



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:08 AM UTC

PDB ID : 8BWY / pdb_00008bwy
EMDB ID : EMD-16304
Title : In situ outer dynein arm from *Chlamydomonas reinhardtii* in a pre-power stroke state
Authors : Zimmermann, N.E.L.; Noga, A.; Obbineni, J.M.; Ishikawa, T.
Deposited on : 2022-12-07
Resolution : 38.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

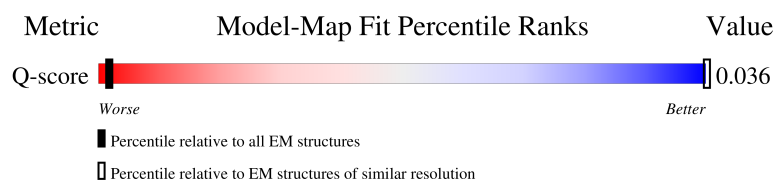
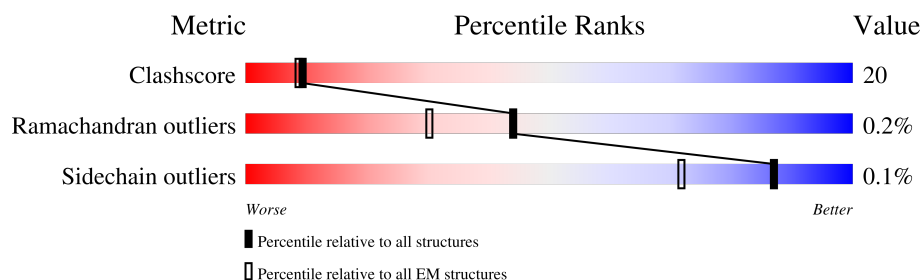
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 38.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2 (38.00 - 38.00)

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

Mol	Chain	Length	Quality of chain
1	A	4168	27% 73% 9% 17%
2	B	4595	33% 73% 18% 6%
3	C	4620	28% 75% 17% 8%
4	d	667	5% 33% 36% 31%

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Mol	Chain	Length	Quality of chain
5	e	670	
6	F	133	
7	G	159	
8	H	92	
9	I	110	
10	J	93	
11	K	111	
12	L	111	
13	M	87	
14	N	132	
15	O	117	
16	P	110	
17	T	309	
18	V	130	
18	x	130	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 87003 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 Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3455	Total	C	N	O	S	0	0
			18127	10919	3573	3623	12		

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4299	Total	C	N	O	S	0	0
			25545	15697	4785	5025	38		

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	4264	Total	C	N	O	S	0	0
			25046	15335	4744	4923	44		

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	459	Total	C	N	O	S	0	0
			3626	2316	609	680	21		

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	545	Total	C	N	O	S	0	0
			3948	2473	697	759	19		

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	98	Total	C	N	O	S	0	0
			781	493	137	149	2		

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	N	O	S	0	0
			744	468	128	147	1		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	85	Total	C	N	O	S	0	0
			702	453	115	130	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	89	Total	C	N	O	S	0	0
			694	443	111	136	4		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	84	Total	C	N	O	S	0	0
			702	459	114	125	4		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			803	525	134	139	5		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	97	Total	C	N	O	S	0	0
			773	506	131	133	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	86	Total	C	N	O	S	0	0
			726	472	122	128	4		

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total	C	N	O	S	0	0
			897	581	154	159	3		

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	111	Total	C	N	O	S	0	0
			878	558	143	174	3		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	103	Total	C	N	O	S	0	0
			847	549	134	161	3		

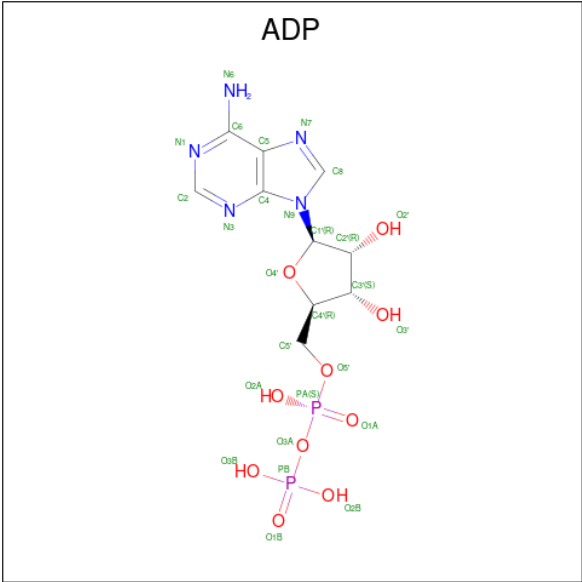
- Molecule 17 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	131	Total	C	N	O	S	0	0
			1057	655	181	215	6		

- Molecule 18 is a protein called Docking complex 1/2 protein.

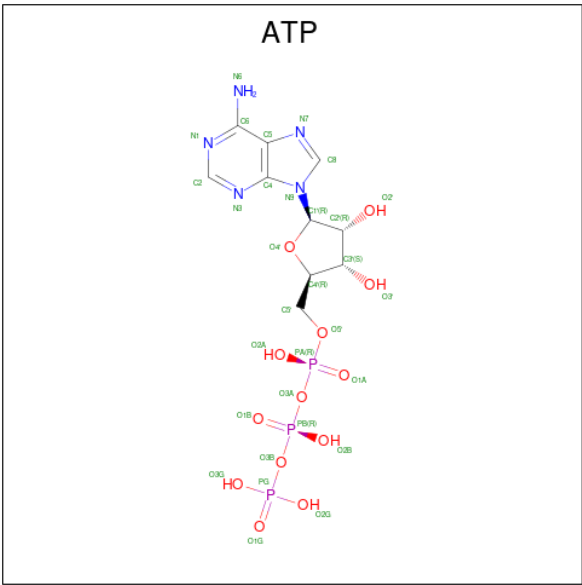
Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	98	Total	C	N	O	0	0
			490	294	98	98		
18	x	101	Total	C	N	O	0	0
			505	303	101	101		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



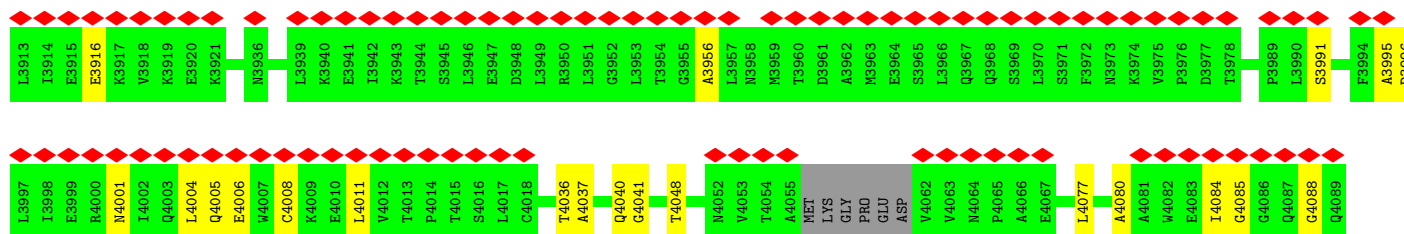
Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

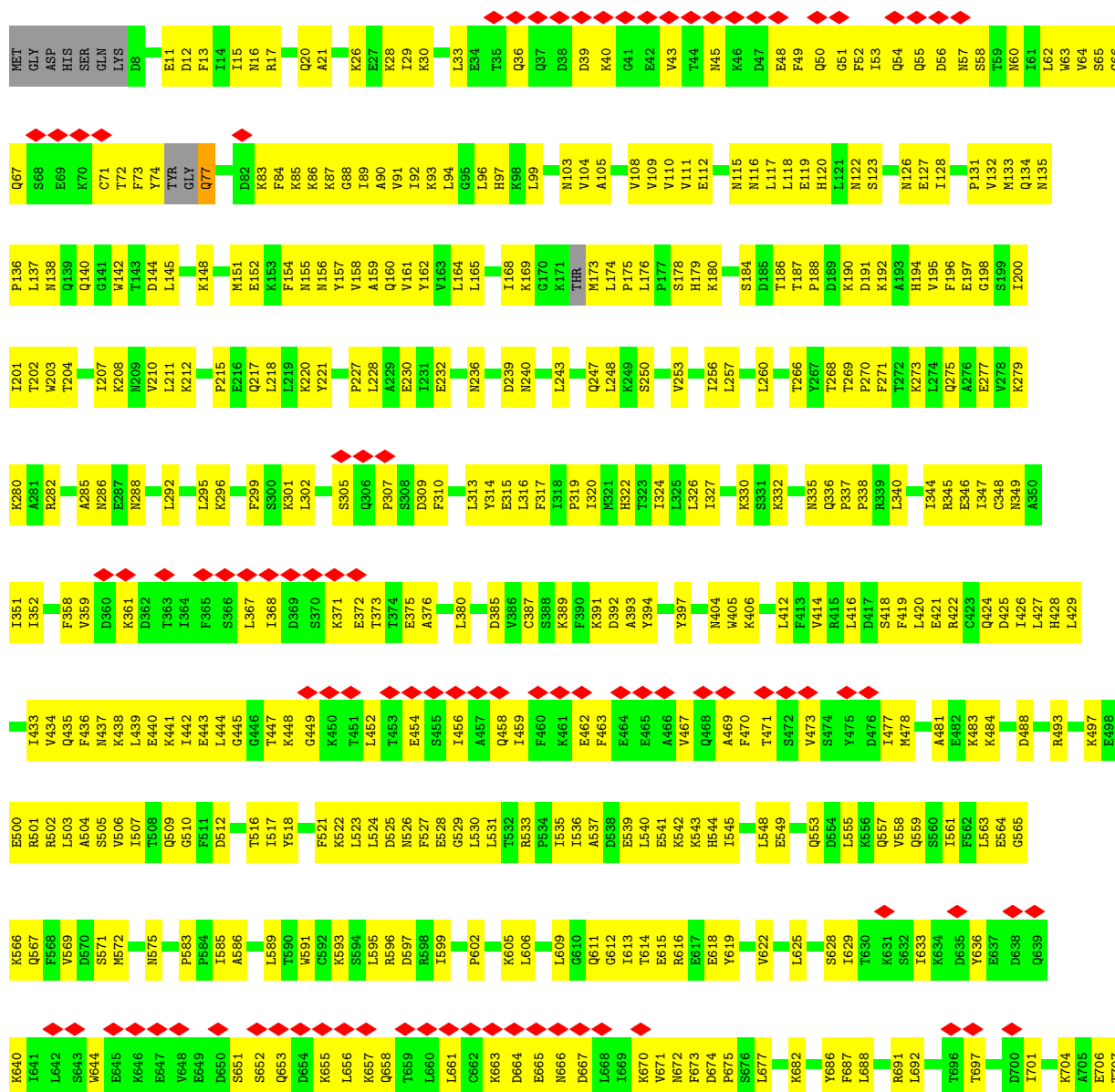


Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			31	10	5	13	3	





• Molecule 2: Outer arm dynein beta heavy chain

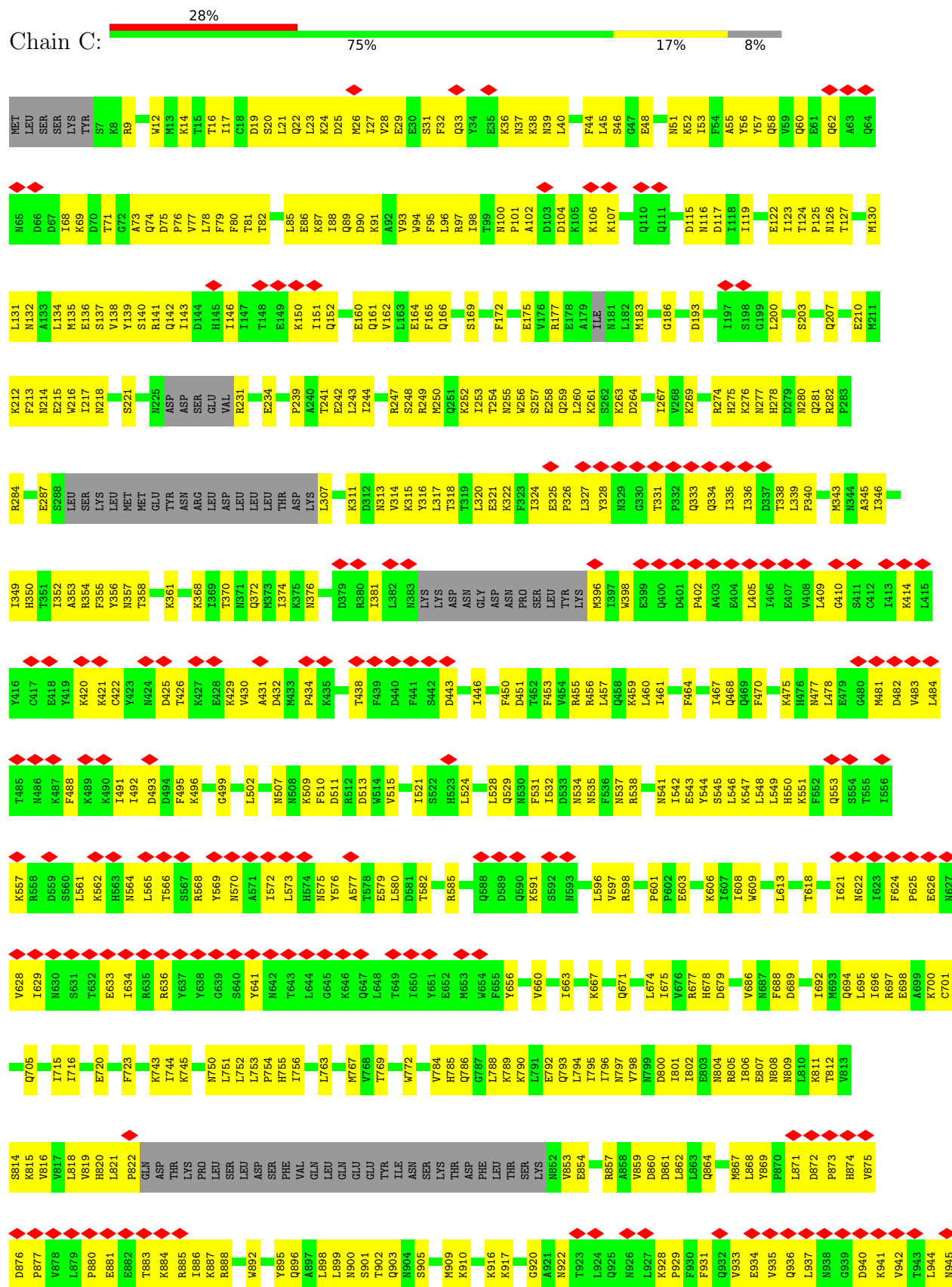


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PRO	LEU	VAL	SER	ALA	LEU	HIS	SER	GLU	PHE	MET	GLU	ASP	ARG	HIS	TRP	SER	GLN	LEU	LYS	GLN	ILE	THR	GLY	THR	VAL	PHE	ASP	HIS	ASN	LEU	ALA	P1353	P1354	E1355	L1356	R1357	N1358	F1359	G1360	G1361	Y1362	N1363	V1364	GLU	ILE	GLU	VAL	ASP	VAL	ALA	GLN	LYS							
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V926	R927	N928	I929	R930	R931	N932	N933	I934	D936	N939	I940	P952	F955	L956	Q957	E958	R959	R960	S961	F962	F963	E964	P965	Q967	C968	L969	A970	M971	I972	N975	C983	N984	Q985	F986	A988	R989	F990	D991	Q908	S909	I910	I911	Q912	F913	D914	P915	E916	E999	D1000	E1001	GLN	ILE	SER						
D861	Y862	V863	N864	V865	L866	V867	I868	S872	T873	A874	I875	T877	L880	H881	L882	N883	E884	Q885	I886	N887	P888	V889	F890	I891	K892	R893	N894	D895	I896	S897	P898	L899	F900	D901	I902	R903	L904	E905	L906	G907	Q908	S909	I910	I911	Q912	F913	D914	P915	E916	E999	D1000	E1001	GLN	ILE	SER				
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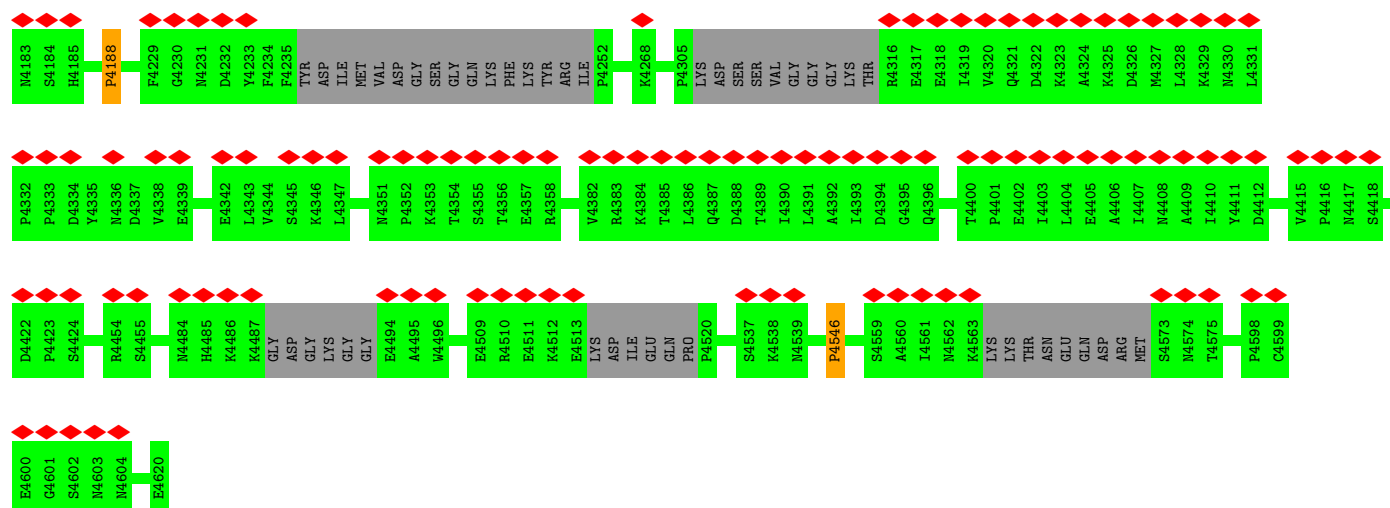
• Molecule 3: Dynein heavy chain, outer arm protein

Chain C:

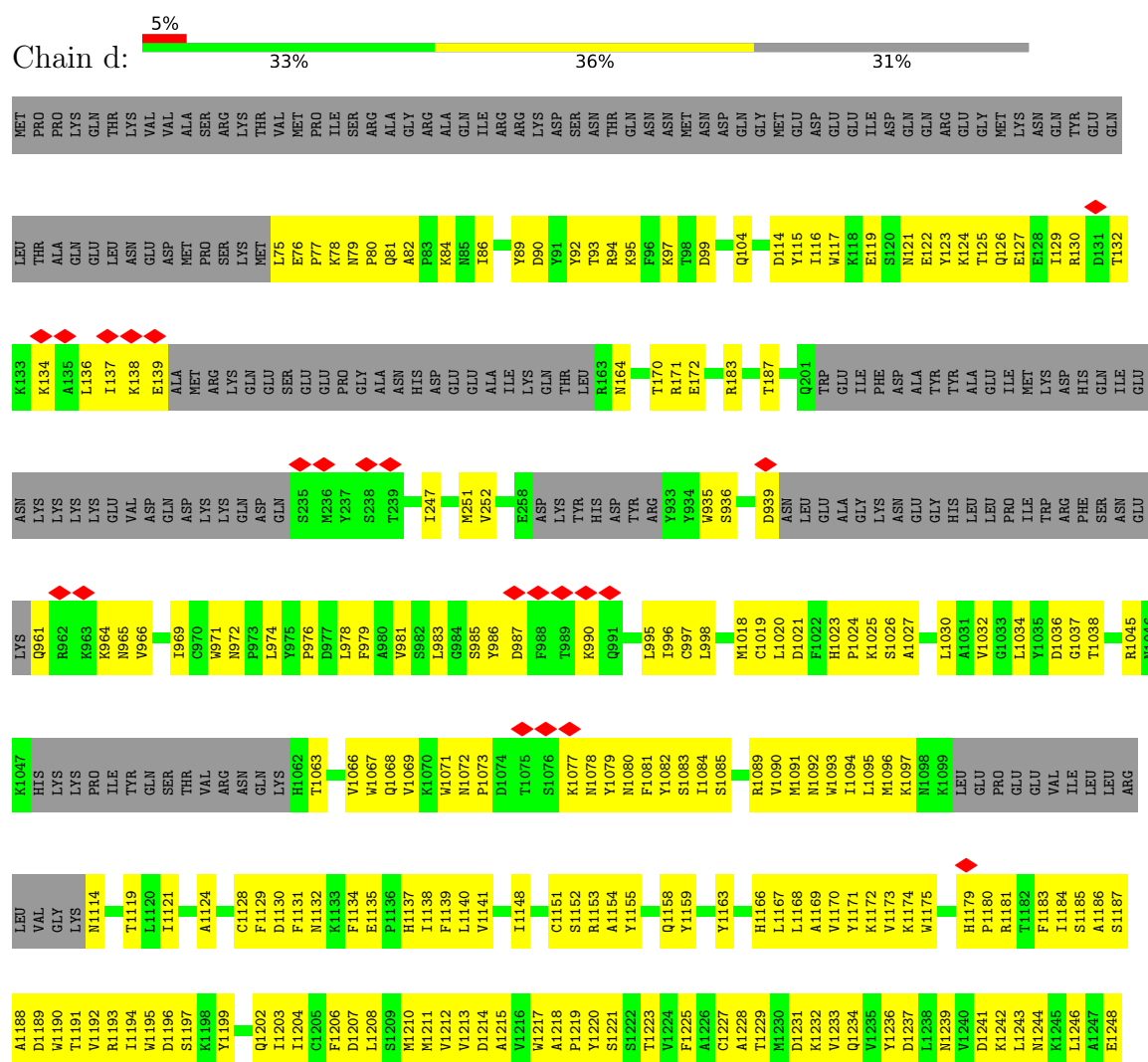




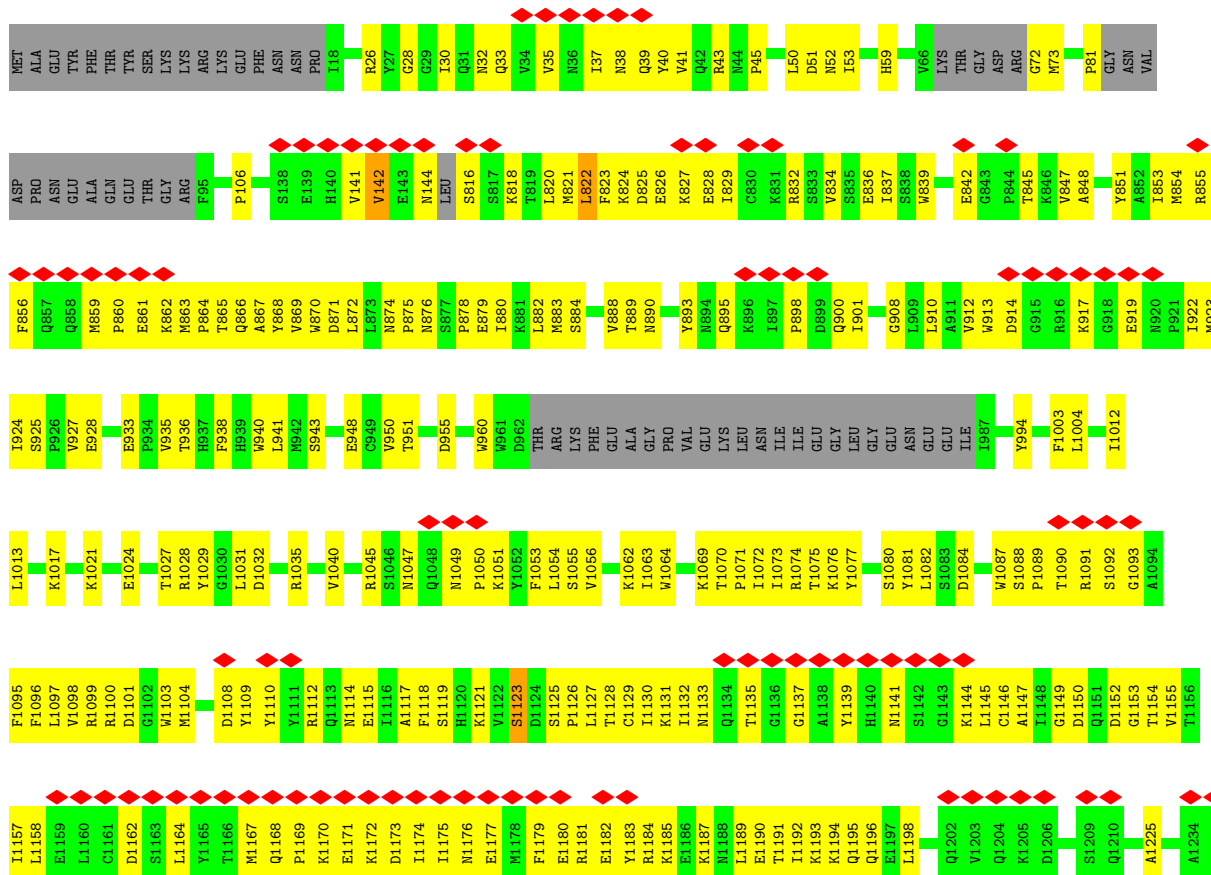
W4040	W4041	I4042	L4043	Q4044	M4045	C4046	H4047	L4048	G4049	L4050	K4051	F4052	M4053	E4054	E4055	V4056	E4057	T4058	L4059	V4060	S4061	P4062	L4063	M4064	I4066	H4067	E4068	D4069	F4070	R4071	L4072	L4073	I4074	T4075	E4076	A4077	Q4078	H4079	P4080	G4081	F4082	P4083	L4084	G4085	L4086	L4087	Q4088	K4089	T4090	L4091	K4092	V4093	V4121	P4180	Q4181	P4182			
S3927	Q3930	E3931	E3966	V3979	Q3980	E3981	S3982	S3983	N3984	M3985	D3986	P3987	V3988	L3989	F3990	L3991	L3992	S3993	A3994	G3995	A3996	D3997	P3998	T3999	I4002	D4003	F4012	P4013	C4014	E4015	K4016	V4017	S4018	M4019	G4020	E4021	G4022	Q4023	E4024	R4025	V4026	A4027	R4028	Q4029	V4030	I4031	M4032	K4033	G4034	F4035	V4036	E4037	G4038	G4039					
N3797	R3798	V3799	K3800	N3801	L3802	L3803	S3804	F3805	L3806	T3807	F3808	H3809	S3852	GLY	ASP	ALA	LEU	ASP	ILE	LYS	SER	GLU	ARG	Q3863	E3870	V3874	K3882	HIS	THR	PHE	SER	GLY	GLN	THR	LEU	P3891	E3895	L3899	I3900	S3903	E3904	N3905	Q3906	F3919	P3920	I3921	P3922	D3923	F3919	P3920	I3921	P3922	D3923	E3926					
N3694	L3695	L3696	E3697	R3698	L3699	I3700	N3701	S3702	Q3703	G3704	N3705	L3706	L3707	D3708	D3709	T3710	E3711	L3712	N3713	V3714	V3715	V3726	L3730	I3740	E3742	K3743	R3744	E3745	Q3746	I3747	R3748	W3769	K3770	I3771	N3772	S3773	E3776	Q3777	F3778	L3779	K3780	L3781	F3782	I3783	S3785	I3786	D3787	L3788	S3789	E3790	K3791	A3792							
N3505	Q3506	G3507	N3539	V3540	I3541	R3542	N3543	K3544	L3545	S3546	A3547	SER	ILE	PRO	GLU	ARG	CYS	I3555	T3556	L3557	L3558	S3559	H3560	P3561	K3562	F3563	K3564	D3565	H3566	F3567	L3568	K3569	C3571	M3572	E3573	S3574	G3575	L3576	T3577	L3578	I3579	V3580	E3581	N3582	E3586	V3587	D3588	D3592	L3595	E3596	ARG	GLN	ILE						
ILE	VAL	LYS	THR	GLN	PHE	ASN	VAL	ALA	THR	GLU	MET	L3617	S3618	K3619	E3620	F3621	Q3657	L3658	L3659	G3660	K3661	V3662	I3663	S3664	K3665	E3666	Q3667	K3668	A3669	L3670	E3671	D3672	S3673	L3674	N3675	Q3676	L3677	L3678	A3679	D3680	V3681	N3682	Q3683	N3684	Q3685	K3686	D3687	L3688	Q3689	K3690	L3691	D3692	K3693						
N3317	A3318	Q3319	T3320	F3321	A3322	T3323	K3324	A3325	S3326	K3327	A3328	A3329	A3330	G3331	L3332	L3333	K3334	A3335	F3336	A3337	A3338	Y3339	Y3340	E3341	H3342	H3343	Q3344	K3345	S3346	K3347	T3348	V3349	F3351	K3352	K3353	Q3354	V3355	A3356	A3357	T3358	E3359	A3360	G3361	R3362	Q3363	A3364	T3365	L3366	E3367	A3368	E3369	D3370							
VAL	PHE	ASN	LYS	GLY	LYS	ALA	VAL	LEU	PHE	LEU	LYS	S3272	Y3273	D3274	E3275	S3276	G3277	I3278	Q3279	T3280	L3281	G3282	D3283	M3284	N3285	F3286	K3287	K3288	K3289	L3290	K3291	E3292	F3293	E3294	K3295	D3296	S3297	I3298	N3299	E3300	E3301	T3302	I3303	E3304	L3305	E3306	E3307	P3308	Y3309	L3310	ILE	PRO	ILE	GLN	ILE	GLU	ASP	TRP	
E3197	L3198	E3199	A3200	A3201	L3202	F3203	A3204	R3205	R3206	R3207	A3208	Q3209	E3210	A3211	V3212	D3213	S3214	I3215	E3216	S3217	K3218	D3219	I3220	V3221	E3222	L3223	K3224	A3225	N3226	K3227	K3228	P3229	L3230	E3231	I3232	I3233	K3234	Y3235	I3236	M3237	D3238	A3239	V3240	L3241	V3242	F3243	F3244	K3245	A3246	R3247	L3248	ILE	PRO	ILE	GLN	ILE	GLU	ASP	TRP
S3137	L3138	K3139	E3140	E3141	E3142	I3143	Q3144	L3145	N3146	E3147	A3148	T3149	E3150	K3151	T3152	N3153	Q3154	L3155	L3156	A3157	D3158	L3159	D3160	K3161	E3162	S3163	K3164	A3165	A3166	N3167	Q3168	Q3170	E3171	E3172	V3173	A3174	A3175	T3176	N3177	K3178	Q3179	C3180	E3181	I3182	Q3183	Q3184	E3185	Q3186	I3187	I3188	S3189	E3190	K3191	E3192	E3193	A3194	E3195	R3196	
A2913	G2914	K2918	E2932	L2935	V2958	G2961	D2962	I2963	S2964	Q2965	A2966	Y2967	C2968	K2969	N2972	L2973	G2974	N2975	I2976	D2977	S2978	P2979	Q2980	T3023	K3048	T3051	K3052	E3053	E3054	T3055	K3056	Q3057	E3058	F3117	N3122	Q3125	E3126	A3127	T3128	I3129	T3130	I3131	N3132	Q3133	N3134	E3135	I3136	F2910	D2911	D2912									
V2754	H2755	G2756	V2757	I2758	Q2759	E2760	V2761	L2762	L2763	E2764	S2765	F2766	S2767	Q2768	I2769	E2770	N2771	E2772	I2773	L2774	E2775	K2776	V2777	S2778	P2779	E2780	K2781	T2782	V2793	I2794	N2795	E2796	D2797	G2798	I2799	L2800	E2801	E2802	E2803	K2804	F2805	T2815	E2816	V2830	L2864	T2884	K2885	T2886	Y2887	S2888	F2910	D2911	D2912						



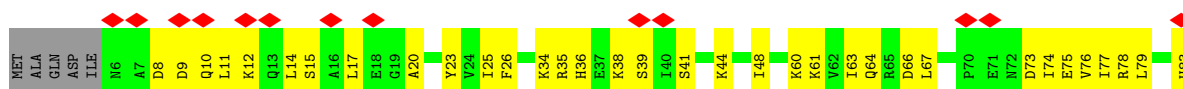
• Molecule 4: Dynein intermediate chain 2



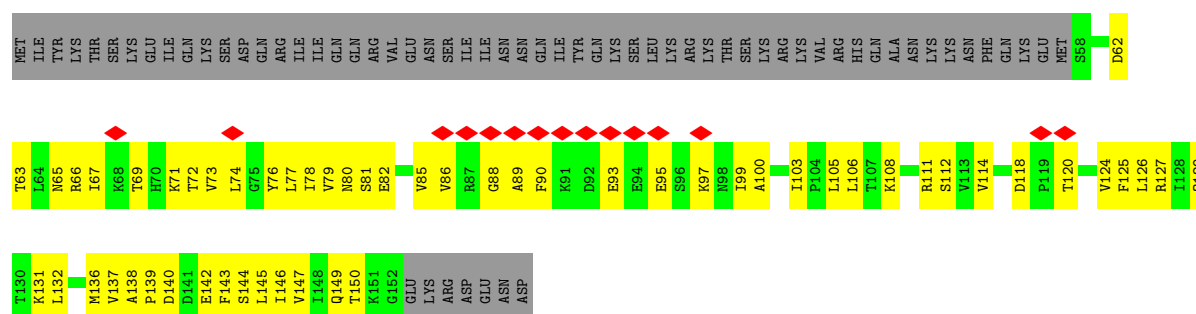
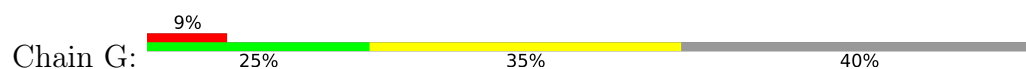
- Molecule 5: Flagellar outer dynein arm intermediate protein, putative



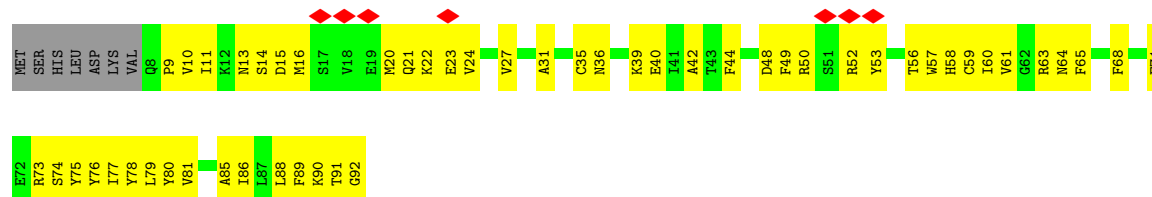
- Molecule 6: Dynein light chain roadblock-type 2 protein



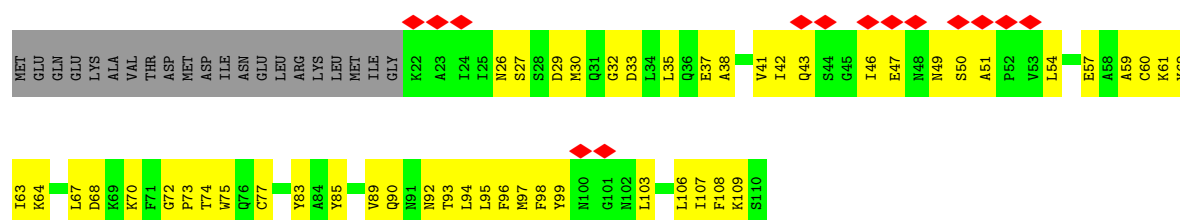
- Molecule 7: Dynein light chain roadblock-type 2 protein



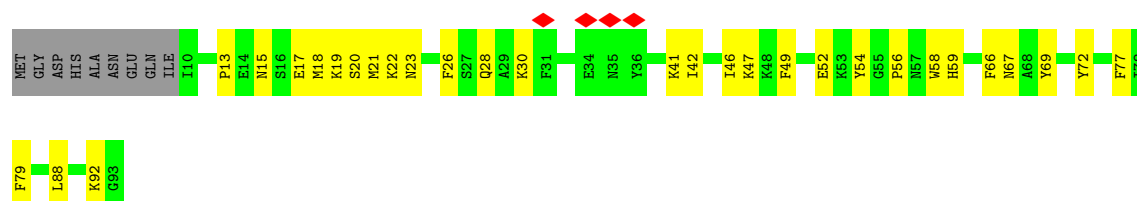
- Molecule 8: Dynein light chain



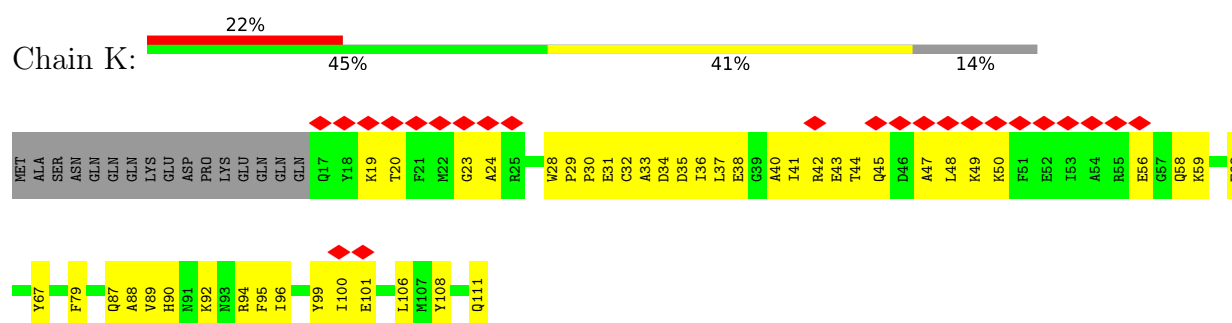
- Molecule 9: Dynein light chain



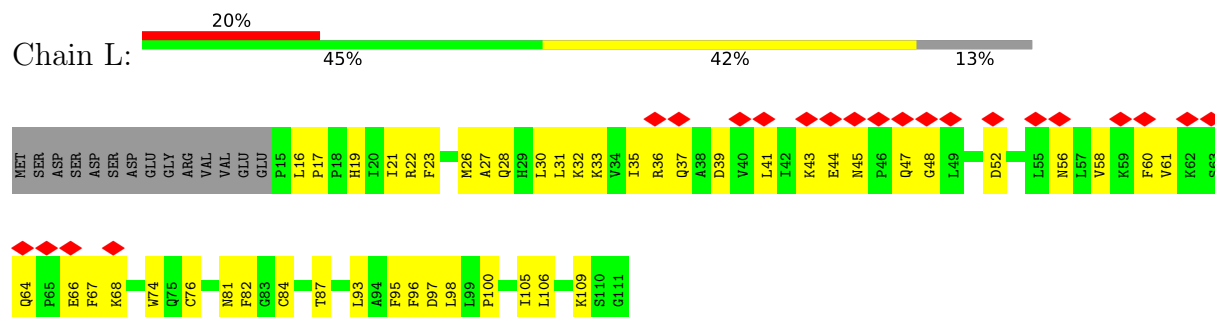
- Molecule 10: Dynein light chain



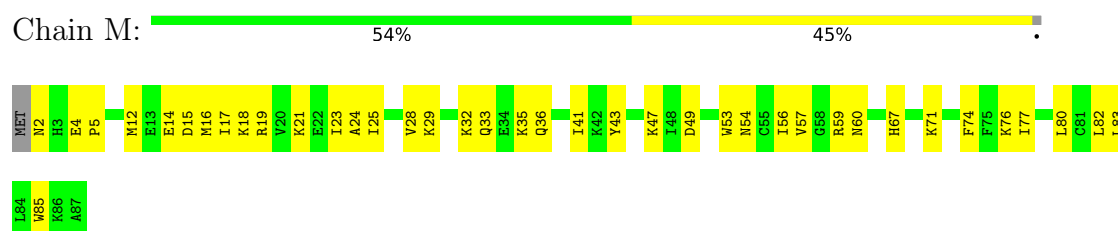
- Molecule 11: Dynein light chain



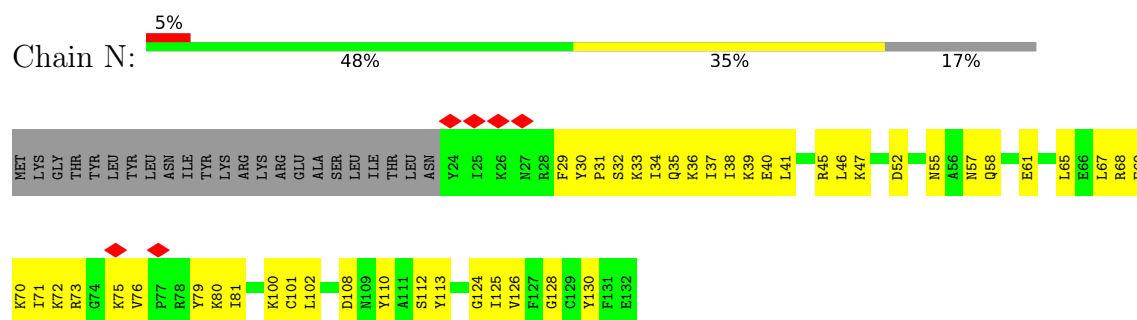
• Molecule 12: Dynein light chain



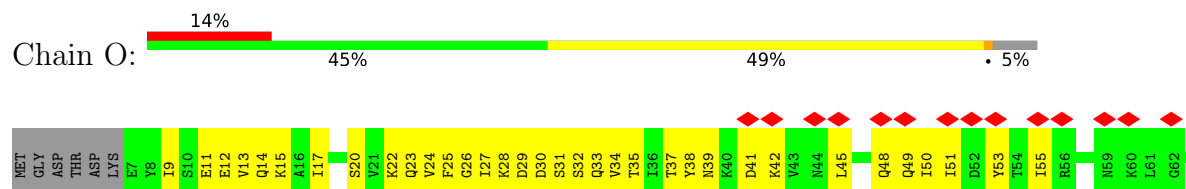
• Molecule 13: Dynein light chain



• Molecule 14: Dynein light chain 2A



• Molecule 15: Dynein light chain tctex-type 1 protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80.0	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.252	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	629.0, 629.0, 629.0	wwPDB
Map dimensions	74, 74, 74	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	8.5, 8.5, 8.5	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/18167	0.78	9/25169 (0.0%)
2	B	1.01	266/25709 (1.0%)	0.87	88/35300 (0.2%)
3	C	1.07	303/25227 (1.2%)	0.85	198/34687 (0.6%)
4	d	0.24	0/3710	0.51	0/5026
5	e	0.24	0/4021	0.57	5/5463 (0.1%)
6	F	0.23	0/793	0.54	0/1070
7	G	0.20	0/751	0.45	0/1014
8	H	0.16	0/718	0.38	0/965
9	I	0.19	0/705	0.46	0/954
10	J	0.16	0/723	0.41	0/966
11	K	0.25	0/828	0.59	0/1114
12	L	0.19	0/790	0.44	0/1063
13	M	0.20	0/743	0.42	0/996
14	N	0.26	0/915	0.58	0/1229
15	O	0.19	0/891	0.47	0/1209
16	P	3.92	186/866 (21.5%)	2.58	62/1171 (5.3%)
17	T	0.19	0/1070	0.44	0/1436
All	All	0.90	755/86627 (0.9%)	0.83	362/118832 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
3	C	0	5
All	All	0	8

