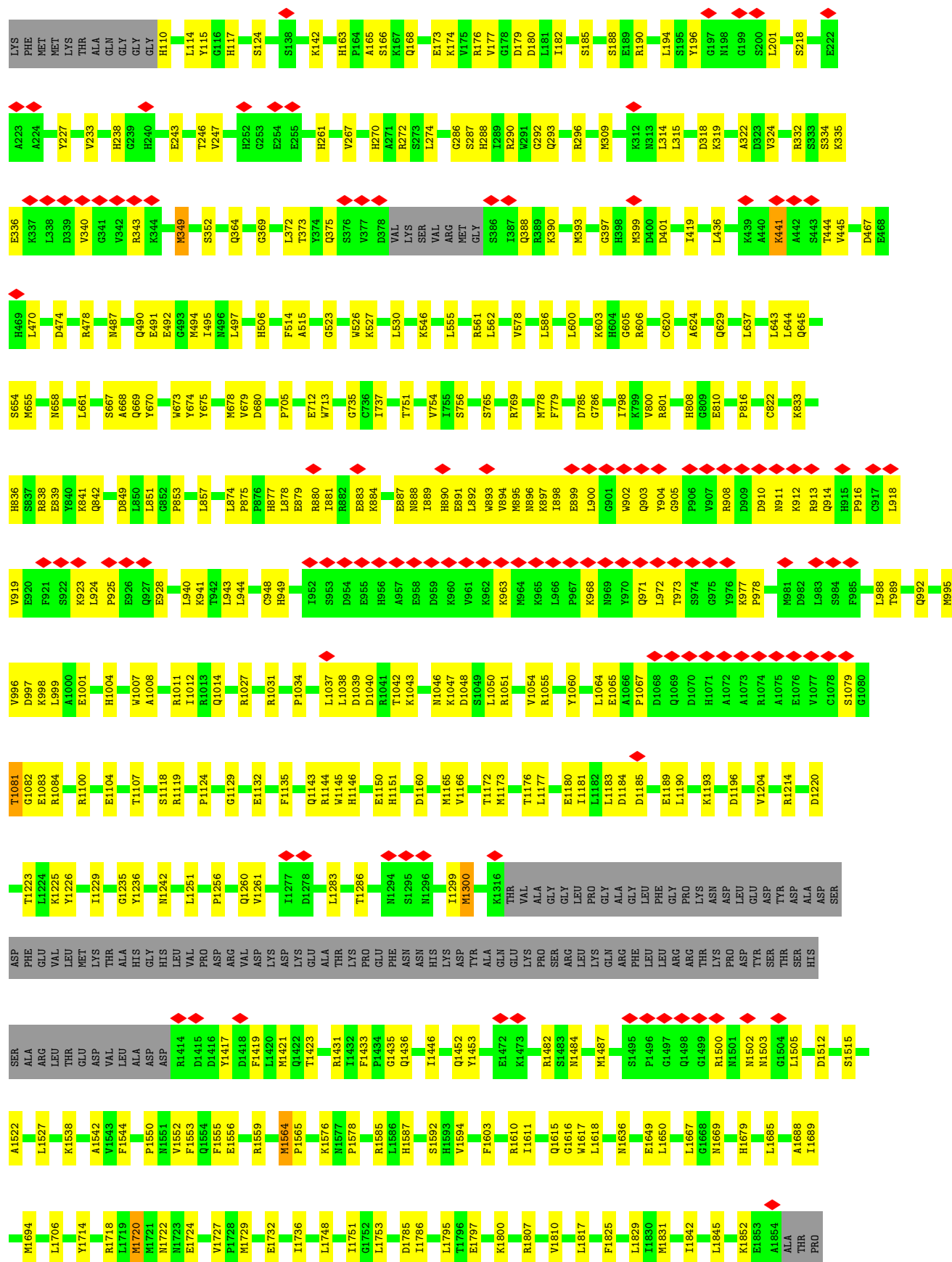


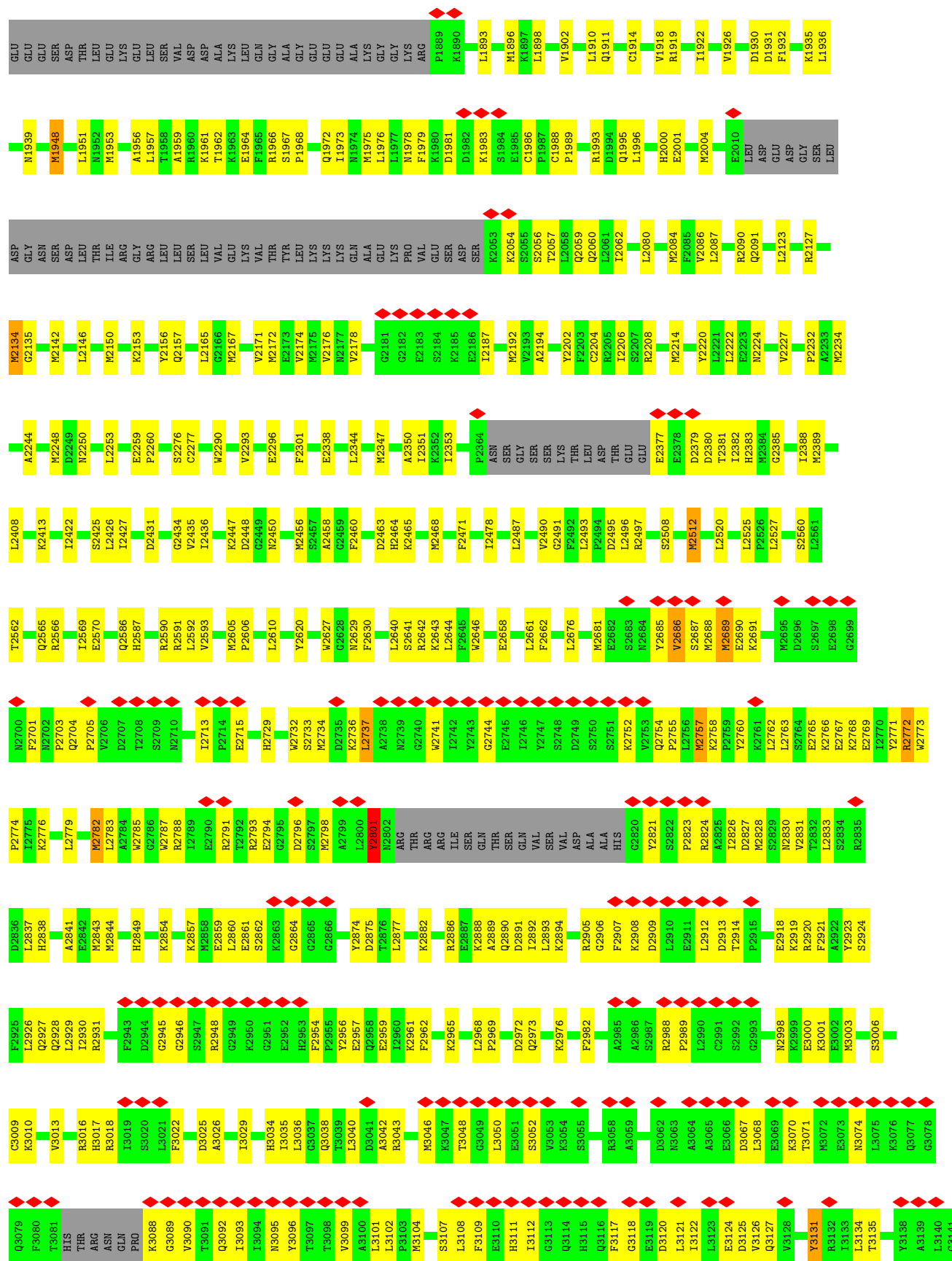




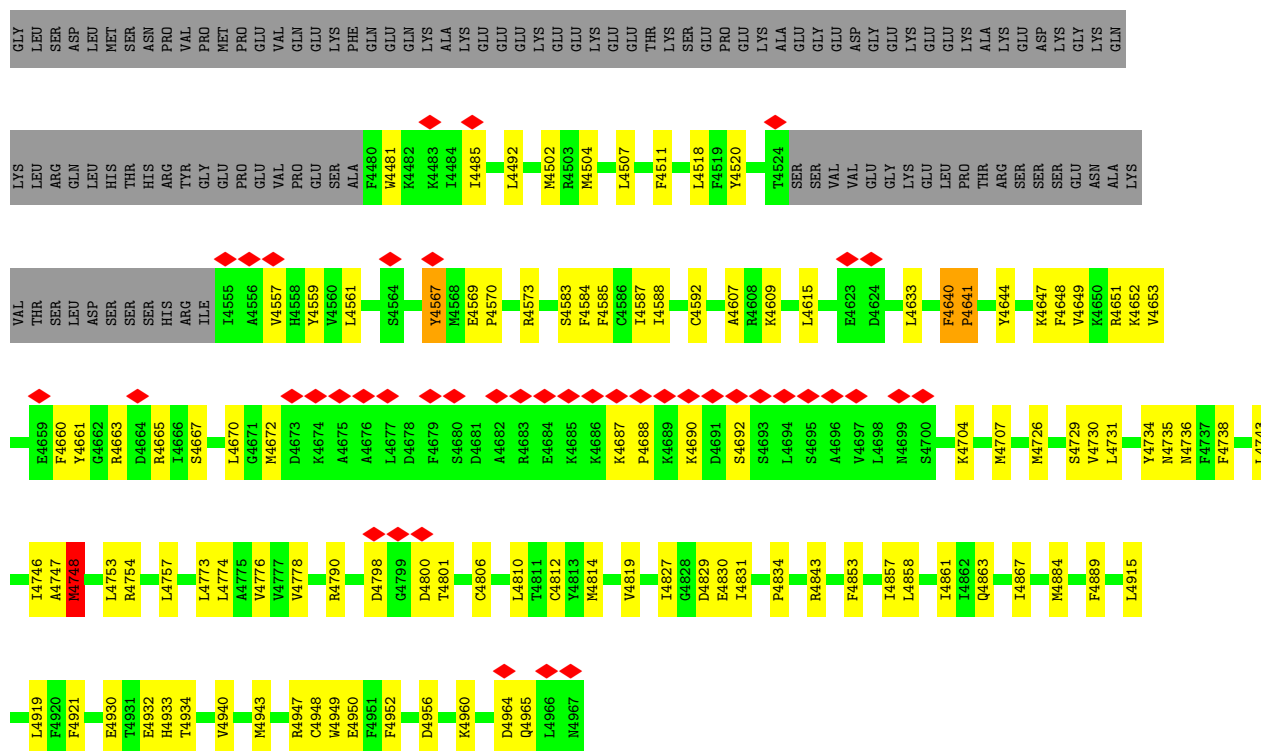
• Molecule 2: Ryanodine receptor 2



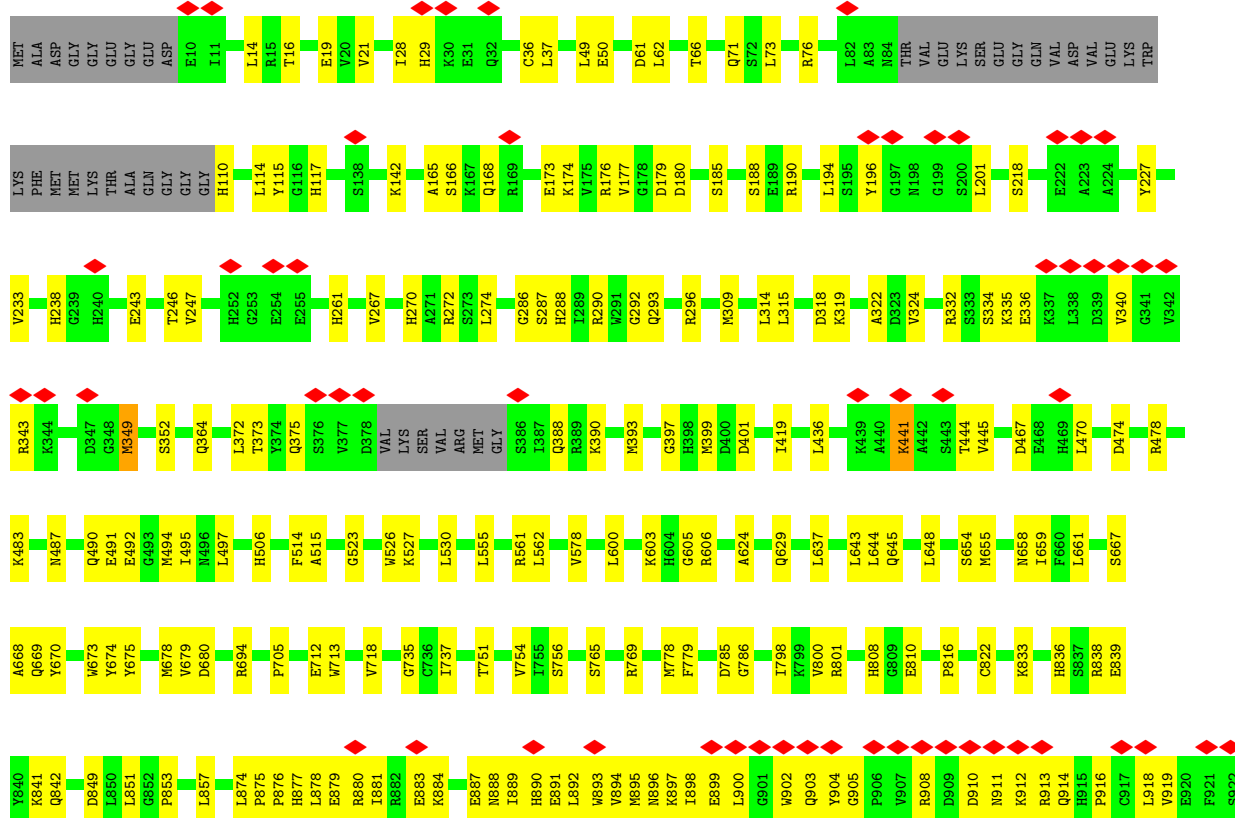


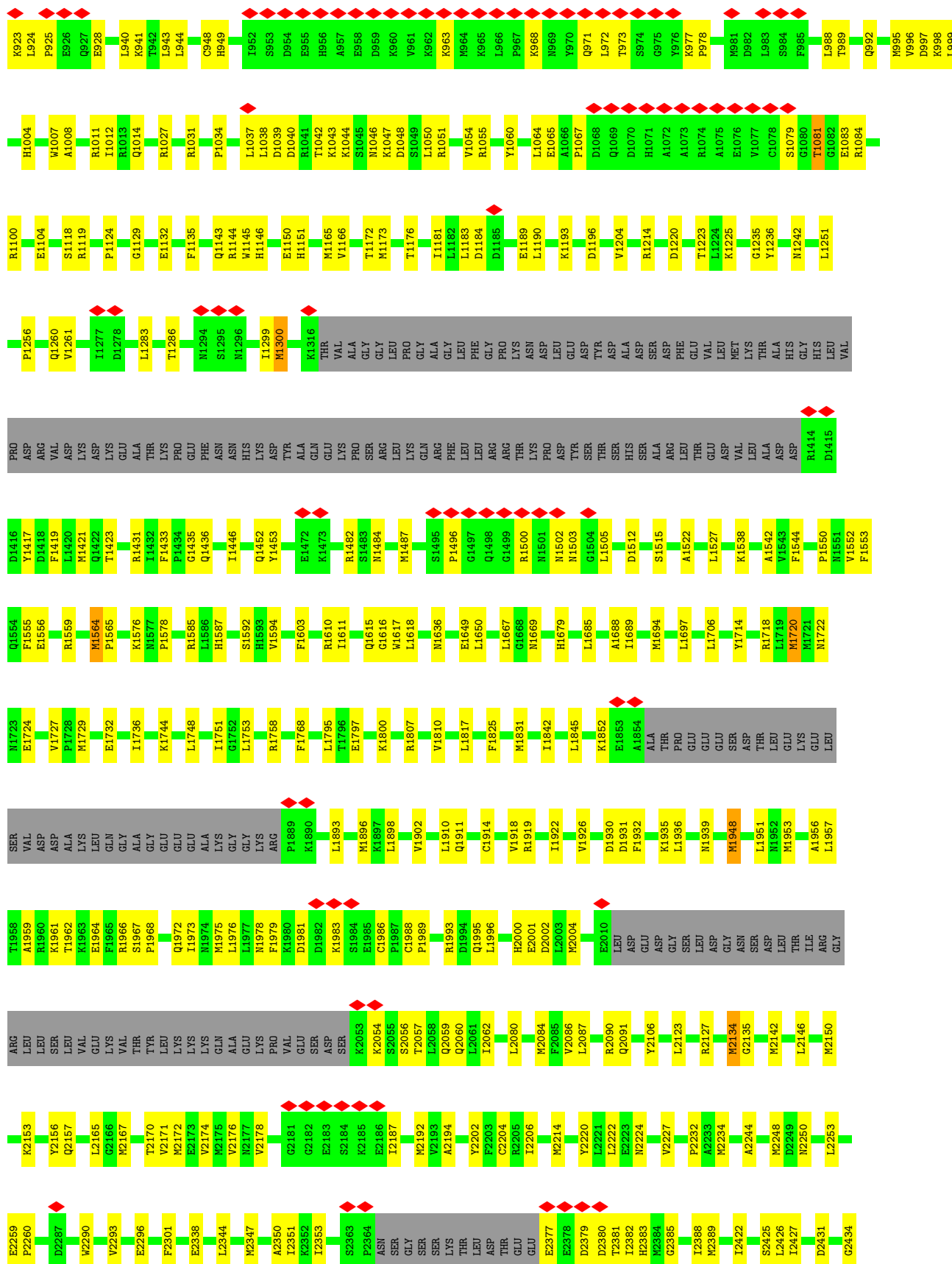






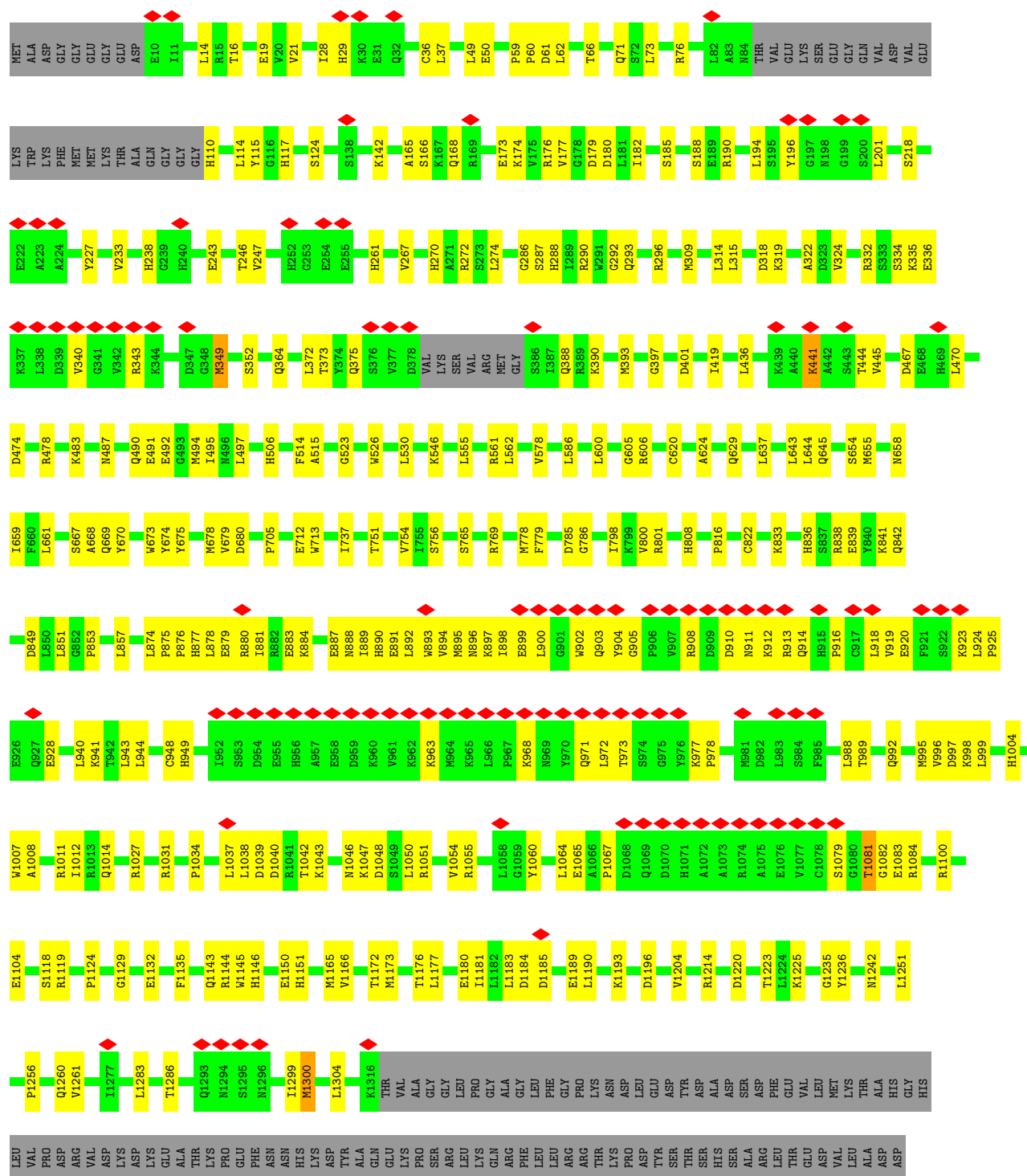
• Molecule 2: Ryanodine receptor 2





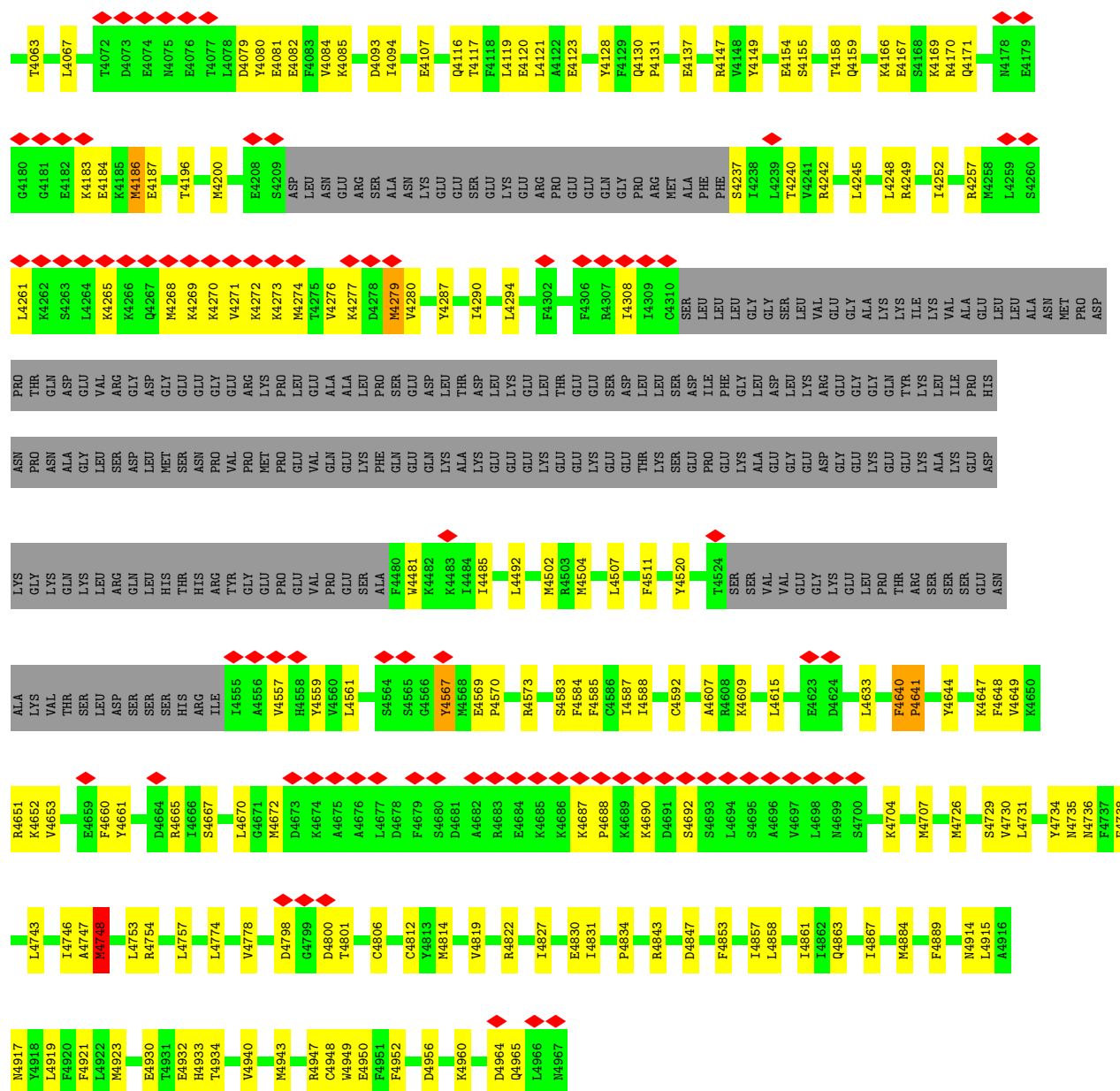
VAL	ASP	N3287	A3222	C3158	I3094	I3029	E2952	K2863	R2793	H2729	V2593	I2435
ALA	MET	L3288	E3223	L3159	N3095	I3029	H2953	G2864	E2794	W2732	P2606	I2436
LEU	SER	G3289	S3224	F3162	H3034	H3034	F2954	G2865	G2795	D2733	K2447	K2447
LYS	ALA	I3290	G3225	A3163	I3035	I3035	Y2955	G2866	D2796	S2733	L2610	D2448
ARG	PHE	D3291	I3226	G3164	T3097	L3036	Y2956		S2797	D2734	G2449	G2449
LEU	LEU	A3165	I3227	A3165	T3098	G3037	E2957		W2798	K2735	Y2620	N2450
LEU	LEU	F3166	Y3228	F3166	Q3038	Q3038	Q2958	Y2874	A2799	K2736	W2627	N2456
PRO	ILE	P3167	T3229	P3167	T3039	T3039	E2959	D2875	L2800	L2737	N2628	S2457
ILE	LEU	F3170	Q3230	F3170	L3101	L3040	T2960	T2876	Y2801	A2738	N2629	K2458
ASP	ASP	L3171	Q3231	L3171	L3102	L3041	K2961	L2877	N2802	N2739	F2630	G2459
GLY	GLY	M3231	Q3232	M3231	A3042	A3042	F2962	K2882	ARG	G2740		F2460
ASN	PHE	K3297	H3233	K3297	R3043	R3043			THR	W2741	L2640	
ASN	THR	F3173	V3234	F3173	T3044	T3044	K2965	R2886	ARG	I2742	S2641	D2463
VAL	THR	H3174	M3235	H3174	V3045	V3045	L2968	E2887	ARG	I2743	R2642	D2464
CYS	LEU	K3177			M3046	M3046	F2969	K2888	ILE	G2744	K2643	K2465
PRO	ALA				K3047	K3047	D2972	Q2958	GLN	E2745	F2645	
PRO	ALA				T3048	T3048	Q2973	D2891	THR	I2746	W2646	K2468
GLY	GLY				G3049	G3049	K2976	L2892	GLN	I2747		F2471
ASP	ASP				L3050	L3050		L2893	VAL	S2748	E2658	I2478
GLN	ASP				E3051	E3051	F2982	K2894	SER	S2750	E2660	L2487
ASN	LEU				S3052	S3052	A2985		VAL	S2751	E2661	
LEU	LEU				V3053	V3053	A2986	R2905	ASP	K2752	F2682	
LEU	LEU				K3054	K3054	S2987	G2906	ALA	W2753		
LEU	LEU				R3058	R3058	R2988	F2907	HIS	K2754	M2681	F2492
VAL	VAL				A3059	A3059	R2989	D2909		L2755	L2493	L2493
ASP	ASP				G3113	G3113	L2990	D2910		P2755	F2494	
TYR	TYR				Q3114	Q3114	C2991	E2911		M2757	D2495	D2495
LEU	LEU				H3115	H3115	S2992	L2912		K2758	N2684	L2496
LEU	LEU				Q3116	Q3116	G2993	D2913		Y2760	Y2685	R2497
ASN	ASN				F3117	F3117	G2994	T2914		S2686	S2687	S2508
ASN	ASN				G3118	G3118	H2995	P2915		L2762	M2688	
VAL	VAL				E3119	E3119	N2998	E2918		L2763	E2690	K2512
ASP	ASP				D3120	D3120	K2999	R2919		S2764	M2689	L2520
TYR	TYR				L3121	L3121	E3000	R2920		E2765	K2699	L2520
LEU	LEU				I3122	I3122	K3001	F2921		K2766	S2697	L2525
LEU	LEU				L3123	L3123	E3002	A2922		E2767	F2526	F2526
ASP	ASP				E3124	E3124	K3003	Y2923		E2768	L2527	L2527
ASP	ASP				D3125	D3125	S3006	S2924		E2769	S2560	S2560
GLY	GLY				V3126	V3126		F2925		Y2771	L2561	L2561
VAL	VAL				Q3127	Q3127	N2998	R2931		I2772	T2562	T2562
LEU	LEU				Y3131	Y3131	K2999	F2925		W2772	F2701	F2701
LEU	LEU				L3132	L3132	E3000	L2926		K2773	N2702	N2702
ASN	ASN				I3133	I3133	K3001	Q2927		P2703	Q2703	Q2703
ASN	ASN				T3134	T3134	E3002	Q2928		I2775	R2566	R2566
GLY	GLY				L3135	L3135	S3006	L2929		K2776	P2705	P2705
LEU	LEU				A3139	A3139	C3009	R2930		L2779	V2706	V2706
LEU	LEU				L3140	L3140	K3010	R2931		M2782	D2707	D2707
LEU	LEU				G3141	G3141	Q3077	F2943		L2783	T2708	T2708
LEU	LEU				T3142	T3142	Q3079	D2944		S2709	S2709	S2709
ALA	ALA				S3143	S3143	F3080	K3016		N2710	N2710	N2710
ALA	ALA				K3144	K3144	T3081	H3017		I2713	P2714	P2714
ALA	ALA				S3145	S3145	HIS	R3018		E2715	E2715	E2715
THR	THR				I3146	I3146	THR	F2943				
THR	THR				Y3147	Y3147	ARG	D2944				
LEU	LEU				V3148	V3148	ASN	G2945				
LEU	LEU				E3149	E3149	GLN	G2946				
ASP	ASP				R3150	R3150	PRO	S2947				
ASP	ASP				Q3151	Q3151	K3088	R2948				
LEU	LEU				V3152	V3152	G3089	G2949				
LEU	LEU				S3153	S3153	V3090	K2950				
ALA	ALA				L3155	L3155	T3091	G2951				
ALA	ALA				G3156	G3156	Q3092	K2951				
GLY	GLY				L3221	L3221	I3093					

C4812	E4684	E4569	ALA	GLU	V4084	V3979	F3854	M3719	L3590	GLN
T4813	K4685	P4570	F4480	ARG	K4085	V3979	Q3855	M3719	L3590	MET
M4814	K4686	R4573	K4483	SER	R4086	G3996	Q3861	A3729	L3591	ALA
				ALA	D4093	K3997			S3592	LEU
Y4818	K4687		L4492	LYS	D4094			H3732	R3595	TYR
V4819	P4688	S4583	M4502	ASP	E4107	V4000	I3870	T3743	K3596	LYS
T4827	K4689	F4584	R4503	LEU	E4116	D4001		I3744	A3601	ASP
E4830	K4690	F4585	R4503	LEU	T4117	M4008	L3879	T3743		LEU
L4831	L4587	C4586	M4504	GLU	F4118	N4009		I3744		PRO
L4831	L4588	L4588		LYS	L4120	E4011		S3747	R3604	ASN
P4834	S4692	C4592	L4507	GLU	F4119	V4010	Q3882	P3753	M3605	ARG
	S4693		C4310	THR	L4121	E4011	S3884	M3754		THR
R4843	L4694			GLU	L4122	L4021			L3608	ASP
	S4695			SER	E4123	L4026	D3887	T3758	R3615	THR
F4853	A4696	L4615	Y4520	GLU	E4123	L4026	F3888	I3763		SER
T4857	V4697	E4623	T4524	GLN	Y4128	T4027	Y3889	L3763	A3649	PRO
L4858	L4698	D4624		LYS	F4129	D4030	W3890	L3778	E3650	GLU
	N4699			ARG	Q4130	E4034	E3900		P3651	LYS
S4700	S4700			MET	P4131	F4035	Q3901	E3783	P3652	THR
				ALA	E4137	P4036		K3784	E3653	VAL
K4704	M4707	L4633	S4237	PHE	E4137	P4037	R3904	M3797	E3654	GLU
M4726			I4238	GLY	R4147	D4038	N3905		D3655	ARG
S4729	V4730	F4640	L4239	LEU	Y4148	D4038	F3906	L3803	E3656	LEU
L4731	L4731	ARG	T4240	LYS	Y4149	G4039		D3804	G3657	ASP
Y4734	K4650	THR	V4241	ILE	E4154	K4040	L3920	D3804	T3668	ILE
N4735	K4651	GLY	R4242	LYS	S4155	V4042	T3921	L3805	T3668	ALA
N4736	K4652	GLY		VAL	T4158	V4043	E3922	N3806	K3659	ASN
F4737	V4653	GLN	R4249	ALA	Q4159	S4044	I3924	R3810	R3660	VAL
F4738		TYR		LEU	Q4159	S4044	Q3925	Q3810		LEU
L4743		LYS	I4252	LEU	K4166	K4045	P3927	Q3811	L3664	PHE
I4746	P4660	ASP	L4253	ALA	K4167	H4049		N3812	I3668	HIS
A4747	P4661	PRO	R4257	ASN	S4168	H4052	L3935	E3815	I3668	GLU
M4748	C4662	HIS	M4258	MET	K4169	M4053	R3939	G3816	T3677	LYS
R4754	R4663	ASN	L4259	ASP	R4170	S4054		G3817	E3678	SER
L4757	D4664	THR	S4260	PRO	Q4171	H4055	D3942	G3818	K3679	LYS
L4773	R4665	ALA	L4261	ALA	M4178	K4056		M3819	L3687	ARG
L4774	S4667	GLY	K4262	GLN	E4179	H4057	G3946	V3820	Y3688	VAL
V4778		LEU	S4263	ASP	G4180	Y4058	Y3950	T3821	M3689	GLY
R4790		ARG	L4264	GLU	E4182		M3954	E3822	D3693	ARG
D4798	L4677	LEU	K4265	LEU	E4183	T4063	Q3955	G3824		HIS
G4799	S4564	THR	K4266	ASP	K4184	L4067		S3825	D3697	TYR
D4800	S4565	ASN	Q4267	GLY	E4184		L3958	G3826	K3697	CYS
T4801	G4566	PRO	M4274	GLU	K4185			H3700	H3700	VAL
C4806	Y4567	VAL	T4276	LEU	M4186	T4072	S3963	D3701	D3701	GLU
M4809	M4568	GLN	V4276	ALA	E4187	D4073	Q3964	E3702	E3702	HIS
		LYS	D4278	LEU	T4196	E4074	I3965	ASP	ASP	PRO
			M4279	ALA	E4208	M4075	E3966	ASP	ASP	GLN
			V4280	LEU	S4209	E4076	L3967	ASP	ASP	ARG
				ASN	ASP	T4078	M3972	GLY	GLY	SER
					LEU	D4079	Q3975	GLU	GLU	LYS
						Y4080		E3710	E3710	K3584
						E4081		V3711	V3711	W3587
						F4082				
						F4083				









• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 81% 17%



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 81% 18%



- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:  81% 18% ..



- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  81% 17% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.594	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	I	0.29	0/1143	0.68	3/1534 (0.2%)
1	J	0.29	0/1143	0.68	3/1534 (0.2%)
1	K	0.29	0/1143	0.68	3/1534 (0.2%)
1	L	0.29	0/1143	0.68	3/1534 (0.2%)
2	A	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
2	B	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
2	C	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
2	D	0.37	7/34594 (0.0%)	0.45	6/46723 (0.0%)
3	E	0.16	0/834	0.41	0/1123
3	F	0.16	0/834	0.41	0/1123
3	G	0.16	0/834	0.41	0/1123
3	H	0.16	0/834	0.41	0/1123
All	All	0.37	28/146284 (0.0%)	0.46	36/197520 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3205	CYS	CB-SG	54.55	3.61	1.81
2	A	3205	CYS	CB-SG	54.53	3.61	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3205	CYS	CB-SG	54.53	3.61	1.81
2	C	3205	CYS	CB-SG	54.50	3.61	1.81
2	B	3131	TYR	CD2-CE2	15.06	1.83	1.38
2	A	3131	TYR	CD2-CE2	15.06	1.83	1.38
2	D	3131	TYR	CD2-CE2	15.05	1.83	1.38
2	C	3131	TYR	CD2-CE2	15.04	1.83	1.38
2	B	3131	TYR	CD1-CE1	14.56	1.82	1.38
2	C	3131	TYR	CD1-CE1	14.55	1.82	1.38
2	A	3131	TYR	CD1-CE1	14.54	1.82	1.38
2	D	3131	TYR	CD1-CE1	14.52	1.82	1.38
2	B	3131	TYR	CE2-CZ	11.96	1.67	1.38
2	C	3131	TYR	CE2-CZ	11.96	1.67	1.38
2	A	3131	TYR	CE2-CZ	11.93	1.66	1.38
2	D	3131	TYR	CE2-CZ	11.92	1.66	1.38
2	D	3131	TYR	CE1-CZ	11.79	1.66	1.38
2	A	3131	TYR	CE1-CZ	11.77	1.66	1.38
2	B	3131	TYR	CE1-CZ	11.75	1.66	1.38
2	C	3131	TYR	CE1-CZ	11.74	1.66	1.38
2	B	3131	TYR	CG-CD2	10.23	1.60	1.39
2	D	3131	TYR	CG-CD2	10.23	1.60	1.39
2	C	3131	TYR	CG-CD2	10.22	1.60	1.39
2	A	3131	TYR	CG-CD2	10.21	1.60	1.39
2	A	3131	TYR	CG-CD1	10.05	1.60	1.39
2	B	3131	TYR	CG-CD1	10.04	1.60	1.39
2	D	3131	TYR	CG-CD1	10.05	1.60	1.39
2	C	3131	TYR	CG-CD1	10.02	1.60	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3205	CYS	CA-CB-SG	9.28	135.73	114.40
2	A	3205	CYS	CA-CB-SG	9.27	135.71	114.40
2	B	3205	CYS	CA-CB-SG	9.25	135.68	114.40
2	D	3205	CYS	CA-CB-SG	9.25	135.68	114.40
1	K	124	GLU	N-CA-C	-7.28	102.52	111.40
1	L	124	GLU	N-CA-C	-7.27	102.53	111.40
1	I	124	GLU	N-CA-C	-7.24	102.56	111.40
1	J	124	GLU	N-CA-C	-7.23	102.58	111.40
1	J	77	MET	CB-CG-SD	5.68	129.75	112.70
1	I	77	MET	CB-CG-SD	5.68	129.74	112.70
1	K	77	MET	CB-CG-SD	5.68	129.74	112.70
1	L	77	MET	CB-CG-SD	5.68	129.73	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3923	TYR	CA-C-N	-5.39	114.62	122.28
2	C	3923	TYR	C-N-CA	-5.39	114.62	122.28
2	D	3923	TYR	CA-C-N	-5.39	114.62	122.28
2	D	3923	TYR	C-N-CA	-5.39	114.62	122.28
1	I	132	ASP	N-CA-C	-5.37	105.99	112.54
1	K	132	ASP	N-CA-C	-5.37	105.99	112.54
1	L	132	ASP	N-CA-C	-5.36	106.00	112.54
2	A	3923	TYR	CA-C-N	-5.36	114.67	122.28
2	A	3923	TYR	C-N-CA	-5.36	114.67	122.28
2	B	3923	TYR	CA-C-N	-5.36	114.67	122.28
2	B	3923	TYR	C-N-CA	-5.36	114.67	122.28
1	J	132	ASP	N-CA-C	-5.33	106.03	112.54
2	B	4748	MET	CB-CG-SD	5.24	128.43	112.70
2	C	4748	MET	CB-CG-SD	5.23	128.39	112.70
2	A	4748	MET	CB-CG-SD	5.23	128.38	112.70
2	D	4748	MET	CB-CG-SD	5.22	128.35	112.70
2	B	4567	TYR	CA-CB-CG	5.14	123.15	113.90
2	C	4567	TYR	CA-CB-CG	5.13	123.14	113.90
2	A	4567	TYR	CA-CB-CG	5.13	123.13	113.90
2	D	4567	TYR	CA-CB-CG	5.13	123.13	113.90
2	D	2686	VAL	N-CA-C	-5.10	101.35	108.80
2	A	2686	VAL	N-CA-C	-5.10	101.35	108.80
2	B	2686	VAL	N-CA-C	-5.09	101.37	108.80
2	C	2686	VAL	N-CA-C	-5.09	101.37	108.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2801	TYR	Peptide
2	A	4640	PHE	Peptide
2	B	2801	TYR	Peptide
2	B	4640	PHE	Peptide
2	C	2801	TYR	Peptide
2	C	4640	PHE	Peptide
2	D	2801	TYR	Peptide
2	D	4640	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1131	0	1058	56	0
1	J	1131	0	1058	52	0
1	K	1131	0	1058	51	0
1	L	1131	0	1058	49	0
2	A	33849	0	33549	855	0
2	B	33849	0	33549	849	0
2	C	33849	0	33549	830	0
2	D	33849	0	33549	850	0
3	E	818	0	821	10	0
3	F	818	0	821	11	0
3	G	818	0	821	13	0
3	H	818	0	821	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	62	0	24	1	0
6	B	62	0	24	1	0
6	C	62	0	24	1	0
6	D	62	0	24	1	0
All	All	143464	0	141808	3551	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 12.