All (755) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1075	TRP	C-O	24.46	1.54	1.24
3	C	3345	LYS	C-O	-18.77	1.00	1.24
2	B	1244	LEU	N-CA	-16.00	1.35	1.46
3	C	3307	GLU	N-CA	-15.79	1.33	1.46
3	C	3331	GLY	CA-C	15.63	1.69	1.52
3	C	3215	ILE	CA-CB	14.87	1.71	1.54
3	C	3355	GLN	C-N	14.87	1.52	1.33
3	C	3212	VAL	CA-CB	13.98	1.70	1.54
3	C	3228	LYS	C-O	13.80	1.38	1.24
3	C	3280	THR	CA-C	13.78	1.70	1.52
3	C	3238	ASP	N-CA	13.63	1.62	1.46
3	C	3273	TYR	CA-C	13.54	1.70	1.52
3	C	3274	ASP	N-CA	13.53	1.63	1.46
3	C	3229	PRO	CA-C	-13.52	1.38	1.52
3	C	3336	ALA	N-CA	13.46	1.62	1.46
3	C	3208	ALA	CA-C	-13.40	1.35	1.52
3	C	3343	HIS	N-CA	13.37	1.62	1.46
3	C	3281	LEU	N-CA	13.09	1.63	1.46
2	B	1245	PRO	CA-CB	13.06	1.67	1.53
3	C	3286	PHE	N-CA	-13.05	1.30	1.46
3	C	3332	ILE	N-CA	13.03	1.62	1.46
3	C	3335	TRP	CA-C	12.91	1.69	1.52
3	C	3236	ILE	CA-CB	12.87	1.71	1.54
3	C	3337	PHE	N-CA	-12.73	1.30	1.46
3	C	3209	GLN	N-CA	-12.69	1.30	1.46
3	C	3321	PHE	CA-C	-12.63	1.36	1.52
3	C	3235	TYR	C-N	12.44	1.49	1.33
3	C	3205	LEU	N-CA	-12.32	1.31	1.46
3	C	3336	ALA	CA-C	-12.21	1.36	1.52
3	C	3285	ASN	CA-C	-12.21	1.36	1.52
3	C	3210	GLU	N-CA	12.13	1.61	1.46
3	C	3237	MET	CA-C	12.12	1.69	1.52
3	C	3324	LYS	C-N	12.03	1.49	1.33
3	C	3220	ILE	N-CA	12.03	1.60	1.46
16	P	80	VAL	CA-CB	12.01	1.68	1.54
3	C	3283	ASP	C-O	-11.89	1.09	1.23
3	C	3207	ARG	C-N	11.87	1.49	1.33
3	C	3219	ASP	CA-C	11.86	1.68	1.52
3	C	3215	ILE	CA-C	-11.84	1.38	1.52
3	C	3303	ILE	C-N	11.81	1.49	1.33
3	C	3240	VAL	CA-CB	11.67	1.69	1.54
3	C	3342	TYR	CA-C	11.61	1.68	1.52
3	C	3225	ALA	C-N	-11.60	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3299	ASN	N-CA	11.57	1.59	1.45
3	C	3290	LEU	C-O	-11.57	1.10	1.24
3	C	3334	LYS	C-N	-11.57	1.18	1.33
3	C	3214	SER	C-N	11.54	1.48	1.33
3	C	3247	ARG	C-O	11.52	1.36	1.23
3	C	3204	ALA	CA-C	-11.43	1.37	1.52
3	C	3272	SER	C-N	-11.42	1.18	1.33
3	C	3290	LEU	N-CA	-11.39	1.32	1.46
3	C	3306	LEU	N-CA	11.32	1.60	1.46
3	C	3275	GLU	N-CA	-11.29	1.32	1.46
3	C	3317	PHE	C-O	-11.28	1.10	1.23
16	P	77	LEU	N-CA	-11.28	1.38	1.46
3	C	3230	LEU	N-CA	-11.27	1.30	1.45
3	C	3322	ALA	N-CA	-11.25	1.31	1.46
2	B	1319	HIS	CE1-NE2	11.23	1.43	1.32
3	C	3234	LYS	C-N	-11.23	1.18	1.33
3	C	3308	PRO	CA-CB	11.21	1.69	1.53
3	C	3312	GLN	C-O	11.19	1.38	1.24
16	P	17	ILE	N-CA	11.10	1.59	1.46
3	C	3216	GLU	C-N	-11.06	1.18	1.33
3	C	3248	LEU	C-O	11.03	1.37	1.23
3	C	3325	ALA	CA-CB	10.98	1.70	1.53
3	C	3227	LYS	C-N	-10.96	1.19	1.32
3	C	3237	MET	N-CA	-10.94	1.32	1.46
3	C	3295	LYS	CA-C	10.93	1.68	1.52
3	C	3309	TYR	CA-C	10.93	1.67	1.52
3	C	3209	GLN	CA-C	10.92	1.66	1.52
3	C	3305	LEU	CA-C	10.92	1.67	1.52
3	C	3234	LYS	N-CA	10.90	1.59	1.46
16	P	58	VAL	N-CA	10.89	1.59	1.46
3	C	3296	ASP	N-CA	10.85	1.60	1.46
3	C	3286	PHE	C-O	-10.84	1.11	1.24
3	C	3334	LYS	CA-CB	10.78	1.70	1.53
2	B	1298	LEU	CA-C	10.76	1.65	1.52
3	C	3311	ASN	C-N	-10.76	1.19	1.34
16	P	16	ASP	CA-C	10.74	1.67	1.52
3	C	3304	GLU	C-N	-10.69	1.18	1.33
3	C	3313	SER	C-O	10.65	1.37	1.24
3	C	3299	ASN	CA-C	-10.64	1.40	1.52
3	C	3330	ALA	N-CA	-10.64	1.33	1.46
16	P	57	LYS	CA-C	10.63	1.65	1.52
3	C	3281	LEU	C-O	10.58	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3310	LEU	N-CA	10.53	1.59	1.46
3	C	3226	ASN	CA-CB	-10.51	1.35	1.53
3	C	3226	ASN	CA-C	10.51	1.66	1.52
3	C	3335	TRP	CA-CB	-10.45	1.37	1.53
3	C	3216	GLU	N-CA	-10.44	1.32	1.45
3	C	3322	ALA	C-O	-10.41	1.10	1.24
3	C	3224	LYS	C-O	10.40	1.37	1.24
3	C	3298	ILE	CA-C	10.37	1.66	1.52
3	C	3218	LYS	C-N	-10.33	1.19	1.33
3	C	3289	LYS	CA-C	-10.27	1.38	1.52
2	B	1369	VAL	CA-C	10.24	1.65	1.52
16	P	7	GLU	CA-C	10.21	1.64	1.52
3	C	3300	GLU	N-CA	-10.17	1.34	1.46
3	C	3246	ALA	C-N	10.15	1.46	1.33
3	C	3211	ALA	C-N	10.13	1.46	1.33
3	C	3221	VAL	N-CA	-10.13	1.34	1.46
2	B	77	GLN	N-CA	10.13	1.65	1.46
3	C	3296	ASP	C-O	10.04	1.36	1.24
16	P	79	HIS	CA-CB	10.03	1.66	1.52
3	C	3227	LYS	N-CA	10.01	1.58	1.46
3	C	3333	LEU	C-N	10.01	1.47	1.33
3	C	3304	GLU	CA-CB	9.98	1.68	1.53
16	P	21	ASN	N-CA	9.96	1.57	1.45
3	C	3306	LEU	CA-C	-9.95	1.39	1.52
16	P	24	VAL	CA-CB	9.94	1.67	1.54
3	C	3291	LYS	CA-CB	9.89	1.69	1.53
16	P	8	ILE	N-CA	9.88	1.57	1.46
16	P	25	LEU	CA-CB	9.85	1.66	1.53
3	C	3330	ALA	CA-CB	9.83	1.68	1.53
3	C	3243	PHE	CA-C	-9.80	1.39	1.52
16	P	26	VAL	CA-CB	9.78	1.66	1.54
3	C	3209	GLN	C-O	-9.78	1.12	1.24
3	C	3218	LYS	CA-CB	9.77	1.68	1.53
3	C	3236	ILE	CA-C	-9.71	1.40	1.52
3	C	3274	ASP	CA-C	-9.69	1.39	1.52
3	C	3220	ILE	C-O	9.66	1.35	1.24
3	C	3208	ALA	CA-CB	9.66	1.68	1.53
3	C	3233	ILE	CA-C	9.65	1.65	1.52
3	C	3214	SER	N-CA	9.64	1.58	1.46
3	C	3213	ASP	CA-C	9.61	1.65	1.52
2	B	1297	GLN	N-CA	9.60	1.57	1.46
3	C	3305	LEU	CA-CB	-9.60	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3248	LEU	CA-CB	-9.58	1.37	1.53
3	C	3241	LEU	CA-C	9.57	1.65	1.52
3	C	3279	GLN	CA-CB	9.53	1.68	1.53
3	C	3219	ASP	CA-CB	-9.52	1.38	1.53
3	C	3339	ILE	CA-CB	-9.50	1.40	1.54
3	C	3293	PHE	CA-C	-9.50	1.40	1.52
3	C	3292	GLU	CA-CB	-9.49	1.40	1.53
2	B	1296	LYS	CA-C	9.48	1.65	1.52
3	C	3340	TYR	CA-C	-9.47	1.40	1.52
3	C	3345	LYS	N-CA	-9.45	1.33	1.46
3	C	3310	LEU	C-O	-9.44	1.13	1.24
3	C	3340	TYR	C-N	9.44	1.47	1.33
16	P	60	ILE	C-O	9.37	1.35	1.24
2	B	1301	CYS	CA-C	9.37	1.64	1.52
3	C	3314	GLU	C-O	9.37	1.35	1.24
3	C	3279	GLN	C-N	-9.36	1.21	1.33
3	C	3227	LYS	C-O	9.33	1.35	1.24
2	B	1366	VAL	N-CA	9.31	1.57	1.46
3	C	3207	ARG	CA-CB	-9.30	1.38	1.53
16	P	55	ILE	CA-CB	9.30	1.65	1.54
3	C	3328	ALA	CA-CB	-9.27	1.37	1.53
2	B	1274	ILE	N-CA	9.25	1.57	1.46
3	C	3217	SER	C-N	9.25	1.45	1.33
16	P	6	ILE	N-CA	9.21	1.57	1.46
3	C	3220	ILE	CA-C	-9.20	1.41	1.52
16	P	20	LYS	CA-C	9.18	1.65	1.52
2	B	1342	ASN	N-CA	-9.18	1.35	1.46
3	C	3329	ALA	C-N	9.17	1.45	1.33
3	C	3278	ILE	C-N	9.17	1.45	1.33
3	C	3235	TYR	CA-CB	-9.11	1.38	1.53
16	P	54	THR	CA-CB	9.11	1.64	1.52
3	C	3244	PHE	N-CA	-9.10	1.32	1.46
16	P	59	ASN	CA-C	9.07	1.63	1.52
16	P	101	TRP	NE1-CE2	-9.05	1.27	1.37
3	C	3307	GLU	C-N	9.03	1.46	1.33
3	C	3354	ILE	C-O	-8.99	1.13	1.24
16	P	30	ALA	C-O	8.98	1.35	1.23
2	B	1220	GLN	C-N	8.98	1.45	1.33
3	C	3333	LEU	C-O	8.97	1.34	1.24
16	P	69	VAL	C-N	8.96	1.45	1.33
2	B	1368	LYS	CA-CB	8.89	1.67	1.53
16	P	49	ASP	C-N	8.89	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3205	LEU	C-O	-8.88	1.13	1.24
2	B	1341	THR	CA-C	-8.87	1.41	1.52
2	B	1330	TRP	N-CA	8.83	1.58	1.46
3	C	3239	ALA	CA-CB	-8.82	1.39	1.53
3	C	3311	ASN	C-O	8.78	1.34	1.23
3	C	3244	PHE	C-O	-8.76	1.09	1.24
16	P	15	GLU	CA-CB	8.76	1.67	1.53
2	B	1231	LYS	C-N	8.73	1.45	1.33
3	C	3239	ALA	C-N	8.73	1.45	1.33
3	C	3309	TYR	CA-CB	-8.73	1.38	1.53
16	P	77	LEU	CA-C	8.72	1.62	1.52
3	C	3242	VAL	N-CA	8.70	1.57	1.46
2	B	1330	TRP	C-O	8.69	1.35	1.24
16	P	84	HIS	CE1-NE2	-8.64	1.24	1.32
2	B	1302	MET	N-CA	8.64	1.57	1.46
2	B	1253	GLY	C-N	8.63	1.45	1.34
3	C	3320	THR	CA-CB	-8.59	1.39	1.53
3	C	3343	HIS	CA-C	-8.59	1.41	1.52
3	C	3325	ALA	C-O	-8.58	1.14	1.24
3	C	3339	ILE	N-CA	8.57	1.57	1.46
2	B	1240	PHE	C-N	8.57	1.45	1.33
16	P	88	VAL	C-N	8.55	1.43	1.33
3	C	3277	GLY	N-CA	8.54	1.56	1.45
2	B	1250	GLU	C-N	8.51	1.46	1.33
16	P	14	PHE	C-N	8.50	1.44	1.33
2	B	1215	GLN	CA-C	8.49	1.64	1.52
3	C	3320	THR	N-CA	8.49	1.56	1.46
2	B	1282	ASN	C-N	8.46	1.45	1.33
3	C	3294	GLU	N-CA	-8.46	1.34	1.45
16	P	72	HIS	CG-ND1	-8.43	1.28	1.38
3	C	3320	THR	C-N	8.40	1.45	1.33
16	P	86	LYS	N-CA	8.38	1.56	1.46
3	C	3230	LEU	C-N	-8.38	1.23	1.33
16	P	91	GLN	CA-CB	8.36	1.67	1.53
3	C	3245	LYS	N-CA	8.33	1.57	1.46
2	B	1294	ASN	C-N	8.30	1.45	1.33
3	C	3288	LYS	C-N	8.30	1.45	1.33
16	P	21	ASN	C-N	8.29	1.44	1.33
16	P	44	GLU	CA-C	8.29	1.63	1.52
2	B	1305	LEU	N-CA	8.27	1.56	1.46
16	P	100	LEU	C-N	8.25	1.44	1.33
3	C	3319	ASP	C-O	-8.25	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3244	PHE	C-N	8.24	1.43	1.33
3	C	3287	MET	N-CA	8.24	1.56	1.46
16	P	72	HIS	CD2-NE2	-8.23	1.28	1.37
2	B	1364	VAL	CA-C	-8.22	1.42	1.52
16	P	53	LEU	C-N	8.22	1.45	1.33
2	B	1329	PRO	CA-C	8.21	1.64	1.52
3	C	3289	LYS	C-N	8.21	1.44	1.33
2	B	1273	ALA	CA-C	8.20	1.63	1.52
2	B	1299	LYS	N-CA	8.20	1.56	1.46
3	C	3302	THR	N-CA	8.18	1.56	1.46
3	C	3274	ASP	C-O	8.17	1.34	1.24
3	C	3329	ALA	CA-C	-8.15	1.41	1.52
2	B	1245	PRO	C-N	8.14	1.45	1.33
2	B	1264	ILE	C-N	8.12	1.44	1.33
3	C	3290	LEU	CA-CB	8.11	1.66	1.53
2	B	1224	ARG	CZ-NH1	8.11	1.44	1.32
16	P	79	HIS	CE1-NE2	8.10	1.40	1.32
2	B	1315	ILE	C-N	8.09	1.44	1.34
3	C	3344	GLN	C-N	8.09	1.45	1.33
16	P	95	ASN	CA-C	8.08	1.62	1.53
2	B	1363	ASN	C-N	8.07	1.44	1.33
3	C	3217	SER	CA-CB	-8.07	1.39	1.53
3	C	3314	GLU	N-CA	-8.04	1.36	1.46
2	B	1367	GLU	C-N	8.03	1.44	1.33
16	P	63	GLU	N-CA	8.03	1.56	1.46
16	P	55	ILE	C-O	-8.02	1.15	1.24
3	C	3305	LEU	C-N	8.01	1.45	1.33
3	C	3317	PHE	C-N	8.00	1.44	1.33
16	P	85	LYS	CA-C	7.99	1.63	1.53
16	P	89	VAL	C-O	-7.95	1.15	1.23
3	C	3223	LEU	C-O	7.94	1.34	1.24
3	C	3297	SER	C-N	-7.94	1.24	1.33
2	B	1303	ASN	N-CA	-7.94	1.36	1.46
2	B	1318	ILE	N-CA	7.94	1.55	1.46
2	B	1335	ALA	CA-C	7.93	1.62	1.52
3	C	3229	PRO	CA-CB	7.91	1.62	1.54
16	P	92	PHE	CA-CB	7.91	1.67	1.53
2	B	1339	LEU	CA-C	-7.90	1.42	1.52
16	P	84	HIS	CG-ND1	-7.90	1.29	1.38
2	B	1314	ALA	C-N	-7.90	1.24	1.34
2	B	1255	GLU	N-CA	-7.89	1.37	1.46
2	B	1259	ASN	N-CA	-7.87	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1325	TRP	NE1-CE2	-7.87	1.28	1.37
2	B	1243	LYS	CA-C	-7.87	1.41	1.52
2	B	1281	TYR	N-CA	7.86	1.56	1.46
16	P	38	ILE	C-O	7.84	1.34	1.24
3	C	3294	GLU	C-N	-7.84	1.22	1.33
2	B	1365	ILE	N-CA	-7.83	1.35	1.46
16	P	50	HIS	C-O	7.83	1.33	1.23
2	B	1356	ILE	CA-CB	-7.82	1.45	1.54
16	P	21	ASN	CA-C	-7.81	1.43	1.52
16	P	76	SER	CA-C	-7.80	1.42	1.52
2	B	1237	ARG	NE-CZ	-7.80	1.24	1.33
2	B	1213	PRO	C-O	7.79	1.34	1.24
3	C	3230	LEU	CA-CB	7.79	1.65	1.53
2	B	1355	GLU	C-N	-7.78	1.24	1.33
2	B	1358	ASN	CA-C	7.76	1.63	1.52
3	C	3308	PRO	C-N	-7.76	1.22	1.33
2	B	1233	VAL	N-CA	-7.75	1.37	1.46
2	B	1336	ASP	N-CA	7.74	1.56	1.46
2	B	1322	TYR	C-N	7.74	1.44	1.33
3	C	3319	ASP	CA-C	7.73	1.62	1.52
16	P	91	GLN	C-O	-7.73	1.15	1.23
16	P	43	PHE	CA-CB	7.73	1.65	1.53
2	B	1356	ILE	C-N	7.71	1.44	1.33
2	B	1297	GLN	CA-C	-7.70	1.43	1.52
2	B	1316	ALA	CA-C	-7.70	1.42	1.52
3	C	3325	ALA	CA-C	-7.70	1.43	1.52
3	C	3242	VAL	C-N	7.68	1.44	1.34
3	C	3222	GLU	CA-C	7.66	1.63	1.52
2	B	1254	TYR	CA-CB	7.65	1.66	1.53
3	C	3231	ASP	C-N	7.64	1.43	1.33
2	B	1317	LEU	N-CA	-7.63	1.36	1.46
3	C	3276	SER	CA-C	7.62	1.63	1.52
3	C	3333	LEU	N-CA	-7.61	1.37	1.46
3	C	3341	GLU	N-CA	-7.61	1.35	1.46
2	B	1252	MET	C-N	-7.60	1.24	1.33
2	B	1315	ILE	CA-CB	-7.59	1.43	1.54
2	B	1349	ILE	C-N	7.59	1.43	1.33
2	B	1340	ASP	N-CA	-7.58	1.36	1.46
3	C	3233	ILE	N-CA	-7.57	1.37	1.46
3	C	3284	MET	C-N	7.57	1.44	1.34
2	B	1269	HIS	CD2-NE2	-7.56	1.29	1.37
3	C	3336	ALA	C-O	7.55	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1252	MET	N-CA	-7.54	1.36	1.45
2	B	1340	ASP	C-N	7.54	1.44	1.33
2	B	1359	PHE	N-CA	7.53	1.55	1.46
2	B	1271	LEU	C-N	7.52	1.44	1.33
16	P	36	CYS	CA-C	-7.51	1.43	1.52
3	C	3284	MET	N-CA	7.51	1.56	1.46
2	B	1309	LYS	CA-CB	7.51	1.65	1.53
3	C	3201	ALA	CA-CB	-7.51	1.40	1.53
3	C	3247	ARG	C-N	7.50	1.43	1.33
2	B	1266	VAL	C-N	7.50	1.44	1.33
2	B	1249	THR	CA-C	-7.49	1.42	1.52
3	C	3278	ILE	C-O	7.49	1.32	1.24
3	C	3213	ASP	C-O	-7.49	1.14	1.24
16	P	90	LYS	CA-CB	7.48	1.68	1.54
2	B	1283	ASN	CA-CB	7.47	1.65	1.53
16	P	37	LYS	N-CA	-7.46	1.35	1.45
2	B	1240	PHE	N-CA	-7.44	1.37	1.46
3	C	3341	GLU	CA-CB	7.43	1.66	1.53
2	B	1258	ASN	CA-C	-7.42	1.43	1.52
2	B	1223	LYS	N-CA	7.42	1.55	1.46
3	C	3288	LYS	C-O	-7.41	1.15	1.24
3	C	3286	PHE	C-N	7.38	1.43	1.33
2	B	1342	ASN	C-N	7.37	1.44	1.33
2	B	1364	VAL	CA-CB	7.36	1.64	1.54
3	C	3312	GLN	CA-CB	-7.35	1.41	1.53
2	B	1241	MET	CA-CB	7.35	1.64	1.53
3	C	3282	GLY	C-O	7.33	1.32	1.23
2	B	1332	GLN	CA-CB	7.33	1.65	1.53
2	B	1256	ASN	N-CA	7.31	1.55	1.46
3	C	3282	GLY	N-CA	-7.30	1.36	1.45
2	B	1221	ASN	CA-CB	7.29	1.64	1.53
16	P	59	ASN	C-N	-7.29	1.25	1.34
3	C	3246	ALA	CA-CB	7.28	1.62	1.52
16	P	31	SER	C-N	-7.27	1.24	1.33
2	B	1252	MET	CA-CB	7.26	1.67	1.53
2	B	1306	LYS	C-N	7.24	1.43	1.33
2	B	1300	ASP	C-N	-7.24	1.24	1.33
3	C	3217	SER	C-O	7.24	1.33	1.24
2	B	1269	HIS	CG-ND1	-7.23	1.30	1.38
16	P	12	LYS	CA-C	7.22	1.62	1.52
16	P	81	PHE	CA-CB	7.22	1.66	1.53
3	C	3223	LEU	CA-CB	-7.21	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	87	THR	C-O	7.19	1.32	1.23
2	B	1254	TYR	CA-C	-7.18	1.43	1.52
3	C	3247	ARG	CA-CB	7.18	1.62	1.52
16	P	80	VAL	C-O	-7.17	1.16	1.24
3	C	3206	ARG	C-O	-7.16	1.15	1.24
3	C	3312	GLN	CA-C	7.13	1.62	1.52
2	B	1334	LYS	N-CA	7.12	1.54	1.46
2	B	1247	ASP	C-N	7.12	1.44	1.33
2	B	1365	ILE	CA-C	7.12	1.62	1.52
2	B	1312	TRP	NE1-CE2	7.11	1.45	1.37
3	C	3214	SER	C-O	7.11	1.33	1.24
16	P	98	ASP	C-N	7.11	1.43	1.33
16	P	10	SER	N-CA	7.07	1.54	1.46
16	P	42	GLN	C-N	7.07	1.44	1.33
3	C	3216	GLU	CA-CB	7.07	1.65	1.53
2	B	1232	GLU	CA-CB	7.06	1.64	1.53
3	C	3232	ILE	CA-CB	7.06	1.62	1.54
2	B	1363	ASN	N-CA	7.05	1.55	1.46
3	C	3206	ARG	C-N	-7.03	1.24	1.33
16	P	70	GLU	CA-CB	7.02	1.64	1.53
2	B	1290	LEU	C-O	-7.01	1.15	1.23
3	C	3322	ALA	C-N	6.99	1.43	1.34
2	B	1302	MET	C-O	6.99	1.33	1.24
3	C	3313	SER	N-CA	6.96	1.55	1.46
3	C	3238	ASP	C-N	-6.95	1.24	1.33
3	C	3235	TYR	C-O	6.94	1.32	1.24
16	P	38	ILE	CA-CB	-6.94	1.46	1.54
2	B	1302	MET	CA-C	-6.93	1.43	1.52
16	P	78	PRO	C-O	-6.93	1.15	1.24
16	P	13	GLN	N-CA	6.92	1.54	1.46
16	P	60	ILE	N-CA	6.92	1.55	1.46
2	B	1232	GLU	CA-C	-6.92	1.43	1.52
16	P	66	GLU	C-O	-6.91	1.15	1.24
3	C	3298	ILE	C-N	6.90	1.43	1.33
16	P	70	GLU	C-O	-6.90	1.16	1.24
2	B	1289	GLU	C-O	-6.89	1.15	1.23
3	C	3212	VAL	C-O	-6.89	1.16	1.24
16	P	60	ILE	CA-CB	-6.89	1.44	1.54
16	P	33	CYS	CA-CB	6.87	1.64	1.53
3	C	3223	LEU	N-CA	6.86	1.55	1.46
3	C	3326	SER	N-CA	-6.85	1.38	1.46
3	C	3319	ASP	C-N	-6.85	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1304	ASP	CA-C	6.85	1.61	1.52
2	B	1358	ASN	N-CA	-6.83	1.37	1.46
2	B	1316	ALA	CA-CB	6.82	1.64	1.53
2	B	1317	LEU	CA-C	6.82	1.62	1.52
2	B	1222	ILE	C-N	6.82	1.42	1.33
3	C	3301	GLU	CA-C	6.81	1.62	1.52
2	B	1344	THR	C-N	6.81	1.43	1.34
2	B	1222	ILE	N-CA	-6.80	1.38	1.46
2	B	1255	GLU	CA-C	6.79	1.61	1.52
16	P	101	TRP	CA-CB	6.79	1.63	1.53
2	B	1298	LEU	CB-CG	6.79	1.67	1.53
3	C	3236	ILE	C-N	-6.78	1.24	1.34
3	C	3346	SER	CA-C	-6.76	1.44	1.52
3	C	3226	ASN	C-O	6.75	1.32	1.23
16	P	44	GLU	N-CA	-6.75	1.39	1.46
16	P	86	LYS	CA-CB	6.74	1.62	1.54
16	P	76	SER	N-CA	6.74	1.54	1.46
2	B	1230	MET	C-N	-6.73	1.24	1.33
2	B	1251	SER	CA-C	-6.73	1.43	1.52
2	B	1213	PRO	CA-CB	-6.73	1.44	1.53
2	B	1216	ALA	N-CA	6.72	1.54	1.46
2	B	1300	ASP	CA-CB	6.71	1.64	1.53
2	B	1349	ILE	N-CA	-6.71	1.38	1.46
2	B	1229	PHE	C-N	6.71	1.42	1.33
2	B	1176	VAL	CA-CB	6.70	1.58	1.53
2	B	1266	VAL	N-CA	-6.70	1.38	1.46
2	B	1298	LEU	N-CA	-6.70	1.37	1.46
16	P	15	GLU	C-N	-6.69	1.24	1.34
16	P	87	THR	N-CA	-6.68	1.37	1.45
3	C	3281	LEU	CA-C	-6.67	1.43	1.52
3	C	3283	ASP	CA-CB	6.67	1.64	1.53
3	C	3280	THR	CA-CB	-6.65	1.43	1.53
2	B	1250	GLU	N-CA	-6.65	1.37	1.46
16	P	75	SER	C-N	6.63	1.42	1.33
2	B	1309	LYS	CA-C	-6.63	1.44	1.52
3	C	3241	LEU	C-N	-6.63	1.25	1.34
3	C	3354	ILE	CA-C	-6.63	1.44	1.52
16	P	65	LEU	CA-CB	6.62	1.64	1.53
2	B	1288	PHE	N-CA	6.61	1.54	1.46
2	B	1327	THR	CA-CB	6.60	1.64	1.53
3	C	3287	MET	C-O	-6.60	1.16	1.24
3	C	3232	ILE	CA-C	-6.59	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1280	GLU	CA-C	6.59	1.61	1.52
16	P	45	PRO	N-CA	6.58	1.56	1.47
16	P	100	LEU	N-CA	-6.58	1.38	1.46
16	P	68	ILE	CA-C	-6.58	1.44	1.52
16	P	62	GLU	CA-C	6.58	1.61	1.52
2	B	1319	HIS	CA-CB	-6.57	1.43	1.53
2	B	1282	ASN	N-CA	-6.55	1.38	1.46
2	B	1320	PHE	CA-C	-6.55	1.43	1.52
16	P	93	ILE	C-O	6.55	1.31	1.23
16	P	6	ILE	C-O	-6.54	1.16	1.24
16	P	56	VAL	CA-CB	6.54	1.62	1.54
16	P	26	VAL	C-O	-6.53	1.16	1.24
2	B	1341	THR	CB-OG1	-6.53	1.33	1.43
2	B	1325	TRP	CD2-CE3	-6.53	1.29	1.40
2	B	1343	LYS	CA-CB	6.53	1.64	1.53
2	B	1273	ALA	C-N	6.52	1.42	1.33
2	B	1222	ILE	CA-CB	-6.52	1.46	1.54
16	P	27	ASP	C-O	-6.52	1.16	1.23
3	C	3245	LYS	C-N	6.51	1.42	1.33
3	C	3242	VAL	CA-CB	-6.50	1.45	1.54
2	B	1301	CYS	CA-CB	-6.50	1.43	1.53
2	B	1308	LEU	CA-CB	-6.49	1.42	1.53
2	B	1351	ASN	CA-CB	-6.49	1.42	1.53
3	C	3231	ASP	C-O	6.49	1.31	1.24
2	B	1214	LEU	CA-CB	-6.49	1.46	1.54
16	P	22	GLU	CA-CB	6.49	1.63	1.53
2	B	1324	ASP	N-CA	-6.49	1.38	1.46
2	B	1357	ARG	CZ-NH2	-6.48	1.25	1.33
16	P	65	LEU	CA-C	-6.47	1.43	1.52
3	C	3286	PHE	CA-C	6.46	1.61	1.52
2	B	1255	GLU	C-N	6.46	1.42	1.34
3	C	3283	ASP	CA-C	6.46	1.61	1.52
16	P	7	GLU	C-O	-6.46	1.16	1.24
2	B	1221	ASN	CA-C	-6.46	1.44	1.52
2	B	1359	PHE	C-O	-6.46	1.16	1.24
2	B	1258	ASN	CA-CB	6.45	1.63	1.53
2	B	1325	TRP	C-N	-6.44	1.25	1.34
3	C	3277	GLY	C-O	6.44	1.31	1.23
2	B	1266	VAL	CA-CB	-6.44	1.46	1.54
2	B	1242	GLN	CA-CB	-6.42	1.43	1.53
16	P	39	LEU	CA-C	-6.42	1.43	1.52
16	P	32	TRP	CD2-CE2	6.41	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3278	ILE	CA-C	-6.41	1.44	1.52
16	P	35	PRO	CA-C	6.41	1.61	1.52
16	P	23	TYR	CA-CB	6.41	1.65	1.53
16	P	36	CYS	C-O	6.41	1.32	1.24
16	P	41	GLU	N-CA	6.41	1.54	1.46
16	P	37	LYS	CA-CB	6.40	1.63	1.53
2	B	1274	ILE	CA-C	-6.40	1.45	1.52
16	P	40	ALA	N-CA	-6.39	1.38	1.46
2	B	1272	THR	C-N	-6.38	1.25	1.33
16	P	36	CYS	N-CA	6.38	1.54	1.46
16	P	79	HIS	ND1-CE1	-6.38	1.26	1.32
2	B	1348	GLN	CA-C	-6.36	1.44	1.52
3	C	3338	ALA	CA-CB	6.36	1.64	1.53
2	B	1222	ILE	CA-C	6.36	1.60	1.52
2	B	1312	TRP	CD2-CE3	6.36	1.50	1.40
16	P	69	VAL	N-CA	-6.35	1.39	1.46
2	B	1277	ARG	CZ-NH1	-6.33	1.23	1.32
2	B	1257	ILE	CA-CB	-6.33	1.45	1.54
2	B	1234	GLU	N-CA	6.32	1.53	1.46
3	C	3329	ALA	N-CA	6.32	1.54	1.46
16	P	9	THR	CA-C	6.32	1.60	1.52
3	C	3318	ASN	C-O	-6.31	1.16	1.24
16	P	78	PRO	N-CA	6.31	1.55	1.47
3	C	3285	ASN	CA-CB	6.30	1.63	1.53
3	C	3273	TYR	CA-CB	-6.29	1.42	1.53
2	B	1320	PHE	CA-CB	6.29	1.64	1.53
16	P	56	VAL	N-CA	6.29	1.53	1.46
2	B	1362	TYR	CA-C	6.28	1.60	1.52
3	C	3229	PRO	C-O	6.28	1.30	1.23
2	B	1287	LEU	CA-C	6.28	1.60	1.52
3	C	3206	ARG	CA-C	6.28	1.60	1.52
3	C	3343	HIS	C-N	6.27	1.42	1.33
2	B	1357	ARG	CA-C	-6.27	1.43	1.52
2	B	1327	THR	CA-C	-6.27	1.44	1.52
2	B	1336	ASP	CA-C	-6.27	1.43	1.52
16	P	22	GLU	N-CA	-6.26	1.38	1.46
2	B	1370	LYS	N-CA	6.24	1.58	1.46
16	P	79	HIS	CG-ND1	6.24	1.45	1.38
16	P	56	VAL	C-O	-6.23	1.17	1.24
16	P	101	TRP	C-N	-6.23	1.25	1.33
2	B	1252	MET	CG-SD	6.22	1.96	1.80
2	B	1339	LEU	N-CA	6.21	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3297	SER	C-O	6.19	1.32	1.24
2	B	1324	ASP	C-N	6.18	1.42	1.33
2	B	1284	LEU	CA-C	6.17	1.61	1.52
16	P	43	PHE	CA-C	-6.17	1.44	1.52
16	P	81	PHE	C-O	-6.17	1.16	1.24
2	B	1289	GLU	N-CA	6.14	1.54	1.46
2	B	1314	ALA	N-CA	6.14	1.53	1.46
16	P	93	ILE	CA-C	6.14	1.60	1.53
2	B	1293	SER	C-N	-6.13	1.25	1.34
16	P	67	SER	C-N	6.13	1.41	1.33
2	B	1358	ASN	C-N	6.12	1.42	1.33
2	B	1265	MET	C-N	-6.12	1.26	1.33
2	B	1275	GLU	N-CA	-6.12	1.38	1.46
3	C	3293	PHE	C-O	6.12	1.31	1.23
16	P	29	PHE	C-O	6.12	1.31	1.23
2	B	1345	LEU	CA-CB	6.10	1.63	1.53
2	B	1338	LEU	CA-C	6.10	1.60	1.52
3	C	3323	THR	C-O	-6.08	1.16	1.24
3	C	3330	ALA	C-N	-6.08	1.26	1.33
16	P	41	GLU	CD-OE1	6.08	1.36	1.25
16	P	88	VAL	C-O	-6.05	1.18	1.24
3	C	3233	ILE	C-N	6.04	1.41	1.33
2	B	1238	LYS	C-N	6.04	1.42	1.33
2	B	1221	ASN	C-N	-6.04	1.26	1.33
2	B	1350	LYS	C-N	-6.04	1.25	1.34
3	C	3292	GLU	N-CA	6.03	1.53	1.46
3	C	3211	ALA	CA-C	-6.03	1.44	1.52
3	C	3205	LEU	CA-CB	6.03	1.62	1.53
3	C	3326	SER	C-N	6.01	1.41	1.33
2	B	1337	ILE	N-CA	-6.00	1.39	1.46
3	C	3327	LYS	CA-CB	6.00	1.62	1.53
2	B	1255	GLU	CD-OE2	6.00	1.36	1.25
16	P	102	GLU	CA-CB	-6.00	1.43	1.53
2	B	1278	ALA	C-N	5.99	1.42	1.33
2	B	1265	MET	CA-C	-5.98	1.45	1.52
16	P	8	ILE	C-O	-5.98	1.18	1.24
16	P	99	GLN	CA-C	-5.98	1.45	1.52
3	C	3173	VAL	C-O	-5.98	1.17	1.24
16	P	48	LYS	C-N	-5.96	1.24	1.33
2	B	1241	MET	C-N	-5.96	1.25	1.33
3	C	3291	LYS	C-N	5.95	1.42	1.33
3	C	3293	PHE	N-CA	5.95	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3231	ASP	CA-CB	-5.95	1.44	1.53
3	C	3214	SER	CA-CB	-5.95	1.43	1.53
3	C	3224	LYS	C-N	5.95	1.42	1.33
2	B	1295	TYR	CA-C	-5.95	1.45	1.52
2	B	1319	HIS	CG-CD2	5.94	1.42	1.35
16	P	35	PRO	CA-CB	-5.93	1.45	1.53
2	B	1333	ILE	CA-CB	-5.92	1.48	1.54
16	P	71	SER	C-N	5.92	1.42	1.33
2	B	1344	THR	CA-CB	-5.92	1.44	1.53
2	B	1266	VAL	CA-C	5.91	1.60	1.52
2	B	1231	LYS	CA-CB	-5.91	1.43	1.53
3	C	3338	ALA	CA-C	5.91	1.60	1.52
2	B	1345	LEU	CA-C	-5.91	1.44	1.52
2	B	1357	ARG	CA-CB	5.91	1.63	1.53
16	P	34	GLY	N-CA	-5.89	1.36	1.44
2	B	1341	THR	N-CA	5.89	1.53	1.46
3	C	3207	ARG	N-CA	5.88	1.53	1.46
2	B	1242	GLN	C-N	5.88	1.42	1.33
2	B	1265	MET	SD-CE	5.87	1.94	1.79
16	P	62	GLU	CD-OE1	5.86	1.36	1.25
3	C	3314	GLU	CA-C	5.86	1.60	1.52
2	B	1352	LEU	CA-C	-5.85	1.45	1.53
16	P	37	LYS	C-N	-5.84	1.26	1.33
2	B	1337	ILE	CB-CG1	5.84	1.65	1.53
16	P	16	ASP	CG-OD2	5.84	1.36	1.25
3	C	3303	ILE	N-CA	-5.83	1.39	1.46
3	C	3318	ASN	N-CA	5.83	1.53	1.46
16	P	17	ILE	C-O	5.83	1.30	1.24
2	B	1357	ARG	CD-NE	-5.82	1.38	1.46
16	P	74	VAL	C-O	5.81	1.30	1.24
3	C	3219	ASP	C-O	5.80	1.31	1.24
16	P	102	GLU	C-N	5.79	1.41	1.33
3	C	3212	VAL	N-CA	-5.78	1.39	1.46
3	C	3206	ARG	N-CA	5.78	1.53	1.46
2	B	1288	PHE	CA-C	5.77	1.59	1.52
3	C	3306	LEU	C-O	5.77	1.31	1.24
2	B	1340	ASP	CA-C	5.77	1.60	1.52
2	B	1239	GLU	CA-C	-5.76	1.45	1.52
2	B	1298	LEU	C-N	-5.75	1.25	1.33
16	P	51	LYS	C-O	5.75	1.31	1.24
3	C	3323	THR	N-CA	5.75	1.53	1.46
16	P	8	ILE	C-N	5.74	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	23	TYR	C-O	-5.74	1.17	1.24
2	B	1263	THR	C-N	-5.72	1.27	1.34
2	B	1275	GLU	C-N	5.72	1.41	1.33
3	C	3175	ALA	C-O	5.72	1.30	1.24
16	P	10	SER	C-O	5.71	1.31	1.24
16	P	97	LYS	C-N	-5.71	1.26	1.33
2	B	1330	TRP	CD2-CE2	-5.70	1.31	1.41
2	B	1341	THR	CA-CB	5.70	1.62	1.53
3	C	3223	LEU	C-N	-5.70	1.26	1.34
16	P	71	SER	CB-OG	5.70	1.53	1.42
2	B	1294	ASN	CG-OD1	5.70	1.34	1.23
3	C	3329	ALA	C-O	5.69	1.31	1.24
16	P	68	ILE	N-CA	5.69	1.53	1.46
3	C	3345	LYS	CA-C	-5.68	1.45	1.52
3	C	3279	GLN	N-CA	-5.68	1.39	1.46
16	P	25	LEU	C-O	-5.65	1.17	1.24
2	B	1353	PRO	N-CD	5.64	1.55	1.47
2	B	1308	LEU	C-N	5.64	1.41	1.33
2	B	1299	LYS	C-N	5.63	1.41	1.33
16	P	18	LEU	N-CA	-5.62	1.39	1.46
2	B	1325	TRP	CZ2-CH2	-5.61	1.26	1.37
2	B	1233	VAL	C-N	5.61	1.41	1.33
16	P	96	GLN	C-N	5.61	1.41	1.33
2	B	1261	TYR	CG-CD2	5.60	1.51	1.39
16	P	14	PHE	C-O	5.60	1.30	1.24
16	P	74	VAL	CA-CB	-5.60	1.47	1.54
2	B	1281	TYR	C-N	-5.59	1.26	1.33
3	C	3346	SER	C-O	-5.58	1.17	1.24
16	P	11	THR	N-CA	-5.58	1.39	1.46
2	B	1350	LYS	CA-CB	5.58	1.62	1.53
16	P	75	SER	CA-C	5.57	1.59	1.52
2	B	1232	GLU	CG-CD	5.57	1.66	1.52
2	B	1305	LEU	C-O	5.56	1.30	1.24
16	P	67	SER	C-O	-5.56	1.17	1.24
3	C	3288	LYS	CA-CB	-5.56	1.44	1.53
16	P	20	LYS	CA-CB	-5.56	1.44	1.53
16	P	91	GLN	CG-CD	5.55	1.66	1.52
16	P	41	GLU	C-N	-5.54	1.25	1.33
3	C	3344	GLN	C-O	-5.54	1.17	1.24
16	P	101	TRP	CD2-CE3	-5.54	1.31	1.40
3	C	3344	GLN	N-CA	-5.52	1.39	1.46
16	P	95	ASN	C-O	5.52	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	19	GLU	CA-CB	5.51	1.62	1.53
2	B	1366	VAL	C-N	-5.51	1.26	1.33
2	B	1326	LYS	CA-CB	-5.50	1.44	1.53
3	C	3341	GLU	C-N	-5.50	1.25	1.33
2	B	1215	GLN	CD-NE2	5.50	1.44	1.33
16	P	66	GLU	CD-OE1	5.49	1.35	1.25
16	P	14	PHE	CG-CD1	5.49	1.50	1.38
2	B	1214	LEU	CB-CG	5.48	1.64	1.53
3	C	3317	PHE	N-CA	5.48	1.52	1.46
16	P	103	MET	N-CA	5.48	1.52	1.46
16	P	84	HIS	CA-C	5.48	1.59	1.52
3	C	3240	VAL	CA-C	-5.48	1.45	1.52
3	C	3276	SER	C-N	-5.47	1.27	1.33
16	P	17	ILE	CA-C	-5.47	1.45	1.52
16	P	106	LEU	CA-CB	-5.47	1.44	1.53
2	B	1300	ASP	CG-OD2	5.46	1.35	1.25
16	P	71	SER	CA-CB	-5.46	1.44	1.53
3	C	3339	ILE	C-O	5.46	1.30	1.23
16	P	24	VAL	C-O	-5.45	1.18	1.24
2	B	1269	HIS	CA-CB	5.45	1.61	1.53
2	B	1265	MET	N-CA	5.44	1.52	1.46
3	C	3243	PHE	CA-CB	5.43	1.62	1.53
16	P	99	GLN	C-N	-5.43	1.26	1.33
3	C	3353	ARG	CA-C	-5.43	1.45	1.52
3	C	3326	SER	C-O	-5.43	1.17	1.23
2	B	1299	LYS	C-O	5.42	1.31	1.23
3	C	3318	ASN	C-N	5.42	1.40	1.33
16	P	43	PHE	C-N	-5.42	1.26	1.33
16	P	99	GLN	N-CA	5.42	1.53	1.46
2	B	1351	ASN	C-N	5.42	1.42	1.33
2	B	1219	THR	C-N	-5.40	1.26	1.33
2	B	1277	ARG	CA-C	5.40	1.59	1.52
2	B	1248	TYR	C-N	5.40	1.40	1.33
2	B	1352	LEU	CA-CB	5.40	1.61	1.53
3	C	3350	LYS	C-N	5.39	1.41	1.34
2	B	1267	TYR	N-CA	5.39	1.53	1.46
2	B	1268	TYR	CA-CB	-5.38	1.44	1.53
3	C	3307	GLU	C-O	5.38	1.30	1.24
2	B	1224	ARG	C-N	5.37	1.40	1.33
2	B	1239	GLU	N-CA	5.37	1.52	1.46
16	P	106	LEU	C-N	-5.36	1.25	1.33
16	P	42	GLN	CA-CB	-5.36	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1313	ASP	C-N	5.35	1.40	1.33
2	B	1235	SER	CB-OG	5.35	1.52	1.42
3	C	3291	LYS	CA-C	5.35	1.60	1.52
16	P	40	ALA	CA-C	5.35	1.60	1.52
2	B	1362	TYR	C-N	-5.33	1.25	1.33
2	B	1307	ASN	CA-CB	5.33	1.62	1.53
16	P	103	MET	CA-C	-5.33	1.45	1.52
3	C	3321	PHE	CA-CB	5.32	1.61	1.53
16	P	62	GLU	C-N	5.31	1.40	1.33
16	P	61	ASP	C-O	5.31	1.30	1.24
16	P	104	ALA	N-CA	-5.31	1.39	1.46
3	C	3223	LEU	CA-C	5.31	1.60	1.52
3	C	3324	LYS	CA-C	-5.31	1.45	1.52
3	C	3332	ILE	CA-C	-5.29	1.46	1.52
2	B	1347	THR	C-N	5.29	1.40	1.33
16	P	5	TYR	CA-C	5.27	1.64	1.52
2	B	1265	MET	CA-CB	5.27	1.61	1.53
3	C	3289	LYS	CA-CB	5.26	1.62	1.53
2	B	1220	GLN	CA-CB	-5.26	1.45	1.53
2	B	1273	ALA	CA-CB	-5.26	1.45	1.53
2	B	1267	TYR	CA-CB	5.25	1.62	1.53
2	B	1286	LYS	C-N	-5.25	1.26	1.33
2	B	1367	GLU	CA-CB	-5.25	1.45	1.53
3	C	3311	ASN	CA-CB	-5.25	1.46	1.53
16	P	59	ASN	CA-CB	-5.24	1.45	1.53
2	B	1354	LYS	C-N	5.22	1.40	1.33
2	B	1367	GLU	CD-OE2	5.21	1.35	1.25
3	C	3293	PHE	C-N	5.21	1.41	1.33
16	P	73	ASN	N-CA	-5.20	1.39	1.46
2	B	1259	ASN	CB-CG	5.19	1.65	1.52
2	B	1323	ASN	N-CA	5.19	1.52	1.46
3	C	3205	LEU	C-N	5.19	1.40	1.33
2	B	1337	ILE	C-N	-5.19	1.26	1.33
3	C	3313	SER	CA-C	-5.18	1.45	1.52
3	C	3317	PHE	CA-CB	5.18	1.61	1.53
16	P	79	HIS	CB-CG	-5.17	1.43	1.50
2	B	1257	ILE	C-N	5.17	1.41	1.33
2	B	1319	HIS	CG-ND1	5.17	1.44	1.38
2	B	1346	GLY	C-O	-5.17	1.17	1.23
3	C	3296	ASP	C-N	-5.15	1.26	1.33
3	C	3311	ASN	CA-C	5.15	1.59	1.53
16	P	66	GLU	N-CA	-5.14	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1325	TRP	N-CA	5.14	1.52	1.46
16	P	72	HIS	CA-C	-5.13	1.44	1.52
3	C	3328	ALA	CA-C	5.13	1.59	1.52
2	B	1340	ASP	CB-CG	-5.12	1.39	1.52
16	P	100	LEU	CB-CG	-5.12	1.43	1.53
2	B	1274	ILE	CA-CB	5.12	1.60	1.54
2	B	1363	ASN	CB-CG	5.12	1.64	1.52
3	C	3273	TYR	C-N	5.11	1.40	1.34
3	C	3332	ILE	C-O	5.11	1.30	1.24
3	C	3343	HIS	C-O	-5.11	1.17	1.23
2	B	1243	LYS	N-CA	5.11	1.52	1.46
16	P	106	LEU	CA-C	5.11	1.60	1.52
2	B	1346	GLY	N-CA	-5.11	1.39	1.45
2	B	1280	GLU	C-N	5.10	1.41	1.34
16	P	44	GLU	CA-CB	-5.10	1.46	1.53
16	P	72	HIS	C-N	5.09	1.40	1.33
2	B	1332	GLN	CG-CD	5.09	1.64	1.52
3	C	3211	ALA	CA-CB	-5.09	1.45	1.53
2	B	1295	TYR	CA-CB	5.08	1.60	1.53
3	C	3324	LYS	CA-CB	-5.08	1.45	1.53
16	P	62	GLU	C-O	-5.08	1.17	1.23
16	P	71	SER	C-O	-5.08	1.18	1.24
2	B	1312	TRP	CZ2-CH2	5.08	1.46	1.37
16	P	73	ASN	CA-C	5.07	1.59	1.52
3	C	3212	VAL	CA-C	-5.07	1.46	1.52
2	B	1268	TYR	N-CA	-5.06	1.39	1.46
16	P	102	GLU	CA-C	5.06	1.59	1.52
2	B	1256	ASN	CA-CB	5.05	1.61	1.53
2	B	1297	GLN	C-O	-5.05	1.17	1.24
16	P	90	LYS	C-O	-5.05	1.17	1.23
2	B	1250	GLU	CD-OE1	5.04	1.34	1.25
3	C	3295	LYS	C-O	5.04	1.30	1.24
16	P	36	CYS	C-N	5.04	1.40	1.33
2	B	1233	VAL	CA-C	5.03	1.58	1.52
2	B	1325	TRP	CA-CB	5.02	1.61	1.53
3	C	3242	VAL	C-O	5.02	1.30	1.24
16	P	73	ASN	CA-CB	-5.02	1.45	1.53
2	B	1284	LEU	CA-CB	-5.01	1.45	1.53
2	B	1352	LEU	C-O	5.00	1.30	1.23
16	P	96	GLN	CA-CB	-5.00	1.46	1.53

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3355	GLN	CA-C-N	-18.06	95.72	120.46
3	C	3355	GLN	C-N-CA	-18.06	95.72	120.46
3	C	3345	LYS	N-CA-C	-14.17	80.62	110.80
5	e	106	PRO	N-CA-CB	13.43	110.44	102.92
3	C	3212	VAL	N-CA-C	-12.76	98.17	110.42
3	C	3354	ILE	CA-C-O	-12.69	104.92	120.78
3	C	3345	LYS	CA-C-O	-12.47	102.67	120.51
2	B	1075	TRP	O-C-N	-12.16	107.31	122.27
3	C	3281	LEU	CA-C-N	-10.49	108.33	119.98
3	C	3281	LEU	C-N-CA	-10.49	108.33	119.98
2	B	3951	PRO	N-CA-CB	10.22	109.66	102.81
2	B	4432	PRO	N-CA-CB	10.07	113.83	103.25
3	C	3303	ILE	N-CA-C	-9.93	100.69	110.72
3	C	3311	ASN	CA-C-O	9.88	131.51	120.84
2	B	1330	TRP	CA-CB-CG	9.81	132.24	113.60
3	C	3227	LYS	CA-C-O	9.67	130.80	120.55
3	C	3325	ALA	N-CA-C	-9.61	100.79	111.07
3	C	3240	VAL	N-CA-C	-9.35	101.08	110.62
3	C	3205	LEU	N-CA-C	-9.24	101.21	111.28
3	C	3324	LYS	CA-C-O	-9.13	110.11	120.24
3	C	3213	ASP	O-C-N	-9.01	111.68	122.22
3	C	3216	GLU	CA-C-O	8.91	131.28	121.56
3	C	3319	ASP	O-C-N	-8.88	112.79	122.03
3	C	3378	ALA	O-C-N	-8.69	111.03	122.59
3	C	3331	GLY	O-C-N	-8.68	113.85	122.18
3	C	3332	ILE	CB-CA-C	-8.58	100.56	112.14
3	C	3314	GLU	N-CA-CB	-8.45	97.62	110.13
3	C	3223	LEU	N-CA-C	8.40	123.31	112.89
3	C	3332	ILE	N-CA-C	8.31	119.09	110.62
3	C	3241	LEU	N-CA-C	8.30	120.41	111.36
3	C	3307	GLU	N-CA-CB	-8.26	100.67	110.42
3	C	3227	LYS	N-CA-C	8.26	120.28	111.28
3	C	3295	LYS	N-CA-CB	-8.24	97.96	110.33
3	C	3220	ILE	O-C-N	8.19	129.82	121.87
3	C	3206	ARG	O-C-N	-8.16	113.66	122.07
3	C	3340	TYR	N-CA-C	-8.13	102.38	111.82
3	C	2978	PRO	N-CA-CB	8.06	110.89	103.08
3	C	3354	ILE	N-CA-C	-8.05	92.59	109.34
3	C	3336	ALA	O-C-N	8.04	130.64	122.12
3	C	3339	ILE	N-CA-C	7.99	120.05	111.58
3	C	3343	HIS	CA-C-O	-7.98	112.22	121.16
3	C	3277	GLY	N-CA-C	7.97	122.97	112.77
3	C	3322	ALA	N-CA-C	-7.84	102.97	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3317	PHE	CA-C-O	-7.83	111.81	120.81
3	C	3278	ILE	O-C-N	7.83	129.46	121.87
3	C	3286	PHE	CA-C-N	7.82	130.76	120.28
3	C	3286	PHE	C-N-CA	7.82	130.76	120.28
3	C	3302	THR	N-CA-C	7.79	119.55	111.14
3	C	3312	GLN	N-CA-CB	-7.78	98.24	110.22
3	C	3228	LYS	O-C-N	7.78	127.61	121.55
3	C	3289	LYS	CA-C-O	-7.76	109.83	119.38
3	C	3234	LYS	N-CA-C	7.75	119.36	111.07
16	P	50	HIS	CA-CB-CG	-7.74	106.06	113.80
3	C	3339	ILE	CB-CA-C	-7.71	102.23	111.94
1	A	1185	PRO	N-CA-CB	7.70	110.16	103.31
3	C	4188	PRO	N-CA-CB	7.70	111.33	103.25
3	C	2805	PRO	N-CA-CB	7.69	110.04	103.35
3	C	4182	PRO	N-CA-CB	7.62	111.25	103.25
3	C	3233	ILE	CB-CA-C	7.58	122.37	112.14
3	C	3234	LYS	CA-C-O	7.56	128.76	120.82
3	C	3219	ASP	N-CA-C	7.56	119.60	111.36
3	C	3207	ARG	CA-C-O	-7.50	112.47	120.42
3	C	3287	MET	N-CA-CB	7.49	121.13	110.12
3	C	3345	LYS	CA-C-N	7.42	130.09	120.44
3	C	3345	LYS	C-N-CA	7.42	130.09	120.44
2	B	1259	ASN	OD1-CG-ND2	-7.41	115.19	122.60
3	C	3289	LYS	N-CA-C	-7.38	103.53	112.54
2	B	1363	ASN	OD1-CG-ND2	-7.35	115.25	122.60
3	C	3293	PHE	O-C-N	7.34	131.53	122.86
3	C	3211	ALA	CA-C-O	-7.32	112.12	120.24
3	C	3232	ILE	N-CA-C	7.31	117.40	110.53
3	C	3340	TYR	O-C-N	7.29	131.23	122.27
2	B	1305	LEU	N-CA-C	7.28	118.85	111.07
3	C	3306	LEU	CA-C-N	-7.26	110.78	119.78
3	C	3306	LEU	C-N-CA	-7.26	110.78	119.78
3	C	3218	LYS	CA-C-O	7.25	128.66	120.90
3	C	3344	GLN	CA-C-O	-7.25	110.15	120.51
3	C	3244	PHE	N-CA-C	-7.23	104.89	113.21
3	C	3209	GLN	O-C-N	-7.22	113.92	122.15
2	B	1304	ASP	CA-CB-CG	7.21	119.81	112.60
2	B	1313	ASP	N-CA-C	-7.20	103.46	111.82
2	B	1309	LYS	N-CA-C	-7.19	103.52	111.36
2	B	4008	PRO	N-CA-CB	7.19	110.80	103.25
2	B	3703	PRO	N-CA-CB	7.18	110.79	103.25
16	P	59	ASN	CA-C-O	7.17	127.93	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4180	PRO	N-CA-CB	7.17	110.78	103.25
3	C	3297	SER	N-CA-C	7.16	121.60	113.01
3	C	3323	THR	N-CA-CB	7.14	121.22	110.22
3	C	3203	PRO	CA-C-O	7.12	133.56	120.60
2	B	1369	VAL	O-C-N	-7.12	114.50	121.90
3	C	4546	PRO	N-CA-CB	7.12	110.72	103.25
3	C	2979	PRO	N-CA-CB	7.11	110.72	103.25
3	C	3241	LEU	O-C-N	-7.11	114.05	122.15
3	C	3483	PRO	N-CA-CB	7.11	109.94	103.19
3	C	3278	ILE	N-CA-C	-7.10	103.38	110.62
16	P	69	VAL	CA-C-O	-7.09	113.70	121.29
5	e	81	PRO	N-CA-CB	7.08	110.79	103.00
2	B	1075	TRP	CA-C-O	-7.06	111.85	119.97
3	C	3288	LYS	CA-C-O	-7.03	112.44	120.24
3	C	3209	GLN	CA-C-N	7.02	129.69	120.28
3	C	3209	GLN	C-N-CA	7.02	129.69	120.28
2	B	1247	ASP	N-CA-C	-7.01	104.81	113.15
3	C	3322	ALA	CA-C-N	7.00	130.37	120.28
3	C	3322	ALA	C-N-CA	7.00	130.37	120.28
2	B	1325	TRP	CD2-CE2-CZ2	7.00	129.40	122.40
3	C	3221	VAL	N-CA-CB	-6.98	101.63	110.57
3	C	3292	GLU	CB-CA-C	-6.97	97.73	109.03
2	B	1229	PHE	N-CA-C	-6.97	103.74	111.82
3	C	3336	ALA	CA-C-N	-6.96	110.41	120.29
3	C	3336	ALA	C-N-CA	-6.96	110.41	120.29
2	B	4431	ASP	CA-C-N	6.95	128.52	119.84
2	B	4431	ASP	C-N-CA	6.95	128.52	119.84
3	C	3334	LYS	CA-C-O	6.93	127.89	120.55
3	C	3340	TYR	CA-C-O	-6.92	112.01	119.97
2	B	1323	ASN	CA-CB-CG	-6.89	105.71	112.60
3	C	3302	THR	CB-CA-C	-6.87	100.04	110.90
3	C	3317	PHE	CA-C-N	6.86	134.64	121.54
3	C	3317	PHE	C-N-CA	6.86	134.64	121.54
3	C	3272	SER	N-CA-C	6.86	121.66	113.16
3	C	3220	ILE	CA-C-N	-6.84	111.81	120.56
3	C	3220	ILE	C-N-CA	-6.84	111.81	120.56
2	B	1320	PHE	N-CA-C	-6.78	104.97	113.18
3	C	3274	ASP	O-C-N	6.76	130.13	122.22
3	C	3329	ALA	O-C-N	6.75	131.16	122.39
16	P	98	ASP	CA-CB-CG	-6.74	105.86	112.60
16	P	91	GLN	OE1-CD-NE2	-6.71	115.89	122.60
3	C	3346	SER	CA-C-O	-6.70	113.78	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3286	PHE	CA-C-O	-6.70	113.45	120.55
2	B	1218	GLU	N-CA-C	-6.70	104.05	111.82
3	C	3309	TYR	N-CA-C	6.68	121.26	113.18
2	B	1652	PRO	N-CA-CB	6.67	110.25	103.25
3	C	3216	GLU	N-CA-C	-6.67	101.10	110.50
3	C	3325	ALA	CA-C-O	-6.67	113.82	120.82
16	P	13	GLN	N-CA-C	6.64	118.60	111.36
2	B	1262	ASP	N-CA-C	-6.63	103.97	111.07
16	P	29	PHE	CA-CB-CG	-6.63	107.17	113.80
2	B	1325	TRP	CE2-CD2-CG	6.62	115.15	107.20
3	C	3303	ILE	CA-C-O	-6.60	113.85	120.85
2	B	1349	ILE	N-CA-C	-6.56	103.93	110.62
2	B	1244	LEU	O-C-N	6.55	124.79	120.27
3	C	3215	ILE	CA-C-O	-6.51	113.58	121.13
16	P	47	LYS	N-CA-C	-6.50	104.11	111.07
3	C	3284	MET	N-CA-CB	6.49	121.16	110.39
3	C	3274	ASP	CA-C-N	-6.46	111.12	120.29
3	C	3274	ASP	C-N-CA	-6.46	111.12	120.29
3	C	3225	ALA	N-CA-C	6.45	120.77	113.02
2	B	1236	PHE	N-CA-C	-6.45	104.29	111.71
3	C	3244	PHE	CA-C-N	6.45	136.38	125.02
3	C	3244	PHE	C-N-CA	6.45	136.38	125.02
3	C	3296	ASP	CA-C-O	6.45	127.29	119.49
16	P	57	LYS	O-C-N	-6.44	115.64	123.30
3	C	3313	SER	CA-C-N	-6.44	109.96	120.71
3	C	3313	SER	C-N-CA	-6.44	109.96	120.71
3	C	3228	LYS	CA-C-N	-6.40	112.44	120.51
3	C	3228	LYS	C-N-CA	-6.40	112.44	120.51
2	B	1362	TYR	N-CA-C	6.37	118.23	111.28
2	B	956	LEU	CA-CB-CG	-6.34	94.12	116.30
1	A	1188	LEU	N-CA-C	-6.33	97.54	108.56
3	C	3272	SER	CA-C-O	6.32	126.93	119.28
2	B	1247	ASP	CA-CB-CG	6.31	118.91	112.60
2	B	1335	ALA	CA-C-O	6.31	125.72	118.97
2	B	1301	CYS	N-CA-C	6.29	117.80	111.07
16	P	79	HIS	CG-CD2-NE2	-6.28	100.92	107.20
2	B	1228	ILE	CB-CA-C	-6.27	103.95	111.97
2	B	1271	LEU	N-CA-C	-6.24	104.93	112.54
2	B	1319	HIS	ND1-CG-CD2	6.23	112.33	106.10
2	B	1362	TYR	O-C-N	-6.22	115.53	122.12
3	C	3286	PHE	N-CA-C	-6.21	104.51	111.28
3	C	3297	SER	N-CA-CB	-6.21	99.52	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3275	GLU	N-CA-CB	-6.21	100.97	110.16
3	C	3304	GLU	CA-C-O	6.19	127.11	120.55
3	C	3237	MET	N-CA-CB	-6.17	100.71	110.22
3	C	3273	TYR	N-CA-CB	-6.17	100.89	109.97
16	P	61	ASP	CA-CB-CG	6.17	118.77	112.60
3	C	3223	LEU	CA-C-O	6.17	126.96	119.31
2	B	1278	ALA	N-CA-C	-6.16	104.63	111.71
2	B	1313	ASP	CA-CB-CG	6.14	118.74	112.60
3	C	3322	ALA	CA-C-O	-6.12	111.86	119.38
5	e	1237	PRO	N-CA-CB	6.09	110.03	103.33
3	C	3240	VAL	CB-CA-C	6.08	120.36	112.14
3	C	3289	LYS	O-C-N	6.03	130.51	122.43
3	C	3210	GLU	N-CA-CB	6.03	118.98	110.12
5	e	1249	PRO	N-CA-CB	6.02	110.18	103.44
3	C	3299	ASN	N-CA-CB	6.02	120.48	110.85
3	C	3212	VAL	CA-C-O	-6.02	114.79	121.17
3	C	3222	GLU	CB-CA-C	6.00	120.88	110.68
3	C	3229	PRO	O-C-N	6.00	131.09	123.05
3	C	3283	ASP	CA-C-N	6.00	130.74	120.72
3	C	3283	ASP	C-N-CA	6.00	130.74	120.72
2	B	1245	PRO	CA-C-O	-5.96	114.97	121.77
2	B	1229	PHE	CA-CB-CG	5.95	119.75	113.80
3	C	3343	HIS	CA-C-N	5.93	132.86	121.54
3	C	3343	HIS	C-N-CA	5.93	132.86	121.54
3	C	3205	LEU	CA-C-N	5.92	128.14	120.44
3	C	3205	LEU	C-N-CA	5.92	128.14	120.44
2	B	1928	SER	N-CA-C	5.91	118.75	108.76
2	B	2085	GLN	N-CA-CB	5.91	118.58	110.01
2	B	1345	LEU	N-CA-C	-5.91	104.92	111.71
16	P	81	PHE	CA-CB-CG	5.90	119.70	113.80
3	C	3333	LEU	O-C-N	5.88	128.37	122.08
16	P	32	TRP	CH2-CZ2-CE2	-5.86	109.88	117.50
3	C	3344	GLN	CA-C-N	-5.85	110.37	121.54
3	C	3344	GLN	C-N-CA	-5.85	110.37	121.54
3	C	3211	ALA	CB-CA-C	-5.82	100.04	110.70
16	P	78	PRO	N-CA-CB	5.81	109.35	103.25
3	C	3208	ALA	N-CA-C	-5.81	104.87	111.14
3	C	3290	LEU	CA-C-O	-5.80	114.40	120.55
2	B	2557	PRO	N-CA-CB	5.80	109.34	103.25
3	C	3321	PHE	O-C-N	5.80	128.76	122.15
1	A	1365	TYR	CA-C-N	5.79	128.31	120.44
1	A	1365	TYR	C-N-CA	5.79	128.31	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3281	LEU	N-CA-C	5.79	120.19	113.18
2	B	1312	TRP	CB-CA-C	-5.79	101.75	110.90
3	C	3230	LEU	CA-C-O	5.78	128.57	121.87
2	B	1269	HIS	ND1-CE1-NE2	5.77	114.17	108.40
2	B	1364	VAL	CA-CB-CG1	5.76	120.20	110.40
2	B	1321	GLN	OE1-CD-NE2	-5.76	116.84	122.60
2	B	1307	ASN	OD1-CG-ND2	5.76	128.36	122.60
3	C	3237	MET	O-C-N	-5.75	115.49	122.22
3	C	3233	ILE	N-CA-C	-5.75	104.75	110.62
3	C	3378	ALA	CA-C-O	-5.75	112.29	120.51
16	P	35	PRO	N-CA-C	5.74	121.09	113.57
2	B	1359	PHE	N-CA-CB	5.74	118.58	109.51
3	C	3289	LYS	N-CA-CB	5.73	119.91	110.39
2	B	1342	ASN	CA-C-O	-5.71	115.00	121.00
3	C	3285	ASN	CA-C-O	-5.71	113.40	119.97
16	P	75	SER	CA-C-N	5.71	128.94	120.95
16	P	75	SER	C-N-CA	5.71	128.94	120.95
16	P	48	LYS	N-CA-C	5.71	119.34	112.38
16	P	20	LYS	N-CA-C	5.69	120.29	113.23
2	B	1358	ASN	OD1-CG-ND2	-5.69	116.91	122.60
3	C	3215	ILE	O-C-N	5.68	128.47	122.67
3	C	3272	SER	N-CA-CB	-5.67	101.77	110.44
3	C	3208	ALA	O-C-N	5.66	128.21	122.09
2	B	1298	LEU	CA-C-O	5.66	126.71	120.71
3	C	3292	GLU	N-CA-C	5.64	120.82	113.88
3	C	3298	ILE	CB-CA-C	5.64	120.51	111.32
2	B	1325	TRP	CE3-CZ3-CH2	5.63	128.43	121.10
3	C	3329	ALA	N-CA-C	-5.63	105.51	112.38
2	B	1224	ARG	NE-CZ-NH2	-5.63	114.14	119.20
16	P	64	ASP	CA-CB-CG	-5.63	106.97	112.60
2	B	1240	PHE	CA-C-O	-5.62	114.92	120.82
16	P	79	HIS	ND1-CG-CD2	5.60	111.70	106.10
16	P	53	LEU	CA-C-O	-5.59	114.29	120.38
16	P	32	TRP	CD2-CE3-CZ3	-5.58	111.34	118.60
3	C	3208	ALA	CA-C-O	-5.58	114.95	120.70
3	C	3327	LYS	O-C-N	-5.58	116.21	122.12
16	P	36	CYS	O-C-N	5.58	130.20	122.78
3	C	3311	ASN	CA-C-N	-5.57	112.26	120.28
3	C	3311	ASN	C-N-CA	-5.57	112.26	120.28
2	B	1300	ASP	CA-CB-CG	5.55	118.15	112.60
16	P	72	HIS	N-CA-CB	5.55	118.52	110.47
2	B	1285	GLU	N-CA-C	-5.55	105.38	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2556	ARG	CA-C-N	5.54	126.76	119.84
2	B	2556	ARG	C-N-CA	5.54	126.76	119.84
2	B	1225	ASP	CA-CB-CG	5.53	118.13	112.60
16	P	32	TRP	CG-CD2-CE3	-5.53	128.37	133.90
2	B	1292	LYS	N-CA-C	-5.52	105.26	111.28
2	B	1225	ASP	N-CA-C	-5.52	104.49	111.11
3	C	3332	ILE	O-C-N	5.52	127.22	121.87
3	C	3276	SER	CB-CA-C	5.51	120.05	110.68
3	C	3219	ASP	N-CA-CB	-5.50	102.02	110.16
16	P	92	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	3545	ILE	N-CA-C	-5.50	108.14	113.53
2	B	1244	LEU	CA-C-O	-5.50	114.08	119.13
2	B	1291	GLN	N-CA-CB	5.50	116.50	110.35
2	B	1269	HIS	N-CA-C	-5.49	105.38	111.36
2	B	1347	THR	N-CA-C	-5.48	105.41	111.71
16	P	32	TRP	CG-CD1-NE1	5.48	117.32	110.20
16	P	65	LEU	N-CA-C	-5.47	106.45	113.23
3	C	3293	PHE	N-CA-C	-5.46	102.80	110.50
2	B	1332	GLN	OE1-CD-NE2	-5.45	117.15	122.60
16	P	68	ILE	CB-CA-C	-5.44	104.79	112.14
16	P	7	GLU	O-C-N	-5.44	115.94	123.12
3	C	3279	GLN	CA-C-O	5.42	126.51	120.82
3	C	3313	SER	CA-C-O	5.42	126.23	120.10
16	P	68	ILE	N-CA-CB	5.40	117.88	110.54
16	P	8	ILE	CA-C-O	-5.40	115.02	121.28
2	B	1237	ARG	NH1-CZ-NH2	5.39	126.31	119.30
2	B	1333	ILE	N-CA-C	5.38	117.37	109.63
2	B	1164	MET	CB-CG-SD	-5.37	96.58	112.70
16	P	62	GLU	N-CA-C	5.37	118.02	109.96
3	C	3337	PHE	N-CA-CB	-5.35	102.24	110.16
3	C	3225	ALA	CA-C-O	5.34	125.89	119.43
2	B	1277	ARG	N-CA-C	5.33	117.17	111.36
3	C	3326	SER	N-CA-CB	-5.33	101.86	110.71
16	P	69	VAL	N-CA-C	-5.33	105.13	110.30
2	B	1238	LYS	N-CA-C	-5.33	105.47	111.28
3	C	3297	SER	CA-C-O	5.33	125.97	119.05
3	C	3299	ASN	O-C-N	5.32	129.87	123.16
3	C	3276	SER	O-C-N	-5.31	116.49	122.12
16	P	89	VAL	N-CA-CB	5.31	118.81	110.31
1	A	340	GLY	N-CA-C	5.30	118.21	111.85
3	C	3321	PHE	CA-C-O	-5.30	114.80	120.42
16	P	21	ASN	CA-C-O	-5.29	115.16	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	76	SER	N-CA-CB	5.29	117.73	109.85
3	C	3285	ASN	O-C-N	5.28	128.77	122.27
2	B	1298	LEU	O-C-N	-5.28	116.51	123.21
3	C	3296	ASP	N-CA-C	5.27	118.81	112.38
3	C	3325	ALA	N-CA-CB	5.27	117.65	110.01
16	P	13	GLN	CG-CD-NE2	5.27	124.31	116.40
16	P	105	LYS	N-CA-C	-5.27	105.71	111.82
1	A	903	PRO	N-CA-C	-5.25	106.56	113.65
3	C	3303	ILE	CB-CA-C	5.25	119.46	112.22
3	C	3294	GLU	N-CA-C	-5.24	102.41	109.95
16	P	69	VAL	CA-C-N	5.23	127.29	120.28
16	P	69	VAL	C-N-CA	5.23	127.29	120.28
2	B	1306	LYS	O-C-N	5.23	128.12	122.15
3	C	3321	PHE	CB-CA-C	-5.23	101.95	110.85
16	P	93	ILE	CA-CB-CG1	-5.22	101.53	110.40
16	P	55	ILE	CA-C-N	5.21	129.82	123.10
16	P	55	ILE	C-N-CA	5.21	129.82	123.10
3	C	3228	LYS	CB-CA-C	5.21	117.13	109.22
16	P	51	LYS	N-CA-CB	-5.21	101.92	110.40
3	C	3235	TYR	N-CA-CB	-5.20	102.47	110.16
2	B	1245	PRO	N-CD-CG	5.19	110.99	103.20
3	C	3309	TYR	CA-C-O	5.19	125.75	119.11
3	C	3284	MET	CA-C-O	-5.18	113.00	119.38
16	P	88	VAL	CA-C-N	5.18	129.32	121.65
16	P	88	VAL	C-N-CA	5.18	129.32	121.65
3	C	3276	SER	CA-C-O	5.17	126.22	120.63
2	B	1300	ASP	CA-C-O	5.17	126.21	120.63
16	P	55	ILE	CB-CA-C	5.17	117.21	110.96
2	B	1361	GLY	N-CA-C	-5.16	100.95	113.18
3	C	3283	ASP	O-C-N	-5.16	116.55	122.95
2	B	1226	LEU	N-CA-C	5.16	116.59	111.07
1	A	3916	GLU	N-CA-C	-5.15	100.11	108.41
16	P	88	VAL	N-CA-CB	-5.15	104.57	110.49
16	P	21	ASN	OD1-CG-ND2	5.15	127.75	122.60
2	B	1302	MET	O-C-N	5.14	129.32	122.43
16	P	28	PHE	N-CA-C	-5.14	102.44	110.10
2	B	1262	ASP	CA-CB-CG	5.14	117.74	112.60
3	C	3294	GLU	CA-C-O	5.14	128.67	121.73
5	e	822	LEU	CB-CG-CD1	-5.13	95.30	110.70
3	C	3204	ALA	O-C-N	5.12	129.41	122.59
16	P	62	GLU	CA-C-N	5.12	127.13	120.28
16	P	62	GLU	C-N-CA	5.12	127.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	89	VAL	CB-CA-C	-5.11	105.22	111.92
3	C	3228	LYS	N-CA-C	-5.11	100.21	109.09
3	C	3206	ARG	N-CA-CB	5.10	117.40	110.01
16	P	67	SER	CA-C-N	5.10	127.44	120.46
16	P	67	SER	C-N-CA	5.10	127.44	120.46
2	B	1366	VAL	CA-C-O	5.09	126.16	120.71
3	C	3329	ALA	CA-C-O	-5.09	113.33	119.49
16	P	14	PHE	O-C-N	5.07	127.49	122.12
3	C	3280	THR	O-C-N	-5.06	116.75	122.12
3	C	3355	GLN	CB-CA-C	5.06	120.50	110.42
3	C	3224	LYS	O-C-N	5.06	128.14	122.22
2	B	1264	ILE	N-CA-C	-5.05	104.96	112.04
2	B	1367	GLU	O-C-N	5.05	127.91	122.15
3	C	3222	GLU	CA-C-O	5.05	126.08	120.63
16	P	50	HIS	CB-CA-C	-5.05	104.10	111.77
2	B	1348	GLN	CB-CA-C	-5.05	102.96	110.88
16	P	60	ILE	N-CA-C	5.05	117.36	111.05
3	C	3230	LEU	N-CA-C	-5.04	103.87	110.53
3	C	3246	ALA	N-CA-CB	-5.04	104.38	110.53
3	C	3320	THR	CA-C-O	-5.04	115.08	120.42
16	P	71	SER	CA-C-O	-5.04	115.51	120.70
16	P	21	ASN	O-C-N	5.04	129.60	123.10
2	B	1338	LEU	CB-CA-C	5.03	118.05	109.80
1	A	1366	ASN	N-CA-C	5.01	116.55	111.14
2	B	1221	ASN	OD1-CG-ND2	5.01	127.61	122.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Peptide
2	B	1075	TRP	Mainchain
2	B	966	LYS	Peptide
3	C	3201	ALA	Mainchain
3	C	3344	GLN	Mainchain
3	C	3354	ILE	Mainchain
3	C	3378	ALA	Mainchain
3	C	974	GLN	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	A	18127	0	9379	321	0
2	B	25545	0	17415	984	0
3	C	25046	0	16445	750	0
4	d	3626	0	3455	256	0
5	e	3948	0	3485	302	0
6	F	781	0	791	46	0
7	G	744	0	771	47	0
8	H	702	0	686	55	0
9	I	694	0	684	46	0
10	J	702	0	671	27	0
11	K	803	0	766	79	0
12	L	773	0	806	54	0
13	M	726	0	726	36	0
14	N	897	0	911	71	0
15	O	878	0	868	57	0
16	P	847	0	836	77	0
17	T	1057	0	1033	37	0
18	V	490	0	102	5	0
18	x	505	0	105	7	0
19	C	81	0	36	0	0
20	C	31	0	12	0	0
All	All	87003	0	59983	2970	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 20.