All (3551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3131:TYR:CD1	2:D:3131:TYR:CE1	1.82	1.68
2:A:3131:TYR:CD1	2:A:3131:TYR:CE1	1.82	1.63
2:C:3131:TYR:CD2	2:C:3131:TYR:CE2	1.83	1.61
2:C:3131:TYR:CE1	2:C:3131:TYR:CD1	1.82	1.61
2:D:3131:TYR:CE2	2:D:3131:TYR:CD2	1.83	1.61
2:B:3131:TYR:CD2	2:B:3131:TYR:CE2	1.83	1.58
2:B:3131:TYR:CD1	2:B:3131:TYR:CE1	1.82	1.58
2:A:3131:TYR:CE2	2:A:3131:TYR:CD2	1.83	1.58
1:J:127:ARG:NH1	1:J:135:GLY:CA	1.70	1.53
1:K:127:ARG:NH1	1:K:135:GLY:CA	1.70	1.53
1:L:127:ARG:NH1	1:L:135:GLY:CA	1.70	1.50
1:I:127:ARG:NH1	1:I:135:GLY:CA	1.70	1.48
2:A:3848:GLU:OE1	2:A:3922:GLU:CD	1.87	1.18
2:A:3131:TYR:CZ	2:A:3205:CYS:SG	2.37	1.17
2:B:3131:TYR:CZ	2:B:3205:CYS:SG	2.37	1.17
2:C:3131:TYR:CZ	2:C:3205:CYS:SG	2.37	1.17
2:C:3848:GLU:OE1	2:C:3922:GLU:CD	1.87	1.17
2:A:3131:TYR:CE2	2:A:3205:CYS:SG	2.38	1.17
2:B:3131:TYR:CE2	2:B:3205:CYS:SG	2.38	1.17
2:C:3131:TYR:CE2	2:C:3205:CYS:SG	2.38	1.17
2:D:3131:TYR:CE2	2:D:3205:CYS:SG	2.38	1.17
2:D:3131:TYR:CZ	2:D:3205:CYS:SG	2.37	1.17
2:B:3848:GLU:OE1	2:B:3922:GLU:CD	1.87	1.16
2:D:3848:GLU:OE1	2:D:3922:GLU:CD	1.87	1.16
2:B:3131:TYR:CE1	2:B:3205:CYS:SG	2.42	1.13
2:A:3131:TYR:CE1	2:A:3205:CYS:SG	2.42	1.12
2:C:3131:TYR:CE1	2:C:3205:CYS:SG	2.42	1.11
2:D:3131:TYR:CE1	2:D:3205:CYS:SG	2.42	1.11
2:A:3131:TYR:CD2	2:A:3205:CYS:SG	2.44	1.11
2:B:3131:TYR:CD2	2:B:3205:CYS:SG	2.43	1.11
2:C:3131:TYR:CD2	2:C:3205:CYS:SG	2.43	1.11
2:D:3131:TYR:CD2	2:D:3205:CYS:SG	2.44	1.10
2:C:3131:TYR:CD1	2:C:3205:CYS:SG	2.46	1.09
2:D:3131:TYR:CD1	2:D:3205:CYS:SG	2.46	1.09
2:A:3131:TYR:CD1	2:A:3205:CYS:SG	2.46	1.08
2:B:3131:TYR:CD1	2:B:3205:CYS:SG	2.46	1.08
1:L:127:ARG:NH1	1:L:135:GLY:HA2	0.74	1.07
1:I:127:ARG:NH1	1:I:135:GLY:HA2	0.74	1.07
1:J:127:ARG:NH1	1:J:135:GLY:HA2	0.74	1.06
1:K:127:ARG:NH1	1:K:135:GLY:HA2	0.74	1.06
1:K:127:ARG:CZ	1:K:135:GLY:HA2	1.88	1.03
1:J:127:ARG:CZ	1:J:135:GLY:HA2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:ARG:CZ	1:I:135:GLY:HA2	1.88	1.02
1:L:127:ARG:CZ	1:L:135:GLY:HA2	1.88	1.01
2:C:3131:TYR:CG	2:C:3205:CYS:SG	2.53	1.01
2:B:3131:TYR:CG	2:B:3205:CYS:SG	2.53	1.01
2:D:3131:TYR:CG	2:D:3205:CYS:SG	2.53	1.01
2:A:3131:TYR:CG	2:A:3205:CYS:SG	2.53	1.01
2:C:3131:TYR:CZ	2:C:3205:CYS:CB	2.51	0.94
2:A:3131:TYR:CZ	2:A:3205:CYS:CB	2.51	0.94
2:A:3131:TYR:CE1	2:A:3205:CYS:CB	2.51	0.94
2:B:3131:TYR:CE1	2:B:3205:CYS:CB	2.51	0.94
2:C:3131:TYR:CE2	2:C:3205:CYS:CB	2.51	0.93
2:D:3131:TYR:CE1	2:D:3205:CYS:CB	2.51	0.93
2:A:3131:TYR:CE2	2:A:3205:CYS:CB	2.51	0.93
2:B:3131:TYR:CZ	2:B:3205:CYS:CB	2.51	0.93
2:D:3131:TYR:CE2	2:D:3205:CYS:CB	2.51	0.93
1:I:127:ARG:HH11	1:I:135:GLY:HA2	1.27	0.93
2:D:3131:TYR:CZ	2:D:3205:CYS:CB	2.51	0.93
1:K:127:ARG:HH11	1:K:135:GLY:HA2	1.27	0.93
2:C:3131:TYR:CD2	2:C:3205:CYS:CB	2.52	0.93
2:C:3131:TYR:CE1	2:C:3205:CYS:CB	2.51	0.93
2:A:3131:TYR:CD2	2:A:3205:CYS:CB	2.52	0.92
2:B:3131:TYR:CE2	2:B:3205:CYS:CB	2.51	0.92
1:J:127:ARG:HH11	1:J:135:GLY:HA2	1.27	0.92
2:B:3131:TYR:CD2	2:B:3205:CYS:CB	2.52	0.92
2:D:3131:TYR:CD2	2:D:3205:CYS:CB	2.52	0.91
2:B:3131:TYR:CD1	2:B:3205:CYS:CB	2.54	0.91
2:C:3131:TYR:CD1	2:C:3205:CYS:CB	2.54	0.91
2:A:3131:TYR:CD1	2:A:3205:CYS:CB	2.54	0.90
2:D:3131:TYR:CD1	2:D:3205:CYS:CB	2.54	0.90
1:L:127:ARG:HH11	1:L:135:GLY:HA2	1.27	0.90
2:C:3131:TYR:CG	2:C:3205:CYS:CB	2.56	0.89
2:D:3131:TYR:CG	2:D:3205:CYS:CB	2.56	0.89
2:B:3131:TYR:CG	2:B:3205:CYS:CB	2.56	0.89
2:C:4834:PRO:HB3	2:C:4843:ARG:HD3	1.55	0.88
2:A:3131:TYR:CG	2:A:3205:CYS:CB	2.56	0.88
2:A:4834:PRO:HB3	2:A:4843:ARG:HD3	1.55	0.88
2:D:4834:PRO:HB3	2:D:4843:ARG:HD3	1.55	0.86
2:B:4834:PRO:HB3	2:B:4843:ARG:HD3	1.55	0.85
2:C:2425:SER:O	2:D:142:LYS:NZ	2.08	0.85
2:A:142:LYS:NZ	2:D:2425:SER:O	2.11	0.84
2:B:2788:ARG:NH1	2:B:2905:ARG:O	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2512:MET:HA	2:D:2512:MET:HE2	1.61	0.83
2:A:2512:MET:HE2	2:A:2512:MET:HA	1.61	0.82
2:A:2788:ARG:NH1	2:A:2905:ARG:O	2.12	0.82
2:A:888:ASN:ND2	2:A:1060:TYR:OH	2.13	0.82
2:C:2788:ARG:NH1	2:C:2905:ARG:O	2.12	0.82
2:D:888:ASN:ND2	2:D:1060:TYR:OH	2.13	0.82
2:B:2773:TRP:HE3	2:B:2776:LYS:HZ3	1.27	0.81
2:D:2788:ARG:NH1	2:D:2905:ARG:O	2.12	0.81
2:C:888:ASN:ND2	2:C:1060:TYR:OH	2.13	0.81
2:C:3890:TRP:HB3	2:D:76:ARG:HG2	1.61	0.81
2:B:2512:MET:HE2	2:B:2512:MET:HA	1.61	0.81
2:C:2512:MET:HE2	2:C:2512:MET:HA	1.61	0.81
2:B:888:ASN:ND2	2:B:1060:TYR:OH	2.13	0.80
2:C:3067:ASP:HA	2:C:3070:LYS:HZ3	1.46	0.80
2:D:3067:ASP:HA	2:D:3070:LYS:HZ3	1.46	0.80
2:D:2773:TRP:HE3	2:D:2776:LYS:HZ3	1.27	0.80
2:B:3067:ASP:HA	2:B:3070:LYS:HZ3	1.46	0.80
2:C:1559:ARG:HD2	2:C:1565:PRO:HD3	1.64	0.80
2:B:1559:ARG:HD2	2:B:1565:PRO:HD3	1.64	0.80
2:C:2773:TRP:HE3	2:C:2776:LYS:HZ3	1.27	0.79
2:A:76:ARG:HG2	2:D:3890:TRP:HB3	1.64	0.79
2:D:2794:GLU:HB2	2:D:2798:MET:HE1	1.65	0.79
2:D:1559:ARG:HD2	2:D:1565:PRO:HD3	1.64	0.78
2:A:1559:ARG:HD2	2:A:1565:PRO:HD3	1.64	0.78
2:C:2794:GLU:HB2	2:C:2798:MET:HE1	1.65	0.78
2:B:3183:ILE:HG23	2:B:3184:TYR:HD1	1.49	0.78
2:D:1729:MET:HE1	2:D:1930:ASP:HB2	1.66	0.78
2:A:2773:TRP:HE3	2:A:2776:LYS:HZ3	1.29	0.78
3:G:12:ASP:OD2	3:G:15:THR:OG1	2.03	0.77
2:B:2794:GLU:HB2	2:B:2798:MET:HE1	1.65	0.77
2:A:2794:GLU:HB2	2:A:2798:MET:HE1	1.65	0.77
2:B:1729:MET:HE1	2:B:1930:ASP:HB2	1.65	0.77
2:A:3183:ILE:HG23	2:A:3184:TYR:HD1	1.49	0.77
2:C:3183:ILE:HG23	2:C:3184:TYR:HD1	1.49	0.77
2:A:3067:ASP:HA	2:A:3070:LYS:HZ3	1.50	0.77
2:C:3122:ILE:HD11	2:C:3167:PRO:HD3	1.67	0.77
2:D:3122:ILE:HD11	2:D:3167:PRO:HD3	1.67	0.77
2:A:1729:MET:HE1	2:A:1930:ASP:HB2	1.65	0.76
2:C:1729:MET:HE1	2:C:1930:ASP:HB2	1.65	0.76
2:D:3183:ILE:HG23	2:D:3184:TYR:HD1	1.49	0.76
3:E:12:ASP:OD2	3:E:15:THR:OG1	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:ASP:OD2	3:H:15:THR:OG1	2.03	0.76
2:C:3783:GLU:OE1	2:C:3784:LYS:NZ	2.18	0.76
2:B:2957:GLU:OE1	2:B:2961:LYS:NZ	2.18	0.76
2:B:3122:ILE:HD11	2:B:3167:PRO:HD3	1.67	0.76
3:F:12:ASP:OD2	3:F:15:THR:OG1	2.02	0.76
2:B:2923:TYR:O	2:B:2927:GLN:NE2	2.19	0.76
2:C:2923:TYR:O	2:C:2927:GLN:NE2	2.19	0.76
2:D:2923:TYR:O	2:D:2927:GLN:NE2	2.19	0.75
2:A:2923:TYR:O	2:A:2927:GLN:NE2	2.19	0.75
2:D:2957:GLU:OE1	2:D:2961:LYS:NZ	2.18	0.75
2:A:3122:ILE:HD11	2:A:3167:PRO:HD3	1.67	0.75
2:B:3050:LEU:HD23	2:B:3052:SER:H	1.51	0.75
2:C:3689:MET:HE1	2:C:3753:PRO:HB2	1.68	0.75
2:D:3050:LEU:HD23	2:D:3052:SER:H	1.51	0.75
2:C:3050:LEU:HD23	2:C:3052:SER:H	1.51	0.75
2:D:3689:MET:HE1	2:D:3753:PRO:HB2	1.68	0.75
2:A:2957:GLU:OE1	2:A:2961:LYS:NZ	2.18	0.74
2:A:3222:ALA:O	2:A:3282:LYS:NZ	2.20	0.74
2:B:3783:GLU:OE1	2:B:3784:LYS:NZ	2.18	0.74
2:A:3050:LEU:HD23	2:A:3052:SER:H	1.51	0.74
2:B:4641:PRO:HB3	2:B:4644:TYR:HB3	1.69	0.74
2:C:4641:PRO:HB3	2:C:4644:TYR:HB3	1.69	0.74
2:C:4667:SER:HA	2:C:4672:MET:HE3	1.70	0.74
2:D:4667:SER:HA	2:D:4672:MET:HE3	1.70	0.74
2:A:3689:MET:HE1	2:A:3753:PRO:HB2	1.68	0.74
2:B:3689:MET:HE1	2:B:3753:PRO:HB2	1.68	0.74
2:D:3222:ALA:O	2:D:3282:LYS:NZ	2.20	0.74
2:D:4641:PRO:HB3	2:D:4644:TYR:HB3	1.69	0.74
2:C:2957:GLU:OE1	2:C:2961:LYS:NZ	2.18	0.73
2:B:895:MET:HE3	2:B:978:PRO:HG3	1.70	0.73
2:B:4667:SER:HA	2:B:4672:MET:HE3	1.70	0.73
2:A:4641:PRO:HB3	2:A:4644:TYR:HB3	1.69	0.73
2:A:4667:SER:HA	2:A:4672:MET:HE3	1.70	0.73
1:K:73:MET:HE3	1:K:78:LYS:HZ1	1.54	0.73
2:A:895:MET:HE3	2:A:978:PRO:HG3	1.70	0.73
2:C:895:MET:HE3	2:C:978:PRO:HG3	1.70	0.73
1:K:117:LEU:HD22	1:K:122:VAL:HG23	1.71	0.73
2:C:3131:TYR:CG	2:C:3205:CYS:HB3	2.23	0.73
2:D:4670:LEU:HB2	2:D:4672:MET:HE2	1.70	0.73
1:K:72:MET:HA	1:K:75:ARG:HG2	1.71	0.72
2:D:3131:TYR:CG	2:D:3205:CYS:HB3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:895:MET:HE3	2:D:978:PRO:HG3	1.70	0.72
2:D:1079:SER:OG	2:D:1084:ARG:NH2	2.22	0.72
2:A:3131:TYR:CG	2:A:3205:CYS:HB3	2.23	0.72
1:L:73:MET:HE3	1:L:78:LYS:HZ1	1.55	0.72
2:B:4670:LEU:HB2	2:B:4672:MET:HE2	1.70	0.72
2:C:2830:ASN:HB3	2:D:1435:GLY:HA3	1.71	0.72
2:C:1079:SER:OG	2:C:1084:ARG:NH2	2.22	0.72
1:L:117:LEU:HD22	1:L:122:VAL:HG23	1.71	0.72
2:B:1079:SER:OG	2:B:1084:ARG:NH2	2.22	0.72
2:C:3222:ALA:O	2:C:3282:LYS:NZ	2.20	0.72
1:J:117:LEU:HD22	1:J:122:VAL:HG23	1.71	0.72
1:L:72:MET:HA	1:L:75:ARG:HG2	1.71	0.72
1:K:137:VAL:HG13	1:K:141:GLU:HB2	1.72	0.71
2:C:4670:LEU:HB2	2:C:4672:MET:HE2	1.70	0.71
2:D:3184:TYR:HB3	2:D:3192:ARG:HH21	1.55	0.71
2:A:3783:GLU:OE1	2:A:3784:LYS:NZ	2.18	0.71
2:B:3131:TYR:CG	2:B:3205:CYS:HB3	2.23	0.71
2:D:3131:TYR:CE1	2:D:3205:CYS:HB2	2.25	0.71
1:I:73:MET:HE3	1:I:78:LYS:HZ1	1.55	0.71
2:D:3247:SER:HA	2:D:3250:TRP:HD1	1.56	0.71
2:A:1079:SER:OG	2:A:1084:ARG:NH2	2.22	0.71
2:A:2703:PRO:O	2:A:2854:LYS:NZ	2.23	0.71
2:A:4670:LEU:HB2	2:A:4672:MET:HE2	1.70	0.71
1:J:137:VAL:HG13	1:J:141:GLU:HB2	1.72	0.71
2:C:2703:PRO:O	2:C:2854:LYS:NZ	2.23	0.71
2:B:3131:TYR:CE1	2:B:3205:CYS:HB2	2.25	0.71
2:D:2703:PRO:O	2:D:2854:LYS:NZ	2.23	0.71
1:J:72:MET:HA	1:J:75:ARG:HG2	1.71	0.71
2:A:3184:TYR:HB3	2:A:3192:ARG:HH21	1.55	0.71
1:I:137:VAL:HG13	1:I:141:GLU:HB2	1.72	0.70
2:A:3247:SER:HA	2:A:3250:TRP:HD1	1.56	0.70
2:C:3184:TYR:HB3	2:C:3192:ARG:HH21	1.55	0.70
1:J:73:MET:HE3	1:J:78:LYS:HZ1	1.56	0.70
2:B:188:SER:HB2	2:B:190:ARG:HH11	1.56	0.70
1:I:117:LEU:HD22	1:I:122:VAL:HG23	1.71	0.70
2:C:3247:SER:HA	2:C:3250:TRP:HD1	1.56	0.70
2:A:3131:TYR:CE1	2:A:3205:CYS:HB2	2.25	0.70
2:B:2703:PRO:O	2:B:2854:LYS:NZ	2.23	0.70
1:I:72:MET:HA	1:I:75:ARG:HG2	1.71	0.70
2:B:3222:ALA:O	2:B:3282:LYS:NZ	2.20	0.70
2:B:3247:SER:HA	2:B:3250:TRP:HD1	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2998:ASN:ND2	2:A:3048:THR:OG1	2.25	0.70
2:C:3131:TYR:CE1	2:C:3205:CYS:HB2	2.25	0.70
2:A:188:SER:HB2	2:A:190:ARG:HH11	1.57	0.70
1:L:137:VAL:HG13	1:L:141:GLU:HB2	1.72	0.69
2:B:875:PRO:HD2	2:B:878:LEU:HD12	1.74	0.69
2:C:188:SER:HB2	2:C:190:ARG:HH11	1.57	0.69
2:D:2998:ASN:ND2	2:D:3048:THR:OG1	2.25	0.69
2:B:2998:ASN:ND2	2:B:3048:THR:OG1	2.25	0.69
2:B:3184:TYR:HB3	2:B:3192:ARG:HH21	1.55	0.69
2:B:2172:MET:HA	2:B:2172:MET:HE3	1.74	0.69
2:C:2998:ASN:ND2	2:C:3048:THR:OG1	2.25	0.69
2:D:188:SER:HB2	2:D:190:ARG:HH11	1.57	0.69
2:D:4687:LYS:HD2	2:D:4688:PRO:HD2	1.75	0.69
2:A:2172:MET:HA	2:A:2172:MET:HE3	1.74	0.69
2:C:288:HIS:O	2:C:290:ARG:NH1	2.26	0.69
2:A:4726:MET:HE2	2:A:4730:VAL:HG23	1.75	0.69
2:D:3783:GLU:OE1	2:D:3784:LYS:NZ	2.18	0.69
2:B:4726:MET:HE2	2:B:4730:VAL:HG23	1.75	0.68
2:D:875:PRO:HD2	2:D:878:LEU:HD12	1.74	0.68
2:D:4747:ALA:HB1	2:D:4757:LEU:HD11	1.75	0.68
2:B:4687:LYS:HD2	2:B:4688:PRO:HD2	1.75	0.68
2:C:4726:MET:HE2	2:C:4730:VAL:HG23	1.75	0.68
2:C:875:PRO:HD2	2:C:878:LEU:HD12	1.74	0.68
2:C:4687:LYS:HD2	2:C:4688:PRO:HD2	1.75	0.68
2:C:988:LEU:HD13	2:C:1055:ARG:HE	1.59	0.68
2:D:4237:SER:N	2:D:4240:THR:HG1	1.91	0.68
2:C:2172:MET:HE3	2:C:2172:MET:HA	1.74	0.68
2:A:4687:LYS:HD2	2:A:4688:PRO:HD2	1.75	0.68
2:D:4726:MET:HE2	2:D:4730:VAL:HG23	1.75	0.68
2:B:988:LEU:HD13	2:B:1055:ARG:HE	1.59	0.68
2:B:4186:MET:HA	2:B:4186:MET:HE3	1.75	0.68
2:A:288:HIS:O	2:A:290:ARG:NH1	2.26	0.68
2:C:4747:ALA:HB1	2:C:4757:LEU:HD11	1.75	0.68
2:A:875:PRO:HD2	2:A:878:LEU:HD12	1.74	0.67
2:B:679:VAL:HG22	2:B:800:VAL:HG12	1.76	0.67
2:B:3890:TRP:HB3	2:C:76:ARG:HG2	1.76	0.67
2:D:2172:MET:HA	2:D:2172:MET:HE3	1.74	0.67
2:A:3118:GLY:HA2	2:A:3121:LEU:HB3	1.76	0.67
2:A:1435:GLY:H	2:A:1500:ARG:HH22	1.43	0.67
2:C:4640:PHE:CD2	2:C:4641:PRO:HD3	2.30	0.67
2:D:4640:PHE:CD2	2:D:4641:PRO:HD3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:988:LEU:HD13	2:A:1055:ARG:HE	1.59	0.67
2:A:4186:MET:HA	2:A:4186:MET:HE3	1.75	0.67
2:B:4237:SER:N	2:B:4240:THR:HG1	1.92	0.67
2:C:679:VAL:HG22	2:C:800:VAL:HG12	1.77	0.67
2:C:4831:ILE:HG13	2:C:4843:ARG:HH21	1.59	0.67
1:J:137:VAL:HG21	2:B:3587:TRP:CH2	2.30	0.67
2:B:288:HIS:O	2:B:290:ARG:NH1	2.26	0.67
2:B:897:LYS:HD2	2:B:902:TRP:NE1	2.10	0.67
2:A:4237:SER:N	2:A:4240:THR:HG1	1.92	0.67
2:A:4270:LYS:HA	2:A:4273:LYS:HE2	1.77	0.67
2:A:4640:PHE:CD2	2:A:4641:PRO:HD3	2.30	0.67
2:B:4831:ILE:HG13	2:B:4843:ARG:HH21	1.59	0.67
2:C:4186:MET:HA	2:C:4186:MET:HE3	1.75	0.67
2:D:988:LEU:HD13	2:D:1055:ARG:HE	1.59	0.67
2:D:3253:GLY:HA2	2:D:3264:CYS:HB3	1.77	0.67
2:A:4747:ALA:HB1	2:A:4757:LEU:HD11	1.75	0.67
2:C:897:LYS:HD2	2:C:902:TRP:NE1	2.10	0.67
2:C:3118:GLY:HA2	2:C:3121:LEU:HB3	1.76	0.67
2:D:4651:ARG:NH2	2:D:4672:MET:SD	2.68	0.67
2:A:3253:GLY:HA2	2:A:3264:CYS:HB3	1.77	0.67
2:B:1435:GLY:H	2:B:1500:ARG:HH22	1.43	0.67
2:B:4747:ALA:HB1	2:B:4757:LEU:HD11	1.75	0.67
2:C:3253:GLY:HA2	2:C:3264:CYS:HB3	1.77	0.67
2:D:288:HIS:O	2:D:290:ARG:NH1	2.26	0.67
2:D:3118:GLY:HA2	2:D:3121:LEU:HB3	1.76	0.67
1:I:101:ILE:N	1:I:137:VAL:O	2.25	0.67
2:A:679:VAL:HG22	2:A:800:VAL:HG12	1.77	0.67
2:A:2760:TYR:HA	2:A:2763:LEU:HD13	1.78	0.67
2:D:897:LYS:HD2	2:D:902:TRP:NE1	2.10	0.67
2:D:1435:GLY:H	2:D:1500:ARG:HH22	1.43	0.67
2:D:3142:THR:O	2:D:3144:LYS:NZ	2.28	0.67
2:A:897:LYS:HD2	2:A:902:TRP:NE1	2.10	0.66
2:C:2760:TYR:HA	2:C:2763:LEU:HD13	1.77	0.66
2:D:3848:GLU:OE1	2:D:3922:GLU:OE2	2.13	0.66
2:D:4186:MET:HA	2:D:4186:MET:HE3	1.75	0.66
2:C:3142:THR:O	2:C:3144:LYS:NZ	2.28	0.66
2:C:4818:TYR:OH	2:D:4847:ASP:OD2	2.08	0.66
2:D:679:VAL:HG22	2:D:800:VAL:HG12	1.77	0.66
2:A:4120:GLU:HA	2:A:4123:GLU:HG2	1.78	0.66
2:B:4270:LYS:HA	2:B:4273:LYS:HE2	1.77	0.66
2:D:4831:ILE:HG13	2:D:4843:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4640:PHE:CD2	2:B:4641:PRO:HD3	2.30	0.66
2:C:3250:TRP:HZ2	2:C:3309:LYS:HE3	1.60	0.66
2:A:3848:GLU:OE1	2:A:3922:GLU:OE2	2.13	0.66
2:B:3253:GLY:HA2	2:B:3264:CYS:HB3	1.77	0.66
2:C:2824:ARG:NH2	2:D:1502:ASN:HB3	2.10	0.66
2:C:4270:LYS:HA	2:C:4273:LYS:HE2	1.77	0.66
2:C:4651:ARG:NH2	2:C:4672:MET:SD	2.68	0.66
2:A:1172:THR:HB	2:A:1190:LEU:HD11	1.78	0.66
2:A:4831:ILE:HG13	2:A:4843:ARG:HH21	1.59	0.66
2:B:606:ARG:HH11	2:B:644:LEU:HD21	1.61	0.66
2:B:897:LYS:HD2	2:B:902:TRP:CE2	2.31	0.66
2:B:1172:THR:HB	2:B:1190:LEU:HD11	1.78	0.66
2:B:2760:TYR:HA	2:B:2763:LEU:HD13	1.77	0.66
2:B:4651:ARG:NH2	2:B:4672:MET:SD	2.68	0.66
2:C:2928:GLN:OE1	2:C:2931:ARG:NH2	2.29	0.66
2:A:897:LYS:HD2	2:A:902:TRP:CE2	2.31	0.66
2:B:3118:GLY:HA2	2:B:3121:LEU:HB3	1.76	0.66
2:B:3848:GLU:OE1	2:B:3922:GLU:OE2	2.13	0.66
2:C:1172:THR:HB	2:C:1190:LEU:HD11	1.78	0.66
2:C:1242:ASN:HB3	2:C:1807:ARG:HG3	1.77	0.66
2:D:1172:THR:HB	2:D:1190:LEU:HD11	1.78	0.66
2:A:4651:ARG:NH2	2:A:4672:MET:SD	2.68	0.66
2:D:3250:TRP:HZ2	2:D:3309:LYS:HE3	1.60	0.66
2:B:2830:ASN:HB3	2:C:1435:GLY:HA3	1.76	0.66
2:C:3848:GLU:OE1	2:C:3922:GLU:OE2	2.13	0.66
1:J:101:ILE:N	1:J:137:VAL:O	2.25	0.66
2:B:3997:LYS:NZ	2:B:4001:ASP:OD2	2.29	0.66
2:C:606:ARG:HH11	2:C:644:LEU:HD21	1.61	0.66
2:D:606:ARG:HH11	2:D:644:LEU:HD21	1.61	0.66
2:D:2760:TYR:HA	2:D:2763:LEU:HD13	1.78	0.66
2:D:4270:LYS:HA	2:D:4273:LYS:HE2	1.77	0.66
2:A:2928:GLN:OE1	2:A:2931:ARG:NH2	2.29	0.65
2:C:1435:GLY:H	2:C:1500:ARG:HH22	1.43	0.65
2:B:1242:ASN:HB3	2:B:1807:ARG:HG3	1.77	0.65
2:B:2928:GLN:OE1	2:B:2931:ARG:NH2	2.29	0.65
2:C:874:LEU:HD13	2:C:940:LEU:HD13	1.79	0.65
2:D:897:LYS:HD2	2:D:902:TRP:CE2	2.31	0.65
2:A:606:ARG:HH11	2:A:644:LEU:HD21	1.61	0.65
2:A:1910:LEU:HD13	2:A:2062:ILE:HG12	1.79	0.65
1:K:101:ILE:N	1:K:137:VAL:O	2.25	0.65
2:B:3847:CYS:HB3	2:B:3855:GLN:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:897:LYS:HD2	2:C:902:TRP:CE2	2.31	0.65
2:D:16:THR:HG1	2:D:110:HIS:N	1.94	0.65
2:D:4120:GLU:HA	2:D:4123:GLU:HG2	1.78	0.65
2:B:1910:LEU:HD13	2:B:2062:ILE:HG12	1.79	0.65
2:B:3250:TRP:HZ2	2:B:3309:LYS:HE3	1.60	0.65
2:B:4120:GLU:HA	2:B:4123:GLU:HG2	1.78	0.65
2:B:16:THR:HG1	2:B:110:HIS:N	1.95	0.65
2:C:2389:MET:HE1	2:C:2460:PHE:HA	1.79	0.65
2:D:2928:GLN:OE1	2:D:2931:ARG:NH2	2.29	0.65
1:L:101:ILE:N	1:L:137:VAL:O	2.25	0.65
2:C:3847:CYS:HB3	2:C:3855:GLN:HG3	1.78	0.65
2:A:2389:MET:HE1	2:A:2460:PHE:HA	1.79	0.65
2:B:1936:LEU:HD11	2:B:1976:LEU:HD22	1.79	0.65
2:B:2389:MET:HE1	2:B:2460:PHE:HA	1.79	0.65
2:B:2831:VAL:HB	2:B:2894:LYS:HE3	1.79	0.65
2:C:1910:LEU:HD13	2:C:2062:ILE:HG12	1.79	0.65
2:D:4052:MET:HE1	2:D:4063:THR:HA	1.79	0.65
2:A:1242:ASN:HB3	2:A:1807:ARG:HG3	1.78	0.65
2:C:4120:GLU:HA	2:C:4123:GLU:HG2	1.78	0.65
2:A:4822:ARG:NH1	2:B:4829:ASP:OD1	2.29	0.65
2:B:2187:ILE:HG13	2:B:2227:VAL:HG13	1.79	0.65
2:B:2801:TYR:OH	2:C:1496:PRO:O	2.14	0.65
2:D:1910:LEU:HD13	2:D:2062:ILE:HG12	1.79	0.65
2:D:3246:MET:HG2	2:D:3309:LYS:NZ	2.12	0.65
2:A:1936:LEU:HD11	2:A:1976:LEU:HD22	1.79	0.64
2:A:3250:TRP:HZ2	2:A:3309:LYS:HE3	1.60	0.64
2:D:1242:ASN:HB3	2:D:1807:ARG:HG3	1.77	0.64
2:A:874:LEU:HD13	2:A:940:LEU:HD13	1.79	0.64
2:A:3142:THR:O	2:A:3144:LYS:NZ	2.28	0.64
2:C:2831:VAL:HB	2:C:2894:LYS:HE3	1.79	0.64
2:D:2831:VAL:HB	2:D:2894:LYS:HE3	1.79	0.64
2:B:874:LEU:HD13	2:B:940:LEU:HD13	1.79	0.64
2:C:16:THR:HG1	2:C:110:HIS:N	1.94	0.64
2:D:1936:LEU:HD11	2:D:1976:LEU:HD22	1.79	0.64
2:D:2389:MET:HE1	2:D:2460:PHE:HA	1.79	0.64
2:A:16:THR:HG1	2:A:110:HIS:N	1.95	0.64
2:C:2187:ILE:HG13	2:C:2227:VAL:HG13	1.79	0.64
2:C:3997:LYS:NZ	2:C:4001:ASP:OD2	2.29	0.64
2:A:2187:ILE:HG13	2:A:2227:VAL:HG13	1.79	0.64
2:A:3848:GLU:OE1	2:A:3848:GLU:HA	1.97	0.64
2:B:902:TRP:CD1	2:B:918:LEU:HD12	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3246:MET:HG2	2:B:3309:LYS:NZ	2.12	0.64
2:B:4052:MET:HE1	2:B:4063:THR:HA	1.79	0.64
2:C:4690:LYS:HE3	2:C:4692:SER:HB2	1.80	0.64
2:A:2831:VAL:HB	2:A:2894:LYS:HE3	1.79	0.64
2:A:3246:MET:HG2	2:A:3309:LYS:NZ	2.12	0.64
2:D:2187:ILE:HG13	2:D:2227:VAL:HG13	1.79	0.64
2:A:3260:ARG:HG2	2:A:3263:MET:HB3	1.80	0.64
2:C:3246:MET:HG2	2:C:3309:LYS:NZ	2.12	0.64
2:A:3847:CYS:HB3	2:A:3855:GLN:HG3	1.78	0.64
2:C:4052:MET:HE1	2:C:4063:THR:HA	1.79	0.64
2:D:3260:ARG:HG2	2:D:3263:MET:HB3	1.80	0.64
2:D:3848:GLU:OE1	2:D:3848:GLU:HA	1.97	0.64
2:D:3997:LYS:NZ	2:D:4001:ASP:OD2	2.29	0.64
2:A:902:TRP:CD1	2:A:918:LEU:HD12	2.33	0.64
2:B:4889:PHE:HD2	2:B:4915:LEU:HD21	1.63	0.64
2:D:3847:CYS:HB3	2:D:3855:GLN:HG3	1.78	0.64
2:A:3997:LYS:NZ	2:A:4001:ASP:OD2	2.29	0.64
2:C:801:ARG:NH1	2:C:1615:GLN:O	2.30	0.64
2:C:3848:GLU:OE1	2:C:3848:GLU:HA	1.97	0.64
2:A:801:ARG:NH1	2:A:1615:GLN:O	2.30	0.63
2:A:4753:LEU:HD23	2:B:4773:LEU:HD13	1.80	0.63
2:B:3142:THR:O	2:B:3144:LYS:NZ	2.28	0.63
2:C:3172:GLU:HG2	2:C:3211:LEU:HD12	1.81	0.63
2:A:3172:GLU:HG2	2:A:3211:LEU:HD12	1.80	0.63
2:B:3260:ARG:HG2	2:B:3263:MET:HB3	1.80	0.63
2:C:1936:LEU:HD11	2:C:1976:LEU:HD22	1.79	0.63
2:D:4690:LYS:HE3	2:D:4692:SER:HB2	1.80	0.63
2:C:3260:ARG:HG2	2:C:3263:MET:HB3	1.80	0.63
2:D:902:TRP:CD1	2:D:918:LEU:HD12	2.33	0.63
2:A:1720:MET:HE3	2:A:2127:ARG:HD3	1.80	0.63
2:C:902:TRP:CD1	2:C:918:LEU:HD12	2.33	0.63
2:C:4276:VAL:O	2:C:4279:MET:HG3	1.99	0.63
2:D:4889:PHE:HD2	2:D:4915:LEU:HD21	1.63	0.63
2:B:3172:GLU:HG2	2:B:3211:LEU:HD12	1.81	0.63
2:C:1720:MET:HE3	2:C:2127:ARG:HD3	1.80	0.63
2:D:3172:GLU:HG2	2:D:3211:LEU:HD12	1.80	0.63
2:A:4276:VAL:O	2:A:4279:MET:HG3	1.99	0.63
2:B:309:MET:HE3	2:B:315:LEU:HB3	1.81	0.63
2:B:3848:GLU:OE1	2:B:3848:GLU:HA	1.97	0.63
2:C:893:TRP:O	2:C:897:LYS:HG2	1.99	0.63
2:A:4052:MET:HE1	2:A:4063:THR:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4889:PHE:HD2	2:A:4915:LEU:HD21	1.63	0.62
2:C:2465:LYS:NZ	2:C:2495:ASP:OD2	2.30	0.62
2:C:2758:LYS:HB2	2:C:2762:LEU:HD23	1.81	0.62
2:C:4045:LYS:HD2	2:C:4067:LEU:HD22	1.81	0.62
2:D:309:MET:HE3	2:D:315:LEU:HB3	1.81	0.62
2:A:4690:LYS:HE3	2:A:4692:SER:HB2	1.80	0.62
2:B:4276:VAL:O	2:B:4279:MET:HG3	1.99	0.62
2:B:4690:LYS:HE3	2:B:4692:SER:HB2	1.80	0.62
2:B:1720:MET:HE3	2:B:2127:ARG:HD3	1.80	0.62
2:B:4045:LYS:HD2	2:B:4067:LEU:HD22	1.81	0.62
2:D:874:LEU:HD13	2:D:940:LEU:HD13	1.79	0.62
2:D:3188:SER:OG	2:D:3190:ARG:NH1	2.32	0.62
2:B:999:LEU:HB3	2:B:1050:LEU:HD11	1.82	0.62
2:C:309:MET:HE3	2:C:315:LEU:HB3	1.81	0.62
2:C:2969:PRO:O	2:C:2973:GLN:NE2	2.33	0.62
2:D:999:LEU:HB3	2:D:1050:LEU:HD11	1.82	0.62
2:A:309:MET:HE3	2:A:315:LEU:HB3	1.81	0.62
2:A:2969:PRO:O	2:A:2973:GLN:NE2	2.33	0.62
2:A:3211:LEU:O	2:A:3215:MET:HG2	1.99	0.62
1:L:110:MET:HA	2:D:3590:LEU:HD21	1.82	0.62
2:B:2833:LEU:HB3	2:B:2837:LEU:HD11	1.82	0.62
2:C:999:LEU:HB3	2:C:1050:LEU:HD11	1.82	0.62
2:C:4889:PHE:HD2	2:C:4915:LEU:HD21	1.63	0.62
2:D:893:TRP:O	2:D:897:LYS:HG2	1.99	0.62
2:D:4276:VAL:O	2:D:4279:MET:HG3	1.99	0.62
2:A:999:LEU:HB3	2:A:1050:LEU:HD11	1.82	0.62
2:A:3188:SER:OG	2:A:3190:ARG:NH1	2.32	0.62
2:B:3188:SER:OG	2:B:3190:ARG:NH1	2.32	0.62
2:C:2833:LEU:HB3	2:C:2837:LEU:HD11	1.82	0.62
2:D:1048:ASP:HA	2:D:1051:ARG:HG2	1.81	0.62
2:A:2827:ASP:OD2	2:A:2830:ASN:ND2	2.32	0.62
2:B:2758:LYS:HB2	2:B:2762:LEU:HD23	1.81	0.62
2:B:2827:ASP:OD2	2:B:2830:ASN:ND2	2.32	0.62
2:B:3211:LEU:O	2:B:3215:MET:HG2	1.99	0.62
2:C:3188:SER:OG	2:C:3190:ARG:NH1	2.32	0.62
2:D:801:ARG:NH1	2:D:1615:GLN:O	2.30	0.62
2:D:1031:ARG:NH1	6:D:5004:ATP:O3G	2.33	0.62
2:D:2827:ASP:OD2	2:D:2830:ASN:ND2	2.32	0.62
2:D:2969:PRO:O	2:D:2973:GLN:NE2	2.33	0.62
2:A:174:LYS:O	2:A:176:ARG:NH1	2.33	0.62
2:A:1031:ARG:NH1	6:A:5004:ATP:O3G	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:ASN:OD1	2:B:897:LYS:N	2.33	0.62
2:B:3848:GLU:OE2	2:B:3922:GLU:OE1	2.03	0.62
2:D:1720:MET:HE3	2:D:2127:ARG:HD3	1.80	0.62
2:D:3211:LEU:O	2:D:3215:MET:HG2	1.99	0.62
2:B:893:TRP:O	2:B:897:LYS:HG2	1.99	0.62
2:D:896:ASN:OD1	2:D:897:LYS:N	2.33	0.62
2:A:1119:ARG:NH2	2:A:1196:ASP:OD1	2.33	0.61
2:A:1502:ASN:OD1	2:A:1503:ASN:N	2.33	0.61
2:A:2244:ALA:O	2:A:2248:MET:HB2	2.00	0.61
2:A:2758:LYS:HB2	2:A:2762:LEU:HD23	1.81	0.61
2:A:4748:MET:HA	2:A:4748:MET:HE3	1.82	0.61
2:C:2827:ASP:OD2	2:C:2830:ASN:ND2	2.32	0.61
2:C:2857:LYS:HA	2:C:2860:LEU:HG	1.82	0.61
2:C:4748:MET:HA	2:C:4748:MET:HE3	1.82	0.61
2:D:1119:ARG:NH2	2:D:1196:ASP:OD1	2.33	0.61
2:A:893:TRP:O	2:A:897:LYS:HG2	1.99	0.61
2:C:896:ASN:OD1	2:C:897:LYS:N	2.33	0.61
2:C:1048:ASP:HA	2:C:1051:ARG:HG2	1.81	0.61
2:C:1502:ASN:OD1	2:C:1503:ASN:N	2.33	0.61
2:D:4045:LYS:HD2	2:D:4067:LEU:HD22	1.81	0.61
2:A:896:ASN:OD1	2:A:897:LYS:N	2.33	0.61
2:B:1119:ARG:NH2	2:B:1196:ASP:OD1	2.33	0.61
2:A:1048:ASP:HA	2:A:1051:ARG:HG2	1.81	0.61
2:A:3803:LEU:HB2	2:A:3884:SER:HB2	1.83	0.61
2:A:4045:LYS:HD2	2:A:4067:LEU:HD22	1.81	0.61
1:J:137:VAL:HG21	2:B:3587:TRP:HH2	1.66	0.61
2:B:1048:ASP:HA	2:B:1051:ARG:HG2	1.81	0.61
2:B:3192:ARG:HA	2:B:3197:LEU:HD12	1.83	0.61
2:D:174:LYS:O	2:D:176:ARG:NH1	2.33	0.61
2:A:3034:HIS:CE1	2:A:3038:GLN:HE22	2.18	0.61
2:A:3192:ARG:HA	2:A:3197:LEU:HD12	1.83	0.61
2:C:878:LEU:HA	2:C:881:ILE:HG22	1.83	0.61
2:D:878:LEU:HA	2:D:881:ILE:HG22	1.83	0.61
2:B:878:LEU:HA	2:B:881:ILE:HG22	1.83	0.61
2:B:1502:ASN:OD1	2:B:1503:ASN:N	2.33	0.61
2:B:2232:PRO:HB3	2:B:2382:ILE:HD11	1.83	0.61
2:C:3192:ARG:HA	2:C:3197:LEU:HD12	1.83	0.61
2:C:3211:LEU:O	2:C:3215:MET:HG2	2.00	0.61
2:D:2857:LYS:HA	2:D:2860:LEU:HG	1.82	0.61
2:D:3803:LEU:HB2	2:D:3884:SER:HB2	1.83	0.61
2:D:4748:MET:HA	2:D:4748:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2841:ALA:HB1	2:A:2889:ALA:HB1	1.83	0.61
2:B:2733:SER:O	2:B:2737:LEU:HG	2.01	0.61
2:B:2969:PRO:O	2:B:2973:GLN:NE2	2.33	0.61
2:C:2244:ALA:O	2:C:2248:MET:HB2	2.00	0.61
2:C:3034:HIS:CE1	2:C:3038:GLN:HE22	2.18	0.61
2:D:185:SER:HG	2:D:188:SER:HG	1.44	0.61
2:D:2244:ALA:O	2:D:2248:MET:HB2	2.00	0.61
2:D:3034:HIS:CE1	2:D:3038:GLN:HE22	2.18	0.61
2:A:2773:TRP:HB3	2:A:2774:PRO:HD3	1.83	0.61
2:A:2833:LEU:HB3	2:A:2837:LEU:HD11	1.82	0.61
2:B:2841:ALA:HB1	2:B:2889:ALA:HB1	1.83	0.61
2:D:2232:PRO:HB3	2:D:2382:ILE:HD11	1.83	0.61
2:D:2465:LYS:NZ	2:D:2495:ASP:OD2	2.30	0.61
2:D:2758:LYS:HB2	2:D:2762:LEU:HD23	1.81	0.61
2:D:4748:MET:O	2:D:4754:ARG:NH2	2.34	0.61
2:B:3148:VAL:HG13	2:B:3151:GLN:HE21	1.66	0.61
2:C:373:THR:HG21	2:C:397:GLY:HA2	1.83	0.61
2:A:1129:GLY:HA3	2:A:1145:TRP:HB3	1.83	0.61
2:A:2478:ILE:HD13	2:A:2527:LEU:HD11	1.83	0.61
2:A:2857:LYS:HA	2:A:2860:LEU:HG	1.82	0.61
2:A:4187:GLU:OE2	2:A:4947:ARG:NH2	2.34	0.61
2:A:4930:GLU:HA	2:A:4933:HIS:HD2	1.66	0.61
2:B:2244:ALA:O	2:B:2248:MET:HB2	2.00	0.61
2:C:561:ARG:HH11	2:C:561:ARG:HG3	1.66	0.61
2:C:4930:GLU:HA	2:C:4933:HIS:CD2	2.36	0.61
2:C:4930:GLU:HA	2:C:4933:HIS:HD2	1.65	0.61
2:D:2833:LEU:HB3	2:D:2837:LEU:HD11	1.82	0.61
2:A:878:LEU:HA	2:A:881:ILE:HG22	1.83	0.60
2:A:3070:LYS:O	2:A:3074:ASN:ND2	2.34	0.60
2:A:3848:GLU:OE2	2:A:3922:GLU:OE1	2.03	0.60
2:A:4748:MET:O	2:A:4754:ARG:NH2	2.34	0.60
2:B:4748:MET:HA	2:B:4748:MET:HE3	1.82	0.60
2:C:2733:SER:O	2:C:2737:LEU:HG	2.01	0.60
2:C:3848:GLU:OE1	2:C:3922:GLU:CG	2.49	0.60
2:D:1502:ASN:OD1	2:D:1503:ASN:N	2.33	0.60
2:A:997:ASP:OD1	2:A:1047:LYS:NZ	2.32	0.60
1:J:127:ARG:NH1	1:J:135:GLY:C	2.58	0.60
2:B:1129:GLY:HA3	2:B:1145:TRP:HB3	1.83	0.60
2:B:3070:LYS:O	2:B:3074:ASN:ND2	2.34	0.60
2:C:174:LYS:O	2:C:176:ARG:NH1	2.33	0.60
2:C:3148:VAL:HG13	2:C:3151:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2773:TRP:HB3	2:D:2774:PRO:HD3	1.83	0.60
2:D:3070:LYS:O	2:D:3074:ASN:ND2	2.34	0.60
2:D:3148:VAL:HG13	2:D:3151:GLN:HE21	1.66	0.60
2:A:2232:PRO:HB3	2:A:2382:ILE:HD11	1.83	0.60
1:J:110:MET:HA	2:B:3590:LEU:HD21	1.82	0.60
2:B:1031:ARG:NH1	6:B:5004:ATP:O3G	2.33	0.60
2:B:2773:TRP:HB3	2:B:2774:PRO:HD3	1.83	0.60
2:B:2857:LYS:HA	2:B:2860:LEU:HG	1.82	0.60
2:B:3183:ILE:HG23	2:B:3184:TYR:CD1	2.36	0.60
2:B:3253:GLY:C	2:B:3255:GLU:H	2.09	0.60
2:B:3939:ARG:NH2	2:B:3942:ASP:OD2	2.34	0.60
2:B:4137:GLU:HG2	2:B:4147:ARG:HG2	1.83	0.60
2:C:2232:PRO:HB3	2:C:2382:ILE:HD11	1.83	0.60
2:D:561:ARG:HH11	2:D:561:ARG:HG3	1.66	0.60
2:D:2478:ILE:HD13	2:D:2527:LEU:HD11	1.83	0.60
2:A:4271:VAL:HG12	2:A:4274:MET:HE3	1.84	0.60
2:B:561:ARG:HG3	2:B:561:ARG:HH11	1.66	0.60
2:B:2425:SER:O	2:C:142:LYS:NZ	2.33	0.60
2:C:3070:LYS:O	2:C:3074:ASN:ND2	2.34	0.60
2:C:4187:GLU:OE2	2:C:4947:ARG:NH2	2.34	0.60
2:A:3253:GLY:C	2:A:3255:GLU:H	2.09	0.60
2:C:349:MET:HE3	2:C:349:MET:HA	1.83	0.60
2:C:1031:ARG:NH1	6:C:5004:ATP:O3G	2.33	0.60
2:C:3253:GLY:C	2:C:3255:GLU:H	2.09	0.60
2:C:3803:LEU:HB2	2:C:3884:SER:HB2	1.83	0.60
2:C:4049:HIS:HD2	2:C:4067:LEU:HD11	1.67	0.60
2:C:4137:GLU:HG2	2:C:4147:ARG:HG2	1.83	0.60
2:D:895:MET:HE3	2:D:978:PRO:CG	2.32	0.60
2:D:2733:SER:O	2:D:2737:LEU:HG	2.01	0.60
2:A:373:THR:HG21	2:A:397:GLY:HA2	1.83	0.60
2:A:3148:VAL:HG13	2:A:3151:GLN:HE21	1.66	0.60
2:A:4049:HIS:HD2	2:A:4067:LEU:HD11	1.67	0.60
2:A:4829:ASP:OD1	2:D:4822:ARG:NH1	2.35	0.60
2:B:174:LYS:O	2:B:176:ARG:NH1	2.33	0.60
2:B:349:MET:HA	2:B:349:MET:HE3	1.84	0.60
2:B:3803:LEU:HB2	2:B:3884:SER:HB2	1.83	0.60
2:B:4271:VAL:HG12	2:B:4274:MET:HE3	1.84	0.60
2:D:3192:ARG:HA	2:D:3197:LEU:HD12	1.83	0.60
2:D:4271:VAL:HG12	2:D:4274:MET:HE3	1.84	0.60
2:D:4930:GLU:HA	2:D:4933:HIS:HD2	1.66	0.60
2:B:3034:HIS:CE1	2:B:3038:GLN:HE22	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4187:GLU:OE2	2:B:4947:ARG:NH2	2.34	0.60
2:C:3183:ILE:HG23	2:C:3184:TYR:CD1	2.35	0.60
2:C:4748:MET:O	2:C:4754:ARG:NH2	2.34	0.60
2:D:373:THR:HG21	2:D:397:GLY:HA2	1.83	0.60
2:A:2465:LYS:NZ	2:A:2495:ASP:OD2	2.30	0.60
2:A:4930:GLU:HA	2:A:4933:HIS:CD2	2.36	0.60
2:B:2478:ILE:HD13	2:B:2527:LEU:HD11	1.83	0.60
2:B:4049:HIS:HD2	2:B:4067:LEU:HD11	1.67	0.60
2:C:1119:ARG:NH2	2:C:1196:ASP:OD1	2.33	0.60
2:C:2773:TRP:HB3	2:C:2774:PRO:HD3	1.83	0.60
2:D:3304:GLN:HA	2:D:3307:ILE:HG12	1.84	0.60
2:D:4187:GLU:OE2	2:D:4947:ARG:NH2	2.34	0.60
2:A:4137:GLU:HG2	2:A:4147:ARG:HG2	1.83	0.60
2:B:3304:GLN:HA	2:B:3307:ILE:HG12	1.84	0.60
2:C:1129:GLY:HA3	2:C:1145:TRP:HB3	1.83	0.60
2:A:4831:ILE:HG13	2:A:4843:ARG:NH2	2.17	0.60
2:B:4107:GLU:OE2	2:B:4149:TYR:OH	2.15	0.60
2:C:4818:TYR:OH	2:D:4843:ARG:NH1	2.35	0.60
2:A:2733:SER:O	2:A:2737:LEU:HG	2.01	0.59
2:A:3848:GLU:OE1	2:A:3922:GLU:CG	2.49	0.59
2:B:4831:ILE:HG13	2:B:4843:ARG:NH2	2.17	0.59
2:C:2194:ALA:HB2	2:C:2234:MET:HE3	1.84	0.59
2:D:2841:ALA:HB1	2:D:2889:ALA:HB1	1.83	0.59
2:D:4831:ILE:HG13	2:D:4843:ARG:NH2	2.17	0.59
2:A:561:ARG:HH11	2:A:561:ARG:HG3	1.66	0.59
2:B:902:TRP:HD1	2:B:918:LEU:HD12	1.67	0.59
2:B:904:TYR:HB2	2:B:918:LEU:HD22	1.85	0.59
2:B:4748:MET:O	2:B:4754:ARG:NH2	2.34	0.59
2:C:2841:ALA:HB1	2:C:2889:ALA:HB1	1.83	0.59
2:C:4492:LEU:HD12	2:C:4592:CYS:SG	2.43	0.59
2:D:997:ASP:HA	2:D:1047:LYS:HE2	1.84	0.59
2:A:895:MET:HE3	2:A:978:PRO:CG	2.32	0.59
2:A:2641:SER:HB3	2:A:2676:LEU:HD21	1.84	0.59
2:A:3183:ILE:HG23	2:A:3184:TYR:CD1	2.35	0.59
2:C:4271:VAL:HG12	2:C:4274:MET:HE3	1.84	0.59
2:D:490:GLN:HG2	2:D:495:ILE:HD12	1.84	0.59
2:D:4930:GLU:HA	2:D:4933:HIS:CD2	2.36	0.59
2:A:902:TRP:HD1	2:A:918:LEU:HD12	1.67	0.59
2:A:2338:GLU:OE1	2:A:2338:GLU:N	2.36	0.59
2:B:801:ARG:NH1	2:B:1615:GLN:O	2.30	0.59
2:B:2214:MET:HA	2:B:2214:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3848:GLU:OE1	2:B:3922:GLU:CG	2.49	0.59
2:D:349:MET:HA	2:D:349:MET:HE3	1.84	0.59
2:A:2214:MET:HA	2:A:2214:MET:HE3	1.85	0.59
1:L:5:LEU:HD23	1:L:10:ILE:HG13	1.84	0.59
1:K:5:LEU:HD23	1:K:10:ILE:HG13	1.85	0.59
2:B:2194:ALA:HB2	2:B:2234:MET:HE3	1.84	0.59
2:C:490:GLN:HG2	2:C:495:ILE:HD12	1.84	0.59
2:D:2641:SER:HB3	2:D:2676:LEU:HD21	1.84	0.59
2:B:2641:SER:HB3	2:B:2676:LEU:HD21	1.85	0.59
2:C:3304:GLN:HA	2:C:3307:ILE:HG12	1.84	0.59
2:C:3317:THR:H	2:C:3320:LEU:HD23	1.67	0.59
2:D:2338:GLU:OE1	2:D:2338:GLU:N	2.36	0.59
2:D:3317:THR:H	2:D:3320:LEU:HD23	1.67	0.59
2:D:4049:HIS:HD2	2:D:4067:LEU:HD11	1.67	0.59
2:A:349:MET:HA	2:A:349:MET:HE3	1.84	0.59
2:A:997:ASP:HA	2:A:1047:LYS:HE2	1.84	0.59
2:B:2338:GLU:OE1	2:B:2338:GLU:N	2.36	0.59
2:B:3317:THR:H	2:B:3320:LEU:HD23	1.67	0.59
2:B:4492:LEU:HD12	2:B:4592:CYS:SG	2.43	0.59
2:B:4930:GLU:HA	2:B:4933:HIS:HD2	1.66	0.59
2:C:997:ASP:HA	2:C:1047:LYS:HE2	1.84	0.59
2:D:902:TRP:HD1	2:D:918:LEU:HD12	1.67	0.59
2:D:1129:GLY:HA3	2:D:1145:TRP:HB3	1.83	0.59
1:I:5:LEU:HD23	1:I:10:ILE:HG13	1.85	0.59
2:A:1165:MET:HE1	2:A:1176:THR:HG23	1.85	0.59
2:A:3304:GLN:HA	2:A:3307:ILE:HG12	1.84	0.59
2:B:373:THR:HG21	2:B:397:GLY:HA2	1.83	0.59
2:B:4930:GLU:HA	2:B:4933:HIS:CD2	2.36	0.59
2:C:185:SER:HG	2:C:188:SER:HG	1.51	0.59
2:C:2478:ILE:HD13	2:C:2527:LEU:HD11	1.83	0.59
2:C:3939:ARG:NH2	2:C:3942:ASP:OD2	2.34	0.59
2:B:894:VAL:O	2:B:898:ILE:HG12	2.03	0.59
2:B:997:ASP:HA	2:B:1047:LYS:HE2	1.84	0.59
2:B:3131:TYR:CD2	2:B:3205:CYS:HB3	2.38	0.59
2:C:185:SER:OG	2:C:188:SER:OG	2.20	0.59
2:C:902:TRP:HD1	2:C:918:LEU:HD12	1.67	0.59
2:C:904:TYR:HB2	2:C:918:LEU:HD22	1.85	0.59
2:C:1038:LEU:O	2:C:1043:LYS:NZ	2.36	0.59
2:D:3253:GLY:C	2:D:3255:GLU:H	2.09	0.59
2:D:3848:GLU:OE1	2:D:3922:GLU:CG	2.49	0.59
2:A:904:TYR:HB2	2:A:918:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3159:LEU:HD12	2:A:3241:MET:HE2	1.85	0.59
2:A:4057:HIS:CE1	2:B:4660:PHE:HZ	2.21	0.59
2:A:4492:LEU:HD12	2:A:4592:CYS:SG	2.42	0.59
2:D:4137:GLU:HG2	2:D:4147:ARG:HG2	1.83	0.59
2:C:894:VAL:O	2:C:898:ILE:HG12	2.03	0.58
2:C:2338:GLU:N	2:C:2338:GLU:OE1	2.36	0.58
2:D:4492:LEU:HD12	2:D:4592:CYS:SG	2.43	0.58
2:A:884:LYS:HA	2:A:887:GLU:HG3	1.86	0.58
2:A:2640:LEU:HA	2:A:2643:LYS:HZ1	1.68	0.58
2:B:1165:MET:HE1	2:B:1176:THR:HG23	1.85	0.58
2:B:3159:LEU:HD12	2:B:3241:MET:HE2	1.85	0.58
2:B:2926:LEU:O	2:B:2930:ILE:HD12	2.04	0.58
2:C:895:MET:HE3	2:C:978:PRO:CG	2.32	0.58
2:C:4818:TYR:HE1	2:D:4847:ASP:HB2	1.68	0.58
2:D:2194:ALA:HB2	2:D:2234:MET:HE3	1.84	0.58
2:D:3939:ARG:NH2	2:D:3942:ASP:OD2	2.34	0.58
2:A:1722:ASN:O	2:A:1919:ARG:NH2	2.36	0.58
2:C:2734:MET:HE2	2:C:2737:LEU:HD11	1.86	0.58
2:D:884:LYS:HA	2:D:887:GLU:HG3	1.86	0.58
2:D:1722:ASN:O	2:D:1919:ARG:NH2	2.36	0.58
2:D:2734:MET:HE2	2:D:2737:LEU:HD11	1.86	0.58
2:D:3159:LEU:HD12	2:D:3241:MET:HE2	1.85	0.58
2:D:3173:THR:O	2:D:3177:LYS:NZ	2.36	0.58
2:A:494:MET:HE1	2:A:497:LEU:HD23	1.86	0.58
2:A:2734:MET:HE2	2:A:2737:LEU:HD11	1.86	0.58
2:A:3317:THR:H	2:A:3320:LEU:HD23	1.67	0.58
1:J:5:LEU:HD23	1:J:10:ILE:HG13	1.85	0.58
2:B:1722:ASN:O	2:B:1919:ARG:NH2	2.36	0.58
2:D:894:VAL:O	2:D:898:ILE:HG12	2.03	0.58
2:D:1100:ARG:HH22	2:D:1235:GLY:HA3	1.69	0.58
2:A:3131:TYR:CD2	2:A:3205:CYS:HB3	2.38	0.58
2:B:494:MET:HE1	2:B:497:LEU:HD23	1.86	0.58
2:B:2057:THR:OG1	2:B:2060:GLN:OE1	2.20	0.58
2:C:667:SER:HB2	2:C:669:GLN:HE22	1.69	0.58
2:C:884:LYS:HA	2:C:887:GLU:HG3	1.86	0.58
2:C:2982:PHE:O	2:C:3001:LYS:NZ	2.37	0.58
2:C:4831:ILE:HG13	2:C:4843:ARG:NH2	2.17	0.58
2:D:667:SER:HB2	2:D:669:GLN:HE22	1.69	0.58
2:D:904:TYR:HB2	2:D:918:LEU:HD22	1.85	0.58
2:A:490:GLN:HG2	2:A:495:ILE:HD12	1.84	0.58
2:A:2194:ALA:HB2	2:A:2234:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2982:PHE:O	2:A:3001:LYS:NZ	2.37	0.58
2:B:490:GLN:HG2	2:B:495:ILE:HD12	1.84	0.58
2:B:895:MET:HE3	2:B:978:PRO:CG	2.32	0.58
2:B:903:GLN:H	2:B:913:ARG:HE	1.52	0.58
2:C:2202:TYR:O	2:C:2206:ILE:HG12	2.04	0.58
2:C:2641:SER:HB3	2:C:2676:LEU:HD21	1.84	0.58
2:D:2202:TYR:O	2:D:2206:ILE:HG12	2.04	0.58
2:D:2736:LYS:HB3	2:D:2741:TRP:HB2	1.86	0.58
2:D:2982:PHE:O	2:D:3001:LYS:NZ	2.37	0.58
2:A:963:LYS:HB3	2:A:977:LYS:HE2	1.86	0.58
1:L:42:GLN:HE21	2:D:1957:LEU:HD21	1.68	0.58
2:B:2982:PHE:O	2:B:3001:LYS:NZ	2.37	0.58
2:C:903:GLN:H	2:C:913:ARG:HE	1.52	0.58
2:C:2926:LEU:O	2:C:2930:ILE:HD12	2.04	0.58
2:D:2214:MET:HA	2:D:2214:MET:HE3	1.85	0.58
2:A:335:LYS:NZ	2:A:401:ASP:OD2	2.37	0.58
2:A:4518:LEU:HG	2:B:4810:LEU:HD13	1.85	0.58
2:B:3173:THR:O	2:B:3177:LYS:NZ	2.36	0.58
2:D:903:GLN:H	2:D:913:ARG:HE	1.52	0.58
2:D:905:GLY:HA3	2:D:914:GLN:HB3	1.86	0.58
2:A:1898:LEU:HD22	2:A:1902:VAL:HG11	1.86	0.58
2:A:2736:LYS:HB3	2:A:2741:TRP:HB2	1.86	0.58
2:B:884:LYS:HA	2:B:887:GLU:HG3	1.86	0.58
2:C:1722:ASN:O	2:C:1919:ARG:NH2	2.36	0.58
2:C:2214:MET:HA	2:C:2214:MET:HE3	1.85	0.58
2:C:3173:THR:O	2:C:3177:LYS:NZ	2.36	0.58
2:D:247:VAL:O	2:D:272:ARG:NH1	2.37	0.58
2:D:963:LYS:HB3	2:D:977:LYS:HE2	1.86	0.58
2:D:3112:ILE:HG23	2:D:3118:GLY:HA3	1.86	0.58
2:A:247:VAL:O	2:A:272:ARG:NH1	2.37	0.57
2:A:3173:THR:O	2:A:3177:LYS:NZ	2.36	0.57
2:B:667:SER:HB2	2:B:669:GLN:HE22	1.69	0.57
2:B:963:LYS:HB3	2:B:977:LYS:HE2	1.86	0.57
2:B:997:ASP:OD1	2:B:1047:LYS:NZ	2.32	0.57
2:B:1100:ARG:HH22	2:B:1235:GLY:HA3	1.69	0.57
2:C:1100:ARG:HH22	2:C:1235:GLY:HA3	1.69	0.57
2:D:335:LYS:NZ	2:D:401:ASP:OD2	2.37	0.57
2:A:270:HIS:CD2	2:A:491:GLU:HG3	2.39	0.57
2:A:891:GLU:O	2:A:894:VAL:HG22	2.04	0.57
2:A:894:VAL:O	2:A:898:ILE:HG12	2.03	0.57
2:A:3677:THR:O	2:A:3679:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:HIS:CD2	2:B:491:GLU:HG3	2.39	0.57
2:B:2465:LYS:NZ	2:B:2495:ASP:OD2	2.30	0.57
2:C:247:VAL:O	2:C:272:ARG:NH1	2.37	0.57
2:C:494:MET:HE1	2:C:497:LEU:HD23	1.86	0.57
2:C:2123:LEU:HD13	2:C:2167:MET:HG2	1.87	0.57
2:C:3321:PRO:O	2:C:3325:LYS:HG2	2.04	0.57
2:A:903:GLN:H	2:A:913:ARG:HE	1.52	0.57
2:A:4719:PHE:CE2	2:D:4294:LEU:HD22	2.39	0.57
1:J:102:SER:OG	1:J:105:GLU:OE1	2.22	0.57
1:J:106:LEU:HD22	2:B:3587:TRP:HE1	1.70	0.57
2:B:670:TYR:O	2:B:673:TRP:NE1	2.38	0.57
2:B:891:GLU:O	2:B:894:VAL:HG22	2.04	0.57
2:B:2734:MET:HE2	2:B:2737:LEU:HD11	1.86	0.57
2:C:891:GLU:O	2:C:894:VAL:HG22	2.04	0.57
2:C:905:GLY:HA3	2:C:914:GLN:HB3	1.86	0.57
2:C:2972:ASP:HA	2:C:3035:ILE:HD11	1.87	0.57
2:C:3112:ILE:HG23	2:C:3118:GLY:HA3	1.86	0.57
2:C:3159:LEU:HD12	2:C:3241:MET:HE2	1.85	0.57
2:D:1165:MET:HE1	2:D:1176:THR:HG23	1.85	0.57
2:D:1898:LEU:HD22	2:D:1902:VAL:HG11	1.86	0.57
2:B:335:LYS:NZ	2:B:401:ASP:OD2	2.37	0.57
2:B:2202:TYR:O	2:B:2206:ILE:HG12	2.04	0.57
2:D:2972:ASP:HA	2:D:3035:ILE:HD11	1.87	0.57
2:A:667:SER:HB2	2:A:669:GLN:HE22	1.69	0.57
2:A:1100:ARG:HH22	2:A:1235:GLY:HA3	1.69	0.57
2:A:2972:ASP:HA	2:A:3035:ILE:HD11	1.87	0.57
2:A:3321:PRO:O	2:A:3325:LYS:HG2	2.04	0.57
2:B:247:VAL:O	2:B:272:ARG:NH1	2.37	0.57
2:B:2640:LEU:HA	2:B:2643:LYS:HZ1	1.69	0.57
2:B:3321:PRO:O	2:B:3325:LYS:HG2	2.04	0.57
2:C:1165:MET:HE1	2:C:1176:THR:HG23	1.85	0.57
2:C:2057:THR:OG1	2:C:2060:GLN:OE1	2.20	0.57
2:D:2123:LEU:HD13	2:D:2167:MET:HG2	1.86	0.57
2:A:924:LEU:HD12	2:A:925:PRO:HD2	1.86	0.57
2:A:1286:THR:OG1	2:A:1550:PRO:O	2.22	0.57
2:A:2926:LEU:O	2:A:2930:ILE:HD12	2.04	0.57
2:B:1898:LEU:HD22	2:B:1902:VAL:HG11	1.86	0.57
2:C:670:TYR:O	2:C:673:TRP:NE1	2.38	0.57
2:C:3677:THR:O	2:C:3679:LYS:NZ	2.37	0.57
2:D:670:TYR:O	2:D:673:TRP:NE1	2.38	0.57
2:D:2627:TRP:HB2	2:D:2630:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3321:PRO:O	2:D:3325:LYS:HG2	2.04	0.57
1:I:102:SER:HA	1:I:136:GLN:HG3	1.87	0.57
2:A:2202:TYR:O	2:A:2206:ILE:HG12	2.04	0.57
2:B:1989:PRO:O	2:B:1993:ARG:HG3	2.05	0.57
2:B:3131:TYR:OH	2:B:3205:CYS:O	2.23	0.57
2:C:1989:PRO:O	2:C:1993:ARG:HG3	2.05	0.57
2:D:2926:LEU:O	2:D:2930:ILE:HD12	2.04	0.57
2:D:3677:THR:O	2:D:3679:LYS:NZ	2.37	0.57
2:A:4583:SER:O	2:A:4587:ILE:HD12	2.05	0.57
2:B:3677:THR:O	2:B:3679:LYS:NZ	2.37	0.57
2:C:1898:LEU:HD22	2:C:1902:VAL:HG11	1.86	0.57
2:C:3958:LEU:HD22	2:C:3964:GLN:HG3	1.87	0.57
2:D:3183:ILE:HG23	2:D:3184:TYR:CD1	2.35	0.57
2:A:3112:ILE:HG23	2:A:3118:GLY:HA3	1.86	0.57
1:L:127:ARG:NH1	1:L:135:GLY:C	2.58	0.57
2:B:2972:ASP:HA	2:B:3035:ILE:HD11	1.87	0.57
2:C:924:LEU:HD12	2:C:925:PRO:HD2	1.86	0.57
2:C:963:LYS:HB3	2:C:977:LYS:HE2	1.86	0.57
2:C:3163:ALA:HB1	2:C:3245:TYR:HD1	1.70	0.57
2:D:4583:SER:O	2:D:4587:ILE:HD12	2.05	0.57
2:A:3131:TYR:CZ	2:A:3205:CYS:O	2.58	0.57
2:A:3131:TYR:OH	2:A:3205:CYS:O	2.23	0.57
2:B:1951:LEU:HD11	2:B:1961:LYS:HE3	1.87	0.57
2:C:335:LYS:NZ	2:C:401:ASP:OD2	2.37	0.57
2:D:494:MET:HE1	2:D:497:LEU:HD23	1.86	0.57
2:D:3163:ALA:HB1	2:D:3245:TYR:HD1	1.70	0.57
2:A:4827:ILE:O	2:A:4831:ILE:HG12	2.05	0.56
2:B:924:LEU:HD12	2:B:925:PRO:HD2	1.86	0.56
2:B:968:LYS:NZ	2:B:971:GLN:O	2.38	0.56
2:B:3958:LEU:HD22	2:B:3964:GLN:HG3	1.87	0.56
2:C:968:LYS:NZ	2:C:971:GLN:O	2.38	0.56
2:C:4040:LYS:NZ	2:C:4042:VAL:O	2.38	0.56
2:D:924:LEU:HD12	2:D:925:PRO:HD2	1.86	0.56
2:D:968:LYS:NZ	2:D:971:GLN:O	2.38	0.56
2:D:2146:LEU:O	2:D:2150:MET:HG2	2.05	0.56
2:D:3823:GLU:HG3	2:D:3826:GLY:H	1.70	0.56
2:A:670:TYR:O	2:A:673:TRP:NE1	2.38	0.56
2:A:3797:MET:HE1	2:A:3870:ILE:HG23	1.87	0.56
2:A:3920:LEU:HD22	2:A:3935:LEU:HD11	1.87	0.56
2:B:1795:LEU:HD23	2:B:1842:ILE:HD11	1.87	0.56
2:B:2610:LEU:HD13	2:B:2644:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3026:ALA:HA	2:B:3029:ILE:HD12	1.87	0.56
2:C:1732:GLU:HB3	2:C:1753:LEU:HD21	1.87	0.56
2:C:1795:LEU:HD23	2:C:1842:ILE:HD11	1.87	0.56
2:C:3797:MET:HE1	2:C:3870:ILE:HG23	1.87	0.56
2:D:3920:LEU:HD22	2:D:3935:LEU:HD11	1.87	0.56
2:D:4040:LYS:NZ	2:D:4042:VAL:O	2.38	0.56
2:A:705:PRO:HD3	2:A:857:LEU:HD13	1.87	0.56
2:A:905:GLY:HA3	2:A:914:GLN:HB3	1.86	0.56
2:A:1435:GLY:HA3	2:D:2830:ASN:HB3	1.87	0.56
2:A:1732:GLU:HB3	2:A:1753:LEU:HD21	1.87	0.56
2:A:2123:LEU:HD13	2:A:2167:MET:HG2	1.87	0.56
2:A:2627:TRP:HB2	2:A:2630:PHE:HB2	1.87	0.56
2:A:3823:GLU:HG3	2:A:3826:GLY:H	1.70	0.56
1:L:102:SER:HA	1:L:136:GLN:HG3	1.87	0.56
1:L:102:SER:OG	1:L:105:GLU:OE1	2.22	0.56
2:B:905:GLY:HA3	2:B:914:GLN:HB3	1.86	0.56
2:B:4827:ILE:O	2:B:4831:ILE:HG12	2.05	0.56
2:C:270:HIS:CD2	2:C:491:GLU:HG3	2.39	0.56
2:C:3823:GLU:HG3	2:C:3826:GLY:H	1.70	0.56
2:C:4237:SER:N	2:C:4240:THR:HG1	2.03	0.56
2:C:4827:ILE:O	2:C:4831:ILE:HG12	2.05	0.56
2:D:270:HIS:CD2	2:D:491:GLU:HG3	2.39	0.56
2:D:1038:LEU:O	2:D:1043:LYS:NZ	2.36	0.56
2:D:3026:ALA:HA	2:D:3029:ILE:HD12	1.87	0.56
2:A:2142:MET:HB3	2:A:2192:MET:HE1	1.88	0.56
2:A:3163:ALA:HB1	2:A:3245:TYR:HD1	1.70	0.56
2:B:2123:LEU:HD13	2:B:2167:MET:HG2	1.87	0.56
2:B:3823:GLU:HG3	2:B:3826:GLY:H	1.70	0.56
2:C:1951:LEU:HD11	2:C:1961:LYS:HE3	1.87	0.56
2:C:4819:VAL:HG12	2:C:4830:GLU:HG3	1.88	0.56
2:D:3131:TYR:CZ	2:D:3205:CYS:O	2.58	0.56
2:A:3939:ARG:NH2	2:A:3942:ASP:OD2	2.34	0.56
2:B:1732:GLU:HB3	2:B:1753:LEU:HD21	1.87	0.56
2:B:3246:MET:HG2	2:B:3309:LYS:HZ2	1.68	0.56
2:B:4040:LYS:NZ	2:B:4042:VAL:O	2.38	0.56
2:C:4583:SER:O	2:C:4587:ILE:HD12	2.05	0.56
2:D:891:GLU:O	2:D:894:VAL:HG22	2.04	0.56
2:A:968:LYS:NZ	2:A:971:GLN:O	2.38	0.56
2:B:4583:SER:O	2:B:4587:ILE:HD12	2.05	0.56
2:C:705:PRO:HD3	2:C:857:LEU:HD13	1.87	0.56
2:C:3846:LEU:HB3	2:C:3854:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3152:ARG:HD2	2:D:3232:PRO:HB2	1.87	0.56
2:A:2610:LEU:HD13	2:A:2644:LEU:HD21	1.87	0.56
2:A:3152:ARG:HD2	2:A:3232:PRO:HB2	1.87	0.56
2:A:4040:LYS:NZ	2:A:4042:VAL:O	2.38	0.56
1:K:102:SER:OG	1:K:105:GLU:OE1	2.22	0.56
2:B:1500:ARG:HG3	2:B:1505:LEU:HB2	1.88	0.56
2:B:2736:LYS:HB3	2:B:2741:TRP:HB2	1.86	0.56
2:B:3112:ILE:HG23	2:B:3118:GLY:HA3	1.86	0.56
2:B:3163:ALA:HB1	2:B:3245:TYR:HD1	1.70	0.56
2:B:3846:LEU:HB3	2:B:3854:PHE:CE2	2.41	0.56
2:C:2627:TRP:HB2	2:C:2630:PHE:HB2	1.87	0.56
2:C:2736:LYS:HB3	2:C:2741:TRP:HB2	1.86	0.56
2:D:2610:LEU:HD13	2:D:2644:LEU:HD21	1.87	0.56
2:D:3958:LEU:HD22	2:D:3964:GLN:HG3	1.87	0.56
1:J:102:SER:HA	1:J:136:GLN:HG3	1.87	0.56
1:K:102:SER:HA	1:K:136:GLN:HG3	1.87	0.56
2:B:705:PRO:HD3	2:B:857:LEU:HD13	1.87	0.56
2:B:4819:VAL:HG12	2:B:4830:GLU:HG3	1.88	0.56
2:C:2610:LEU:HD13	2:C:2644:LEU:HD21	1.87	0.56
2:C:3152:ARG:HD2	2:C:3232:PRO:HB2	1.87	0.56
2:C:3235:MET:HB2	2:C:3239:LEU:HD12	1.88	0.56
2:D:891:GLU:HB3	2:D:895:MET:HE1	1.88	0.56
2:A:2146:LEU:O	2:A:2150:MET:HG2	2.05	0.56
2:A:3026:ALA:HA	2:A:3029:ILE:HD12	1.87	0.56
1:J:122:VAL:O	1:J:126:ILE:HG23	2.06	0.56
1:K:122:VAL:O	1:K:126:ILE:HG23	2.06	0.56
2:C:1500:ARG:HG3	2:C:1505:LEU:HB2	1.88	0.56
2:C:3729:ALA:HA	2:C:3732:HIS:CD2	2.41	0.56
2:A:3729:ALA:HA	2:A:3732:HIS:CD2	2.41	0.56
2:B:3013:VAL:O	2:B:3018:ARG:NH2	2.40	0.56
2:B:3797:MET:HE1	2:B:3870:ILE:HG23	1.87	0.56
2:C:3920:LEU:HD22	2:C:3935:LEU:HD11	1.87	0.56
2:D:3192:ARG:HD3	2:D:3199:THR:HG22	1.87	0.56
2:D:3235:MET:HB2	2:D:3239:LEU:HD12	1.88	0.56
2:D:3846:LEU:HB3	2:D:3854:PHE:CE2	2.41	0.56
1:I:5:LEU:HB3	1:I:10:ILE:HD11	1.88	0.55
2:A:1989:PRO:O	2:A:1993:ARG:HG3	2.05	0.55
2:A:3013:VAL:O	2:A:3018:ARG:NH2	2.39	0.55
2:A:3846:LEU:HB3	2:A:3854:PHE:CE2	2.41	0.55
3:F:83:TYR:HB3	3:F:87:GLY:HA2	1.88	0.55
1:J:5:LEU:HB3	1:J:10:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:THR:OG1	2:B:110:HIS:N	2.39	0.55
2:B:2146:LEU:O	2:B:2150:MET:HG2	2.05	0.55
2:D:2142:MET:HB3	2:D:2192:MET:HE1	1.88	0.55
1:I:122:VAL:O	1:I:126:ILE:HG23	2.06	0.55
2:A:1951:LEU:HD11	2:A:1961:LYS:HE3	1.87	0.55
2:A:2057:THR:OG1	2:A:2060:GLN:OE1	2.20	0.55
2:B:514:PHE:CD2	2:B:526:TRP:HB2	2.41	0.55
2:B:2627:TRP:HB2	2:B:2630:PHE:HB2	1.87	0.55
2:B:3131:TYR:CZ	2:B:3205:CYS:O	2.58	0.55
2:C:2961:LYS:HB2	2:C:2965:LYS:NZ	2.21	0.55
2:C:3192:ARG:HD3	2:C:3199:THR:HG22	1.87	0.55
2:D:705:PRO:HD3	2:D:857:LEU:HD13	1.87	0.55
2:D:1795:LEU:HD23	2:D:1842:ILE:HD11	1.87	0.55
2:D:1989:PRO:O	2:D:1993:ARG:HG3	2.05	0.55
2:D:2961:LYS:HB2	2:D:2965:LYS:NZ	2.21	0.55
2:D:3729:ALA:HA	2:D:3732:HIS:CD2	2.41	0.55
2:D:3848:GLU:OE2	2:D:3922:GLU:OE1	2.03	0.55
2:A:3958:LEU:HD22	2:A:3964:GLN:HG3	1.87	0.55
2:B:2961:LYS:HB2	2:B:2965:LYS:NZ	2.21	0.55
2:C:798:ILE:HD12	2:C:800:VAL:HG22	1.88	0.55
2:A:1795:LEU:HD23	2:A:1842:ILE:HD11	1.87	0.55
2:A:2961:LYS:HB2	2:A:2965:LYS:NZ	2.21	0.55
3:G:83:TYR:HB3	3:G:87:GLY:HA2	1.89	0.55
3:H:83:TYR:HB3	3:H:87:GLY:HA2	1.88	0.55
1:L:122:VAL:O	1:L:126:ILE:HG23	2.06	0.55
1:K:107:ARG:NH2	1:K:119:ASP:OD2	2.40	0.55
2:B:2142:MET:HB3	2:B:2192:MET:HE1	1.88	0.55
2:C:3131:TYR:CZ	2:C:3205:CYS:O	2.58	0.55
2:D:514:PHE:CD2	2:D:526:TRP:HB2	2.41	0.55
2:D:3591:LEU:HB3	2:D:3595:ARG:NH1	2.22	0.55
2:D:3797:MET:HE1	2:D:3870:ILE:HG23	1.87	0.55
2:A:891:GLU:HB3	2:A:895:MET:HE1	1.88	0.55
2:A:3131:TYR:CD1	2:A:3205:CYS:HB2	2.41	0.55
2:B:2512:MET:HA	2:B:2512:MET:CE	2.35	0.55
2:C:514:PHE:CD2	2:C:526:TRP:HB2	2.41	0.55
2:D:1732:GLU:HB3	2:D:1753:LEU:HD21	1.87	0.55
2:B:1487:MET:HE1	2:B:1544:PHE:CD2	2.42	0.55
2:B:3152:ARG:HD2	2:B:3232:PRO:HB2	1.87	0.55
2:B:3591:LEU:HB3	2:B:3595:ARG:NH1	2.22	0.55
2:B:3920:LEU:HD22	2:B:3935:LEU:HD11	1.87	0.55
2:C:891:GLU:HB3	2:C:895:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2146:LEU:O	2:C:2150:MET:HG2	2.05	0.55
2:D:798:ILE:HD12	2:D:800:VAL:HG22	1.88	0.55
2:D:1487:MET:HE1	2:D:1544:PHE:CD2	2.42	0.55
2:D:3013:VAL:O	2:D:3018:ARG:NH2	2.40	0.55
2:A:1487:MET:HE1	2:A:1544:PHE:CD2	2.42	0.55
1:L:107:ARG:NH2	1:L:119:ASP:OD2	2.40	0.55
1:K:5:LEU:HB3	1:K:10:ILE:HD11	1.88	0.55
2:B:3192:ARG:HD3	2:B:3199:THR:HG22	1.87	0.55
2:C:2448:ASP:OD2	2:C:2450:ASN:ND2	2.40	0.55
2:D:2640:LEU:HA	2:D:2643:LYS:HZ1	1.71	0.55
2:D:4819:VAL:HG12	2:D:4830:GLU:HG3	1.88	0.55
2:D:4827:ILE:O	2:D:4831:ILE:HG12	2.05	0.55
2:A:1500:ARG:HG3	2:A:1505:LEU:HB2	1.88	0.55
2:C:2435:VAL:HG11	2:C:2468:MET:HE3	1.89	0.55
2:C:3026:ALA:HA	2:C:3029:ILE:HD12	1.87	0.55
2:C:3227:ARG:HD2	2:C:3228:TYR:H	1.72	0.55
2:D:2435:VAL:HG11	2:D:2468:MET:HE3	1.89	0.55
2:D:2448:ASP:OD2	2:D:2450:ASN:ND2	2.40	0.55
2:D:2732:TRP:O	2:D:2736:LYS:HG3	2.07	0.55
2:A:514:PHE:CD2	2:A:526:TRP:HB2	2.41	0.55
2:A:1007:TRP:O	2:A:1011:ARG:HG2	2.07	0.55
2:A:2448:ASP:OD2	2:A:2450:ASN:ND2	2.40	0.55
1:K:127:ARG:NH1	1:K:135:GLY:C	2.58	0.55
2:B:3729:ALA:HA	2:B:3732:HIS:CD2	2.41	0.55
2:C:2512:MET:HA	2:C:2512:MET:CE	2.35	0.55
2:C:3322:LEU:HD12	2:C:3323:MET:HG3	1.89	0.55
2:D:1951:LEU:HD11	2:D:1961:LYS:HE3	1.87	0.55
2:A:185:SER:OG	2:A:188:SER:OG	2.20	0.55
2:A:246:THR:HG21	2:A:267:VAL:HG11	1.89	0.55
2:A:4819:VAL:HG12	2:A:4830:GLU:HG3	1.88	0.55
1:J:107:ARG:NH2	1:J:119:ASP:OD2	2.40	0.55
2:B:891:GLU:HB3	2:B:895:MET:HE1	1.88	0.55
2:B:2732:TRP:O	2:B:2736:LYS:HG3	2.07	0.55
2:B:3227:ARG:HD2	2:B:3228:TYR:H	1.72	0.55
2:B:3235:MET:HB2	2:B:3239:LEU:HD12	1.88	0.55
2:C:2142:MET:HB3	2:C:2192:MET:HE1	1.88	0.55
2:C:2436:ILE:HG22	2:C:2491:GLY:HA3	1.89	0.55
2:D:1007:TRP:O	2:D:1011:ARG:HG2	2.07	0.55
2:D:2918:GLU:HA	2:D:2923:TYR:CD1	2.42	0.55
2:D:3227:ARG:HD2	2:D:3228:TYR:H	1.72	0.55
1:I:102:SER:OG	1:I:105:GLU:OE1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:629:GLN:OE1	2:A:1669:ASN:ND2	2.37	0.54
2:A:2732:TRP:O	2:A:2736:LYS:HG3	2.07	0.54
2:A:2918:GLU:HA	2:A:2923:TYR:CD1	2.42	0.54
2:A:4169:LYS:HE3	2:A:4170:ARG:HH22	1.72	0.54
3:E:83:TYR:HB3	3:E:87:GLY:HA2	1.89	0.54
2:D:3131:TYR:OH	2:D:3205:CYS:O	2.23	0.54
2:A:16:THR:OG1	2:A:110:HIS:N	2.39	0.54
2:A:849:ASP:OD1	2:A:1214:ARG:NE	2.37	0.54
2:A:3192:ARG:HD3	2:A:3199:THR:HG22	1.87	0.54
2:B:2918:GLU:HA	2:B:2923:TYR:CD1	2.42	0.54
2:C:997:ASP:OD1	2:C:1047:LYS:NZ	2.32	0.54
2:C:2171:VAL:HA	2:C:2174:VAL:HG22	1.89	0.54
2:C:3591:LEU:HB3	2:C:3595:ARG:NH1	2.22	0.54
2:D:4169:LYS:HE3	2:D:4170:ARG:HH22	1.72	0.54
2:A:562:LEU:HG	2:A:600:LEU:HD13	1.89	0.54
2:A:2436:ILE:HG22	2:A:2491:GLY:HA3	1.89	0.54
2:A:3591:LEU:HB3	2:A:3595:ARG:NH1	2.22	0.54
1:L:5:LEU:HB3	1:L:10:ILE:HD11	1.88	0.54
2:B:296:ARG:HH21	2:B:324:VAL:HA	1.73	0.54
2:B:839:GLU:HB3	2:B:851:LEU:HD12	1.88	0.54
2:C:1487:MET:HE1	2:C:1544:PHE:CD2	2.42	0.54
2:C:3901:GLN:OE1	2:C:3904:ARG:NH1	2.40	0.54
2:D:1500:ARG:HG3	2:D:1505:LEU:HB2	1.88	0.54
2:D:2057:THR:OG1	2:D:2060:GLN:OE1	2.20	0.54
2:D:3322:LEU:HD12	2:D:3323:MET:HG3	1.89	0.54
1:I:134:ASP:OD1	2:A:3298:ARG:NH1	2.39	0.54
2:A:555:LEU:HD21	2:A:578:VAL:HG11	1.90	0.54
2:A:798:ILE:HD12	2:A:800:VAL:HG22	1.88	0.54
2:A:3322:LEU:HD12	2:A:3323:MET:HG3	1.89	0.54
2:A:4107:GLU:OE2	2:A:4149:TYR:OH	2.15	0.54
2:B:246:THR:HG21	2:B:267:VAL:HG11	1.89	0.54
2:B:555:LEU:HD21	2:B:578:VAL:HG11	1.90	0.54
2:B:798:ILE:HD12	2:B:800:VAL:HG22	1.88	0.54
2:B:2436:ILE:HG22	2:B:2491:GLY:HA3	1.90	0.54
2:B:3322:LEU:HD12	2:B:3323:MET:HG3	1.89	0.54
2:B:4169:LYS:HE3	2:B:4170:ARG:HH22	1.72	0.54
2:D:2171:VAL:HA	2:D:2174:VAL:HG22	1.89	0.54
2:D:2436:ILE:HG22	2:D:2491:GLY:HA3	1.89	0.54
2:A:839:GLU:HB3	2:A:851:LEU:HD12	1.88	0.54
2:A:3235:MET:HB2	2:A:3239:LEU:HD12	1.88	0.54
2:A:3312:PRO:HA	2:A:3315:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2171:VAL:HA	2:B:2174:VAL:HG22	1.89	0.54
2:C:16:THR:OG1	2:C:110:HIS:N	2.39	0.54
2:C:562:LEU:HG	2:C:600:LEU:HD13	1.89	0.54
2:C:3283:ILE:O	2:C:3287:ASN:HB2	2.08	0.54
2:C:4169:LYS:HE3	2:C:4170:ARG:HH22	1.72	0.54
2:D:1842:ILE:HD12	2:D:1845:LEU:HD12	1.90	0.54
1:I:127:ARG:NH1	1:I:135:GLY:C	2.58	0.54
2:A:1124:PRO:HD2	2:A:1594:VAL:HG23	1.90	0.54
2:A:2171:VAL:HA	2:A:2174:VAL:HG22	1.89	0.54
1:J:100:TYR:CD1	1:J:138:ASN:HB3	2.43	0.54
2:B:238:HIS:HB3	2:B:243:GLU:HG3	1.90	0.54
2:B:562:LEU:HG	2:B:600:LEU:HD13	1.89	0.54
2:D:16:THR:OG1	2:D:110:HIS:N	2.39	0.54
2:D:839:GLU:HB3	2:D:851:LEU:HD12	1.88	0.54
2:D:4633:LEU:O	2:D:4704:LYS:NZ	2.41	0.54
2:A:2134:MET:HE3	2:A:2135:GLY:H	1.73	0.54
2:B:1007:TRP:O	2:B:1011:ARG:HG2	2.07	0.54
2:B:2134:MET:HE3	2:B:2135:GLY:H	1.73	0.54
2:B:2448:ASP:OD2	2:B:2450:ASN:ND2	2.40	0.54
2:B:3901:GLN:OE1	2:B:3904:ARG:NH1	2.41	0.54
2:C:2918:GLU:HA	2:C:2923:TYR:CD1	2.42	0.54
2:D:842:GLN:HB2	2:D:1603:PHE:HB2	1.90	0.54
2:D:3283:ILE:O	2:D:3287:ASN:HB2	2.08	0.54
2:D:3950:VAL:O	2:D:3954:MET:HB2	2.08	0.54
2:A:296:ARG:HH21	2:A:324:VAL:HA	1.72	0.54
2:C:238:HIS:HB3	2:C:243:GLU:HG3	1.90	0.54
2:C:849:ASP:OD1	2:C:1214:ARG:NE	2.37	0.54
2:C:2732:TRP:O	2:C:2736:LYS:HG3	2.07	0.54
2:C:3131:TYR:CD2	2:C:3205:CYS:HB3	2.38	0.54
2:C:3131:TYR:OH	2:C:3205:CYS:O	2.23	0.54
2:C:3950:VAL:O	2:C:3954:MET:HB2	2.08	0.54
2:D:1184:ASP:OD2	2:D:1193:LYS:NZ	2.38	0.54
1:I:107:ARG:NH2	1:I:119:ASP:OD2	2.40	0.54
2:A:3227:ARG:HD2	2:A:3228:TYR:H	1.72	0.54
2:B:842:GLN:HB2	2:B:1603:PHE:HB2	1.90	0.54
2:C:2134:MET:HE3	2:C:2135:GLY:H	1.73	0.54
2:D:2134:MET:HE3	2:D:2135:GLY:H	1.73	0.54
2:A:1435:GLY:H	2:A:1500:ARG:NH2	2.06	0.54
2:A:3950:VAL:O	2:A:3954:MET:HB2	2.08	0.54
1:J:77:MET:HA	1:J:77:MET:HE3	1.90	0.54
1:K:100:TYR:CD1	1:K:138:ASN:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:296:ARG:HH21	2:C:324:VAL:HA	1.72	0.54
2:C:839:GLU:HB3	2:C:851:LEU:HD12	1.89	0.54
2:C:1007:TRP:CD1	2:C:1011:ARG:HH11	2.26	0.54
2:C:1124:PRO:HD2	2:C:1594:VAL:HG23	1.90	0.54
2:C:1286:THR:OG1	2:C:1550:PRO:O	2.22	0.54
2:C:1842:ILE:HD12	2:C:1845:LEU:HD12	1.90	0.54
2:D:296:ARG:HH21	2:D:324:VAL:HA	1.72	0.54
2:D:562:LEU:HG	2:D:600:LEU:HD13	1.89	0.54
2:D:996:VAL:HG22	2:D:1054:VAL:HG21	1.89	0.54
2:D:1007:TRP:CD1	2:D:1011:ARG:HH11	2.26	0.54
2:D:2593:VAL:HG12	2:D:2644:LEU:HB2	1.90	0.54
2:D:3901:GLN:OE1	2:D:3904:ARG:NH1	2.41	0.54
1:I:19:LEU:HD11	2:A:3595:ARG:HH21	1.73	0.53
2:A:605:GLY:HA2	2:A:1585:ARG:HD2	1.91	0.53
2:A:1038:LEU:O	2:A:1043:LYS:NZ	2.36	0.53
2:A:2435:VAL:HG11	2:A:2468:MET:HE3	1.89	0.53
2:A:3901:GLN:OE1	2:A:3904:ARG:NH1	2.41	0.53
2:B:713:TRP:HH2	2:B:1251:LEU:HD21	1.73	0.53
2:C:246:THR:HG21	2:C:267:VAL:HG11	1.89	0.53
2:C:555:LEU:HD21	2:C:578:VAL:HG11	1.90	0.53
2:C:842:GLN:HB2	2:C:1603:PHE:HB2	1.90	0.53
2:C:2640:LEU:HA	2:C:2643:LYS:HZ1	1.72	0.53
2:C:3312:PRO:HA	2:C:3315:LEU:HB2	1.89	0.53
2:D:2562:THR:O	2:D:2566:ARG:HG3	2.08	0.53
2:A:238:HIS:HB3	2:A:243:GLU:HG3	1.90	0.53
2:B:1979:PHE:CD1	2:B:1993:ARG:HG2	2.44	0.53
2:B:3283:ILE:O	2:B:3287:ASN:HB2	2.08	0.53
2:C:436:LEU:HG	2:C:445:VAL:HG11	1.91	0.53
2:C:713:TRP:HH2	2:C:1251:LEU:HD21	1.73	0.53
2:D:238:HIS:HB3	2:D:243:GLU:HG3	1.90	0.53
2:D:555:LEU:HD21	2:D:578:VAL:HG11	1.90	0.53
2:D:605:GLY:HA2	2:D:1585:ARG:HD2	1.90	0.53
2:D:1256:PRO:HG3	2:D:1453:TYR:HB2	1.90	0.53
2:D:3900:GLU:OE2	2:D:3904:ARG:NH2	2.41	0.53
1:L:42:GLN:HE21	2:D:1957:LEU:CD2	2.21	0.53
1:L:100:TYR:CD1	1:L:138:ASN:HB3	2.43	0.53
2:B:28:ILE:HG22	2:B:29:HIS:HD2	1.73	0.53
2:B:629:GLN:OE1	2:B:1669:ASN:ND2	2.37	0.53
2:B:1842:ILE:HD12	2:B:1845:LEU:HD12	1.90	0.53
2:B:2435:VAL:HG11	2:B:2468:MET:HE3	1.89	0.53
2:B:2926:LEU:HD12	2:B:3003:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4633:LEU:O	2:B:4704:LYS:NZ	2.41	0.53
2:C:801:ARG:HG2	2:C:1618:LEU:HA	1.91	0.53
2:C:1979:PHE:CD1	2:C:1993:ARG:HG2	2.44	0.53
2:C:3216:GLU:HA	2:C:3219:VAL:HG22	1.90	0.53
2:A:28:ILE:HG22	2:A:29:HIS:HD2	1.73	0.53
2:A:996:VAL:HG22	2:A:1054:VAL:HG21	1.90	0.53
2:A:1256:PRO:HG3	2:A:1453:TYR:HB2	1.90	0.53
2:A:1936:LEU:HD21	2:A:1976:LEU:HD13	1.91	0.53
2:B:1124:PRO:HD2	2:B:1594:VAL:HG23	1.90	0.53
2:C:2562:THR:O	2:C:2566:ARG:HG3	2.08	0.53
2:C:2859:GLU:O	2:C:2862:SER:OG	2.23	0.53
2:C:3900:GLU:OE2	2:C:3904:ARG:NH2	2.41	0.53
2:D:71:GLN:HB3	2:D:73:LEU:HD23	1.90	0.53
2:D:246:THR:HG21	2:D:267:VAL:HG11	1.89	0.53
1:I:77:MET:HE3	1:I:77:MET:HA	1.90	0.53
1:I:100:TYR:CD1	1:I:138:ASN:HB3	2.43	0.53
2:A:3246:MET:HG2	2:A:3309:LYS:HZ1	1.72	0.53
2:A:3900:GLU:OE2	2:A:3904:ARG:NH2	2.41	0.53
2:B:996:VAL:HG22	2:B:1054:VAL:HG21	1.89	0.53
2:B:3312:PRO:HA	2:B:3315:LEU:HB2	1.89	0.53
2:C:4049:HIS:CD2	2:C:4067:LEU:HD11	2.43	0.53
2:C:4633:LEU:O	2:C:4704:LYS:NZ	2.41	0.53
2:D:1144:ARG:NE	2:D:1150:GLU:OE2	2.42	0.53
2:D:2512:MET:HA	2:D:2512:MET:CE	2.35	0.53
2:D:3131:TYR:CD2	2:D:3205:CYS:HB3	2.38	0.53
2:A:1007:TRP:CD1	2:A:1011:ARG:HH11	2.26	0.53
2:A:1144:ARG:NE	2:A:1150:GLU:OE2	2.42	0.53
2:A:2593:VAL:HG12	2:A:2644:LEU:HB2	1.90	0.53
1:L:77:MET:HA	1:L:77:MET:HE3	1.90	0.53
1:K:134:ASP:OD1	2:C:3298:ARG:NH1	2.42	0.53
2:B:801:ARG:HG2	2:B:1618:LEU:HA	1.91	0.53
2:B:1936:LEU:HD21	2:B:1976:LEU:HD13	1.91	0.53
2:B:3861:GLN:H	2:B:3867:THR:HG23	1.74	0.53
2:B:3900:GLU:OE2	2:B:3904:ARG:NH2	2.41	0.53
2:B:3950:VAL:O	2:B:3954:MET:HB2	2.08	0.53
2:C:1007:TRP:O	2:C:1011:ARG:HG2	2.07	0.53
2:C:1256:PRO:HG3	2:C:1453:TYR:HB2	1.90	0.53
2:C:1957:LEU:HB2	2:C:3601:ALA:HB2	1.91	0.53
2:C:3013:VAL:O	2:C:3018:ARG:NH2	2.39	0.53
2:D:2779:LEU:O	2:D:2783:LEU:HD12	2.08	0.53
2:A:173:GLU:OE2	2:A:176:ARG:NH2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2290:TRP:CZ2	2:A:2388:ILE:HG12	2.44	0.53
2:A:4633:LEU:O	2:A:4704:LYS:NZ	2.41	0.53
1:K:77:MET:HA	1:K:77:MET:HE3	1.90	0.53
2:B:71:GLN:HB3	2:B:73:LEU:HD23	1.90	0.53
2:B:436:LEU:HG	2:B:445:VAL:HG11	1.91	0.53
2:B:1007:TRP:CD1	2:B:1011:ARG:HH11	2.26	0.53
2:B:2493:LEU:HG	2:B:2497:ARG:HH21	1.74	0.53
2:B:2779:LEU:O	2:B:2783:LEU:HD12	2.08	0.53
2:D:801:ARG:HG2	2:D:1618:LEU:HA	1.91	0.53
2:D:849:ASP:OD1	2:D:1214:ARG:NE	2.37	0.53
2:D:1124:PRO:HD2	2:D:1594:VAL:HG23	1.90	0.53
2:D:2290:TRP:CZ2	2:D:2388:ILE:HG12	2.44	0.53
2:D:2779:LEU:HA	2:D:2782:MET:HG2	1.91	0.53
2:A:842:GLN:HB2	2:A:1603:PHE:HB2	1.90	0.53
2:A:3216:GLU:HA	2:A:3219:VAL:HG22	1.90	0.53
2:A:3283:ILE:O	2:A:3287:ASN:HB2	2.08	0.53
2:A:4049:HIS:CD2	2:A:4067:LEU:HD11	2.43	0.53
2:A:4559:TYR:OH	2:B:4790:ARG:NH2	2.42	0.53
2:B:1144:ARG:NE	2:B:1150:GLU:OE2	2.42	0.53
2:B:2973:GLN:HA	2:B:2976:LYS:HZ3	1.74	0.53
2:C:1144:ARG:NE	2:C:1150:GLU:OE2	2.42	0.53
2:D:1431:ARG:NH1	2:D:1556:GLU:OE2	2.42	0.53
2:D:2905:ARG:HE	2:D:2906:GLY:H	1.57	0.53
2:D:3125:ASP:HB2	2:D:3195:LEU:HD22	1.91	0.53
2:D:4049:HIS:CD2	2:D:4067:LEU:HD11	2.43	0.53
2:A:1979:PHE:CD1	2:A:1993:ARG:HG2	2.44	0.53
2:A:2493:LEU:HG	2:A:2497:ARG:HH21	1.74	0.53
2:A:2905:ARG:HE	2:A:2906:GLY:H	1.57	0.53
2:A:3125:ASP:HB2	2:A:3195:LEU:HD22	1.91	0.53
2:B:185:SER:OG	2:B:188:SER:OG	2.20	0.53
2:B:3102:LEU:HD21	2:B:3155:LEU:HD23	1.91	0.53
2:C:28:ILE:HG22	2:C:29:HIS:HD2	1.73	0.53
2:C:2779:LEU:O	2:C:2783:LEU:HD12	2.09	0.53
2:C:2905:ARG:HE	2:C:2906:GLY:H	1.57	0.53