All (2970) 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:B:1212:ILE:CG2	2:B:1213:PRO:HD3	1.22	1.64
2:B:814:TYR:CA	2:B:1075:TRP:CZ2	1.79	1.58
2:B:814:TYR:HB2	2:B:1075:TRP:CE2	1.39	1.56
2:B:1148:SER:CB	2:B:1214:LEU:HB2	1.35	1.56
2:B:1148:SER:H	2:B:1214:LEU:CD1	1.01	1.55
2:B:1212:ILE:CG2	2:B:1213:PRO:CD	1.88	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:814:TYR:HA	2:B:1075:TRP:CZ2	0.99	1.50
2:B:814:TYR:CB	2:B:1075:TRP:CE2	1.91	1.50
2:B:814:TYR:CA	2:B:1075:TRP:CE2	1.99	1.45
3:C:3354:ILE:C	3:C:3358:ILE:H	1.25	1.39
2:B:1148:SER:OG	2:B:1214:LEU:CB	1.75	1.34
3:C:3343:HIS:HA	3:C:3346:SER:CB	1.58	1.32
2:B:813:ASP:OD2	2:B:1076:LEU:CD1	1.78	1.31
3:C:3194:ALA:HB2	3:C:3352:LYS:O	1.35	1.27
2:B:1136:ASP:OD2	2:B:1221:ASN:ND2	1.65	1.27
3:C:3343:HIS:C	3:C:3346:SER:H	1.44	1.25
2:B:814:TYR:HB2	2:B:1075:TRP:CD2	1.20	1.24
2:B:1212:ILE:HG22	2:B:1213:PRO:CG	1.58	1.24
2:B:814:TYR:N	2:B:1075:TRP:NE1	1.86	1.23
1:A:357:ILE:HG21	1:A:379:LYS:C	1.64	1.22
3:C:3187:ILE:CB	3:C:3360:GLU:N	2.03	1.21
3:C:3343:HIS:CA	3:C:3346:SER:H	1.55	1.19
2:B:898:PRO:HG2	2:B:1074:SER:OG	1.43	1.19
2:B:813:ASP:OD2	2:B:1076:LEU:HD12	1.43	1.19
2:B:1212:ILE:HG23	2:B:1213:PRO:CD	1.60	1.18
2:B:1148:SER:N	2:B:1214:LEU:HD13	0.84	1.17
2:B:1148:SER:CB	2:B:1214:LEU:CB	2.20	1.16
3:C:3354:ILE:C	3:C:3358:ILE:N	2.06	1.12
1:A:357:ILE:CG2	1:A:379:LYS:C	2.23	1.11
2:B:1147:ILE:N	2:B:1214:LEU:HD11	1.63	1.11
1:A:357:ILE:CG2	1:A:379:LYS:O	1.99	1.10
2:B:814:TYR:H	2:B:1075:TRP:NE1	1.45	1.09
2:B:813:ASP:OD2	2:B:1076:LEU:HD11	1.47	1.07
2:B:1148:SER:OG	2:B:1214:LEU:HB2	0.90	1.07
3:C:3343:HIS:C	3:C:3346:SER:N	2.14	1.06
2:B:1147:ILE:C	2:B:1214:LEU:HD13	1.81	1.05
2:B:898:PRO:HG2	2:B:1074:SER:CB	1.87	1.05
2:B:814:TYR:N	2:B:1075:TRP:CE2	2.22	1.04
2:B:814:TYR:HA	2:B:1075:TRP:CH2	1.93	1.03
3:C:3194:ALA:HB1	3:C:3353:ARG:HA	1.38	1.03
3:C:3194:ALA:CB	3:C:3353:ARG:HA	1.87	1.03
2:B:1148:SER:HB2	2:B:1214:LEU:HB2	1.39	1.03
2:B:2379:GLU:CB	3:C:1536:LEU:HA	1.89	1.02
3:C:3354:ILE:O	3:C:3358:ILE:N	1.88	1.02
3:C:3342:TYR:O	3:C:3346:SER:N	1.93	1.02
2:B:1148:SER:HB2	2:B:1214:LEU:CB	1.86	1.01
2:B:1212:ILE:HG22	2:B:1213:PRO:CD	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1148:SER:OG	2:B:1213:PRO:C	2.02	1.01
3:C:3354:ILE:O	3:C:3357:ALA:N	1.93	1.01
1:A:357:ILE:HG21	1:A:379:LYS:CA	1.58	0.99
2:B:814:TYR:CG	2:B:1075:TRP:CH2	2.16	0.99
3:C:805:ARG:HB3	5:e:822:LEU:HB2	1.43	0.98
4:d:117:TRP:HB2	15:O:34:VAL:HB	1.42	0.98
2:B:814:TYR:CB	2:B:1075:TRP:CZ2	2.30	0.98
2:B:1212:ILE:HG22	2:B:1213:PRO:HG3	1.46	0.98
2:B:814:TYR:CB	2:B:1075:TRP:CD2	2.07	0.97
3:C:175:GLU:O	3:C:177:ARG:NH1	1.98	0.97
3:C:3344:GLN:C	3:C:3348:ILE:H	1.73	0.97
4:d:1193:ARG:HG2	4:d:1202:GLN:HG3	1.47	0.96
2:B:1214:LEU:HG	2:B:1215:GLN:HG3	1.47	0.96
2:B:814:TYR:HB2	2:B:1075:TRP:CG	2.00	0.96
5:e:824:LYS:HD2	5:e:1154:THR:HB	1.48	0.95
1:A:222:PHE:HB2	2:B:952:PRO:HB3	1.49	0.94
2:B:814:TYR:N	2:B:1075:TRP:HE1	1.60	0.94
2:B:1343:LYS:HA	2:B:1369:VAL:HG13	1.48	0.94
3:C:3194:ALA:CB	3:C:3352:LYS:O	2.14	0.94
2:B:1359:PHE:HB2	2:B:1362:TYR:HD2	1.32	0.94
3:C:3180:CYS:HA	3:C:3366:ALA:HB1	1.50	0.93
3:C:3344:GLN:H	3:C:3347:LYS:H	1.15	0.93
4:d:1194:ILE:H	4:d:1202:GLN:NE2	1.66	0.93
3:C:928:LYS:HD2	3:C:957:ARG:HH22	1.34	0.92
2:B:1147:ILE:H	2:B:1214:LEU:HD11	1.26	0.92
2:B:94:LEU:HD13	3:C:124:THR:HG23	1.49	0.91
4:d:116:ILE:HD13	5:e:43:ARG:HB3	1.52	0.91
2:B:1147:ILE:N	2:B:1214:LEU:CD1	2.33	0.91
3:C:3194:ALA:HB1	3:C:3353:ARG:CA	2.01	0.91
3:C:3192:GLU:N	3:C:3356:VAL:CB	1.71	0.91
2:B:1243:LYS:HG3	2:B:1264:ILE:HG12	1.51	0.91
2:B:2379:GLU:CB	3:C:1536:LEU:CB	2.48	0.90
13:M:49:ASP:HB2	13:M:53:TRP:HE1	1.37	0.89
2:B:1283:ASN:HA	2:B:1286:LYS:HD2	1.54	0.89
3:C:3190:GLU:CB	3:C:3355:GLN:C	2.46	0.89
2:B:1317:LEU:HB3	16:P:32:TRP:HH2	1.35	0.89
3:C:3194:ALA:HB2	3:C:3352:LYS:C	1.98	0.89
1:A:60:LEU:HD11	1:A:67:CYS:HB3	1.53	0.88
6:F:67:LEU:HD11	7:G:95:GLU:HB3	1.55	0.88
1:A:220:TRP:HE1	2:B:956:LEU:HD13	1.37	0.88
2:B:1317:LEU:HD13	16:P:77:LEU:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1155:TYR:HB2	4:d:1158:GLN:HB3	1.53	0.87
3:C:535:ASN:HA	3:C:548:LEU:HD23	1.56	0.87
2:B:435:GLN:HG3	2:B:533:ARG:HG3	1.55	0.87
2:B:1148:SER:N	2:B:1214:LEU:CD1	1.81	0.87
2:B:67:GLN:H	2:B:85:LYS:HZ3	1.20	0.87
2:B:1359:PHE:HB2	2:B:1362:TYR:CD2	2.09	0.87
2:B:2379:GLU:CB	3:C:1536:LEU:CA	2.52	0.86
3:C:805:ARG:NH2	5:e:824:LYS:HG2	1.90	0.86
4:d:1170:VAL:HA	4:d:1187:SER:HA	1.56	0.86
5:e:820:LEU:HG	5:e:1158:LEU:HB3	1.58	0.86
4:d:1194:ILE:N	4:d:1202:GLN:HE21	1.74	0.86
4:d:1194:ILE:H	4:d:1202:GLN:HE21	0.91	0.86
3:C:667:LYS:HA	3:C:671:GLN:HB2	1.58	0.86
4:d:983:LEU:HB2	4:d:995:LEU:HD13	1.58	0.86
3:C:3378:ALA:O	3:C:3380:ILE:N	2.09	0.85
5:e:26:ARG:HE	15:O:12:GLU:HG2	1.40	0.85
2:B:483:LYS:HD3	2:B:484:LYS:HD3	1.56	0.85
3:C:633:GLU:HA	3:C:636:ARG:HD3	1.58	0.85
14:N:32:SER:HA	14:N:35:GLN:HB3	1.58	0.85
2:B:529:GLY:H	5:e:1194:LYS:HB3	1.42	0.85
11:K:33:ALA:HA	14:N:36:LYS:HA	1.58	0.85
2:B:1135:HIS:CG	2:B:1217:GLU:OE2	2.18	0.85
1:A:357:ILE:HG21	1:A:379:LYS:O	1.65	0.85
2:B:1148:SER:HB2	2:B:1214:LEU:HD22	1.57	0.85
11:K:37:LEU:HD13	14:N:36:LYS:HZ3	1.42	0.85
1:A:342:ALA:HB3	1:A:346:LEU:HD21	1.56	0.85
5:e:51:ASP:HB3	13:M:35:LYS:HD3	1.57	0.85
11:K:34:ASP:HB2	14:N:36:LYS:C	2.02	0.85
3:C:3344:GLN:N	3:C:3347:LYS:H	1.73	0.84
2:B:1245:PRO:HA	2:B:1360:LYS:HB2	1.59	0.84
5:e:832:ARG:NH1	5:e:868:TYR:OH	2.10	0.84
3:C:3194:ALA:CB	3:C:3352:LYS:C	2.50	0.84
11:K:36:ILE:HG22	11:K:96:ILE:HD11	1.59	0.84
3:C:862:LEU:HD13	3:C:972:TRP:HE1	1.40	0.84
2:B:157:TYR:HA	2:B:178:SER:HB2	1.60	0.84
3:C:3343:HIS:HA	3:C:3346:SER:CA	2.08	0.84
3:C:3344:GLN:N	3:C:3346:SER:N	2.25	0.83
5:e:842:GLU:HG2	5:e:898:PRO:HD3	1.59	0.83
3:C:3343:HIS:CA	3:C:3346:SER:N	2.36	0.83
11:K:34:ASP:HB3	14:N:40:GLU:HB2	1.59	0.83
3:C:793:GLN:O	5:e:1123:SER:OG	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1346:GLY:HA3	2:B:1369:VAL:HG11	1.59	0.83
3:C:89:GLN:HA	3:C:126:ASN:HD21	1.40	0.83
2:B:477:ILE:HG13	2:B:481:ALA:HA	1.61	0.83
2:B:1148:SER:OG	2:B:1214:LEU:CA	2.26	0.82
2:B:1146:VAL:CG1	2:B:1215:GLN:CD	2.50	0.82
2:B:1176:VAL:HG13	2:B:1188:GLN:HG2	1.61	0.82
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.82
4:d:1202:GLN:HE22	4:d:1204:ILE:C	1.88	0.82
2:B:175:PRO:HG2	2:B:210:VAL:HG12	1.60	0.82
2:B:902:ILE:HA	2:B:915:PRO:HG2	1.60	0.82
3:C:242:GLU:HG3	3:C:368:LYS:HE3	1.58	0.82
1:A:282:ARG:O	1:A:284:ASN:N	2.11	0.82
3:C:3190:GLU:CB	3:C:3355:GLN:O	2.28	0.82
3:C:3202:LEU:O	3:C:3204:ALA:N	2.13	0.82
1:A:220:TRP:NE1	2:B:956:LEU:HD13	1.94	0.82
2:B:173:MET:HE1	2:B:218:LEU:HA	1.61	0.82
2:B:1148:SER:HB2	2:B:1214:LEU:CD2	2.09	0.82
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.82
3:C:3187:ILE:CB	3:C:3359:ALA:O	0.82	0.81
3:C:456:ARG:HA	3:C:459:LYS:HD2	1.62	0.81
5:e:1167:MET:HG2	5:e:1169:PRO:HD2	1.62	0.81
1:A:357:ILE:HG22	1:A:379:LYS:O	1.79	0.81
2:B:1212:ILE:CB	2:B:1213:PRO:CD	2.39	0.81
2:B:296:LYS:HE2	5:e:1225:ALA:HB1	1.63	0.81
2:B:898:PRO:HG2	2:B:1074:SER:HB3	1.62	0.81
2:B:898:PRO:CG	2:B:1074:SER:OG	2.28	0.80
2:B:1317:LEU:HB3	16:P:32:TRP:CH2	2.16	0.80
2:B:449:GLY:HA3	5:e:1183:TYR:HB3	1.62	0.80
2:B:509:GLN:HA	2:B:512:ASP:HB2	1.62	0.80
3:C:1071:ILE:HG13	3:C:1074:MET:HB2	1.64	0.80
5:e:43:ARG:HG3	5:e:45:PRO:HD2	1.61	0.80
1:A:2611:LYS:O	1:A:2613:THR:N	2.15	0.80
3:C:3187:ILE:CB	3:C:3359:ALA:C	0.85	0.80
1:A:250:LYS:HD3	1:A:251:TRP:HB2	1.62	0.79
4:d:126:GLN:HE21	5:e:45:PRO:HD3	1.45	0.79
5:e:910:LEU:HD21	5:e:951:THR:HG21	1.65	0.79
2:B:4032:GLY:O	2:B:4036:GLY:N	2.15	0.79
16:P:37:LYS:O	16:P:95:ASN:ND2	2.15	0.79
1:A:4124:TYR:N	1:A:4146:MET:O	2.15	0.79
5:e:1062:LYS:HG2	5:e:1074:ARG:HD3	1.65	0.79
2:B:94:LEU:HD11	2:B:109:VAL:HG23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:814:TYR:HA	2:B:1075:TRP:HZ2	0.99	0.79
1:A:4048:THR:O	1:A:4110:ALA:N	2.16	0.79
3:C:804:ASN:HB3	5:e:821:MET:HA	1.65	0.79
2:B:3830:PHE:O	2:B:3839:ASP:N	2.16	0.78
3:C:3194:ALA:CB	3:C:3353:ARG:CA	2.60	0.78
3:C:31:SER:O	3:C:37:ASN:ND2	2.14	0.78
3:C:269:LYS:HD2	3:C:281:GLN:HA	1.66	0.78
4:d:966:VAL:HA	4:d:983:LEU:HG	1.63	0.78
1:A:5:LEU:HB2	1:A:352:LEU:HD11	1.64	0.78
3:C:502:LEU:HB2	3:C:509:LYS:HD2	1.64	0.78
2:B:1147:ILE:H	2:B:1214:LEU:CD1	1.94	0.78
15:O:22:LYS:HD2	15:O:26:GLY:HA3	1.64	0.78
1:A:256:ILE:HD11	1:A:322:GLU:HB2	1.66	0.78
1:A:2631:ALA:O	1:A:2635:LYS:N	2.16	0.78
2:B:1136:ASP:CG	2:B:1221:ASN:HD21	1.91	0.78
3:C:3202:LEU:O	3:C:3205:LEU:N	2.16	0.78
11:K:30:PRO:HD2	14:N:33:LYS:HB2	1.65	0.78
2:B:112:GLU:O	2:B:120:HIS:NE2	2.16	0.78
3:C:805:ARG:NH2	5:e:822:LEU:HB3	1.97	0.78
2:B:137:LEU:HB3	2:B:142:TRP:HD1	1.49	0.78
3:C:60:GLN:HB3	3:C:62:GLN:HE22	1.47	0.78
2:B:1136:ASP:CG	2:B:1221:ASN:ND2	2.40	0.77
5:e:1168:GLN:HE21	5:e:1172:LYS:HB3	1.46	0.77
4:d:117:TRP:NE1	15:O:30:ASP:O	2.18	0.77
3:C:381:ILE:O	3:C:396:MET:N	2.17	0.77
3:C:3344:GLN:O	3:C:3348:ILE:N	2.18	0.77
3:C:101:PRO:HG2	3:C:104:ASP:HB3	1.67	0.77
2:B:1148:SER:OG	2:B:1213:PRO:O	2.02	0.77
2:B:1360:LYS:O	2:B:1364:VAL:HB	1.84	0.77
2:B:708:TYR:HE1	2:B:756:ARG:HB3	1.51	0.76
2:B:1340:ASP:OD2	2:B:1343:LYS:HB3	1.86	0.76
2:B:3546:ARG:O	2:B:3550:GLY:N	2.19	0.76
2:B:3552:ASN:O	2:B:3553:LEU:N	2.18	0.76
1:A:6:VAL:HB	1:A:353:ASN:HB3	1.68	0.76
2:B:1178:ILE:HA	2:B:1181:LYS:HE2	1.66	0.76
5:e:859:MET:SD	5:e:862:LYS:NZ	2.53	0.76
2:B:841:LYS:HA	2:B:844:LEU:HD12	1.66	0.76
4:d:92:TYR:O	13:M:2:ASN:N	2.19	0.76
1:A:344:ASN:HD21	2:B:969:LEU:HB3	1.50	0.76
2:B:2201:TYR:O	2:B:2205:GLY:N	2.19	0.76
2:B:1148:SER:HG	2:B:1214:LEU:HB2	1.46	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:477:ASN:HD22	3:C:528:LEU:HD23	1.49	0.76
5:e:1103:TRP:HA	5:e:1121:LYS:HA	1.67	0.76
2:B:1107:ARG:HD3	2:B:1190:ILE:HG12	1.67	0.76
4:d:1148:ILE:HD11	4:d:1170:VAL:HG21	1.68	0.76
2:B:459:ILE:HG23	2:B:499:LEU:HD22	1.68	0.76
2:B:1120:THR:OG1	2:B:1157:ARG:NH1	2.19	0.76
2:B:794:LEU:HD21	2:B:867:VAL:HA	1.68	0.75
2:B:1146:VAL:HG13	2:B:1215:GLN:HG3	1.68	0.75
3:C:542:ILE:HD13	3:C:576:TYR:HA	1.68	0.75
2:B:215:PRO:HA	2:B:218:LEU:HD12	1.67	0.75
3:C:3343:HIS:C	3:C:3345:LYS:N	2.44	0.75
1:A:22:SER:OG	1:A:321:ARG:NH1	2.20	0.75
3:C:973:ASP:HB3	3:C:981:ASP:HB3	1.69	0.75
3:C:3342:TYR:O	3:C:3346:SER:CA	2.34	0.75
16:P:36:CYS:HB2	16:P:95:ASN:HD21	1.51	0.75
1:A:221:SER:HB2	1:A:226:TYR:HE1	1.52	0.74
3:C:3344:GLN:CA	3:C:3347:LYS:H	2.00	0.74
3:C:1146:GLN:HB3	3:C:1187:TRP:CH2	2.22	0.74
2:B:373:THR:HA	2:B:376:ALA:HB3	1.70	0.74
3:C:857:ARG:HG2	5:e:875:PRO:HB2	1.69	0.74
3:C:1105:ARG:NH2	3:C:1176:GLU:OE2	2.19	0.74
3:C:3343:HIS:HA	3:C:3346:SER:H	1.50	0.74
3:C:3354:ILE:HA	3:C:3357:ALA:HB3	1.70	0.74
14:N:102:LEU:HD23	15:O:90:ASP:O	1.88	0.74
2:B:1146:VAL:HG13	2:B:1215:GLN:CG	2.18	0.74
2:B:814:TYR:CG	2:B:1075:TRP:CZ2	2.61	0.74
1:A:332:GLU:O	1:A:334:ARG:NH1	2.21	0.74
2:B:1148:SER:CA	2:B:1214:LEU:HD13	2.09	0.74
5:e:828:GLU:O	5:e:832:ARG:NH1	2.21	0.74
1:A:2297:GLY:N	1:A:2375:PHE:O	2.21	0.73
3:C:948:LEU:HA	3:C:951:ILE:HD12	1.68	0.73
2:B:2228:THR:O	2:B:2231:LYS:N	2.21	0.73
3:C:1141:GLN:HA	3:C:1144:LYS:HD2	1.70	0.73
1:A:2496:MET:O	1:A:2500:ALA:N	2.20	0.73
2:B:1148:SER:H	2:B:1214:LEU:CG	1.96	0.73
2:B:1240:PHE:O	2:B:1244:LEU:HB2	1.88	0.73
2:B:2396:MET:N	2:B:2447:PRO:O	2.22	0.73
3:C:801:ILE:HD13	3:C:868:LEU:HD21	1.69	0.73
2:B:1148:SER:HB2	2:B:1214:LEU:CG	2.17	0.73
5:e:1131:LYS:HE2	5:e:1147:ALA:HB3	1.71	0.73
3:C:859:VAL:HA	3:C:975:GLN:HE22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:87:THR:OG1	13:M:54:ASN:ND2	2.19	0.73
2:B:802:ILE:HG12	2:B:877:THR:HG21	1.69	0.73
2:B:1148:SER:OG	2:B:1214:LEU:N	2.22	0.73
2:B:1568:SER:O	2:B:1572:ALA:N	2.21	0.73
2:B:1219:THR:HA	2:B:1222:ILE:HD12	1.71	0.73
3:C:805:ARG:HH22	5:e:824:LYS:HG2	1.52	0.73
9:I:89:VAL:HG21	9:I:94:LEU:HB2	1.69	0.73
1:A:4004:LEU:O	1:A:4008:CYS:N	2.21	0.72
3:C:880:PRO:HB2	3:C:883:THR:HB	1.71	0.72
7:G:136:MET:O	7:G:146:ILE:HA	1.89	0.72
2:B:301:LYS:HE3	2:B:320:ILE:HG21	1.70	0.72
2:B:516:THR:HG21	5:e:1076:LYS:H	1.54	0.72
2:B:924:LEU:HD12	2:B:926:VAL:H	1.53	0.72
2:B:1149:ASP:OD1	2:B:1214:LEU:CD2	2.37	0.72
3:C:210:GLU:OE1	3:C:277:ASN:ND2	2.23	0.72
5:e:832:ARG:HD3	5:e:851:TYR:HB3	1.71	0.72
2:B:64:VAL:HA	2:B:83:LYS:HZ1	1.54	0.72
2:B:548:LEU:HD21	2:B:613:ILE:HD13	1.71	0.72
2:B:1285:GLU:HG3	2:B:1290:LEU:HD12	1.70	0.72
3:C:895:TYR:HA	3:C:898:LEU:HD12	1.72	0.72
4:d:1163:TYR:CZ	4:d:1195:TRP:HD1	2.07	0.72
9:I:51:ALA:H	9:I:54:LEU:HD23	1.54	0.72
3:C:14:LYS:HG3	3:C:24:LYS:HE3	1.70	0.72
3:C:971:ASN:ND2	3:C:986:TYR:OH	2.23	0.72
1:A:343:ASN:HD21	2:B:931:ARG:HE	1.38	0.72
2:B:64:VAL:HG13	2:B:86:LYS:HD3	1.72	0.72
2:B:447:THR:O	5:e:1187:LYS:NZ	2.15	0.72
2:B:1650:ALA:N	2:B:1653:ALA:O	2.22	0.72
2:B:2221:ASP:O	2:B:2225:GLY:N	2.23	0.72
3:C:3344:GLN:HA	3:C:3347:LYS:CB	2.19	0.72
11:K:20:THR:O	14:N:75:LYS:NZ	2.22	0.72
1:A:1954:SER:O	1:A:1957:SER:N	2.22	0.72
2:B:1113:LEU:HD22	2:B:1164:MET:HE1	1.72	0.72
2:B:518:TYR:OH	5:e:1031:LEU:O	2.07	0.71
2:B:1146:VAL:HG13	2:B:1215:GLN:CD	2.14	0.71
4:d:1203:ILE:HG22	4:d:1204:ILE:HG13	1.72	0.71
2:B:1360:LYS:HD2	2:B:1363:ASN:HB3	1.71	0.71
3:C:534:ASN:HA	3:C:537:ASN:HB2	1.70	0.71
3:C:3194:ALA:HB3	3:C:3353:ARG:HA	1.70	0.71
16:P:28:PHE:CZ	16:P:74:VAL:HG21	2.25	0.71
1:A:2627:LYS:O	1:A:2631:ALA:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LEU:O	2:B:77:GLN:NE2	2.24	0.71
2:B:1271:LEU:HD21	2:B:1301:CYS:HB2	1.71	0.71
3:C:3180:CYS:HA	3:C:3366:ALA:CB	2.20	0.71
4:d:1228:ALA:HB1	4:d:1257:LEU:HD11	1.72	0.71
14:N:41:LEU:HD11	14:N:70:LYS:HG3	1.73	0.71
3:C:3187:ILE:O	3:C:3356:VAL:O	2.07	0.71
6:F:14:LEU:HA	6:F:17:LEU:HD23	1.71	0.71
3:C:3187:ILE:C	3:C:3360:GLU:N	2.49	0.71
1:A:322:GLU:HG3	1:A:340:GLY:HA3	1.71	0.71
2:B:734:GLU:HB2	2:B:737:VAL:HG22	1.73	0.71
2:B:1315:ILE:HD13	2:B:1318:ILE:HD12	1.70	0.71
5:e:870:TRP:HB3	5:e:878:PRO:HA	1.73	0.71
5:e:1062:LYS:HE2	5:e:1064:TRP:HE1	1.54	0.71
7:G:76:TYR:H	7:G:89:ALA:HB3	1.56	0.70
1:A:22:SER:HB3	1:A:340:GLY:HA2	1.72	0.70
2:B:1136:ASP:OD2	2:B:1218:GLU:OE1	1.80	0.70
3:C:853:VAL:O	3:C:857:ARG:HD3	1.90	0.70
2:B:526:ASN:HA	5:e:1191:THR:HB	1.73	0.70
2:B:117:LEU:HD13	3:C:146:ILE:HG13	1.71	0.70
2:B:442:ILE:HD12	5:e:1194:LYS:HG2	1.73	0.70
2:B:3848:ASP:O	2:B:3853:CYS:N	2.25	0.70
5:e:1137:GLY:H	5:e:1141:ASN:HD22	1.37	0.70
1:A:3895:MET:O	1:A:3899:THR:N	2.24	0.70
3:C:350:HIS:HB2	18:x:151:UNK:HA	1.74	0.70
3:C:3194:ALA:HB1	3:C:3353:ARG:N	2.06	0.70
5:e:52:ASN:HA	12:L:22:ARG:HD3	1.73	0.70
5:e:1087:TRP:HE1	5:e:1093:GLY:HA2	1.56	0.70
1:A:319:ARG:HB2	1:A:322:GLU:OE2	1.91	0.70
1:A:1400:ALA:N	1:A:1524:ARG:O	2.22	0.70
2:B:1048:ASP:OD1	2:B:1173:LYS:NZ	2.25	0.70
2:B:1249:THR:OG1	2:B:1259:ASN:ND2	2.24	0.70
2:B:2209:GLU:N	2:B:2258:HIS:O	2.25	0.70
4:d:1024:PRO:HD3	4:d:1071:TRP:CE3	2.26	0.70
4:d:1066:VAL:HA	4:d:1085:SER:HA	1.74	0.70
2:B:208:LYS:HB3	2:B:212:LYS:HE2	1.73	0.70
2:B:1147:ILE:CA	2:B:1214:LEU:CD1	2.70	0.70
2:B:1301:CYS:SG	2:B:1302:MET:N	2.65	0.70
1:A:339:GLY:C	1:A:346:LEU:HB2	2.17	0.69
4:d:1188:ALA:HA	4:d:1212:VAL:HG22	1.74	0.69
2:B:55:GLN:O	2:B:93:LYS:NZ	2.25	0.69
2:B:422:ARG:HD3	2:B:478:MET:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1310:THR:O	16:P:76:SER:HB3	1.92	0.69
3:C:3343:HIS:HA	3:C:3346:SER:N	2.05	0.69
2:B:1277:ARG:HH12	2:B:1280:GLU:HB2	1.57	0.69
12:L:28:GLN:HG3	12:L:32:LYS:HE3	1.72	0.69
2:B:1150:VAL:HA	2:B:1153:VAL:HG12	1.72	0.69
3:C:248:SER:O	3:C:252:LYS:HB2	1.92	0.69
4:d:1151:CYS:SG	4:d:1152:SER:N	2.63	0.69
5:e:59:HIS:ND1	11:K:90:HIS:HB3	2.07	0.69
1:A:124:PRO:HB3	1:A:185:PHE:HE2	1.57	0.69
1:A:3594:ARG:O	1:A:3621:TRP:N	2.26	0.69
1:A:208:MET:HG3	1:A:296:ILE:HD13	1.73	0.69
1:A:2044:TYR:O	1:A:2086:GLN:N	2.26	0.69
1:A:3519:LEU:O	1:A:3523:LEU:N	2.26	0.69
2:B:533:ARG:HE	2:B:535:ILE:HD11	1.57	0.69
2:B:3833:MET:O	2:B:3839:ASP:N	2.25	0.69
3:C:809:ASN:HD21	5:e:876:ASN:HD21	1.40	0.69
10:J:26:PHE:O	10:J:30:LYS:HG2	1.93	0.69
2:B:169:LYS:HZ1	3:C:150:LYS:HB2	1.58	0.69
2:B:380:LEU:HD11	2:B:427:LEU:HB2	1.74	0.69
1:A:3384:SER:O	1:A:3388:ARG:N	2.26	0.69
2:B:493:ARG:NH2	2:B:500:GLU:OE2	2.26	0.69
3:C:784:VAL:O	3:C:788:LEU:HG	1.92	0.69
2:B:1137:LYS:HB3	2:B:1215:GLN:NE2	2.08	0.68
2:B:1310:THR:HA	16:P:93:ILE:HG21	1.75	0.68
2:B:4123:ASP:O	2:B:4126:ILE:N	2.26	0.68
4:d:247:ILE:HA	7:G:125:PHE:CE1	2.26	0.68
5:e:1109:TYR:OH	5:e:1184:ARG:NH1	2.26	0.68
1:A:3221:SER:O	1:A:3225:ARG:N	2.25	0.68
2:B:20:GLN:HG2	3:C:16:THR:HG22	1.75	0.68
4:d:1166:HIS:H	4:d:1193:ARG:HD2	1.58	0.68
5:e:1098:VAL:HG22	5:e:1104:MET:HG3	1.74	0.68
2:B:445:GLY:HA2	2:B:506:VAL:HG21	1.73	0.68
2:B:1070:PRO:HB3	2:B:1079:ASN:HA	1.74	0.68
3:C:857:ARG:HE	5:e:875:PRO:HB2	1.59	0.68
2:B:420:LEU:O	2:B:424:GLN:HG2	1.93	0.68
3:C:177:ARG:HE	3:C:259:GLN:HA	1.59	0.68
3:C:871:LEU:HD22	3:C:875:VAL:HG23	1.75	0.68
8:H:16:MET:HE1	8:H:77:ILE:HB	1.75	0.68
2:B:536:ILE:HG22	2:B:540:LEU:HG	1.74	0.68
3:C:3192:GLU:H	3:C:3356:VAL:CB	2.01	0.68
6:F:20:ALA:HA	6:F:101:GLN:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:MET:HB2	12:L:30:LEU:HD22	1.75	0.68
2:B:510:GLY:HA2	2:B:523:LEU:HD23	1.74	0.68
1:A:2893:LEU:O	1:A:2898:ARG:N	2.26	0.68
2:B:1229:PHE:O	2:B:1233:VAL:HG23	1.94	0.68
5:e:1110:TYR:CZ	5:e:1174:ILE:HG12	2.29	0.68
1:A:3470:LEU:O	1:A:3473:ILE:N	2.28	0.67
5:e:37:ILE:N	5:e:39:GLN:OE1	2.27	0.67
1:A:189:ARG:NH1	1:A:190:LEU:O	2.27	0.67
4:d:961:GLN:HB3	4:d:964:LYS:HB2	1.75	0.67
4:d:1172:LYS:HZ1	4:d:1174:LYS:HB3	1.59	0.67
1:A:3:GLN:N	1:A:305:ASN:O	2.23	0.67
1:A:3835:GLU:O	1:A:3839:LYS:N	2.27	0.67
3:C:1065:ILE:HD13	3:C:1082:CYS:HB2	1.76	0.67
3:C:3741:ASN:O	3:C:3745:GLU:N	2.27	0.67
1:A:1931:LYS:O	1:A:1939:LYS:N	2.28	0.67
2:B:596:ARG:NH1	2:B:597:ASP:OD1	2.27	0.67
3:C:79:PHE:O	3:C:82:THR:OG1	2.11	0.67
3:C:3344:GLN:H	3:C:3347:LYS:N	1.90	0.67
1:A:329:ASP:O	1:A:334:ARG:NH1	2.27	0.67
2:B:1054:ILE:HD13	2:B:1057:LEU:HD12	1.77	0.67
2:B:1113:LEU:HD21	2:B:1160:ILE:HB	1.76	0.67
2:B:1226:LEU:HD11	2:B:1285:GLU:OE2	1.93	0.67
3:C:935:VAL:HG21	3:C:1076:LEU:HB2	1.75	0.67
2:B:439:LEU:HB3	2:B:533:ARG:HH11	1.59	0.67
2:B:1047:LEU:HD22	2:B:1106:PHE:HE2	1.60	0.67
3:C:96:LEU:HB3	3:C:119:ILE:HB	1.77	0.67
2:B:4441:ILE:N	2:B:4494:TYR:O	2.28	0.67
17:T:33:VAL:O	17:T:37:THR:HG23	1.94	0.67
1:A:3781:TYR:O	1:A:3785:GLU:N	2.26	0.67
3:C:57:TYR:HB2	3:C:91:LYS:HB2	1.77	0.67
3:C:531:PHE:HA	3:C:534:ASN:HB2	1.76	0.67
4:d:1184:ILE:HD13	4:d:1194:ILE:HA	1.76	0.67
2:B:470:PHE:CE1	2:B:488:ASP:HB3	2.29	0.67
2:B:1047:LEU:HD22	2:B:1106:PHE:CE2	2.30	0.67
3:C:3353:ARG:O	3:C:3354:ILE:O	2.13	0.67
2:B:1149:ASP:H	2:B:1214:LEU:HD22	1.58	0.66
2:B:1340:ASP:CG	2:B:1343:LYS:HB3	2.21	0.66
5:e:828:GLU:O	5:e:868:TYR:OH	2.10	0.66
3:C:1112:THR:HG21	3:C:1179:ALA:HA	1.78	0.66
1:A:1484:GLU:O	1:A:1495:LEU:N	2.27	0.66
1:A:2495:ASP:O	1:A:2496:MET:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:PRO:O	9:I:109:LYS:NZ	2.27	0.66
9:I:99:TYR:HD2	9:I:103:LEU:HB2	1.61	0.66
2:B:1277:ARG:NH1	2:B:1280:GLU:HB2	2.10	0.66
2:B:1343:LYS:HA	2:B:1369:VAL:CG1	2.24	0.66
2:B:449:GLY:HA3	5:e:1183:TYR:CG	2.31	0.66
7:G:62:ASP:HB3	7:G:66:ARG:HH21	1.61	0.66
16:P:24:VAL:HG22	16:P:54:THR:HB	1.78	0.66
1:A:274:GLY:O	1:A:282:ARG:NH1	2.27	0.66
1:A:1592:ARG:O	1:A:1593:SER:N	2.29	0.66
2:B:2890:GLY:N	2:B:3022:PHE:O	2.29	0.66
15:O:51:ILE:O	15:O:55:ILE:HG12	1.96	0.66
2:B:1315:ILE:HG12	2:B:1362:TYR:HD1	1.61	0.66
3:C:621:ILE:HA	3:C:624:PHE:CD2	2.31	0.66
3:C:884:LYS:HG3	3:C:885:ARG:HD2	1.78	0.66
4:d:1067:TRP:N	4:d:1084:ILE:O	2.20	0.66
4:d:1089:ARG:HD3	4:d:1121:ILE:HG23	1.77	0.66
4:d:1273:ASP:OD1	4:d:1277:GLY:N	2.29	0.66
3:C:243:LEU:HD22	3:C:320:LEU:HD13	1.78	0.66
4:d:1175:TRP:HA	4:d:1183:PHE:HA	1.78	0.66
2:B:1212:ILE:HG23	2:B:1213:PRO:HD3	0.66	0.66
3:C:210:GLU:HG3	3:C:280:ASN:ND2	2.11	0.66
3:C:624:PHE:HB3	3:C:634:ILE:HG23	1.77	0.66
4:d:95:LYS:NZ	10:J:52:GLU:OE2	2.29	0.66
2:B:132:VAL:HG11	3:C:77:VAL:HG22	1.78	0.66
2:B:674:ASP:HB3	2:B:675:PRO:HD3	1.76	0.66
2:B:677:LEU:HD11	2:B:712:ILE:HD12	1.79	0.66
3:C:608:ILE:HD13	3:C:705:GLN:HG2	1.77	0.66
3:C:3353:ARG:O	3:C:3357:ALA:N	2.28	0.65
1:A:166:GLY:HA2	1:A:171:ARG:H	1.59	0.65
3:C:903:GLN:NE2	3:C:994:GLU:OE2	2.28	0.65
4:d:1081:PHE:O	4:d:1092:ASN:HA	1.97	0.65
5:e:883:MET:HG3	5:e:919:GLU:HG3	1.76	0.65
2:B:217:GLN:HA	2:B:220:LYS:HD3	1.77	0.65
3:C:336:ILE:O	3:C:340:PRO:HD2	1.97	0.65
2:B:572:MET:HG3	2:B:575:ASN:H	1.61	0.65
2:B:1283:ASN:CA	2:B:1286:LYS:HD2	2.27	0.65
2:B:1804:PHE:O	2:B:1808:LYS:N	2.28	0.65
3:C:52:LYS:NZ	3:C:75:ASP:OD2	2.29	0.65
4:d:76:GLU:H	15:O:86:THR:HG21	1.61	0.65
5:e:823:PHE:CE1	5:e:875:PRO:HA	2.32	0.65
1:A:283:THR:HG21	2:B:939:ASN:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2465:TRP:O	2:B:2469:ALA:N	2.30	0.65
11:K:30:PRO:O	14:N:32:SER:HB3	1.97	0.65
2:B:454:GLU:O	2:B:458:GLN:CB	2.45	0.65
2:B:716:ASP:HA	2:B:719:VAL:HG12	1.78	0.65
2:B:752:ILE:HD13	2:B:765:PHE:HB3	1.77	0.65
2:B:806:ASN:OD1	2:B:881:HIS:NE2	2.30	0.65
2:B:851:LYS:HD2	2:B:851:LYS:O	1.97	0.65
2:B:1107:ARG:HG3	2:B:1111:LYS:HE3	1.78	0.65
2:B:1317:LEU:HD22	16:P:32:TRP:HZ3	1.62	0.65
3:C:1182:LEU:HD12	3:C:1185:ARG:HE	1.62	0.65
3:C:2492:ILE:O	3:C:2634:MET:N	2.29	0.65
16:P:47:LYS:HD3	16:P:55:ILE:CG1	2.27	0.65
1:A:2374:SER:O	1:A:2378:GLY:N	2.29	0.65
2:B:663:LYS:HG2	2:B:664:ASP:H	1.61	0.65
2:B:1346:GLY:HA2	2:B:1349:ILE:HD12	1.78	0.65
3:C:601:PRO:HD2	3:C:701:CYS:SG	2.37	0.65
9:I:30:MET:HG3	9:I:35:LEU:HD22	1.78	0.65
2:B:652:SER:O	2:B:672:ASN:ND2	2.30	0.65
3:C:542:ILE:HG23	3:C:575:ASN:HB2	1.79	0.65
9:I:59:ALA:O	9:I:63:ILE:HG12	1.97	0.65
2:B:65:SER:HB2	2:B:87:LYS:H	1.62	0.65
2:B:530:LEU:HD21	2:B:536:ILE:HG21	1.77	0.65
2:B:1243:LYS:HE2	2:B:1264:ILE:HA	1.78	0.65
2:B:1802:GLU:O	2:B:1806:ILE:N	2.30	0.65
2:B:1176:VAL:O	2:B:1179:THR:OG1	2.12	0.64
3:C:696:ILE:HG23	3:C:700:LYS:HE2	1.79	0.64
3:C:1144:LYS:HE2	4:d:171:ARG:HG2	1.79	0.64
2:B:688:LEU:O	2:B:691:ARG:NH1	2.30	0.64
3:C:313:ASN:HD21	3:C:355:PHE:HB3	1.62	0.64
3:C:942:VAL:HB	3:C:1017:LEU:HD11	1.80	0.64
3:C:3194:ALA:HB1	3:C:3352:LYS:C	2.23	0.64
7:G:103:ILE:HD13	7:G:106:LEU:HD12	1.79	0.64
2:B:1244:LEU:HB3	2:B:1245:PRO:HD3	1.78	0.64
17:T:43:ASN:HA	17:T:46:LYS:HE3	1.79	0.64
3:C:819:VAL:HG12	3:C:909:MET:HG2	1.78	0.64
5:e:845:THR:HA	5:e:872:LEU:HD12	1.79	0.64
6:F:75:GLU:OE2	7:G:131:LYS:NZ	2.31	0.64
2:B:1245:PRO:CA	2:B:1360:LYS:HB2	2.27	0.64
1:A:256:ILE:HG23	1:A:324:ALA:HB2	1.78	0.64
2:B:1283:ASN:O	2:B:1287:LEU:HG	1.98	0.64
2:B:1359:PHE:O	2:B:1363:ASN:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:282:ARG:NH2	18:x:125:UNK:O	2.27	0.64
3:C:3870:GLU:O	3:C:3874:TRP:N	2.31	0.64
2:B:345:ARG:HG3	2:B:414:VAL:HG12	1.79	0.64
2:B:656:LEU:HD22	2:B:756:ARG:HD2	1.78	0.64
3:C:951:ILE:HD13	3:C:1074:MET:HE2	1.80	0.64
2:B:2285:LEU:N	2:B:2293:ILE:O	2.30	0.64
3:C:77:VAL:HG11	3:C:94:TRP:HZ2	1.63	0.64
3:C:3354:ILE:CA	3:C:3358:ILE:N	2.61	0.64
11:K:111:GLN:OE1	11:K:111:GLN:N	2.30	0.64
16:P:60:ILE:HG23	16:P:69:VAL:HG21	1.80	0.64
2:B:165:LEU:HA	2:B:168:ILE:HB	1.78	0.64
2:B:528:GLU:HB3	5:e:1198:LEU:HD22	1.80	0.64
16:P:6:ILE:O	16:P:57:LYS:N	2.26	0.64
2:B:1161:ILE:HG13	2:B:1197:PHE:CZ	2.33	0.63
3:C:2910:PHE:O	3:C:2914:GLY:N	2.31	0.63
3:C:3353:ARG:O	3:C:3357:ALA:CB	2.46	0.63
3:C:3354:ILE:O	3:C:3357:ALA:CA	2.45	0.63
4:d:1163:TYR:HD2	4:d:1193:ARG:HH21	1.45	0.63
1:A:222:PHE:O	1:A:223:THR:OG1	2.14	0.63
3:C:1026:LEU:HD13	3:C:1088:TRP:CG	2.33	0.63
10:J:67:ASN:HB2	11:K:58:GLN:HB2	1.80	0.63
13:M:5:PRO:HA	13:M:77:ILE:HG22	1.80	0.63
16:P:42:GLN:C	16:P:45:PRO:HD2	2.24	0.63
2:B:1748:ASP:O	2:B:1752:GLY:N	2.31	0.63
3:C:601:PRO:HG3	3:C:697:ARG:HD3	1.80	0.63
3:C:1227:ARG:HG3	3:C:1228:ARG:HH22	1.62	0.63
3:C:3354:ILE:C	3:C:3358:ILE:CB	2.71	0.63
14:N:76:VAL:HB	14:N:79:TYR:HB2	1.79	0.63
2:B:658:GLN:NE2	2:B:746:GLU:OE1	2.32	0.63
3:C:546:LEU:HD12	3:C:549:LEU:HD23	1.79	0.63
1:A:220:TRP:HB2	1:A:253:LEU:HD13	1.81	0.63
2:B:161:VAL:O	2:B:164:LEU:HB3	1.98	0.63
3:C:700:LYS:HE3	4:d:1063:THR:HB	1.80	0.63
1:A:2175:SER:O	1:A:2177:ILE:N	2.32	0.63
3:C:862:LEU:HB2	3:C:972:TRP:CD1	2.33	0.63
12:L:21:ILE:HG12	12:L:31:LEU:HD21	1.80	0.63
1:A:42:ASP:HB2	1:A:48:ASP:HB3	1.80	0.63
1:A:357:ILE:HG23	1:A:379:LYS:C	2.23	0.63
2:B:66:GLY:HA2	2:B:86:LYS:HG2	1.81	0.63
2:B:1147:ILE:HB	2:B:1214:LEU:HD12	1.81	0.63
3:C:317:LEU:HD23	3:C:356:TYR:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:667:LYS:HD2	3:C:716:ILE:HD12	1.81	0.63
3:C:872:ASP:O	3:C:888:ARG:NH2	2.31	0.63
8:H:10:VAL:N	8:H:80:TYR:O	2.29	0.63
1:A:341:TRP:CE2	1:A:344:ASN:HA	2.34	0.63
2:B:92:ILE:HB	2:B:109:VAL:HB	1.81	0.63
2:B:156:ASN:HB2	2:B:180:LYS:HE2	1.81	0.63
2:B:228:LEU:O	2:B:232:GLU:HG2	1.98	0.63
2:B:449:GLY:HA3	5:e:1183:TYR:CB	2.28	0.63
5:e:927:VAL:HG23	5:e:928:GLU:H	1.62	0.63
1:A:223:THR:HA	2:B:956:LEU:HD11	1.81	0.63
1:A:1398:GLY:O	1:A:1524:ARG:N	2.32	0.63
1:A:199:PRO:O	1:A:221:SER:OG	2.16	0.62
2:B:425:ASP:OD1	2:B:426:ILE:N	2.32	0.62
8:H:9:PRO:HA	8:H:81:VAL:HA	1.80	0.62
2:B:801:ILE:HG21	2:B:874:ALA:HB1	1.79	0.62
2:B:1243:LYS:HZ3	2:B:1264:ILE:HG23	1.64	0.62
3:C:3180:CYS:CA	3:C:3366:ALA:HB1	2.26	0.62
11:K:37:LEU:HD13	14:N:36:LYS:NZ	2.12	0.62
2:B:1318:ILE:HG12	2:B:1345:LEU:HD13	1.79	0.62
3:C:343:MET:HG2	3:C:422:CYS:HB2	1.80	0.62
3:C:618:THR:HA	3:C:621:ILE:HG12	1.81	0.62
16:P:26:VAL:O	16:P:80:VAL:HA	1.99	0.62
1:A:264:TRP:HB3	1:A:296:ILE:HD12	1.81	0.62
2:B:797:PHE:CE1	2:B:829:VAL:HA	2.34	0.62
3:C:56:TYR:OH	3:C:74:GLN:NE2	2.32	0.62
3:C:177:ARG:NH2	3:C:258:GLU:HB2	2.14	0.62
3:C:797:ASN:ND2	5:e:1123:SER:HB2	2.14	0.62
2:B:1365:ILE:O	2:B:1369:VAL:HG23	2.00	0.62
2:B:3590:LEU:O	2:B:3594:LEU:N	2.31	0.62
3:C:793:GLN:C	5:e:1123:SER:HG	2.06	0.62
3:C:3344:GLN:CA	3:C:3347:LYS:N	2.62	0.62
8:H:40:GLU:OE1	8:H:40:GLU:N	2.32	0.62
9:I:99:TYR:CD2	9:I:103:LEU:HB2	2.35	0.62
2:B:196:PHE:O	2:B:200:ILE:HG12	2.00	0.62
2:B:507:ILE:HD11	2:B:536:ILE:HG23	1.80	0.62
2:B:701:ILE:HA	2:B:704:LYS:HD2	1.80	0.62
3:C:28:VAL:HG22	3:C:69:LYS:HD3	1.81	0.62
3:C:85:LEU:HG	3:C:87:LYS:H	1.63	0.62
3:C:805:ARG:HG3	3:C:806:ILE:HG13	1.81	0.62
4:d:1148:ILE:HD12	4:d:1193:ARG:CZ	2.30	0.62
2:B:439:LEU:HB3	2:B:533:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:GLU:HB2	5:e:1194:LYS:HZ3	1.65	0.62
2:B:565:GLY:HA2	2:B:571:SER:H	1.63	0.62
2:B:1284:LEU:HD23	2:B:1287:LEU:HD12	1.81	0.62
2:B:3516:PRO:O	2:B:3519:LEU:N	2.32	0.62
12:L:82:PHE:HB3	13:M:60:ASN:O	1.99	0.62
4:d:1174:LYS:HD2	4:d:1217:TRP:CD1	2.35	0.62
4:d:1203:ILE:HG23	4:d:1308:ASN:HD21	1.64	0.62
2:B:30:LYS:HA	2:B:33:LEU:HD23	1.81	0.62
2:B:1138:LYS:HG2	2:B:1145:LYS:O	2.00	0.62
3:C:244:ILE:HG23	3:C:247:ARG:HH21	1.64	0.62
3:C:317:LEU:HA	3:C:352:ILE:HG23	1.80	0.62
5:e:1097:LEU:HG	5:e:1099:ARG:NH1	2.15	0.62
1:A:345:TRP:CD1	2:B:970:ALA:HB1	2.34	0.62
5:e:1133:ASN:HB2	5:e:1145:LEU:HD11	1.82	0.62
11:K:32:CYS:SG	11:K:33:ALA:N	2.63	0.62
15:O:74:GLN:HB3	15:O:107:TYR:HB2	1.82	0.62
17:T:166:LYS:HE3	17:T:168:ASN:HD21	1.65	0.62
2:B:833:GLY:HA2	2:B:836:ILE:HG12	1.81	0.61
1:A:96:LEU:HD23	1:A:113:ILE:HG22	1.81	0.61
2:B:875:ILE:HB	2:B:962:PHE:CZ	2.35	0.61
2:B:2189:GLY:O	2:B:2193:VAL:N	2.31	0.61
5:e:1063:ILE:HD13	5:e:1073:ILE:HB	1.81	0.61
2:B:677:LEU:HD11	2:B:712:ILE:CD1	2.30	0.61
2:B:1079:ASN:OD1	2:B:1080:LEU:N	2.33	0.61
4:d:1148:ILE:HD12	4:d:1193:ARG:NH2	2.16	0.61
3:C:952:GLN:HG2	3:C:1006:ILE:HD13	1.81	0.61
3:C:3344:GLN:N	3:C:3347:LYS:N	2.45	0.61
1:A:144:GLN:HE21	1:A:171:ARG:HH11	1.48	0.61
2:B:503:LEU:O	2:B:507:ILE:HG13	2.01	0.61
2:B:518:TYR:HE2	5:e:1031:LEU:HB3	1.65	0.61
2:B:665:GLU:HB3	2:B:726:LYS:HG3	1.82	0.61
3:C:243:LEU:HB3	3:C:322:LYS:HD2	1.82	0.61
17:T:104:ALA:O	17:T:177:ARG:HD3	2.00	0.61
1:A:334:ARG:HD3	1:A:351:ALA:HB1	1.82	0.61
2:B:123:SER:O	2:B:127:GLU:HB2	2.01	0.61
2:B:452:LEU:HD11	5:e:1187:LYS:HG3	1.82	0.61
5:e:941:LEU:HD13	5:e:950:VAL:HG21	1.83	0.61
8:H:16:MET:HB3	8:H:20:MET:HB2	1.82	0.61
8:H:77:ILE:HG12	8:H:79:LEU:HD22	1.82	0.61
2:B:454:GLU:O	2:B:458:GLN:HB2	2.00	0.61
2:B:1148:SER:CB	2:B:1214:LEU:CG	2.76	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1311:MET:O	2:B:1314:ALA:HB3	2.00	0.61
2:B:1340:ASP:O	2:B:1344:THR:OG1	2.14	0.61
3:C:398:TRP:CD1	3:C:496:LYS:HB2	2.36	0.61
3:C:596:LEU:HD11	3:C:598:ARG:HE	1.65	0.61
3:C:3354:ILE:CB	3:C:3358:ILE:CB	2.79	0.61
3:C:3355:GLN:O	3:C:3359:ALA:CB	2.49	0.61
7:G:81:SER:N	7:G:142:GLU:O	2.33	0.61
2:B:64:VAL:HG22	2:B:83:LYS:HZ2	1.65	0.61
3:C:562:LYS:HA	3:C:565:LEU:HB2	1.81	0.61
4:d:972:ASN:HD22	4:d:978:LEU:HD23	1.66	0.61
7:G:138:ALA:HB3	7:G:145:LEU:HB2	1.82	0.61
2:B:315:GLU:O	2:B:319:PRO:HD2	2.00	0.61
2:B:452:LEU:HD21	5:e:1187:LYS:HZ3	1.66	0.61
2:B:531:LEU:HD13	2:B:609:LEU:HB3	1.83	0.61
3:C:511:ASP:O	3:C:515:VAL:HG23	2.01	0.61
16:P:60:ILE:HA	16:P:65:LEU:HD22	1.83	0.61
1:A:5:LEU:H	1:A:306:LEU:HD22	1.66	0.61
2:B:422:ARG:HG2	2:B:477:ILE:HG23	1.83	0.61
2:B:439:LEU:HD22	2:B:530:LEU:HA	1.82	0.61
2:B:497:LYS:O	4:d:1155:TYR:OH	2.14	0.61
3:C:535:ASN:HB3	3:C:568:ARG:HH12	1.66	0.61
4:d:123:TYR:O	4:d:127:GLU:HG2	2.01	0.61
4:d:1308:ASN:HA	4:d:1311:ILE:HD12	1.82	0.61
11:K:37:LEU:HB2	14:N:36:LYS:HD2	1.81	0.61
2:B:115:ASN:HD21	3:C:98:ILE:HG23	1.66	0.60
2:B:2904:THR:O	2:B:2908:GLY:N	2.34	0.60
4:d:95:LYS:HG2	10:J:52:GLU:HG2	1.83	0.60
4:d:136:LEU:HD23	4:d:164:ASN:HD22	1.66	0.60
16:P:82:LEU:HG	16:P:89:VAL:HB	1.83	0.60
1:A:3487:VAL:O	1:A:3491:LYS:N	2.33	0.60
3:C:3344:GLN:O	3:C:3348:ILE:CB	2.50	0.60
4:d:116:ILE:O	5:e:41:VAL:HG11	2.01	0.60
4:d:1170:VAL:HG11	4:d:1185:SER:HB2	1.83	0.60
6:F:88:ILE:O	6:F:98:LEU:HA	2.01	0.60
11:K:29:PRO:HG2	14:N:30:TYR:H	1.65	0.60
11:K:33:ALA:C	14:N:36:LYS:HD3	2.27	0.60
2:B:26:LYS:H	2:B:29:ILE:HD12	1.67	0.60
2:B:161:VAL:HG13	2:B:164:LEU:HD13	1.83	0.60
2:B:433:ILE:HA	2:B:463:PHE:CZ	2.36	0.60
2:B:435:GLN:HA	2:B:438:LYS:HE2	1.83	0.60
2:B:1149:ASP:N	2:B:1214:LEU:HD22	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HB3	1:A:185:PHE:CE2	2.34	0.60
3:C:405:LEU:HD21	3:C:464:PHE:HB3	1.83	0.60
4:d:1180:PRO:HG3	4:d:1301:LYS:HD3	1.82	0.60
5:e:26:ARG:NE	15:O:12:GLU:HG2	2.13	0.60
6:F:76:VAL:HG22	6:F:90:THR:HG23	1.84	0.60
12:L:22:ARG:NH1	12:L:97:ASP:OD2	2.33	0.60
12:L:33:LYS:HD3	12:L:60:PHE:CZ	2.36	0.60
1:A:192:PRO:HA	1:A:239:TRP:HE1	1.65	0.60
1:A:1616:ALA:O	1:A:1620:LEU:N	2.32	0.60
1:A:1915:ALA:O	1:A:1919:SER:N	2.33	0.60
2:B:165:LEU:O	2:B:169:LYS:N	2.27	0.60
2:B:555:LEU:HD21	2:B:602:PRO:HG2	1.83	0.60
2:B:1328:LYS:HG2	2:B:1332:GLN:HE21	1.65	0.60
3:C:1081:ILE:O	3:C:1085:LEU:HG	2.01	0.60
4:d:1091:MET:HE1	4:d:1093:TRP:HE1	1.67	0.60
6:F:9:ASP:OD1	6:F:10:GLN:N	2.34	0.60
1:A:1348:TYR:O	1:A:1355:LYS:N	2.34	0.60
2:B:473:VAL:HG23	2:B:488:ASP:OD1	2.02	0.60
3:C:678:HIS:HD2	3:C:686:VAL:HA	1.65	0.60
3:C:678:HIS:CD2	3:C:686:VAL:HA	2.36	0.60
5:e:33:GLN:H	15:O:28:LYS:HE2	1.66	0.60
5:e:1090:THR:HG22	5:e:1164:LEU:HD12	1.84	0.60
1:A:3214:GLU:O	1:A:3218:ASN:N	2.35	0.60
2:B:1196:ASN:O	2:B:1200:ILE:HG12	2.02	0.60
3:C:3344:GLN:C	3:C:3345:LYS:O	2.23	0.60
5:e:867:ALA:HB3	5:e:882:LEU:HB3	1.82	0.60
5:e:871:ASP:HB2	5:e:874:ASN:HB2	1.83	0.60
8:H:14:SER:HA	8:H:77:ILE:HA	1.83	0.60
9:I:67:LEU:HB3	9:I:75:TRP:CD1	2.37	0.60
12:L:37:GLN:HE22	12:L:41:LEU:HD12	1.65	0.60
1:A:341:TRP:NE1	1:A:343:ASN:O	2.34	0.60
3:C:143:ILE:HG21	3:C:162:VAL:HG21	1.83	0.60
2:B:1106:PHE:HD2	2:B:1171:LEU:HB2	1.65	0.60
2:B:3393:ARG:O	2:B:3396:GLU:N	2.34	0.60
4:d:1152:SER:HB3	4:d:1158:GLN:NE2	2.17	0.60
17:T:45:LYS:O	17:T:49:LYS:HG2	2.00	0.60
2:B:433:ILE:HA	2:B:463:PHE:HZ	1.67	0.60
2:B:707:THR:O	2:B:710:THR:OG1	2.18	0.60
7:G:126:LEU:O	7:G:137:VAL:HB	2.01	0.60
2:B:299:PHE:HD1	2:B:302:LEU:HD12	1.67	0.59
2:B:1145:LYS:HZ1	2:B:1150:VAL:HG11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:316:TYR:HB2	3:C:353:ALA:HB2	1.84	0.59
3:C:3353:ARG:O	3:C:3357:ALA:HB3	2.02	0.59
2:B:814:TYR:HB2	2:B:1075:TRP:NE1	2.07	0.59
2:B:429:LEU:O	2:B:433:ILE:HG13	2.01	0.59
2:B:1068:LYS:HD3	2:B:1069:THR:O	2.02	0.59
2:B:1240:PHE:HE1	2:B:1267:TYR:HB3	1.68	0.59
4:d:1073:PRO:HA	4:d:1079:TYR:HD2	1.67	0.59
16:P:58:VAL:HG22	16:P:65:LEU:HD21	1.83	0.59
3:C:750:ASN:HB2	3:C:887:LYS:HD3	1.85	0.59
3:C:1039:SER:HB3	3:C:1103:ARG:NH2	2.18	0.59
5:e:853:ILE:HB	5:e:864:PRO:HA	1.84	0.59
14:N:108:ASP:OD1	14:N:130:TYR:N	2.28	0.59
1:A:200:ARG:HH22	1:A:228:ASN:ND2	2.01	0.59
1:A:288:VAL:HG12	1:A:290:ASP:H	1.66	0.59
1:A:3406:ARG:O	1:A:3688:ALA:N	2.33	0.59
2:B:359:VAL:HG21	2:B:419:PHE:HZ	1.68	0.59
2:B:1311:MET:SD	2:B:1356:ILE:HG13	2.43	0.59
3:C:321:GLU:HB2	3:C:345:ALA:HB1	1.82	0.59
3:C:3354:ILE:CA	3:C:3357:ALA:HB3	2.32	0.59
5:e:72:GLY:HA2	8:H:73:ARG:HH11	1.68	0.59
5:e:1012:ILE:HD11	5:e:1040:VAL:HG21	1.85	0.59
7:G:127:ARG:HG2	7:G:129:GLN:HE22	1.67	0.59
9:I:93:THR:HB	9:I:109:LYS:HB2	1.85	0.59
16:P:65:LEU:O	16:P:69:VAL:HG23	2.02	0.59
3:C:77:VAL:HG11	3:C:94:TRP:CZ2	2.38	0.59
3:C:812:THR:HA	3:C:815:LYS:HE3	1.85	0.59
3:C:970:TYR:CE1	3:C:977:LYS:HD2	2.38	0.59
3:C:3343:HIS:CA	3:C:3346:SER:CB	2.54	0.59
3:C:577:ALA:HA	3:C:641:TYR:OH	2.03	0.59
3:C:755:HIS:CE1	3:C:794:LEU:HD13	2.37	0.59
3:C:861:ASP:OD1	5:e:876:ASN:ND2	2.36	0.59
4:d:1179:HIS:ND1	4:d:1298:GLU:OE2	2.35	0.59
1:A:144:GLN:HE21	1:A:171:ARG:NH1	2.01	0.59
1:A:320:PRO:HD2	1:A:341:TRP:O	2.03	0.59
1:A:3206:LYS:O	1:A:3210:ALA:N	2.33	0.59
2:B:203:TRP:HZ3	2:B:253:VAL:HG13	1.68	0.59
2:B:367:LEU:HD11	2:B:375:GLU:HB2	1.84	0.59
2:B:433:ILE:HG23	2:B:463:PHE:HE2	1.67	0.59
3:C:346:ILE:O	3:C:349:ILE:HG13	2.03	0.59
3:C:807:GLU:O	3:C:811:LYS:NZ	2.35	0.59
4:d:1148:ILE:O	4:d:1163:TYR:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:827:LYS:HE3	5:e:878:PRO:HD2	1.84	0.59
3:C:495:PHE:CE1	3:C:513:ASP:HB3	2.38	0.59
2:B:336:GLN:OE1	2:B:406:LYS:NZ	2.36	0.58
2:B:586:ALA:HB1	2:B:686:TYR:CZ	2.38	0.58
2:B:1246:PHE:CG	2:B:1360:LYS:HB3	2.38	0.58
2:B:2657:LYS:O	2:B:2660:SER:N	2.36	0.58
3:C:544:TYR:CG	4:d:1207:ASP:HB3	2.39	0.58
3:C:1009:THR:HA	3:C:1012:LYS:HE2	1.85	0.58
2:B:1245:PRO:C	2:B:1360:LYS:HB2	2.28	0.58
2:B:1660:ILE:O	2:B:1672:PHE:N	2.35	0.58
3:C:857:ARG:HG3	5:e:876:ASN:N	2.19	0.58
3:C:3343:HIS:O	3:C:3345:LYS:N	2.34	0.58
4:d:965:ASN:OD1	4:d:1258:THR:HG21	2.03	0.58
1:A:2628:GLN:O	1:A:2632:GLU:N	2.34	0.58
2:B:273:LYS:HB3	2:B:282:ARG:HH12	1.66	0.58
3:C:1144:LYS:HB3	4:d:172:GLU:O	2.03	0.58
4:d:1241:ASP:HB2	4:d:1246:LEU:HD11	1.83	0.58
8:H:13:ASN:O	8:H:78:TYR:N	2.33	0.58
11:K:19:LYS:HG2	11:K:28:TRP:HB2	1.86	0.58
11:K:38:GLU:O	11:K:42:ARG:HG2	2.04	0.58
2:B:671:VAL:HG11	2:B:673:PHE:CE2	2.38	0.58
2:B:1218:GLU:O	2:B:1222:ILE:HG13	2.04	0.58
3:C:21:LEU:HD22	3:C:91:LYS:HG3	1.85	0.58
3:C:931:PHE:HD1	3:C:1074:MET:HE1	1.68	0.58
3:C:934:GLU:O	3:C:945:ASN:N	2.24	0.58
4:d:1223:THR:N	4:d:1239:ASN:OD1	2.36	0.58
14:N:33:LYS:HD3	14:N:36:LYS:HG3	1.84	0.58
1:A:10:LEU:HG	1:A:65:ASN:HB3	1.86	0.58
1:A:38:GLY:O	1:A:53:PRO:HB3	2.04	0.58
1:A:2928:VAL:O	1:A:2932:SER:N	2.29	0.58
2:B:1175:ASN:O	2:B:1179:THR:HG23	2.03	0.58
3:C:931:PHE:CD1	3:C:1074:MET:HE1	2.38	0.58
4:d:117:TRP:HH2	5:e:40:TYR:N	2.02	0.58
5:e:824:LYS:HB3	5:e:1155:VAL:H	1.66	0.58
7:G:71:LYS:HD3	7:G:72:THR:HG23	1.85	0.58
7:G:111:ARG:HA	7:G:114:VAL:HG12	1.84	0.58
7:G:136:MET:HB3	7:G:147:VAL:HG12	1.85	0.58
12:L:31:LEU:O	12:L:35:ILE:HG12	2.03	0.58
1:A:284:ASN:HA	2:B:935:ASN:HD21	1.68	0.58
1:A:3023:ARG:O	1:A:3027:LYS:N	2.37	0.58
2:B:1250:GLU:HA	2:B:1256:ASN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:561:LEU:O	3:C:565:LEU:N	2.23	0.58
3:C:561:LEU:HG	3:C:565:LEU:HG	1.84	0.58
3:C:797:ASN:CG	5:e:1123:SER:HB2	2.29	0.58
3:C:899:LEU:HD13	3:C:989:ILE:HD11	1.85	0.58
3:C:1095:GLN:O	3:C:1098:GLN:HG3	2.03	0.58
5:e:837:ILE:HG13	5:e:1129:CYS:HB3	1.84	0.58
1:A:3135:LEU:O	1:A:3139:VAL:N	2.35	0.58
2:B:64:VAL:O	2:B:74:TYR:HA	2.03	0.58
2:B:1224:ARG:O	2:B:1228:ILE:HG12	2.02	0.58
2:B:4547:VAL:O	2:B:4558:VAL:N	2.36	0.58
4:d:89:TYR:CE2	10:J:56:PRO:HA	2.39	0.58
5:e:908:GLY:HA2	5:e:935:VAL:HG13	1.86	0.58
2:B:1314:ALA:HB2	16:P:75:SER:C	2.29	0.58
8:H:9:PRO:HG3	8:H:81:VAL:HG13	1.86	0.58
2:B:336:GLN:HG3	2:B:338:PRO:HG2	1.85	0.58
2:B:814:TYR:HB2	2:B:1075:TRP:CD1	2.36	0.58
2:B:1072:ASP:HB3	2:B:1077:ARG:HA	1.86	0.58
2:B:1215:GLN:HB3	2:B:1218:GLU:HB2	1.85	0.58
3:C:933:VAL:HG21	3:C:944:LEU:HB3	1.86	0.58
3:C:2912:ASP:O	3:C:2918:LYS:N	2.37	0.58
5:e:38:ASN:N	5:e:39:GLN:OE1	2.37	0.58
6:F:34:LYS:HE3	6:F:36:HIS:CE1	2.39	0.58
8:H:16:MET:O	8:H:21:GLN:NE2	2.36	0.58
11:K:23:GLY:HA3	11:K:41:ILE:HG23	1.85	0.58
16:P:32:TRP:CH2	16:P:77:LEU:HG	2.38	0.58
1:A:225:GLN:HG3	1:A:282:ARG:HH11	1.69	0.58
2:B:429:LEU:HB2	2:B:470:PHE:CE2	2.39	0.58
2:B:2781:ASP:O	2:B:3047:TRP:N	2.37	0.58
3:C:44:PHE:HE1	3:C:51:ASN:C	2.12	0.58
3:C:1095:GLN:OE1	3:C:1098:GLN:NE2	2.37	0.58
2:B:55:GLN:HE21	2:B:57:ASN:HB3	1.68	0.57
2:B:503:LEU:HD11	2:B:533:ARG:HH21	1.68	0.57
2:B:1734:THR:O	2:B:1737:VAL:N	2.37	0.57
3:C:801:ILE:HA	5:e:822:LEU:HD11	1.85	0.57
3:C:3203:PRO:O	3:C:3204:ALA:HB2	2.04	0.57
5:e:35:VAL:HG12	5:e:37:ILE:HG12	1.85	0.57
1:A:1701:GLN:O	1:A:1705:ASN:N	2.35	0.57
2:B:134:GLN:HE21	3:C:79:PHE:HZ	1.51	0.57
3:C:210:GLU:HG3	3:C:280:ASN:HD21	1.69	0.57
3:C:580:LEU:HD22	3:C:641:TYR:CE1	2.39	0.57
1:A:51:ILE:HA	1:A:82:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:HD1	1:A:177:LEU:HB3	1.70	0.57
1:A:3615:CYS:O	1:A:3619:GLY:N	2.37	0.57
2:B:200:ILE:HG21	2:B:257:LEU:HD21	1.85	0.57
2:B:1354:LYS:HG2	2:B:1357:ARG:NH1	2.19	0.57
3:C:805:ARG:CZ	5:e:822:LEU:HB3	2.34	0.57
4:d:247:ILE:O	4:d:251:MET:CB	2.52	0.57
5:e:1182:GLU:HA	5:e:1185:LYS:HD2	1.86	0.57
1:A:195:ASN:N	1:A:196:PRO:HD2	2.19	0.57
2:B:2376:SER:CB	3:C:1540:GLN:HA	2.34	0.57
3:C:104:ASP:OD2	3:C:107:LYS:HE3	2.05	0.57
3:C:3378:ALA:O	3:C:3379:GLN:C	2.48	0.57
4:d:1166:HIS:N	4:d:1193:ARG:HD2	2.19	0.57
4:d:1268:ILE:HD13	4:d:1282:LYS:HB2	1.85	0.57
5:e:818:LYS:NZ	5:e:1118:PHE:HD2	2.03	0.57
6:F:87:TYR:HH	6:F:98:LEU:HD13	1.69	0.57
16:P:47:LYS:HD3	16:P:55:ILE:HG12	1.86	0.57
2:B:422:ARG:NE	2:B:478:MET:HA	2.20	0.57
2:B:1315:ILE:HG23	2:B:1365:ILE:HG13	1.86	0.57
2:B:1325:TRP:HA	2:B:1328:LYS:HG3	1.86	0.57
3:C:1144:LYS:NZ	4:d:170:THR:O	2.31	0.57
12:L:96:PHE:CE2	12:L:105:ILE:HD11	2.39	0.57
16:P:11:THR:O	16:P:15:GLU:HG2	2.05	0.57
1:A:276:PHE:HE2	1:A:284:ASN:HB2	1.70	0.57
1:A:1400:ALA:O	1:A:1526:ILE:N	2.38	0.57
2:B:609:LEU:HD13	2:B:614:THR:HG23	1.86	0.57
2:B:810:SER:HB3	2:B:815:ASP:HA	1.87	0.57
2:B:1357:ARG:HG3	2:B:1358:ASN:OD1	2.05	0.57
2:B:653:GLN:HG3	2:B:655:LYS:H	1.69	0.57
2:B:1268:TYR:HB3	2:B:1305:LEU:HD21	1.86	0.57
3:C:529:GLN:HA	3:C:532:ILE:HD12	1.87	0.57
3:C:796:ILE:HG21	5:e:1121:LYS:O	2.05	0.57
5:e:854:MET:HB3	5:e:855:ARG:CZ	2.35	0.57
5:e:1081:TYR:HB2	5:e:1100:ARG:HG3	1.85	0.57
7:G:78:ILE:HG23	7:G:86:VAL:HB	1.87	0.57
11:K:41:ILE:O	11:K:45:GLN:NE2	2.37	0.57
1:A:99:GLY:HA3	1:A:149:HIS:HE1	1.69	0.57
1:A:225:GLN:HB2	1:A:251:TRP:CD1	2.40	0.57
2:B:956:LEU:O	2:B:960:ARG:HD3	2.05	0.57
3:C:1111:LEU:HB3	3:C:1183:LEU:HD21	1.87	0.57
3:C:1195:GLU:O	3:C:1199:LYS:HD3	2.04	0.57
3:C:3186:GLN:O	3:C:3359:ALA:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:32:SER:O	14:N:36:LYS:HG2	2.05	0.57
1:A:69:TRP:O	1:A:70:ARG:NE	2.30	0.57
1:A:2417:PHE:N	1:A:2487:ALA:O	2.38	0.57
2:B:738:LYS:O	2:B:741:ILE:HG22	2.05	0.57
2:B:813:ASP:CG	2:B:1075:TRP:HE1	2.12	0.57
2:B:1107:ARG:NH1	2:B:1111:LYS:HB3	2.19	0.57
2:B:1117:ILE:HG22	2:B:1200:ILE:HG22	1.87	0.57
2:B:2818:LEU:N	2:B:2835:THR:O	2.38	0.57
3:C:972:TRP:HA	3:C:975:GLN:HE21	1.70	0.57
4:d:1225:PHE:HB3	4:d:1236:TYR:HB2	1.85	0.57
13:M:23:ILE:HG22	13:M:41:ILE:HG12	1.87	0.57
2:B:227:PRO:HD3	2:B:346:GLU:HB3	1.86	0.57
2:B:929:THR:HG22	2:B:930:ILE:H	1.68	0.57
3:C:1223:VAL:HG22	3:C:1259:LYS:HE2	1.87	0.57
5:e:30:ILE:HG12	15:O:22:LYS:HG3	1.87	0.57
9:I:38:ALA:O	9:I:42:ILE:HG13	2.04	0.57
1:A:203:HIS:HB3	1:A:219:GLY:HA3	1.87	0.56
2:B:1225:ASP:HB3	2:B:1281:TYR:CZ	2.40	0.56
2:B:1250:GLU:OE2	2:B:1256:ASN:ND2	2.38	0.56
2:B:4191:GLY:O	2:B:4196:GLY:N	2.38	0.56
3:C:278:HIS:HD2	3:C:282:ARG:NH1	2.03	0.56
4:d:1071:TRP:HE3	4:d:1079:TYR:HB2	1.70	0.56
5:e:943:SER:HB2	5:e:948:GLU:H	1.70	0.56
9:I:57:GLU:O	9:I:61:LYS:HG2	2.05	0.56
11:K:31:GLU:HA	14:N:32:SER:HB3	1.87	0.56
2:B:1276:GLY:O	2:B:1280:GLU:HG2	2.05	0.56
3:C:789:LYS:O	5:e:1121:LYS:NZ	2.37	0.56
3:C:1116:LYS:O	3:C:1120:THR:HG23	2.05	0.56
4:d:1139:PHE:CE1	4:d:1151:CYS:HB3	2.39	0.56
4:d:1196:ASP:HB3	4:d:1199:TYR:HD2	1.70	0.56
5:e:1090:THR:HG22	5:e:1164:LEU:HA	1.87	0.56
1:A:232:TYR:HB2	1:A:239:TRP:CZ3	2.39	0.56
2:B:16:ASN:HB2	2:B:17:ARG:HH11	1.71	0.56
2:B:51:GLY:HA2	2:B:54:GLN:HE21	1.71	0.56
2:B:310:PHE:HA	2:B:313:LEU:HD12	1.86	0.56
2:B:425:ASP:OD1	2:B:426:ILE:HG13	2.04	0.56
2:B:1051:ASP:OD1	2:B:1174:HIS:NE2	2.38	0.56
3:C:1057:GLN:NE2	3:C:1061:GLU:OE2	2.36	0.56
4:d:84:LYS:HE3	11:K:92:LYS:HE2	1.87	0.56
11:K:45:GLN:O	11:K:49:LYS:HG2	2.04	0.56
1:A:62:LEU:HD13	1:A:327:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:988:ALA:O	2:B:992:THR:HG23	2.04	0.56
4:d:1206:PHE:CG	4:d:1207:ASP:N	2.73	0.56
6:F:74:ILE:HD12	6:F:77:ILE:HD11	1.87	0.56
1:A:3492:LYS:O	1:A:3496:GLU:N	2.39	0.56
1:A:4135:GLY:O	1:A:4140:PHE:N	2.38	0.56
2:B:380:LEU:HD21	2:B:427:LEU:HA	1.86	0.56
2:B:839:LEU:O	2:B:842:GLU:HG2	2.06	0.56
2:B:3579:ILE:O	2:B:3625:MET:N	2.39	0.56
3:C:562:LYS:HA	3:C:565:LEU:HD12	1.88	0.56
3:C:857:ARG:HH21	5:e:875:PRO:HD2	1.71	0.56
3:C:3342:TYR:O	3:C:3345:LYS:C	2.48	0.56
4:d:1168:LEU:HD13	4:d:1189:ASP:HB2	1.86	0.56
5:e:1181:ARG:O	5:e:1185:LYS:HG3	2.05	0.56
12:L:74:TRP:CD2	12:L:109:LYS:HD3	2.41	0.56
13:M:76:LYS:HA	13:M:80:LEU:O	2.05	0.56
15:O:99:GLN:NE2	15:O:100:CYS:O	2.39	0.56
16:P:33:CYS:SG	16:P:38:ILE:HG23	2.45	0.56
1:A:255:GLY:HA3	1:A:268:ILE:HD11	1.87	0.56
1:A:341:TRP:HH2	2:B:967:GLN:HE22	1.53	0.56
2:B:658:GLN:HB3	2:B:667:ASP:HB3	1.86	0.56
2:B:918:GLY:HA2	2:B:921:SER:HB2	1.87	0.56
2:B:1325:TRP:HE1	2:B:1333:ILE:HG23	1.71	0.56
3:C:910:LYS:HB3	3:C:998:VAL:HG11	1.87	0.56
3:C:3378:ALA:C	3:C:3380:ILE:N	2.63	0.56
4:d:935:TRP:CD1	4:d:1279:THR:HA	2.39	0.56
15:O:32:SER:HA	15:O:35:THR:OG1	2.05	0.56
2:B:133:MET:HB3	2:B:137:LEU:HD11	1.86	0.56
2:B:541:GLU:HA	2:B:616:ARG:HH12	1.71	0.56
3:C:874:HIS:HB3	3:C:884:LYS:HD2	1.87	0.56
3:C:1055:PHE:HE2	3:C:1093:LYS:HE3	1.70	0.56
5:e:924:ILE:HG22	5:e:925:SER:H	1.71	0.56
14:N:80:LYS:O	14:N:128:GLY:HA2	2.05	0.56
16:P:43:PHE:HD1	16:P:100:LEU:HD21	1.69	0.56
2:B:110:VAL:HG12	3:C:122:GLU:HG2	1.86	0.56
2:B:928:ASN:OD1	2:B:932:ASN:ND2	2.39	0.56
2:B:1037:LEU:O	2:B:1041:ARG:HG2	2.06	0.56
2:B:1117:ILE:HG13	2:B:1197:PHE:CE2	2.41	0.56
2:B:1124:ILE:HG22	2:B:1207:VAL:HG12	1.88	0.56
3:C:78:LEU:HD12	3:C:131:LEU:HD12	1.88	0.56
5:e:863:MET:HB2	5:e:866:GLN:HE21	1.71	0.56
5:e:924:ILE:HG22	5:e:925:SER:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:45:LEU:HA	15:O:48:GLN:HE21	1.70	0.56
2:B:158:VAL:HA	2:B:161:VAL:HB	1.88	0.56
2:B:1047:LEU:HG	2:B:1047:LEU:O	2.06	0.56
3:C:3117:PHE:CB	3:C:3433:ALA:HB2	2.36	0.56
3:C:3355:GLN:O	3:C:3359:ALA:HB3	2.05	0.56
4:d:117:TRP:N	4:d:119:GLU:OE1	2.39	0.56
5:e:872:LEU:HD13	5:e:1145:LEU:HD21	1.88	0.56
5:e:1056:VAL:HG11	5:e:1082:LEU:HD13	1.88	0.56
5:e:1072:ILE:HD11	5:e:1185:LYS:HE2	1.88	0.56
5:e:1080:SER:HB2	5:e:1099:ARG:HD2	1.88	0.56
16:P:39:LEU:HG	16:P:95:ASN:HB2	1.87	0.56
2:B:176:LEU:HD22	2:B:243:LEU:HD21	1.87	0.56
2:B:544:HIS:CG	2:B:613:ILE:HG22	2.41	0.56
2:B:1243:LYS:NZ	2:B:1264:ILE:HG23	2.21	0.56
3:C:807:GLU:N	3:C:807:GLU:OE2	2.39	0.56
5:e:922:ILE:HG13	5:e:923:MET:H	1.71	0.56
8:H:22:LYS:NZ	8:H:23:GLU:OE2	2.38	0.56
16:P:36:CYS:CB	16:P:95:ASN:HD21	2.19	0.56
1:A:44:ASN:HB2	1:A:48:ASP:OD2	2.05	0.55
2:B:656:LEU:HD12	2:B:752:ILE:O	2.05	0.55
2:B:721:ASN:OD1	2:B:770:LYS:NZ	2.39	0.55
3:C:40:LEU:HD11	3:C:73:ALA:HB2	1.87	0.55
3:C:542:ILE:HD12	3:C:576:TYR:CD1	2.41	0.55
3:C:3180:CYS:CB	3:C:3366:ALA:C	2.79	0.55
4:d:1237:ASP:H	4:d:1246:LEU:HD23	1.71	0.55
4:d:1242:LYS:HE2	4:d:1243:LEU:HB2	1.88	0.55
11:K:100:ILE:HG12	11:K:101:GLU:OE1	2.05	0.55
16:P:42:GLN:HG2	16:P:97:LYS:HG3	1.87	0.55
1:A:194:GLY:H	1:A:239:TRP:HD1	1.54	0.55
2:B:1126:LYS:HZ1	2:B:1138:LYS:HB3	1.70	0.55
2:B:1172:LYS:HA	2:B:1176:VAL:HB	1.87	0.55
2:B:1240:PHE:HA	2:B:1243:LYS:HZ2	1.71	0.55
5:e:72:GLY:HA2	8:H:73:ARG:NH1	2.22	0.55
2:B:52:PHE:O	2:B:93:LYS:NZ	2.40	0.55
2:B:134:GLN:HB2	3:C:79:PHE:CZ	2.41	0.55
2:B:327:ILE:HD11	2:B:397:TYR:CE1	2.40	0.55
12:L:21:ILE:HA	12:L:96:PHE:HB3	1.88	0.55
12:L:33:LYS:HD3	12:L:60:PHE:HZ	1.70	0.55
16:P:63:GLU:HA	16:P:66:GLU:CD	2.30	0.55
1:A:170:GLN:HB2	2:B:861:ASP:HB3	1.88	0.55
1:A:272:SER:HA	1:A:287:PHE:HD1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1689:GLY:O	1:A:1693:THR:N	2.38	0.55
2:B:625:LEU:O	2:B:628:SER:OG	2.23	0.55
3:C:430:VAL:O	3:C:434:PRO:HD3	2.06	0.55
3:C:541:ASN:HB2	3:C:544:TYR:CD2	2.41	0.55
5:e:1168:GLN:HG3	5:e:1172:LYS:HE2	1.89	0.55
16:P:28:PHE:HB2	16:P:79:HIS:HB3	1.88	0.55
1:A:75:GLN:O	1:A:121:TRP:N	2.39	0.55
1:A:272:SER:HA	1:A:287:PHE:CD1	2.42	0.55
2:B:275:GLN:OE1	2:B:275:GLN:N	2.40	0.55
2:B:962:PHE:O	2:B:967:GLN:N	2.40	0.55
2:B:1099:THR:O	2:B:1103:VAL:HG23	2.07	0.55
12:L:84:CYS:HA	13:M:56:ILE:HG23	1.88	0.55
1:A:169:TYR:HB2	1:A:171:ARG:NE	2.22	0.55
1:A:257:MET:HE3	1:A:258:ALA:H	1.70	0.55
2:B:326:LEU:HD22	2:B:330:LYS:HG3	1.89	0.55
2:B:1277:ARG:HH11	2:B:1277:ARG:HA	1.71	0.55
3:C:405:LEU:HD23	3:C:468:GLN:HE21	1.72	0.55
3:C:1032:GLN:HG3	3:C:1036:LYS:HG2	1.89	0.55
1:A:4080:ALA:HB1	1:A:4092:TYR:O	2.07	0.55
2:B:84:PHE:HZ	3:C:150:LYS:HD3	1.72	0.55
2:B:344:ILE:HD13	2:B:394:TYR:OH	2.05	0.55
2:B:429:LEU:HD13	2:B:470:PHE:CG	2.42	0.55
2:B:876:GLN:CD	2:B:966:LYS:HB3	2.31	0.55
2:B:1285:GLU:HG3	2:B:1290:LEU:CD1	2.36	0.55
3:C:135:MET:HG3	3:C:165:PHE:HE2	1.71	0.55
3:C:544:TYR:CD2	4:d:1207:ASP:HB3	2.42	0.55
11:K:37:LEU:CD1	14:N:36:LYS:HZ3	2.18	0.55
13:M:17:ILE:O	13:M:21:LYS:HG2	2.06	0.55
14:N:37:ILE:HG23	14:N:70:LYS:HZ3	1.72	0.55
1:A:2176:THR:O	1:A:2177:ILE:N	2.40	0.55
2:B:118:LEU:HD13	2:B:158:VAL:HG12	1.88	0.55
2:B:123:SER:HB3	3:C:96:LEU:HD21	1.88	0.55
2:B:269:THR:HB	2:B:270:PRO:HD3	1.89	0.55
2:B:589:LEU:HD21	2:B:640:LYS:HB2	1.89	0.55
2:B:615:GLU:HA	2:B:619:TYR:CD2	2.42	0.55
2:B:987:ARG:HA	2:B:990:PHE:CD2	2.41	0.55
2:B:1123:GLY:O	2:B:1138:LYS:NZ	2.40	0.55
3:C:624:PHE:HB3	3:C:634:ILE:CG2	2.37	0.55
5:e:834:VAL:H	5:e:1153:GLY:HA2	1.71	0.55
5:e:1075:THR:HG21	5:e:1114:ASN:HB2	1.87	0.55
5:e:1077:TYR:HD2	5:e:1080:SER:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:81:ASN:HB3	13:M:60:ASN:HD21	1.72	0.55
16:P:8:ILE:HD11	16:P:14:PHE:HD1	1.72	0.55
2:B:1154:GLU:HB3	2:B:1155:PRO:HD3	1.87	0.55
2:B:1311:MET:C	2:B:1362:TYR:HE1	2.14	0.55
4:d:1134:PHE:HB2	4:d:1181:ARG:HH12	1.72	0.55
5:e:1013:LEU:HD21	5:e:1035:ARG:HH22	1.71	0.55
5:e:1088:SER:HB2	5:e:1096:PHE:HE2	1.71	0.55
3:C:1112:THR:OG1	3:C:1179:ALA:O	2.20	0.55
3:C:1211:GLU:HG3	3:C:1214:GLN:HE21	1.72	0.55
4:d:1132:ASN:HB3	4:d:1135:GLU:O	2.06	0.55
2:B:179:HIS:HB3	2:B:203:TRP:CE2	2.42	0.54
3:C:457:LEU:HD23	3:C:460:LEU:HD12	1.89	0.54
3:C:1253:GLU:HA	3:C:1256:TYR:CE1	2.42	0.54
5:e:1147:ALA:HA	5:e:1157:ILE:HA	1.89	0.54
7:G:125:PHE:HA	7:G:139:PRO:HD2	1.88	0.54
15:O:13:VAL:O	15:O:17:ILE:HG12	2.07	0.54
1:A:1727:ASN:O	1:A:1731:LYS:N	2.39	0.54
2:B:45:ASN:HD21	2:B:48:GLU:CD	2.15	0.54
2:B:173:MET:HE3	2:B:221:TYR:HD2	1.72	0.54
2:B:718:ILE:HD11	2:B:766:ILE:O	2.07	0.54
2:B:862:TYR:O	2:B:866:ILE:HG12	2.07	0.54
2:B:1109:THR:HG23	2:B:1164:MET:HG3	1.89	0.54
3:C:936:GLN:HB3	3:C:1080:ASN:ND2	2.23	0.54
12:L:39:ASP:O	12:L:43:LYS:HG2	2.08	0.54
1:A:99:GLY:HA3	1:A:149:HIS:CE1	2.42	0.54
1:A:2406:CYS:O	1:A:2410:GLU:N	2.38	0.54
2:B:190:LYS:O	2:B:194:HIS:HB2	2.07	0.54
2:B:1061:GLN:HA	2:B:1064:ILE:HD12	1.89	0.54
3:C:928:LYS:HD2	3:C:957:ARG:NH2	2.15	0.54
4:d:86:ILE:O	4:d:99:ASP:N	2.41	0.54
4:d:1089:ARG:NH1	4:d:1091:MET:HB3	2.22	0.54
2:B:344:ILE:HD11	2:B:397:TYR:HE2	1.70	0.54
2:B:1148:SER:HG	2:B:1213:PRO:C	1.93	0.54
2:B:1317:LEU:HD22	16:P:32:TRP:CZ3	2.43	0.54
3:C:1144:LYS:HD3	4:d:171:ARG:HA	1.89	0.54
4:d:79:ASN:HB2	4:d:104:GLN:HB3	1.89	0.54
5:e:1170:LYS:O	5:e:1174:ILE:HG13	2.07	0.54
2:B:160:GLN:HB3	2:B:178:SER:OG	2.06	0.54
2:B:198:GLY:O	2:B:202:THR:HG23	2.06	0.54
2:B:836:ILE:HD13	2:B:839:LEU:HD21	1.90	0.54
2:B:939:ASN:OD1	2:B:940:ILE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1325:TRP:NE1	2:B:1333:ILE:HG23	2.22	0.54
2:B:1814:SER:O	2:B:1818:LEU:N	2.39	0.54
3:C:134:LEU:O	3:C:138:VAL:HG12	2.08	0.54
3:C:809:ASN:ND2	5:e:876:ASN:HD21	2.06	0.54
3:C:3332:ILE:O	3:C:3333:LEU:C	2.49	0.54
4:d:1045:ARG:HD2	5:e:141:VAL:H	1.73	0.54
4:d:1194:ILE:O	4:d:1202:GLN:HG2	2.08	0.54
5:e:863:MET:HB2	5:e:866:GLN:NE2	2.21	0.54
6:F:25:ILE:HD11	6:F:95:PHE:HB3	1.88	0.54
1:A:3438:HIS:O	1:A:3442:GLY:N	2.41	0.54
2:B:843:VAL:HG11	2:B:859:TYR:CE2	2.43	0.54
2:B:1240:PHE:CE2	2:B:1271:LEU:HD22	2.43	0.54
2:B:1317:LEU:CD1	16:P:77:LEU:H	2.20	0.54
3:C:349:ILE:HG23	3:C:357:ASN:HD21	1.73	0.54
3:C:970:TYR:HE1	3:C:977:LYS:HD2	1.73	0.54
5:e:30:ILE:HD11	15:O:23:GLN:N	2.23	0.54
1:A:2102:LEU:O	1:A:2106:GLY:N	2.40	0.54
2:B:137:LEU:HG	2:B:145:LEU:HB2	1.90	0.54
3:C:793:GLN:C	5:e:1123:SER:OG	2.49	0.54
3:C:3378:ALA:O	3:C:3381:GLN:N	2.39	0.54
5:e:59:HIS:CE1	11:K:88:ALA:HB3	2.43	0.54
16:P:13:GLN:HA	16:P:16:ASP:OD1	2.08	0.54
17:T:179:CYS:HB3	17:T:192:TYR:CZ	2.42	0.54
1:A:194:GLY:N	1:A:239:TRP:HD1	2.06	0.54
1:A:219:GLY:O	1:A:226:TYR:N	2.41	0.54
2:B:335:ASN:HD21	2:B:340:LEU:HD13	1.73	0.54
2:B:1280:GLU:HA	2:B:1283:ASN:OD1	2.07	0.54
3:C:867:MET:HB2	5:e:826:GLU:OE2	2.08	0.54
3:C:3187:ILE:CB	3:C:3360:GLU:CA	2.84	0.54
3:C:3343:HIS:C	3:C:3345:LYS:H	2.15	0.54
5:e:30:ILE:HG12	15:O:22:LYS:CG	2.38	0.54
7:G:93:GLU:O	7:G:97:LYS:HG2	2.08	0.54
8:H:57:TRP:CE2	8:H:90:LYS:HD2	2.43	0.54
1:A:169:TYR:HB2	1:A:171:ARG:HE	1.73	0.54
1:A:2499:ARG:O	1:A:2503:PHE:N	2.40	0.54
2:B:118:LEU:HD12	2:B:162:TYR:HD1	1.72	0.54
2:B:527:PHE:HB3	2:B:530:LEU:HD13	1.90	0.54
2:B:1107:ARG:HG3	2:B:1111:LYS:CE	2.38	0.54
3:C:580:LEU:HD13	3:C:641:TYR:CD2	2.42	0.54
8:H:24:VAL:HA	8:H:49:PHE:HZ	1.73	0.54
15:O:9:ILE:HG23	15:O:12:GLU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:LEU:O	2:B:168:ILE:HG12	2.08	0.54
2:B:1054:ILE:HD11	2:B:1098:TYR:HB2	1.90	0.54
2:B:1126:LYS:HZ2	2:B:1134:LEU:HD22	1.73	0.54
3:C:123:ILE:HD11	3:C:134:LEU:HD12	1.90	0.54
3:C:325:GLU:HB3	3:C:338:THR:OG1	2.08	0.54
3:C:352:ILE:HB	3:C:357:ASN:HD22	1.72	0.54
3:C:715:ILE:HD11	18:V:222:UNK:HA	1.90	0.54
3:C:716:ILE:O	3:C:720:GLU:HG2	2.07	0.54
3:C:1124:LYS:HB3	3:C:1125:PRO:HD3	1.90	0.54
3:C:3342:TYR:O	3:C:3346:SER:HA	2.06	0.54
2:B:1110:GLN:HA	2:B:1164:MET:SD	2.48	0.53
2:B:1264:ILE:HG22	2:B:1268:TYR:CE2	2.43	0.53
2:B:1291:GLN:CD	2:B:1291:GLN:H	2.15	0.53
3:C:410:GLY:O	3:C:414:LYS:HG2	2.06	0.53
3:C:818:LEU:H	3:C:909:MET:HE3	1.73	0.53
3:C:1037:LYS:HA	3:C:1040:LYS:HE2	1.90	0.53
3:C:1139:LEU:O	3:C:1143:ARG:HG3	2.08	0.53
4:d:126:GLN:HE21	5:e:45:PRO:CD	2.18	0.53
16:P:90:LYS:HB3	16:P:103:MET:HE2	1.89	0.53
1:A:18:PRO:HB2	1:A:338:PHE:CE2	2.43	0.53
2:B:240:ASN:O	2:B:243:LEU:HG	2.07	0.53
2:B:449:GLY:HA2	2:B:452:LEU:HG	1.89	0.53
2:B:730:LEU:HG	2:B:731:PRO:HD3	1.89	0.53
2:B:812:ASP:HB2	2:B:900:PHE:CE2	2.42	0.53
2:B:904:LEU:HG	2:B:913:PHE:CE1	2.43	0.53
2:B:936:ASP:HA	2:B:939:ASN:ND2	2.23	0.53
2:B:1229:PHE:HE2	2:B:1277:ARG:HG3	1.72	0.53
3:C:1184:ARG:HA	3:C:1187:TRP:HD1	1.72	0.53
3:C:2324:GLY:O	3:C:2327:LEU:N	2.41	0.53
4:d:1300:LYS:O	4:d:1304:GLU:HG3	2.08	0.53
12:L:52:ASP:OD1	12:L:56:ASN:ND2	2.41	0.53
15:O:38:TYR:HD1	15:O:106:ILE:HG22	1.73	0.53
17:T:131:PHE:CD1	17:T:172:PHE:HE2	2.25	0.53
1:A:3048:SER:O	1:A:3052:GLY:N	2.41	0.53
1:A:4006:GLU:O	1:A:4011:LEU:N	2.41	0.53
2:B:133:MET:HG3	2:B:148:LYS:HG3	1.90	0.53
2:B:671:VAL:HG11	2:B:673:PHE:CZ	2.43	0.53
2:B:1057:LEU:HD13	2:B:1094:TRP:HB3	1.90	0.53
2:B:1212:ILE:HG22	2:B:1213:PRO:HG2	1.73	0.53
3:C:17:ILE:O	3:C:20:SER:OG	2.26	0.53
3:C:674:LEU:HB2	18:V:232:UNK:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:982:LYS:HG3	3:C:984:THR:HG22	1.91	0.53
4:d:1175:TRP:HB3	4:d:1183:PHE:CD2	2.43	0.53
14:N:34:ILE:HD12	14:N:71:ILE:HG13	1.90	0.53
16:P:16:ASP:OD2	16:P:17:ILE:N	2.41	0.53
17:T:107:LYS:HB2	17:T:177:ARG:HG2	1.90	0.53
2:B:16:ASN:HB2	2:B:17:ARG:NH1	2.24	0.53
2:B:84:PHE:CZ	3:C:150:LYS:HD3	2.44	0.53
2:B:197:GLU:O	2:B:201:ILE:HG12	2.08	0.53
2:B:387:CYS:HB3	2:B:391:LYS:HZ3	1.74	0.53
2:B:653:GLN:HG2	2:B:671:VAL:HA	1.90	0.53
2:B:1366:VAL:HA	2:B:1369:VAL:HB	1.89	0.53
3:C:478:LEU:HD23	3:C:484:LEU:HB2	1.88	0.53