2:C:2926:LEU:HD12	2:C:3003:MET:HE3	1.90	0.53
2:D:658:ASN:ND2	2:D:833:LYS:HG2	2.24	0.53
2:D:3312:PRO:HA	2:D:3315:LEU:HB2	1.89	0.53
2:A:919:VAL:HB	2:A:923:LYS:HE3	1.91	0.53
2:A:2562:THR:O	2:A:2566:ARG:HG3	2.08	0.53
1:J:10:ILE:O	1:J:14:LYS:N	2.38	0.53
1:J:114:GLY:O	1:J:116:LYS:NZ	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1256:PRO:HG3	2:B:1453:TYR:HB2	1.90	0.53
2:B:3125:ASP:HB2	2:B:3195:LEU:HD22	1.91	0.53
2:B:3131:TYR:CD1	2:B:3205:CYS:HB2	2.41	0.53
2:C:71:GLN:HB3	2:C:73:LEU:HD23	1.90	0.53
2:C:173:GLU:OE2	2:C:176:ARG:NH2	2.36	0.53
2:C:3125:ASP:HB2	2:C:3195:LEU:HD22	1.91	0.53
2:C:3861:GLN:H	2:C:3867:THR:HG23	1.74	0.53
2:D:233:VAL:HG12	2:D:274:LEU:HD22	1.91	0.53
2:D:1419:PHE:O	2:D:1423:THR:HB	2.09	0.53
2:D:1978:ASN:HB2	2:D:1986:CYS:HB3	1.91	0.53
1:I:69:PHE:O	1:I:73:MET:HG2	2.10	0.52
2:A:713:TRP:HH2	2:A:1251:LEU:HD21	1.73	0.52
2:A:801:ARG:HG2	2:A:1618:LEU:HA	1.91	0.52
2:A:2512:MET:HA	2:A:2512:MET:CE	2.35	0.52
2:A:3102:LEU:HD21	2:A:3155:LEU:HD23	1.91	0.52
2:A:3890:TRP:HB3	2:B:76:ARG:HG2	1.90	0.52
3:G:50:ARG:HH21	3:G:53:LYS:HZ2	1.57	0.52
1:J:76:LYS:HB2	1:J:78:LYS:HZ2	1.73	0.52
2:B:605:GLY:HA2	2:B:1585:ARG:HD2	1.91	0.52
2:B:1611:ILE:HB	2:B:1615:GLN:HB2	1.91	0.52
2:B:2059:GLN:NE2	2:B:2091:GLN:O	2.42	0.52
2:B:2593:VAL:HG12	2:B:2644:LEU:HB2	1.90	0.52
2:B:3016:ARG:O	2:B:3018:ARG:NE	2.32	0.52
2:C:668:ALA:HB2	2:C:1012:ILE:HD11	1.92	0.52
2:C:996:VAL:HG22	2:C:1054:VAL:HG21	1.90	0.52
2:D:713:TRP:HH2	2:D:1251:LEU:HD21	1.73	0.52
2:D:2923:TYR:HA	2:D:3003:MET:HE1	1.92	0.52
2:A:28:ILE:HG22	2:A:29:HIS:CD2	2.44	0.52
2:A:334:SER:OG	2:A:336:GLU:OE1	2.22	0.52
2:A:1184:ASP:OD2	2:A:1193:LYS:NZ	2.38	0.52
2:A:1419:PHE:O	2:A:1423:THR:HB	2.09	0.52
2:B:28:ILE:HG22	2:B:29:HIS:CD2	2.45	0.52
2:B:919:VAL:HB	2:B:923:LYS:HE3	1.91	0.52
2:B:1957:LEU:HB2	2:B:3601:ALA:HB2	1.91	0.52
2:B:2905:ARG:HE	2:B:2906:GLY:H	1.57	0.52
2:C:629:GLN:OE1	2:C:1669:ASN:ND2	2.37	0.52
2:C:658:ASN:ND2	2:C:833:LYS:HG2	2.24	0.52
2:C:1419:PHE:O	2:C:1423:THR:HB	2.09	0.52
2:D:1435:GLY:H	2:D:1500:ARG:NH2	2.06	0.52
2:D:2859:GLU:O	2:D:2862:SER:OG	2.23	0.52
2:D:3861:GLN:H	2:D:3867:THR:HG23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:233:VAL:HG12	2:A:274:LEU:HD22	1.91	0.52
1:K:69:PHE:O	1:K:73:MET:HG2	2.10	0.52
2:C:3246:MET:HG2	2:C:3309:LYS:HZ1	1.75	0.52
2:D:668:ALA:HB2	2:D:1012:ILE:HD11	1.92	0.52
2:D:1979:PHE:CD1	2:D:1993:ARG:HG2	2.44	0.52
2:A:71:GLN:HB3	2:A:73:LEU:HD23	1.90	0.52
2:A:185:SER:HG	2:A:188:SER:HG	1.51	0.52
2:A:1978:ASN:HB2	2:A:1986:CYS:HB3	1.91	0.52
2:A:2923:TYR:HA	2:A:3003:MET:HE1	1.92	0.52
2:A:4790:ARG:HH22	2:D:4557:VAL:HG21	1.74	0.52
2:C:2831:VAL:CG2	2:D:1435:GLY:HA2	2.39	0.52
2:D:28:ILE:HG22	2:D:29:HIS:HD2	1.73	0.52
2:D:1936:LEU:HD21	2:D:1976:LEU:HD13	1.91	0.52
2:A:1957:LEU:HB2	2:A:3601:ALA:HB2	1.91	0.52
1:K:110:MET:HA	2:C:3590:LEU:HD21	1.92	0.52
2:B:3216:GLU:HA	2:B:3219:VAL:HG22	1.90	0.52
2:C:1431:ARG:NH1	2:C:1556:GLU:OE2	2.42	0.52
2:C:2290:TRP:CZ2	2:C:2388:ILE:HG12	2.44	0.52
2:C:3109:PHE:HB3	2:C:3162:PHE:HA	1.91	0.52
2:D:1286:THR:OG1	2:D:1550:PRO:O	2.22	0.52
2:D:4081:GLU:O	2:D:4085:LYS:HG3	2.10	0.52
2:D:4520:TYR:CE2	2:D:4559:TYR:HB3	2.45	0.52
2:A:658:ASN:ND2	2:A:833:LYS:HG2	2.24	0.52
2:A:1842:ILE:HD12	2:A:1845:LEU:HD12	1.90	0.52
2:B:658:ASN:ND2	2:B:833:LYS:HG2	2.24	0.52
2:B:903:GLN:N	2:B:913:ARG:HE	2.07	0.52
2:B:2562:THR:O	2:B:2566:ARG:HG3	2.08	0.52
2:B:4049:HIS:CD2	2:B:4067:LEU:HD11	2.43	0.52
2:C:897:LYS:HD2	2:C:902:TRP:CD1	2.45	0.52
2:C:2593:VAL:HG12	2:C:2644:LEU:HB2	1.90	0.52
2:D:1611:ILE:HB	2:D:1615:GLN:HB2	1.91	0.52
2:A:2779:LEU:O	2:A:2783:LEU:HD12	2.08	0.52
2:A:3319:PHE:O	2:A:3322:LEU:HG	2.10	0.52
2:A:3861:GLN:H	2:A:3867:THR:HG23	1.74	0.52
2:B:467:ASP:HB3	2:B:470:LEU:HG	1.92	0.52
2:B:1038:LEU:O	2:B:1043:LYS:NZ	2.36	0.52
2:B:4518:LEU:HD12	2:C:4809:MET:HG3	1.92	0.52
2:C:1936:LEU:HD21	2:C:1976:LEU:HD13	1.91	0.52
2:C:3108:LEU:HA	2:C:3111:HIS:CD2	2.45	0.52
2:C:3134:LEU:HD22	2:C:3162:PHE:HE2	1.74	0.52
2:C:4081:GLU:O	2:C:4085:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:436:LEU:HG	2:D:445:VAL:HG11	1.91	0.52
2:D:919:VAL:HB	2:D:923:LYS:HE3	1.91	0.52
2:D:2059:GLN:NE2	2:D:2091:GLN:O	2.42	0.52
2:D:3319:PHE:O	2:D:3322:LEU:HG	2.10	0.52
2:A:37:LEU:HA	2:A:49:LEU:HD23	1.92	0.52
2:A:114:LEU:HB2	2:A:117:HIS:CE1	2.45	0.52
2:A:1431:ARG:NH1	2:A:1556:GLU:OE2	2.42	0.52
2:A:1611:ILE:HB	2:A:1615:GLN:HB2	1.91	0.52
2:A:2926:LEU:HD12	2:A:3003:MET:HE3	1.90	0.52
2:A:4520:TYR:CE2	2:A:4559:TYR:HB3	2.45	0.52
3:E:24:VAL:HG22	3:E:48:LYS:HG2	1.92	0.52
2:B:114:LEU:HB2	2:B:117:HIS:CE1	2.45	0.52
2:B:173:GLU:OE2	2:B:176:ARG:NH2	2.36	0.52
2:B:1431:ARG:NH1	2:B:1556:GLU:OE2	2.42	0.52
2:B:2729:HIS:HB2	2:B:2771:TYR:HE2	1.75	0.52
2:B:2779:LEU:HA	2:B:2782:MET:HG2	1.91	0.52
2:B:3134:LEU:HD22	2:B:3162:PHE:HE2	1.74	0.52
2:B:3319:PHE:O	2:B:3322:LEU:HG	2.10	0.52
2:C:233:VAL:HG12	2:C:274:LEU:HD22	1.91	0.52
2:C:2059:GLN:NE2	2:C:2091:GLN:O	2.42	0.52
2:C:4584:PHE:O	2:C:4588:ILE:HG13	2.10	0.52
2:D:2172:MET:SD	2:D:2214:MET:HE1	2.50	0.52
2:A:903:GLN:N	2:A:913:ARG:HE	2.07	0.52
2:A:2059:GLN:NE2	2:A:2091:GLN:O	2.42	0.52
2:A:2763:LEU:HD23	2:A:2767:GLU:HG2	1.92	0.52
2:B:4584:PHE:O	2:B:4588:ILE:HG13	2.10	0.52
2:C:605:GLY:HA2	2:C:1585:ARG:HD2	1.91	0.52
2:C:1435:GLY:H	2:C:1500:ARG:NH2	2.06	0.52
2:D:114:LEU:HB2	2:D:117:HIS:CE1	2.45	0.52
2:D:2926:LEU:HD12	2:D:3003:MET:HE3	1.90	0.52
2:D:3216:GLU:HA	2:D:3219:VAL:HG22	1.90	0.52
2:A:1135:PHE:CE2	2:A:1146:HIS:CD2	2.98	0.52
2:A:3125:ASP:H	2:A:3183:ILE:HD11	1.75	0.52
2:B:3109:PHE:HB3	2:B:3162:PHE:HA	1.91	0.52
2:C:114:LEU:HB2	2:C:117:HIS:CE1	2.45	0.52
2:C:1135:PHE:CE2	2:C:1146:HIS:CD2	2.98	0.52
2:C:4520:TYR:CE2	2:C:4559:TYR:HB3	2.45	0.52
2:D:1957:LEU:HB2	2:D:3601:ALA:HB2	1.91	0.52
2:D:3109:PHE:HB3	2:D:3162:PHE:HA	1.91	0.52
2:A:436:LEU:HG	2:A:445:VAL:HG11	1.91	0.51
2:A:2729:HIS:HB2	2:A:2771:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3925:GLN:NE2	2:A:4934:THR:HA	2.26	0.51
2:B:2290:TRP:CZ2	2:B:2388:ILE:HG12	2.44	0.51
2:B:2763:LEU:HD23	2:B:2767:GLU:HG2	1.92	0.51
2:C:925:PRO:HB2	2:C:928:GLU:OE1	2.10	0.51
2:C:3131:TYR:CD1	2:C:3205:CYS:HB2	2.41	0.51
2:D:467:ASP:HB3	2:D:470:LEU:HG	1.92	0.51
2:D:925:PRO:HB2	2:D:928:GLU:OE1	2.10	0.51
2:D:1685:LEU:O	2:D:1689:ILE:HG12	2.10	0.51
2:D:2729:HIS:HB2	2:D:2771:TYR:HE2	1.75	0.51
2:A:1685:LEU:O	2:A:1689:ILE:HG12	2.10	0.51
1:K:42:GLN:HE21	2:C:1957:LEU:HD21	1.75	0.51
2:B:1135:PHE:CE2	2:B:1146:HIS:CD2	2.98	0.51
2:B:1419:PHE:O	2:B:1423:THR:HB	2.09	0.51
2:C:2172:MET:SD	2:C:2214:MET:HE1	2.50	0.51
2:C:3183:ILE:HD12	2:C:3187:LYS:HE3	1.93	0.51
2:C:3230:GLN:O	2:C:3231:MET:HE2	2.10	0.51
2:D:185:SER:OG	2:D:188:SER:OG	2.20	0.51
2:D:897:LYS:HD2	2:D:902:TRP:CD1	2.45	0.51
2:A:897:LYS:HD2	2:A:902:TRP:CD1	2.45	0.51
2:A:3108:LEU:HA	2:A:3111:HIS:CD2	2.45	0.51
1:J:69:PHE:O	1:J:73:MET:HG2	2.10	0.51
2:B:1978:ASN:HB2	2:B:1986:CYS:HB3	1.91	0.51
2:B:2172:MET:SD	2:B:2214:MET:HE1	2.50	0.51
2:C:919:VAL:HB	2:C:923:LYS:HE3	1.92	0.51
2:C:1611:ILE:HB	2:C:1615:GLN:HB2	1.91	0.51
2:C:2493:LEU:HG	2:C:2497:ARG:HH21	1.74	0.51
2:C:2779:LEU:HA	2:C:2782:MET:HG2	1.91	0.51
2:C:4252:ILE:HG21	2:D:4707:MET:HG2	1.92	0.51
2:D:3921:THR:O	2:D:3925:GLN:HG2	2.10	0.51
2:D:4026:LEU:HD13	2:D:4058:TYR:CE2	2.46	0.51
2:A:3183:ILE:HD12	2:A:3187:LYS:HE3	1.93	0.51
1:L:69:PHE:O	1:L:73:MET:HG2	2.10	0.51
2:B:233:VAL:HG12	2:B:274:LEU:HD22	1.91	0.51
2:B:3125:ASP:H	2:B:3183:ILE:HD11	1.75	0.51
2:C:2973:GLN:HA	2:C:2976:LYS:HZ3	1.76	0.51
2:C:3925:GLN:NE2	2:C:4934:THR:HA	2.26	0.51
2:D:37:LEU:HA	2:D:49:LEU:HD23	1.92	0.51
2:D:3102:LEU:HD21	2:D:3155:LEU:HD23	1.91	0.51
2:D:3108:LEU:HA	2:D:3111:HIS:CD2	2.45	0.51
2:A:2172:MET:SD	2:A:2214:MET:HE1	2.50	0.51
2:A:2785:TRP:HD1	2:A:2905:ARG:HH22	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3151:GLN:HE22	2:A:3155:LEU:HD11	1.76	0.51
2:A:4196:THR:HB	2:A:4919:LEU:HD11	1.93	0.51
2:A:4584:PHE:O	2:A:4588:ILE:HG13	2.10	0.51
2:A:4661:TYR:HB3	2:A:4665:ARG:NH2	2.26	0.51
2:B:1922:ILE:O	2:B:1926:VAL:HG23	2.11	0.51
2:B:3151:GLN:HE22	2:B:3155:LEU:HD11	1.76	0.51
2:B:3183:ILE:HD12	2:B:3187:LYS:HE3	1.93	0.51
2:C:28:ILE:HG22	2:C:29:HIS:CD2	2.44	0.51
2:C:1978:ASN:HB2	2:C:1986:CYS:HB3	1.91	0.51
2:C:2923:TYR:HA	2:C:3003:MET:HE1	1.92	0.51
2:D:2785:TRP:HD1	2:D:2905:ARG:HH22	1.59	0.51
2:D:3000:GLU:HG2	2:D:3003:MET:HE2	1.92	0.51
2:D:3131:TYR:CD1	2:D:3205:CYS:HB2	2.41	0.51
2:D:3925:GLN:NE2	2:D:4934:THR:HA	2.26	0.51
2:D:4661:TYR:HB3	2:D:4665:ARG:NH2	2.26	0.51
2:A:2779:LEU:HA	2:A:2782:MET:HG2	1.91	0.51
2:A:3879:LEU:O	2:A:3882:GLN:HG3	2.11	0.51
2:B:2923:TYR:HA	2:B:3003:MET:HE1	1.92	0.51
2:B:4196:THR:HB	2:B:4919:LEU:HD11	1.93	0.51
2:C:903:GLN:N	2:C:913:ARG:HE	2.07	0.51
2:C:1685:LEU:O	2:C:1689:ILE:HG12	2.10	0.51
2:C:2729:HIS:HB2	2:C:2771:TYR:HE2	1.75	0.51
2:C:4011:GLU:HG2	2:C:4121:LEU:HD13	1.93	0.51
2:D:1135:PHE:CE2	2:D:1146:HIS:CD2	2.98	0.51
2:D:2134:MET:HG2	2:D:2178:VAL:HG22	1.93	0.51
2:D:3183:ILE:HD12	2:D:3187:LYS:HE3	1.93	0.51
2:A:3000:GLU:HG2	2:A:3003:MET:HE2	1.93	0.51
2:A:3134:LEU:HD22	2:A:3162:PHE:HE2	1.74	0.51
2:B:668:ALA:HB2	2:B:1012:ILE:HD11	1.92	0.51
2:B:925:PRO:HB2	2:B:928:GLU:OE1	2.10	0.51
2:B:3230:GLN:O	2:B:3231:MET:HE2	2.10	0.51
2:B:4011:GLU:HG2	2:B:4121:LEU:HD13	1.93	0.51
2:D:62:LEU:O	2:D:66:THR:HG23	2.11	0.51
2:D:2493:LEU:HG	2:D:2497:ARG:HH21	1.74	0.51
2:D:2587:HIS:HA	2:D:2590:ARG:HG2	1.93	0.51
2:D:3134:LEU:HD22	2:D:3162:PHE:HE2	1.74	0.51
2:D:3230:GLN:O	2:D:3231:MET:HE2	2.10	0.51
2:D:4196:THR:HB	2:D:4919:LEU:HD11	1.93	0.51
2:D:4584:PHE:O	2:D:4588:ILE:HG13	2.10	0.51
2:A:467:ASP:HB3	2:A:470:LEU:HG	1.92	0.51
2:A:3921:THR:O	2:A:3925:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:897:LYS:HD2	2:B:902:TRP:CD1	2.45	0.51
2:B:2080:LEU:O	2:B:2084:MET:HG3	2.11	0.51
2:B:3108:LEU:HA	2:B:3111:HIS:CD2	2.45	0.51
2:B:4026:LEU:HD13	2:B:4058:TYR:CE2	2.46	0.51
2:B:4661:TYR:HB3	2:B:4665:ARG:NH2	2.26	0.51
2:C:62:LEU:O	2:C:66:THR:HG23	2.11	0.51
2:C:1922:ILE:O	2:C:1926:VAL:HG23	2.11	0.51
2:C:2134:MET:HG2	2:C:2178:VAL:HG22	1.93	0.51
2:C:2905:ARG:HG3	2:C:2907:PHE:H	1.76	0.51
2:D:903:GLN:N	2:D:913:ARG:HE	2.07	0.51
2:D:2250:ASN:HB3	2:D:2253:LEU:HB2	1.93	0.51
2:D:2758:LYS:NZ	2:D:2763:LEU:HA	2.26	0.51
2:D:3151:GLN:HE22	2:D:3155:LEU:HD11	1.76	0.51
2:A:668:ALA:HB2	2:A:1012:ILE:HD11	1.92	0.51
2:A:2587:HIS:HA	2:A:2590:ARG:HG2	1.93	0.51
2:A:2765:GLU:HG3	2:A:2769:GLU:OE2	2.11	0.51
2:A:3109:PHE:HB3	2:A:3162:PHE:HA	1.91	0.51
2:A:4081:GLU:O	2:A:4085:LYS:HG3	2.10	0.51
3:F:24:VAL:HG22	3:F:48:LYS:HG2	1.92	0.51
3:H:24:VAL:HG22	3:H:48:LYS:HG2	1.92	0.51
2:B:2988:ARG:HB2	2:B:2989:PRO:HD3	1.93	0.51
2:C:2785:TRP:HD1	2:C:2905:ARG:HH22	1.59	0.51
2:C:3921:THR:O	2:C:3925:GLN:HG2	2.10	0.51
2:D:28:ILE:HG22	2:D:29:HIS:CD2	2.44	0.51
2:D:2763:LEU:HD23	2:D:2767:GLU:HG2	1.92	0.51
2:D:4011:GLU:HG2	2:D:4121:LEU:HD13	1.93	0.51
1:I:10:ILE:O	1:I:14:LYS:N	2.38	0.51
1:I:134:ASP:HA	2:A:3298:ARG:HG3	1.93	0.51
2:A:3230:GLN:O	2:A:3231:MET:HE2	2.10	0.51
2:A:3805:LEU:HD11	2:A:3887:ASP:HB3	1.93	0.51
2:A:4026:LEU:HD13	2:A:4058:TYR:CE2	2.46	0.51
2:A:4569:GLU:HB3	2:A:4570:PRO:HD3	1.93	0.51
2:C:2080:LEU:O	2:C:2084:MET:HG3	2.11	0.51
2:C:2765:GLU:HG3	2:C:2769:GLU:OE2	2.11	0.51
2:C:3151:GLN:HE22	2:C:3155:LEU:HD11	1.76	0.51
2:C:4026:LEU:HD13	2:C:4058:TYR:CE2	2.46	0.51
2:D:629:GLN:OE1	2:D:1669:ASN:ND2	2.37	0.51
2:D:3805:LEU:HD11	2:D:3887:ASP:HB3	1.93	0.51
2:A:3215:MET:O	2:A:3219:VAL:HG13	2.11	0.50
2:A:4011:GLU:HG2	2:A:4121:LEU:HD13	1.93	0.50
2:B:37:LEU:HA	2:B:49:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1435:GLY:H	2:B:1500:ARG:NH2	2.06	0.50
2:B:3925:GLN:NE2	2:B:4934:THR:HA	2.26	0.50
2:B:4520:TYR:CE2	2:B:4559:TYR:HB3	2.45	0.50
2:C:3016:ARG:O	2:C:3018:ARG:NE	2.32	0.50
2:C:3102:LEU:HD21	2:C:3155:LEU:HD23	1.91	0.50
2:C:3125:ASP:H	2:C:3183:ILE:HD11	1.75	0.50
2:C:3319:PHE:O	2:C:3322:LEU:HG	2.10	0.50
2:D:674:TYR:HE1	2:D:756:SER:HB3	1.76	0.50
2:A:925:PRO:HB2	2:A:928:GLU:OE1	2.10	0.50
2:A:2988:ARG:HB2	2:A:2989:PRO:HD3	1.93	0.50
3:G:24:VAL:HG22	3:G:48:LYS:HG2	1.92	0.50
2:B:1685:LEU:O	2:B:1689:ILE:HG12	2.10	0.50
2:B:1935:LYS:HE3	2:B:1995:GLN:HE22	1.76	0.50
2:B:3879:LEU:O	2:B:3882:GLN:HG3	2.11	0.50
2:C:4661:TYR:HB3	2:C:4665:ARG:NH2	2.26	0.50
2:D:2988:ARG:HB2	2:D:2989:PRO:HD3	1.93	0.50
2:D:3125:ASP:H	2:D:3183:ILE:HD11	1.76	0.50
2:D:4166:LYS:O	2:D:4170:ARG:HG2	2.11	0.50
2:A:674:TYR:HE1	2:A:756:SER:HB3	1.76	0.50
2:A:1922:ILE:O	2:A:1926:VAL:HG23	2.11	0.50
2:A:2758:LYS:NZ	2:A:2763:LEU:HA	2.26	0.50
2:B:2905:ARG:HG3	2:B:2907:PHE:H	1.76	0.50
2:B:3000:GLU:HG2	2:B:3003:MET:HE2	1.93	0.50
2:B:3215:MET:O	2:B:3219:VAL:HG13	2.11	0.50
2:B:3921:THR:O	2:B:3925:GLN:HG2	2.10	0.50
2:C:1935:LYS:HE3	2:C:1995:GLN:HE22	1.76	0.50
2:C:3215:MET:O	2:C:3219:VAL:HG13	2.11	0.50
2:C:4154:GLU:O	2:C:4158:THR:HG23	2.12	0.50
2:D:3016:ARG:O	2:D:3018:ARG:NE	2.32	0.50
2:D:4055:HIS:CE1	2:D:4057:HIS:CD2	3.00	0.50
2:A:4057:HIS:HE1	2:B:4660:PHE:HZ	1.57	0.50
2:A:4154:GLU:O	2:A:4158:THR:HG23	2.12	0.50
2:B:1184:ASP:OD2	2:B:1193:LYS:NZ	2.38	0.50
2:B:4081:GLU:O	2:B:4085:LYS:HG3	2.10	0.50
2:B:4166:LYS:O	2:B:4170:ARG:HG2	2.11	0.50
2:C:2763:LEU:HD23	2:C:2767:GLU:HG2	1.92	0.50
2:D:1922:ILE:O	2:D:1926:VAL:HG23	2.11	0.50
2:D:4569:GLU:HB3	2:D:4570:PRO:HD3	1.94	0.50
2:A:62:LEU:O	2:A:66:THR:HG23	2.11	0.50
2:A:2134:MET:HG2	2:A:2178:VAL:HG22	1.93	0.50
2:A:2250:ASN:HB3	2:A:2253:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4166:LYS:O	2:A:4170:ARG:HG2	2.11	0.50
2:B:2782:MET:HB2	2:B:2787:TRP:HE3	1.76	0.50
2:C:4569:GLU:HB3	2:C:4570:PRO:HD3	1.94	0.50
2:D:1564:MET:SD	2:D:1565:PRO:HD2	2.52	0.50
2:A:3001:LYS:NZ	2:A:3041:ASP:OD2	2.33	0.50
2:A:4055:HIS:CE1	2:A:4057:HIS:CD2	3.00	0.50
1:J:106:LEU:HD22	2:B:3587:TRP:NE1	2.25	0.50
2:B:2758:LYS:NZ	2:B:2763:LEU:HA	2.26	0.50
2:B:2765:GLU:HG3	2:B:2769:GLU:OE2	2.11	0.50
2:B:2833:LEU:HB2	2:B:2838[A]:HIS:NE2	2.27	0.50
2:B:4154:GLU:O	2:B:4158:THR:HG23	2.12	0.50
2:B:4569:GLU:HB3	2:B:4570:PRO:HD3	1.94	0.50
2:C:37:LEU:HA	2:C:49:LEU:HD23	1.92	0.50
2:C:1014:GLN:O	2:C:1027:ARG:NH2	2.45	0.50
2:C:2054:LYS:HE2	2:C:2056:SER:HA	1.94	0.50
2:C:2250:ASN:HB3	2:C:2253:LEU:HB2	1.93	0.50
2:C:2782:MET:HB2	2:C:2787:TRP:HE3	1.76	0.50
2:D:506:HIS:CE1	2:D:530:LEU:HD21	2.47	0.50
2:D:1935:LYS:HE3	2:D:1995:GLN:HE22	1.76	0.50
2:D:2591:ARG:HH22	2:D:2875:ASP:CG	2.20	0.50
2:A:1748:LEU:HB3	2:A:1751:ILE:HD13	1.94	0.50
2:A:2080:LEU:O	2:A:2084:MET:HG3	2.11	0.50
2:A:2782:MET:HB2	2:A:2787:TRP:HE3	1.76	0.50
2:A:2830:ASN:HB3	2:B:1435:GLY:HA3	1.94	0.50
2:B:1286:THR:OG1	2:B:1550:PRO:O	2.22	0.50
2:B:2134:MET:HG2	2:B:2178:VAL:HG22	1.93	0.50
2:B:2250:ASN:HB3	2:B:2253:LEU:HB2	1.93	0.50
2:B:2859:GLU:O	2:B:2862:SER:OG	2.23	0.50
2:B:4055:HIS:CE1	2:B:4057:HIS:CD2	3.00	0.50
2:C:467:ASP:HB3	2:C:470:LEU:HG	1.92	0.50
2:C:3996:GLY:O	2:C:4000:VAL:HG23	2.12	0.50
2:C:4196:THR:HB	2:C:4919:LEU:HD11	1.93	0.50
2:D:997:ASP:OD1	2:D:1047:LYS:NZ	2.32	0.50
2:D:1299:ILE:HD11	2:D:1544:PHE:HB3	1.94	0.50
2:D:3215:MET:O	2:D:3219:VAL:HG13	2.11	0.50
2:D:3246:MET:HG2	2:D:3309:LYS:HZ1	1.75	0.50
2:D:3879:LEU:O	2:D:3882:GLN:HG3	2.11	0.50
2:A:874:LEU:CD1	2:A:940:LEU:HD13	2.42	0.50
2:A:2591:ARG:HH22	2:A:2875:ASP:CG	2.20	0.50
2:B:506:HIS:CE1	2:B:530:LEU:HD21	2.47	0.50
2:B:1014:GLN:O	2:B:1027:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1104:GLU:OE1	2:B:1225:LYS:NZ	2.44	0.50
2:B:2587:HIS:HA	2:B:2590:ARG:HG2	1.93	0.50
2:B:2785:TRP:HD1	2:B:2905:ARG:HH22	1.59	0.50
2:C:2831:VAL:HG22	2:D:1435:GLY:HA2	1.94	0.50
2:C:2988:ARG:HB2	2:C:2989:PRO:HD3	1.93	0.50
2:C:3000:GLU:HG2	2:C:3003:MET:HE2	1.92	0.50
2:C:3295:TRP:CD1	2:C:3296:MET:SD	3.05	0.50
2:D:874:LEU:CD1	2:D:940:LEU:HD13	2.42	0.50
2:D:2080:LEU:O	2:D:2084:MET:HG3	2.11	0.50
2:D:2765:GLU:HG3	2:D:2769:GLU:OE2	2.11	0.50
2:D:4154:GLU:O	2:D:4158:THR:HG23	2.12	0.50
2:A:318:ASP:O	2:A:322:ALA:HB2	2.12	0.50
2:A:1564:MET:SD	2:A:1565:PRO:HD2	2.52	0.50
2:A:3089:GLY:O	2:A:3093:ILE:HG12	2.12	0.50
2:A:3122:ILE:HA	2:A:3126:VAL:HB	1.94	0.50
2:B:66:THR:OG1	2:B:124:SER:OG	2.24	0.50
2:B:674:TYR:HE1	2:B:756:SER:HB3	1.77	0.50
2:B:2591:ARG:HH22	2:B:2875:ASP:CG	2.20	0.50
2:B:3089:GLY:O	2:B:3093:ILE:HG12	2.12	0.50
2:B:3118:GLY:O	2:B:3122:ILE:HG12	2.12	0.50
2:B:4863:GLN:O	2:B:4867:ILE:HG12	2.12	0.50
2:C:2758:LYS:NZ	2:C:2763:LEU:HA	2.26	0.50
2:C:4055:HIS:CE1	2:C:4057:HIS:CD2	3.00	0.50
2:C:4166:LYS:O	2:C:4170:ARG:HG2	2.11	0.50
2:D:238:HIS:ND1	2:D:243:GLU:OE2	2.45	0.50
2:D:2054:LYS:HE2	2:D:2056:SER:HA	1.94	0.50
2:D:3089:GLY:O	2:D:3093:ILE:HG12	2.12	0.50
2:A:474:ASP:O	2:A:478:ARG:HG2	2.12	0.49
2:A:3295:TRP:CD1	2:A:3296:MET:SD	3.05	0.49
2:B:3046:MET:HG3	2:B:3121:LEU:HA	1.94	0.49
2:B:3295:TRP:CD1	2:B:3296:MET:SD	3.05	0.49
2:C:1564:MET:SD	2:C:1565:PRO:HD2	2.52	0.49
2:C:2591:ARG:HH22	2:C:2875:ASP:CG	2.20	0.49
2:C:3118:GLY:O	2:C:3122:ILE:HG12	2.12	0.49
2:C:3805:LEU:HD21	2:C:3888:PHE:HA	1.94	0.49
2:D:334:SER:OG	2:D:336:GLU:OE1	2.22	0.49
2:D:1014:GLN:O	2:D:1027:ARG:NH2	2.45	0.49
2:A:506:HIS:CE1	2:A:530:LEU:HD21	2.47	0.49
2:B:62:LEU:O	2:B:66:THR:HG23	2.11	0.49
2:C:674:TYR:HE1	2:C:756:SER:HB3	1.76	0.49
2:C:1299:ILE:HD11	2:C:1544:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3805:LEU:HD11	2:C:3887:ASP:HB3	1.93	0.49
2:D:474:ASP:O	2:D:478:ARG:HG2	2.12	0.49
2:D:2833:LEU:HB2	2:D:2838[A]:HIS:NE2	2.27	0.49
2:D:3122:ILE:HA	2:D:3126:VAL:HB	1.94	0.49
2:A:2905:ARG:HG3	2:A:2907:PHE:H	1.76	0.49
2:A:3996:GLY:O	2:A:4000:VAL:HG23	2.12	0.49
2:A:4507:LEU:HD21	2:A:4746:ILE:HG22	1.94	0.49
2:B:995:MET:HA	2:B:998:LYS:HD3	1.94	0.49
2:B:2833:LEU:HB2	2:B:2838[B]:HIS:NE2	2.28	0.49
2:C:238:HIS:ND1	2:C:243:GLU:OE2	2.45	0.49
2:C:506:HIS:CE1	2:C:530:LEU:HD21	2.47	0.49
2:C:874:LEU:CD1	2:C:940:LEU:HD13	2.42	0.49
2:C:3848:GLU:OE2	2:C:3922:GLU:OE1	2.03	0.49
2:C:3879:LEU:O	2:C:3882:GLN:HG3	2.11	0.49
2:D:2924:SER:O	2:D:2928:GLN:HG2	2.12	0.49
2:D:3295:TRP:CD1	2:D:3296:MET:SD	3.05	0.49
2:D:3805:LEU:HD21	2:D:3888:PHE:HA	1.94	0.49
2:A:995:MET:HA	2:A:998:LYS:HD3	1.94	0.49
2:A:1014:GLN:O	2:A:1027:ARG:NH2	2.45	0.49
2:A:2768:LYS:HB3	2:A:2772:ARG:HH21	1.77	0.49
2:B:115:TYR:OH	2:B:179:ASP:OD2	2.31	0.49
2:B:4021:LEU:HD22	2:B:4128:TYR:CE2	2.48	0.49
2:C:2587:HIS:HA	2:C:2590:ARG:HG2	1.93	0.49
2:C:3089:GLY:O	2:C:3093:ILE:HG12	2.12	0.49
2:D:318:ASP:O	2:D:322:ALA:HB2	2.12	0.49
2:D:2905:ARG:HG3	2:D:2907:PHE:H	1.76	0.49
2:D:4863:GLN:O	2:D:4867:ILE:HG12	2.12	0.49
2:A:1040:ASP:HA	2:A:1043:LYS:HG2	1.95	0.49
2:A:2833:LEU:HB2	2:A:2838[A]:HIS:NE2	2.27	0.49
2:A:3046:MET:HG3	2:A:3121:LEU:HA	1.94	0.49
2:A:3118:GLY:O	2:A:3122:ILE:HG12	2.12	0.49
2:A:4769:LEU:HB3	2:D:4753:LEU:HD11	1.94	0.49
2:B:318:ASP:O	2:B:322:ALA:HB2	2.12	0.49
2:B:2691:LYS:HA	2:B:2704:GLN:HE22	1.78	0.49
2:B:3805:LEU:HD11	2:B:3887:ASP:HB3	1.93	0.49
2:B:4753:LEU:HG	2:C:4773:LEU:HD22	1.94	0.49
2:C:318:ASP:O	2:C:322:ALA:HB2	2.12	0.49
2:C:1685:LEU:HD22	2:C:1706:LEU:HB2	1.95	0.49
2:C:4055:HIS:CE1	2:C:4057:HIS:HD2	2.31	0.49
2:C:4268:MET:HA	2:C:4271:VAL:HG22	1.94	0.49
2:D:3996:GLY:O	2:D:4000:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4271:VAL:HA	2:D:4274:MET:HG2	1.95	0.49
2:A:1299:ILE:HD11	2:A:1544:PHE:HB3	1.94	0.49
2:A:1935:LYS:HE3	2:A:1995:GLN:HE22	1.76	0.49
2:B:238:HIS:ND1	2:B:243:GLU:OE2	2.45	0.49
2:C:474:ASP:O	2:C:478:ARG:HG2	2.12	0.49
2:D:1040:ASP:HA	2:D:1043:LYS:HG2	1.95	0.49
2:D:1948:MET:HA	2:D:1948:MET:HE3	1.95	0.49
2:D:2691:LYS:HA	2:D:2704:GLN:HE22	1.78	0.49
2:A:115:TYR:OH	2:A:179:ASP:OD2	2.31	0.49
2:A:1948:MET:HA	2:A:1948:MET:HE3	1.95	0.49
2:A:2087:LEU:O	2:A:2091:GLN:HG2	2.13	0.49
2:A:4271:VAL:HA	2:A:4274:MET:HG2	1.95	0.49
2:B:1299:ILE:HD11	2:B:1544:PHE:HB3	1.94	0.49
2:B:3996:GLY:O	2:B:4000:VAL:HG23	2.12	0.49
2:B:4507:LEU:HD21	2:B:4746:ILE:HG22	1.94	0.49
2:C:2924:SER:O	2:C:2928:GLN:HG2	2.12	0.49
2:D:2961:LYS:HB2	2:D:2965:LYS:HZ3	1.78	0.49
2:D:4507:LEU:HD21	2:D:4746:ILE:HG22	1.94	0.49
2:A:889:ILE:HA	2:A:892:LEU:HD12	1.95	0.49
2:A:1948:MET:HE1	2:A:1956:ALA:HB2	1.94	0.49
2:A:2859:GLU:O	2:A:2862:SER:OG	2.23	0.49
2:B:2054:LYS:HE2	2:B:2056:SER:HA	1.94	0.49
2:C:2833:LEU:HB2	2:C:2838[A]:HIS:NE2	2.27	0.49
2:D:1948:MET:HE1	2:D:1956:ALA:HB2	1.94	0.49
2:D:2496:LEU:HD23	2:D:2520:LEU:HD13	1.95	0.49
2:D:2768:LYS:HB3	2:D:2772:ARG:HH21	1.77	0.49
2:D:3046:MET:HG3	2:D:3121:LEU:HA	1.94	0.49
2:A:2691:LYS:HA	2:A:2704:GLN:HE22	1.78	0.49
2:A:2833:LEU:HB2	2:A:2838[B]:HIS:NE2	2.28	0.49
1:J:59:ASP:N	1:J:68:GLU:OE2	2.33	0.49
2:B:1564:MET:SD	2:B:1565:PRO:HD2	2.52	0.49
2:B:2768:LYS:HB3	2:B:2772:ARG:HH21	1.77	0.49
2:B:3096:TYR:CE2	2:B:3101:LEU:HD13	2.48	0.49
2:B:4155:SER:O	2:B:4159:GLN:HG2	2.13	0.49
2:B:4573:ARG:NH2	2:B:4736:ASN:OD1	2.46	0.49
2:C:115:TYR:OH	2:C:179:ASP:OD2	2.31	0.49
2:C:1004:HIS:NE2	2:C:1038:LEU:HD21	2.28	0.49
2:C:1040:ASP:HA	2:C:1043:LYS:HG2	1.95	0.49
2:C:1522:ALA:HB3	2:C:1527:LEU:HD21	1.95	0.49
2:C:2156:TYR:HE1	2:C:2202:TYR:HE2	1.60	0.49
2:C:3046:MET:HG3	2:C:3121:LEU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3096:TYR:CE2	2:C:3101:LEU:HD13	2.48	0.49
2:C:3719:MET:HA	2:C:3719:MET:HE3	1.95	0.49
2:D:1685:LEU:HD22	2:D:1706:LEU:HB2	1.95	0.49
2:D:3096:TYR:CE2	2:D:3101:LEU:HD13	2.48	0.49
2:D:3118:GLY:O	2:D:3122:ILE:HG12	2.12	0.49
2:D:4055:HIS:CE1	2:D:4057:HIS:HD2	2.31	0.49
2:D:4814:MET:HA	2:D:4814:MET:HE3	1.95	0.49
2:A:606:ARG:NH1	2:A:644:LEU:HD21	2.25	0.49
2:A:1081:THR:HG23	2:A:1083:GLU:H	1.78	0.49
2:A:3036:LEU:O	2:A:3040:LEU:HG	2.12	0.49
2:A:4863:GLN:O	2:A:4867:ILE:HG12	2.12	0.49
2:B:474:ASP:O	2:B:478:ARG:HG2	2.12	0.49
2:B:1004:HIS:NE2	2:B:1038:LEU:HD21	2.28	0.49
2:B:1081:THR:HG23	2:B:1083:GLU:H	1.78	0.49
2:B:1522:ALA:HB3	2:B:1527:LEU:HD21	1.95	0.49
2:B:3042:ALA:HB1	2:B:3121:LEU:HB2	1.95	0.49
2:B:3211:LEU:HD21	2:B:3245:TYR:CE2	2.48	0.49
2:B:3238:ILE:O	2:B:3241:MET:HB3	2.13	0.49
2:B:4268:MET:HA	2:B:4271:VAL:HG22	1.94	0.49
2:C:2496:LEU:HD23	2:C:2520:LEU:HD13	1.95	0.49
2:C:2691:LYS:HA	2:C:2704:GLN:HE22	1.78	0.49
2:C:3238:ILE:O	2:C:3241:MET:HB3	2.13	0.49
2:C:4021:LEU:HD22	2:C:4128:TYR:CE2	2.48	0.49
2:D:1081:THR:HG23	2:D:1083:GLU:H	1.78	0.49
2:D:2782:MET:HB2	2:D:2787:TRP:HE3	1.76	0.49
2:D:4573:ARG:NH2	2:D:4736:ASN:OD1	2.46	0.49
2:A:2156:TYR:HE1	2:A:2202:TYR:HE2	1.60	0.48
2:A:2924:SER:O	2:A:2928:GLN:HG2	2.12	0.48
2:A:3096:TYR:CE2	2:A:3101:LEU:HD13	2.48	0.48
2:A:4021:LEU:HD22	2:A:4128:TYR:CE2	2.48	0.48
2:B:889:ILE:HA	2:B:892:LEU:HD12	1.95	0.48
2:B:3171:LEU:HD13	2:B:3214:LEU:HD12	1.95	0.48
2:C:889:ILE:HA	2:C:892:LEU:HD12	1.95	0.48
2:C:995:MET:HA	2:C:998:LYS:HD3	1.94	0.48
2:C:2831:VAL:HG22	2:D:1435:GLY:O	2.13	0.48
2:C:2857:LYS:O	2:C:2860:LEU:HG	2.13	0.48
2:C:3036:LEU:O	2:C:3040:LEU:HG	2.12	0.48
2:C:4507:LEU:HD21	2:C:4746:ILE:HG22	1.94	0.48
2:D:889:ILE:HA	2:D:892:LEU:HD12	1.95	0.48
2:D:4155:SER:O	2:D:4159:GLN:HG2	2.13	0.48
2:A:2054:LYS:HE2	2:A:2056:SER:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3171:LEU:HD13	2:A:3214:LEU:HD12	1.95	0.48
2:A:3211:LEU:HD21	2:A:3245:TYR:CE2	2.48	0.48
1:L:134:ASP:OD1	2:D:3298:ARG:NH1	2.46	0.48
1:L:137:VAL:HG21	2:D:3587:TRP:CH2	2.47	0.48
2:B:874:LEU:CD1	2:B:940:LEU:HD13	2.42	0.48
2:B:913:ARG:HG3	2:B:913:ARG:O	2.13	0.48
2:B:2729:HIS:CE1	2:B:2763:LEU:HD11	2.49	0.48
2:B:3036:LEU:O	2:B:3040:LEU:HG	2.12	0.48
2:B:3122:ILE:HA	2:B:3126:VAL:HB	1.94	0.48
2:B:3805:LEU:HD21	2:B:3888:PHE:HA	1.94	0.48
2:B:4055:HIS:CE1	2:B:4057:HIS:HD2	2.31	0.48
2:B:4271:VAL:HA	2:B:4274:MET:HG2	1.95	0.48
2:C:1748:LEU:HB3	2:C:1751:ILE:HD13	1.94	0.48
2:D:995:MET:HA	2:D:998:LYS:HD3	1.94	0.48
2:D:1004:HIS:NE2	2:D:1038:LEU:HD21	2.28	0.48
2:D:1748:LEU:HB3	2:D:1751:ILE:HD13	1.94	0.48
2:D:2565:GLN:O	2:D:2569:ILE:HG12	2.14	0.48
2:D:2733:SER:HA	2:D:2736:LYS:NZ	2.28	0.48
2:D:3255:GLU:OE1	2:D:3273:MET:HE2	2.14	0.48
2:D:4021:LEU:HD22	2:D:4128:TYR:CE2	2.48	0.48
2:A:238:HIS:ND1	2:A:243:GLU:OE2	2.45	0.48
2:D:883:GLU:HG2	2:D:884:LYS:N	2.28	0.48
2:D:1522:ALA:HB3	2:D:1527:LEU:HD21	1.95	0.48
2:D:2087:LEU:O	2:D:2091:GLN:HG2	2.13	0.48
2:D:2729:HIS:CE1	2:D:2763:LEU:HD11	2.49	0.48
2:D:3036:LEU:O	2:D:3040:LEU:HG	2.12	0.48
2:D:3238:ILE:O	2:D:3241:MET:HB3	2.13	0.48
2:D:3269:ASN:O	2:D:3273:MET:HG3	2.14	0.48
2:D:4268:MET:HA	2:D:4271:VAL:HG22	1.94	0.48
2:A:2733:SER:HA	2:A:2736:LYS:HZ3	1.78	0.48
2:A:3238:ILE:O	2:A:3241:MET:HB3	2.13	0.48
2:A:4573:ARG:NH2	2:A:4736:ASN:OD1	2.46	0.48
2:B:606:ARG:NH1	2:B:644:LEU:HD21	2.26	0.48
2:B:1040:ASP:HA	2:B:1043:LYS:HG2	1.95	0.48
2:B:1748:LEU:HB3	2:B:1751:ILE:HD13	1.94	0.48
2:B:1797:GLU:HA	2:B:1800:LYS:HE3	1.96	0.48
2:B:1948:MET:HE1	2:B:1956:ALA:HB2	1.94	0.48
2:B:3255:GLU:OE1	2:B:3273:MET:HE2	2.13	0.48
2:C:913:ARG:HG3	2:C:913:ARG:O	2.12	0.48
2:C:1948:MET:HA	2:C:1948:MET:HE3	1.95	0.48
2:C:2224:ASN:O	2:C:2227:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2733:SER:HA	2:C:2736:LYS:NZ	2.28	0.48
2:C:3122:ILE:HA	2:C:3126:VAL:HB	1.94	0.48
2:C:3269:ASN:O	2:C:3273:MET:HG3	2.14	0.48
2:C:4271:VAL:HA	2:C:4274:MET:HG2	1.95	0.48
2:C:4573:ARG:NH2	2:C:4736:ASN:OD1	2.46	0.48
2:D:2857:LYS:O	2:D:2860:LEU:HG	2.13	0.48
2:D:3043:ARG:HA	2:D:3120:ASP:OD2	2.13	0.48
1:I:76:LYS:HB2	1:I:78:LYS:HZ2	1.78	0.48
2:A:913:ARG:HG3	2:A:913:ARG:O	2.13	0.48
2:A:1004:HIS:NE2	2:A:1038:LEU:HD21	2.28	0.48
2:A:2701:PHE:CE2	2:A:2703:PRO:HG3	2.49	0.48
2:A:3295:TRP:HB3	2:A:3298:ARG:HH21	1.79	0.48
2:A:3805:LEU:HD21	2:A:3888:PHE:HA	1.94	0.48
2:A:4055:HIS:CE1	2:A:4057:HIS:HD2	2.31	0.48
2:A:4814:MET:HA	2:A:4814:MET:HE3	1.95	0.48
3:G:88:HIS:HD2	3:G:89:PRO:HD2	1.79	0.48
2:B:2496:LEU:HD23	2:B:2520:LEU:HD13	1.95	0.48
2:B:2733:SER:HA	2:B:2736:LYS:NZ	2.28	0.48
2:B:2924:SER:O	2:B:2928:GLN:HG2	2.12	0.48
2:B:4814:MET:HA	2:B:4814:MET:HE3	1.95	0.48
2:C:2385:GLY:O	2:C:2389:MET:HG3	2.13	0.48
2:C:2833:LEU:HB2	2:C:2838[B]:HIS:NE2	2.28	0.48
2:C:4155:SER:O	2:C:4159:GLN:HG2	2.13	0.48
2:C:4863:GLN:O	2:C:4867:ILE:HG12	2.12	0.48
2:D:115:TYR:OH	2:D:179:ASP:OD2	2.31	0.48
2:D:3246:MET:HG2	2:D:3309:LYS:HZ2	1.78	0.48
2:A:2224:ASN:O	2:A:2227:VAL:HG23	2.14	0.48
2:A:2729:HIS:CE1	2:A:2763:LEU:HD11	2.49	0.48
2:A:3043:ARG:HA	2:A:3120:ASP:OD2	2.13	0.48
2:A:3253:GLY:C	2:A:3255:GLU:N	2.72	0.48
1:L:76:LYS:HB2	1:L:78:LYS:HZ2	1.78	0.48
1:L:127:ARG:HD3	1:L:127:ARG:HA	1.41	0.48
2:B:292:GLY:HA3	2:B:340:VAL:HG21	1.96	0.48
2:B:874:LEU:HD12	2:B:875:PRO:HD2	1.95	0.48
2:B:2565:GLN:O	2:B:2569:ILE:HG12	2.14	0.48
2:B:3963:SER:OG	2:B:3964:GLN:OE1	2.30	0.48
2:C:883:GLU:HG2	2:C:884:LYS:N	2.28	0.48
2:C:1081:THR:HG23	2:C:1083:GLU:H	1.78	0.48
2:D:661:LEU:HD23	2:D:673:TRP:CD1	2.49	0.48
2:D:1034:PRO:HD2	2:D:1037:LEU:HD12	1.96	0.48
2:D:3211:LEU:HD21	2:D:3245:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3295:TRP:HB3	2:D:3298:ARG:HH21	1.78	0.48
2:D:3689:MET:HE2	2:D:3754:MET:HG2	1.96	0.48
2:A:292:GLY:HA3	2:A:340:VAL:HG21	1.96	0.48
2:A:375:GLN:HB2	2:A:390:LYS:HB3	1.95	0.48
2:A:883:GLU:HG2	2:A:884:LYS:N	2.28	0.48
2:A:1797:GLU:HA	2:A:1800:LYS:HE3	1.96	0.48
1:J:36:VAL:O	1:J:39:SER:OG	2.27	0.48
2:B:165:ALA:HB3	2:B:180:ASP:HB3	1.96	0.48
2:B:849:ASP:OD1	2:B:1214:ARG:NE	2.37	0.48
2:B:3269:ASN:O	2:B:3273:MET:HG3	2.14	0.48
2:C:375:GLN:HB2	2:C:390:LYS:HB3	1.95	0.48
2:C:441:LYS:HG3	2:C:444:THR:HG23	1.96	0.48
2:C:2087:LEU:O	2:C:2091:GLN:HG2	2.13	0.48
2:C:2701:PHE:CE2	2:C:2703:PRO:HG3	2.49	0.48
2:C:3200:ASN:CB	2:C:3203:ASP:HB2	2.44	0.48
2:C:3211:LEU:HD21	2:C:3245:TYR:CE2	2.49	0.48
2:D:3068:LEU:O	2:D:3071:THR:OG1	2.27	0.48
2:D:3719:MET:HA	2:D:3719:MET:HE3	1.95	0.48
2:A:2733:SER:HA	2:A:2736:LYS:NZ	2.28	0.48
2:A:2968:LEU:HD13	2:A:3029:ILE:HG12	1.96	0.48
3:H:88:HIS:HD2	3:H:89:PRO:HD2	1.79	0.48
2:B:1685:LEU:HD22	2:B:1706:LEU:HB2	1.95	0.48
2:B:2156:TYR:HE1	2:B:2202:TYR:HE2	1.60	0.48
2:B:3295:TRP:HB3	2:B:3298:ARG:HH21	1.78	0.48
2:C:2729:HIS:CE1	2:C:2763:LEU:HD11	2.49	0.48
2:C:3131:TYR:O	2:C:3135:THR:HG23	2.14	0.48
2:C:3744:ILE:O	2:C:3747:SER:OG	2.31	0.48
2:D:2946:GLY:HA3	2:D:2954:PHE:HZ	1.79	0.48
2:D:2968:LEU:HD13	2:D:3029:ILE:HG12	1.96	0.48
2:A:3689:MET:HE2	2:A:3754:MET:HG2	1.96	0.48
3:E:88:HIS:HD2	3:E:89:PRO:HD2	1.79	0.48
2:B:1948:MET:HA	2:B:1948:MET:HE3	1.95	0.48
2:B:2385:GLY:O	2:B:2389:MET:HG3	2.13	0.48
2:B:2857:LYS:O	2:B:2860:LEU:HG	2.13	0.48
2:B:3043:ARG:HA	2:B:3120:ASP:OD2	2.13	0.48
2:B:3719:MET:HA	2:B:3719:MET:HE3	1.95	0.48
2:C:318:ASP:OD1	2:C:319:LYS:N	2.45	0.48
2:C:1435:GLY:N	2:C:1500:ARG:HH22	2.11	0.48
2:C:1967:SER:O	2:C:1972:GLN:NE2	2.41	0.48
2:C:2768:LYS:HB3	2:C:2772:ARG:HH21	1.77	0.48
2:C:3042:ALA:HB1	2:C:3121:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:606:ARG:NH1	2:D:644:LEU:HD21	2.25	0.48
2:D:2385:GLY:O	2:D:2389:MET:HG3	2.13	0.48
2:A:1685:LEU:HD22	2:A:1706:LEU:HB2	1.95	0.48
2:A:2857:LYS:O	2:A:2860:LEU:HG	2.13	0.48
2:A:3106:SER:OG	2:A:3157:GLU:OE1	2.21	0.48
2:A:4155:SER:O	2:A:4159:GLN:HG2	2.13	0.48
2:A:4800:ASP:OD1	2:A:4801:THR:N	2.47	0.48
2:B:2968:LEU:HD13	2:B:3029:ILE:HG12	1.96	0.48
2:B:3131:TYR:O	2:B:3135:THR:HG23	2.14	0.48
2:C:606:ARG:NH1	2:C:644:LEU:HD21	2.26	0.48
2:C:661:LEU:HD23	2:C:673:TRP:CD1	2.49	0.48
2:C:1034:PRO:HD2	2:C:1037:LEU:HD12	1.96	0.48
2:C:2565:GLN:O	2:C:2569:ILE:HG12	2.14	0.48
2:C:2681:MET:HE1	2:C:2920:ARG:HG2	1.96	0.48
2:C:3184:TYR:CG	2:C:3201:VAL:HG22	2.49	0.48
2:D:318:ASP:OD1	2:D:319:LYS:N	2.45	0.48
2:D:375:GLN:HB2	2:D:390:LYS:HB3	1.95	0.48
2:D:3200:ASN:CB	2:D:3203:ASP:HB2	2.44	0.48
2:A:165:ALA:HB3	2:A:180:ASP:HB3	1.96	0.47
2:A:874:LEU:HD12	2:A:875:PRO:HD2	1.95	0.47
2:A:3006:SER:C	2:A:3010:LYS:HZ2	2.22	0.47
2:A:3255:GLU:OE1	2:A:3273:MET:HE2	2.13	0.47
2:A:3269:ASN:O	2:A:3273:MET:HG3	2.14	0.47
2:B:2087:LEU:O	2:B:2091:GLN:HG2	2.13	0.47
2:B:2701:PHE:CE2	2:B:2703:PRO:HG3	2.49	0.47
2:C:19:GLU:HG2	2:C:66:THR:HB	1.95	0.47
2:C:1948:MET:HE1	2:C:1956:ALA:HB2	1.94	0.47
2:C:2968:LEU:HD13	2:C:3029:ILE:HG12	1.96	0.47
2:C:3295:TRP:HB3	2:C:3298:ARG:HH21	1.79	0.47
2:D:19:GLU:HG2	2:D:66:THR:HB	1.96	0.47
2:D:913:ARG:HG3	2:D:913:ARG:O	2.13	0.47
2:D:1797:GLU:HA	2:D:1800:LYS:HE3	1.96	0.47
2:D:2156:TYR:HE1	2:D:2202:TYR:HE2	1.60	0.47
2:D:3184:TYR:CG	2:D:3201:VAL:HG22	2.49	0.47
2:A:1143:GLN:HG3	2:A:1151:HIS:HA	1.96	0.47
2:A:1522:ALA:HB3	2:A:1527:LEU:HD21	1.95	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HB2	1.95	0.47
2:A:3166:PHE:CD2	2:A:3170:PHE:HB3	2.50	0.47
2:A:4268:MET:HA	2:A:4271:VAL:HG22	1.94	0.47
2:B:441:LYS:HG3	2:B:444:THR:HG23	1.96	0.47
2:B:661:LEU:HD23	2:B:673:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2431:ASP:O	2:B:2435:VAL:HG23	2.14	0.47
2:C:912:LYS:HE3	2:C:914:GLN:HG3	1.96	0.47
2:C:2431:ASP:O	2:C:2435:VAL:HG23	2.14	0.47
2:C:2912:LEU:HB3	2:C:2914:THR:HG23	1.96	0.47
2:C:3253:GLY:C	2:C:3255:GLU:N	2.72	0.47
2:D:441:LYS:HG3	2:D:444:THR:HG23	1.96	0.47
2:D:2224:ASN:O	2:D:2227:VAL:HG23	2.14	0.47
2:D:2701:PHE:CE2	2:D:2703:PRO:HG3	2.49	0.47
2:D:2833:LEU:HB2	2:D:2838[B]:HIS:NE2	2.28	0.47
2:A:19:GLU:HG2	2:A:66:THR:HB	1.96	0.47
2:A:661:LEU:HD23	2:A:673:TRP:CD1	2.49	0.47
2:A:769:ARG:NH2	2:A:816:PRO:HG3	2.30	0.47
2:A:912:LYS:HE3	2:A:914:GLN:HG3	1.96	0.47
2:A:2565:GLN:O	2:A:2569:ILE:HG12	2.14	0.47
2:A:3719:MET:HA	2:A:3719:MET:HE3	1.95	0.47
2:B:2828:MET:O	2:B:2894:LYS:NZ	2.42	0.47
2:B:3200:ASN:CB	2:B:3203:ASP:HB2	2.44	0.47
2:C:874:LEU:HD12	2:C:875:PRO:HD2	1.95	0.47
2:C:1797:GLU:HA	2:C:1800:LYS:HE3	1.96	0.47
2:C:3166:PHE:CD2	2:C:3170:PHE:HB3	2.50	0.47
2:C:3255:GLU:OE1	2:C:3273:MET:HE2	2.13	0.47
2:D:4027:THR:HG21	2:D:4084:VAL:HG11	1.97	0.47
1:I:50:GLN:NE2	1:I:54:ASN:HD21	2.13	0.47
2:A:1104:GLU:OE1	2:A:1225:LYS:NZ	2.44	0.47
2:A:2385:GLY:O	2:A:2389:MET:HG3	2.13	0.47
2:A:2496:LEU:HD23	2:A:2520:LEU:HD13	1.95	0.47
2:A:2713:ILE:HG12	2:A:2776:LYS:HB2	1.97	0.47
1:L:50:GLN:NE2	1:L:54:ASN:HD21	2.13	0.47
2:B:2224:ASN:O	2:B:2227:VAL:HG23	2.14	0.47
2:C:1039:ASP:C	2:C:1043:LYS:HZ2	2.23	0.47
2:C:2744:GLY:H	2:C:2755:PRO:HA	1.79	0.47
2:C:4735:ASN:HB3	2:C:4738:PHE:HD2	1.79	0.47
2:D:165:ALA:HB3	2:D:180:ASP:HB3	1.96	0.47
2:D:1552:VAL:HG12	2:D:1553:PHE:HD1	1.80	0.47
2:A:1034:PRO:HD2	2:A:1037:LEU:HD12	1.96	0.47
2:A:1564:MET:HE1	2:A:1578:PRO:HA	1.97	0.47
2:A:2350:ALA:HA	2:A:2353:ILE:HG22	1.96	0.47
2:A:2658:GLU:OE1	2:A:2661:LEU:N	2.37	0.47
2:A:3200:ASN:CB	2:A:3203:ASP:HB2	2.44	0.47
2:A:4567:TYR:O	2:A:4567:TYR:CD1	2.68	0.47
3:F:88:HIS:HD2	3:F:89:PRO:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3068:LEU:O	2:B:3071:THR:OG1	2.27	0.47
2:C:904:TYR:HE1	2:C:916:PRO:HA	1.80	0.47
2:C:2713:ILE:HG12	2:C:2776:LYS:HB2	1.97	0.47
2:C:3043:ARG:HA	2:C:3120:ASP:OD2	2.13	0.47
2:C:4814:MET:HA	2:C:4814:MET:HE3	1.95	0.47
2:D:769:ARG:NH2	2:D:816:PRO:HG3	2.30	0.47
2:D:912:LYS:HE3	2:D:914:GLN:HG3	1.96	0.47
2:D:2431:ASP:O	2:D:2435:VAL:HG23	2.14	0.47
2:D:2886:ARG:HG2	2:D:2890:GLN:OE1	2.15	0.47
2:D:3042:ALA:HB1	2:D:3121:LEU:HB2	1.95	0.47
2:D:3131:TYR:O	2:D:3135:THR:HG23	2.14	0.47
2:D:4520:TYR:HD1	2:D:4561:LEU:HD13	1.79	0.47
2:D:4735:ASN:HB3	2:D:4738:PHE:HD2	1.79	0.47
2:A:4276:VAL:O	2:A:4280:VAL:HG23	2.15	0.47
2:A:4707:MET:HG2	2:D:4252:ILE:HG21	1.97	0.47
2:B:375:GLN:HB2	2:B:390:LYS:HB3	1.95	0.47
2:B:769:ARG:NH2	2:B:816:PRO:HG3	2.29	0.47
2:B:2681:MET:HE1	2:B:2920:ARG:HG2	1.96	0.47
2:B:2892:ILE:HG13	2:B:2893:LEU:N	2.30	0.47
2:B:4027:THR:HG21	2:B:4084:VAL:HG11	1.97	0.47
2:C:769:ARG:NH2	2:C:816:PRO:HG3	2.30	0.47
2:D:293:GLN:HG3	2:D:343:ARG:NH1	2.29	0.47
2:D:874:LEU:HD12	2:D:875:PRO:HD2	1.95	0.47
2:D:3171:LEU:HD13	2:D:3214:LEU:HD12	1.95	0.47
2:D:4800:ASP:OD1	2:D:4801:THR:N	2.47	0.47
1:I:126:ILE:O	1:I:130:ASP:N	2.48	0.47
2:A:624:ALA:HB2	2:A:1667:LEU:HD12	1.97	0.47
2:A:2293:VAL:O	2:A:2296:GLU:HG2	2.15	0.47
2:A:2886:ARG:HG2	2:A:2890:GLN:OE1	2.15	0.47
2:A:2892:ILE:HG13	2:A:2893:LEU:N	2.30	0.47
2:A:2946:GLY:HA3	2:A:2954:PHE:HZ	1.79	0.47
2:A:3184:TYR:CG	2:A:3201:VAL:HG22	2.49	0.47
2:A:4520:TYR:HD1	2:A:4561:LEU:HD13	1.79	0.47
2:B:883:GLU:HG2	2:B:884:LYS:N	2.28	0.47
2:B:996:VAL:HG13	2:B:1050:LEU:HD22	1.97	0.47
2:B:2001:GLU:OE1	2:B:2001:GLU:N	2.48	0.47
2:B:2886:ARG:HG2	2:B:2890:GLN:OE1	2.15	0.47
2:B:3006:SER:C	2:B:3010:LYS:HZ2	2.22	0.47
2:B:3042:ALA:HB1	2:B:3121:LEU:HD13	1.97	0.47
2:B:3184:TYR:HB3	2:B:3192:ARG:NH2	2.27	0.47
2:B:3184:TYR:CG	2:B:3201:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3689:MET:HE2	2:B:3754:MET:HG2	1.96	0.47
2:B:4557:VAL:HG21	2:C:4790:ARG:HH22	1.80	0.47
2:B:4567:TYR:O	2:B:4567:TYR:CD1	2.68	0.47
2:C:334:SER:OG	2:C:336:GLU:OE1	2.22	0.47
2:C:514:PHE:HD2	2:C:526:TRP:HB2	1.80	0.47
2:C:1552:VAL:HG12	2:C:1553:PHE:HD1	1.80	0.47
2:C:3006:SER:C	2:C:3010:LYS:HZ2	2.22	0.47
2:C:3246:MET:HG2	2:C:3309:LYS:HZ2	1.78	0.47
2:C:3689:MET:HE2	2:C:3754:MET:HG2	1.96	0.47
2:C:3715:GLU:OE2	2:C:4647:LYS:HE2	2.15	0.47
2:C:4800:ASP:OD1	2:C:4801:THR:N	2.47	0.47
2:D:50:GLU:CD	2:D:61:ASP:H	2.22	0.47
2:D:292:GLY:HA3	2:D:340:VAL:HG21	1.96	0.47
2:D:1143:GLN:HG3	2:D:1151:HIS:HA	1.96	0.47
2:D:1564:MET:HE1	2:D:1578:PRO:HA	1.97	0.47
2:D:3166:PHE:CD2	2:D:3170:PHE:HB3	2.50	0.47
2:A:441:LYS:HG3	2:A:444:THR:HG23	1.96	0.47
1:K:50:GLN:NE2	1:K:54:ASN:HD21	2.13	0.47
2:B:514:PHE:HD2	2:B:526:TRP:HB2	1.80	0.47
2:B:912:LYS:HE3	2:B:914:GLN:HG3	1.96	0.47
2:B:1718:ARG:HD3	2:B:1831:MET:HA	1.97	0.47
2:B:2153:LYS:HD3	2:B:2156:TYR:HD2	1.80	0.47
2:B:2744:GLY:H	2:B:2755:PRO:HA	1.79	0.47
2:B:2824:ARG:NH2	2:C:1502:ASN:HB3	2.30	0.47
2:B:4026:LEU:HD13	2:B:4058:TYR:HE2	1.80	0.47
2:C:293:GLN:HG3	2:C:343:ARG:NH1	2.30	0.47
2:C:1732:GLU:O	2:C:1736:ILE:HG13	2.15	0.47
2:C:2422:ILE:O	2:C:2426:LEU:HG	2.15	0.47
2:C:2946:GLY:HA3	2:C:2954:PHE:HZ	1.79	0.47
2:C:3171:LEU:HD13	2:C:3214:LEU:HD12	1.95	0.47
2:C:4567:TYR:CD1	2:C:4567:TYR:O	2.68	0.47
2:D:904:TYR:HE1	2:D:916:PRO:HA	1.79	0.47
2:A:293:GLN:HG3	2:A:343:ARG:NH1	2.29	0.47
2:A:1552:VAL:HG12	2:A:1553:PHE:HD1	1.80	0.47
2:A:4806:CYS:HA	2:A:4812:CYS:HB2	1.97	0.47
2:B:1034:PRO:HD2	2:B:1037:LEU:HD12	1.96	0.47
2:B:1435:GLY:N	2:B:1500:ARG:HH22	2.11	0.47
2:B:1564:MET:HE1	2:B:1578:PRO:HA	1.97	0.47
2:B:2685:TYR:HD2	2:B:2686:VAL:O	1.98	0.47
2:B:3166:PHE:CD2	2:B:3170:PHE:HB3	2.50	0.47
2:B:4800:ASP:OD1	2:B:4801:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:165:ALA:HB3	2:C:180:ASP:HB3	1.96	0.47
2:C:292:GLY:HA3	2:C:340:VAL:HG21	1.96	0.47
2:C:2293:VAL:O	2:C:2296:GLU:HG2	2.15	0.47
2:C:2662:PHE:HE2	2:C:2962:PHE:HD1	1.62	0.47
2:C:3042:ALA:HB1	2:C:3121:LEU:HD13	1.97	0.47
2:C:3164:GLY:C	2:C:3248:ARG:HH12	2.23	0.47
2:D:913:ARG:HA	2:D:913:ARG:HD2	1.74	0.47
2:D:1176:THR:HG22	2:D:1181:ILE:HA	1.97	0.47
2:D:1435:GLY:N	2:D:1500:ARG:HH22	2.11	0.47
2:D:2642:ARG:HH12	2:D:2921:PHE:HA	1.80	0.47
2:D:2658:GLU:OE1	2:D:2661:LEU:N	2.37	0.47
2:D:2662:PHE:HE2	2:D:2962:PHE:HD1	1.62	0.47
2:D:2713:ILE:HG12	2:D:2776:LYS:HB2	1.97	0.47
2:D:3164:GLY:C	2:D:3248:ARG:HH12	2.23	0.47
2:D:3166:PHE:O	2:D:3248:ARG:NH1	2.48	0.47
2:D:3715:GLU:OE2	2:D:4647:LYS:HE2	2.15	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HD13	1.97	0.47
2:A:3131:TYR:O	2:A:3135:THR:HG23	2.14	0.47
2:A:3166:PHE:O	2:A:3248:ARG:NH1	2.48	0.47
2:A:3744:ILE:O	2:A:3747:SER:OG	2.31	0.47
2:A:4853:PHE:HA	2:A:4857:ILE:HD12	1.97	0.47
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.97	0.47
2:B:293:GLN:HG3	2:B:343:ARG:NH1	2.29	0.47
2:B:2293:VAL:O	2:B:2296:GLU:HG2	2.15	0.47
2:B:4648:PHE:CD1	2:B:4651:ARG:HG3	2.50	0.47
2:C:911:ASN:OD1	2:C:912:LYS:N	2.48	0.47
2:C:996:VAL:HG13	2:C:1050:LEU:HD22	1.97	0.47
2:C:1417:TYR:O	2:C:1421:MET:HG2	2.15	0.47
2:C:1564:MET:HE1	2:C:1578:PRO:HA	1.97	0.47
2:C:2350:ALA:HA	2:C:2353:ILE:HG22	1.96	0.47
2:C:4026:LEU:HD13	2:C:4058:TYR:HE2	1.80	0.47
2:C:4276:VAL:O	2:C:4280:VAL:HG23	2.15	0.47
2:D:972:LEU:HD23	2:D:973:THR:N	2.30	0.47
2:D:2422:ILE:O	2:D:2426:LEU:HG	2.15	0.47
2:D:3006:SER:C	2:D:3010:LYS:HZ2	2.22	0.47
2:D:4567:TYR:O	2:D:4567:TYR:CD1	2.68	0.47
2:D:4648:PHE:CD1	2:D:4651:ARG:HG3	2.50	0.47
2:A:1718:ARG:HD3	2:A:1831:MET:HA	1.97	0.46
2:A:4648:PHE:CD1	2:A:4651:ARG:HG3	2.50	0.46
2:A:4956:ASP:HA	2:A:4960:LYS:HD3	1.97	0.46
1:J:50:GLN:NE2	1:J:54:ASN:HD21	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:LEU:HD23	2:B:973:THR:N	2.30	0.46
2:B:1732:GLU:O	2:B:1736:ILE:HG13	2.15	0.46
2:B:1981:ASP:OD2	2:B:1983:LYS:NZ	2.48	0.46
2:B:2713:ILE:HG12	2:B:2776:LYS:HB2	1.97	0.46
2:B:3164:GLY:C	2:B:3248:ARG:HH12	2.23	0.46
2:B:3310:VAL:HG13	2:B:3314:LEU:HD12	1.97	0.46
2:B:4276:VAL:O	2:B:4280:VAL:HG23	2.15	0.46
2:C:1184:ASP:OD2	2:C:1193:LYS:NZ	2.38	0.46
2:C:2642:ARG:HH12	2:C:2921:PHE:HA	1.80	0.46
2:D:1417:TYR:O	2:D:1421:MET:HG2	2.15	0.46
2:D:1718:ARG:HD3	2:D:1831:MET:HA	1.97	0.46
2:D:2001:GLU:OE1	2:D:2001:GLU:N	2.48	0.46
2:D:2153:LYS:HD3	2:D:2156:TYR:HD2	1.80	0.46
2:D:2681:MET:HE1	2:D:2920:ARG:HG2	1.96	0.46
2:D:2733:SER:HA	2:D:2736:LYS:HZ3	1.78	0.46
2:D:2744:GLY:H	2:D:2755:PRO:HA	1.79	0.46
2:D:2892:ILE:HG13	2:D:2893:LEU:N	2.30	0.46
2:D:3042:ALA:HB1	2:D:3121:LEU:HD13	1.97	0.46
2:D:3106:SER:OG	2:D:3157:GLU:OE1	2.21	0.46
2:D:4079:ASP:O	2:D:4082:GLU:HG3	2.15	0.46
2:D:4276:VAL:O	2:D:4280:VAL:HG23	2.15	0.46
2:A:1732:GLU:O	2:A:1736:ILE:HG13	2.15	0.46
2:A:1981:ASP:OD2	2:A:1983:LYS:NZ	2.48	0.46
2:A:2001:GLU:OE1	2:A:2001:GLU:N	2.48	0.46
2:A:2422:ILE:O	2:A:2426:LEU:HG	2.15	0.46
2:A:2431:ASP:O	2:A:2435:VAL:HG23	2.14	0.46
2:A:3043:ARG:HB3	2:A:3117:PHE:CD1	2.51	0.46
2:A:3310:VAL:HG13	2:A:3314:LEU:HD12	1.97	0.46
2:B:1143:GLN:HG3	2:B:1151:HIS:HA	1.96	0.46
2:B:2891:ASP:OD1	2:B:2892:ILE:N	2.48	0.46
2:B:3253:GLY:C	2:B:3255:GLU:N	2.72	0.46
2:B:4079:ASP:O	2:B:4082:GLU:HG3	2.16	0.46
2:B:4853:PHE:HA	2:B:4857:ILE:HD12	1.97	0.46
2:C:1610:ARG:HA	2:C:1617:TRP:HA	1.98	0.46
2:C:2001:GLU:N	2:C:2001:GLU:OE1	2.48	0.46
2:C:2153:LYS:HD3	2:C:2156:TYR:HD2	1.80	0.46
2:C:2891:ASP:OD1	2:C:2892:ILE:N	2.48	0.46
2:C:3043:ARG:HB3	2:C:3117:PHE:CD1	2.50	0.46
2:C:3166:PHE:O	2:C:3248:ARG:NH1	2.48	0.46
2:C:4079:ASP:O	2:C:4082:GLU:HG3	2.16	0.46
2:C:4853:PHE:HA	2:C:4857:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4806:CYS:HA	2:D:4812:CYS:HB2	1.97	0.46
1:I:10:ILE:HA	1:I:13:PHE:HB2	1.97	0.46
2:A:2787:TRP:CZ2	2:A:2843:MET:HE1	2.51	0.46
2:A:2972:ASP:OD1	2:A:2976:LYS:NZ	2.49	0.46
2:A:3164:GLY:C	2:A:3248:ARG:HH12	2.23	0.46
2:A:4079:ASP:O	2:A:4082:GLU:HG3	2.15	0.46
1:K:125:MET:HE3	1:K:125:MET:HB3	1.71	0.46
2:B:50:GLU:CD	2:B:61:ASP:H	2.22	0.46
2:B:904:TYR:HE1	2:B:916:PRO:HA	1.80	0.46
2:B:2787:TRP:CZ2	2:B:2843:MET:HE1	2.51	0.46
2:B:2912:LEU:HB3	2:B:2914:THR:HG23	1.96	0.46
2:B:3166:PHE:O	2:B:3248:ARG:NH1	2.48	0.46
2:B:3715:GLU:OE2	2:B:4647:LYS:HE2	2.15	0.46
2:C:419:ILE:HD13	2:C:492:GLU:HG3	1.97	0.46
2:C:436:LEU:HD23	2:C:436:LEU:HA	1.81	0.46
2:C:4520:TYR:HD1	2:C:4561:LEU:HD13	1.80	0.46
2:C:4774:LEU:O	2:C:4778:VAL:HG23	2.16	0.46
2:D:173:GLU:OE2	2:D:176:ARG:NH2	2.36	0.46
2:D:1694:MET:HE2	2:D:1694:MET:HB2	1.84	0.46
2:D:2972:ASP:OD1	2:D:2976:LYS:NZ	2.49	0.46
2:A:2891:ASP:OD1	2:A:2892:ILE:N	2.48	0.46
2:A:4026:LEU:HD13	2:A:4058:TYR:HE2	1.80	0.46
3:E:19:LYS:HB2	3:E:19:LYS:HE3	1.84	0.46
1:L:10:ILE:HA	1:L:13:PHE:HB2	1.98	0.46
1:K:137:VAL:HG21	2:C:3587:TRP:CH2	2.49	0.46
2:B:19:GLU:HG2	2:B:66:THR:HB	1.96	0.46
2:B:3925:GLN:HE22	2:B:4934:THR:HA	1.80	0.46
2:B:4806:CYS:HA	2:B:4812:CYS:HB2	1.97	0.46
2:C:2685:TYR:HD2	2:C:2686:VAL:O	1.98	0.46
2:C:4648:PHE:CD1	2:C:4651:ARG:HG3	2.50	0.46
2:D:1610:ARG:HA	2:D:1617:TRP:HA	1.97	0.46
2:D:2912:LEU:HB3	2:D:2914:THR:HG23	1.96	0.46
2:D:2973:GLN:HA	2:D:2976:LYS:HZ3	1.79	0.46
2:D:4008:ASN:OD1	2:D:4009:ASN:N	2.49	0.46
2:D:4026:LEU:HD13	2:D:4058:TYR:HE2	1.80	0.46
2:D:4853:PHE:HA	2:D:4857:ILE:HD12	1.97	0.46
2:A:2646:TRP:CH2	2:A:2928:GLN:HG3	2.51	0.46
2:A:2685:TYR:HD2	2:A:2686:VAL:O	1.98	0.46
2:A:2912:LEU:HB3	2:A:2914:THR:HG23	1.96	0.46
2:A:3604:ARG:O	2:A:3604:ARG:HD3	2.16	0.46
2:A:4008:ASN:OD1	2:A:4009:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1176:THR:HG22	2:B:1181:ILE:HA	1.97	0.46
2:B:2946:GLY:HA3	2:B:2954:PHE:HZ	1.79	0.46
2:B:4774:LEU:O	2:B:4778:VAL:HG23	2.16	0.46
2:C:1143:GLN:HG3	2:C:1151:HIS:HA	1.96	0.46
2:C:1718:ARG:HD3	2:C:1831:MET:HA	1.97	0.46
2:C:4027:THR:HG21	2:C:4084:VAL:HG11	1.97	0.46
2:D:624:ALA:HB2	2:D:1667:LEU:HD12	1.97	0.46
2:D:2293:VAL:O	2:D:2296:GLU:HG2	2.15	0.46
2:D:2350:ALA:HA	2:D:2353:ILE:HG22	1.96	0.46
2:D:3925:GLN:HE22	2:D:4934:THR:HA	1.80	0.46
2:A:2681:MET:HE1	2:A:2920:ARG:HG2	1.96	0.46
2:A:2744:GLY:H	2:A:2755:PRO:HA	1.79	0.46
2:A:2772:ARG:HG3	2:A:2776:LYS:HZ2	1.80	0.46
2:B:334:SER:OG	2:B:336:GLU:OE1	2.22	0.46
2:B:1552:VAL:HG12	2:B:1553:PHE:HD1	1.80	0.46
2:B:2422:ILE:O	2:B:2426:LEU:HG	2.15	0.46
2:B:3604:ARG:O	2:B:3604:ARG:HD3	2.16	0.46
2:B:4956:ASP:HA	2:B:4960:LYS:HD3	1.97	0.46
2:C:972:LEU:HD23	2:C:973:THR:N	2.30	0.46
2:C:1014:GLN:HB3	2:C:1027:ARG:HH21	1.81	0.46
2:C:2886:ARG:HG2	2:C:2890:GLN:OE1	2.15	0.46
2:C:3184:TYR:HB3	2:C:3192:ARG:NH2	2.27	0.46
2:C:3925:GLN:HE22	2:C:4934:THR:HA	1.80	0.46
2:C:4008:ASN:OD1	2:C:4009:ASN:N	2.49	0.46
2:C:4116:GLN:HA	2:C:4119:LEU:HD12	1.98	0.46
2:D:419:ILE:HD13	2:D:492:GLU:HG3	1.97	0.46
2:D:514:PHE:HD2	2:D:526:TRP:HB2	1.80	0.46
2:D:1300:MET:HA	2:D:1300:MET:HE3	1.97	0.46
2:D:2891:ASP:OD1	2:D:2892:ILE:N	2.48	0.46
2:D:3156:GLY:O	2:D:3240:PRO:HB2	2.16	0.46
2:A:902:TRP:CD1	2:A:913:ARG:NH2	2.84	0.46
2:A:972:LEU:HD23	2:A:973:THR:N	2.30	0.46
2:A:2525:LEU:HG	2:A:2569:ILE:HD13	1.98	0.46
2:A:2779:LEU:O	2:A:2782:MET:HG3	2.16	0.46
2:A:2828:MET:O	2:A:2894:LYS:NZ	2.42	0.46
2:A:2946:GLY:HA3	2:A:2954:PHE:CZ	2.51	0.46
2:A:3022:PHE:HB3	2:A:3025:ASP:OD1	2.16	0.46
2:A:3715:GLU:OE2	2:A:4647:LYS:HE2	2.15	0.46
2:A:4027:THR:HG21	2:A:4084:VAL:HG11	1.97	0.46
2:A:4735:ASN:HB3	2:A:4738:PHE:HD2	1.79	0.46
2:A:4921:PHE:HE2	2:A:4940:VAL:HG11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1417:TYR:O	2:B:1421:MET:HG2	2.15	0.46
2:B:3022:PHE:HB3	2:B:3025:ASP:OD1	2.16	0.46
2:C:3156:GLY:O	2:C:3240:PRO:HB2	2.16	0.46
2:C:3293:GLY:HA3	2:C:3295:TRP:CZ3	2.51	0.46
2:C:4806:CYS:HA	2:C:4812:CYS:HB2	1.97	0.46
2:C:4956:ASP:HA	2:C:4960:LYS:HD3	1.97	0.46
2:D:902:TRP:CD1	2:D:913:ARG:NH2	2.84	0.46
2:D:2685:TYR:HD2	2:D:2686:VAL:O	1.98	0.46
1:I:110:MET:HA	2:A:3590:LEU:HD21	1.97	0.46
2:A:218:SER:HB3	2:A:286:GLY:HA3	1.98	0.46
2:A:1008:ALA:O	2:A:1012:ILE:HG12	2.16	0.46
2:A:2642:ARG:HH12	2:A:2921:PHE:HA	1.80	0.46
1:J:127:ARG:HD3	1:J:127:ARG:HA	1.41	0.46
2:B:1014:GLN:HB3	2:B:1027:ARG:HH21	1.81	0.46
2:B:2350:ALA:HA	2:B:2353:ILE:HG22	1.96	0.46
2:B:2629:ASN:OD1	2:B:2630:PHE:N	2.49	0.46
2:B:2689:MET:HE3	2:B:2689:MET:HB3	1.59	0.46
2:B:2779:LEU:O	2:B:2782:MET:HG3	2.16	0.46
2:B:3127:GLN:HG3	2:B:3183:ILE:HB	1.98	0.46
2:B:4008:ASN:OD1	2:B:4009:ASN:N	2.49	0.46
2:D:2525:LEU:HG	2:D:2569:ILE:HD13	1.98	0.46
2:D:2629:ASN:OD1	2:D:2630:PHE:N	2.49	0.46
2:D:2785:TRP:CD1	2:D:2905:ARG:HH22	2.34	0.46
2:D:3604:ARG:O	2:D:3604:ARG:HD3	2.16	0.46
2:D:4116:GLN:HA	2:D:4119:LEU:HD12	1.98	0.46
2:A:514:PHE:HD2	2:A:526:TRP:HB2	1.80	0.46
2:A:1014:GLN:HB3	2:A:1027:ARG:HH21	1.81	0.46
2:B:658:ASN:HD21	2:B:833:LYS:HG2	1.81	0.46
2:B:2946:GLY:HA3	2:B:2954:PHE:CZ	2.51	0.46
2:B:2956:TYR:HA	2:B:2959:GLU:OE1	2.16	0.46
2:B:3293:GLY:HA3	2:B:3295:TRP:CZ3	2.51	0.46
2:B:4520:TYR:HD1	2:B:4561:LEU:HD13	1.79	0.46
2:B:4921:PHE:HE2	2:B:4940:VAL:HG11	1.81	0.46
2:C:678:MET:HB2	2:C:754:VAL:HG22	1.98	0.46
2:C:2892:ILE:HG13	2:C:2893:LEU:N	2.30	0.46
2:C:2946:GLY:HA3	2:C:2954:PHE:CZ	2.51	0.46
2:D:1008:ALA:O	2:D:1012:ILE:HG12	2.16	0.46
2:D:1967:SER:O	2:D:1972:GLN:NE2	2.41	0.46
2:D:2779:LEU:O	2:D:2782:MET:HG3	2.16	0.46
2:D:3293:GLY:HA3	2:D:3295:TRP:CZ3	2.51	0.46
2:A:50:GLU:CD	2:A:61:ASP:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:166:SER:OG	2:A:168:GLN:OE1	2.34	0.46
2:A:1176:THR:HG22	2:A:1181:ILE:HA	1.97	0.46
2:A:2629:ASN:OD1	2:A:2630:PHE:N	2.49	0.46
2:A:2662:PHE:HE2	2:A:2962:PHE:HD1	1.62	0.46
2:A:2689:MET:HB3	2:A:2689:MET:HE3	1.59	0.46
1:J:68:GLU:O	1:J:71:THR:OG1	2.33	0.46
2:B:908:ARG:NH2	2:B:928:GLU:OE2	2.49	0.46
2:B:3316:LYS:O	2:B:3317:THR:OG1	2.33	0.46
2:C:785:ASP:OD1	2:C:786:GLY:N	2.49	0.46
2:C:2447:LYS:HE2	2:C:2864:GLY:HA3	1.98	0.46
2:C:2629:ASN:OD1	2:C:2630:PHE:N	2.49	0.46
2:C:2785:TRP:CD1	2:C:2905:ARG:HH22	2.34	0.46
2:C:2787:TRP:CZ2	2:C:2843:MET:HE1	2.50	0.46
2:D:194:LEU:HD11	2:D:201:LEU:HB3	1.98	0.46
2:D:658:ASN:HD21	2:D:833:LYS:HG2	1.81	0.46
2:D:785:ASP:OD1	2:D:786:GLY:N	2.49	0.46
2:D:3043:ARG:HB3	2:D:3117:PHE:CD1	2.51	0.46
1:I:68:GLU:O	1:I:71:THR:OG1	2.33	0.45
1:L:48:GLU:O	1:L:52:MET:HG2	2.17	0.45
1:K:126:ILE:O	1:K:130:ASP:N	2.48	0.45
2:B:2642:ARG:HH12	2:B:2921:PHE:HA	1.80	0.45
2:B:4735:ASN:HB3	2:B:4738:PHE:HD2	1.79	0.45
2:C:1300:MET:HA	2:C:1300:MET:HE3	1.97	0.45
2:C:1981:ASP:OD2	2:C:1983:LYS:NZ	2.48	0.45
2:C:3127:GLN:HG3	2:C:3183:ILE:HB	1.98	0.45
2:D:911:ASN:OD1	2:D:912:LYS:N	2.48	0.45
2:D:996:VAL:HG13	2:D:1050:LEU:HD22	1.97	0.45
2:D:1039:ASP:C	2:D:1043:LYS:HZ2	2.24	0.45
2:D:1732:GLU:O	2:D:1736:ILE:HG13	2.15	0.45
2:D:2646:TRP:CH2	2:D:2928:GLN:HG3	2.51	0.45
2:D:4269:LYS:HA	2:D:4272:LYS:HE2	1.98	0.45
2:D:4774:LEU:O	2:D:4778:VAL:HG23	2.16	0.45
1:I:48:GLU:O	1:I:52:MET:HG2	2.17	0.45
1:I:61:ASN:ND2	1:I:63:THR:O	2.50	0.45
1:I:106:LEU:HD22	2:A:3587:TRP:HE1	1.82	0.45
2:A:66:THR:OG1	2:A:124:SER:OG	2.24	0.45
2:A:654:SER:O	2:A:655:MET:HE2	2.17	0.45
2:A:1151:HIS:ND1	2:A:1185:ASP:OD1	2.32	0.45
2:A:1417:TYR:O	2:A:1421:MET:HG2	2.15	0.45
2:A:1435:GLY:N	2:A:1500:ARG:HH22	2.12	0.45
1:J:61:ASN:ND2	1:J:63:THR:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:THR:OG1	1:K:83:GLU:OE2	2.32	0.45
2:B:624:ALA:HB2	2:B:1667:LEU:HD12	1.97	0.45
2:B:1300:MET:HA	2:B:1300:MET:HE3	1.98	0.45
2:B:1610:ARG:HA	2:B:1617:TRP:HA	1.98	0.45
2:B:2703:PRO:HB2	2:B:2854:LYS:HE2	1.99	0.45
2:B:2821:TYR:CE2	2:B:2823:PRO:HG3	2.51	0.45
2:B:3043:ARG:HB3	2:B:3117:PHE:CD1	2.50	0.45
2:B:3253:GLY:O	2:B:3257:ASN:HB3	2.16	0.45
2:C:658:ASN:HD21	2:C:833:LYS:HG2	1.82	0.45
2:C:1176:THR:HG22	2:C:1181:ILE:HA	1.97	0.45
2:C:2791:ARG:NH1	2:C:2796:ASP:OD2	2.50	0.45
2:C:4921:PHE:HE2	2:C:4940:VAL:HG11	1.81	0.45
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.97	0.45
2:D:989:THR:HG22	2:D:992:GLN:HG2	1.98	0.45
2:D:3022:PHE:HB3	2:D:3025:ASP:OD1	2.16	0.45
2:D:3310:VAL:HG13	2:D:3314:LEU:HD12	1.97	0.45
2:D:4956:ASP:HA	2:D:4960:LYS:HD3	1.97	0.45
2:A:887:GLU:O	2:A:891:GLU:HG2	2.17	0.45
2:A:911:ASN:OD1	2:A:912:LYS:N	2.48	0.45
2:A:3963:SER:OG	2:A:3964:GLN:OE1	2.30	0.45
2:A:4774:LEU:O	2:A:4778:VAL:HG23	2.16	0.45
3:E:78:THR:O	3:E:81:VAL:HG12	2.17	0.45
1:J:10:ILE:HA	1:J:13:PHE:HB2	1.98	0.45
2:B:1008:ALA:O	2:B:1012:ILE:HG12	2.16	0.45
2:B:3156:GLY:O	2:B:3240:PRO:HB2	2.16	0.45
2:C:908:ARG:NH2	2:C:928:GLU:OE2	2.49	0.45
2:C:2592:LEU:HD22	2:C:2606:PRO:HB3	1.98	0.45
2:C:2956:TYR:HA	2:C:2959:GLU:OE1	2.16	0.45
2:C:2961:LYS:HB2	2:C:2965:LYS:HZ3	1.81	0.45
2:D:66:THR:OG1	2:D:124:SER:OG	2.24	0.45
2:D:166:SER:OG	2:D:168:GLN:OE1	2.34	0.45
2:D:2956:TYR:HA	2:D:2959:GLU:OE1	2.16	0.45
2:D:4921:PHE:HE2	2:D:4940:VAL:HG11	1.81	0.45
2:A:785:ASP:OD1	2:A:786:GLY:N	2.49	0.45
2:A:1118:SER:HB2	2:A:1204:VAL:HG11	1.98	0.45
2:A:1979:PHE:HE1	2:A:1988:CYS:HB3	1.82	0.45
2:A:2791:ARG:NH1	2:A:2796:ASP:OD2	2.50	0.45
2:A:3156:GLY:O	2:A:3240:PRO:HB2	2.16	0.45
2:A:3293:GLY:HA3	2:A:3295:TRP:CZ3	2.51	0.45
3:H:78:THR:O	3:H:81:VAL:HG12	2.17	0.45
1:L:36:VAL:O	1:L:39:SER:OG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:ASP:N	1:L:68:GLU:OE2	2.33	0.45
2:B:2785:TRP:CD1	2:B:2905:ARG:HH22	2.34	0.45
2:B:2857:LYS:O	2:B:2861:GLU:OE1	2.34	0.45
2:B:4269:LYS:HA	2:B:4272:LYS:HE2	1.99	0.45
2:B:4609:LYS:HE3	2:B:4615:LEU:HD13	1.99	0.45
2:C:50:GLU:CD	2:C:61:ASP:H	2.22	0.45
2:C:902:TRP:CD1	2:C:913:ARG:NH2	2.84	0.45
2:C:2646:TRP:CH2	2:C:2928:GLN:HG3	2.51	0.45
2:C:2779:LEU:O	2:C:2782:MET:HG3	2.16	0.45
2:C:2821:TYR:CE2	2:C:2823:PRO:HG3	2.51	0.45
2:C:2857:LYS:O	2:C:2861:GLU:OE1	2.34	0.45
2:C:3022:PHE:HB3	2:C:3025:ASP:OD1	2.16	0.45
2:C:4242:ARG:HH22	2:C:4249:ARG:NH1	2.15	0.45
2:D:50:GLU:OE2	2:D:61:ASP:N	2.48	0.45
2:D:654:SER:O	2:D:655:MET:HE2	2.17	0.45
2:D:1981:ASP:OD2	2:D:1983:LYS:NZ	2.48	0.45
2:D:4242:ARG:HH22	2:D:4249:ARG:NH1	2.15	0.45
2:D:4858:LEU:HD23	2:D:4861:ILE:HD12	1.98	0.45
2:A:989:THR:HG22	2:A:992:GLN:HG2	1.98	0.45
2:A:1610:ARG:HA	2:A:1617:TRP:HA	1.98	0.45
2:A:2153:LYS:HD3	2:A:2156:TYR:HD2	1.80	0.45
2:A:2425:SER:O	2:B:142:LYS:NZ	2.49	0.45
2:A:2426:LEU:HB2	2:A:2427:ILE:HD12	1.99	0.45
2:A:3276:LEU:O	2:A:3280:ILE:HG12	2.17	0.45
2:A:3664:LEU:O	2:A:3668:ILE:HG13	2.17	0.45
1:L:10:ILE:O	1:L:14:LYS:N	2.38	0.45
2:B:654:SER:O	2:B:655:MET:HE2	2.17	0.45
2:B:887:GLU:O	2:B:891:GLU:HG2	2.17	0.45
2:B:902:TRP:CD1	2:B:913:ARG:NH2	2.84	0.45
2:B:1979:PHE:HE1	2:B:1988:CYS:HB3	1.82	0.45
2:C:227:TYR:CG	2:C:352:SER:HB2	2.52	0.45
2:C:1008:ALA:O	2:C:1012:ILE:HG12	2.16	0.45
2:C:3310:VAL:HG13	2:C:3314:LEU:HD12	1.97	0.45
2:D:908:ARG:NH2	2:D:928:GLU:OE2	2.49	0.45
2:D:2592:LEU:HD22	2:D:2606:PRO:HB3	1.98	0.45
2:D:3253:GLY:O	2:D:3257:ASN:HB3	2.16	0.45
2:A:658:ASN:HD21	2:A:833:LYS:HG2	1.82	0.45
2:A:678:MET:HB2	2:A:754:VAL:HG22	1.98	0.45
2:A:904:TYR:HE1	2:A:916:PRO:HA	1.80	0.45
2:A:1694:MET:HE2	2:A:1694:MET:HB2	1.84	0.45
2:A:2821:TYR:CE2	2:A:2823:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3107:SER:O	2:A:3111:HIS:HD2	2.00	0.45
2:A:4117:THR:O	2:A:4120:GLU:HG3	2.16	0.45
2:A:4269:LYS:HA	2:A:4272:LYS:HE2	1.99	0.45
2:A:4719:PHE:HE2	2:D:4294:LEU:HD22	1.79	0.45
1:K:10:ILE:HA	1:K:13:PHE:HB2	1.97	0.45
1:K:48:GLU:O	1:K:52:MET:HG2	2.17	0.45
1:K:127:ARG:HD3	1:K:127:ARG:HA	1.41	0.45
2:B:194:LEU:HD11	2:B:201:LEU:HB3	1.98	0.45
2:B:785:ASP:OD1	2:B:786:GLY:N	2.49	0.45
2:B:911:ASN:OD1	2:B:912:LYS:N	2.48	0.45
2:B:2646:TRP:CH2	2:B:2928:GLN:HG3	2.51	0.45
2:B:3107:SER:O	2:B:3111:HIS:HD2	2.00	0.45
2:B:3276:LEU:O	2:B:3280:ILE:HG12	2.17	0.45
2:B:4117:THR:O	2:B:4120:GLU:HG3	2.17	0.45
2:C:654:SER:O	2:C:655:MET:HE2	2.17	0.45
2:C:2849:HIS:NE2	2:C:2877:LEU:HD11	2.32	0.45
2:C:3604:ARG:O	2:C:3604:ARG:HD3	2.16	0.45
2:C:3649:ALA:C	2:C:3652:PRO:HD2	2.42	0.45
2:C:4257:ARG:O	2:C:4261:LEU:HG	2.17	0.45
2:D:2782:MET:HB2	2:D:2782:MET:HE2	1.82	0.45
2:D:2787:TRP:CZ2	2:D:2843:MET:HE1	2.51	0.45
2:A:314:LEU:HD11	2:A:372:LEU:HD13	1.99	0.45
2:A:908:ARG:NH2	2:A:928:GLU:OE2	2.49	0.45
2:A:2849:HIS:NE2	2:A:2877:LEU:HD11	2.32	0.45
2:A:3187:LYS:O	2:A:3191:GLU:HB2	2.17	0.45
2:A:3812:ASN:HA	2:A:3815:GLU:CD	2.42	0.45
2:A:3925:GLN:HE22	2:A:4934:THR:HA	1.80	0.45
2:A:4714:PHE:CG	2:D:4294:LEU:HD13	2.51	0.45
3:F:78:THR:O	3:F:81:VAL:HG12	2.17	0.45
2:B:419:ILE:HD13	2:B:492:GLU:HG3	1.97	0.45
2:B:2791:ARG:NH1	2:B:2796:ASP:OD2	2.50	0.45
2:C:624:ALA:HB2	2:C:1667:LEU:HD12	1.97	0.45
2:C:1964:GLU:OE2	2:C:1975:MET:HE3	2.17	0.45
2:C:2658:GLU:OE1	2:C:2661:LEU:N	2.37	0.45
2:C:4287:TYR:HA	2:C:4290:ILE:HD12	1.99	0.45
2:C:4609:LYS:HE3	2:C:4615:LEU:HD13	1.99	0.45
2:D:887:GLU:O	2:D:891:GLU:HG2	2.17	0.45
2:D:1151:HIS:ND1	2:D:1185:ASP:OD1	2.32	0.45
2:D:2426:LEU:HB2	2:D:2427:ILE:HD12	1.99	0.45
2:D:2791:ARG:NH1	2:D:2796:ASP:OD2	2.50	0.45
2:D:2849:HIS:NE2	2:D:2877:LEU:HD11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3276:LEU:O	2:D:3280:ILE:HG12	2.17	0.45
2:D:3812:ASN:HA	2:D:3815:GLU:CD	2.42	0.45
2:D:3963:SER:OG	2:D:3964:GLN:OE1	2.30	0.45
2:D:4257:ARG:O	2:D:4261:LEU:HG	2.17	0.45
2:A:436:LEU:HD23	2:A:436:LEU:HA	1.81	0.45
2:A:2347:MET:O	2:A:2351:ILE:HG12	2.17	0.45
2:A:2956:TYR:HA	2:A:2959:GLU:OE1	2.16	0.45
2:A:2973:GLN:HA	2:A:2976:LYS:HZ3	1.81	0.45
2:A:4257:ARG:O	2:A:4261:LEU:HG	2.17	0.45
2:B:2662:PHE:HE2	2:B:2962:PHE:HD1	1.62	0.45
2:B:2849:HIS:NE2	2:B:2877:LEU:HD11	2.32	0.45
2:B:3184:TYR:CE2	2:B:3197:LEU:HB3	2.52	0.45
2:B:4287:TYR:HA	2:B:4290:ILE:HD12	1.99	0.45
2:C:2447:LYS:HD3	2:C:2447:LYS:HA	1.80	0.45
2:D:1014:GLN:HB3	2:D:1027:ARG:HH21	1.81	0.45
2:D:3067:ASP:O	2:D:3071:THR:HG23	2.17	0.45
2:D:3184:TYR:HB3	2:D:3192:ARG:NH2	2.27	0.45
1:I:133:GLY:O	2:A:3298:ARG:HG2	2.17	0.45
2:A:419:ILE:HD13	2:A:492:GLU:HG3	1.97	0.45
2:A:1300:MET:HA	2:A:1300:MET:HE3	1.98	0.45
2:A:4277:LYS:HD3	2:A:4277:LYS:HA	1.75	0.45
2:A:4609:LYS:HE3	2:A:4615:LEU:HD13	1.99	0.45
3:F:3:VAL:HG21	3:F:59:GLY:HA2	1.98	0.45
2:B:314:LEU:HD11	2:B:372:LEU:HD13	1.99	0.45
2:B:318:ASP:OD1	2:B:319:LYS:N	2.45	0.45
2:B:527:LYS:HE2	2:B:527:LYS:HB2	1.82	0.45
2:B:989:THR:HG22	2:B:992:GLN:HG2	1.98	0.45
2:B:2447:LYS:HE2	2:B:2864:GLY:HA3	1.99	0.45
2:B:2525:LEU:HG	2:B:2569:ILE:HD13	1.98	0.45
2:B:2620:TYR:HB2	2:B:2627:TRP:HD1	1.82	0.45