4:d:119:GLU:CD	15:O:34:VAL:HG11	2.34	0.53
5:e:1080:SER:HB2	5:e:1099:ARG:CD	2.38	0.53
17:T:152:ILE:O	17:T:156:ILE:HG12	2.09	0.53
1:A:5:LEU:HD23	1:A:304:ILE:O	2.09	0.53
1:A:316:CYS:HB3	1:A:350:TRP:CD2	2.44	0.53
1:A:3733:SER:O	1:A:3737:GLY:N	2.41	0.53
3:C:135:MET:HG2	3:C:139:TYR:HD2	1.73	0.53
3:C:1235:PRO:HB3	3:C:1249:LEU:HD11	1.90	0.53
4:d:1080:ASN:HA	4:d:1094:ILE:HB	1.89	0.53
5:e:1088:SER:O	5:e:1090:THR:N	2.39	0.53
9:I:64:LYS:HE2	9:I:75:TRP:O	2.09	0.53
11:K:42:ARG:NH2	11:K:67:TYR:OH	2.42	0.53
11:K:95:PHE:CZ	11:K:106:LEU:HD11	2.43	0.53
1:A:60:LEU:HD13	1:A:69:TRP:CE2	2.44	0.53
2:B:203:TRP:CZ3	2:B:253:VAL:HG13	2.43	0.53
2:B:437:ASN:HA	2:B:441:LYS:HZ3	1.73	0.53
2:B:893:ARG:NH1	2:B:895:ASP:O	2.40	0.53
2:B:1325:TRP:HA	2:B:1328:LYS:CG	2.37	0.53
3:C:543:GLU:OE1	3:C:576:TYR:OH	2.21	0.53
3:C:596:LEU:HD21	3:C:598:ARG:HD2	1.90	0.53
3:C:1140:GLU:HA	3:C:1143:ARG:HD2	1.91	0.53
4:d:1124:ALA:HB1	4:d:1129:PHE:CZ	2.42	0.53
5:e:1146:CYS:O	5:e:1158:LEU:HD23	2.09	0.53
6:F:61:LYS:HB2	8:H:36:ASN:ND2	2.24	0.53
8:H:71:PHE:O	8:H:73:ARG:NH2	2.41	0.53
11:K:44:THR:O	11:K:48:LEU:HG	2.09	0.53
14:N:33:LYS:O	14:N:36:LYS:HB2	2.08	0.53
15:O:14:GLN:HB2	15:O:97:LEU:HD11	1.91	0.53
16:P:25:LEU:HB2	16:P:55:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:915:PRO:HA	2:B:927:ARG:HH21	1.74	0.53
2:B:1260:ALA:O	2:B:1264:ILE:HG13	2.08	0.53
3:C:547:LYS:O	3:C:551:LYS:HG2	2.09	0.53
3:C:750:ASN:HD21	3:C:886:ILE:HG22	1.74	0.53
3:C:945:ASN:HB3	3:C:946:PRO:HD3	1.91	0.53
4:d:966:VAL:HG21	4:d:1272:GLY:HA3	1.90	0.53
8:H:16:MET:SD	8:H:76:TYR:N	2.82	0.53
13:M:71:LYS:O	13:M:85:TRP:HA	2.07	0.53
2:B:105:ALA:HA	2:B:108:VAL:HG22	1.91	0.53
2:B:537:ALA:HA	2:B:540:LEU:HB2	1.91	0.53
2:B:1350:LYS:HE2	2:B:1370:LYS:HE3	1.91	0.53
3:C:1091:GLU:O	3:C:1094:LEU:HG	2.08	0.53
4:d:82:ALA:O	11:K:92:LYS:HG2	2.08	0.53
5:e:1187:LYS:O	5:e:1191:THR:HG23	2.09	0.53
12:L:67:PHE:HB3	12:L:74:TRP:HZ2	1.74	0.53
16:P:80:VAL:HG12	16:P:103:MET:SD	2.48	0.53
1:A:266:TYR:O	1:A:293:VAL:HA	2.09	0.53
2:B:814:TYR:N	2:B:1075:TRP:CZ2	2.57	0.53
2:B:1285:GLU:HG3	2:B:1290:LEU:HB2	1.90	0.53
3:C:98:ILE:HG13	3:C:116:ASN:O	2.09	0.53
5:e:950:VAL:HG13	5:e:1017:LYS:HZ1	1.74	0.53
6:F:44:LYS:HE3	6:F:48:ILE:HD11	1.91	0.53
14:N:29:PHE:HD1	14:N:76:VAL:HG11	1.74	0.53
16:P:65:LEU:HG	16:P:68:ILE:HD12	1.91	0.53
1:A:256:ILE:O	1:A:268:ILE:HA	2.08	0.53
2:B:436:PHE:O	2:B:533:ARG:NH1	2.42	0.53
2:B:470:PHE:CZ	2:B:488:ASP:HB3	2.43	0.53
2:B:1170:LYS:O	2:B:1173:LYS:HE2	2.09	0.53
3:C:127:THR:HB	3:C:130:MET:HB3	1.90	0.53
11:K:24:ALA:HB2	11:K:100:ILE:HD12	1.91	0.53
1:A:283:THR:HA	2:B:955:PHE:CZ	2.44	0.52
2:B:1090:ARG:HA	2:B:1093:ARG:HE	1.74	0.52
2:B:1271:LEU:HD12	2:B:1274:ILE:HG21	1.91	0.52
3:C:857:ARG:HG3	5:e:876:ASN:H	1.73	0.52
11:K:28:TRP:CE2	14:N:33:LYS:HE3	2.43	0.52
1:A:345:TRP:CZ2	2:B:967:GLN:HG2	2.45	0.52
1:A:3764:LEU:O	1:A:3768:LEU:N	2.38	0.52
1:A:3991:SER:O	1:A:3995:ALA:HB3	2.10	0.52
2:B:1147:ILE:C	2:B:1214:LEU:CD1	2.59	0.52
3:C:269:LYS:HE3	3:C:284:ARG:HD3	1.92	0.52
3:C:1055:PHE:CE2	3:C:1093:LYS:HE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1204:ILE:HG21	4:d:1243:LEU:HD21	1.90	0.52
5:e:895:GLN:NE2	5:e:940:TRP:O	2.42	0.52
1:A:143:PRO:HD3	1:A:187:TRP:CD1	2.44	0.52
2:B:60:ASN:ND2	3:C:137:SER:O	2.42	0.52
2:B:67:GLN:HA	2:B:71:CYS:O	2.10	0.52
2:B:1356:ILE:HA	2:B:1359:PHE:HD2	1.75	0.52
3:C:48:GLU:HG3	3:C:100:ASN:O	2.08	0.52
3:C:478:LEU:HB3	3:C:484:LEU:HD22	1.90	0.52
3:C:944:LEU:HD11	3:C:1071:ILE:HD11	1.92	0.52
6:F:86:GLU:O	6:F:100:ILE:HA	2.10	0.52
7:G:79:VAL:HG11	7:G:100:ALA:HB1	1.91	0.52
12:L:28:GLN:O	12:L:32:LYS:HG2	2.09	0.52
2:B:21:ALA:C	3:C:115:ASP:HB3	2.34	0.52
2:B:88:GLY:O	2:B:89:ILE:HD13	2.10	0.52
2:B:545:ILE:O	2:B:549:GLU:HG2	2.09	0.52
2:B:1151:LYS:HG3	2:B:1208:LYS:HE3	1.90	0.52
2:B:1315:ILE:CG1	2:B:1362:TYR:HD1	2.22	0.52
2:B:1982:THR:O	2:B:1994:LEU:N	2.42	0.52
2:B:2372:ARG:CB	3:C:1543:GLY:HA2	2.39	0.52
2:B:3874:ILE:O	2:B:3878:ILE:N	2.40	0.52
3:C:544:TYR:CD1	4:d:1207:ASP:HB3	2.44	0.52
3:C:696:ILE:O	3:C:700:LYS:HD3	2.10	0.52
7:G:71:LYS:O	7:G:72:THR:OG1	2.21	0.52
11:K:29:PRO:HD2	14:N:30:TYR:HD2	1.75	0.52
11:K:30:PRO:HG3	14:N:36:LYS:NZ	2.24	0.52
1:A:10:LEU:HD22	1:A:349:LEU:HD22	1.91	0.52
1:A:22:SER:HB3	1:A:340:GLY:CA	2.39	0.52
2:B:656:LEU:O	2:B:756:ARG:NH2	2.42	0.52
2:B:885:GLN:HA	2:B:894:ASN:ND2	2.25	0.52
2:B:1130:ASP:OD1	2:B:1135:HIS:NE2	2.39	0.52
3:C:269:LYS:CD	3:C:281:GLN:HA	2.38	0.52
3:C:470:PHE:CZ	3:C:524:LEU:HD13	2.45	0.52
3:C:548:LEU:HD12	3:C:551:LYS:HG3	1.91	0.52
3:C:853:VAL:HG23	3:C:854:GLU:H	1.74	0.52
3:C:1099:ASP:O	3:C:1103:ARG:HG2	2.10	0.52
4:d:1135:GLU:OE2	4:d:1137:HIS:HB2	2.10	0.52
4:d:1236:TYR:HE1	4:d:1243:LEU:O	1.93	0.52
5:e:1092:SER:N	5:e:1170:LYS:HD3	2.25	0.52
6:F:83:HIS:N	6:F:103:CYS:SG	2.83	0.52
2:B:596:ARG:HB3	2:B:633:ILE:HG21	1.91	0.52
2:B:1052:GLU:O	2:B:1056:HIS:ND1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:SER:HA	3:C:106:LYS:HZ1	1.75	0.52
3:C:200:LEU:HB3	3:C:275:HIS:NE2	2.24	0.52
3:C:745:LYS:HZ1	3:C:756:ILE:HD13	1.75	0.52
3:C:969:LEU:HB2	3:C:974:GLN:HE22	1.75	0.52
4:d:1077:LYS:HG2	4:d:1078:ASN:H	1.75	0.52
5:e:870:TRP:HZ2	5:e:1155:VAL:HG11	1.73	0.52
11:K:47:ALA:HA	11:K:50:LYS:HE2	1.91	0.52
16:P:28:PHE:HA	16:P:58:VAL:O	2.10	0.52
17:T:186:LEU:HA	17:T:189:ARG:HG2	1.90	0.52
1:A:322:GLU:OE2	1:A:341:TRP:N	2.42	0.52
2:B:247:GLN:O	2:B:250:SER:OG	2.24	0.52
2:B:418:SER:O	2:B:422:ARG:HG3	2.10	0.52
2:B:1256:ASN:OD1	2:B:1257:ILE:N	2.43	0.52
3:C:624:PHE:HE2	3:C:641:TYR:CD2	2.27	0.52
4:d:1215:ALA:HB1	4:d:1225:PHE:CE1	2.45	0.52
5:e:825:ASP:HB3	5:e:878:PRO:HD3	1.91	0.52
5:e:853:ILE:HG23	5:e:856:PHE:H	1.74	0.52
5:e:1088:SER:HA	5:e:1132:ILE:HD12	1.91	0.52
5:e:1169:PRO:HA	5:e:1172:LYS:HG2	1.92	0.52
6:F:34:LYS:HG2	6:F:35:ARG:H	1.74	0.52
11:K:35:ASP:OD2	14:N:39:LYS:HE2	2.10	0.52
2:B:319:PRO:HA	2:B:322:HIS:HB2	1.91	0.52
2:B:523:LEU:O	2:B:526:ASN:HB2	2.10	0.52
3:C:542:ILE:HD11	3:C:579:GLU:OE1	2.10	0.52
3:C:566:THR:HA	3:C:569:TYR:CD2	2.45	0.52
3:C:793:GLN:HB3	5:e:1123:SER:HA	1.91	0.52
5:e:1135:THR:HG23	5:e:1145:LEU:HD23	1.90	0.52
16:P:39:LEU:HD11	16:P:96:GLN:N	2.25	0.52
1:A:7:TRP:CZ3	1:A:350:TRP:HB3	2.45	0.52
1:A:220:TRP:HE1	2:B:956:LEU:CD1	2.16	0.52
1:A:1327:ARG:O	1:A:1330:ASN:N	2.42	0.52
2:B:28:LYS:HD3	2:B:73:PHE:HD1	1.75	0.52
2:B:1291:GLN:OE1	2:B:1291:GLN:N	2.38	0.52
2:B:3985:PHE:N	2:B:4076:LEU:O	2.42	0.52
2:B:4390:SER:O	2:B:4394:SER:N	2.43	0.52
3:C:1133:GLY:HA3	3:C:1268:ARG:HD3	1.92	0.52
4:d:116:ILE:HG12	5:e:43:ARG:HE	1.75	0.52
4:d:116:ILE:HG23	4:d:119:GLU:CD	2.34	0.52
5:e:832:ARG:NH2	5:e:853:ILE:HD11	2.25	0.52
5:e:890:ASN:ND2	5:e:936:THR:O	2.43	0.52
5:e:910:LEU:HG	5:e:938:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:1029:TYR:HB3	5:e:1032:ASP:HB2	1.91	0.52
9:I:99:TYR:HB2	9:I:103:LEU:H	1.75	0.52
13:M:67:HIS:HB3	13:M:85:TRP:HB2	1.91	0.52
16:P:24:VAL:HA	16:P:54:THR:O	2.09	0.52
1:A:60:LEU:HD13	1:A:69:TRP:CD2	2.45	0.52
1:A:3615:CYS:O	1:A:3620:HIS:N	2.43	0.52
2:B:525:ASP:O	2:B:528:GLU:HG3	2.10	0.52
2:B:737:VAL:HG12	2:B:740:LYS:HD2	1.92	0.52
2:B:789:LYS:HE2	2:B:839:LEU:HB3	1.92	0.52
3:C:331:THR:HB	3:C:334:GLN:HG3	1.92	0.52
3:C:800:ASP:O	5:e:822:LEU:HD11	2.10	0.52
3:C:903:GLN:HE21	3:C:994:GLU:CD	2.18	0.52
4:d:1171:TYR:CE2	4:d:1188:ALA:HB2	2.45	0.52
5:e:1112:ARG:NH1	5:e:1115:GLU:HG3	2.25	0.52
6:F:78:ARG:HB2	6:F:88:ILE:HG22	1.91	0.52
7:G:65:ASN:O	7:G:69:THR:HG23	2.10	0.52
2:B:260:LEU:HD13	2:B:268:THR:HG21	1.91	0.51
2:B:503:LEU:O	2:B:506:VAL:HG12	2.10	0.51
2:B:1318:ILE:HG22	2:B:1322:TYR:CE2	2.45	0.51
5:e:1027:THR:HB	5:e:1064:TRP:CE3	2.45	0.51
13:M:74:PHE:HD2	13:M:83:LEU:HB2	1.74	0.51
16:P:6:ILE:HB	16:P:56:VAL:HG22	1.92	0.51
17:T:103:SER:O	17:T:107:LYS:HG3	2.10	0.51
1:A:162:GLY:HA2	1:A:174:PHE:O	2.10	0.51
1:A:344:ASN:ND2	2:B:969:LEU:HB3	2.23	0.51
2:B:544:HIS:O	2:B:548:LEU:HD13	2.10	0.51
2:B:1148:SER:CB	2:B:1214:LEU:HD22	2.33	0.51
3:C:81:THR:HA	3:C:126:ASN:HA	1.91	0.51
3:C:234:GLU:O	3:C:368:LYS:NZ	2.43	0.51
3:C:1076:LEU:HD23	3:C:1076:LEU:H	1.74	0.51
3:C:1164:ASP:HA	3:C:1167:LEU:O	2.10	0.51
4:d:1213:VAL:HG22	4:d:1214:ASP:H	1.74	0.51
6:F:87:TYR:OH	6:F:98:LEU:HD13	2.11	0.51
2:B:569:VAL:HB	5:e:1100:ARG:HD3	1.92	0.51
2:B:671:VAL:HG12	2:B:673:PHE:H	1.75	0.51
2:B:709:ARG:O	2:B:713:VAL:HG23	2.10	0.51
2:B:813:ASP:C	2:B:1075:TRP:HE1	2.15	0.51
2:B:862:TYR:O	2:B:865:VAL:HG12	2.10	0.51
3:C:488:PHE:HA	3:C:491:ILE:HD12	1.91	0.51
8:H:63:ARG:HH21	8:H:85:ALA:N	2.09	0.51
16:P:15:GLU:O	16:P:19:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASP:H	1:A:334:ARG:NH1	2.08	0.51
1:A:1302:ASP:O	1:A:1304:SER:N	2.44	0.51
1:A:3409:PHE:O	1:A:3413:LYS:N	2.43	0.51
2:B:1154:GLU:CD	2:B:1204:VAL:HG11	2.35	0.51
3:C:9:ARG:NH2	3:C:117:ASP:OD2	2.40	0.51
14:N:81:ILE:HG23	14:N:126:VAL:HG13	1.91	0.51
2:B:1145:LYS:HE2	2:B:1150:VAL:HG21	1.93	0.51
2:B:1271:LEU:O	2:B:1274:ILE:HB	2.11	0.51
3:C:203:SER:O	3:C:207:GLN:HG2	2.11	0.51
3:C:582:THR:O	3:C:585:ARG:HG3	2.11	0.51
3:C:789:LYS:O	3:C:793:GLN:HG2	2.11	0.51
3:C:2397:GLY:O	3:C:2633:ASN:N	2.43	0.51
4:d:1167:LEU:H	4:d:1193:ARG:NH1	2.07	0.51
5:e:848:ALA:HB2	5:e:893:TYR:OH	2.10	0.51
15:O:20:SER:HA	15:O:53:TYR:HE2	1.75	0.51
3:C:53:ILE:HB	3:C:95:PHE:HB2	1.92	0.51
3:C:752:LEU:HD13	3:C:795:ILE:HG12	1.93	0.51
3:C:1120:THR:O	3:C:1124:LYS:HB2	2.11	0.51
5:e:1110:TYR:CE2	5:e:1174:ILE:HG12	2.46	0.51
6:F:73:ASP:OD1	6:F:74:ILE:N	2.43	0.51
15:O:94:ASP:OD1	15:O:116:ALA:N	2.43	0.51
2:B:91:VAL:HA	2:B:109:VAL:O	2.10	0.51
2:B:1459:THR:N	2:B:1466:THR:O	2.43	0.51
3:C:12:TRP:O	3:C:16:THR:HG23	2.10	0.51
4:d:1297:THR:O	4:d:1301:LYS:HG3	2.10	0.51
5:e:1047:ASN:HB3	5:e:1087:TRP:CZ3	2.46	0.51
1:A:209:ALA:HB3	1:A:264:TRP:CD1	2.46	0.51
2:B:1250:GLU:HG3	2:B:1256:ASN:HD22	1.74	0.51
3:C:902:THR:O	3:C:905:SER:OG	2.27	0.51
3:C:3354:ILE:O	3:C:3357:ALA:C	2.53	0.51
4:d:978:LEU:HD11	4:d:998:LEU:HG	1.92	0.51
4:d:1190:TRP:CD1	4:d:1212:VAL:HG23	2.45	0.51
7:G:80:ASN:HA	7:G:143:PHE:HA	1.92	0.51
12:L:33:LYS:HZ1	12:L:67:PHE:HE2	1.57	0.51
17:T:186:LEU:H	17:T:189:ARG:HH11	1.58	0.51
1:A:2891:ARG:O	1:A:2895:LEU:N	2.44	0.51
1:A:3850:PRO:O	1:A:3855:MET:N	2.43	0.51
2:B:151:MET:O	2:B:151:MET:HE3	2.11	0.51
2:B:563:LEU:HB2	2:B:564:GLU:OE1	2.09	0.51
2:B:653:GLN:HE21	2:B:655:LYS:H	1.57	0.51
2:B:927:ARG:NH1	2:B:929:THR:OG1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1071:TRP:CE2	4:d:1081:PHE:HE1	2.28	0.51
16:P:28:PHE:CD2	16:P:74:VAL:HG11	2.45	0.51
1:A:175:ASN:HB3	1:A:198:ASP:C	2.36	0.51
3:C:78:LEU:HD23	3:C:78:LEU:O	2.11	0.51
3:C:336:ILE:O	3:C:339:LEU:N	2.44	0.51
3:C:374:ILE:HD11	3:C:453:PHE:CE2	2.46	0.51
3:C:596:LEU:HG	3:C:598:ARG:HG2	1.92	0.51
4:d:972:ASN:HD21	4:d:1027:ALA:HB2	1.76	0.51
5:e:28:GLY:H	15:O:15:LYS:HE2	1.76	0.51
5:e:1108:ASP:H	5:e:1117:ALA:HB2	1.75	0.51
11:K:37:LEU:HB2	14:N:36:LYS:CD	2.41	0.51
2:B:155:ASN:OD1	2:B:180:LYS:NZ	2.44	0.50
2:B:720:ASP:HB3	2:B:724:HIS:CE1	2.45	0.50
2:B:876:GLN:HG3	2:B:966:LYS:HD2	1.93	0.50
3:C:193:ASP:OD1	3:C:267:ILE:HG21	2.10	0.50
3:C:892:TRP:O	3:C:896:GLN:HG2	2.11	0.50
4:d:82:ALA:H	11:K:92:LYS:HG3	1.76	0.50
11:K:94:ARG:O	11:K:108:TYR:HA	2.11	0.50
1:A:287:PHE:C	1:A:318:PRO:HB3	2.36	0.50
2:B:1240:PHE:HD1	2:B:1243:LYS:NZ	2.08	0.50
2:B:1361:GLY:O	2:B:1364:VAL:HG12	2.12	0.50
3:C:263:LYS:HG3	3:C:264:ASP:N	2.26	0.50
3:C:576:TYR:CD1	3:C:624:PHE:HE1	2.29	0.50
3:C:790:LYS:O	3:C:793:GLN:HB2	2.11	0.50
5:e:832:ARG:HD3	5:e:851:TYR:CB	2.38	0.50
5:e:943:SER:HB2	5:e:948:GLU:N	2.26	0.50
6:F:85:TYR:HE2	6:F:87:TYR:HB2	1.76	0.50
8:H:15:ASP:N	8:H:76:TYR:O	2.36	0.50
16:P:9:THR:HA	16:P:65:LEU:HD12	1.94	0.50
1:A:190:LEU:HD13	1:A:232:TYR:CZ	2.47	0.50
2:B:110:VAL:H	3:C:122:GLU:HG2	1.75	0.50
2:B:301:LYS:HA	2:B:316:LEU:HD23	1.93	0.50
2:B:449:GLY:HA2	2:B:452:LEU:CG	2.41	0.50
2:B:859:TYR:CE2	2:B:863:VAL:HG21	2.47	0.50
3:C:1109:ASP:O	3:C:1113:GLU:HG2	2.11	0.50
6:F:97:MET:N	6:F:97:MET:SD	2.84	0.50
14:N:101:CYS:C	14:N:102:LEU:HD12	2.36	0.50
1:A:4036:THR:O	1:A:4040:GLN:N	2.45	0.50
3:C:260:LEU:HD22	3:C:307:LEU:HD22	1.93	0.50
3:C:1107:LEU:HB3	3:C:1156:VAL:HG21	1.93	0.50
3:C:3355:GLN:O	3:C:3356:VAL:C	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3378:ALA:C	3:C:3380:ILE:H	2.20	0.50
4:d:964:LYS:HG3	4:d:985:SER:HB2	1.93	0.50
4:d:969:ILE:HG12	4:d:981:VAL:HG13	1.92	0.50
4:d:1186:ALA:HB1	4:d:1211:MET:HG3	1.93	0.50
5:e:1069:LYS:HG3	5:e:1070:THR:HG23	1.92	0.50
5:e:1127:LEU:HD23	5:e:1150:ASP:OD1	2.12	0.50
7:G:72:THR:HB	7:G:150:THR:OG1	2.12	0.50
16:P:17:ILE:HD13	16:P:20:LYS:HE3	1.93	0.50
2:B:135:ASN:HB3	3:C:82:THR:HG21	1.93	0.50
2:B:797:PHE:HE1	2:B:829:VAL:HA	1.77	0.50
3:C:58:GLN:HA	3:C:90:ASP:CG	2.36	0.50
9:I:43:GLN:NE2	9:I:47:GLU:OE2	2.33	0.50
12:L:28:GLN:HE22	12:L:31:LEU:HD23	1.75	0.50
15:O:101:TYR:HB3	15:O:108:ALA:HB3	1.93	0.50
17:T:41:SER:O	17:T:45:LYS:HG2	2.11	0.50
1:A:18:PRO:HB2	1:A:338:PHE:HE2	1.77	0.50
1:A:192:PRO:CA	1:A:239:TRP:HE1	2.25	0.50
1:A:334:ARG:CB	1:A:353:ASN:HA	2.42	0.50
2:B:462:GLU:HG2	2:B:499:LEU:HD21	1.92	0.50
2:B:533:ARG:HB3	2:B:535:ILE:HG12	1.94	0.50
2:B:877:THR:HG22	2:B:881:HIS:CE1	2.47	0.50
3:C:177:ARG:NE	3:C:259:GLN:HA	2.25	0.50
3:C:282:ARG:NH2	18:x:125:UNK:C	2.75	0.50
3:C:1026:LEU:HD12	3:C:1027:CYS:N	2.25	0.50
3:C:1228:ARG:HA	3:C:1228:ARG:NE	2.27	0.50
4:d:1305:GLU:HA	4:d:1308:ASN:ND2	2.27	0.50
5:e:870:TRP:CZ2	5:e:1155:VAL:HG11	2.47	0.50
5:e:1103:TRP:HD1	5:e:1121:LYS:N	2.09	0.50
1:A:213:GLN:HB2	1:A:232:TYR:O	2.12	0.50
1:A:3840:TYR:O	1:A:3844:LYS:N	2.45	0.50
2:B:1114:LEU:O	2:B:1118:GLU:HG2	2.12	0.50
2:B:1328:LYS:HG2	2:B:1332:GLN:HG2	1.93	0.50
3:C:44:PHE:HB2	3:C:53:ILE:HD11	1.92	0.50
3:C:91:LYS:HD3	3:C:125:PRO:HD3	1.93	0.50
3:C:250:MET:HA	3:C:314:VAL:HG11	1.93	0.50
3:C:499:GLY:HA2	3:C:509:LYS:HG3	1.93	0.50
3:C:1211:GLU:HG3	3:C:1214:GLN:NE2	2.27	0.50
5:e:829:ILE:HD12	5:e:1153:GLY:O	2.11	0.50
6:F:25:ILE:HD13	6:F:97:MET:HG3	1.93	0.50
9:I:33:ASP:N	9:I:33:ASP:OD1	2.44	0.50
15:O:27:ILE:HG21	15:O:32:SER:OG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:MET:HE1	1:A:266:TYR:HB3	1.93	0.50
1:A:310:GLU:HG3	1:A:311:THR:H	1.76	0.50
1:A:3552:ILE:O	1:A:3556:PHE:N	2.43	0.50
2:B:387:CYS:O	2:B:391:LYS:HD2	2.10	0.50
3:C:44:PHE:CZ	3:C:97:ARG:HB3	2.46	0.50
3:C:1235:PRO:HD3	3:C:1252:PHE:CE2	2.47	0.50
3:C:3343:HIS:C	3:C:3345:LYS:C	2.78	0.50
5:e:1073:ILE:HD11	5:e:1184:ARG:CZ	2.41	0.50
5:e:1189:LEU:O	5:e:1193:LYS:HG3	2.11	0.50
11:K:90:HIS:HE2	11:K:95:PHE:HB2	1.77	0.50
2:B:119:GLU:O	2:B:122:ASN:HB3	2.12	0.50
2:B:332:LYS:HB3	2:B:405:TRP:CD1	2.46	0.50
2:B:454:GLU:O	2:B:458:GLN:HB3	2.10	0.50
2:B:1138:LYS:HE3	2:B:1145:LYS:HD3	1.93	0.50
2:B:1222:ILE:HG12	2:B:1284:LEU:HD13	1.93	0.50
2:B:1252:MET:HB3	2:B:1255:GLU:OE1	2.11	0.50
3:C:27:ILE:HG12	3:C:68:ILE:HA	1.93	0.50
3:C:370:THR:HG21	3:C:450:PHE:HB2	1.94	0.50
3:C:971:ASN:H	3:C:974:GLN:HE21	1.60	0.50
3:C:1184:ARG:HA	3:C:1187:TRP:CD1	2.47	0.50
4:d:1152:SER:OG	4:d:1153:ARG:N	2.44	0.50
6:F:77:ILE:O	6:F:89:ILE:HB	2.11	0.50
14:N:39:LYS:HA	14:N:113:TYR:CE2	2.47	0.50
2:B:26:LYS:HD3	2:B:74:TYR:HE1	1.77	0.49
2:B:309:ASP:HA	2:B:358:PHE:CE2	2.47	0.49
2:B:1040:CYS:O	2:B:1045:PRO:HD3	2.11	0.49
2:B:1317:LEU:HD13	16:P:77:LEU:H	1.76	0.49
3:C:254:THR:O	3:C:258:GLU:HG3	2.12	0.49
3:C:278:HIS:HB2	3:C:282:ARG:HD3	1.94	0.49
3:C:532:ILE:HG21	3:C:564:ASN:HB3	1.94	0.49
3:C:633:GLU:HA	3:C:636:ARG:HH11	1.77	0.49
3:C:857:ARG:CG	5:e:875:PRO:HB2	2.38	0.49
3:C:1035:ILE:HG21	3:C:1095:GLN:HG2	1.94	0.49
4:d:94:ARG:HG2	13:M:2:ASN:HB2	1.93	0.49
5:e:1088:SER:HB2	5:e:1096:PHE:CE2	2.46	0.49
12:L:16:LEU:HD22	12:L:17:PRO:HD2	1.93	0.49
1:A:144:GLN:NE2	1:A:145:PRO:O	2.46	0.49
1:A:276:PHE:HB2	1:A:282:ARG:CG	2.41	0.49
2:B:187:THR:HB	2:B:188:PRO:HD3	1.95	0.49
2:B:1261:TYR:O	2:B:1265:MET:N	2.44	0.49
3:C:45:LEU:O	3:C:106:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1068:GLN:OE1	4:d:1129:PHE:N	2.44	0.49
5:e:912:VAL:O	5:e:922:ILE:HG12	2.12	0.49
6:F:87:TYR:HA	6:F:99:ALA:O	2.12	0.49
1:A:221:SER:HB2	1:A:226:TYR:CE1	2.40	0.49
1:A:2827:ILE:O	1:A:2831:GLU:N	2.45	0.49
1:A:3217:ILE:O	1:A:3221:SER:N	2.40	0.49
1:A:4001:ASN:O	1:A:4005:GLN:N	2.39	0.49
1:A:4085:GLY:O	1:A:4088:GLY:N	2.46	0.49
2:B:137:LEU:HB3	2:B:142:TRP:CD1	2.37	0.49
2:B:296:LYS:HE2	5:e:1225:ALA:CB	2.38	0.49
2:B:606:LEU:HD13	2:B:612:GLY:HA2	1.94	0.49
2:B:663:LYS:HD3	2:B:666:ASN:HB3	1.94	0.49
2:B:688:LEU:HD12	2:B:691:ARG:HH22	1.77	0.49
3:C:89:GLN:HE22	3:C:91:LYS:NZ	2.09	0.49
3:C:443:ASP:OD2	3:C:443:ASP:N	2.45	0.49
4:d:1036:ASP:OD1	4:d:1038:THR:OG1	2.30	0.49
5:e:816:SER:N	5:e:1162:ASP:HB3	2.28	0.49
8:H:73:ARG:HH11	8:H:73:ARG:HG2	1.76	0.49
1:A:53:PRO:O	1:A:82:ARG:HB3	2.12	0.49
1:A:4155:LYS:O	1:A:4159:SER:N	2.45	0.49
2:B:127:GLU:OE1	2:B:127:GLU:N	2.45	0.49
2:B:132:VAL:HG22	3:C:75:ASP:O	2.12	0.49
2:B:892:LYS:HG2	2:B:893:ARG:H	1.78	0.49
2:B:1324:ASP:O	2:B:1328:LYS:HG3	2.12	0.49
3:C:591:LYS:HE3	3:C:596:LEU:HD22	1.95	0.49
3:C:715:ILE:HG12	18:V:221:UNK:O	2.13	0.49
3:C:896:GLN:O	3:C:900:ASN:ND2	2.39	0.49
3:C:1101:HIS:O	3:C:1105:ARG:HG2	2.12	0.49
3:C:3344:GLN:C	3:C:3348:ILE:N	2.58	0.49
4:d:1296:GLN:OE1	4:d:1296:GLN:N	2.45	0.49
5:e:910:LEU:O	5:e:924:ILE:HA	2.13	0.49
11:K:30:PRO:HG3	14:N:36:LYS:HZ2	1.77	0.49
1:A:48:ASP:HA	1:A:51:ILE:HG12	1.94	0.49
1:A:2324:ASN:HA	1:A:2327:ASN:O	2.13	0.49
2:B:96:LEU:HD23	2:B:99:LEU:HD23	1.94	0.49
2:B:337:PRO:HD3	2:B:404:ASN:HB2	1.93	0.49
2:B:351:ILE:HG21	2:B:416:LEU:HD22	1.95	0.49
2:B:876:GLN:CG	2:B:966:LYS:HD2	2.42	0.49
2:B:1034:ASN:O	2:B:1038:LYS:HG2	2.13	0.49
3:C:21:LEU:HD21	3:C:57:TYR:CD1	2.48	0.49
3:C:46:SER:HA	3:C:106:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:805:ARG:O	3:C:809:ASN:ND2	2.46	0.49
3:C:1054:LYS:O	3:C:1058:ILE:HG12	2.12	0.49
3:C:1143:ARG:O	3:C:1146:GLN:HB2	2.13	0.49
3:C:1146:GLN:HA	3:C:1149:ILE:HD12	1.94	0.49
5:e:1144:LYS:HD2	5:e:1164:LEU:HD13	1.94	0.49
8:H:49:PHE:HA	8:H:52:ARG:HG2	1.93	0.49
8:H:60:ILE:HG21	8:H:65:PHE:CE2	2.47	0.49
17:T:163:LEU:HD22	17:T:166:LYS:HB2	1.94	0.49
2:B:211:LEU:HD12	2:B:277:GLU:HB3	1.94	0.49
2:B:436:PHE:HA	2:B:533:ARG:NH1	2.28	0.49
2:B:524:LEU:HB3	2:B:611:GLN:HG3	1.93	0.49
2:B:1152:ASP:O	2:B:1155:PRO:HD2	2.12	0.49
2:B:1325:TRP:HA	2:B:1328:LYS:CD	2.42	0.49
3:C:241:THR:HA	3:C:244:ILE:HD12	1.95	0.49
3:C:409:LEU:HD11	3:C:461:ILE:HG12	1.93	0.49
3:C:482:ASP:OD1	3:C:483:VAL:N	2.45	0.49
3:C:948:LEU:HD13	3:C:1010:LYS:HG2	1.95	0.49
3:C:3439:GLN:O	3:C:3443:LEU:N	2.42	0.49
4:d:981:VAL:HB	4:d:997:CYS:SG	2.53	0.49
4:d:1267:PRO:HD3	4:d:1287:LEU:HD21	1.94	0.49
5:e:818:LYS:HZ2	5:e:1118:PHE:HD2	1.60	0.49
5:e:1082:LEU:HA	5:e:1099:ARG:NH1	2.28	0.49
1:A:225:GLN:HG3	1:A:282:ARG:NH1	2.27	0.49
2:B:17:ARG:NH1	3:C:19:ASP:OD2	2.46	0.49
2:B:839:LEU:O	2:B:843:VAL:HG23	2.12	0.49
3:C:663:ILE:HG22	3:C:667:LYS:NZ	2.28	0.49
4:d:1163:TYR:CZ	4:d:1195:TRP:CD1	2.96	0.49
6:F:94:ASP:OD1	6:F:94:ASP:N	2.46	0.49
9:I:83:TYR:CE2	9:I:85:TYR:HD1	2.30	0.49
16:P:72:HIS:HB2	16:P:74:VAL:HG23	1.95	0.49
2:B:285:ALA:O	2:B:288:ASN:HB2	2.13	0.49
2:B:736:LEU:HA	2:B:739:LYS:HD2	1.94	0.49
2:B:811:PRO:HB3	2:B:900:PHE:HA	1.94	0.49
2:B:872:SER:HB3	2:B:966:LYS:HE3	1.94	0.49
3:C:135:MET:HA	3:C:139:TYR:CD2	2.47	0.49
3:C:1116:LYS:HG2	3:C:1182:LEU:HD21	1.95	0.49
5:e:1045:ARG:NH2	5:e:1051:LYS:HA	2.27	0.49
17:T:154:GLN:O	17:T:158:GLU:HG2	2.13	0.49
1:A:158:VAL:HB	1:A:180:LEU:HB3	1.93	0.49
2:B:137:LEU:HD21	2:B:145:LEU:HD22	1.94	0.49
2:B:248:LEU:HA	2:B:253:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:GLU:HG2	2:B:535:ILE:HB	1.95	0.49
2:B:788:GLN:HA	2:B:791:HIS:CD2	2.47	0.49
3:C:52:LYS:HA	3:C:95:PHE:O	2.11	0.49
3:C:56:TYR:HE1	3:C:76:PRO:HD2	1.78	0.49
3:C:210:GLU:HG3	3:C:280:ASN:CG	2.37	0.49
3:C:626:GLU:H	3:C:629:ILE:HG13	1.78	0.49
3:C:3194:ALA:CB	3:C:3353:ARG:N	2.71	0.49
12:L:95:PHE:HD1	12:L:106:LEU:HB2	1.78	0.49
13:M:5:PRO:HD3	13:M:25:ILE:HD11	1.94	0.49
16:P:7:GLU:HA	16:P:57:LYS:O	2.12	0.49
1:A:174:PHE:C	1:A:199:PRO:HA	2.38	0.49
1:A:334:ARG:HB3	1:A:353:ASN:HA	1.95	0.49
1:A:1300:GLN:O	1:A:1302:ASP:N	2.44	0.49
2:B:467:VAL:O	2:B:471:THR:HG23	2.13	0.49
2:B:1146:VAL:HG11	2:B:1215:GLN:CD	2.36	0.49
2:B:1315:ILE:HG12	2:B:1362:TYR:CD1	2.46	0.49
3:C:420:LYS:HD3	3:C:421:LYS:HZ2	1.76	0.49
3:C:572:ILE:O	3:C:576:TYR:HD2	1.95	0.49
3:C:580:LEU:HD13	3:C:641:TYR:CE2	2.48	0.49
4:d:1231:ASP:O	4:d:1250:LYS:HA	2.13	0.49
5:e:39:GLN:OE1	5:e:39:GLN:N	2.46	0.49
5:e:39:GLN:HG3	15:O:31:SER:OG	2.12	0.49
5:e:922:ILE:O	5:e:924:ILE:HD12	2.12	0.49
11:K:29:PRO:HB2	14:N:30:TYR:HB2	1.95	0.49
13:M:14:GLU:OE2	13:M:18:LYS:HD3	2.13	0.49
15:O:68:CYS:SG	15:O:113:PHE:HB2	2.53	0.49
1:A:205:ALA:HA	1:A:215:MET:O	2.13	0.48
3:C:136:GLU:OE2	3:C:166:GLN:NE2	2.45	0.48
3:C:674:LEU:HD21	3:C:769:THR:HG21	1.95	0.48
3:C:820:HIS:HB3	3:C:920:GLY:O	2.12	0.48
7:G:74:LEU:HD11	7:G:150:THR:HG23	1.95	0.48
8:H:16:MET:HG3	8:H:74:SER:O	2.13	0.48
9:I:68:ASP:HA	9:I:72:GLY:O	2.12	0.48
11:K:29:PRO:HD2	14:N:30:TYR:CD2	2.48	0.48
16:P:59:ASN:O	16:P:65:LEU:HD13	2.13	0.48
2:B:92:ILE:HD13	2:B:109:VAL:HG12	1.94	0.48
2:B:144:ASP:O	2:B:148:LYS:HG2	2.13	0.48
2:B:2888:LEU:O	2:B:3022:PHE:N	2.46	0.48
2:B:3533:LEU:N	2:B:3642:THR:O	2.43	0.48
3:C:426:THR:O	3:C:430:VAL:HG23	2.14	0.48
3:C:446:ILE:HG23	3:C:450:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:818:LEU:HB3	3:C:962:VAL:HG11	1.93	0.48
4:d:1193:ARG:HG2	4:d:1202:GLN:CG	2.32	0.48
5:e:142:VAL:O	5:e:144:ASN:N	2.46	0.48
5:e:848:ALA:HB2	5:e:869:VAL:HG22	1.95	0.48
5:e:1082:LEU:HD12	5:e:1099:ARG:HH12	1.78	0.48
5:e:1185:LYS:O	5:e:1189:LEU:HG	2.13	0.48
9:I:26:ASN:HD21	9:I:98:PHE:HB2	1.79	0.48
10:J:20:SER:O	10:J:54:TYR:OH	2.28	0.48
1:A:2287:GLU:N	1:A:2305:ASP:O	2.43	0.48
2:B:13:PHE:O	2:B:17:ARG:HG2	2.13	0.48
2:B:500:GLU:HA	2:B:503:LEU:HD12	1.94	0.48
2:B:813:ASP:CG	2:B:1075:TRP:NE1	2.72	0.48
2:B:968:CYS:O	2:B:972:ILE:HG12	2.14	0.48
2:B:1113:LEU:HA	2:B:1116:PHE:CD1	2.48	0.48
3:C:102:ALA:O	3:C:106:LYS:HE2	2.13	0.48
3:C:358:THR:HB	3:C:361:LYS:HG3	1.94	0.48
3:C:876:ASP:HB2	3:C:877:PRO:HD3	1.94	0.48
3:C:1227:ARG:HG3	3:C:1228:ARG:NH2	2.27	0.48
3:C:3353:ARG:C	3:C:3354:ILE:O	2.53	0.48
4:d:996:ILE:HD11	4:d:1032:VAL:HG11	1.95	0.48
4:d:1172:LYS:HZ1	4:d:1174:LYS:CB	2.26	0.48
5:e:960:TRP:HB3	5:e:1017:LYS:HZ1	1.78	0.48
11:K:48:LEU:HB2	11:K:49:LYS:NZ	2.28	0.48
12:L:68:LYS:H	12:L:68:LYS:HD2	1.77	0.48
2:B:873:THR:O	2:B:876:GLN:HB2	2.13	0.48
2:B:1120:THR:HG21	2:B:1154:GLU:OE1	2.14	0.48
2:B:1271:LEU:O	2:B:1275:GLU:HG2	2.12	0.48
3:C:100:ASN:OD1	3:C:101:PRO:HD3	2.14	0.48
3:C:493:ASP:O	3:C:496:LYS:HG2	2.13	0.48
3:C:1200:GLU:HA	3:C:1203:HIS:CD2	2.48	0.48
3:C:2864:LEU:N	3:C:3023:THR:O	2.45	0.48
4:d:137:ILE:HG23	4:d:138:LYS:HD2	1.94	0.48
4:d:1213:VAL:HG11	4:d:1229:THR:HG23	1.95	0.48
6:F:87:TYR:HD1	6:F:100:ILE:HG13	1.79	0.48
1:A:1399:CYS:HA	1:A:1524:ARG:C	2.39	0.48
2:B:105:ALA:HB3	3:C:20:SER:O	2.13	0.48
2:B:613:ILE:HD12	2:B:616:ARG:HB2	1.96	0.48
2:B:729:LEU:HB3	2:B:737:VAL:HG23	1.95	0.48
2:B:1568:SER:O	2:B:1571:GLU:N	2.44	0.48
3:C:29:GLU:OE2	3:C:33:GLN:NE2	2.46	0.48
3:C:446:ILE:HG23	3:C:450:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:935:VAL:H	3:C:1077:MET:HB2	1.78	0.48
4:d:1183:PHE:HB2	4:d:1195:TRP:HE3	1.77	0.48
5:e:1092:SER:OG	5:e:1108:ASP:OD1	2.30	0.48
1:A:277:GLU:HG2	1:A:280:GLY:H	1.79	0.48
1:A:4124:TYR:O	1:A:4146:MET:N	2.46	0.48
2:B:228:LEU:HD13	2:B:302:LEU:HD13	1.95	0.48
2:B:469:ALA:O	2:B:473:VAL:HG22	2.13	0.48
2:B:477:ILE:HB	2:B:484:LYS:HB2	1.96	0.48
2:B:1069:THR:OG1	2:B:1070:PRO:HD2	2.13	0.48
3:C:257:SER:O	3:C:261:LYS:HG2	2.13	0.48
3:C:339:LEU:O	3:C:343:MET:HG3	2.13	0.48
3:C:805:ARG:HG3	3:C:806:ILE:N	2.27	0.48
4:d:75:LEU:HD13	14:N:101:CYS:SG	2.54	0.48
4:d:82:ALA:H	11:K:92:LYS:CG	2.26	0.48
4:d:1166:HIS:CE1	4:d:1168:LEU:HB2	2.49	0.48
4:d:1172:LYS:HD2	4:d:1215:ALA:HB3	1.96	0.48
8:H:50:ARG:HH22	8:H:56:THR:HG23	1.78	0.48
14:N:102:LEU:HG	15:O:89:GLN:HE21	1.79	0.48
1:A:3468:LYS:O	1:A:3472:THR:N	2.44	0.48
2:B:615:GLU:HA	2:B:619:TYR:HD2	1.78	0.48
2:B:725:ILE:HD12	2:B:728:CYS:HB3	1.95	0.48
2:B:814:TYR:H	2:B:1075:TRP:CD1	2.28	0.48
2:B:1106:PHE:CD2	2:B:1171:LEU:HB2	2.48	0.48
2:B:1126:LYS:NZ	2:B:1134:LEU:HD22	2.29	0.48
2:B:1271:LEU:HA	2:B:1274:ILE:HB	1.95	0.48
3:C:276:LYS:O	3:C:278:HIS:N	2.46	0.48
3:C:314:VAL:HA	3:C:317:LEU:HG	1.94	0.48
3:C:818:LEU:HB3	3:C:962:VAL:CG1	2.44	0.48
3:C:1108:LEU:HD21	3:C:1180:ARG:HB2	1.95	0.48
4:d:1221:SER:OG	4:d:1294:ILE:HA	2.13	0.48
5:e:824:LYS:CB	5:e:1155:VAL:H	2.26	0.48
6:F:60:LYS:NZ	6:F:64:GLN:OE1	2.47	0.48
12:L:81:ASN:HD21	13:M:59:ARG:NE	2.11	0.48
15:O:20:SER:HA	15:O:53:TYR:CE2	2.49	0.48
2:B:56:ASP:HA	2:B:97:HIS:NE2	2.28	0.48
2:B:128:ILE:O	2:B:132:VAL:HG23	2.14	0.48
2:B:156:ASN:HA	2:B:159:ALA:CB	2.44	0.48
2:B:447:THR:OG1	2:B:448:LYS:N	2.46	0.48
2:B:1148:SER:HG	2:B:1214:LEU:CB	2.12	0.48
3:C:160:GLU:O	3:C:164:GLU:HG2	2.14	0.48
4:d:1218:ALA:HB1	4:d:1220:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:38:ILE:HD11	14:N:124:GLY:HA3	1.96	0.48
1:A:154:PHE:C	1:A:156:GLY:H	2.21	0.48
2:B:120:HIS:CE1	3:C:119:ILE:HD13	2.48	0.48
2:B:191:ASP:O	2:B:195:VAL:HG13	2.14	0.48
2:B:789:LYS:NZ	2:B:835:GLN:OE1	2.46	0.48
2:B:790:ILE:HG13	2:B:859:TYR:OH	2.14	0.48
2:B:885:GLN:HA	2:B:894:ASN:HD21	1.79	0.48
2:B:1318:ILE:HG23	2:B:1345:LEU:HD13	1.96	0.48
3:C:172:PHE:HA	3:C:175:GLU:HB2	1.95	0.48
3:C:603:GLU:HA	3:C:606:LYS:HE2	1.96	0.48
3:C:805:ARG:HB3	5:e:822:LEU:HD12	1.95	0.48
3:C:973:ASP:O	3:C:981:ASP:N	2.47	0.48
4:d:97:LYS:HE2	13:M:32:LYS:HD3	1.96	0.48
4:d:1173:VAL:HA	4:d:1184:ILE:O	2.14	0.48
7:G:79:VAL:HG23	7:G:144:SER:HB2	1.95	0.48
7:G:124:VAL:HG12	7:G:125:PHE:CE1	2.48	0.48
16:P:6:ILE:HB	16:P:56:VAL:HA	1.95	0.48
1:A:322:GLU:HG3	1:A:339:GLY:O	2.14	0.48
2:B:335:ASN:ND2	2:B:340:LEU:HD13	2.28	0.48
2:B:706:GLU:O	2:B:710:THR:HG23	2.14	0.48
2:B:1256:ASN:OD1	2:B:1257:ILE:HG13	2.13	0.48
3:C:314:VAL:O	3:C:317:LEU:HG	2.13	0.48
3:C:350:HIS:CB	18:x:151:UNK:HA	2.41	0.48
3:C:1185:ARG:HA	3:C:1188:ASP:OD2	2.13	0.48
5:e:865:THR:HG21	5:e:888:VAL:H	1.78	0.48
7:G:77:LEU:HD22	7:G:146:ILE:HB	1.95	0.48
1:A:154:PHE:CE1	1:A:234:ILE:HD11	2.49	0.47
2:B:507:ILE:HG22	2:B:543:LYS:HD2	1.96	0.47
2:B:521:PHE:HA	2:B:524:LEU:HB2	1.96	0.47
2:B:1120:THR:O	2:B:1124:ILE:HG13	2.14	0.47
2:B:1329:PRO:HD2	2:B:1332:GLN:OE1	2.14	0.47
3:C:80:PHE:CD2	3:C:90:ASP:HB2	2.49	0.47
5:e:33:GLN:N	15:O:28:LYS:HE2	2.28	0.47
7:G:63:THR:O	7:G:66:ARG:HG2	2.14	0.47
9:I:97:MET:HE2	9:I:97:MET:HB2	1.71	0.47
14:N:41:LEU:HB3	14:N:45:ARG:CZ	2.44	0.47
17:T:49:LYS:HA	17:T:52:GLU:CD	2.39	0.47
1:A:154:PHE:CE1	1:A:207:MET:HE2	2.49	0.47
1:A:157:LYS:HB2	1:A:159:TYR:HE1	1.80	0.47
1:A:256:ILE:CD1	1:A:322:GLU:HB2	2.41	0.47
2:B:26:LYS:HB2	2:B:29:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:LYS:HE3	2:B:666:ASN:HD22	1.79	0.47
2:B:930:ILE:O	2:B:934:ILE:HG12	2.14	0.47
2:B:1102:LEU:HA	2:B:1105:GLN:HG2	1.95	0.47
2:B:1107:ARG:CD	2:B:1190:ILE:HG12	2.41	0.47
2:B:1360:LYS:HG3	2:B:1364:VAL:N	2.28	0.47
3:C:1129:ILE:O	3:C:1201:TYR:OH	2.31	0.47
4:d:137:ILE:HA	4:d:164:ASN:ND2	2.29	0.47
8:H:58:HIS:HB2	8:H:89:PHE:CZ	2.48	0.47
9:I:29:ASP:OD2	9:I:92:ASN:N	2.42	0.47
12:L:81:ASN:HD21	13:M:59:ARG:HE	1.62	0.47
15:O:27:ILE:HD13	15:O:32:SER:OG	2.14	0.47
16:P:28:PHE:CE1	16:P:74:VAL:HG21	2.49	0.47
1:A:153:PHE:O	1:A:207:MET:HE1	2.14	0.47
2:B:136:PRO:HG3	3:C:78:LEU:HD13	1.96	0.47
2:B:156:ASN:HA	2:B:159:ALA:HB3	1.96	0.47
2:B:433:ILE:HG23	2:B:463:PHE:CE2	2.47	0.47
2:B:851:LYS:NZ	2:B:854:ASN:OD1	2.47	0.47
3:C:1143:ARG:HG2	3:C:1190:LEU:HD11	1.96	0.47
3:C:1180:ARG:HA	3:C:1183:LEU:HD12	1.94	0.47
3:C:3592:ASP:O	3:C:3595:LEU:N	2.47	0.47
4:d:81:GLN:N	11:K:92:LYS:HG3	2.30	0.47
5:e:1077:TYR:CD2	5:e:1080:SER:HB3	2.50	0.47
9:I:83:TYR:HE2	9:I:85:TYR:HD1	1.61	0.47
2:B:118:LEU:HD12	2:B:162:TYR:CD1	2.49	0.47
2:B:368:ILE:HG12	2:B:371:LYS:HB2	1.96	0.47
2:B:524:LEU:HD13	2:B:611:GLN:HG3	1.96	0.47
2:B:1352:LEU:HB3	2:B:1353:PRO:HD2	1.96	0.47
3:C:256:TRP:HA	3:C:259:GLN:HG3	1.96	0.47
3:C:507:ASN:O	3:C:511:ASP:HB2	2.14	0.47
3:C:1096:TYR:HA	3:C:1099:ASP:OD2	2.15	0.47
3:C:1112:THR:HG23	3:C:1182:LEU:HB3	1.97	0.47
4:d:1217:TRP:CZ3	4:d:1223:THR:HB	2.49	0.47
5:e:59:HIS:CD2	11:K:108:TYR:CZ	3.02	0.47
5:e:1087:TRP:CZ3	5:e:1089:PRO:HA	2.49	0.47
7:G:76:TYR:CE2	7:G:78:ILE:HB	2.50	0.47
7:G:82:GLU:OE1	7:G:82:GLU:N	2.46	0.47
9:I:37:GLU:O	9:I:41:VAL:HG23	2.14	0.47
10:J:15:ASN:HD21	10:J:22:LYS:HB2	1.80	0.47
12:L:41:LEU:HA	12:L:44:GLU:HG3	1.94	0.47
12:L:74:TRP:CE2	12:L:109:LYS:HD3	2.50	0.47
14:N:52:ASP:HB3	14:N:55:ASN:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:186:LEU:H	17:T:189:ARG:HD3	1.79	0.47
1:A:317:LYS:HG3	1:A:342:ALA:HB1	1.96	0.47
1:A:4037:ALA:O	1:A:4041:GLY:N	2.41	0.47
2:B:26:LYS:HE2	2:B:72:THR:HG21	1.96	0.47
2:B:126:ASN:HB2	2:B:156:ASN:HD21	1.78	0.47
2:B:137:LEU:HD21	2:B:145:LEU:HD13	1.97	0.47
2:B:653:GLN:H	2:B:757:TRP:HE1	1.62	0.47
2:B:721:ASN:HB3	2:B:777:PHE:HE2	1.78	0.47
2:B:1171:LEU:HG	2:B:1176:VAL:HG23	1.96	0.47
3:C:135:MET:HE2	3:C:165:PHE:CD2	2.49	0.47
3:C:317:LEU:HD23	3:C:356:TYR:CD2	2.46	0.47
3:C:456:ARG:HG2	3:C:502:LEU:HD11	1.95	0.47
3:C:936:GLN:O	3:C:942:VAL:HA	2.15	0.47
3:C:944:LEU:HD11	3:C:948:LEU:HD12	1.97	0.47
6:F:26:PHE:CE1	6:F:98:LEU:HD11	2.50	0.47
16:P:12:LYS:HD2	16:P:12:LYS:C	2.39	0.47
16:P:79:HIS:CG	16:P:93:ILE:HG22	2.50	0.47
17:T:44:LEU:O	17:T:48:GLU:HG2	2.13	0.47
1:A:95:MET:O	1:A:113:ILE:HA	2.14	0.47
1:A:200:ARG:HA	1:A:220:TRP:O	2.13	0.47
1:A:342:ALA:HB2	1:A:346:LEU:HD11	1.96	0.47
1:A:3996:ASP:HA	1:A:4168:ASP:HA	1.96	0.47
2:B:524:LEU:HA	2:B:524:LEU:HD23	1.68	0.47
2:B:656:LEU:HB3	2:B:756:ARG:CZ	2.44	0.47
2:B:1145:LYS:CE	2:B:1150:VAL:HG21	2.45	0.47
3:C:51:ASN:HA	3:C:97:ARG:HD2	1.95	0.47
3:C:869:TYR:CG	3:C:869:TYR:O	2.68	0.47
3:C:951:ILE:HG21	3:C:1074:MET:SD	2.54	0.47
3:C:1115:THR:HG21	3:C:1183:LEU:HD23	1.96	0.47
3:C:1173:ASP:HB2	3:C:1177:MET:HE3	1.96	0.47
4:d:134:LYS:HA	4:d:134:LYS:HE3	1.96	0.47
4:d:134:LYS:O	4:d:138:LYS:HG2	2.15	0.47
4:d:1183:PHE:HB2	4:d:1195:TRP:CE3	2.49	0.47
5:e:1055:SER:HG	5:e:1064:TRP:CD1	2.33	0.47
9:I:73:PRO:O	9:I:74:THR:HG22	2.15	0.47
10:J:21:MET:HG2	10:J:54:TYR:CZ	2.50	0.47
11:K:35:ASP:OD1	11:K:36:ILE:N	2.48	0.47
12:L:47:GLN:CD	12:L:48:GLY:H	2.22	0.47
15:O:76:THR:HG22	15:O:78:HIS:H	1.79	0.47
17:T:176:TYR:OH	17:T:199:MET:SD	2.60	0.47
1:A:196:PRO:N	1:A:197:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:TYR:H	2:B:180:LYS:CE	2.27	0.47
2:B:271:PHE:HA	2:B:275:GLN:OE1	2.15	0.47
2:B:439:LEU:CD2	2:B:530:LEU:HA	2.45	0.47
2:B:505:SER:O	2:B:509:GLN:HG3	2.15	0.47
2:B:697:THR:O	2:B:701:ILE:HG13	2.15	0.47
2:B:854:ASN:HA	2:B:857:LYS:HE2	1.95	0.47
2:B:969:LEU:O	2:B:972:ILE:HB	2.15	0.47
2:B:1040:CYS:HA	2:B:1043:LYS:HD2	1.97	0.47
2:B:1057:LEU:O	2:B:1091:VAL:HG11	2.15	0.47
3:C:464:PHE:O	3:C:468:GLN:HG2	2.13	0.47
3:C:535:ASN:O	3:C:545:SER:HA	2.15	0.47
3:C:663:ILE:HG21	3:C:698:GLU:OE1	2.14	0.47
3:C:864:GLN:NE2	5:e:824:LYS:HG3	2.30	0.47
3:C:864:GLN:NE2	5:e:826:GLU:HG3	2.30	0.47
3:C:1099:ASP:HA	3:C:1102:LYS:HZ3	1.79	0.47
4:d:124:LYS:HD2	4:d:125:THR:N	2.30	0.47
4:d:936:SER:H	4:d:1278:VAL:HB	1.79	0.47
4:d:939:ASP:H	4:d:961:GLN:N	2.13	0.47
4:d:974:LEU:HD22	4:d:1026:SER:HB2	1.96	0.47
8:H:59:CYS:HB2	8:H:88:LEU:HD13	1.96	0.47
10:J:13:PRO:HG2	10:J:79:PHE:HB3	1.96	0.47
15:O:30:ASP:C	15:O:33:GLN:HE21	2.22	0.47
17:T:51:SER:O	17:T:55:ILE:HG12	2.14	0.47
1:A:3894:VAL:O	1:A:3898:LEU:N	2.39	0.47
2:B:1073:ILE:HG23	2:B:1078:ILE:HD12	1.97	0.47
3:C:24:LYS:NZ	3:C:29:GLU:HB2	2.30	0.47
3:C:459:LYS:HD3	3:C:510:PHE:CG	2.50	0.47
3:C:688:PHE:O	3:C:692:ILE:HG13	2.15	0.47
3:C:864:GLN:NE2	5:e:824:LYS:O	2.48	0.47
3:C:948:LEU:HD22	3:C:1010:LYS:HD3	1.97	0.47
3:C:1006:ILE:O	3:C:1009:THR:OG1	2.26	0.47
3:C:1105:ARG:NH1	3:C:1175:ASP:HB2	2.30	0.47
4:d:84:LYS:CG	11:K:89:VAL:HB	2.45	0.47
4:d:1300:LYS:O	4:d:1303:MET:HE3	2.14	0.47
5:e:933:GLU:HG2	5:e:955:ASP:H	1.79	0.47
8:H:35:CYS:SG	8:H:40:GLU:HB3	2.55	0.47
1:A:220:TRP:CE2	2:B:956:LEU:HD13	2.50	0.47
2:B:473:VAL:O	2:B:484:LYS:HD2	2.15	0.47
2:B:1303:ASN:O	2:B:1307:ASN:HB2	2.14	0.47
3:C:331:THR:HG22	3:C:333:GLN:H	1.78	0.47
4:d:117:TRP:CZ2	5:e:41:VAL:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:847:VAL:HG21	5:e:1131:LYS:HZ3	1.78	0.47
5:e:859:MET:HG3	5:e:860:PRO:HD2	1.97	0.47
5:e:1054:LEU:HD22	5:e:1095:PHE:CE2	2.49	0.47
1:A:146:ARG:HH22	1:A:176:ASP:CG	2.22	0.47
2:B:117:LEU:CD1	3:C:146:ILE:HG13	2.43	0.47
2:B:917:ILE:HG12	2:B:983:CYS:HB3	1.97	0.47
2:B:1146:VAL:CG1	2:B:1215:GLN:HG3	2.42	0.47
3:C:177:ARG:HE	3:C:259:GLN:CA	2.27	0.47
3:C:213:PHE:O	3:C:217:ILE:HG12	2.15	0.47
3:C:321:GLU:OE2	3:C:321:GLU:N	2.48	0.47
3:C:597:VAL:HG22	4:d:986:TYR:HE2	1.80	0.47
3:C:1107:LEU:HD13	3:C:1156:VAL:HG22	1.97	0.47
3:C:1209:LEU:O	3:C:1213:LYS:HG2	2.15	0.47
3:C:3203:PRO:O	3:C:3204:ALA:CB	2.63	0.47
5:e:53:ILE:HG13	13:M:33:GLN:HE21	1.80	0.47
8:H:31:ALA:HB2	8:H:44:PHE:CD2	2.50	0.47
11:K:37:LEU:HD22	14:N:33:LYS:HZ2	1.80	0.47
12:L:22:ARG:HD2	12:L:95:PHE:CE2	2.50	0.47
1:A:2955:MET:O	1:A:2959:LYS:N	2.47	0.46
1:A:3817:ASN:O	1:A:3821:ALA:N	2.41	0.46
2:B:164:LEU:HD22	2:B:165:LEU:HD22	1.96	0.46
2:B:443:GLU:O	2:B:444:LEU:HD23	2.16	0.46
2:B:528:GLU:OE1	5:e:1195:GLN:HA	2.14	0.46
2:B:856:TRP:O	2:B:860:ASN:ND2	2.48	0.46
2:B:1126:LYS:NZ	2:B:1138:LYS:HB3	2.30	0.46
3:C:601:PRO:HG3	3:C:697:ARG:HB3	1.96	0.46
3:C:751:LEU:HD13	3:C:869:TYR:O	2.14	0.46
4:d:90:ASP:HB2	4:d:93:THR:O	2.15	0.46
5:e:834:VAL:O	5:e:1128:THR:HG21	2.15	0.46
5:e:1071:PRO:CG	5:e:1074:ARG:HE	2.29	0.46
14:N:32:SER:CA	14:N:35:GLN:HB3	2.38	0.46
14:N:57:ASN:HD22	14:N:58:GLN:NE2	2.13	0.46
14:N:68:ARG:O	14:N:72:LYS:HG2	2.16	0.46
16:P:84:HIS:HB3	16:P:89:VAL:HG21	1.96	0.46
1:A:283:THR:HG23	2:B:955:PHE:HE1	1.79	0.46
1:A:329:ASP:H	1:A:334:ARG:HH11	1.62	0.46
1:A:4077:LEU:O	1:A:4102:HIS:N	2.47	0.46
2:B:605:LYS:HB3	2:B:611:GLN:HB3	1.96	0.46
2:B:1285:GLU:CG	2:B:1290:LEU:HB2	2.44	0.46
2:B:4412:GLN:O	2:B:4414:TRP:N	2.49	0.46
2:B:4548:TYR:HA	2:B:4557:TYR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:LYS:NZ	3:C:71:THR:O	2.29	0.46
3:C:743:LYS:HZ2	3:C:795:ILE:HD13	1.81	0.46
3:C:937:LEU:HD12	3:C:940:ASP:O	2.15	0.46
3:C:1145:GLU:O	3:C:1148:GLU:N	2.48	0.46
4:d:1037:GLY:HA2	4:d:1066:VAL:HG13	1.97	0.46
4:d:1190:TRP:HD1	4:d:1212:VAL:HG23	1.80	0.46
12:L:36:ARG:HD2	12:L:37:GLN:N	2.31	0.46
2:B:157:TYR:H	2:B:180:LYS:HE2	1.80	0.46
2:B:1302:MET:HA	2:B:1305:LEU:HD12	1.97	0.46
2:B:1311:MET:O	2:B:1362:TYR:HE1	1.98	0.46
3:C:420:LYS:HB3	3:C:421:LYS:HZ2	1.80	0.46
3:C:477:ASN:ND2	3:C:528:LEU:HA	2.30	0.46
3:C:801:ILE:CA	5:e:822:LEU:HD11	2.46	0.46
3:C:854:GLU:HA	3:C:857:ARG:HB2	1.97	0.46
3:C:3232:ILE:O	3:C:3233:ILE:C	2.59	0.46
4:d:1068:GLN:O	4:d:1083:SER:HA	2.15	0.46
4:d:1190:TRP:HB3	4:d:1208:LEU:O	2.14	0.46
5:e:834:VAL:N	5:e:1153:GLY:HA2	2.30	0.46
5:e:893:TYR:CE2	5:e:901:ILE:HD12	2.50	0.46
5:e:1021:LYS:HE3	5:e:1024:GLU:HA	1.96	0.46
5:e:1091:ARG:HH21	5:e:1171:GLU:HG3	1.81	0.46
6:F:60:LYS:HA	6:F:63:ILE:HG22	1.96	0.46
14:N:35:GLN:O	14:N:38:ILE:HG22	2.15	0.46
2:B:91:VAL:HG13	2:B:108:VAL:HB	1.97	0.46
2:B:613:ILE:HD11	2:B:619:TYR:HB2	1.96	0.46
2:B:801:ILE:HD13	2:B:874:ALA:C	2.40	0.46
2:B:1255:GLU:OE1	2:B:1255:GLU:N	2.48	0.46
3:C:80:PHE:CD1	3:C:87:LYS:HB3	2.51	0.46
3:C:874:HIS:CD2	3:C:881:GLU:HG3	2.50	0.46
3:C:896:GLN:O	3:C:900:ASN:HB2	2.15	0.46
4:d:122:GLU:HA	4:d:125:THR:HG22	1.97	0.46
4:d:1138:ILE:HG12	4:d:1152:SER:HB2	1.96	0.46
5:e:821:MET:HG3	5:e:1157:ILE:HG23	1.97	0.46
5:e:1176:ASN:HA	5:e:1179:PHE:CD2	2.50	0.46
9:I:89:VAL:HG11	9:I:94:LEU:HD22	1.98	0.46
18:x:125:UNK:O	18:x:126:UNK:C	2.63	0.46
1:A:32:THR:HG22	1:A:34:ILE:HG12	1.96	0.46
1:A:2077:TYR:N	1:A:2123:GLN:O	2.43	0.46
2:B:156:ASN:C	2:B:159:ALA:H	2.23	0.46
2:B:527:PHE:HA	5:e:1194:LYS:HZ2	1.81	0.46
2:B:786:SER:O	2:B:790:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2631:GLY:O	2:B:2645:LEU:N	2.42	0.46
3:C:940:ASP:O	3:C:941:LYS:HE2	2.15	0.46
3:C:1111:LEU:HG	3:C:1153:PHE:CD1	2.51	0.46
4:d:1140:LEU:HD22	4:d:1195:TRP:CZ3	2.50	0.46
8:H:16:MET:HE2	8:H:16:MET:HB2	1.88	0.46
9:I:97:MET:HE1	9:I:99:TYR:CE1	2.49	0.46
12:L:81:ASN:O	13:M:60:ASN:N	2.48	0.46
1:A:345:TRP:O	1:A:346:LEU:HD23	2.16	0.46
2:B:28:LYS:HD3	2:B:73:PHE:CD1	2.51	0.46
2:B:122:ASN:HB2	2:B:159:ALA:HB2	1.98	0.46
2:B:633:ILE:HA	2:B:636:TYR:HD2	1.81	0.46
2:B:670:LYS:HD3	2:B:670:LYS:HA	1.69	0.46
2:B:718:ILE:HD13	2:B:769:SER:HB3	1.98	0.46
2:B:1121:LYS:NZ	2:B:1200:ILE:HD12	2.31	0.46
2:B:1236:PHE:HA	2:B:1239:GLU:OE1	2.14	0.46
2:B:1328:LYS:CG	2:B:1332:GLN:HG2	2.45	0.46
2:B:1577:ARG:O	2:B:1579:ASP:N	2.45	0.46
3:C:25:ASP:HB2	3:C:28:VAL:HG23	1.97	0.46
3:C:568:ARG:HD2	3:C:572:ILE:HG13	1.97	0.46
3:C:972:TRP:O	3:C:975:GLN:HG2	2.15	0.46
7:G:99:ILE:HG23	7:G:103:ILE:HG13	1.97	0.46
12:L:58:VAL:HG23	12:L:76:CYS:SG	2.55	0.46
1:A:26:ILE:HG13	1:A:323:SER:OG	2.16	0.46
1:A:248:ILE:HG22	1:A:301:TRP:HD1	1.79	0.46
2:B:501:ARG:HB2	4:d:1155:TYR:CE1	2.51	0.46
2:B:593:LYS:HA	2:B:596:ARG:HG2	1.97	0.46
2:B:2446:GLY:O	2:B:2675:SER:N	2.43	0.46
3:C:326:PRO:HG2	3:C:372:GLN:OE1	2.15	0.46
3:C:786:GLN:HA	3:C:789:LYS:HG2	1.97	0.46
3:C:1187:TRP:O	3:C:1190:LEU:HB3	2.15	0.46
4:d:1130:ASP:OD1	4:d:1131:PHE:N	2.49	0.46
4:d:1169:ALA:C	4:d:1187:SER:HG	2.23	0.46
12:L:33:LYS:O	12:L:36:ARG:HG3	2.16	0.46
14:N:70:LYS:O	14:N:73:ARG:HG3	2.16	0.46
15:O:24:VAL:HG22	15:O:49:GLN:HE22	1.81	0.46
2:B:66:GLY:O	2:B:72:THR:HA	2.16	0.46
2:B:419:PHE:HA	2:B:422:ARG:CD	2.46	0.46
2:B:540:LEU:O	2:B:544:HIS:N	2.45	0.46
2:B:913:PHE:HB2	2:B:916:GLU:HA	1.97	0.46
3:C:488:PHE:O	3:C:492:ILE:HG12	2.15	0.46
3:C:814:SER:CA	3:C:901:SER:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:1193:LYS:HA	5:e:1196:GLN:OE1	2.16	0.46
6:F:85:TYR:CE2	6:F:87:TYR:HB2	2.50	0.46
11:K:34:ASP:N	14:N:36:LYS:HA	2.31	0.46
16:P:28:PHE:CE2	16:P:74:VAL:HG21	2.50	0.46
16:P:79:HIS:CD2	16:P:93:ILE:HG22	2.51	0.46
1:A:39:LEU:HD11	2:B:964:GLU:O	2.15	0.46
1:A:177:LEU:HD13	1:A:239:TRP:HH2	1.81	0.46
1:A:1721:LYS:O	1:A:1725:GLY:N	2.45	0.46
2:B:104:VAL:O	2:B:108:VAL:HG22	2.16	0.46
2:B:207:ILE:HG23	2:B:211:LEU:HD23	1.97	0.46
2:B:883:ASN:ND2	2:B:972:ILE:HD13	2.31	0.46
3:C:434:PRO:O	3:C:438:THR:N	2.49	0.46
3:C:1060:GLU:O	3:C:1063:GLU:HG3	2.15	0.46
3:C:1105:ARG:NH2	3:C:1176:GLU:HB2	2.31	0.46
3:C:3744:ARG:O	3:C:3748:ARG:N	2.43	0.46
4:d:121:ASN:OD1	4:d:122:GLU:HG2	2.16	0.46
5:e:1125:SER:O	5:e:1126:PRO:C	2.58	0.46
5:e:1129:CYS:SG	5:e:1130:ILE:N	2.89	0.46
8:H:24:VAL:HG11	8:H:77:ILE:HD13	1.97	0.46
8:H:71:PHE:CD1	8:H:76:TYR:HB2	2.51	0.46
9:I:46:ILE:O	9:I:50:SER:HB3	2.16	0.46
1:A:7:TRP:CD1	1:A:315:VAL:HG13	2.51	0.46
1:A:2638:ALA:HB2	1:A:2875:ALA:HB1	1.97	0.46
2:B:160:GLN:HE22	2:B:243:LEU:HD13	1.80	0.46
3:C:269:LYS:CE	3:C:284:ARG:HD3	2.46	0.46
3:C:1058:ILE:O	3:C:1062:ILE:HG13	2.16	0.46
3:C:1182:LEU:CD1	3:C:1185:ARG:HE	2.28	0.46
8:H:42:ALA:HB2	8:H:61:VAL:HG22	1.98	0.46
10:J:28:GLN:HG3	10:J:49:PHE:CE2	2.51	0.46
11:K:40:ALA:O	11:K:44:THR:HG22	2.16	0.46
13:M:57:VAL:HG22	13:M:82:LEU:HD22	1.97	0.46
16:P:16:ASP:OD2	16:P:16:ASP:C	2.58	0.46
1:A:10:LEU:HD21	1:A:329:ASP:OD2	2.16	0.45
2:B:60:ASN:HD21	3:C:141:ARG:HE	1.64	0.45
2:B:292:LEU:O	2:B:295:LEU:HG	2.16	0.45
2:B:437:ASN:O	2:B:441:LYS:HG2	2.16	0.45
2:B:516:THR:HG21	5:e:1076:LYS:HB3	1.97	0.45
2:B:1246:PHE:CE2	2:B:1257:ILE:HG12	2.51	0.45
2:B:1268:TYR:HB3	2:B:1305:LEU:CD2	2.46	0.45
3:C:21:LEU:HD12	3:C:22:GLN:HB2	1.97	0.45
3:C:81:THR:HG22	3:C:126:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:864:GLN:CG	5:e:824:LYS:HE3	2.46	0.45
3:C:1111:LEU:HG	3:C:1153:PHE:HB2	1.98	0.45
4:d:117:TRP:CG	15:O:31:SER:HA	2.51	0.45
4:d:1153:ARG:HD3	4:d:1153:ARG:HA	1.60	0.45
5:e:832:ARG:HH11	5:e:868:TYR:HH	1.63	0.45
5:e:900:GLN:HB2	5:e:912:VAL:CG1	2.46	0.45
9:I:37:GLU:HB3	9:I:70:LYS:HZ2	1.81	0.45
9:I:75:TRP:CD1	9:I:109:LYS:HZ2	2.34	0.45
1:A:53:PRO:C	1:A:82:ARG:HB3	2.40	0.45
2:B:49:PHE:O	2:B:53:ILE:HG13	2.17	0.45
2:B:1102:LEU:HD12	2:B:1103:VAL:N	2.32	0.45
2:B:1189:GLN:HE21	2:B:1190:ILE:HG13	1.81	0.45
3:C:58:GLN:HB3	3:C:68:ILE:HG23	1.99	0.45
3:C:274:ARG:HH11	3:C:275:HIS:CD2	2.35	0.45
3:C:1142:ILE:O	3:C:1146:GLN:HG3	2.17	0.45
9:I:32:GLY:O	9:I:35:LEU:HB2	2.17	0.45
11:K:34:ASP:HB2	14:N:36:LYS:HB3	1.98	0.45
13:M:33:GLN:OE1	13:M:36:GLN:NE2	2.38	0.45
2:B:1164:MET:HB2	2:B:1164:MET:HE3	1.63	0.45
3:C:57:TYR:HD1	3:C:69:LYS:HE2	1.81	0.45
3:C:177:ARG:HH21	3:C:259:GLN:HG2	1.80	0.45
3:C:264:ASP:HA	3:C:267:ILE:HD12	1.98	0.45
3:C:821:LEU:HD23	3:C:922:ASN:HB3	1.98	0.45
3:C:1264:LYS:HD3	3:C:1264:LYS:HA	1.66	0.45
4:d:1073:PRO:HA	4:d:1079:TYR:CD2	2.49	0.45
4:d:1192:VAL:HB	4:d:1211:MET:SD	2.56	0.45
5:e:1175:ILE:HG22	5:e:1179:PHE:CZ	2.51	0.45
8:H:24:VAL:HA	8:H:49:PHE:CZ	2.52	0.45
17:T:103:SER:OG	17:T:107:LYS:HE3	2.15	0.45
2:B:159:ALA:O	2:B:162:TYR:HB3	2.16	0.45
2:B:392:ASP:OD1	2:B:393:ALA:N	2.49	0.45
2:B:591:TRP:CZ2	2:B:595:LEU:HD11	2.52	0.45
2:B:752:ILE:CD1	2:B:765:PHE:HB3	2.45	0.45
2:B:1320:PHE:HA	2:B:1323:ASN:HB2	1.98	0.45
3:C:151:ILE:O	3:C:152:GLN:NE2	2.50	0.45
3:C:253:ILE:HG22	3:C:311:LYS:HE2	1.99	0.45
3:C:3180:CYS:CB	3:C:3366:ALA:HB1	2.47	0.45
4:d:84:LYS:HG3	11:K:89:VAL:HB	1.98	0.45
4:d:1020:LEU:HD11	4:d:1030:LEU:HD11	1.99	0.45
4:d:1072:ASN:HB2	4:d:1080:ASN:HB2	1.98	0.45
4:d:1297:THR:OG1	4:d:1301:LYS:NZ	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:1135:THR:O	5:e:1141:ASN:ND2	2.50	0.45
6:F:11:LEU:HD21	6:F:34:LYS:HE2	1.98	0.45
10:J:42:ILE:O	10:J:46:ILE:HG13	2.17	0.45
14:N:32:SER:HA	14:N:35:GLN:CB	2.39	0.45
17:T:31:PRO:HA	17:T:197:PHE:CZ	2.51	0.45
1:A:80:LEU:H	1:A:80:LEU:HD12	1.82	0.45
1:A:1338:GLU:O	1:A:1341:TRP:N	2.50	0.45
2:B:103:ASN:ND2	3:C:21:LEU:O	2.49	0.45
2:B:134:GLN:HB2	3:C:79:PHE:HZ	1.81	0.45
2:B:164:LEU:HD23	2:B:168:ILE:CG1	2.45	0.45
2:B:394:TYR:HE2	2:B:412:LEU:HD13	1.81	0.45
2:B:756:ARG:HA	2:B:762:ILE:HD13	1.97	0.45
2:B:836:ILE:HA	2:B:839:LEU:HG	1.97	0.45
2:B:1147:ILE:HB	2:B:1214:LEU:CD1	2.47	0.45
3:C:55:ALA:O	3:C:93:VAL:HG12	2.16	0.45
3:C:177:ARG:NH2	3:C:255:ASN:O	2.50	0.45
3:C:807:GLU:O	3:C:811:LYS:HG2	2.17	0.45
3:C:1115:THR:HB	3:C:1186:ASN:HD22	1.80	0.45
3:C:2932:GLU:O	3:C:2935:LEU:N	2.42	0.45
4:d:115:TYR:C	4:d:116:ILE:HD12	2.41	0.45
6:F:67:LEU:HG	7:G:99:ILE:HG12	1.98	0.45
14:N:31:PRO:HB3	14:N:110:TYR:O	2.16	0.45
17:T:115:LYS:HG3	17:T:176:TYR:CZ	2.51	0.45
1:A:166:GLY:HA2	1:A:171:ARG:N	2.28	0.45
2:B:279:LYS:HB3	2:B:286:ASN:HB2	1.97	0.45
2:B:419:PHE:CD2	2:B:422:ARG:HD2	2.51	0.45
2:B:1227:ASP:O	2:B:1231:LYS:HG2	2.16	0.45
2:B:1345:LEU:O	2:B:1349:ILE:HG13	2.16	0.45
3:C:51:ASN:O	3:C:96:LEU:HD12	2.16	0.45
3:C:576:TYR:CG	3:C:624:PHE:HE1	2.35	0.45
3:C:792:GLU:HA	3:C:795:ILE:HD12	1.99	0.45
3:C:793:GLN:O	3:C:796:ILE:N	2.49	0.45
3:C:864:GLN:HA	5:e:826:GLU:OE2	2.15	0.45
3:C:871:LEU:HD12	3:C:871:LEU:O	2.16	0.45
3:C:1055:PHE:CE1	3:C:1089:ALA:HB1	2.51	0.45
4:d:84:LYS:HE3	11:K:92:LYS:CE	2.46	0.45
5:e:1173:ASP:O	5:e:1177:GLU:HB2	2.16	0.45
11:K:31:GLU:HA	14:N:32:SER:CB	2.47	0.45
1:A:230:MET:HE1	1:A:241:ASP:HB2	1.98	0.45
1:A:1338:GLU:O	1:A:1342:GLN:N	2.45	0.45
1:A:1826:GLN:O	1:A:1829:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2920:GLN:O	1:A:2924:MET:N	2.41	0.45
1:A:3996:ASP:HA	1:A:4168:ASP:O	2.17	0.45
2:B:40:LYS:HA	2:B:43:VAL:HG22	1.98	0.45
2:B:230:GLU:OE2	2:B:346:GLU:HG3	2.17	0.45
2:B:236:ASN:HA	2:B:239:ASP:OD2	2.17	0.45
2:B:442:ILE:HA	5:e:1190:GLU:HB3	1.99	0.45
2:B:901:ASP:HB2	2:B:903:ARG:NH1	2.32	0.45
2:B:1311:MET:C	2:B:1362:TYR:CE1	2.95	0.45
3:C:785:HIS:C	3:C:789:LYS:HZ1	2.24	0.45
3:C:786:GLN:HB3	3:C:790:LYS:NZ	2.31	0.45
3:C:1018:SER:HA	3:C:1021:THR:HG23	1.99	0.45
3:C:1125:PRO:HG2	3:C:1128:ASP:HB2	1.97	0.45
4:d:116:ILE:HG21	4:d:122:GLU:HB2	1.98	0.45
4:d:247:ILE:HA	7:G:125:PHE:HE1	1.78	0.45
4:d:1171:TYR:HE2	4:d:1188:ALA:HB2	1.81	0.45
10:J:59:HIS:CD2	10:J:92:LYS:HB3	2.52	0.45
11:K:47:ALA:HA	11:K:50:LYS:CE	2.47	0.45
15:O:34:VAL:HG22	15:O:104:ASN:CG	2.42	0.45
2:B:1814:SER:O	2:B:1817:TRP:N	2.50	0.45
3:C:535:ASN:CB	3:C:568:ARG:HH12	2.28	0.45
3:C:656:TYR:O	3:C:660:VAL:HG22	2.16	0.45
3:C:822:PRO:HG3	3:C:920:GLY:HA3	1.97	0.45
3:C:860:ASP:HB3	5:e:825:ASP:HA	1.99	0.45
5:e:919:GLU:HG2	5:e:919:GLU:O	2.17	0.45
8:H:24:VAL:HG11	8:H:77:ILE:HG21	1.99	0.45
8:H:50:ARG:NH1	8:H:56:THR:HA	2.31	0.45
8:H:50:ARG:NH2	8:H:57:TRP:O	2.50	0.45
11:K:96:ILE:O	11:K:106:LEU:HD12	2.17	0.45
16:P:39:LEU:HD11	16:P:96:GLN:C	2.41	0.45
1:A:282:ARG:C	1:A:284:ASN:H	2.14	0.45
2:B:184:SER:HA	2:B:192:LYS:HE2	1.98	0.45
2:B:186:THR:HG22	2:B:188:PRO:HD2	1.99	0.45
2:B:553:GLN:NE2	2:B:557:GLN:HB2	2.32	0.45
2:B:914:ASP:HB2	2:B:915:PRO:HD3	1.98	0.45
2:B:1136:ASP:OD2	2:B:1218:GLU:HA	2.16	0.45
2:B:1146:VAL:HG12	2:B:1214:LEU:HD11	1.11	0.45
2:B:1282:ASN:HA	2:B:1285:GLU:OE1	2.16	0.45
2:B:1313:ASP:O	2:B:1317:LEU:HG	2.17	0.45
3:C:572:ILE:HG23	3:C:576:TYR:CE2	2.52	0.45
5:e:927:VAL:HG23	5:e:928:GLU:N	2.31	0.45
8:H:81:VAL:HG23	8:H:86:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:37:LEU:CB	14:N:36:LYS:HD2	2.45	0.45
11:K:48:LEU:HB2	11:K:49:LYS:HZ2	1.81	0.45
12:L:61:VAL:HG13	12:L:67:PHE:CD2	2.52	0.45
14:N:112:SER:HB2	14:N:125:ILE:HG22	1.98	0.45
15:O:33:GLN:HB2	15:O:103:ILE:HG21	1.99	0.45
1:A:114:LEU:HA	1:A:120:GLN:O	2.16	0.45
1:A:222:PHE:HB2	2:B:952:PRO:CB	2.34	0.45
1:A:334:ARG:HA	1:A:354:VAL:HG23	1.97	0.45
2:B:154:PHE:CZ	3:C:161:GLN:HB3	2.52	0.45
2:B:517:ILE:HG13	2:B:518:TYR:N	2.32	0.45
2:B:583:PRO:HD3	2:B:682:LYS:NZ	2.32	0.45
2:B:1137:LYS:HB3	2:B:1215:GLN:HE21	1.81	0.45
2:B:1322:TYR:HE1	2:B:1342:ASN:CG	2.25	0.45
3:C:21:LEU:HD12	3:C:22:GLN:N	2.32	0.45
3:C:231:ARG:HA	3:C:249:ARG:HH21	1.81	0.45
4:d:1184:ILE:HA	4:d:1193:ARG:O	2.17	0.45
9:I:89:VAL:CG2	9:I:108:PHE:HB2	2.47	0.45
13:M:4:GLU:N	13:M:4:GLU:OE1	2.48	0.45
15:O:77:ASN:HB3	15:O:107:TYR:CZ	2.52	0.45
1:A:63:THR:C	1:A:64:GLN:HG3	2.42	0.44
1:A:223:THR:HG22	2:B:955:PHE:HB3	1.98	0.44
1:A:290:ASP:OD1	1:A:291:SER:N	2.49	0.44
2:B:55:GLN:NE2	2:B:57:ASN:HB3	2.32	0.44
2:B:63:TRP:O	2:B:88:GLY:HA2	2.17	0.44
2:B:504:ALA:CB	2:B:539:GLU:HG3	2.47	0.44
2:B:886:ILE:HG13	2:B:975:ASN:CG	2.42	0.44
2:B:1317:LEU:HD13	16:P:77:LEU:CB	2.35	0.44
2:B:2500:LEU:O	2:B:2504:GLN:N	2.50	0.44
3:C:1178:ASP:O	3:C:1182:LEU:HB2	2.17	0.44
4:d:114:ASP:OD1	4:d:114:ASP:N	2.50	0.44
10:J:72:TYR:CD2	10:J:77:PHE:HB2	2.52	0.44
1:A:3437:ASP:O	1:A:3441:ILE:N	2.44	0.44
2:B:135:ASN:HA	2:B:138:ASN:HD22	1.82	0.44
2:B:332:LYS:C	2:B:405:TRP:HD1	2.25	0.44
2:B:853:GLN:HA	2:B:856:TRP:HD1	1.82	0.44
2:B:1046:ASN:HB2	2:B:1170:LYS:NZ	2.33	0.44
3:C:933:VAL:HG11	3:C:944:LEU:HD13	1.99	0.44
3:C:1234:GLY:HA3	3:C:1252:PHE:HE2	1.83	0.44
5:e:834:VAL:HG23	5:e:1153:GLY:HA2	1.99	0.44
5:e:1081:TYR:CB	5:e:1100:ARG:HG3	2.47	0.44
11:K:24:ALA:HB1	11:K:99:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:O	1:A:21:ARG:HB2	2.17	0.44
1:A:152:THR:OG1	1:A:207:MET:HE3	2.16	0.44
2:B:559:GLN:NE2	2:B:629:ILE:HG23	2.33	0.44
2:B:749:LYS:NZ	2:B:768:LYS:HE2	2.32	0.44
2:B:841:LYS:O	2:B:844:LEU:HB2	2.18	0.44
2:B:875:ILE:HB	2:B:962:PHE:HZ	1.81	0.44
2:B:1118:GLU:OE2	2:B:1200:ILE:HG13	2.18	0.44
3:C:744:ILE:HG21	3:C:756:ILE:HD11	1.99	0.44
4:d:1172:LYS:NZ	4:d:1215:ALA:HB3	2.32	0.44
6:F:23:TYR:O	6:F:35:ARG:HA	2.17	0.44
9:I:46:ILE:HD11	9:I:99:TYR:CE2	2.52	0.44
16:P:25:LEU:HB2	16:P:55:ILE:CD1	2.47	0.44
2:B:152:GLU:C	2:B:180:LYS:HD2	2.42	0.44
2:B:349:ASN:HA	2:B:352:ILE:HG22	1.99	0.44
2:B:1175:ASN:HA	2:B:1178:ILE:HD12	1.98	0.44
2:B:1214:LEU:HG	2:B:1215:GLN:H	1.83	0.44
3:C:32:PHE:O	3:C:38:LYS:HE2	2.17	0.44
3:C:80:PHE:O	3:C:88:ILE:HG13	2.18	0.44
3:C:429:LYS:HA	3:C:432:ASP:OD2	2.17	0.44
3:C:675:ILE:HD12	3:C:772:TRP:CH2	2.52	0.44
4:d:1019:CYS:SG	4:d:1066:VAL:HG23	2.58	0.44
4:d:1128:CYS:O	4:d:1141:VAL:HG23	2.18	0.44
4:d:1154:ALA:HB3	4:d:1158:GLN:OE1	2.17	0.44
5:e:52:ASN:HD22	12:L:22:ARG:HD3	1.82	0.44
5:e:1045:ARG:HA	5:e:1053:PHE:HA	1.98	0.44
5:e:1082:LEU:H	5:e:1099:ARG:HD2	1.81	0.44
9:I:30:MET:HE1	9:I:75:TRP:CH2	2.53	0.44
10:J:17:GLU:CD	10:J:18:MET:H	2.26	0.44
11:K:79:PHE:HE1	11:K:108:TYR:HH	1.64	0.44
12:L:95:PHE:CD1	12:L:106:LEU:HB2	2.52	0.44
14:N:29:PHE:HE1	14:N:34:ILE:HG12	1.82	0.44
1:A:276:PHE:CE2	1:A:284:ASN:HB2	2.51	0.44
1:A:2525:ASN:O	1:A:2529:SER:CB	2.66	0.44
2:B:64:VAL:HG23	2:B:77:GLN:NE2	2.33	0.44
2:B:1149:ASP:H	2:B:1214:LEU:CD2	2.26	0.44
2:B:1271:LEU:HD21	2:B:1301:CYS:CB	2.45	0.44
3:C:55:ALA:HB3	3:C:93:VAL:CG1	2.48	0.44
3:C:139:TYR:HA	3:C:142:GLN:HG2	1.99	0.44
3:C:853:VAL:HG23	3:C:854:GLU:N	2.33	0.44
3:C:2738:GLU:O	3:C:2742:ALA:N	2.49	0.44
4:d:187:THR:OG1	10:J:66:PHE:O	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:872:LEU:H	5:e:872:LEU:HG	1.63	0.44
5:e:1082:LEU:HA	5:e:1099:ARG:HH11	1.81	0.44
7:G:63:THR:O	7:G:67:ILE:HG12	2.17	0.44
9:I:49:ASN:HB3	9:I:54:LEU:HB2	1.99	0.44
11:K:32:CYS:HB3	14:N:36:LYS:HE2	2.00	0.44
11:K:34:ASP:HA	11:K:37:LEU:HB3	1.99	0.44
1:A:79:PRO:HD2	1:A:121:TRP:CZ3	2.52	0.44
2:B:52:PHE:HD1	2:B:58:SER:HB2	1.82	0.44
2:B:174:LEU:CD2	2:B:236:ASN:HB3	2.47	0.44
2:B:204:THR:HG22	2:B:208:LYS:HE3	2.00	0.44
2:B:368:ILE:O	2:B:372:GLU:N	2.51	0.44
2:B:436:PHE:CZ	2:B:499:LEU:HD13	2.53	0.44
3:C:26:MET:O	3:C:26:MET:HE3	2.17	0.44
3:C:56:TYR:CD1	3:C:80:PHE:HZ	2.36	0.44
3:C:794:LEU:O	3:C:798:VAL:HG23	2.18	0.44
3:C:800:ASP:CG	5:e:820:LEU:HD22	2.42	0.44
3:C:864:GLN:HE22	5:e:826:GLU:HG3	1.83	0.44
3:C:981:ASP:OD1	3:C:982:LYS:N	2.48	0.44
3:C:3343:HIS:O	3:C:3345:LYS:CB	2.66	0.44
5:e:994:TYR:CD2	5:e:1003:PHE:HB3	2.53	0.44
5:e:1139:TYR:C	5:e:1141:ASN:H	2.25	0.44
1:A:2044:TYR:HA	1:A:2085:PRO:HA	2.00	0.44
1:A:4114:PRO:O	1:A:4116:ASP:N	2.51	0.44
2:B:309:ASP:HA	2:B:358:PHE:HE2	1.81	0.44
2:B:789:LYS:HD3	2:B:842:GLU:OE1	2.17	0.44
2:B:962:PHE:HA	2:B:966:LYS:HE2	2.00	0.44
2:B:1146:VAL:CG1	2:B:1215:GLN:CG	2.91	0.44
2:B:1215:GLN:HB3	2:B:1218:GLU:CG	2.47	0.44
4:d:971:TRP:HB3	4:d:979:PHE:CE2	2.53	0.44
7:G:118:ASP:HB3	7:G:120:THR:HG23	1.99	0.44
8:H:61:VAL:HG12	8:H:86:ILE:HG13	1.99	0.44
11:K:42:ARG:HG3	11:K:43:GLU:N	2.33	0.44
14:N:46:LEU:O	14:N:47:LYS:HG2	2.17	0.44
17:T:132:THR:OG1	17:T:133:ALA:N	2.50	0.44
1:A:2943:LYS:O	1:A:2947:ASN:N	2.43	0.44
2:B:134:GLN:O	2:B:137:LEU:HB2	2.18	0.44
2:B:326:LEU:HD12	5:e:1225:ALA:HB3	1.99	0.44
2:B:729:LEU:HD22	2:B:737:VAL:HB	2.00	0.44
2:B:744:MET:HE2	2:B:776:LEU:HD22	2.00	0.44
2:B:1259:ASN:OD1	2:B:1260:ALA:N	2.51	0.44
4:d:1132:ASN:HA	4:d:1183:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1163:TYR:CE1	4:d:1195:TRP:HD1	2.36	0.44
5:e:836:GLU:OE2	5:e:889:THR:HA	2.18	0.44
5:e:1099:ARG:HB2	5:e:1101:ASP:OD1	2.17	0.44
5:e:1103:TRP:NE1	5:e:1119:SER:HB3	2.32	0.44
5:e:1171:GLU:OE2	5:e:1171:GLU:N	2.47	0.44
6:F:60:LYS:O	6:F:63:ILE:HG22	2.17	0.44
15:O:11:GLU:O	15:O:15:LYS:HG3	2.18	0.44
16:P:52:ASN:OD1	16:P:52:ASN:N	2.51	0.44
17:T:107:LYS:HD2	17:T:177:ARG:HG2	2.00	0.44
1:A:12:GLN:HE22	1:A:338:PHE:HE1	1.66	0.44
1:A:276:PHE:HB2	1:A:282:ARG:HB2	2.00	0.44
2:B:116:ASN:ND2	2:B:162:TYR:OH	2.41	0.44
2:B:127:GLU:HG3	3:C:51:ASN:HB2	1.99	0.44
2:B:380:LEU:HD21	2:B:427:LEU:HD12	2.00	0.44
2:B:561:ILE:HG12	2:B:566:LYS:HD3	2.00	0.44
2:B:876:GLN:OE1	2:B:966:LYS:HB3	2.18	0.44
3:C:239:PRO:O	3:C:243:LEU:HG	2.18	0.44
4:d:1246:LEU:HA	4:d:1246:LEU:HD13	1.85	0.44
5:e:820:LEU:HA	5:e:1158:LEU:HA	1.99	0.44
5:e:870:TRP:HA	5:e:879:GLU:HG2	2.00	0.44
6:F:15:SER:HA	6:F:23:TYR:CE1	2.53	0.44
9:I:85:TYR:CE1	9:I:106:LEU:HD22	2.53	0.44
1:A:60:LEU:HD22	1:A:69:TRP:CZ2	2.53	0.43
1:A:212:PRO:HG2	1:A:235:GLU:OE2	2.18	0.43
1:A:341:TRP:CZ2	2:B:963:PHE:CG	3.06	0.43
1:A:343:ASN:HD21	2:B:931:ARG:NE	2.11	0.43
2:B:790:ILE:HD11	2:B:839:LEU:HB2	2.00	0.43
2:B:3748:ARG:O	2:B:3751:ALA:HB3	2.18	0.43
3:C:528:LEU:O	3:C:532:ILE:HG13	2.18	0.43
3:C:622:ASN:O	3:C:625:PRO:HD2	2.18	0.43
4:d:1021:ASP:N	4:d:1021:ASP:OD1	2.50	0.43
11:K:90:HIS:NE2	11:K:95:PHE:HB2	2.32	0.43
12:L:98:LEU:HG	12:L:100:PRO:HD2	2.00	0.43
16:P:83:TYR:CD1	16:P:88:VAL:HA	2.53	0.43
17:T:107:LYS:CB	17:T:177:ARG:HG2	2.48	0.43
1:A:2434:LEU:O	1:A:2438:GLY:N	2.48	0.43
2:B:50:GLN:OE1	2:B:50:GLN:N	2.41	0.43
2:B:115:ASN:HB2	2:B:120:HIS:HB2	2.00	0.43
2:B:566:LYS:HG3	2:B:567:GLN:H	1.83	0.43
2:B:813:ASP:CG	2:B:1075:TRP:CD1	2.96	0.43
2:B:1127:ASN:HB2	2:B:1147:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:LEU:HG	3:C:87:LYS:N	2.32	0.43