2:B:4242:ARG:HH22	2:B:4249:ARG:NH1	2.15	0.45
2:C:910:ASP:OD1	2:C:911:ASN:N	2.50	0.45
2:C:3171:LEU:O	2:C:3210:SER:HA	2.17	0.45
2:C:3276:LEU:O	2:C:3280:ILE:HG12	2.17	0.45
2:D:227:TYR:CG	2:D:352:SER:HB2	2.52	0.45
2:D:1104:GLU:OE1	2:D:1225:LYS:NZ	2.44	0.45
2:D:2857:LYS:O	2:D:2861:GLU:OE1	2.35	0.45
2:D:2946:GLY:HA3	2:D:2954:PHE:CZ	2.51	0.45
2:D:3107:SER:O	2:D:3111:HIS:HD2	2.00	0.45
2:D:3184:TYR:CE2	2:D:3197:LEU:HB3	2.52	0.45
2:D:3302:PHE:C	2:D:3305:PRO:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2703:PRO:HB2	2:A:2854:LYS:HE2	1.99	0.45
3:G:3:VAL:HG21	3:G:59:GLY:HA2	1.98	0.45
1:K:68:GLU:O	1:K:71:THR:OG1	2.33	0.45
2:B:3067:ASP:O	2:B:3071:THR:HG23	2.17	0.45
2:B:3302:PHE:C	2:B:3305:PRO:HD2	2.42	0.45
2:B:3664:LEU:O	2:B:3668:ILE:HG13	2.17	0.45
2:B:4116:GLN:HA	2:B:4119:LEU:HD12	1.98	0.45
2:C:218:SER:HB3	2:C:286:GLY:HA3	1.97	0.45
2:C:314:LEU:HD11	2:C:372:LEU:HD13	1.99	0.45
2:C:989:THR:HG22	2:C:992:GLN:HG2	1.98	0.45
2:C:3107:SER:O	2:C:3111:HIS:HD2	2.00	0.45
2:C:3148:VAL:HA	2:C:3151:GLN:HG3	1.99	0.45
2:C:3253:GLY:O	2:C:3257:ASN:HB3	2.16	0.45
2:C:4117:THR:O	2:C:4120:GLU:HG3	2.16	0.45
2:D:2447:LYS:HE2	2:D:2864:GLY:HA3	1.99	0.45
2:D:2821:TYR:CE2	2:D:2823:PRO:HG3	2.51	0.45
2:D:3649:ALA:C	2:D:3652:PRO:HD2	2.42	0.45
2:D:3830:LEU:HB3	2:D:3833:ASP:OD1	2.17	0.45
2:D:4279:MET:HE2	2:D:4279:MET:HB2	1.81	0.45
1:I:40:LEU:HD11	2:A:3596:LYS:HB3	1.99	0.44
2:A:1967:SER:O	2:A:1972:GLN:NE2	2.41	0.44
2:A:2715:GLU:OE1	2:A:2715:GLU:N	2.44	0.44
2:A:3171:LEU:O	2:A:3210:SER:HA	2.17	0.44
2:A:3184:TYR:CE2	2:A:3197:LEU:HB3	2.52	0.44
2:A:4116:GLN:HA	2:A:4119:LEU:HD12	1.98	0.44
2:A:4649:VAL:O	2:A:4653:VAL:HG23	2.17	0.44
3:E:3:VAL:HG21	3:E:59:GLY:HA2	1.98	0.44
1:K:19:LEU:HD11	2:C:3595:ARG:HH21	1.82	0.44
2:B:227:TYR:CG	2:B:352:SER:HB2	2.52	0.44
2:B:3187:LYS:O	2:B:3191:GLU:HB2	2.17	0.44
2:C:2782:MET:HB2	2:C:2782:MET:HE2	1.82	0.44
2:C:3200:ASN:HB3	2:C:3203:ASP:HB2	2.00	0.44
2:C:3302:PHE:C	2:C:3305:PRO:HD2	2.42	0.44
2:D:2176:VAL:HG22	2:D:2220:TYR:CZ	2.53	0.44
2:D:4287:TYR:HA	2:D:4290:ILE:HD12	1.99	0.44
2:D:4609:LYS:HE3	2:D:4615:LEU:HD13	1.99	0.44
1:I:45:THR:HG22	2:A:3817:LEU:HD23	1.99	0.44
2:A:836:HIS:ND1	2:A:841:LYS:HE3	2.32	0.44
2:A:910:ASP:OD1	2:A:911:ASN:N	2.50	0.44
2:A:2757:MET:N	2:A:2757:MET:SD	2.91	0.44
2:A:2785:TRP:CD1	2:A:2905:ARG:HH22	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3067:ASP:O	2:A:3071:THR:HG23	2.17	0.44
2:A:3184:TYR:HB3	2:A:3192:ARG:NH2	2.27	0.44
2:A:4949:TRP:HB3	2:A:4952:PHE:HD2	1.82	0.44
2:B:678:MET:HB2	2:B:754:VAL:HG22	1.98	0.44
2:B:2961:LYS:HB2	2:B:2965:LYS:HZ3	1.82	0.44
2:B:3812:ASN:HA	2:B:3815:GLU:CD	2.42	0.44
2:B:4858:LEU:HD23	2:B:4861:ILE:HD12	1.98	0.44
2:C:1979:PHE:HE1	2:C:1988:CYS:HB3	1.82	0.44
2:C:2715:GLU:OE1	2:C:2715:GLU:N	2.44	0.44
2:C:3184:TYR:CE2	2:C:3197:LEU:HB3	2.52	0.44
2:C:4858:LEU:HD23	2:C:4861:ILE:HD12	1.98	0.44
2:D:314:LEU:HD11	2:D:372:LEU:HD13	1.99	0.44
2:D:890:HIS:O	2:D:894:VAL:HG13	2.18	0.44
2:D:3187:LYS:O	2:D:3191:GLU:HB2	2.17	0.44
2:D:3664:LEU:O	2:D:3668:ILE:HG13	2.17	0.44
2:D:4949:TRP:HB3	2:D:4952:PHE:HD2	1.82	0.44
2:A:194:LEU:HD11	2:A:201:LEU:HB3	1.98	0.44
2:A:2377:GLU:O	2:A:2381:THR:N	2.50	0.44
2:A:2620:TYR:HB2	2:A:2627:TRP:HD1	1.82	0.44
2:A:3127:GLN:HG3	2:A:3183:ILE:HB	1.98	0.44
2:A:3253:GLY:O	2:A:3257:ASN:HB3	2.16	0.44
2:B:1964:GLU:OE2	2:B:1975:MET:HE3	2.17	0.44
2:B:2222:LEU:HD11	2:B:2301:PHE:CZ	2.52	0.44
2:B:3122:ILE:O	2:B:3127:GLN:HG2	2.18	0.44
2:B:3240:PRO:HG3	2:B:3299:LEU:HG	2.00	0.44
2:B:3649:ALA:C	2:B:3652:PRO:HD2	2.42	0.44
2:B:3830:LEU:HB3	2:B:3833:ASP:OD1	2.18	0.44
2:B:4753:LEU:HD23	2:C:4773:LEU:HD13	1.99	0.44
2:C:877:HIS:O	2:C:880:ARG:HG3	2.18	0.44
2:C:1118:SER:HB2	2:C:1204:VAL:HG11	1.98	0.44
2:C:2176:VAL:HG22	2:C:2220:TYR:CZ	2.53	0.44
2:C:2525:LEU:HG	2:C:2569:ILE:HD13	1.98	0.44
2:D:483:LYS:HE2	2:D:483:LYS:HB2	1.68	0.44
2:A:996:VAL:HG13	2:A:1050:LEU:HD22	1.97	0.44
2:A:1852:LYS:NZ	2:A:2054:LYS:HD2	2.32	0.44
2:A:2204:CYS:SG	2:A:2214:MET:HG3	2.58	0.44
2:A:3068:LEU:O	2:A:3071:THR:OG1	2.27	0.44
2:A:4287:TYR:HA	2:A:4290:ILE:HD12	1.99	0.44
3:H:3:VAL:HG21	3:H:59:GLY:HA2	1.98	0.44
2:B:1118:SER:HB2	2:B:1204:VAL:HG11	1.98	0.44
2:B:1694:MET:HE2	2:B:1694:MET:HB2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3200:ASN:HB3	2:B:3203:ASP:HB2	2.00	0.44
2:C:1512:ASP:OD2	2:C:1515:SER:OG	2.26	0.44
2:C:1939:ASN:C	2:C:1939:ASN:HD22	2.25	0.44
2:C:4269:LYS:HA	2:C:4272:LYS:HE2	1.99	0.44
2:C:4649:VAL:O	2:C:4653:VAL:HG23	2.17	0.44
2:D:2831:VAL:HB	2:D:2894:LYS:CE	2.47	0.44
2:D:3171:LEU:O	2:D:3210:SER:HA	2.17	0.44
2:D:3200:ASN:HB3	2:D:3203:ASP:HB2	2.00	0.44
2:D:4117:THR:O	2:D:4120:GLU:HG3	2.17	0.44
2:D:4649:VAL:O	2:D:4653:VAL:HG23	2.17	0.44
2:A:227:TYR:CG	2:A:352:SER:HB2	2.52	0.44
2:A:874:LEU:HB3	2:A:879:GLU:OE2	2.18	0.44
2:A:877:HIS:O	2:A:880:ARG:HG3	2.18	0.44
2:A:1100:ARG:HB3	2:A:1236:TYR:CD2	2.53	0.44
2:A:3830:LEU:HB3	2:A:3833:ASP:OD1	2.17	0.44
2:C:836:HIS:ND1	2:C:841:LYS:HE3	2.32	0.44
2:C:2757:MET:N	2:C:2757:MET:SD	2.91	0.44
2:C:4511:PHE:HZ	2:C:4746:ILE:HG21	1.83	0.44
2:D:1564:MET:CE	2:D:1565:PRO:HD2	2.48	0.44
2:D:1964:GLU:OE2	2:D:1975:MET:HE3	2.17	0.44
2:D:3122:ILE:O	2:D:3127:GLN:HG2	2.18	0.44
2:D:3744:ILE:O	2:D:3747:SER:OG	2.31	0.44
2:D:4093:ASP:OD1	2:D:4094:ILE:HD12	2.18	0.44
2:A:655:MET:HE1	2:A:836:HIS:CD2	2.53	0.44
2:A:2176:VAL:HG22	2:A:2220:TYR:CZ	2.53	0.44
2:A:3649:ALA:C	2:A:3652:PRO:HD2	2.42	0.44
3:G:78:THR:O	3:G:81:VAL:HG12	2.17	0.44
1:J:42:GLN:HE21	2:B:1957:LEU:HD21	1.82	0.44
1:L:126:ILE:O	1:L:130:ASP:N	2.48	0.44
1:K:121:GLU:O	1:K:124:GLU:HB2	2.18	0.44
2:B:1852:LYS:NZ	2:B:2054:LYS:HD2	2.32	0.44
2:B:2176:VAL:HG22	2:B:2220:TYR:CZ	2.53	0.44
2:B:2377:GLU:O	2:B:2381:THR:N	2.50	0.44
2:B:2592:LEU:HD22	2:B:2606:PRO:HB3	1.98	0.44
2:B:4649:VAL:O	2:B:4653:VAL:HG23	2.17	0.44
2:B:4798:ASP:OD1	2:B:4798:ASP:N	2.51	0.44
2:C:194:LEU:HD11	2:C:201:LEU:HB3	1.98	0.44
2:C:1852:LYS:NZ	2:C:2054:LYS:HD2	2.32	0.44
2:C:2377:GLU:O	2:C:2381:THR:N	2.50	0.44
2:C:3067:ASP:O	2:C:3071:THR:HG23	2.17	0.44
2:C:3812:ASN:HA	2:C:3815:GLU:CD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:655:MET:HE1	2:D:836:HIS:CD2	2.53	0.44
2:D:910:ASP:OD1	2:D:911:ASN:N	2.50	0.44
2:D:949:HIS:O	2:D:1065:GLU:N	2.51	0.44
2:D:2347:MET:O	2:D:2351:ILE:HG12	2.17	0.44
2:D:3127:GLN:HG3	2:D:3183:ILE:HB	1.98	0.44
2:D:4511:PHE:HZ	2:D:4746:ILE:HG21	1.83	0.44
2:D:4798:ASP:OD1	2:D:4798:ASP:N	2.51	0.44
2:A:3200:ASN:HB3	2:A:3203:ASP:HB2	2.00	0.44
2:A:3955:GLN:HE21	2:A:3972:MET:HG2	1.83	0.44
1:L:61:ASN:ND2	1:L:63:THR:O	2.50	0.44
2:B:1564:MET:CE	2:B:1565:PRO:HD2	2.48	0.44
2:B:2383:HIS:CG	2:B:2458:ALA:HB2	2.53	0.44
2:B:2426:LEU:HB2	2:B:2427:ILE:HD12	1.99	0.44
2:B:4093:ASP:OD1	2:B:4094:ILE:HD12	2.18	0.44
2:B:4511:PHE:HZ	2:B:4746:ILE:HG21	1.83	0.44
2:C:21:VAL:HB	2:C:36:CYS:SG	2.58	0.44
2:C:2426:LEU:HB2	2:C:2427:ILE:HD12	1.99	0.44
2:D:1100:ARG:HB3	2:D:1236:TYR:CD2	2.53	0.44
2:D:1979:PHE:HE1	2:D:1988:CYS:HB3	1.82	0.44
2:D:2222:LEU:HD11	2:D:2301:PHE:CZ	2.52	0.44
2:A:515:ALA:HB2	2:A:523:GLY:HA3	2.00	0.44
2:A:2222:LEU:HD23	2:A:2222:LEU:HA	1.88	0.44
2:A:2447:LYS:HE2	2:A:2864:GLY:HA3	1.99	0.44
2:A:2857:LYS:O	2:A:2861:GLU:OE1	2.34	0.44
2:A:3122:ILE:O	2:A:3127:GLN:HG2	2.18	0.44
2:A:3246:MET:HG2	2:A:3309:LYS:HZ2	1.81	0.44
2:A:4242:ARG:HH22	2:A:4249:ARG:NH1	2.15	0.44
2:A:4707:MET:HA	2:D:4252:ILE:HG21	2.00	0.44
1:L:121:GLU:O	1:L:124:GLU:HB2	2.18	0.44
1:K:76:LYS:HB2	1:K:78:LYS:HZ2	1.82	0.44
2:B:903:GLN:H	2:B:913:ARG:NE	2.16	0.44
2:B:3955:GLN:HE21	2:B:3972:MET:HG2	1.83	0.44
2:B:4257:ARG:O	2:B:4261:LEU:HG	2.17	0.44
2:C:887:GLU:O	2:C:891:GLU:HG2	2.17	0.44
2:C:2844:MET:SD	2:C:2888:LYS:NZ	2.91	0.44
2:C:3163:ALA:HB1	2:C:3245:TYR:CD1	2.52	0.44
2:C:3955:GLN:HE21	2:C:3972:MET:HG2	1.83	0.44
2:D:836:HIS:ND1	2:D:841:LYS:HE3	2.32	0.44
2:D:2620:TYR:HB2	2:D:2627:TRP:HD1	1.82	0.44
1:I:121:GLU:O	1:I:124:GLU:HB2	2.18	0.44
2:A:1039:ASP:C	2:A:1043:LYS:HZ2	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2926:LEU:HD23	2:A:2929:LEU:HD12	2.00	0.44
2:A:3240:PRO:HG3	2:A:3299:LEU:HG	2.00	0.44
2:A:4591:TYR:CD2	2:D:4287:TYR:HE1	2.36	0.44
2:A:4726:MET:HE3	2:A:4729:SER:HB2	2.00	0.44
3:G:50:ARG:HH21	3:G:53:LYS:NZ	2.16	0.44
2:B:836:HIS:ND1	2:B:841:LYS:HE3	2.33	0.44
2:B:874:LEU:HB3	2:B:879:GLU:OE2	2.18	0.44
2:B:1100:ARG:HB3	2:B:1236:TYR:CD2	2.53	0.44
2:B:2347:MET:O	2:B:2351:ILE:HG12	2.17	0.44
2:B:3171:LEU:O	2:B:3210:SER:HA	2.18	0.44
2:C:637:LEU:HD22	2:C:1679:HIS:CD2	2.53	0.44
2:C:948:CYS:HA	2:C:1067:PRO:HD3	2.00	0.44
2:C:1100:ARG:HB3	2:C:1236:TYR:CD2	2.53	0.44
2:C:1283:LEU:HB2	2:C:1555:PHE:HB2	2.00	0.44
2:C:2620:TYR:HB2	2:C:2627:TRP:HD1	1.82	0.44
2:C:4237:SER:N	2:C:4240:THR:OG1	2.51	0.44
2:C:4731:LEU:HD23	2:C:4734:TYR:HD2	1.83	0.44
2:D:675:TYR:HB3	2:D:822:CYS:SG	2.58	0.44
2:D:874:LEU:HB3	2:D:879:GLU:OE2	2.18	0.44
2:D:948:CYS:HA	2:D:1067:PRO:HD3	2.00	0.44
2:D:1433:PHE:O	2:D:1500:ARG:NH1	2.51	0.44
2:D:1852:LYS:NZ	2:D:2054:LYS:HD2	2.32	0.44
2:D:1939:ASN:C	2:D:1939:ASN:HD22	2.25	0.44
2:D:2926:LEU:HD23	2:D:2929:LEU:HD12	2.00	0.44
2:D:3955:GLN:HE21	2:D:3972:MET:HG2	1.83	0.44
2:D:4731:LEU:HD23	2:D:4734:TYR:HD2	1.83	0.44
2:A:890:HIS:O	2:A:894:VAL:HG13	2.18	0.43
2:A:949:HIS:O	2:A:1065:GLU:N	2.51	0.43
2:A:1964:GLU:OE2	2:A:1975:MET:HE3	2.17	0.43
2:A:2222:LEU:HD11	2:A:2301:PHE:CZ	2.52	0.43
2:A:2383:HIS:CG	2:A:2458:ALA:HB2	2.53	0.43
2:A:3292:GLU:O	2:A:3292:GLU:HG2	2.18	0.43
2:A:3589:LYS:HE2	2:A:3589:LYS:HB2	1.74	0.43
2:A:4858:LEU:HD23	2:A:4861:ILE:HD12	1.98	0.43
1:J:121:GLU:O	1:J:124:GLU:HB2	2.18	0.43
2:B:890:HIS:O	2:B:894:VAL:HG13	2.18	0.43
2:B:910:ASP:OD1	2:B:911:ASN:N	2.50	0.43
2:B:1132:GLU:HA	2:B:1146:HIS:CE1	2.53	0.43
2:B:3697:LYS:HA	2:B:3700:HIS:CD2	2.53	0.43
2:C:874:LEU:HB3	2:C:879:GLU:OE2	2.18	0.43
2:C:1433:PHE:O	2:C:1500:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2204:CYS:SG	2:C:2214:MET:HG3	2.58	0.43
2:C:2824:ARG:O	2:C:2824:ARG:HD2	2.18	0.43
2:C:3664:LEU:O	2:C:3668:ILE:HG13	2.17	0.43
2:C:3830:LEU:HB3	2:C:3833:ASP:OD1	2.17	0.43
2:C:4949:TRP:HB3	2:C:4952:PHE:HD2	1.83	0.43
2:D:637:LEU:HD22	2:D:1679:HIS:CD2	2.53	0.43
2:D:678:MET:HB2	2:D:754:VAL:HG22	1.98	0.43
2:D:2377:GLU:O	2:D:2381:THR:N	2.50	0.43
2:D:2757:MET:SD	2:D:2757:MET:N	2.91	0.43
2:D:3188:SER:O	2:D:3192:ARG:HB2	2.18	0.43
2:A:21:VAL:HB	2:A:36:CYS:SG	2.58	0.43
2:A:675:TYR:HB3	2:A:822:CYS:SG	2.58	0.43
2:A:3000:GLU:HA	2:A:3003:MET:HE2	2.00	0.43
2:A:3148:VAL:HA	2:A:3151:GLN:HG3	2.00	0.43
2:A:3302:PHE:C	2:A:3305:PRO:HD2	2.42	0.43
2:A:4093:ASP:OD1	2:A:4094:ILE:HD12	2.18	0.43
2:A:4630:TRP:HE3	2:D:4245:LEU:HD23	1.81	0.43
2:A:4798:ASP:OD1	2:A:4798:ASP:N	2.51	0.43
3:G:83:TYR:OH	2:C:1768:PHE:O	2.24	0.43
2:B:287:SER:HA	2:B:349:MET:HE3	2.00	0.43
2:B:655:MET:HE1	2:B:836:HIS:CD2	2.53	0.43
2:B:877:HIS:O	2:B:880:ARG:HG3	2.18	0.43
2:B:2204:CYS:SG	2:B:2214:MET:HG3	2.58	0.43
2:B:3148:VAL:HA	2:B:3151:GLN:HG3	1.99	0.43
2:C:1564:MET:CE	2:C:1565:PRO:HD2	2.48	0.43
2:C:2062:ILE:HG21	2:C:2087:LEU:HG	1.99	0.43
2:C:3122:ILE:O	2:C:3127:GLN:HG2	2.18	0.43
2:C:3187:LYS:O	2:C:3191:GLU:HB2	2.17	0.43
2:C:4093:ASP:OD1	2:C:4094:ILE:HD12	2.18	0.43
2:D:853:PRO:HG2	2:D:1084:ARG:O	2.18	0.43
2:D:874:LEU:HD23	2:D:879:GLU:HG3	2.00	0.43
2:D:1118:SER:HB2	2:D:1204:VAL:HG11	1.98	0.43
2:D:2204:CYS:SG	2:D:2214:MET:HG3	2.58	0.43
2:D:2646:TRP:CZ3	2:D:2928:GLN:HG3	2.54	0.43
2:D:2703:PRO:HB2	2:D:2854:LYS:HE2	1.99	0.43
2:D:2828:MET:O	2:D:2894:LYS:NZ	2.42	0.43
1:I:59:ASP:N	1:I:68:GLU:OE2	2.33	0.43
1:I:137:VAL:HG21	2:A:3587:TRP:CH2	2.53	0.43
2:A:2592:LEU:HD22	2:A:2606:PRO:HB3	1.98	0.43
2:A:2646:TRP:CZ3	2:A:2928:GLN:HG3	2.53	0.43
2:A:3946:GLY:O	2:A:3950:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:ILE:O	1:J:130:ASP:N	2.48	0.43
1:L:80:THR:OG1	1:L:83:GLU:OE2	2.32	0.43
2:B:21:VAL:HB	2:B:36:CYS:SG	2.58	0.43
2:B:913:ARG:HA	2:B:913:ARG:HD2	1.74	0.43
2:B:2757:MET:N	2:B:2757:MET:SD	2.91	0.43
2:B:4731:LEU:HD23	2:B:4734:TYR:HD2	1.83	0.43
2:B:4949:TRP:HB3	2:B:4952:PHE:HD2	1.83	0.43
2:C:902:TRP:CD2	2:C:913:ARG:CZ	3.01	0.43
2:C:1132:GLU:HA	2:C:1146:HIS:CE1	2.54	0.43
2:C:2222:LEU:HD11	2:C:2301:PHE:CZ	2.52	0.43
2:C:4277:LYS:HD3	2:C:4277:LYS:HA	1.75	0.43
2:D:877:HIS:O	2:D:880:ARG:HG3	2.18	0.43
2:D:1446:ILE:HG12	2:D:1542:ALA:HB2	2.00	0.43
2:A:1446:ILE:HG12	2:A:1542:ALA:HB2	2.00	0.43
2:A:2000:HIS:O	2:A:2004:MET:HG2	2.18	0.43
2:A:3131:TYR:HE1	2:A:3208:ILE:HB	1.84	0.43
1:L:130:ASP:C	1:L:133:GLY:H	2.26	0.43
1:K:15:GLU:O	1:K:19:LEU:HG	2.19	0.43
2:B:675:TYR:HB3	2:B:822:CYS:SG	2.58	0.43
2:B:1452:GLN:HE22	2:B:1484:ASN:ND2	2.16	0.43
2:B:2150:MET:O	2:B:2156:TYR:OH	2.26	0.43
2:B:2824:ARG:HD2	2:B:2824:ARG:O	2.18	0.43
2:B:3589:LYS:HB2	2:B:3589:LYS:HE2	1.74	0.43
2:C:655:MET:HE1	2:C:836:HIS:CD2	2.53	0.43
2:C:2347:MET:O	2:C:2351:ILE:HG12	2.17	0.43
2:C:2383:HIS:CG	2:C:2458:ALA:HB2	2.53	0.43
2:C:2926:LEU:HD23	2:C:2929:LEU:HD12	2.00	0.43
2:D:2157:GLN:O	2:D:3615:ARG:NH2	2.52	0.43
2:D:3148:VAL:HA	2:D:3151:GLN:HG3	1.99	0.43
1:I:52:MET:HE2	2:A:3603:PHE:HB3	2.00	0.43
2:A:14:LEU:HG	2:A:177:VAL:HA	2.00	0.43
2:A:287:SER:HA	2:A:349:MET:HE3	2.00	0.43
2:A:1132:GLU:HA	2:A:1146:HIS:CE1	2.54	0.43
2:A:4057:HIS:CE1	2:B:4660:PHE:CZ	3.04	0.43
2:A:4630:TRP:CH2	2:D:4248:LEU:HB3	2.54	0.43
2:A:4633:LEU:HD13	2:A:4707:MET:HE1	2.01	0.43
3:H:50:ARG:HH21	3:H:53:LYS:NZ	2.16	0.43
3:H:79:PRO:O	3:H:84:GLY:HA2	2.19	0.43
2:B:897:LYS:HA	2:B:900:LEU:HB2	2.01	0.43
2:B:948:CYS:HA	2:B:1067:PRO:HD3	2.00	0.43
2:B:1039:ASP:OD1	2:B:1042:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2844:MET:SD	2:B:2888:LYS:NZ	2.91	0.43
2:B:3000:GLU:HA	2:B:3003:MET:HE2	2.00	0.43
2:C:648:LEU:HD23	2:C:648:LEU:HA	1.89	0.43
2:C:890:HIS:O	2:C:894:VAL:HG13	2.18	0.43
2:C:1988:CYS:HA	2:C:1989:PRO:HD3	1.87	0.43
2:D:1688:ALA:HA	2:D:1694:MET:HE3	2.01	0.43
2:D:2000:HIS:O	2:D:2004:MET:HG2	2.18	0.43
2:D:4726:MET:HE3	2:D:4729:SER:HB2	2.00	0.43
1:I:130:ASP:C	1:I:133:GLY:H	2.26	0.43
2:A:2926:LEU:HD23	2:A:2926:LEU:HA	1.87	0.43
2:A:3650:GLU:HB2	2:A:3651:PRO:HD3	2.01	0.43
1:J:48:GLU:O	1:J:52:MET:HG2	2.17	0.43
2:B:637:LEU:HD22	2:B:1679:HIS:CD2	2.53	0.43
2:B:2427:ILE:HD13	2:B:2471:PHE:CZ	2.54	0.43
2:B:2926:LEU:HD23	2:B:2929:LEU:HD12	2.00	0.43
2:B:2972:ASP:OD1	2:B:2976:LYS:NZ	2.49	0.43
2:C:483:LYS:HB2	2:C:483:LYS:HE2	1.68	0.43
2:C:897:LYS:HA	2:C:900:LEU:HB2	2.01	0.43
2:C:949:HIS:O	2:C:1065:GLU:N	2.51	0.43
2:C:2646:TRP:CZ3	2:C:2928:GLN:HG3	2.54	0.43
2:D:515:ALA:HB2	2:D:523:GLY:HA3	2.00	0.43
2:D:2689:MET:HE3	2:D:2689:MET:HB3	1.59	0.43
2:D:2785:TRP:HE1	2:D:2905:ARG:HH12	1.67	0.43
2:D:2824:ARG:HD2	2:D:2824:ARG:O	2.18	0.43
2:D:3102:LEU:HD12	2:D:3102:LEU:HA	1.86	0.43
2:D:3240:PRO:HG3	2:D:3299:LEU:HG	2.00	0.43
2:D:4633:LEU:HD13	2:D:4707:MET:HE1	2.01	0.43
2:A:897:LYS:HA	2:A:900:LEU:HB2	2.01	0.43
2:A:3016:ARG:O	2:A:3018:ARG:NE	2.32	0.43
3:F:50:ARG:HH21	3:F:53:LYS:NZ	2.16	0.43
1:K:10:ILE:O	1:K:14:LYS:N	2.38	0.43
2:B:949:HIS:O	2:B:1065:GLU:N	2.51	0.43
2:B:1433:PHE:O	2:B:1500:ARG:NH1	2.51	0.43
2:B:2658:GLU:OE1	2:B:2661:LEU:N	2.37	0.43
2:B:2945:GLY:HA2	2:B:2948:ARG:CZ	2.49	0.43
2:C:675:TYR:HB3	2:C:822:CYS:SG	2.58	0.43
2:C:694:ARG:NH1	2:C:718:VAL:O	2.49	0.43
2:C:968:LYS:HA	2:C:968:LYS:HD2	1.91	0.43
2:C:1183:LEU:HB3	2:C:1189:GLU:OE1	2.19	0.43
2:C:1260:GLN:OE1	2:C:1261:VAL:N	2.52	0.43
2:C:1538:LYS:HD2	2:C:1636:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1724:GLU:HG2	2:C:2165:LEU:HD23	2.00	0.43
2:C:2000:HIS:O	2:C:2004:MET:HG2	2.18	0.43
2:C:2907:PHE:CE2	2:C:2909:ASP:HA	2.54	0.43
2:C:4107:GLU:OE2	2:C:4149:TYR:OH	2.15	0.43
2:D:902:TRP:CD2	2:D:913:ARG:CZ	3.01	0.43
2:D:1436:GLN:H	2:D:1500:ARG:HH12	1.67	0.43
2:D:2222:LEU:HD23	2:D:2222:LEU:HA	1.89	0.43
2:D:3198:PRO:O	2:D:3199:THR:OG1	2.33	0.43
2:D:3697:LYS:HA	2:D:3700:HIS:CD2	2.54	0.43
2:A:483:LYS:HE2	2:A:483:LYS:HB2	1.68	0.43
2:A:637:LEU:HD22	2:A:1679:HIS:CD2	2.53	0.43
2:A:913:ARG:HA	2:A:913:ARG:HD2	1.74	0.43
2:A:1433:PHE:O	2:A:1500:ARG:NH1	2.51	0.43
2:A:1688:ALA:HA	2:A:1694:MET:HE3	2.01	0.43
2:A:1724:GLU:HG2	2:A:2165:LEU:HD23	2.00	0.43
2:A:2436:ILE:HA	2:A:2465:LYS:HE3	2.01	0.43
2:A:3188:SER:O	2:A:3192:ARG:HB2	2.18	0.43
2:A:3697:LYS:HA	2:A:3700:HIS:CD2	2.54	0.43
2:A:4689:LYS:HD2	2:A:4689:LYS:HA	1.82	0.43
3:E:79:PRO:O	3:E:84:GLY:HA2	2.19	0.43
3:F:79:PRO:O	3:F:84:GLY:HA2	2.19	0.43
3:G:79:PRO:O	3:G:84:GLY:HA2	2.19	0.43
1:J:117:LEU:HD23	1:J:118:THR:N	2.34	0.43
1:K:117:LEU:HD23	1:K:118:THR:N	2.34	0.43
2:B:902:TRP:CD2	2:B:913:ARG:CZ	3.01	0.43
2:B:1081:THR:OG1	2:B:1082:GLY:N	2.51	0.43
2:B:1283:LEU:HB2	2:B:1555:PHE:HB2	2.00	0.43
2:B:1538:LYS:HD2	2:B:1636:ASN:ND2	2.34	0.43
2:B:1714:TYR:CE2	2:B:1718:ARG:HD2	2.54	0.43
2:B:4633:LEU:HD13	2:B:4707:MET:HE1	2.01	0.43
2:C:515:ALA:HB2	2:C:523:GLY:HA3	2.00	0.43
2:C:874:LEU:HD23	2:C:879:GLU:HG3	2.01	0.43
2:C:2972:ASP:OD1	2:C:2976:LYS:NZ	2.49	0.43
2:C:3188:SER:O	2:C:3192:ARG:HB2	2.18	0.43
2:C:4943:MET:HE3	2:C:4948:CYS:O	2.19	0.43
2:D:1183:LEU:HB3	2:D:1189:GLU:OE1	2.19	0.43
2:D:1260:GLN:OE1	2:D:1261:VAL:N	2.52	0.43
2:A:902:TRP:CD2	2:A:913:ARG:CZ	3.01	0.43
2:A:1649:GLU:HG2	2:A:1650:LEU:N	2.34	0.43
2:A:2824:ARG:HD2	2:A:2824:ARG:O	2.18	0.43
2:A:2831:VAL:HB	2:A:2894:LYS:CE	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2945:GLY:HA2	2:A:2948:ARG:CZ	2.49	0.43
2:A:3743:THR:HB	2:A:3758:THR:HG21	2.01	0.43
2:A:4237:SER:O	2:A:4240:THR:OG1	2.37	0.43
2:A:4511:PHE:HZ	2:A:4746:ILE:HG21	1.83	0.43
1:J:130:ASP:C	1:J:133:GLY:H	2.26	0.43
1:K:114:GLY:O	1:K:116:LYS:NZ	2.31	0.43
2:B:166:SER:OG	2:B:168:GLN:OE1	2.34	0.43
2:B:1151:HIS:ND1	2:B:1185:ASP:OD1	2.32	0.43
2:B:1183:LEU:HB3	2:B:1189:GLU:OE1	2.19	0.43
2:B:2157:GLN:O	2:B:3615:ARG:NH2	2.52	0.43
2:B:2733:SER:HA	2:B:2736:LYS:HZ3	1.83	0.43
2:B:3188:SER:O	2:B:3192:ARG:HB2	2.18	0.43
2:B:4735:ASN:HB3	2:B:4738:PHE:CD2	2.54	0.43
2:C:940:LEU:HD12	2:C:941:LYS:N	2.34	0.43
2:C:1452:GLN:HE22	2:C:1484:ASN:ND2	2.16	0.43
2:C:2427:ILE:HD13	2:C:2471:PHE:CZ	2.54	0.43
2:C:2945:GLY:HA2	2:C:2948:ARG:CZ	2.49	0.43
2:C:4663:ARG:HA	2:C:4663:ARG:HD2	1.88	0.43
2:D:21:VAL:HB	2:D:36:CYS:SG	2.58	0.43
2:D:940:LEU:HD12	2:D:941:LYS:N	2.34	0.43
2:D:3655:ASP:HB2	2:D:3660:ARG:HE	1.84	0.43
1:I:80:THR:OG1	1:I:83:GLU:OE2	2.32	0.43
1:I:127:ARG:HD3	1:I:127:ARG:HA	1.41	0.43
2:A:1304:LEU:HD23	2:A:1304:LEU:HA	1.90	0.43
2:A:1512:ASP:OD2	2:A:1515:SER:OG	2.26	0.43
2:A:1931:ASP:OD1	2:A:1932:PHE:N	2.52	0.43
2:A:2793:ARG:HD2	2:A:2793:ARG:C	2.44	0.43
3:G:67:MET:HE2	3:G:67:MET:HB3	1.90	0.43
2:B:2062:ILE:HG21	2:B:2087:LEU:HG	2.00	0.43
2:B:3149:GLU:OE2	2:B:3232:PRO:HG2	2.19	0.43
2:B:3292:GLU:O	2:B:3292:GLU:HG2	2.18	0.43
2:B:3946:GLY:O	2:B:3950:VAL:HG23	2.18	0.43
2:B:4726:MET:HE3	2:B:4729:SER:HB2	2.00	0.43
2:C:853:PRO:HG2	2:C:1084:ARG:O	2.18	0.43
2:C:2259:GLU:HB2	2:C:2260:PRO:HD3	2.01	0.43
2:C:2703:PRO:HB2	2:C:2854:LYS:HE2	1.99	0.43
2:C:2733:SER:HA	2:C:2736:LYS:HZ3	1.82	0.43
2:C:3292:GLU:O	2:C:3296:MET:HE2	2.19	0.43
2:C:4726:MET:HE3	2:C:4729:SER:HB2	2.00	0.43
2:D:1714:TYR:CE2	2:D:1718:ARG:HD2	2.54	0.43
2:D:2793:ARG:HD2	2:D:2793:ARG:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2907:PHE:CE2	2:D:2909:ASP:HA	2.54	0.43
1:I:6:THR:O	1:I:10:ILE:HD12	2.19	0.42
2:A:3926:GLY:O	2:A:3927:PRO:C	2.62	0.42
2:A:4731:LEU:HD23	2:A:4734:TYR:HD2	1.83	0.42
1:K:61:ASN:ND2	1:K:63:THR:O	2.50	0.42
2:B:940:LEU:HD12	2:B:941:LYS:N	2.34	0.42
2:B:1107:THR:OG1	2:B:1160:ASP:O	2.26	0.42
2:B:1166:VAL:HG23	2:B:1173:MET:HG2	2.01	0.42
2:B:2232:PRO:C	2:B:2234:MET:H	2.27	0.42
2:B:2259:GLU:HB2	2:B:2260:PRO:HD3	2.01	0.42
2:B:2646:TRP:CZ3	2:B:2928:GLN:HG3	2.53	0.42
2:C:14:LEU:HG	2:C:177:VAL:HA	2.00	0.42
2:C:765:SER:HA	2:C:779:PHE:O	2.19	0.42
2:C:1039:ASP:OD1	2:C:1042:THR:HB	2.18	0.42
2:C:1040:ASP:OD2	2:C:1044:LYS:NZ	2.52	0.42
2:C:1649:GLU:HG2	2:C:1650:LEU:N	2.34	0.42
2:C:2157:GLN:O	2:C:3615:ARG:NH2	2.51	0.42
2:C:3149:GLU:OE2	2:C:3232:PRO:HG2	2.19	0.42
2:C:3697:LYS:HA	2:C:3700:HIS:CD2	2.54	0.42
2:C:4633:LEU:HD13	2:C:4707:MET:HE1	2.01	0.42
2:D:737:ILE:HD13	2:D:1482:ARG:HD3	2.00	0.42
2:D:1132:GLU:HA	2:D:1146:HIS:CE1	2.54	0.42
2:D:2259:GLU:HB2	2:D:2260:PRO:HD3	2.01	0.42
2:D:2436:ILE:HA	2:D:2465:LYS:HE3	2.01	0.42
2:D:2844:MET:SD	2:D:2888:LYS:NZ	2.91	0.42
2:D:2945:GLY:HA2	2:D:2948:ARG:CZ	2.49	0.42
2:D:3292:GLU:HG2	2:D:3292:GLU:O	2.18	0.42
2:D:3946:GLY:O	2:D:3950:VAL:HG23	2.18	0.42
2:D:4735:ASN:HB3	2:D:4738:PHE:CD2	2.54	0.42
2:D:4964:ASP:OD1	2:D:4965:GLN:N	2.52	0.42
2:A:318:ASP:OD1	2:A:319:LYS:N	2.45	0.42
2:A:1039:ASP:OD1	2:A:1042:THR:HB	2.18	0.42
2:A:1166:VAL:HG23	2:A:1173:MET:HG2	2.01	0.42
2:A:1538:LYS:HD2	2:A:1636:ASN:ND2	2.34	0.42
2:A:2259:GLU:HB2	2:A:2260:PRO:HD3	2.01	0.42
2:A:3088:LYS:HG3	2:A:3090:VAL:HG22	2.01	0.42
2:A:3180:ILE:HG23	2:A:3181:TYR:CD1	2.55	0.42
3:F:67:MET:HE2	3:F:67:MET:HB3	1.90	0.42
1:J:15:GLU:O	1:J:19:LEU:HG	2.19	0.42
1:L:19:LEU:HD11	2:D:3595:ARG:HH21	1.84	0.42
1:L:68:GLU:O	1:L:71:THR:OG1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:THR:O	1:K:10:ILE:HD12	2.19	0.42
1:K:36:VAL:O	1:K:39:SER:OG	2.27	0.42
2:B:3180:ILE:HG23	2:B:3181:TYR:CD1	2.54	0.42
2:B:3192:ARG:O	2:B:3197:LEU:HB2	2.20	0.42
2:B:4279:MET:HE2	2:B:4279:MET:HB2	1.80	0.42
2:C:274:LEU:HD23	2:C:274:LEU:HA	1.81	0.42
2:C:1688:ALA:HA	2:C:1694:MET:HE3	2.01	0.42
2:C:1962:THR:HG22	2:C:1966:ARG:HG3	2.02	0.42
2:C:3131:TYR:HE1	2:C:3208:ILE:HB	1.84	0.42
2:C:3134:LEU:HD22	2:C:3162:PHE:CE2	2.54	0.42
2:C:3188:SER:O	2:C:3192:ARG:CB	2.67	0.42
2:C:3946:GLY:O	2:C:3950:VAL:HG23	2.18	0.42
2:D:287:SER:HA	2:D:349:MET:HE3	2.00	0.42
2:D:765:SER:HA	2:D:779:PHE:O	2.19	0.42
2:D:1724:GLU:HG2	2:D:2165:LEU:HD23	2.00	0.42
2:D:2383:HIS:CG	2:D:2458:ALA:HB2	2.53	0.42
2:D:3292:GLU:O	2:D:3296:MET:HE2	2.19	0.42
2:D:3693:ASP:O	2:D:3697:LYS:HG2	2.19	0.42
2:D:4943:MET:HE3	2:D:4948:CYS:O	2.19	0.42
1:I:15:GLU:O	1:I:19:LEU:HG	2.19	0.42
2:A:261:HIS:CE1	2:A:388:GLN:HE22	2.37	0.42
2:A:1183:LEU:HB3	2:A:1189:GLU:OE1	2.19	0.42
2:A:1452:GLN:HE22	2:A:1484:ASN:ND2	2.16	0.42
2:A:1564:MET:CE	2:A:1565:PRO:HD2	2.48	0.42
2:A:1825:PHE:CE1	2:A:1842:ILE:HG12	2.54	0.42
2:A:2062:ILE:HG21	2:A:2087:LEU:HG	2.00	0.42
2:A:2427:ILE:HD13	2:A:2471:PHE:CZ	2.54	0.42
2:A:2785:TRP:NE1	2:A:2905:ARG:HH12	2.17	0.42
2:A:3290:ILE:C	2:A:3292:GLU:H	2.28	0.42
2:A:3655:ASP:HB2	2:A:3660:ARG:HE	1.84	0.42
2:A:4735:ASN:HB3	2:A:4738:PHE:CD2	2.54	0.42
2:A:4809:MET:HB2	2:D:4520:TYR:O	2.19	0.42
2:A:4943:MET:HE3	2:A:4948:CYS:O	2.19	0.42
1:L:89:ALA:HA	1:L:92:VAL:HG22	2.01	0.42
2:B:561:ARG:HG3	2:B:561:ARG:NH1	2.34	0.42
2:B:1446:ILE:HG12	2:B:1542:ALA:HB2	2.00	0.42
2:B:1688:ALA:HA	2:B:1694:MET:HE3	2.01	0.42
2:B:1931:ASP:OD1	2:B:1932:PHE:N	2.52	0.42
2:B:2785:TRP:NE1	2:B:2905:ARG:HH12	2.17	0.42
2:B:3125:ASP:H	2:B:3183:ILE:CD1	2.32	0.42
2:B:3131:TYR:HE1	2:B:3208:ILE:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3171:LEU:C	2:B:3210:SER:HA	2.44	0.42
2:B:3655:ASP:HB2	2:B:3660:ARG:HE	1.84	0.42
2:B:4237:SER:O	2:B:4240:THR:OG1	2.37	0.42
2:C:166:SER:OG	2:C:168:GLN:OE1	2.34	0.42
2:C:603:LYS:HB3	2:C:603:LYS:HE2	1.88	0.42
2:C:712:GLU:HG3	2:C:838:ARG:HB3	2.02	0.42
2:C:1825:PHE:CE1	2:C:1842:ILE:HG12	2.54	0.42
2:C:2086:VAL:HG22	2:C:3687:LEU:HD13	2.01	0.42
2:C:3171:LEU:C	2:C:3210:SER:HA	2.44	0.42
2:C:3240:PRO:HG3	2:C:3299:LEU:HG	2.00	0.42
2:C:3655:ASP:HB2	2:C:3660:ARG:HE	1.84	0.42
2:C:4798:ASP:OD1	2:C:4798:ASP:N	2.51	0.42
2:D:332:ARG:NH1	2:D:364:GLN:OE1	2.52	0.42
2:D:2062:ILE:HG21	2:D:2087:LEU:HG	2.00	0.42
2:D:2741:TRP:HH2	2:D:2752:LYS:HD3	1.84	0.42
2:D:3180:ILE:HG23	2:D:3181:TYR:CD1	2.55	0.42
2:D:3650:GLU:HB2	2:D:3651:PRO:HD3	2.00	0.42
2:D:3743:THR:HB	2:D:3758:THR:HG21	2.01	0.42
2:D:4268:MET:O	2:D:4271:VAL:HG22	2.20	0.42
2:A:1948:MET:HA	2:A:1948:MET:CE	2.50	0.42
2:A:2157:GLN:O	2:A:3615:ARG:NH2	2.52	0.42
2:A:2907:PHE:CE2	2:A:2909:ASP:HA	2.54	0.42
2:A:3125:ASP:H	2:A:3183:ILE:CD1	2.32	0.42
1:L:6:THR:O	1:L:10:ILE:HD12	2.19	0.42
1:L:15:GLU:O	1:L:19:LEU:HG	2.19	0.42
1:L:76:LYS:HB2	1:L:78:LYS:NZ	2.34	0.42
1:K:76:LYS:HB2	1:K:78:LYS:NZ	2.35	0.42
2:B:332:ARG:NH1	2:B:364:GLN:OE1	2.53	0.42
2:B:902:TRP:CE2	2:B:913:ARG:CZ	3.02	0.42
2:B:1512:ASP:OD2	2:B:1515:SER:OG	2.26	0.42
2:B:2907:PHE:CE2	2:B:2909:ASP:HA	2.54	0.42
2:B:3693:ASP:O	2:B:3697:LYS:HG2	2.19	0.42
2:B:3743:THR:HB	2:B:3758:THR:HG21	2.01	0.42
2:B:3955:GLN:NE2	2:B:3972:MET:HG2	2.35	0.42
2:C:902:TRP:CE2	2:C:913:ARG:CZ	3.03	0.42
2:C:2785:TRP:HE1	2:C:2905:ARG:HH12	1.67	0.42
2:C:3292:GLU:O	2:C:3292:GLU:HG2	2.18	0.42
2:D:1039:ASP:OD1	2:D:1042:THR:HB	2.18	0.42
2:D:1825:PHE:CE1	2:D:1842:ILE:HG12	2.54	0.42
2:D:2086:VAL:HG22	2:D:3687:LEU:HD13	2.01	0.42
2:D:2687:SER:HB3	2:D:2690:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2785:TRP:NE1	2:D:2905:ARG:HH12	2.17	0.42
2:D:4277:LYS:HA	2:D:4277:LYS:HD3	1.75	0.42
2:A:940:LEU:HD12	2:A:941:LYS:N	2.34	0.42
2:A:948:CYS:HA	2:A:1067:PRO:HD3	2.00	0.42
2:A:1714:TYR:CE2	2:A:1718:ARG:HD2	2.54	0.42
2:A:2704:GLN:HA	2:A:2705:PRO:HD3	1.91	0.42
2:A:3192:ARG:O	2:A:3197:LEU:HB2	2.20	0.42
2:A:4279:MET:HE2	2:A:4279:MET:HB2	1.80	0.42
1:J:145:MET:HE2	2:B:3588:HIS:CD2	2.55	0.42
2:B:261:HIS:CE1	2:B:388:GLN:HE22	2.37	0.42
2:B:712:GLU:HG3	2:B:838:ARG:HB3	2.02	0.42
2:B:874:LEU:HD23	2:B:879:GLU:HG3	2.01	0.42
2:C:332:ARG:NH1	2:C:364:GLN:OE1	2.52	0.42
2:C:737:ILE:HD13	2:C:1482:ARG:HD3	2.00	0.42
2:C:903:GLN:H	2:C:913:ARG:NE	2.16	0.42
2:C:913:ARG:HA	2:C:913:ARG:HD2	1.74	0.42
2:C:2828:MET:O	2:C:2894:LYS:NZ	2.42	0.42
2:C:3290:ILE:C	2:C:3292:GLU:H	2.28	0.42
2:C:3693:ASP:O	2:C:3697:LYS:HG2	2.19	0.42
2:C:4689:LYS:HA	2:C:4689:LYS:HD2	1.82	0.42
2:C:4735:ASN:HB3	2:C:4738:PHE:CD2	2.54	0.42
2:C:4964:ASP:OD1	2:C:4965:GLN:N	2.52	0.42
2:D:261:HIS:CE1	2:D:388:GLN:HE22	2.37	0.42
2:D:712:GLU:HG3	2:D:838:ARG:HB3	2.02	0.42
2:D:897:LYS:HA	2:D:900:LEU:HB2	2.00	0.42
2:D:1538:LYS:HD2	2:D:1636:ASN:ND2	2.34	0.42
2:D:1810:VAL:HB	2:D:1817:LEU:HD13	2.01	0.42
2:D:2232:PRO:C	2:D:2234:MET:H	2.27	0.42
2:D:3955:GLN:NE2	2:D:3972:MET:HG2	2.35	0.42
2:A:853:PRO:HG2	2:A:1084:ARG:O	2.18	0.42
2:A:2086:VAL:HG22	2:A:3687:LEU:HD13	2.01	0.42
2:A:3188:SER:O	2:A:3192:ARG:CB	2.67	0.42
2:A:3213:LYS:HA	2:A:3216:GLU:CD	2.45	0.42
2:A:3292:GLU:O	2:A:3296:MET:HE2	2.19	0.42
2:A:3693:ASP:O	2:A:3697:LYS:HG2	2.19	0.42
2:A:3955:GLN:NE2	2:A:3972:MET:HG2	2.35	0.42
2:A:4183:LYS:HG3	2:A:4184:GLU:HG3	2.01	0.42
1:J:125:MET:HE3	1:J:125:MET:HB3	1.71	0.42
2:B:1260:GLN:OE1	2:B:1261:VAL:N	2.52	0.42
2:B:1649:GLU:HG2	2:B:1650:LEU:N	2.34	0.42
2:B:2000:HIS:O	2:B:2004:MET:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3650:GLU:HB2	2:B:3651:PRO:HD3	2.00	0.42
2:B:3926:GLY:O	2:B:3927:PRO:C	2.62	0.42
2:B:4036:ASP:HB2	2:B:4043:ILE:HD13	2.02	0.42
2:B:4943:MET:HE3	2:B:4948:CYS:O	2.19	0.42
2:B:4964:ASP:OD1	2:B:4965:GLN:N	2.52	0.42
2:C:1220:ASP:O	2:C:1223:THR:OG1	2.37	0.42
2:C:1714:TYR:CE2	2:C:1718:ARG:HD2	2.54	0.42
2:C:1973:ILE:HG13	2:C:3608:LEU:HD11	2.02	0.42
2:C:2687:SER:HB3	2:C:2690:GLU:CD	2.45	0.42
2:C:2793:ARG:HD2	2:C:2793:ARG:C	2.44	0.42
2:C:2831:VAL:HB	2:C:2894:LYS:CE	2.47	0.42
2:C:3009:CYS:O	2:C:3013:VAL:HG23	2.19	0.42
2:C:3743:THR:HB	2:C:3758:THR:HG21	2.01	0.42
2:D:1452:GLN:HE22	2:D:1484:ASN:ND2	2.16	0.42
2:D:1914:CYS:HB3	2:D:2090:ARG:NH2	2.35	0.42
2:D:3290:ILE:C	2:D:3292:GLU:H	2.28	0.42
2:A:902:TRP:CE2	2:A:913:ARG:CZ	3.03	0.42
2:A:1283:LEU:HB2	2:A:1555:PHE:HB2	2.00	0.42
2:A:1436:GLN:H	2:A:1500:ARG:HH12	1.67	0.42
2:A:1810:VAL:HB	2:A:1817:LEU:HD13	2.01	0.42
2:A:1914:CYS:HB3	2:A:2090:ARG:NH2	2.35	0.42
2:A:1979:PHE:CD2	2:A:1996:LEU:HD23	2.55	0.42
2:A:3763:ILE:HD11	2:A:3838:ASP:O	2.20	0.42
2:A:4660:PHE:HZ	2:D:4057:HIS:CE1	2.37	0.42
2:B:1979:PHE:CD2	2:B:1996:LEU:HD23	2.55	0.42
2:B:2086:VAL:HG22	2:B:3687:LEU:HD13	2.01	0.42
2:B:2831:VAL:HB	2:B:2894:LYS:CE	2.47	0.42
2:B:3095:ASN:O	2:B:3099:VAL:HG22	2.20	0.42
2:B:3188:SER:O	2:B:3192:ARG:CB	2.67	0.42
2:B:3806:ASN:O	2:B:3810:ARG:HG3	2.20	0.42
2:C:261:HIS:CE1	2:C:388:GLN:HE22	2.37	0.42
2:C:287:SER:HA	2:C:349:MET:HE3	2.00	0.42
2:C:1104:GLU:OE1	2:C:1225:LYS:NZ	2.44	0.42
2:C:1729:MET:CE	2:C:1930:ASP:HB2	2.45	0.42
2:C:3125:ASP:H	2:C:3183:ILE:CD1	2.32	0.42
2:C:3192:ARG:O	2:C:3197:LEU:HB2	2.20	0.42
2:C:3806:ASN:O	2:C:3810:ARG:HG3	2.20	0.42
2:D:3926:GLY:O	2:D:3927:PRO:C	2.62	0.42
2:D:4183:LYS:HG3	2:D:4184:GLU:HG3	2.01	0.42
2:A:50:GLU:OE2	2:A:61:ASP:N	2.48	0.42
2:A:737:ILE:HD13	2:A:1482:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:877:HIS:CE1	2:A:878:LEU:HG	2.55	0.42
2:A:3806:ASN:O	2:A:3810:ARG:HG3	2.20	0.42
1:J:89:ALA:HA	1:J:92:VAL:HG22	2.01	0.42
1:K:127:ARG:NH1	1:K:135:GLY:N	2.55	0.42
2:B:50:GLU:OE2	2:B:61:ASP:N	2.48	0.42
2:B:515:ALA:HB2	2:B:523:GLY:HA3	2.00	0.42
2:B:853:PRO:HG2	2:B:1084:ARG:O	2.18	0.42
2:B:877:HIS:CE1	2:B:878:LEU:HG	2.55	0.42
2:B:1220:ASP:O	2:B:1223:THR:OG1	2.37	0.42
2:B:1729:MET:CE	2:B:1930:ASP:HB2	2.45	0.42
2:B:1810:VAL:HB	2:B:1817:LEU:HD13	2.01	0.42
2:B:2793:ARG:HD2	2:B:2793:ARG:C	2.44	0.42
2:C:756:SER:HB2	2:C:769:ARG:HB3	2.02	0.42
2:C:1166:VAL:HG23	2:C:1173:MET:HG2	2.01	0.42
2:C:1446:ILE:HG12	2:C:1542:ALA:HB2	2.00	0.42
2:C:1914:CYS:HB3	2:C:2090:ARG:NH2	2.35	0.42
2:C:2436:ILE:HA	2:C:2465:LYS:HE3	2.01	0.42
2:C:3088:LYS:HG3	2:C:3090:VAL:HG22	2.01	0.42
2:C:3095:ASN:O	2:C:3099:VAL:HG22	2.20	0.42
2:D:436:LEU:HD23	2:D:436:LEU:HA	1.81	0.42
2:D:1979:PHE:CD2	2:D:1996:LEU:HD23	2.55	0.42
2:D:3124:GLU:C	2:D:3126:VAL:H	2.28	0.42
2:D:3134:LEU:HD22	2:D:3162:PHE:CE2	2.54	0.42
2:D:4743:LEU:O	2:D:4746:ILE:HG12	2.20	0.42
2:A:163:HIS:HB2	2:A:182:ILE:HG13	2.02	0.42
2:A:527:LYS:HE2	2:A:527:LYS:HB2	1.82	0.42
2:A:756:SER:HB2	2:A:769:ARG:HB3	2.02	0.42
2:A:1260:GLN:OE1	2:A:1261:VAL:N	2.52	0.42
2:A:1962:THR:HG22	2:A:1966:ARG:HG3	2.02	0.42
2:A:1973:ILE:HG13	2:A:3608:LEU:HD11	2.02	0.42
2:A:2447:LYS:HA	2:A:2447:LYS:HD3	1.80	0.42
2:A:2508:SER:HB3	2:A:2560:SER:HB3	2.02	0.42
2:A:3149:GLU:OE2	2:A:3232:PRO:HG2	2.19	0.42
1:L:117:LEU:HD23	1:L:118:THR:N	2.34	0.42
1:K:130:ASP:C	1:K:133:GLY:H	2.26	0.42
2:B:491:GLU:OE2	2:B:546:LYS:NZ	2.47	0.42
2:B:1724:GLU:HG2	2:B:2165:LEU:HD23	2.00	0.42
2:B:2772:ARG:HG3	2:B:2776:LYS:HZ2	1.85	0.42
2:B:3017:HIS:O	2:B:3092:GLN:NE2	2.53	0.42
2:B:3763:ILE:HD11	2:B:3838:ASP:O	2.20	0.42
2:B:3975:GLN:O	2:B:3979:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:680:ASP:O	2:C:751:THR:HG23	2.20	0.42
2:C:1931:ASP:OD1	2:C:1932:PHE:N	2.52	0.42
2:C:1948:MET:HA	2:C:1948:MET:CE	2.50	0.42
2:C:2379:ASP:OD2	2:C:2380:ASP:N	2.53	0.42
2:C:2741:TRP:HH2	2:C:2752:LYS:HD3	1.84	0.42
2:C:2785:TRP:NE1	2:C:2905:ARG:HH12	2.18	0.42
2:C:3000:GLU:HA	2:C:3003:MET:HE2	2.00	0.42
2:C:3145:SER:H	2:C:3148:VAL:HB	1.85	0.42
2:C:3955:GLN:NE2	2:C:3972:MET:HG2	2.35	0.42
2:C:3975:GLN:O	2:C:3979:VAL:HG23	2.20	0.42
2:C:4240:THR:HG22	2:C:4308:ILE:HD13	2.02	0.42
2:D:680:ASP:O	2:D:751:THR:HG23	2.20	0.42
2:D:877:HIS:CE1	2:D:878:LEU:HG	2.55	0.42
2:D:1081:THR:OG1	2:D:1082:GLY:N	2.51	0.42
2:D:1649:GLU:HG2	2:D:1650:LEU:N	2.34	0.42
2:D:3125:ASP:H	2:D:3183:ILE:CD1	2.32	0.42
2:D:3149:GLU:OE2	2:D:3232:PRO:HG2	2.19	0.42
1:I:89:ALA:HA	1:I:92:VAL:HG22	2.01	0.42
2:A:1914:CYS:O	2:A:1918:VAL:HG23	2.20	0.42
2:A:3017:HIS:O	2:A:3092:GLN:NE2	2.53	0.42
2:A:4240:THR:HG22	2:A:4308:ILE:HD13	2.02	0.42
3:E:50:ARG:HH21	3:E:53:LYS:NZ	2.16	0.42
1:J:6:THR:O	1:J:10:ILE:HD12	2.19	0.42
2:B:14:LEU:HG	2:B:177:VAL:HA	2.00	0.42
2:B:896:ASN:O	2:B:899:GLU:HG3	2.20	0.42
2:B:1973:ILE:HG13	2:B:3608:LEU:HD11	2.02	0.42
2:B:2705:PRO:HG3	2:B:2854:LYS:HZ2	1.85	0.42
2:C:1046:ASN:OD1	2:C:1047:LYS:N	2.53	0.42
2:C:2232:PRO:C	2:C:2234:MET:H	2.27	0.42
2:C:3017:HIS:O	2:C:3092:GLN:NE2	2.53	0.42
2:C:3106:SER:OG	2:C:3157:GLU:OE1	2.21	0.42
2:C:3213:LYS:HA	2:C:3216:GLU:CD	2.45	0.42
2:C:3763:ILE:HD11	2:C:3838:ASP:O	2.20	0.42
2:C:4268:MET:O	2:C:4271:VAL:HG22	2.20	0.42
2:D:14:LEU:HG	2:D:177:VAL:HA	2.00	0.42
2:D:896:ASN:O	2:D:899:GLU:HG3	2.20	0.42
2:D:903:GLN:H	2:D:913:ARG:NE	2.16	0.42
2:D:2736:LYS:HD2	2:D:2754:GLN:OE1	2.20	0.42
2:D:2826:ILE:H	2:D:2826:ILE:HD12	1.85	0.42
2:D:2930:ILE:HG23	2:D:3010:LYS:HE2	2.02	0.42
2:D:3009:CYS:O	2:D:3013:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3095:ASN:O	2:D:3099:VAL:HG22	2.20	0.42
1:I:36:VAL:O	1:I:39:SER:OG	2.27	0.41
1:I:116:LYS:HB2	1:I:116:LYS:HE2	1.85	0.41
2:A:399:MET:SD	2:A:399:MET:N	2.92	0.41
2:A:2844:MET:SD	2:A:2888:LYS:NZ	2.91	0.41
2:A:3145:SER:H	2:A:3148:VAL:HB	1.85	0.41
2:A:3592:SER:O	2:A:3596:LYS:HD3	2.20	0.41
2:A:4237:SER:N	2:A:4240:THR:OG1	2.51	0.41
1:K:42:GLN:HE21	2:C:1957:LEU:CD2	2.33	0.41
1:K:64:ILE:HG23	1:K:68:GLU:HB3	2.02	0.41
2:B:680:ASP:O	2:B:751:THR:HG23	2.20	0.41
2:B:737:ILE:HD13	2:B:1482:ARG:HD3	2.00	0.41
2:B:808:HIS:O	2:B:1616:GLY:HA2	2.20	0.41
2:B:1914:CYS:HB3	2:B:2090:ARG:NH2	2.35	0.41
2:B:1962:THR:HG22	2:B:1966:ARG:HG3	2.02	0.41
2:B:2508:SER:HB3	2:B:2560:SER:HB3	2.02	0.41
2:B:2586:GLN:HE22	2:B:2590:ARG:NH2	2.19	0.41
2:B:3009:CYS:O	2:B:3013:VAL:HG23	2.19	0.41
2:B:3088:LYS:HG3	2:B:3090:VAL:HG22	2.02	0.41
2:B:3163:ALA:HB1	2:B:3245:TYR:CD1	2.52	0.41
2:B:3290:ILE:C	2:B:3292:GLU:H	2.28	0.41
2:B:3292:GLU:O	2:B:3296:MET:HE2	2.19	0.41
2:C:808:HIS:O	2:C:1616:GLY:HA2	2.20	0.41
2:C:943:LEU:HD11	2:C:1064:LEU:HD12	2.02	0.41
2:C:1436:GLN:H	2:C:1500:ARG:HH12	1.67	0.41
2:C:1810:VAL:HB	2:C:1817:LEU:HD13	2.01	0.41
2:C:2153:LYS:HD3	2:C:2153:LYS:HA	1.82	0.41
2:C:2736:LYS:HD2	2:C:2754:GLN:OE1	2.20	0.41
2:C:3001:LYS:NZ	2:C:3041:ASP:OD2	2.33	0.41
2:C:3926:GLY:O	2:C:3927:PRO:C	2.62	0.41
2:C:4183:LYS:HG3	2:C:4184:GLU:HG3	2.01	0.41
2:D:561:ARG:HG3	2:D:561:ARG:NH1	2.34	0.41
2:D:643:LEU:O	2:D:645:GLN:NE2	2.53	0.41
2:D:902:TRP:CE2	2:D:913:ARG:CZ	3.03	0.41
2:D:1046:ASN:OD1	2:D:1047:LYS:N	2.53	0.41
2:D:1283:LEU:HB2	2:D:1555:PHE:HB2	2.00	0.41
2:D:1948:MET:HA	2:D:1948:MET:CE	2.50	0.41
2:D:2427:ILE:HD13	2:D:2471:PHE:CZ	2.54	0.41
2:D:2508:SER:HB3	2:D:2560:SER:HB3	2.02	0.41
2:D:3188:SER:O	2:D:3192:ARG:CB	2.67	0.41
2:D:3806:ASN:O	2:D:3810:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:LYS:HB2	1:I:78:LYS:NZ	2.35	0.41
1:I:123:ASP:HA	1:I:126:ILE:HG23	2.02	0.41
2:A:2785:TRP:HE1	2:A:2905:ARG:HH12	1.67	0.41
2:A:4036:ASP:HB2	2:A:4043:ILE:HD13	2.02	0.41
2:A:4268:MET:O	2:A:4271:VAL:HG22	2.20	0.41
2:A:4743:LEU:O	2:A:4746:ILE:HG12	2.20	0.41
2:A:4964:ASP:OD1	2:A:4965:GLN:N	2.52	0.41
2:B:765:SER:HA	2:B:779:PHE:O	2.19	0.41
2:B:1962:THR:O	2:B:1966:ARG:HG3	2.20	0.41
2:B:2379:ASP:OD2	2:B:2380:ASP:N	2.53	0.41
2:B:2436:ILE:HA	2:B:2465:LYS:HE3	2.01	0.41
2:B:2687:SER:HB3	2:B:2690:GLU:CD	2.45	0.41
2:B:2908:LYS:HE2	2:B:2908:LYS:HB2	1.95	0.41
2:B:2923:TYR:C	2:B:2927:GLN:HE22	2.28	0.41
2:B:3211:LEU:HD21	2:B:3245:TYR:HE2	1.85	0.41
2:B:3906:PHE:HB3	2:B:3967:LEU:HD11	2.02	0.41
2:B:4183:LYS:HG3	2:B:4184:GLU:HG3	2.01	0.41
2:C:399:MET:SD	2:C:399:MET:N	2.92	0.41
2:C:1979:PHE:CD2	2:C:1996:LEU:HD23	2.55	0.41
2:C:2508:SER:HB3	2:C:2560:SER:HB3	2.02	0.41
2:C:3180:ILE:HG23	2:C:3181:TYR:CD1	2.54	0.41
2:C:3650:GLU:HB2	2:C:3651:PRO:HD3	2.00	0.41
2:C:4057:HIS:CE1	2:D:4660:PHE:HZ	2.38	0.41
2:C:4279:MET:HE2	2:C:4279:MET:HB2	1.81	0.41
2:D:808:HIS:O	2:D:1616:GLY:HA2	2.20	0.41
2:D:1220:ASP:O	2:D:1223:THR:OG1	2.37	0.41
2:D:1962:THR:O	2:D:1966:ARG:HG3	2.20	0.41
2:D:2447:LYS:HD3	2:D:2447:LYS:HA	1.80	0.41
2:D:3000:GLU:HA	2:D:3003:MET:HE2	2.00	0.41
2:D:3145:SER:H	2:D:3148:VAL:HB	1.85	0.41
2:D:3192:ARG:O	2:D:3197:LEU:HB2	2.20	0.41
2:D:3592:SER:O	2:D:3596:LYS:HD3	2.20	0.41
2:D:4237:SER:O	2:D:4240:THR:OG1	2.37	0.41
2:A:712:GLU:HG3	2:A:838:ARG:HB3	2.02	0.41
2:A:2687:SER:HB3	2:A:2690:GLU:CD	2.45	0.41
2:A:2736:LYS:HD2	2:A:2754:GLN:OE1	2.20	0.41
2:A:2833:LEU:HB3	2:A:2837:LEU:CD1	2.49	0.41
2:A:2923:TYR:C	2:A:2927:GLN:HE22	2.28	0.41
2:A:3261:ALA:C	2:A:3263:MET:H	2.28	0.41
2:A:3848:GLU:OE1	2:A:3922:GLU:HG3	2.20	0.41
2:B:163:HIS:HB2	2:B:182:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1797:GLU:HA	2:B:1800:LYS:HG2	2.02	0.41
2:B:2741:TRP:HH2	2:B:2752:LYS:HD3	1.84	0.41
2:B:2785:TRP:HE1	2:B:2905:ARG:HH12	1.67	0.41
2:B:3134:LEU:HD22	2:B:3162:PHE:CE2	2.54	0.41
2:B:3246:MET:HG2	2:B:3309:LYS:HZ1	1.85	0.41
2:B:3679:LYS:HE2	2:B:3679:LYS:HB2	1.92	0.41
2:B:3981:MET:HE2	2:B:3981:MET:HB3	1.83	0.41
2:B:4268:MET:O	2:B:4271:VAL:HG22	2.20	0.41
2:C:487:ASN:O	2:C:491:GLU:HG2	2.21	0.41
2:C:896:ASN:O	2:C:899:GLU:HG3	2.20	0.41
2:C:1697:LEU:HD23	2:C:1697:LEU:HA	1.95	0.41
2:C:4130:GLN:HB3	2:C:4131:PRO:HD3	2.02	0.41
2:D:943:LEU:HD11	2:D:1064:LEU:HD12	2.02	0.41
2:D:3017:HIS:O	2:D:3092:GLN:NE2	2.53	0.41
2:D:3651:PRO:HB2	2:D:3652:PRO:HD3	2.03	0.41
2:D:3763:ILE:HD11	2:D:3838:ASP:O	2.20	0.41
1:I:117:LEU:HD23	1:I:118:THR:N	2.34	0.41
2:A:274:LEU:HD23	2:A:274:LEU:HA	1.81	0.41
2:A:874:LEU:HD23	2:A:879:GLU:HG3	2.01	0.41
2:A:943:LEU:HD11	2:A:1064:LEU:HD12	2.02	0.41
2:A:2961:LYS:HB2	2:A:2965:LYS:HZ3	1.85	0.41
2:A:3163:ALA:HB1	2:A:3245:TYR:CD1	2.52	0.41
2:A:4746:ILE:HD11	2:B:4776:VAL:HG21	2.03	0.41
2:A:4753:LEU:HG	2:B:4773:LEU:HD22	2.02	0.41
1:J:51:ASP:CG	2:B:2208:ARG:HH12	2.28	0.41
1:K:89:ALA:HA	1:K:92:VAL:HG22	2.01	0.41
2:B:1039:ASP:C	2:B:1043:LYS:HZ2	2.28	0.41
2:B:1046:ASN:OD1	2:B:1047:LYS:N	2.53	0.41
2:B:1967:SER:O	2:B:1972:GLN:NE2	2.41	0.41
2:B:2344:LEU:HD22	2:B:2434:GLY:HA3	2.02	0.41
2:B:2736:LYS:HD2	2:B:2754:GLN:OE1	2.20	0.41
2:B:2833:LEU:HB3	2:B:2837:LEU:CD1	2.49	0.41
2:B:3145:SER:H	2:B:3148:VAL:HB	1.85	0.41
2:B:3592:SER:O	2:B:3596:LYS:HD3	2.20	0.41
2:B:4743:LEU:O	2:B:4746:ILE:HG12	2.20	0.41
2:C:1592:SER:OG	2:C:1594:VAL:HG12	2.21	0.41
2:C:1797:GLU:HA	2:C:1800:LYS:HG2	2.03	0.41
2:C:2926:LEU:CD1	2:C:3003:MET:HE3	2.50	0.41
2:C:3124:GLU:C	2:C:3126:VAL:H	2.28	0.41
2:D:487:ASN:O	2:D:491:GLU:HG2	2.21	0.41
2:D:1166:VAL:HG23	2:D:1173:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1914:CYS:O	2:D:1918:VAL:HG23	2.20	0.41
2:D:1931:ASP:OD1	2:D:1932:PHE:N	2.52	0.41
2:D:1973:ILE:HG13	2:D:3608:LEU:HD11	2.02	0.41
2:D:3171:LEU:C	2:D:3210:SER:HA	2.44	0.41
2:D:3261:ALA:C	2:D:3263:MET:H	2.28	0.41
2:D:4107:GLU:OE2	2:D:4149:TYR:OH	2.15	0.41
1:I:122:VAL:O	1:I:126:ILE:N	2.43	0.41
2:A:487:ASN:O	2:A:491:GLU:HG2	2.21	0.41
2:A:3124:GLU:C	2:A:3126:VAL:H	2.28	0.41
2:A:3211:LEU:HD21	2:A:3245:TYR:HE2	1.85	0.41
2:A:3679:LYS:HE2	2:A:3679:LYS:HB2	1.92	0.41
2:A:4858:LEU:HD23	2:A:4858:LEU:HA	1.94	0.41
3:F:58:LYS:O	3:F:62:GLU:OE1	2.39	0.41
1:J:123:ASP:HA	1:J:126:ILE:HG23	2.02	0.41
2:B:586:LEU:HD11	2:B:620:CYS:HB2	2.02	0.41
2:B:889:ILE:O	2:B:893:TRP:CE3	2.74	0.41
2:B:1436:GLN:H	2:B:1500:ARG:HH12	1.67	0.41
2:B:2715:GLU:OE1	2:B:2715:GLU:N	2.44	0.41
2:B:2930:ILE:HG23	2:B:3010:LYS:HE2	2.02	0.41
2:B:3744:ILE:O	2:B:3747:SER:OG	2.31	0.41
2:B:4130:GLN:HB3	2:B:4131:PRO:HD3	2.02	0.41
2:C:194:LEU:HD23	2:C:196:TYR:HE1	1.85	0.41
2:C:875:PRO:HA	2:C:876:PRO:HD3	1.94	0.41
2:C:2344:LEU:HD22	2:C:2434:GLY:HA3	2.02	0.41
2:C:3906:PHE:HB3	2:C:3967:LEU:HD11	2.03	0.41
2:D:1758:ARG:HA	2:D:1758:ARG:HD2	1.83	0.41
2:D:2379:ASP:OD2	2:D:2380:ASP:N	2.53	0.41
2:D:2945:GLY:HA2	2:D:2948:ARG:NH2	2.36	0.41
2:A:332:ARG:NH1	2:A:364:GLN:OE1	2.52	0.41
2:A:643:LEU:O	2:A:645:GLN:NE2	2.53	0.41
2:A:1727:VAL:HG11	2:A:1926:VAL:HG21	2.02	0.41
2:A:1962:THR:O	2:A:1966:ARG:HG3	2.20	0.41
2:A:2232:PRO:C	2:A:2234:MET:H	2.27	0.41
2:A:2826:ILE:H	2:A:2826:ILE:HD12	1.85	0.41
2:A:2945:GLY:HA2	2:A:2948:ARG:NH2	2.36	0.41
2:A:4948:CYS:SG	2:A:4950:GLU:HG2	2.61	0.41
3:H:58:LYS:O	3:H:62:GLU:OE1	2.39	0.41
1:L:16:ALA:HA	1:L:19:LEU:HD12	2.03	0.41
1:K:116:LYS:HB2	1:K:116:LYS:HE2	1.85	0.41
2:B:603:LYS:HB3	2:B:603:LYS:HE2	1.88	0.41
2:B:1748:LEU:HD23	2:B:1748:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3213:LYS:HA	2:B:3216:GLU:CD	2.45	0.41
2:B:4649:VAL:HA	2:B:4652:LYS:HE2	2.03	0.41
2:C:877:HIS:CE1	2:C:878:LEU:HG	2.55	0.41
2:C:1585:ARG:O	2:C:1587:HIS:ND1	2.54	0.41
2:C:2824:ARG:CZ	2:D:1502:ASN:HB3	2.50	0.41
2:C:2826:ILE:H	2:C:2826:ILE:HD12	1.85	0.41
2:C:2923:TYR:C	2:C:2927:GLN:HE22	2.28	0.41
2:C:2930:ILE:HG23	2:C:3010:LYS:HE2	2.02	0.41
2:C:3068:LEU:O	2:C:3071:THR:OG1	2.27	0.41
2:C:3592:SER:O	2:C:3596:LYS:HD3	2.20	0.41
2:D:1592:SER:OG	2:D:1594:VAL:HG12	2.21	0.41
2:D:2868:HIS:HB3	2:D:2871:LEU:HD23	2.03	0.41
2:D:2923:TYR:C	2:D:2927:GLN:HE22	2.28	0.41
2:D:3131:TYR:HE1	2:D:3208:ILE:HB	1.84	0.41
2:D:3211:LEU:HD21	2:D:3245:TYR:HE2	1.85	0.41
2:D:4481:TRP:O	2:D:4485:ILE:HG12	2.21	0.41
2:D:4649:VAL:HA	2:D:4652:LYS:HE2	2.03	0.41
2:D:4948:CYS:SG	2:D:4950:GLU:HG2	2.61	0.41
2:A:390:LYS:HD2	2:A:390:LYS:HA	1.86	0.41
2:A:2379:ASP:OD2	2:A:2380:ASP:N	2.53	0.41
2:A:2868:HIS:HB3	2:A:2871:LEU:HD23	2.03	0.41
2:A:2926:LEU:CD1	2:A:3003:MET:HE3	2.50	0.41
2:A:3009:CYS:O	2:A:3013:VAL:HG23	2.19	0.41
2:A:3171:LEU:C	2:A:3210:SER:HA	2.44	0.41
3:E:58:LYS:O	3:E:62:GLU:OE1	2.39	0.41
3:H:43:ARG:HD3	2:D:1766:PRO:HG2	2.02	0.41
2:B:487:ASN:O	2:B:491:GLU:HG2	2.21	0.41
2:B:756:SER:HB2	2:B:769:ARG:HB3	2.02	0.41
2:B:2926:LEU:HD23	2:B:2926:LEU:HA	1.87	0.41
2:B:3124:GLU:C	2:B:3126:VAL:H	2.28	0.41
2:B:3212:GLU:O	2:B:3216:GLU:OE1	2.39	0.41
2:C:659:ILE:HD12	2:C:661:LEU:HD11	2.03	0.41
2:C:972:LEU:HD23	2:C:973:THR:H	1.86	0.41
2:C:1727:VAL:HG11	2:C:1926:VAL:HG21	2.02	0.41
2:C:1911:GLN:OE1	2:C:2090:ARG:NH1	2.54	0.41
2:C:3965:ILE:HG13	2:C:4086:ARG:HH11	1.86	0.41
2:D:491:GLU:OE2	2:D:546:LYS:NZ	2.47	0.41
2:D:1911:GLN:OE1	2:D:2090:ARG:NH1	2.54	0.41
2:D:2106:TYR:OH	2:D:3615:ARG:NH1	2.53	0.41
2:D:3213:LYS:HA	2:D:3216:GLU:CD	2.45	0.41
2:D:3906:PHE:HB3	2:D:3967:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4130:GLN:HB3	2:D:4131:PRO:HD3	2.02	0.41
1:I:64:ILE:HG23	1:I:68:GLU:HB3	2.02	0.41
2:A:694:ARG:NH1	2:A:718:VAL:O	2.49	0.41
2:A:896:ASN:O	2:A:899:GLU:HG3	2.20	0.41
2:A:1046:ASN:OD1	2:A:1047:LYS:N	2.53	0.41
2:A:2408:LEU:HD22	2:A:2413:LYS:HD3	2.03	0.41
2:A:2741:TRP:HH2	2:A:2752:LYS:HD3	1.84	0.41
2:A:2930:ILE:HG23	2:A:3010:LYS:HE2	2.02	0.41
2:A:3651:PRO:HB2	2:A:3652:PRO:HD3	2.03	0.41
2:A:4481:TRP:O	2:A:4485:ILE:HG12	2.21	0.41
2:A:4649:VAL:HA	2:A:4652:LYS:HE2	2.03	0.41
3:G:58:LYS:O	3:G:62:GLU:OE1	2.39	0.41
2:B:643:LEU:O	2:B:645:GLN:NE2	2.53	0.41
2:B:904:TYR:CE1	2:B:916:PRO:HA	2.56	0.41
2:B:972:LEU:HD23	2:B:973:THR:H	1.86	0.41
2:B:1585:ARG:O	2:B:1587:HIS:ND1	2.53	0.41
2:B:2456:MET:SD	2:B:2512:MET:HE1	2.61	0.41
2:B:2593:VAL:HA	2:B:2644:LEU:HD13	2.03	0.41
2:B:3017:HIS:C	2:B:3018:ARG:HD3	2.46	0.41
2:B:3304:GLN:HB3	2:B:3305:PRO:HD3	2.03	0.41
2:C:1744:LYS:NZ	2:C:2002:ASP:OD1	2.54	0.41
2:C:1758:ARG:HA	2:C:1758:ARG:HD2	1.83	0.41
2:C:1962:THR:O	2:C:1966:ARG:HG3	2.20	0.41
2:C:2928:GLN:HA	2:C:2931:ARG:CZ	2.51	0.41
2:C:4649:VAL:HA	2:C:4652:LYS:HE2	2.03	0.41
2:C:4743:LEU:O	2:C:4746:ILE:HG12	2.20	0.41
2:C:4948:CYS:SG	2:C:4950:GLU:HG2	2.61	0.41
2:D:182:ILE:HG13	2:D:182:ILE:O	2.21	0.41
2:D:586:LEU:HD11	2:D:620:CYS:HB2	2.02	0.41
2:D:904:TYR:CE1	2:D:916:PRO:HA	2.56	0.41
2:D:1304:LEU:HD23	2:D:1304:LEU:HA	1.90	0.41
2:D:1421:MET:SD	2:D:1576:LYS:HD2	2.61	0.41
2:D:2833:LEU:HB3	2:D:2837:LEU:CD1	2.48	0.41
2:D:3253:GLY:C	2:D:3255:GLU:N	2.72	0.41
2:D:3924:ILE:HG21	2:D:3935:LEU:HD12	2.03	0.41
2:D:3975:GLN:O	2:D:3979:VAL:HG23	2.20	0.41
2:A:49:LEU:CD1	2:A:194:LEU:HD13	2.51	0.41
2:A:194:LEU:HD23	2:A:196:TYR:HE1	1.85	0.41
2:A:680:ASP:O	2:A:751:THR:HG23	2.20	0.41
2:A:808:HIS:O	2:A:1616:GLY:HA2	2.20	0.41
2:A:889:ILE:O	2:A:893:TRP:CE3	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:972:LEU:HD23	2:A:973:THR:H	1.86	0.41
2:A:1421:MET:SD	2:A:1576:LYS:HD2	2.61	0.41
2:A:1797:GLU:HA	2:A:1800:LYS:HG2	2.03	0.41
2:A:1893:LEU:HD23	2:A:1896:MET:SD	2.60	0.41
2:A:2487:LEU:HA	2:A:2490:VAL:HG22	2.03	0.41
2:A:2586:GLN:HE22	2:A:2590:ARG:NH2	2.19	0.41
2:A:3095:ASN:O	2:A:3099:VAL:HG22	2.20	0.41
2:A:3134:LEU:HD22	2:A:3162:PHE:CE2	2.54	0.41
2:A:3143:SER:O	2:A:3148:VAL:HG11	2.21	0.41
2:A:3965:ILE:HG13	2:A:4086:ARG:HH11	1.86	0.41
2:A:3975:GLN:O	2:A:3979:VAL:HG23	2.20	0.41
2:A:4196:THR:O	2:A:4200:MET:HG3	2.21	0.41
2:A:4914:ASN:HB3	2:A:4917:ASN:ND2	2.36	0.41
3:G:19:LYS:HB2	3:G:19:LYS:HE3	1.84	0.41
1:J:16:ALA:HA	1:J:19:LEU:HD12	2.03	0.41
1:J:76:LYS:HB2	1:J:78:LYS:NZ	2.35	0.41
1:J:116:LYS:HE2	1:J:116:LYS:HB2	1.85	0.41
1:L:64:ILE:HG23	1:L:68:GLU:HB3	2.02	0.41
1:L:122:VAL:O	1:L:126:ILE:N	2.43	0.41
2:B:943:LEU:HD11	2:B:1064:LEU:HD12	2.02	0.41
2:B:1592:SER:OG	2:B:1594:VAL:HG12	2.20	0.41
2:B:1825:PHE:CE1	2:B:1842:ILE:HG12	2.54	0.41
2:B:2253:LEU:HD23	2:B:2253:LEU:HA	1.85	0.41
2:B:2926:LEU:CD1	2:B:3003:MET:HE3	2.50	0.41
2:B:2928:GLN:HA	2:B:2931:ARG:CZ	2.51	0.41
2:B:3261:ALA:C	2:B:3263:MET:H	2.28	0.41
2:B:3310:VAL:HG11	2:B:3319:PHE:CE2	2.56	0.41
2:B:3965:ILE:HG13	2:B:4086:ARG:HH11	1.86	0.41
2:B:4481:TRP:O	2:B:4485:ILE:HG12	2.21	0.41
2:B:4663:ARG:HD2	2:B:4663:ARG:HA	1.89	0.41
2:B:4948:CYS:SG	2:B:4950:GLU:HG2	2.61	0.41
2:C:643:LEU:O	2:C:645:GLN:NE2	2.53	0.41
2:C:2456:MET:SD	2:C:2512:MET:HE1	2.61	0.41
2:C:2945:GLY:HA2	2:C:2948:ARG:NH2	2.36	0.41
2:C:3017:HIS:C	2:C:3018:ARG:HD3	2.46	0.41
2:C:3101:LEU:O	2:C:3104:MET:HB3	2.21	0.41
2:C:3212:GLU:O	2:C:3216:GLU:OE1	2.39	0.41
2:C:3963:SER:OG	2:C:3964:GLN:OE1	2.30	0.41
2:C:4036:ASP:HB2	2:C:4043:ILE:HD13	2.02	0.41
2:C:4914:ASN:HB3	2:C:4917:ASN:ND2	2.36	0.41
2:D:194:LEU:HD23	2:D:196:TYR:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:659:ILE:HD12	2:D:661:LEU:HD11	2.03	0.41
2:D:889:ILE:O	2:D:893:TRP:CE3	2.74	0.41
2:D:1727:VAL:HG11	2:D:1926:VAL:HG21	2.02	0.41
2:D:1893:LEU:HD23	2:D:1896:MET:SD	2.60	0.41
2:D:1988:CYS:HA	2:D:1989:PRO:HD3	1.87	0.41
2:D:2276:SER:OG	2:D:2277:CYS:N	2.54	0.41
2:D:2408:LEU:HD22	2:D:2413:LYS:HD3	2.03	0.41
2:D:2928:GLN:HA	2:D:2931:ARG:CZ	2.51	0.41
2:D:3163:ALA:HB1	2:D:3245:TYR:CD1	2.52	0.41
2:D:4036:ASP:HB2	2:D:4043:ILE:HD13	2.02	0.41
2:D:4041:GLY:HA2	2:D:4080:TYR:HE1	1.86	0.41
2:D:4200:MET:SD	2:D:4923:MET:HE1	2.61	0.41
2:D:4240:THR:HG22	2:D:4308:ILE:HD13	2.02	0.41
2:A:561:ARG:HG3	2:A:561:ARG:NH1	2.34	0.41
2:A:659:ILE:HD12	2:A:661:LEU:HD11	2.03	0.41
2:A:765:SER:HA	2:A:779:PHE:O	2.20	0.41
2:A:844:ARG:HH11	2:A:845:THR:H	1.69	0.41
2:A:1585:ARG:O	2:A:1587:HIS:ND1	2.54	0.41
2:A:1592:SER:OG	2:A:1594:VAL:HG12	2.21	0.41
2:A:1911:GLN:OE1	2:A:2090:ARG:NH1	2.54	0.41
2:A:2497:ARG:NH1	2:A:2881:GLU:OE2	2.53	0.41
2:A:3088:LYS:HA	2:A:3088:LYS:HD3	1.90	0.41
2:A:3191:GLU:HA	2:A:3194:ALA:HB3	2.03	0.41
2:A:4265:LYS:O	2:A:4269:LYS:HG2	2.21	0.41
3:F:19:LYS:HB2	3:F:19:LYS:HE3	1.84	0.41
1:K:16:ALA:HA	1:K:19:LEU:HD12	2.03	0.41
2:B:1948:MET:HA	2:B:1948:MET:CE	2.50	0.41
2:B:4073:ASP:OD2	2:B:4075:ASN:ND2	2.54	0.41
2:C:735:GLY:O	2:C:737:ILE:HD12	2.21	0.41
2:C:889:ILE:O	2:C:893:TRP:CE3	2.74	0.41
2:C:1893:LEU:HD23	2:C:1896:MET:SD	2.60	0.41
2:C:1914:CYS:O	2:C:1918:VAL:HG23	2.20	0.41
2:C:2487:LEU:HA	2:C:2490:VAL:HG22	2.03	0.41
2:C:2586:GLN:HE22	2:C:2590:ARG:NH2	2.19	0.41
2:C:2659:GLN:HG2	2:C:2660:GLU:N	2.36	0.41
2:C:3102:LEU:HD12	2:C:3102:LEU:HA	1.86	0.41
2:C:3651:PRO:HB2	2:C:3652:PRO:HD3	2.03	0.41
2:D:756:SER:HB2	2:D:769:ARG:HB3	2.02	0.41
2:D:2487:LEU:HA	2:D:2490:VAL:HG22	2.03	0.41
2:D:3143:SER:O	2:D:3148:VAL:HG11	2.21	0.41
2:D:3747:SER:OG	2:D:3792:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:ALA:HA	1:I:19:LEU:HD12	2.03	0.40
1:I:37:MET:HG2	1:I:42:GLN:HB2	2.03	0.40
2:A:1220:ASP:O	2:A:1223:THR:OG1	2.37	0.40
2:A:1939:ASN:C	2:A:1939:ASN:HD22	2.25	0.40
2:A:2928:GLN:HA	2:A:2931:ARG:CZ	2.51	0.40
2:A:3924:ILE:HG21	2:A:3935:LEU:HD12	2.03	0.40
2:A:4200:MET:SD	2:A:4923:MET:HE1	2.61	0.40
2:A:4286:SER:O	2:A:4289:SER:OG	2.36	0.40
1:J:64:ILE:HG23	1:J:68:GLU:HB3	2.02	0.40
1:L:37:MET:HG2	1:L:42:GLN:HB2	2.03	0.40
2:B:194:LEU:HD23	2:B:196:TYR:HE1	1.85	0.40
2:B:399:MET:SD	2:B:399:MET:N	2.92	0.40
2:B:810:GLU:N	2:B:810:GLU:OE2	2.54	0.40
2:B:2463:ASP:OD1	2:B:2464:HIS:N	2.55	0.40
2:B:2945:GLY:HA2	2:B:2948:ARG:NH2	2.36	0.40
2:B:3191:GLU:HA	2:B:3194:ALA:HB3	2.03	0.40
2:B:4196:THR:O	2:B:4200:MET:HG3	2.21	0.40
2:B:4265:LYS:O	2:B:4269:LYS:HG2	2.21	0.40
2:C:527:LYS:HE2	2:C:527:LYS:HB2	1.82	0.40
2:C:1011:ARG:HH21	2:C:1014:GLN:CD	2.25	0.40
2:C:2833:LEU:HB3	2:C:2837:LEU:CD1	2.49	0.40
2:C:3261:ALA:C	2:C:3263:MET:H	2.28	0.40
2:C:4502:MET:SD	2:C:4585:PHE:HB3	2.61	0.40
2:D:49:LEU:CD1	2:D:194:LEU:HD13	2.51	0.40
2:D:1968:PRO:O	2:D:1972:GLN:HG3	2.21	0.40
2:D:2463:ASP:OD1	2:D:2464:HIS:N	2.54	0.40
2:D:2592:LEU:HD23	2:D:2592:LEU:HA	1.90	0.40
2:D:2593:VAL:HA	2:D:2644:LEU:HD13	2.03	0.40
2:D:3848:GLU:OE1	2:D:3922:GLU:HG3	2.21	0.40
2:D:4502:MET:SD	2:D:4585:PHE:HB3	2.61	0.40
2:A:648:LEU:HD23	2:A:648:LEU:HA	1.89	0.40
2:A:1176:THR:HG22	2:A:1181:ILE:HG13	2.03	0.40
2:A:1968:PRO:O	2:A:1972:GLN:HG3	2.21	0.40
2:A:2106:TYR:OH	2:A:3615:ARG:NH1	2.53	0.40
2:A:2329:GLU:CD	2:A:2329:GLU:H	2.29	0.40
2:A:2456:MET:SD	2:A:2512:MET:HE1	2.61	0.40
2:A:3906:PHE:HB3	2:A:3967:LEU:HD11	2.02	0.40
1:J:125:MET:HG3	2:B:3584:LYS:HE2	2.02	0.40
1:K:123:ASP:HA	1:K:126:ILE:HG23	2.03	0.40
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.81	0.40
2:B:364:GLN:NE2	2:B:369:GLY:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1421:MET:SD	2:B:1576:LYS:HD2	2.61	0.40
2:B:2447:LYS:HD3	2:B:2447:LYS:HA	1.80	0.40
2:B:2826:ILE:H	2:B:2826:ILE:HD12	1.85	0.40
2:C:49:LEU:CD1	2:C:194:LEU:HD13	2.51	0.40
2:C:1421:MET:SD	2:C:1576:LYS:HD2	2.61	0.40
2:C:1968:PRO:O	2:C:1972:GLN:HG3	2.21	0.40
2:C:2106:TYR:OH	2:C:3615:ARG:NH1	2.53	0.40
2:C:2170:THR:O	2:C:2174:VAL:HG13	2.21	0.40
2:C:3778:LEU:HD13	2:C:3854:PHE:HD1	1.87	0.40
2:C:4167:GLU:O	2:C:4171:GLN:HG2	2.22	0.40
2:D:884:LYS:HA	2:D:887:GLU:CG	2.51	0.40
2:D:920:GLU:O	2:D:924:LEU:N	2.55	0.40
2:D:1797:GLU:HA	2:D:1800:LYS:HG2	2.03	0.40
2:D:2229:LEU:HD11	2:D:2240:LEU:HD22	2.03	0.40
2:D:2344:LEU:HD22	2:D:2434:GLY:HA3	2.02	0.40
2:D:2488:LEU:HD11	2:D:2548:LEU:HD13	2.03	0.40
2:D:3088:LYS:HG3	2:D:3090:VAL:HG22	2.01	0.40
2:D:3101:LEU:O	2:D:3104:MET:HB3	2.21	0.40
2:A:182:ILE:HG13	2:A:182:ILE:O	2.21	0.40
2:A:997:ASP:O	2:A:1001:GLU:OE1	2.40	0.40
2:A:1748:LEU:HD23	2:A:1748:LEU:HA	1.88	0.40
2:A:3101:LEU:O	2:A:3104:MET:HB3	2.21	0.40
2:A:3661:VAL:HG23	2:A:3666:GLN:HG2	2.03	0.40
2:A:4130:GLN:HB3	2:A:4131:PRO:HD3	2.02	0.40
2:B:49:LEU:CD1	2:B:194:LEU:HD13	2.51	0.40
2:B:968:LYS:HA	2:B:968:LYS:HD2	1.91	0.40
2:B:1727:VAL:HG11	2:B:1926:VAL:HG21	2.02	0.40
2:B:1785:ASP:OD1	2:B:1786:ILE:N	2.55	0.40
2:B:1914:CYS:O	2:B:1918:VAL:HG23	2.20	0.40
2:B:2276:SER:OG	2:B:2277:CYS:N	2.54	0.40
2:B:2487:LEU:HA	2:B:2490:VAL:HG22	2.03	0.40
2:B:2874:TYR:O	2:B:2882:LYS:HE2	2.22	0.40
2:B:3651:PRO:HB2	2:B:3652:PRO:HD3	2.03	0.40
2:B:4240:THR:HG22	2:B:4308:ILE:HD13	2.02	0.40
2:C:884:LYS:HA	2:C:887:GLU:CG	2.51	0.40
2:C:3304:GLN:HB3	2:C:3305:PRO:HD3	2.03	0.40
2:D:972:LEU:HD23	2:D:973:THR:H	1.86	0.40
2:D:1585:ARG:O	2:D:1587:HIS:ND1	2.54	0.40
2:D:2170:THR:O	2:D:2174:VAL:HG13	2.21	0.40
2:D:2329:GLU:CD	2:D:2329:GLU:H	2.29	0.40
2:D:2586:GLN:HE22	2:D:2590:ARG:NH2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2659:GLN:HG2	2:D:2660:GLU:N	2.36	0.40
2:D:2913:ASP:HB3	2:D:2919:LYS:HE3	2.03	0.40
2:D:3281:LEU:HD22	2:D:3322:LEU:HD22	2.03	0.40
2:D:4914:ASN:HB3	2:D:4917:ASN:ND2	2.36	0.40
1:I:57:ASP:OD2	1:I:62:GLY:N	2.46	0.40
1:I:125:MET:HE3	1:I:125:MET:HB3	1.71	0.40
2:A:2344:LEU:HD22	2:A:2434:GLY:HA3	2.02	0.40
2:A:2488:LEU:HD11	2:A:2548:LEU:HD13	2.03	0.40
2:A:2691:LYS:HD3	2:A:2704:GLN:NE2	2.37	0.40
2:A:2824:ARG:NH2	2:B:1502:ASN:HB3	2.37	0.40
2:A:3310:VAL:HG11	2:A:3319:PHE:CE2	2.57	0.40
1:L:123:ASP:HA	1:L:126:ILE:HG23	2.03	0.40
2:B:735:GLY:O	2:B:737:ILE:HD12	2.22	0.40
2:B:1226:TYR:HD1	2:B:1229:ILE:HD11	1.87	0.40
2:B:1829:LEU:HD12	2:B:1829:LEU:HA	1.96	0.40
2:B:1893:LEU:HD23	2:B:1896:MET:SD	2.60	0.40
2:B:1968:PRO:O	2:B:1972:GLN:HG3	2.21	0.40
2:B:2570:GLU:HG2	2:B:2605:MET:HG3	2.03	0.40
2:B:2913:ASP:HB3	2:B:2919:LYS:HE3	2.03	0.40
2:B:3183:ILE:HD12	2:B:3187:LYS:CE	2.52	0.40
2:B:3778:LEU:HD13	2:B:3854:PHE:HD1	1.87	0.40
2:B:3924:ILE:HG21	2:B:3935:LEU:HD12	2.03	0.40
2:B:3958:LEU:HB2	2:B:3968:LEU:HD13	2.03	0.40
2:B:4057:HIS:CE1	2:C:4660:PHE:HZ	2.40	0.40
2:C:810:GLU:N	2:C:810:GLU:OE2	2.55	0.40
2:C:2874:TYR:O	2:C:2882:LYS:HE2	2.22	0.40
2:C:3184:TYR:CD1	2:C:3201:VAL:HG22	2.56	0.40
2:C:3211:LEU:HD21	2:C:3245:TYR:HE2	1.86	0.40
2:C:4041:GLY:HA2	2:C:4080:TYR:HE1	1.86	0.40
2:D:59:PRO:HA	2:D:60:PRO:HD3	1.98	0.40
2:D:875:PRO:HA	2:D:876:PRO:HD3	1.94	0.40
2:D:1962:THR:HG22	2:D:1966:ARG:HG3	2.02	0.40
2:D:2327:ARG:HB3	2:D:2329:GLU:OE2	2.21	0.40
2:D:2874:TYR:O	2:D:2882:LYS:HE2	2.22	0.40
2:D:4167:GLU:O	2:D:4171:GLN:HG2	2.22	0.40
2:A:139:SER:O	2:A:141:ASP:N	2.54	0.40
2:A:1848:PRO:HG3	2:A:1890:LYS:NZ	2.37	0.40
2:A:2463:ASP:OD1	2:A:2464:HIS:N	2.55	0.40
2:A:2931:ARG:NH1	2:A:2932:TYR:CE1	2.90	0.40
2:A:2967:VAL:O	2:A:2971:ILE:HG13	2.22	0.40
2:A:3168:VAL:HG12	2:A:3179:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4898:PHE:O	2:A:4904:GLY:HA3	2.22	0.40
1:K:10:ILE:HG22	1:K:14:LYS:NZ	2.37	0.40
2:B:884:LYS:HA	2:B:887:GLU:CG	2.51	0.40
2:B:997:ASP:O	2:B:1001:GLU:OE1	2.40	0.40
2:B:1177:LEU:O	2:B:1180:GLU:HG3	2.22	0.40
2:B:1911:GLN:OE1	2:B:2090:ARG:NH1	2.54	0.40
2:B:1939:ASN:C	2:B:1939:ASN:HD22	2.25	0.40
2:B:2153:LYS:HD3	2:B:2153:LYS:HA	1.83	0.40
2:B:2408:LEU:HD22	2:B:2413:LYS:HD3	2.03	0.40
2:B:3649:ALA:HB1	2:B:3652:PRO:HB2	2.04	0.40
2:B:4502:MET:SD	2:B:4585:PHE:HB3	2.61	0.40
2:B:4607:ALA:HB1	2:B:4649:VAL:HG21	2.04	0.40
2:C:2463:ASP:OD1	2:C:2464:HIS:N	2.55	0.40
2:C:3191:GLU:HA	2:C:3194:ALA:HB3	2.03	0.40
2:D:1177:LEU:O	2:D:1180:GLU:HG3	2.22	0.40
2:D:1711:LEU:HB3	2:D:1831:MET:SD	2.62	0.40
2:D:2687:SER:C	2:D:2688:MET:HE2	2.47	0.40
2:D:2772:ARG:HG3	2:D:2776:LYS:HZ2	1.87	0.40
2:D:3017:HIS:C	2:D:3018:ARG:HD3	2.46	0.40
2:D:3062:ASP:O	2:D:3065:ALA:HB3	2.22	0.40
2:D:3191:GLU:HA	2:D:3194:ALA:HB3	2.03	0.40
2:D:3832:ASP:HB2	2:D:3835:PHE:HB3	2.04	0.40
2:D:4265:LYS:O	2:D:4269:LYS:HG2	2.21	0.40
2:D:4607:ALA:HB1	2:D:4649:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	141/149 (95%)	139 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	K	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	L	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	A	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	B	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	C	4205/4967 (85%)	4082 (97%)	118 (3%)	5 (0%)	48	79
2	D	4205/4967 (85%)	4080 (97%)	120 (3%)	5 (0%)	48	79
3	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17804/20896 (85%)	17292 (97%)	492 (3%)	20 (0%)	49	79

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3927	PRO
2	A	4641	PRO
2	B	3927	PRO
2	B	4641	PRO
2	C	3927	PRO
2	C	4641	PRO
2	D	3927	PRO
2	D	4641	PRO
2	A	1081	THR
2	A	3851	ASN
2	B	1081	THR
2	B	3851	ASN
2	C	1081	THR
2	C	3851	ASN
2	D	1081	THR
2	D	3851	ASN
2	A	1959	ALA
2	B	1959	ALA
2	C	1959	ALA
2	D	1959	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	123/127 (97%)	113 (92%)	10 (8%)	11	36
1	J	123/127 (97%)	113 (92%)	10 (8%)	11	36
1	K	123/127 (97%)	113 (92%)	10 (8%)	11	36
1	L	123/127 (97%)	113 (92%)	10 (8%)	11	36
2	A	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
2	B	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
2	C	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
2	D	3715/4358 (85%)	3684 (99%)	31 (1%)	73	77
3	E	88/89 (99%)	87 (99%)	1 (1%)	65	74
3	F	88/89 (99%)	87 (99%)	1 (1%)	65	74
3	G	88/89 (99%)	87 (99%)	1 (1%)	65	74
3	H	88/89 (99%)	87 (99%)	1 (1%)	65	74
All	All	15704/18296 (86%)	15536 (99%)	168 (1%)	63	74

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	77	MET
1	I	124	GLU
1	I	125	MET
1	I	126	ILE
1	I	127	ARG
1	I	128	GLU
1	I	130	ASP
1	I	143	VAL
1	I	145	MET
1	I	146	MET
2	A	349	MET
2	A	393	MET
2	A	441	LYS
2	A	778	MET

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Mol	Chain	Res	Type
2	A	944	LEU
2	A	1300	MET
2	A	1564	MET
2	A	1720	MET
2	A	1948	MET
2	A	1953	MET
2	A	2134	MET
2	A	2512	MET
2	A	2688	MET
2	A	2689	MET
2	A	2737	LEU
2	A	2757	MET
2	A	2766	LYS
2	A	2772	ARG
2	A	2782	MET
2	A	2801	TYR
2	A	3104	MET
2	A	3584	LYS
2	A	3591	LEU
2	A	3605	MET
2	A	3847	CYS
2	A	4186	MET
2	A	4279	MET
2	A	4504	MET
2	A	4748	MET
2	A	4884	MET
2	A	4932	GLU
3	E	15	THR
3	F	15	THR
3	G	15	THR
3	H	15	THR
1	J	77	MET
1	J	124	GLU
1	J	125	MET
1	J	126	ILE
1	J	127	ARG
1	J	128	GLU
1	J	130	ASP
1	J	143	VAL
1	J	145	MET
1	J	146	MET
1	L	77	MET

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Mol	Chain	Res	Type
1	L	124	GLU
1	L	125	MET
1	L	126	ILE
1	L	127	ARG
1	L	128	GLU
1	L	130	ASP
1	L	143	VAL
1	L	145	MET
1	L	146	MET
1	K	77	MET
1	K	124	GLU
1	K	125	MET
1	K	126	ILE
1	K	127	ARG
1	K	128	GLU
1	K	130	ASP
1	K	143	VAL
1	K	145	MET
1	K	146	MET
2	B	349	MET
2	B	393	MET
2	B	441	LYS
2	B	778	MET
2	B	944	LEU
2	B	1300	MET
2	B	1564	MET
2	B	1720	MET
2	B	1948	MET
2	B	1953	MET
2	B	2134	MET
2	B	2512	MET
2	B	2688	MET
2	B	2689	MET
2	B	2737	LEU
2	B	2757	MET
2	B	2766	LYS
2	B	2772	ARG
2	B	2782	MET
2	B	2801	TYR
2	B	3104	MET
2	B	3584	LYS
2	B	3591	LEU

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Mol	Chain	Res	Type
2	B	3605	MET
2	B	3847	CYS
2	B	4186	MET
2	B	4279	MET
2	B	4504	MET
2	B	4748	MET
2	B	4884	MET
2	B	4932	GLU
2	C	349	MET
2	C	393	MET
2	C	441	LYS
2	C	778	MET
2	C	944	LEU
2	C	1300	MET
2	C	1564	MET
2	C	1720	MET
2	C	1948	MET
2	C	1953	MET
2	C	2134	MET
2	C	2512	MET
2	C	2688	MET
2	C	2689	MET
2	C	2737	LEU
2	C	2757	MET
2	C	2766	LYS
2	C	2772	ARG
2	C	2782	MET
2	C	2801	TYR
2	C	3104	MET
2	C	3584	LYS
2	C	3591	LEU
2	C	3605	MET
2	C	3847	CYS
2	C	4186	MET
2	C	4279	MET
2	C	4504	MET
2	C	4748	MET
2	C	4884	MET
2	C	4932	GLU
2	D	349	MET
2	D	393	MET
2	D	441	LYS

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Mol	Chain	Res	Type
2	D	778	MET
2	D	944	LEU
2	D	1300	MET
2	D	1564	MET
2	D	1720	MET
2	D	1948	MET
2	D	1953	MET
2	D	2134	MET
2	D	2512	MET
2	D	2688	MET
2	D	2689	MET
2	D	2737	LEU
2	D	2757	MET
2	D	2766	LYS
2	D	2772	ARG
2	D	2782	MET
2	D	2801	TYR
2	D	3104	MET
2	D	3584	LYS
2	D	3591	LEU
2	D	3605	MET
2	D	3847	CYS
2	D	4186	MET
2	D	4279	MET
2	D	4504	MET
2	D	4748	MET
2	D	4884	MET
2	D	4932	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (225) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	9	GLN
1	I	54	ASN
1	I	136	GLN
2	A	29	HIS
2	A	71	GLN
2	A	388	GLN
2	A	544	ASN
2	A	645	GLN
2	A	658	ASN
2	A	669	GLN

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Mol	Chain	Res	Type
2	A	776	GLN
2	A	888	ASN
2	A	949	HIS
2	A	992	GLN
2	A	1002	ASN
2	A	1146	HIS
2	A	1211	GLN
2	A	1452	GLN
2	A	1577	ASN
2	A	1581	GLN
2	A	1691	ASN
2	A	1762	GLN
2	A	1844	GLN
2	A	1905	GLN
2	A	2059	GLN
2	A	2224	ASN
2	A	2278	GLN
2	A	2291	ASN
2	A	2540	HIS
2	A	2729	HIS
2	A	2850	ASN
2	A	2927	GLN
2	A	2995	HIS
2	A	2998	ASN
2	A	3017	HIS
2	A	3031	ASN
2	A	3034	HIS
2	A	3038	GLN
2	A	3077	GLN
2	A	3151	GLN
2	A	3272	HIS
2	A	3722	GLN
2	A	3775	GLN
2	A	3812	ASN
2	A	3831	GLN
2	A	3869	ASN
2	A	3915	GLN
2	A	3949	HIS
2	A	3955	GLN
2	A	4049	HIS
2	A	4057	HIS
2	A	4171	GLN

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Mol	Chain	Res	Type
2	A	4706	GLN
2	A	4742	HIS
2	A	4794	ASN
2	A	4863	GLN
2	A	4879	GLN
2	A	4927	ASN
2	A	4933	HIS
2	A	4967	ASN
3	E	71	GLN
3	G	71	GLN
3	H	71	GLN
1	J	9	GLN
1	J	54	ASN
1	J	136	GLN
1	L	54	ASN
1	L	136	GLN
1	K	9	GLN
1	K	54	ASN
1	K	108	HIS
1	K	136	GLN
2	B	29	HIS
2	B	71	GLN
2	B	388	GLN
2	B	544	ASN
2	B	658	ASN
2	B	669	GLN
2	B	776	GLN
2	B	888	ASN
2	B	1002	ASN
2	B	1146	HIS
2	B	1452	GLN
2	B	1577	ASN
2	B	1581	GLN
2	B	1691	ASN
2	B	1762	GLN
2	B	1844	GLN
2	B	2059	GLN
2	B	2224	ASN
2	B	2278	GLN
2	B	2291	ASN
2	B	2540	HIS
2	B	2729	HIS

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Mol	Chain	Res	Type
2	B	2850	ASN
2	B	2927	GLN
2	B	2995	HIS
2	B	2998	ASN
2	B	3017	HIS
2	B	3031	ASN
2	B	3034	HIS
2	B	3038	GLN
2	B	3077	GLN
2	B	3151	GLN
2	B	3722	GLN
2	B	3775	GLN
2	B	3812	ASN
2	B	3831	GLN
2	B	3869	ASN
2	B	3915	GLN
2	B	3949	HIS
2	B	3955	GLN
2	B	4049	HIS
2	B	4057	HIS
2	B	4171	GLN
2	B	4706	GLN
2	B	4794	ASN
2	B	4863	GLN
2	B	4879	GLN
2	B	4927	ASN
2	B	4933	HIS
2	B	4967	ASN
2	C	29	HIS
2	C	71	GLN
2	C	388	GLN
2	C	544	ASN
2	C	658	ASN
2	C	669	GLN
2	C	776	GLN
2	C	888	ASN
2	C	1002	ASN
2	C	1146	HIS
2	C	1452	GLN
2	C	1577	ASN
2	C	1581	GLN
2	C	1691	ASN

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Mol	Chain	Res	Type
2	C	1762	GLN
2	C	1844	GLN
2	C	2224	ASN
2	C	2278	GLN
2	C	2291	ASN
2	C	2540	HIS
2	C	2729	HIS
2	C	2850	ASN
2	C	2927	GLN
2	C	2995	HIS
2	C	2998	ASN
2	C	3017	HIS
2	C	3031	ASN
2	C	3034	HIS
2	C	3038	GLN
2	C	3077	GLN
2	C	3151	GLN
2	C	3722	GLN
2	C	3775	GLN
2	C	3812	ASN
2	C	3831	GLN
2	C	3869	ASN
2	C	3915	GLN
2	C	3949	HIS
2	C	3955	GLN
2	C	4049	HIS
2	C	4057	HIS
2	C	4171	GLN
2	C	4706	GLN
2	C	4742	HIS
2	C	4794	ASN
2	C	4863	GLN
2	C	4879	GLN
2	C	4927	ASN
2	C	4933	HIS
2	C	4967	ASN
2	D	29	HIS
2	D	71	GLN
2	D	388	GLN
2	D	544	ASN
2	D	645	GLN
2	D	658	ASN

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Mol	Chain	Res	Type
2	D	669	GLN
2	D	776	GLN
2	D	888	ASN
2	D	1002	ASN
2	D	1146	HIS
2	D	1452	GLN
2	D	1577	ASN
2	D	1581	GLN
2	D	1691	ASN
2	D	1762	GLN
2	D	1844	GLN
2	D	1970	GLN
2	D	2224	ASN
2	D	2278	GLN
2	D	2291	ASN
2	D	2540	HIS
2	D	2586	GLN
2	D	2850	ASN
2	D	2927	GLN
2	D	2995	HIS
2	D	2998	ASN
2	D	3017	HIS
2	D	3031	ASN
2	D	3034	HIS
2	D	3038	GLN
2	D	3077	GLN
2	D	3151	GLN
2	D	3272	HIS
2	D	3610	ASN
2	D	3722	GLN
2	D	3775	GLN
2	D	3812	ASN
2	D	3831	GLN
2	D	3869	ASN
2	D	3915	GLN
2	D	3949	HIS
2	D	3955	GLN
2	D	4049	HIS
2	D	4057	HIS
2	D	4171	GLN
2	D	4706	GLN
2	D	4742	HIS

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Mol	Chain	Res	Type
2	D	4794	ASN
2	D	4879	GLN
2	D	4927	ASN
2	D	4933	HIS
2	D	4967	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 24 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ATP	A	5002	-	32,33,33	0.54	0	48,52,52	0.56	0
6	ATP	B	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	A	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	B	5002	-	32,33,33	0.54	0	48,52,52	0.56	0
6	ATP	C	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	D	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
6	ATP	C	5002	-	32,33,33	0.54	0	48,52,52	0.56	0
6	ATP	D	5002	-	32,33,33	0.53	0	48,52,52	0.55	0

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
6	ATP	A	5002	-	-	8/22/38/38	0/3/3/3
6	ATP	B	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	A	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	B	5002	-	-	8/22/38/38	0/3/3/3
6	ATP	C	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	D	5004	-	-	11/22/38/38	0/3/3/3
6	ATP	C	5002	-	-	8/22/38/38	0/3/3/3
6	ATP	D	5002	-	-	8/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5002	ATP	C5'-O5'-PA-O1A
6	A	5002	ATP	C5'-O5'-PA-O2A
6	A	5002	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	PB-O3A-PA-O5'
6	A	5004	ATP	C5'-O5'-PA-O1A
6	A	5004	ATP	C5'-O5'-PA-O2A
6	A	5004	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	O4'-C4'-C5'-O5'
6	B	5002	ATP	C5'-O5'-PA-O1A
6	B	5002	ATP	C5'-O5'-PA-O2A
6	B	5002	ATP	C5'-O5'-PA-O3A
6	B	5004	ATP	PB-O3A-PA-O5'
6	B	5004	ATP	C5'-O5'-PA-O1A
6	B	5004	ATP	C5'-O5'-PA-O2A
6	B	5004	ATP	C5'-O5'-PA-O3A
6	B	5004	ATP	O4'-C4'-C5'-O5'
6	C	5002	ATP	C5'-O5'-PA-O1A
6	C	5002	ATP	C5'-O5'-PA-O2A
6	C	5002	ATP	C5'-O5'-PA-O3A
6	C	5004	ATP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
6	C	5004	ATP	C5'-O5'-PA-O1A
6	C	5004	ATP	C5'-O5'-PA-O2A
6	C	5004	ATP	C5'-O5'-PA-O3A
6	C	5004	ATP	O4'-C4'-C5'-O5'
6	D	5002	ATP	C5'-O5'-PA-O1A
6	D	5002	ATP	C5'-O5'-PA-O2A
6	D	5002	ATP	C5'-O5'-PA-O3A
6	D	5004	ATP	PB-O3A-PA-O5'
6	D	5004	ATP	C5'-O5'-PA-O1A
6	D	5004	ATP	C5'-O5'-PA-O2A
6	D	5004	ATP	C5'-O5'-PA-O3A
6	D	5004	ATP	O4'-C4'-C5'-O5'
6	A	5004	ATP	C3'-C4'-C5'-O5'
6	B	5004	ATP	C3'-C4'-C5'-O5'
6	C	5004	ATP	C3'-C4'-C5'-O5'
6	D	5004	ATP	C3'-C4'-C5'-O5'
6	A	5002	ATP	C4'-C5'-O5'-PA
6	B	5002	ATP	C4'-C5'-O5'-PA
6	C	5002	ATP	C4'-C5'-O5'-PA
6	D	5002	ATP	C4'-C5'-O5'-PA
6	A	5002	ATP	O4'-C4'-C5'-O5'
6	B	5002	ATP	O4'-C4'-C5'-O5'
6	C	5002	ATP	O4'-C4'-C5'-O5'
6	D	5002	ATP	O4'-C4'-C5'-O5'
6	A	5004	ATP	PA-O3A-PB-O1B
6	B	5004	ATP	PA-O3A-PB-O1B
6	C	5004	ATP	PA-O3A-PB-O1B
6	D	5004	ATP	PA-O3A-PB-O1B
6	A	5002	ATP	PB-O3B-PG-O3G
6	A	5004	ATP	PB-O3B-PG-O3G
6	B	5002	ATP	PB-O3B-PG-O3G
6	B	5004	ATP	PB-O3B-PG-O3G
6	C	5002	ATP	PB-O3B-PG-O3G
6	C	5004	ATP	PB-O3B-PG-O3G
6	D	5002	ATP	PB-O3B-PG-O3G
6	D	5004	ATP	PB-O3B-PG-O3G
6	A	5004	ATP	PA-O3A-PB-O2B
6	B	5004	ATP	PA-O3A-PB-O2B
6	C	5004	ATP	PA-O3A-PB-O2B
6	D	5004	ATP	PA-O3A-PB-O2B
6	A	5002	ATP	PB-O3B-PG-O1G
6	B	5002	ATP	PB-O3B-PG-O1G

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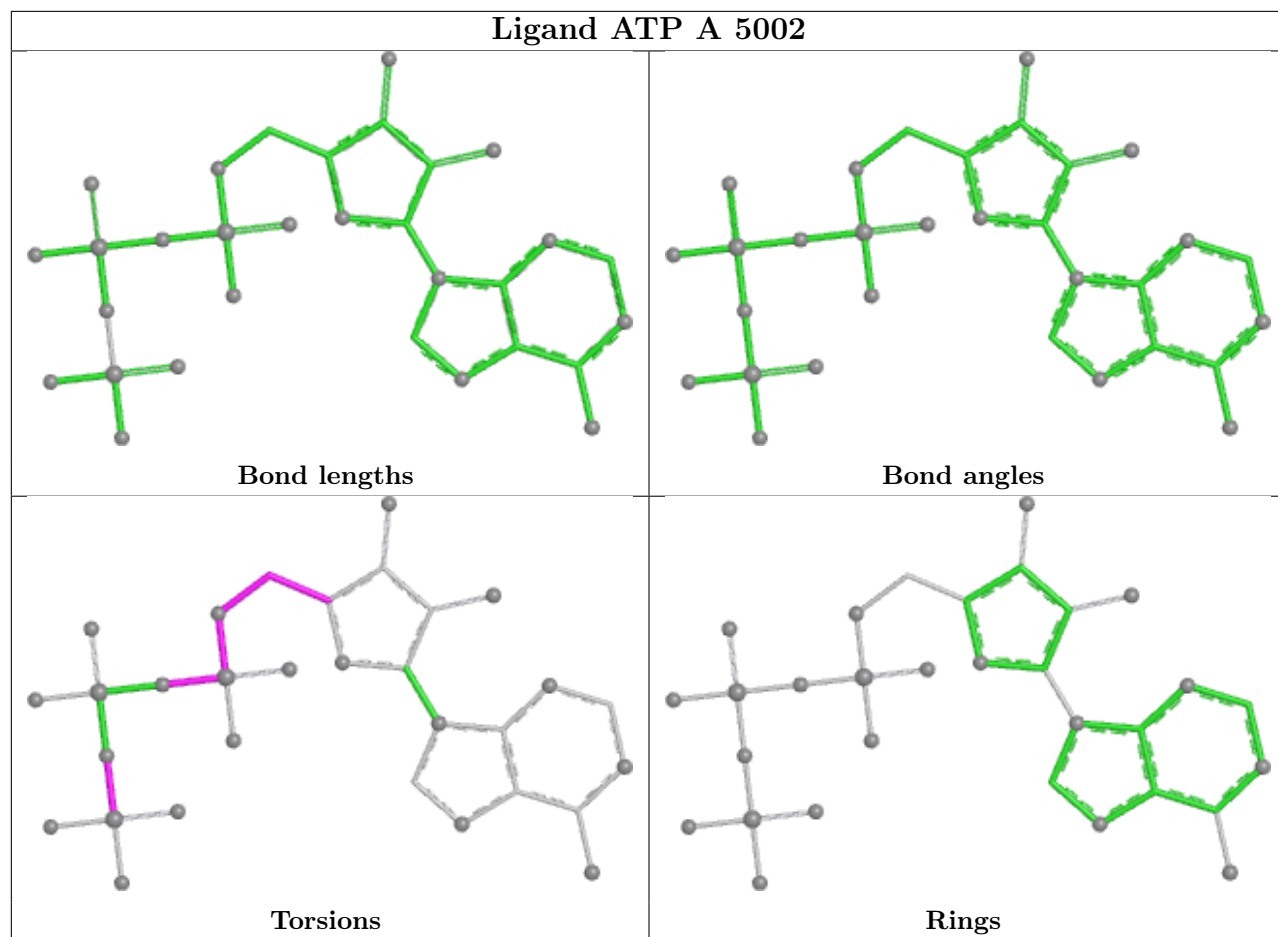
Mol	Chain	Res	Type	Atoms
6	C	5002	ATP	PB-O3B-PG-O1G
6	D	5002	ATP	PB-O3B-PG-O1G
6	A	5002	ATP	PB-O3A-PA-O2A
6	A	5004	ATP	PB-O3A-PA-O1A
6	A	5004	ATP	PB-O3A-PA-O2A
6	B	5002	ATP	PB-O3A-PA-O2A
6	B	5004	ATP	PB-O3A-PA-O1A
6	B	5004	ATP	PB-O3A-PA-O2A
6	C	5002	ATP	PB-O3A-PA-O2A
6	C	5004	ATP	PB-O3A-PA-O1A
6	C	5004	ATP	PB-O3A-PA-O2A
6	D	5002	ATP	PB-O3A-PA-O2A
6	D	5004	ATP	PB-O3A-PA-O1A
6	D	5004	ATP	PB-O3A-PA-O2A

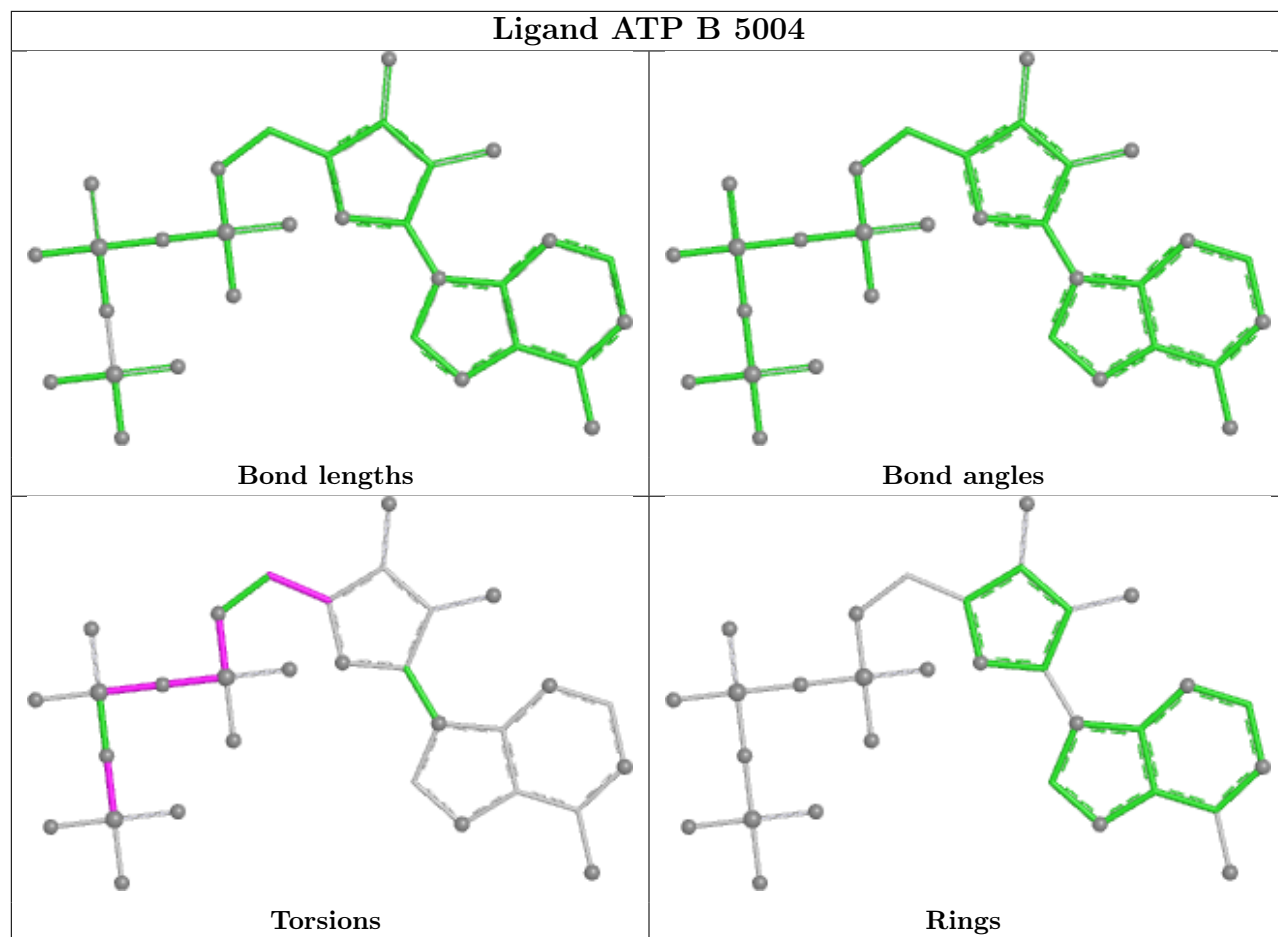
There are no ring outliers.

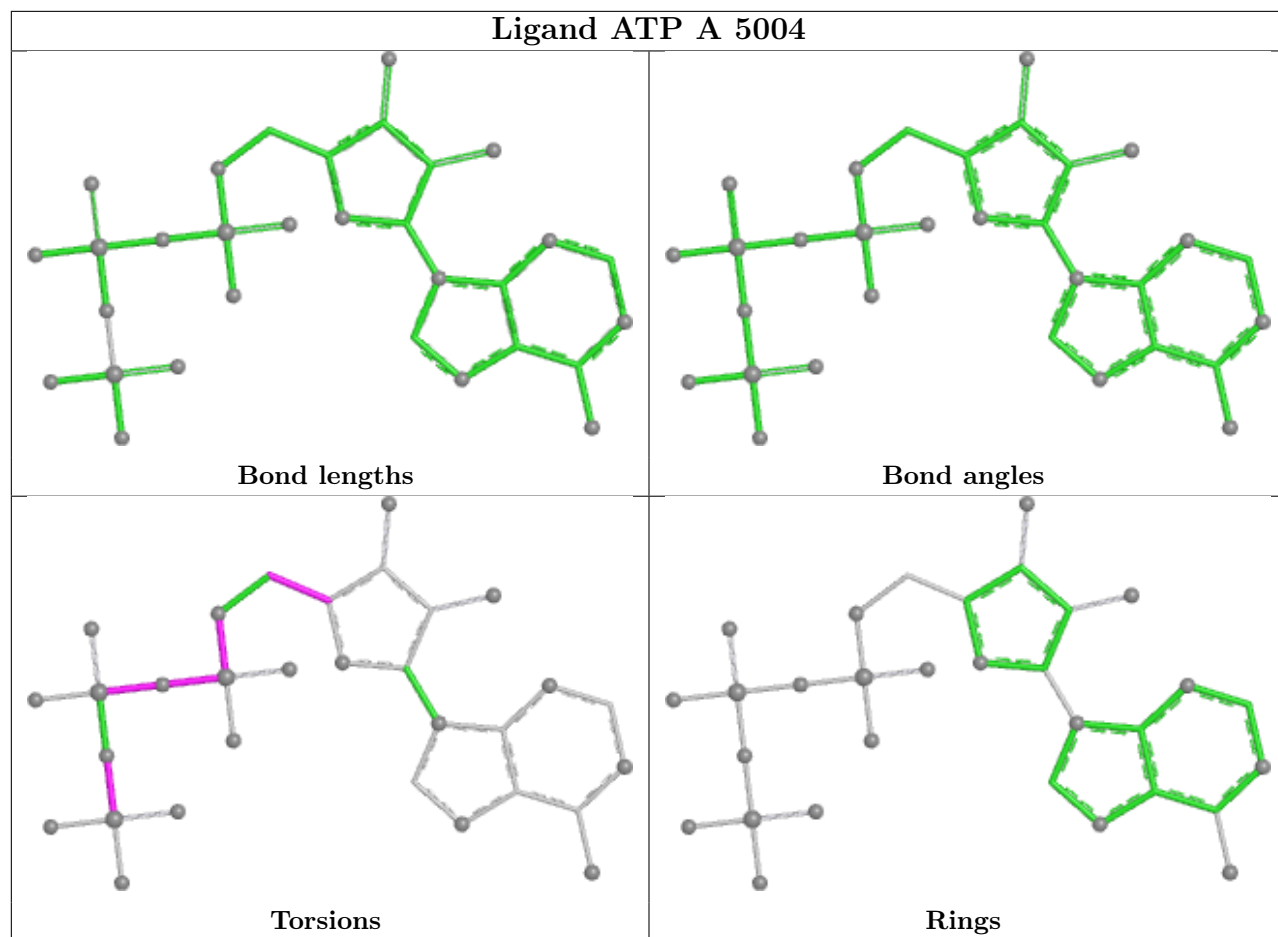
4 monomers are involved in 4 short contacts:

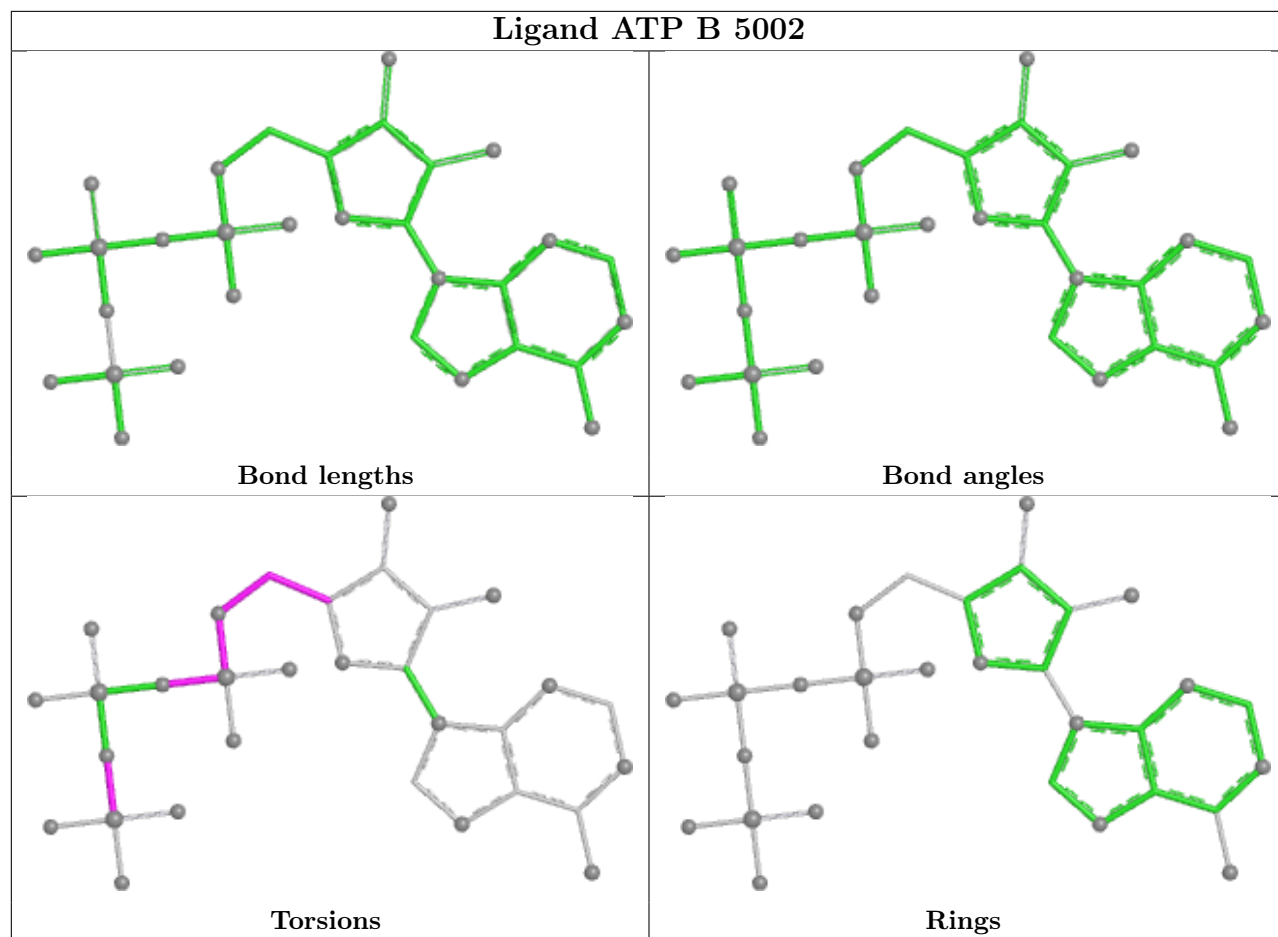
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5004	ATP	1	0
6	A	5004	ATP	1	0
6	C	5004	ATP	1	0
6	D	5004	ATP	1	0

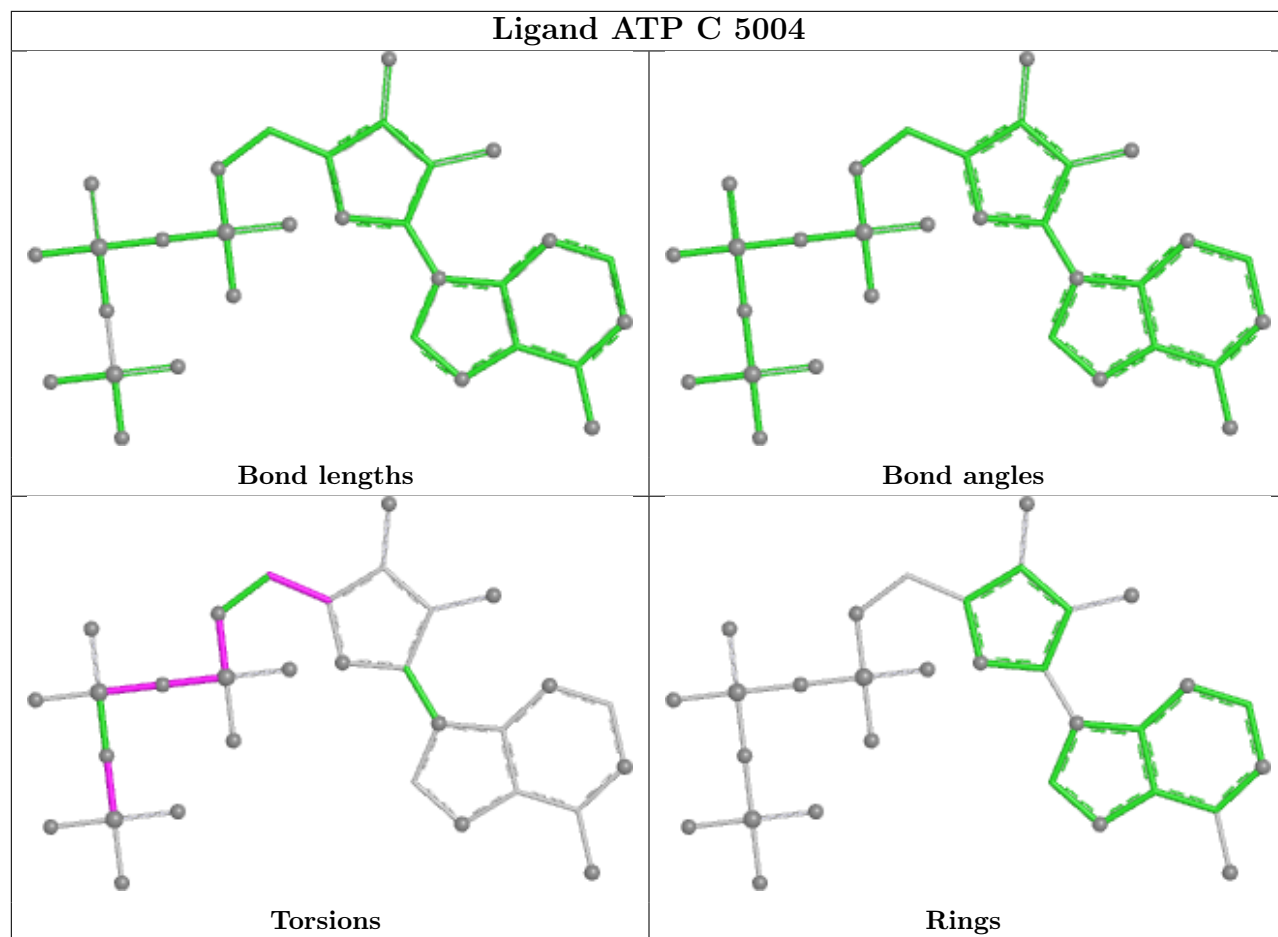
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

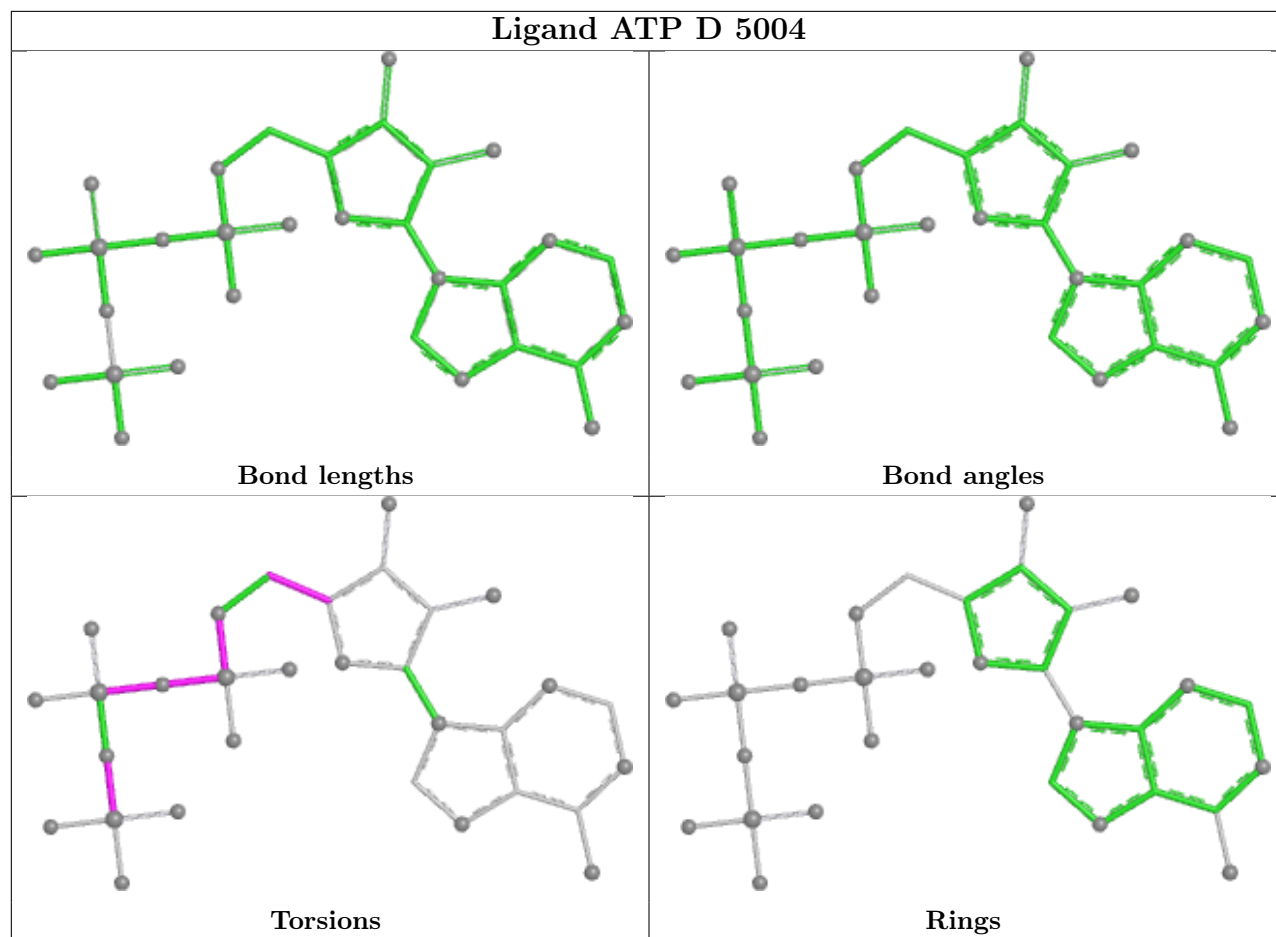


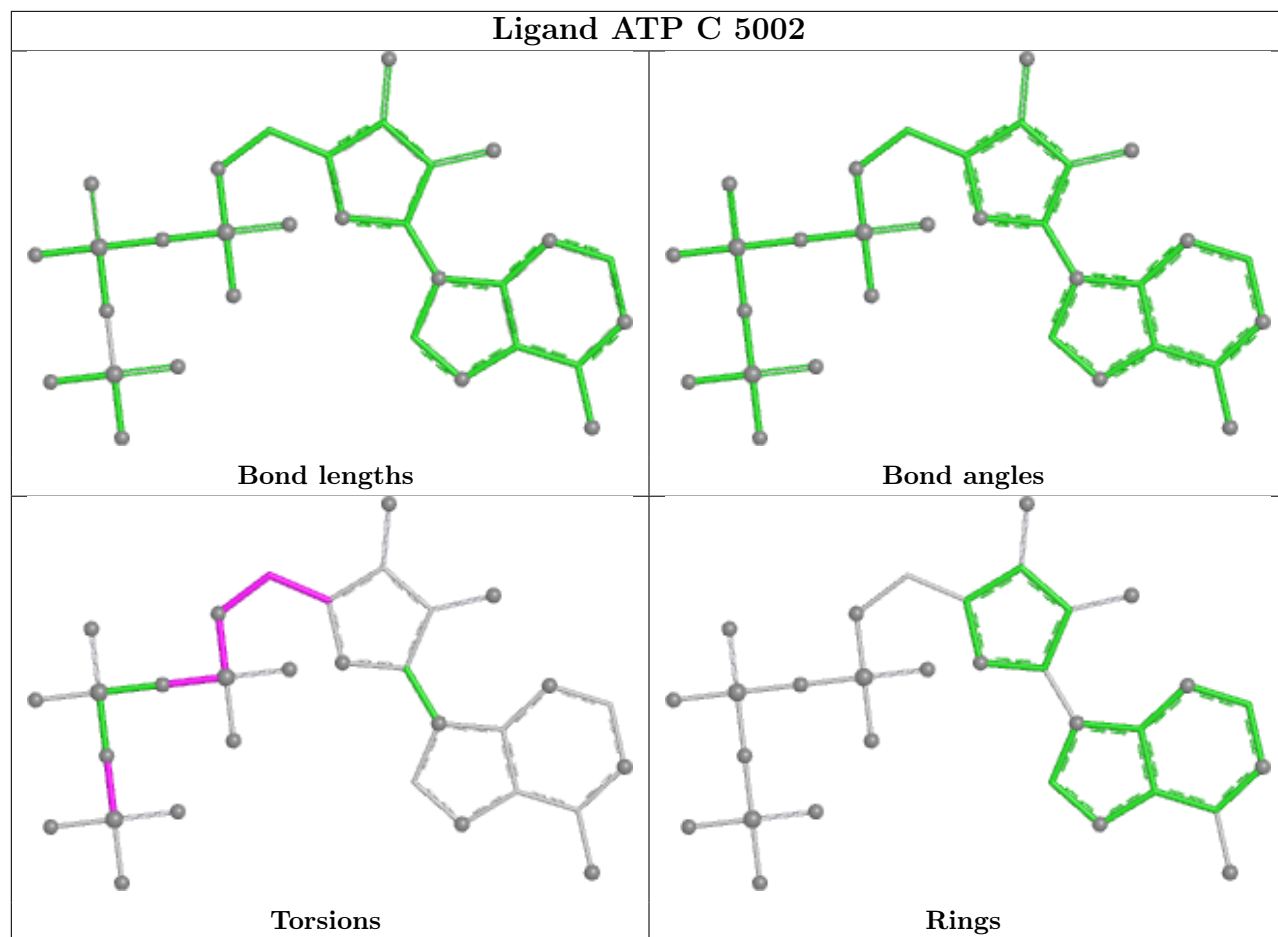


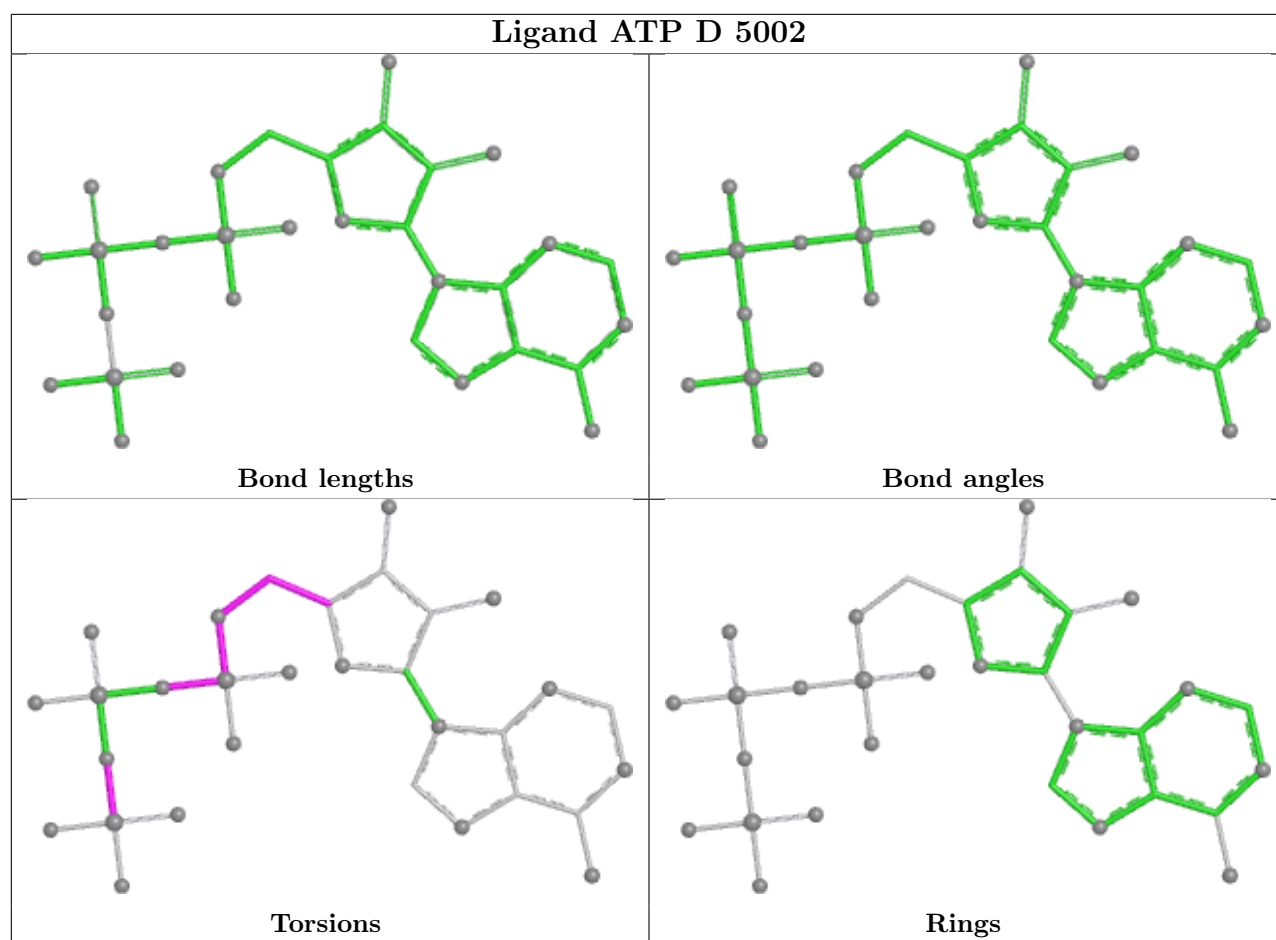












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

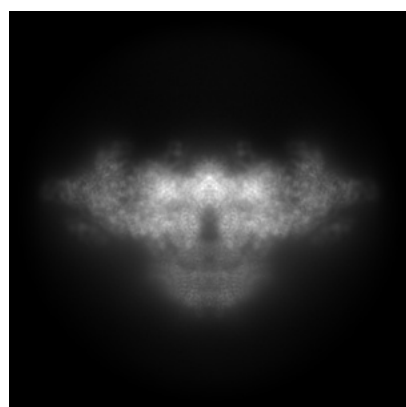
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42769. These allow visual inspection of the internal detail of the map and identification of artifacts.

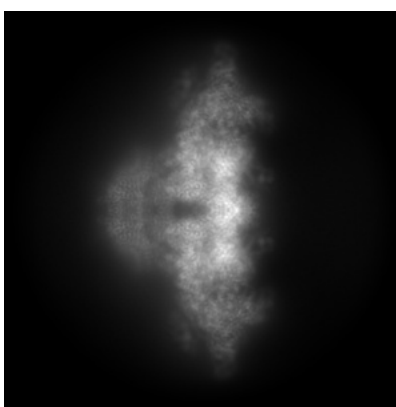
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

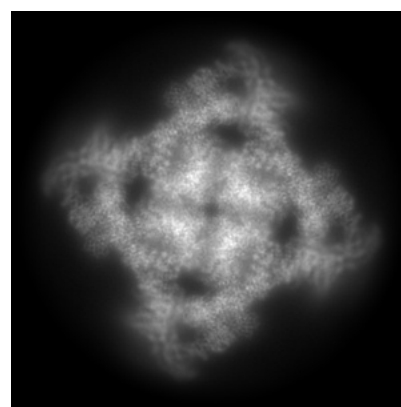
6.1.1 Primary map



X



Y

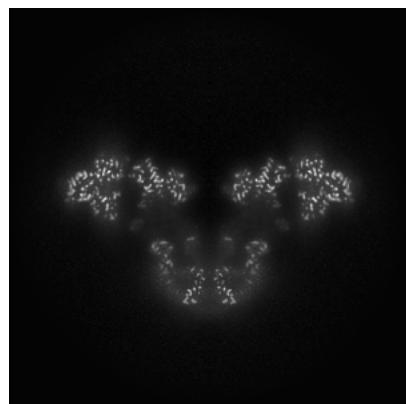


Z

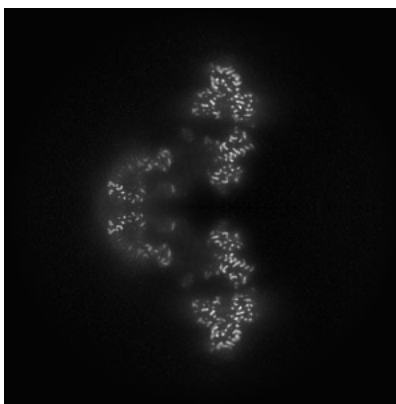
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

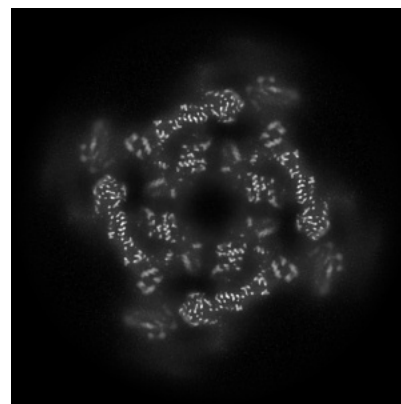
6.2.1 Primary map



X Index: 256



Y Index: 256

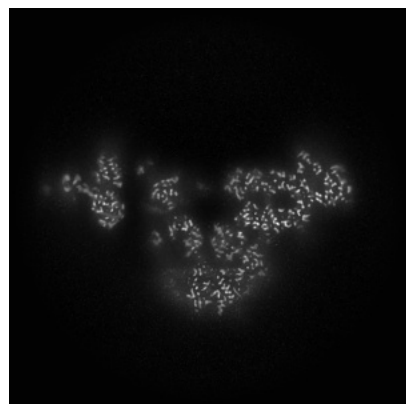


Z Index: 256

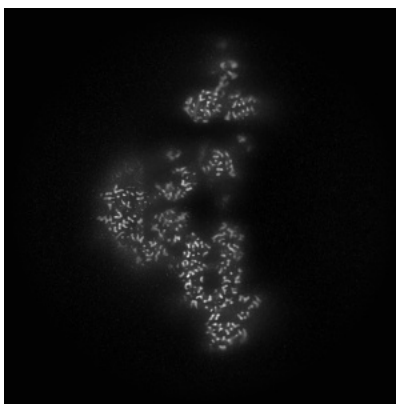
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

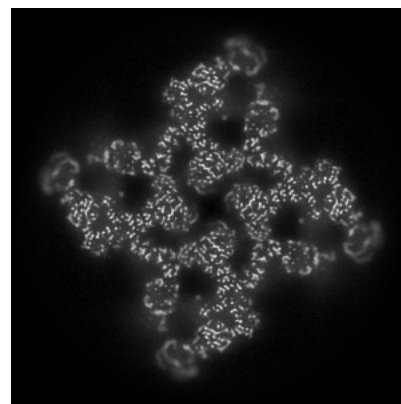
6.3.1 Primary map



X Index: 239



Y Index: 239



Z Index: 283

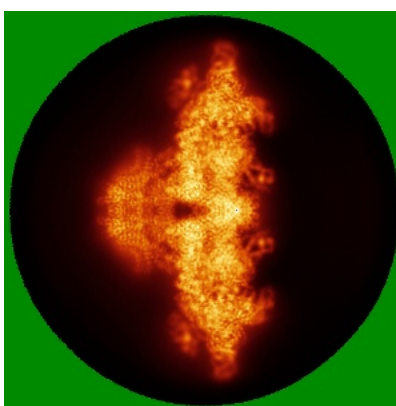
The images above show the largest variance slices of the map in three orthogonal directions.

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

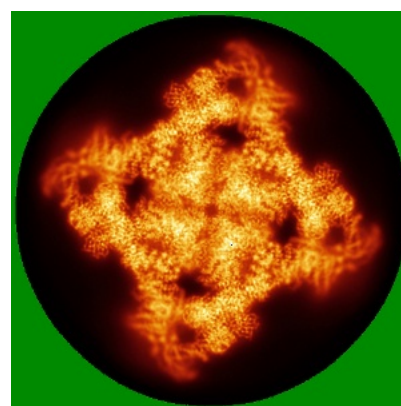
6.4.1 Primary map



X



Y

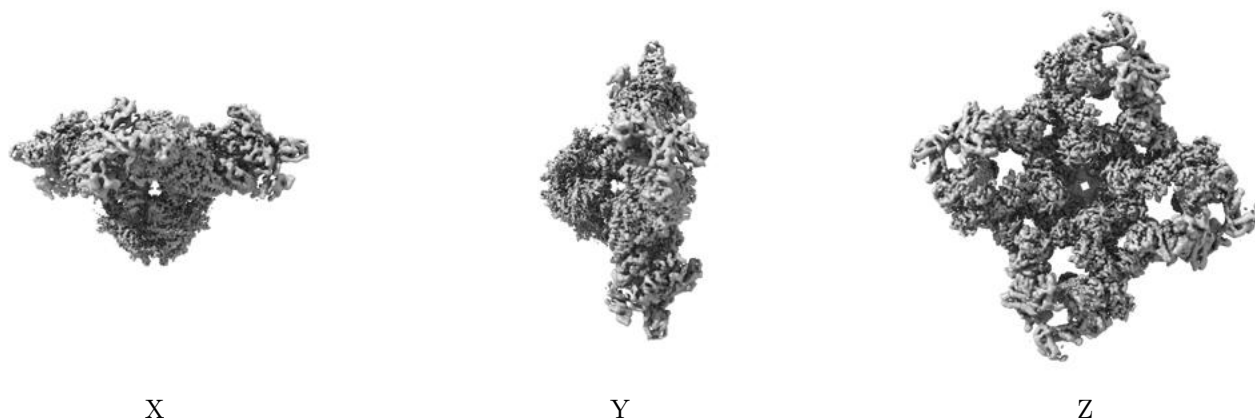


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

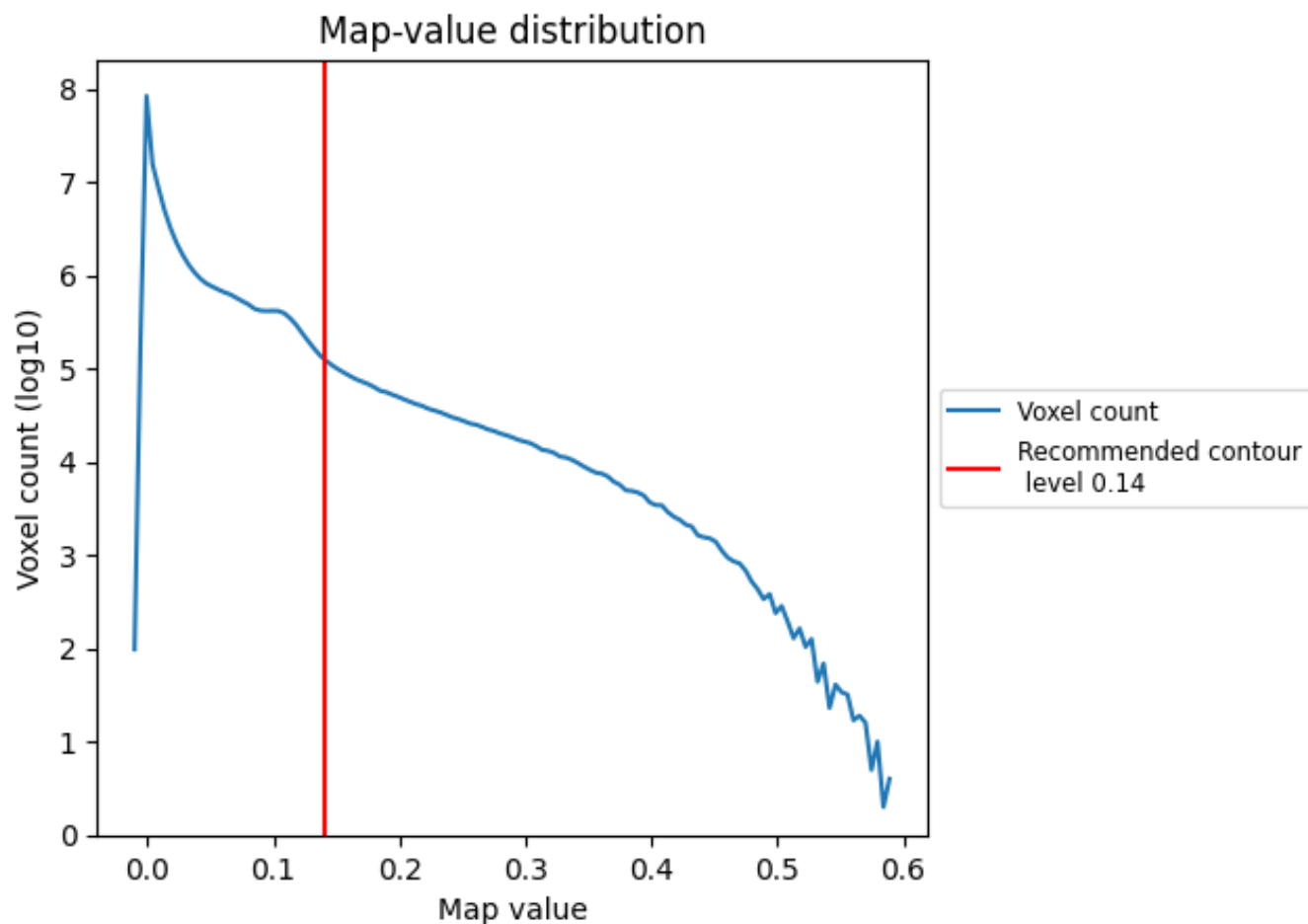
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

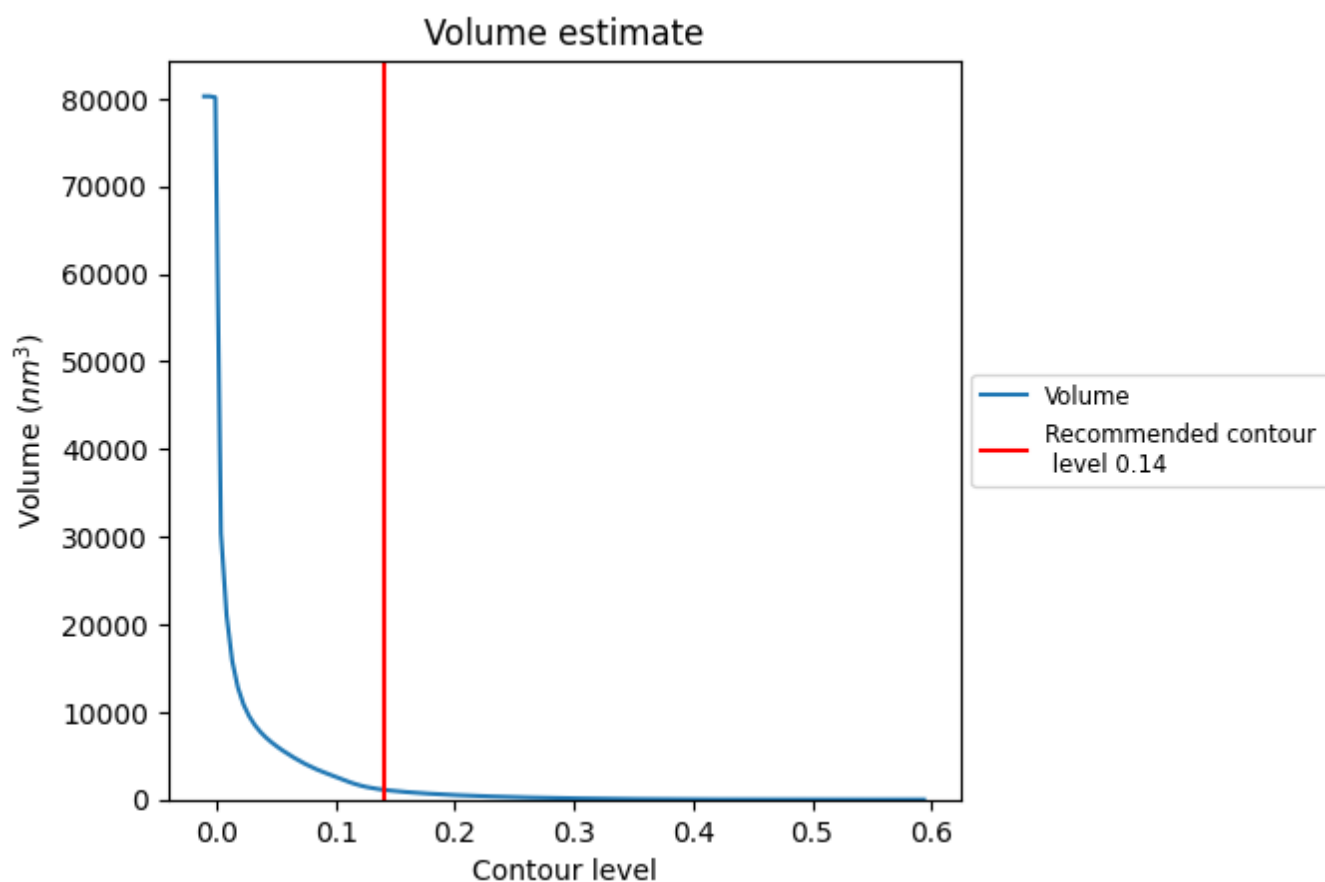
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

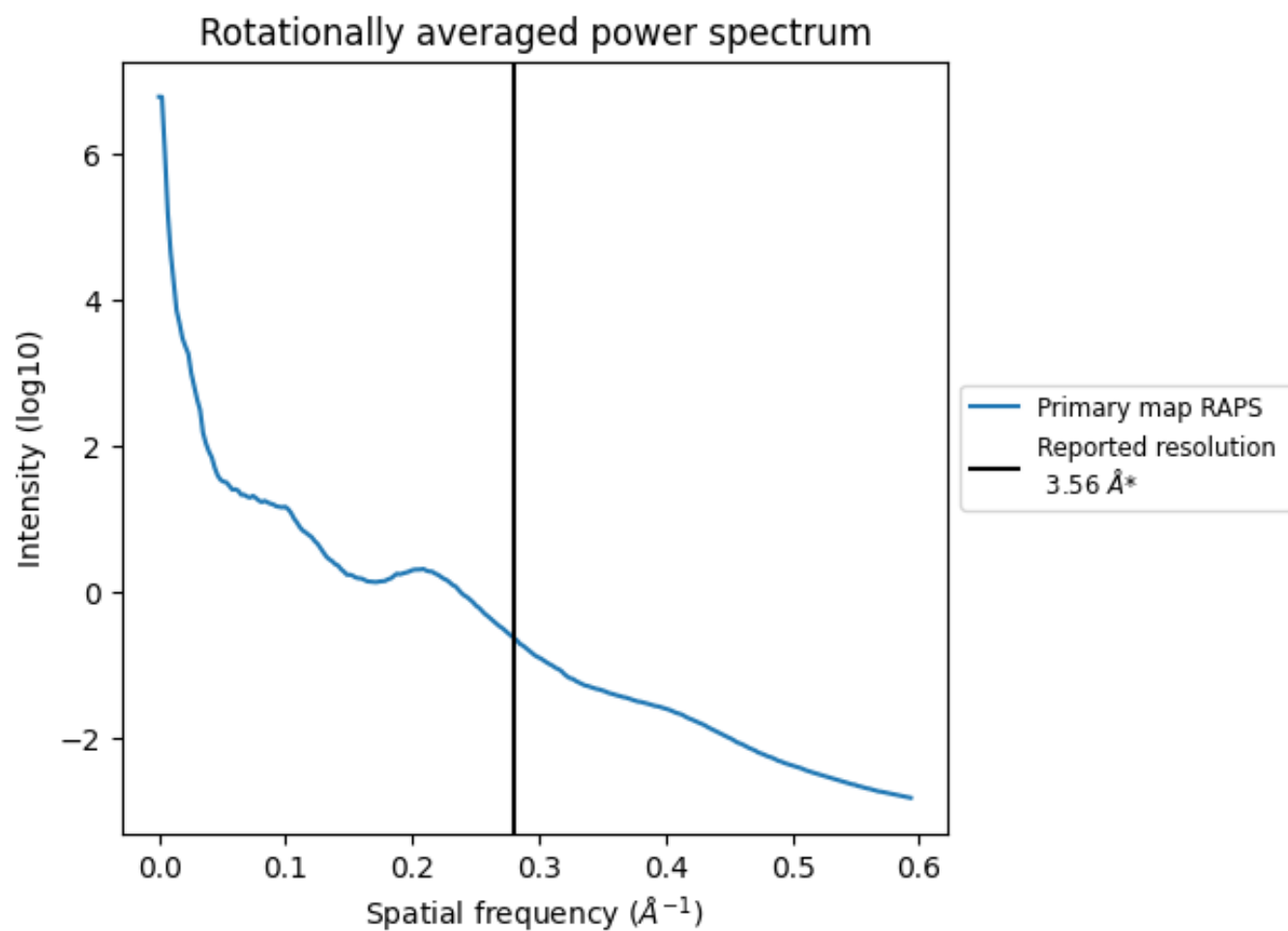
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1122 nm³; this corresponds to an approximate mass of 1014 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

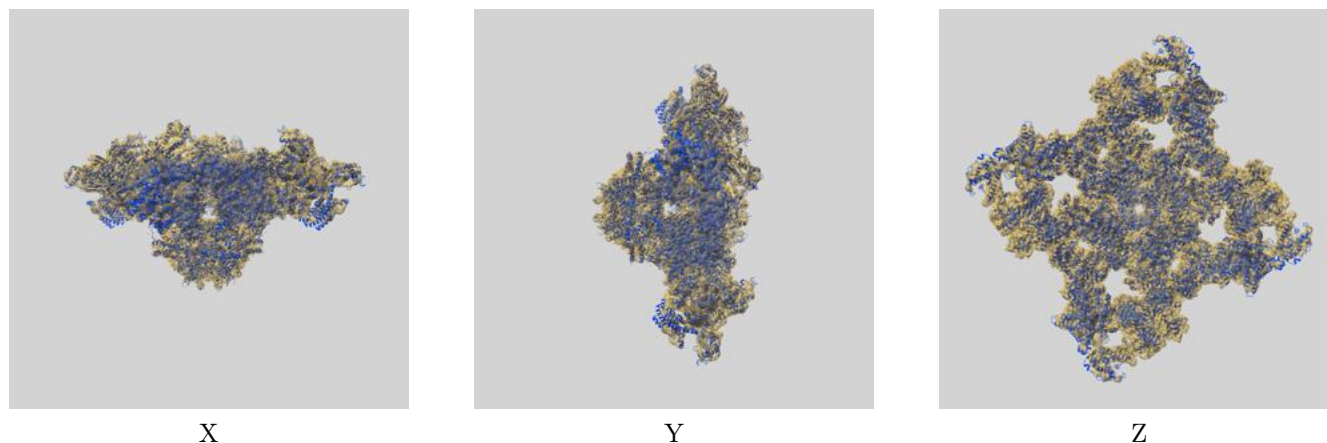
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

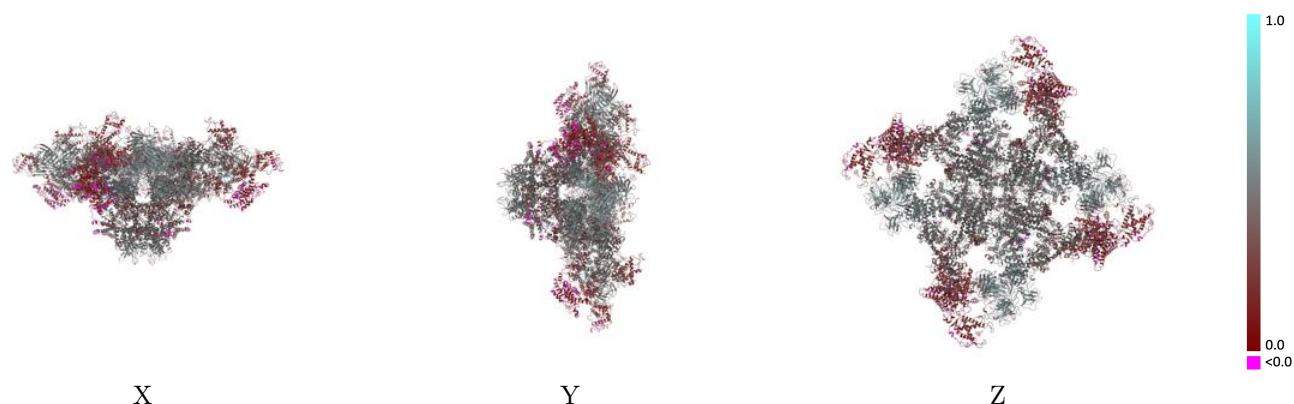
This section contains information regarding the fit between EMDB map EMD-42769 and PDB model 8UXM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



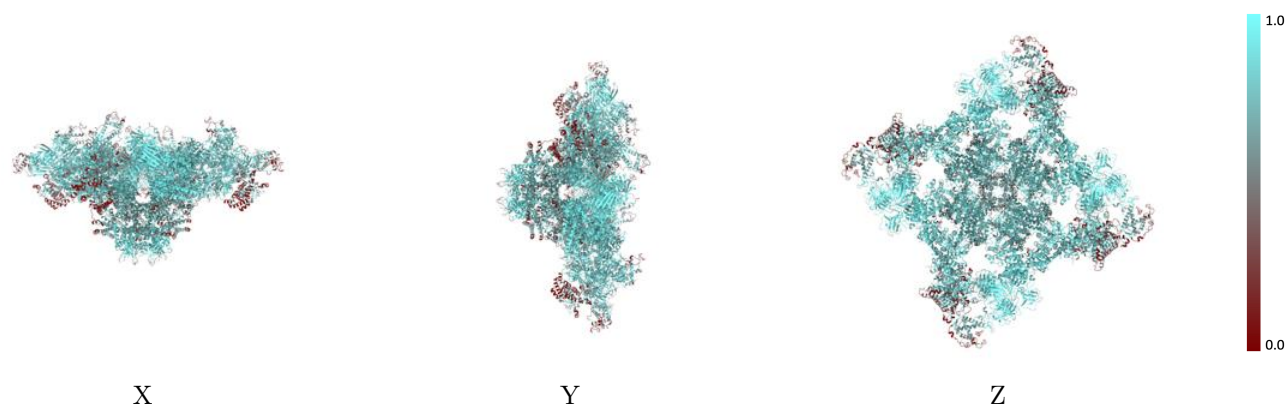
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



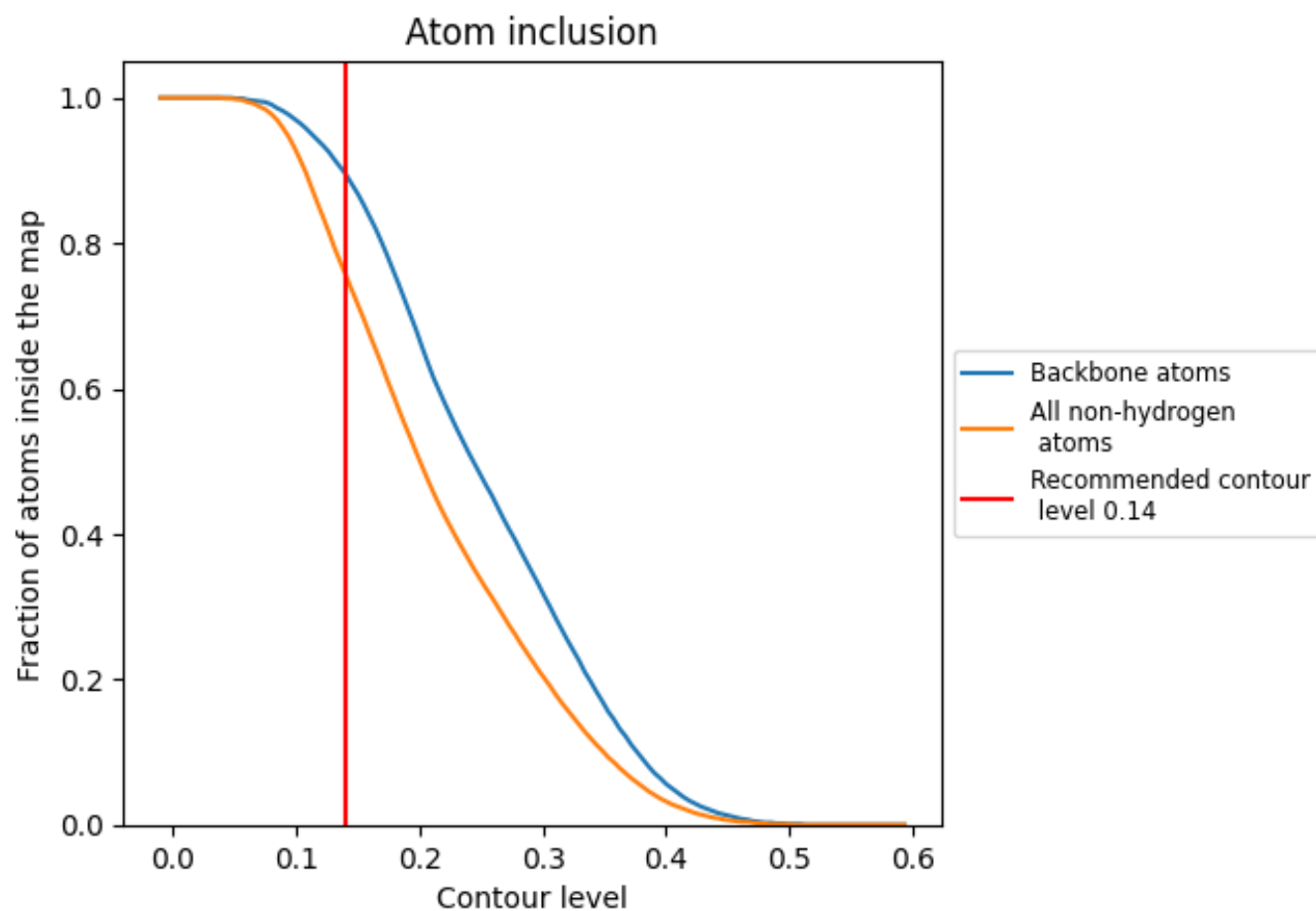
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.3810
A	0.7540	0.3840
B	0.7560	0.3860
C	0.7520	0.3800
D	0.7540	0.3820
E	0.8920	0.5130
F	0.8910	0.5110
G	0.8960	0.5120
H	0.8970	0.5110
I	0.7240	0.2220
J	0.7320	0.2220
K	0.7240	0.2220
L	0.7310	0.2190

1.0

0.0

<0.0