3:C:557:LYS:HB2	3:C:557:LYS:HE3	1.77	0.43
3:C:591:LYS:HB2	3:C:609:TRP:CE3	2.53	0.43
5:e:50:LEU:H	5:e:50:LEU:HD23	1.82	0.43
12:L:61:VAL:HG13	12:L:67:PHE:CE2	2.53	0.43
1:A:51:ILE:HA	1:A:82:ARG:CG	2.47	0.43
2:B:99:LEU:HD12	2:B:99:LEU:HA	1.75	0.43
2:B:109:VAL:HG13	3:C:122:GLU:O	2.19	0.43
2:B:154:PHE:O	2:B:158:VAL:HG23	2.18	0.43
2:B:516:THR:HG21	5:e:1076:LYS:N	2.28	0.43
3:C:123:ILE:HD11	3:C:134:LEU:CD1	2.48	0.43
3:C:550:HIS:O	3:C:553:GLN:HG3	2.18	0.43
3:C:570:ASN:O	3:C:573:LEU:HG	2.17	0.43
4:d:966:VAL:HB	4:d:1258:THR:OG1	2.17	0.43
8:H:50:ARG:HH12	8:H:56:THR:HG23	1.82	0.43
13:M:43:TYR:O	13:M:47:LYS:HD3	2.19	0.43
16:P:43:PHE:HE2	16:P:57:LYS:HG2	1.83	0.43
1:A:164:HIS:CE1	1:A:201:GLY:HA3	2.53	0.43
1:A:222:PHE:O	1:A:222:PHE:CD1	2.70	0.43
1:A:4077:LEU:N	1:A:4102:HIS:O	2.51	0.43
2:B:155:ASN:N	2:B:180:LYS:HZ1	2.17	0.43
2:B:358:PHE:HA	2:B:361:LYS:NZ	2.33	0.43
2:B:801:ILE:HG21	2:B:874:ALA:CB	2.47	0.43
2:B:1748:ASP:O	2:B:1751:GLY:N	2.46	0.43
3:C:132:ASN:ND2	3:C:169:SER:O	2.51	0.43
3:C:857:ARG:NE	5:e:875:PRO:HB2	2.30	0.43
4:d:961:GLN:O	4:d:1276:GLY:HA3	2.19	0.43
4:d:1242:LYS:HD3	4:d:1244:ASN:H	1.82	0.43
5:e:51:ASP:HB3	13:M:35:LYS:CD	2.39	0.43
6:F:8:ASP:O	6:F:12:LYS:HG2	2.18	0.43
9:I:27:SER:OG	9:I:96:PHE:HB3	2.18	0.43
12:L:45:ASN:HD21	12:L:52:ASP:HB3	1.83	0.43
12:L:60:PHE:O	12:L:64:GLN:NE2	2.51	0.43
1:A:904:LEU:O	1:A:908:LEU:N	2.51	0.43
1:A:1399:CYS:HA	1:A:1524:ARG:O	2.19	0.43
2:B:200:ILE:HD11	2:B:256:ILE:HG21	2.00	0.43
2:B:434:VAL:O	2:B:438:LYS:HE2	2.18	0.43
2:B:872:SER:O	2:B:876:GLN:HG2	2.18	0.43
2:B:904:LEU:HD11	2:B:990:PHE:CE2	2.52	0.43
3:C:933:VAL:CG2	3:C:944:LEU:HB3	2.49	0.43
3:C:960:THR:O	3:C:964:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:992:ASP:O	3:C:996:VAL:HG22	2.17	0.43
3:C:3355:GLN:N	3:C:3358:ILE:CB	2.82	0.43
4:d:77:PRO:HD3	15:O:86:THR:OG1	2.19	0.43
4:d:1208:LEU:HD13	4:d:1236:TYR:OH	2.19	0.43
4:d:1239:ASN:HB3	4:d:1300:LYS:NZ	2.33	0.43
4:d:1269:LEU:O	4:d:1280:LEU:HA	2.19	0.43
5:e:73:MET:H	8:H:73:ARG:CZ	2.31	0.43
5:e:834:VAL:HG11	5:e:1149:GLY:HA3	1.99	0.43
6:F:26:PHE:CD1	6:F:98:LEU:HD11	2.53	0.43
11:K:34:ASP:HB3	14:N:40:GLU:CB	2.37	0.43
1:A:397:PHE:O	1:A:405:GLU:HA	2.18	0.43
2:B:154:PHE:CE1	3:C:161:GLN:HB3	2.54	0.43
2:B:340:LEU:HD11	2:B:397:TYR:OH	2.18	0.43
2:B:367:LEU:HB2	2:B:372:GLU:HA	1.99	0.43
2:B:657:LYS:CB	2:B:748:VAL:HB	2.48	0.43
2:B:852:LYS:HB3	2:B:856:TRP:NE1	2.34	0.43
2:B:890:PHE:CE2	2:B:891:ILE:HG12	2.53	0.43
2:B:958:GLU:HB3	2:B:962:PHE:HE2	1.82	0.43
2:B:1138:LYS:O	2:B:1139:LEU:HD23	2.19	0.43
3:C:591:LYS:HG2	3:C:606:LYS:HA	2.00	0.43
3:C:675:ILE:HD12	3:C:772:TRP:HH2	1.84	0.43
9:I:90:GLN:O	9:I:93:THR:OG1	2.26	0.43
11:K:28:TRP:HA	11:K:29:PRO:HA	1.68	0.43
17:T:140:LEU:HB3	17:T:145:TYR:HD2	1.83	0.43
2:B:15:ILE:HD11	2:B:33:LEU:HD21	1.99	0.43
2:B:299:PHE:CD1	2:B:302:LEU:HD12	2.50	0.43
2:B:385:ASP:O	2:B:389:LYS:HG2	2.19	0.43
2:B:428:HIS:CD2	2:B:428:HIS:N	2.86	0.43
2:B:440:GLU:OE1	2:B:441:LYS:NZ	2.50	0.43
2:B:875:ILE:HB	2:B:962:PHE:CE1	2.54	0.43
3:C:102:ALA:O	3:C:106:LYS:HG2	2.19	0.43
3:C:183:MET:HB3	3:C:216:TRP:CE2	2.54	0.43
3:C:269:LYS:HA	3:C:269:LYS:HD3	1.87	0.43
3:C:434:PRO:O	3:C:438:THR:HG23	2.17	0.43
3:C:686:VAL:HG11	3:C:689:ASP:HB2	2.00	0.43
3:C:1147:ALA:O	3:C:1151:MET:HG2	2.18	0.43
4:d:138:LYS:HA	4:d:138:LYS:HE3	2.01	0.43
11:K:29:PRO:CG	14:N:30:TYR:H	2.29	0.43
12:L:81:ASN:HB3	13:M:60:ASN:ND2	2.33	0.43
15:O:37:THR:HG22	15:O:38:TYR:H	1.84	0.43
15:O:37:THR:HG22	15:O:38:TYR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLY:HA2	1:A:288:VAL:O	2.19	0.43
1:A:1758:LEU:N	1:A:1797:LEU:O	2.47	0.43
2:B:128:ILE:O	2:B:131:PRO:HD2	2.18	0.43
2:B:161:VAL:HG22	2:B:164:LEU:HD13	2.00	0.43
2:B:305:SER:OG	2:B:307:PRO:HD2	2.19	0.43
2:B:503:LEU:HD11	2:B:533:ARG:NH2	2.32	0.43
2:B:661:LEU:H	2:B:661:LEU:HD12	1.84	0.43
2:B:1057:LEU:HD22	2:B:1091:VAL:HG13	2.00	0.43
2:B:1232:GLU:CD	2:B:1274:ILE:HD11	2.43	0.43
2:B:1270:LYS:HA	2:B:1270:LYS:HD2	1.67	0.43
2:B:1350:LYS:O	2:B:1357:ARG:NH2	2.47	0.43
2:B:2779:PHE:O	2:B:2783:PHE:N	2.50	0.43
3:C:80:PHE:CE1	3:C:87:LYS:HB3	2.54	0.43
3:C:339:LEU:HA	3:C:339:LEU:HD23	1.86	0.43
3:C:475:LYS:O	4:d:1310:LYS:NZ	2.22	0.43
3:C:542:ILE:CG2	3:C:575:ASN:HB2	2.46	0.43
3:C:859:VAL:HA	3:C:975:GLN:NE2	2.29	0.43
3:C:3177:ASN:HA	3:C:3370:LEU:CB	2.49	0.43
4:d:1163:TYR:CE1	4:d:1195:TRP:CD1	3.07	0.43
4:d:1223:THR:H	4:d:1239:ASN:CG	2.24	0.43
5:e:914:ASP:HB3	5:e:917:LYS:HE2	2.01	0.43
6:F:14:LEU:O	6:F:17:LEU:HB2	2.18	0.43
8:H:64:ASN:OD1	8:H:64:ASN:N	2.51	0.43
9:I:60:CYS:HA	9:I:77:CYS:SG	2.59	0.43
11:K:30:PRO:HD3	14:N:33:LYS:HE2	2.00	0.43
16:P:58:VAL:CG2	16:P:65:LEU:HD11	2.48	0.43
1:A:48:ASP:HA	1:A:51:ILE:CG1	2.49	0.43
1:A:79:PRO:HD3	1:A:112:TYR:CZ	2.54	0.43
1:A:208:MET:CG	1:A:296:ILE:HG21	2.49	0.43
2:B:11:GLU:HB3	2:B:33:LEU:HD13	2.01	0.43
2:B:156:ASN:O	2:B:159:ALA:N	2.52	0.43
2:B:540:LEU:HB3	2:B:544:HIS:NE2	2.34	0.43
2:B:1308:LEU:HD23	2:B:1362:TYR:OH	2.19	0.43
2:B:1318:ILE:HG23	2:B:1345:LEU:CD1	2.49	0.43
3:C:252:LYS:HG2	3:C:256:TRP:CZ2	2.54	0.43
3:C:789:LYS:HB3	3:C:789:LYS:HE3	1.77	0.43
3:C:971:ASN:H	3:C:974:GLN:NE2	2.17	0.43
4:d:972:ASN:HD21	4:d:1027:ALA:CB	2.32	0.43
4:d:1227:CYS:SG	4:d:1234:GLN:HB2	2.58	0.43
5:e:1192:ILE:HA	5:e:1195:GLN:CD	2.43	0.43
6:F:67:LEU:HD13	6:F:67:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:63:THR:HA	7:G:66:ARG:NE	2.33	0.43
8:H:15:ASP:HB2	8:H:76:TYR:HB3	1.99	0.43
17:T:31:PRO:HA	17:T:197:PHE:HZ	1.83	0.43
1:A:89:ALA:N	1:A:96:LEU:O	2.46	0.43
2:B:110:VAL:HG12	3:C:122:GLU:CG	2.49	0.43
2:B:499:LEU:O	2:B:503:LEU:HG	2.18	0.43
2:B:802:ILE:HG12	2:B:877:THR:CG2	2.45	0.43
2:B:837:GLN:O	2:B:840:VAL:HG22	2.19	0.43
2:B:1136:ASP:HA	2:B:1218:GLU:HG2	1.39	0.43
2:B:1153:VAL:HG13	2:B:1157:ARG:NH1	2.34	0.43
2:B:1219:THR:HG23	2:B:1290:LEU:HD21	2.00	0.43
3:C:17:ILE:HD12	3:C:32:PHE:HZ	1.83	0.43
3:C:1183:LEU:O	3:C:1187:TRP:CD1	2.72	0.43
4:d:1045:ARG:HD2	5:e:141:VAL:N	2.34	0.43
5:e:912:VAL:C	5:e:922:ILE:HG21	2.44	0.43
6:F:38:LYS:HA	6:F:41:SER:O	2.18	0.43
10:J:28:GLN:HG3	10:J:49:PHE:CD2	2.54	0.43
11:K:33:ALA:CA	14:N:36:LYS:HD3	2.49	0.43
16:P:12:LYS:HD2	16:P:13:GLN:N	2.34	0.43
17:T:102:SER:HA	17:T:105:GLN:OE1	2.19	0.43
1:A:320:PRO:HG2	1:A:341:TRP:HB3	2.01	0.42
2:B:1115:ASP:HA	2:B:1118:GLU:HG2	2.02	0.42
2:B:2402:ILE:O	2:B:2405:ILE:N	2.52	0.42
3:C:86:GLU:OE2	3:C:87:LYS:HG2	2.19	0.42
3:C:282:ARG:NE	18:x:126:UNK:HA	2.33	0.42
3:C:531:PHE:HE2	3:C:538:ARG:HE	1.67	0.42
3:C:1226:PHE:HZ	3:C:1256:TYR:HB3	1.84	0.42
4:d:961:GLN:HA	4:d:964:LYS:HD3	2.01	0.42
4:d:1166:HIS:CD2	4:d:1193:ARG:HD3	2.53	0.42
5:e:1081:TYR:HB2	5:e:1100:ARG:NE	2.34	0.42
6:F:66:ASP:O	6:F:67:LEU:HD22	2.19	0.42
10:J:77:PHE:CZ	10:J:88:LEU:HD11	2.54	0.42
15:O:41:ASP:OD2	15:O:42:LYS:N	2.52	0.42
16:P:5:TYR:CD1	16:P:57:LYS:HE2	2.55	0.42
17:T:107:LYS:HD3	17:T:178:ARG:HA	2.01	0.42
1:A:268:ILE:O	1:A:291:SER:OG	2.34	0.42
2:B:248:LEU:HD23	2:B:280:LYS:HZ3	1.82	0.42
2:B:380:LEU:CD2	2:B:427:LEU:HA	2.48	0.42
2:B:459:ILE:HG12	2:B:502:ARG:HD2	2.01	0.42
3:C:862:LEU:CD1	3:C:972:TRP:HE1	2.22	0.42
4:d:1158:GLN:HG3	4:d:1159:TYR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1195:TRP:CE2	4:d:1197:SER:HA	2.54	0.42
5:e:832:ARG:NH2	5:e:866:GLN:HG3	2.34	0.42
6:F:36:HIS:O	6:F:39:SER:OG	2.36	0.42
7:G:76:TYR:O	7:G:88:GLY:HA2	2.20	0.42
8:H:68:PHE:HD2	9:I:64:LYS:HE3	1.84	0.42
9:I:89:VAL:HG23	9:I:108:PHE:HB2	2.01	0.42
11:K:32:CYS:O	14:N:32:SER:OG	2.36	0.42
14:N:67:LEU:O	14:N:71:ILE:HD12	2.18	0.42
1:A:48:ASP:OD1	1:A:51:ILE:HD11	2.19	0.42
1:A:225:GLN:OE1	1:A:253:LEU:HG	2.19	0.42
1:A:276:PHE:HB2	1:A:282:ARG:CB	2.49	0.42
1:A:343:ASN:ND2	2:B:931:ARG:HE	2.13	0.42
2:B:26:LYS:HB3	2:B:28:LYS:HG2	2.01	0.42
2:B:348:CYS:HA	2:B:351:ILE:HD12	2.01	0.42
2:B:1121:LYS:HD3	2:B:1203:ARG:HG2	2.01	0.42
3:C:609:TRP:CZ2	3:C:613:LEU:HD11	2.54	0.42
3:C:819:VAL:CG1	3:C:909:MET:HG2	2.47	0.42
3:C:916:LYS:HB2	3:C:1073:ALA:HB1	2.02	0.42
4:d:104:GLN:HB2	15:O:84:GLN:NE2	2.34	0.42
4:d:1268:ILE:HG23	4:d:1280:LEU:HD13	2.02	0.42
5:e:39:GLN:NE2	15:O:29:ASP:OD2	2.52	0.42
7:G:127:ARG:CG	7:G:129:GLN:HE22	2.29	0.42
9:I:95:LEU:HD12	9:I:107:ILE:HD11	2.01	0.42
11:K:33:ALA:CB	14:N:39:LYS:HD3	2.49	0.42
11:K:49:LYS:HA	11:K:49:LYS:HD3	1.91	0.42
12:L:35:ILE:HD13	12:L:96:PHE:CE2	2.54	0.42
17:T:186:LEU:HA	17:T:189:ARG:CG	2.49	0.42
1:A:3777:ASP:O	1:A:3781:TYR:N	2.46	0.42
2:B:337:PRO:N	2:B:338:PRO:HD2	2.34	0.42
2:B:349:ASN:O	2:B:352:ILE:HG22	2.20	0.42
2:B:452:LEU:HD21	5:e:1187:LYS:NZ	2.33	0.42
2:B:1034:ASN:HB2	2:B:1035:PRO:HD3	2.00	0.42
2:B:1083:MET:HE2	2:B:1083:MET:HB2	1.82	0.42
3:C:132:ASN:CB	3:C:169:SER:HB2	2.50	0.42
3:C:135:MET:HG3	3:C:165:PHE:CE2	2.54	0.42
3:C:315:LYS:HA	3:C:315:LYS:HD3	1.74	0.42
3:C:1185:ARG:HH12	3:C:1189:ILE:HD13	1.84	0.42
4:d:138:LYS:O	4:d:139:GLU:HG3	2.19	0.42
4:d:1203:ILE:HA	4:d:1308:ASN:ND2	2.34	0.42
6:F:85:TYR:CD2	6:F:100:ILE:HG23	2.55	0.42
7:G:132:LEU:H	7:G:132:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:30:MET:HE1	9:I:75:TRP:HH2	1.84	0.42
9:I:37:GLU:HB3	9:I:70:LYS:NZ	2.34	0.42
13:M:12:MET:SD	13:M:16:MET:HG3	2.59	0.42
16:P:25:LEU:HD22	16:P:103:MET:SD	2.59	0.42
1:A:2360:GLY:N	1:A:2490:PHE:O	2.50	0.42
2:B:123:SER:CB	3:C:96:LEU:HD21	2.49	0.42
2:B:853:GLN:HA	2:B:856:TRP:HB2	2.02	0.42
2:B:986:PHE:HD1	2:B:989:ARG:HH21	1.67	0.42
2:B:1536:GLU:O	2:B:1539:ARG:N	2.53	0.42
3:C:628:VAL:O	3:C:628:VAL:HG12	2.20	0.42
3:C:1160:TYR:CZ	3:C:1176:GLU:HG2	2.55	0.42
3:C:1183:LEU:O	3:C:1187:TRP:HD1	2.02	0.42
3:C:3726:VAL:O	3:C:3730:LEU:N	2.44	0.42
5:e:861:GLU:O	5:e:862:LYS:HG3	2.18	0.42
5:e:1092:SER:HB2	5:e:1170:LYS:NZ	2.34	0.42
5:e:1097:LEU:HG	5:e:1099:ARG:HH12	1.85	0.42
14:N:61:GLU:O	14:N:65:LEU:HD23	2.19	0.42
16:P:28:PHE:CG	16:P:74:VAL:HG11	2.54	0.42
18:V:221:UNK:O	18:V:222:UNK:C	2.68	0.42
1:A:208:MET:SD	1:A:266:TYR:OH	2.66	0.42
2:B:67:GLN:H	2:B:85:LYS:NZ	2.02	0.42
2:B:389:LYS:HA	2:B:392:ASP:OD2	2.19	0.42
2:B:504:ALA:HB1	2:B:539:GLU:HG3	2.02	0.42
2:B:813:ASP:OD1	2:B:1075:TRP:CD1	2.73	0.42
2:B:1179:THR:HA	2:B:1183:THR:HG22	2.00	0.42
2:B:1229:PHE:HA	2:B:1232:GLU:HG2	2.01	0.42
3:C:409:LEU:HD11	3:C:461:ILE:HA	2.00	0.42
3:C:568:ARG:HD2	3:C:568:ARG:O	2.19	0.42
3:C:3354:ILE:C	3:C:3358:ILE:CA	2.89	0.42
3:C:3503:TRP:O	3:C:3506:GLN:N	2.52	0.42
4:d:1194:ILE:HD12	4:d:1204:ILE:HB	2.01	0.42
4:d:1233:VAL:O	4:d:1248:GLU:HA	2.19	0.42
5:e:853:ILE:HD13	5:e:856:PHE:HB2	2.01	0.42
5:e:1004:LEU:HG	5:e:1012:ILE:CG2	2.49	0.42
5:e:1100:ARG:O	5:e:1126:PRO:HB3	2.19	0.42
12:L:27:ALA:HB3	12:L:30:LEU:HD13	2.00	0.42
14:N:29:PHE:CE1	14:N:34:ILE:HG12	2.54	0.42
15:O:25:PHE:CD2	15:O:50:ILE:HD11	2.54	0.42
1:A:52:ALA:HB3	1:A:53:PRO:HD3	2.02	0.42
1:A:145:PRO:HD2	1:A:171:ARG:HH12	1.85	0.42
2:B:64:VAL:HG22	2:B:83:LYS:NZ	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:LEU:HG	2:B:175:PRO:HA	2.02	0.42
2:B:394:TYR:CE2	2:B:412:LEU:HD13	2.55	0.42
3:C:132:ASN:HB3	3:C:169:SER:HB2	2.02	0.42
3:C:278:HIS:HB2	3:C:282:ARG:CD	2.49	0.42
3:C:315:LYS:HA	3:C:318:THR:HG23	2.02	0.42
3:C:812:THR:O	3:C:816:VAL:HG23	2.20	0.42
4:d:126:GLN:OE1	4:d:130:ARG:HD2	2.20	0.42
4:d:1203:ILE:HG23	4:d:1308:ASN:ND2	2.31	0.42
5:e:52:ASN:CA	12:L:22:ARG:HD3	2.47	0.42
5:e:1064:TRP:CH2	5:e:1071:PRO:HD3	2.55	0.42
5:e:1184:ARG:O	5:e:1187:LYS:HB2	2.19	0.42
10:J:47:LYS:NZ	10:J:58:TRP:O	2.53	0.42
1:A:35:MET:HB3	1:A:58:PHE:HB2	2.01	0.42
1:A:2203:ALA:HB2	1:A:3956:ALA:HA	2.02	0.42
2:B:968:CYS:HA	2:B:971:MET:HE2	2.01	0.42
2:B:1126:LYS:HD2	2:B:1126:LYS:C	2.45	0.42
2:B:1137:LYS:HD3	2:B:1144:MET:HG2	2.00	0.42
2:B:1494:VAL:O	2:B:1498:TYR:N	2.53	0.42
3:C:327:LEU:HA	3:C:376:ASN:OD1	2.20	0.42
3:C:677:ARG:HA	3:C:723:PHE:HE1	1.83	0.42
3:C:745:LYS:HA	3:C:745:LYS:HD3	1.72	0.42
3:C:1105:ARG:HH22	3:C:1176:GLU:HB2	1.84	0.42
3:C:3540:TRP:O	3:C:3544:LYS:N	2.50	0.42
4:d:1267:PRO:O	4:d:1282:LYS:HA	2.19	0.42
6:F:23:TYR:HD1	6:F:36:HIS:CG	2.38	0.42
9:I:41:VAL:O	9:I:62:TYR:HE2	2.02	0.42
9:I:43:GLN:HA	9:I:46:ILE:HD12	2.00	0.42
1:A:63:THR:O	1:A:66:ASN:HB2	2.20	0.42
1:A:288:VAL:CG1	1:A:290:ASP:H	2.31	0.42
1:A:3996:ASP:HA	1:A:4168:ASP:C	2.44	0.42
2:B:376:ALA:O	2:B:380:LEU:CB	2.68	0.42
2:B:418:SER:HA	2:B:421:GLU:OE1	2.20	0.42
2:B:1242:GLN:CD	2:B:1242:GLN:C	2.88	0.42
3:C:23:LEU:HD23	3:C:24:LYS:O	2.18	0.42
3:C:679:ASP:OD1	3:C:679:ASP:N	2.51	0.42
3:C:910:LYS:HE3	3:C:998:VAL:HB	2.01	0.42
3:C:1116:LYS:HA	3:C:1116:LYS:HD2	1.64	0.42
4:d:1208:LEU:HD22	4:d:1236:TYR:OH	2.20	0.42
4:d:1232:LYS:HA	4:d:1249:GLN:O	2.20	0.42
5:e:839:TRP:CG	5:e:1133:ASN:HD21	2.38	0.42
5:e:1073:ILE:HD11	5:e:1184:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:ILE:HD13	7:G:99:ILE:HA	1.87	0.42
10:J:13:PRO:HD2	10:J:79:PHE:O	2.20	0.42
10:J:92:LYS:HD2	10:J:92:LYS:HA	1.88	0.42
13:M:24:ALA:HA	13:M:41:ILE:HD11	2.02	0.42
1:A:46:TYR:OH	1:A:104:SER:HB3	2.19	0.42
2:B:36:GLN:HB3	2:B:39:ASP:HB2	2.02	0.42
2:B:352:ILE:HA	2:B:352:ILE:HD12	1.78	0.42
2:B:796:ASN:HA	2:B:799:VAL:HG22	2.01	0.42
2:B:1208:LYS:O	2:B:1212:ILE:HG13	2.19	0.42
3:C:37:ASN:CG	3:C:71:THR:HB	2.45	0.42
3:C:431:ALA:O	3:C:434:PRO:HD2	2.19	0.42
3:C:928:LYS:N	3:C:929:PRO:HD2	2.35	0.42
5:e:32:ASN:HA	15:O:28:LYS:HD3	2.02	0.42
5:e:1145:LEU:HD13	5:e:1157:ILE:HD11	2.00	0.42
8:H:39:LYS:HB2	8:H:39:LYS:HE2	1.88	0.42
1:A:952:LYS:O	1:A:956:GLU:N	2.35	0.41
2:B:651:SER:OG	2:B:673:PHE:HB3	2.20	0.41
2:B:1045:PRO:HG2	2:B:1050:PHE:CE1	2.55	0.41
2:B:1308:LEU:HD21	2:B:1359:PHE:CE2	2.55	0.41
3:C:572:ILE:HG23	3:C:576:TYR:HE2	1.85	0.41
3:C:763:LEU:HD22	3:C:767:MET:HE3	2.01	0.41
3:C:804:ASN:OD1	3:C:808:ASN:ND2	2.52	0.41
3:C:871:LEU:HB2	3:C:873:PRO:O	2.19	0.41
3:C:3342:TYR:C	3:C:3346:SER:N	2.74	0.41
4:d:1186:ALA:HA	4:d:1191:THR:O	2.20	0.41
5:e:823:PHE:CD1	5:e:875:PRO:HA	2.55	0.41
5:e:853:ILE:HD12	5:e:863:MET:O	2.19	0.41
5:e:865:THR:HB	5:e:884:SER:OG	2.20	0.41
5:e:1028:ARG:HH11	5:e:1069:LYS:HD2	1.84	0.41
7:G:140:ASP:HB3	7:G:143:PHE:C	2.45	0.41
11:K:87:GLN:O	11:K:88:ALA:HB2	2.20	0.41
1:A:277:GLU:H	1:A:277:GLU:CD	2.28	0.41
1:A:1226:LEU:O	1:A:1230:ALA:HB2	2.20	0.41
2:B:835:GLN:OE1	2:B:838:LYS:HB3	2.20	0.41
2:B:875:ILE:HD12	2:B:962:PHE:HZ	1.84	0.41
2:B:880:LEU:HA	2:B:883:ASN:HB2	2.02	0.41
2:B:3652:GLY:O	2:B:3655:GLU:N	2.53	0.41
3:C:89:GLN:OE1	3:C:126:ASN:ND2	2.52	0.41
3:C:805:ARG:HH21	5:e:822:LEU:HB3	1.82	0.41
3:C:809:ASN:HD21	5:e:876:ASN:ND2	2.13	0.41
3:C:1035:ILE:H	3:C:1035:ILE:HG13	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:92:TYR:CD2	13:M:29:LYS:HE2	2.55	0.41
4:d:117:TRP:CH2	5:e:39:GLN:HA	2.55	0.41
4:d:252:VAL:C	7:G:127:ARG:HH12	2.27	0.41
4:d:1023:HIS:HE1	4:d:1025:LYS:HB3	1.85	0.41
8:H:73:ARG:O	8:H:75:TYR:HD1	2.03	0.41
10:J:69:TYR:HB3	11:K:62:GLU:CD	2.45	0.41
11:K:56:GLU:HB2	11:K:59:LYS:HD3	2.02	0.41
1:A:60:LEU:HD11	1:A:67:CYS:CB	2.39	0.41
1:A:3629:LEU:O	1:A:3631:GLN:N	2.53	0.41
2:B:324:ILE:HG23	2:B:397:TYR:CE1	2.55	0.41
2:B:422:ARG:CD	2:B:478:MET:HA	2.50	0.41
2:B:452:LEU:CD1	5:e:1187:LYS:HG3	2.49	0.41
2:B:618:GLU:O	2:B:622:VAL:HG23	2.20	0.41
2:B:1314:ALA:HA	16:P:76:SER:HA	2.00	0.41
2:B:2563:LYS:N	2:B:2601:ILE:O	2.52	0.41
3:C:31:SER:OG	3:C:69:LYS:O	2.34	0.41
3:C:451:ASP:O	3:C:455:ARG:HG2	2.20	0.41
3:C:621:ILE:HG22	3:C:641:TYR:HD2	1.85	0.41
3:C:744:ILE:HD11	3:C:795:ILE:HD11	2.02	0.41
3:C:854:GLU:OE2	5:e:875:PRO:HG2	2.19	0.41
5:e:1091:ARG:NH2	5:e:1171:GLU:HG3	2.35	0.41
8:H:11:ILE:HA	8:H:79:LEU:HB2	2.02	0.41
12:L:16:LEU:HD13	12:L:19:HIS:CE1	2.56	0.41
13:M:15:ASP:OD1	13:M:16:MET:N	2.52	0.41
14:N:100:LYS:HD3	15:O:89:GLN:NE2	2.35	0.41
17:T:56:MET:HE2	17:T:56:MET:HB2	1.94	0.41
17:T:115:LYS:HE3	17:T:115:LYS:HB3	1.90	0.41
2:B:160:GLN:NE2	2:B:243:LEU:HD13	2.35	0.41
2:B:1065:SER:HA	2:B:1084:LYS:HE3	2.02	0.41
2:B:1340:ASP:OD1	2:B:1343:LYS:HB3	2.19	0.41
2:B:3466:ALA:O	2:B:3469:ARG:N	2.53	0.41
3:C:1213:LYS:O	3:C:1217:LYS:HG2	2.20	0.41
3:C:3784:GLU:O	3:C:3787:ASP:N	2.53	0.41
4:d:1069:VAL:HA	4:d:1082:TYR:O	2.20	0.41
4:d:1096:MET:SD	4:d:1097:LYS:N	2.93	0.41
4:d:1219:PRO:O	4:d:1264:TYR:HD1	2.03	0.41
9:I:41:VAL:HG12	9:I:63:ILE:HD12	2.02	0.41
14:N:100:LYS:HD3	15:O:89:GLN:HE22	1.85	0.41
15:O:85:ILE:HG13	15:O:98:ILE:CG2	2.50	0.41
1:A:154:PHE:CZ	1:A:234:ILE:HD11	2.56	0.41
1:A:288:VAL:N	1:A:318:PRO:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:LYS:HB3	2:B:45:ASN:O	2.21	0.41
2:B:173:MET:HG2	2:B:173:MET:O	2.21	0.41
2:B:217:GLN:O	2:B:220:LYS:HG2	2.20	0.41
2:B:687:PHE:HD1	2:B:692:LEU:HB2	1.85	0.41
2:B:832:ASN:O	2:B:836:ILE:HG12	2.21	0.41
2:B:955:PHE:C	2:B:956:LEU:HG	2.42	0.41
2:B:1360:LYS:HD2	2:B:1363:ASN:CB	2.46	0.41
3:C:106:LYS:HA	3:C:106:LYS:HD3	1.86	0.41
3:C:694:GLN:O	3:C:698:GLU:HG3	2.20	0.41
3:C:798:VAL:HG13	3:C:802:ILE:HD12	2.03	0.41
3:C:864:GLN:CD	5:e:824:LYS:HE3	2.45	0.41
3:C:3740:ILE:O	3:C:3744:ARG:N	2.46	0.41
4:d:1210:MET:HG2	4:d:1229:THR:OG1	2.20	0.41
5:e:1072:ILE:HG22	5:e:1073:ILE:HG12	2.02	0.41
8:H:63:ARG:HA	8:H:63:ARG:NE	2.35	0.41
11:K:34:ASP:OD1	11:K:37:LEU:HB3	2.20	0.41
12:L:41:LEU:HD11	12:L:56:ASN:CB	2.51	0.41
1:A:93:ASP:OD1	1:A:94:LYS:HG3	2.21	0.41
2:B:558:VAL:HG13	2:B:595:LEU:HD22	2.03	0.41
2:B:585:ILE:HG21	2:B:644:TRP:HB2	2.02	0.41
2:B:800:LYS:O	2:B:803:GLU:HG3	2.21	0.41
2:B:868:ILE:HG21	2:B:957:GLN:HB3	2.03	0.41
2:B:931:ARG:O	2:B:931:ARG:NH1	2.52	0.41
2:B:1126:LYS:HE3	2:B:1126:LYS:HB3	1.92	0.41
3:C:9:ARG:HE	3:C:45:LEU:HD13	1.86	0.41
3:C:80:PHE:CD1	3:C:80:PHE:N	2.87	0.41
3:C:801:ILE:HA	5:e:822:LEU:CD1	2.49	0.41
3:C:881:GLU:O	3:C:884:LYS:HG2	2.20	0.41
3:C:3354:ILE:O	3:C:3355:GLN:C	2.63	0.41
4:d:1090:VAL:HG21	4:d:1153:ARG:HH22	1.85	0.41
4:d:1095:LEU:HB3	4:d:1114:ASN:OD1	2.21	0.41
5:e:1099:ARG:HH11	5:e:1099:ARG:HD3	1.73	0.41
8:H:73:ARG:NH1	8:H:73:ARG:HG2	2.36	0.41
14:N:69:GLU:O	14:N:72:LYS:HB2	2.20	0.41
1:A:102:TYR:HD2	1:A:107:ARG:HB2	1.86	0.41
2:B:12:ASP:HA	2:B:15:ILE:HD12	2.03	0.41
2:B:63:TRP:HE3	2:B:89:ILE:O	2.04	0.41
2:B:136:PRO:O	2:B:140:GLN:HB2	2.21	0.41
2:B:266:THR:O	2:B:270:PRO:HD2	2.19	0.41
2:B:721:ASN:HB3	2:B:777:PHE:CE2	2.56	0.41
2:B:1329:PRO:HD2	2:B:1332:GLN:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:SER:HA	3:C:162:VAL:HG11	2.03	0.41
3:C:183:MET:HG3	3:C:216:TRP:CG	2.56	0.41
3:C:214:ASN:O	3:C:218:ASN:ND2	2.53	0.41
3:C:354:ARG:HD2	3:C:355:PHE:N	2.36	0.41
3:C:548:LEU:HD12	3:C:548:LEU:HA	1.82	0.41
3:C:984:THR:HA	3:C:987:ASP:OD2	2.21	0.41
3:C:1262:MET:HE3	3:C:1265:ILE:HG13	2.02	0.41
1:A:53:PRO:HD2	1:A:82:ARG:HB2	2.01	0.41
1:A:154:PHE:O	1:A:156:GLY:N	2.53	0.41
1:A:170:GLN:OE1	2:B:861:ASP:HB3	2.20	0.41
1:A:213:GLN:HB2	1:A:232:TYR:C	2.46	0.41
1:A:283:THR:CB	2:B:939:ASN:HB3	2.51	0.41
1:A:283:THR:CG2	2:B:939:ASN:HB3	2.47	0.41
2:B:539:GLU:OE1	2:B:542:LYS:HD3	2.20	0.41
2:B:1363:ASN:HA	2:B:1366:VAL:HB	2.03	0.41
3:C:335:ILE:O	3:C:338:THR:HB	2.21	0.41
3:C:405:LEU:HD23	3:C:468:GLN:NE2	2.34	0.41
3:C:544:TYR:CE2	4:d:1207:ASP:HB3	2.56	0.41
3:C:695:LEU:HA	3:C:698:GLU:CD	2.45	0.41
4:d:78:LYS:O	4:d:80:PRO:HD3	2.21	0.41
4:d:1093:TRP:HB3	4:d:1119:THR:HA	2.03	0.41
4:d:1132:ASN:HA	4:d:1183:PHE:HZ	1.86	0.41
5:e:1049:ASN:N	5:e:1050:PRO:HD2	2.36	0.41
7:G:73:VAL:HA	7:G:149:GLN:HA	2.02	0.41
8:H:73:ARG:HA	8:H:73:ARG:NE	2.36	0.41
13:M:16:MET:SD	13:M:19:ARG:NH2	2.94	0.41
1:A:21:ARG:HA	1:A:39:LEU:O	2.21	0.41
1:A:341:TRP:HH2	2:B:967:GLN:NE2	2.17	0.41
1:A:941:GLU:O	1:A:945:ASP:CB	2.69	0.41
2:B:122:ASN:HB2	2:B:159:ALA:CB	2.51	0.41
2:B:152:GLU:O	2:B:180:LYS:HD2	2.21	0.41
2:B:317:PHE:CE1	2:B:351:ILE:HG12	2.56	0.41
2:B:435:GLN:HA	2:B:438:LYS:CE	2.50	0.41
2:B:444:LEU:HD11	2:B:456:ILE:HD11	2.03	0.41
2:B:715:LEU:HB2	2:B:766:ILE:HD11	2.02	0.41
2:B:765:PHE:CE2	2:B:766:ILE:HG13	2.56	0.41
2:B:931:ARG:HH11	2:B:934:ILE:HB	1.86	0.41
2:B:1044:ILE:O	2:B:1044:ILE:HG22	2.21	0.41
2:B:1172:LYS:C	2:B:1177:PRO:HD3	2.46	0.41
2:B:1317:LEU:CD2	16:P:32:TRP:HZ3	2.31	0.41
2:B:2385:HIS:O	2:B:2388:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:ILE:H	3:C:151:ILE:HD12	1.85	0.41
3:C:221:SER:HG	3:C:287:GLU:CD	2.28	0.41
3:C:324:ILE:O	3:C:328:TYR:HD2	2.03	0.41
3:C:467:ILE:HG12	3:C:488:PHE:HZ	1.86	0.41
3:C:475:LYS:O	3:C:481:MET:HE1	2.21	0.41
3:C:491:ILE:O	3:C:495:PHE:HB2	2.20	0.41
3:C:857:ARG:HE	5:e:875:PRO:CB	2.30	0.41
3:C:875:VAL:HG12	3:C:877:PRO:HD2	2.03	0.41
3:C:1035:ILE:HD13	3:C:1095:GLN:HG2	2.03	0.41
3:C:1062:ILE:O	3:C:1065:ILE:HG23	2.21	0.41
3:C:1084:SER:O	3:C:1088:TRP:CD1	2.74	0.41
4:d:987:ASP:OD2	4:d:990:LYS:HE2	2.20	0.41
4:d:1288:CYS:HB3	4:d:1293:GLU:OE1	2.21	0.41
8:H:27:VAL:HG21	8:H:52:ARG:HH12	1.85	0.41
8:H:52:ARG:HG3	8:H:53:TYR:CD2	2.56	0.41
8:H:89:PHE:HD2	8:H:91:THR:HG23	1.86	0.41
10:J:41:LYS:HD2	10:J:41:LYS:HA	1.91	0.41
10:J:77:PHE:CE1	10:J:88:LEU:HD11	2.56	0.41
11:K:34:ASP:OD1	11:K:38:GLU:HG2	2.20	0.41
12:L:41:LEU:O	12:L:44:GLU:HG3	2.20	0.41
12:L:52:ASP:O	12:L:56:ASN:ND2	2.54	0.41
12:L:64:GLN:HB3	12:L:66:GLU:HG2	2.02	0.41
13:M:28:VAL:HG21	13:M:77:ILE:CD1	2.51	0.41
14:N:33:LYS:HZ2	14:N:36:LYS:NZ	2.19	0.41
16:P:43:PHE:CZ	16:P:55:ILE:HG23	2.55	0.41
16:P:90:LYS:HZ1	16:P:103:MET:HA	1.86	0.41
17:T:49:LYS:NZ	17:T:184:THR:HG23	2.36	0.41
18:x:125:UNK:O	18:x:128:UNK:N	2.53	0.41
1:A:220:TRP:CG	1:A:221:SER:N	2.89	0.41
1:A:2495:ASP:O	1:A:2497:ARG:N	2.54	0.41
2:B:89:ILE:HD12	2:B:112:GLU:HG2	2.02	0.41
2:B:169:LYS:HZ1	3:C:150:LYS:HD2	1.85	0.41
2:B:929:THR:HG22	2:B:930:ILE:N	2.34	0.41
2:B:1197:PHE:CD1	2:B:1197:PHE:C	2.99	0.41
2:B:1214:LEU:HG	2:B:1215:GLN:N	2.36	0.41
2:B:1215:GLN:HB3	2:B:1218:GLU:CB	2.48	0.41
2:B:1243:LYS:HA	2:B:1248:TYR:HE1	1.86	0.41
3:C:56:TYR:HD1	3:C:80:PHE:CZ	2.39	0.41
3:C:989:ILE:HG23	3:C:994:GLU:OE2	2.20	0.41
3:C:1008:GLY:O	3:C:1012:LYS:HG3	2.21	0.41
3:C:1014:ASN:HA	3:C:1017:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1099:ASP:HA	3:C:1102:LYS:HG2	2.02	0.41
3:C:1144:LYS:CE	4:d:171:ARG:HA	2.50	0.41
4:d:1306:PHE:O	4:d:1310:LYS:HG3	2.21	0.41
5:e:1084:ASP:O	5:e:1097:LEU:HD12	2.21	0.41
6:F:74:ILE:HG22	6:F:91:GLN:HG2	2.03	0.41
6:F:77:ILE:HG22	6:F:79:LEU:CD2	2.51	0.41
7:G:77:LEU:HD12	7:G:90:PHE:CE2	2.56	0.41
7:G:108:LYS:O	7:G:112:SER:OG	2.33	0.41
10:J:19:LYS:HB3	10:J:23:ASN:CG	2.46	0.41
13:M:77:ILE:HG13	13:M:80:LEU:HB2	2.02	0.41
17:T:187:GLU:HB2	17:T:188:PRO:CD	2.51	0.41
1:A:45:ASN:OD1	1:A:48:ASP:N	2.49	0.40
2:B:848:LYS:HD3	2:B:848:LYS:HA	1.83	0.40
2:B:1054:ILE:HD13	2:B:1054:ILE:HA	1.84	0.40
2:B:1108:THR:O	2:B:1111:LYS:HG2	2.21	0.40
2:B:1138:LYS:HE3	2:B:1145:LYS:CD	2.51	0.40
2:B:1353:PRO:HG2	2:B:1356:ILE:HG12	2.03	0.40
3:C:186:GLY:HA2	3:C:212:LYS:NZ	2.36	0.40
3:C:327:LEU:HD21	3:C:372:GLN:HG3	2.03	0.40
3:C:917:LYS:HA	3:C:917:LYS:HD2	1.89	0.40
3:C:1037:LYS:HE3	3:C:1037:LYS:HB3	1.77	0.40
4:d:183:ARG:NH2	10:J:72:TYR:OH	2.33	0.40
4:d:1018:MET:N	4:d:1018:MET:SD	2.94	0.40
4:d:1093:TRP:HH2	4:d:1114:ASN:HB3	1.86	0.40
4:d:1206:PHE:CD1	4:d:1243:LEU:HB3	2.56	0.40
4:d:1266:ASP:OD2	4:d:1268:ILE:HG12	2.20	0.40
5:e:938:PHE:CE1	5:e:951:THR:HB	2.57	0.40
7:G:79:VAL:HG12	7:G:85:VAL:HA	2.04	0.40
15:O:37:THR:O	15:O:39:ASN:ND2	2.54	0.40
16:P:60:ILE:HB	16:P:77:LEU:HD13	2.03	0.40
1:A:195:ASN:N	1:A:196:PRO:CD	2.85	0.40
1:A:252:ASN:HA	1:A:272:SER:O	2.22	0.40
1:A:253:LEU:O	1:A:272:SER:N	2.54	0.40
1:A:3742:GLY:O	1:A:3746:TRP:N	2.51	0.40
2:B:277:GLU:HG2	2:B:285:ALA:HB3	2.04	0.40
2:B:347:ILE:O	2:B:351:ILE:HG13	2.21	0.40
2:B:449:GLY:CA	5:e:1183:TYR:HB3	2.44	0.40
2:B:586:ALA:HB1	2:B:686:TYR:CE2	2.56	0.40
2:B:1057:LEU:HA	2:B:1060:ILE:HD12	2.02	0.40
3:C:81:THR:HG22	3:C:126:ASN:N	2.35	0.40
3:C:343:MET:O	3:C:346:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:521:ILE:HD12	3:C:521:ILE:HA	1.95	0.40
3:C:569:TYR:HA	3:C:572:ILE:HD12	2.03	0.40
3:C:601:PRO:CG	3:C:697:ARG:HB3	2.52	0.40
3:C:753:LEU:HB2	3:C:754:PRO:HD3	2.03	0.40
4:d:126:GLN:O	4:d:129:ILE:HG22	2.21	0.40
4:d:1131:PHE:CD1	4:d:1139:PHE:HB3	2.56	0.40
5:e:26:ARG:HE	15:O:12:GLU:CG	2.21	0.40
5:e:883:MET:HE2	5:e:919:GLU:HG2	2.03	0.40
5:e:1145:LEU:HA	5:e:1158:LEU:O	2.20	0.40
5:e:1167:MET:SD	5:e:1167:MET:N	2.91	0.40
12:L:23:PHE:HE2	12:L:93:LEU:HD23	1.86	0.40
14:N:33:LYS:HA	14:N:36:LYS:HG3	2.03	0.40
17:T:47:THR:O	17:T:50:SER:OG	2.37	0.40
1:A:7:TRP:HD1	1:A:315:VAL:HG22	1.85	0.40
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.88	0.40
1:A:287:PHE:CG	1:A:320:PRO:HD3	2.55	0.40
2:B:90:ALA:HB3	2:B:111:VAL:CG2	2.51	0.40
2:B:376:ALA:O	2:B:380:LEU:HB2	2.21	0.40
2:B:653:GLN:HG2	2:B:671:VAL:HG22	2.04	0.40
2:B:788:GLN:HA	2:B:791:HIS:NE2	2.36	0.40
2:B:956:LEU:HD23	2:B:959:ILE:HD12	2.02	0.40
2:B:1144:MET:HE3	2:B:1144:MET:HB3	1.93	0.40
2:B:1264:ILE:HD13	2:B:1264:ILE:HG21	1.87	0.40
3:C:139:TYR:O	3:C:142:GLN:HG2	2.20	0.40
3:C:398:TRP:HB2	3:C:496:LYS:HB2	2.03	0.40
3:C:402:PRO:CA	3:C:468:GLN:HE22	2.35	0.40
3:C:425:ASP:O	3:C:429:LYS:HG2	2.21	0.40
3:C:818:LEU:H	3:C:909:MET:CE	2.34	0.40
3:C:867:MET:HE1	5:e:1152:ASP:O	2.20	0.40
3:C:948:LEU:HD21	3:C:1006:ILE:HG23	2.03	0.40
3:C:995:ILE:O	3:C:999:ILE:HG13	2.22	0.40
3:C:1104:ALA:N	3:C:1159:MET:HE1	2.36	0.40
4:d:1223:THR:HG23	4:d:1239:ASN:HD21	1.86	0.40
5:e:1029:TYR:CB	5:e:1032:ASP:HB2	2.52	0.40
5:e:1097:LEU:O	5:e:1104:MET:HA	2.22	0.40
7:G:108:LYS:HA	7:G:111:ARG:NE	2.36	0.40
8:H:56:THR:N	8:H:92:GLY:O	2.49	0.40
10:J:17:GLU:HB3	10:J:18:MET:SD	2.61	0.40
2:B:314:TYR:CE1	2:B:389:LYS:HB3	2.57	0.40
2:B:444:LEU:HB2	2:B:452:LEU:HD22	2.02	0.40
2:B:444:LEU:CD2	2:B:456:ILE:HG12	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:ILE:HB	2:B:484:LYS:CB	2.52	0.40
2:B:599:ILE:O	2:B:602:PRO:HD2	2.22	0.40
2:B:836:ILE:O	2:B:840:VAL:HG13	2.22	0.40
2:B:851:LYS:CD	2:B:854:ASN:HB3	2.52	0.40
2:B:898:PRO:CG	2:B:1074:SER:HB3	2.43	0.40
2:B:1261:TYR:CE1	2:B:1265:MET:HE3	2.56	0.40
2:B:1305:LEU:HA	2:B:1305:LEU:HD23	1.92	0.40
3:C:221:SER:OG	3:C:287:GLU:OE1	2.38	0.40
3:C:715:ILE:HG12	18:V:221:UNK:C	2.52	0.40
3:C:974:GLN:O	3:C:975:GLN:C	2.64	0.40
3:C:1036:LYS:O	3:C:1040:LYS:HG3	2.22	0.40
3:C:1150:ASP:HA	3:C:1153:PHE:HB3	2.04	0.40
3:C:3311:ASN:O	3:C:3312:GLN:C	2.64	0.40
4:d:130:ARG:O	4:d:134:LYS:HG2	2.21	0.40
4:d:1034:LEU:O	4:d:1066:VAL:HG22	2.22	0.40
4:d:1071:TRP:CE3	4:d:1079:TYR:HB2	2.51	0.40
4:d:1196:ASP:HB2	4:d:1203:ILE:HD11	2.04	0.40
4:d:1218:ALA:HB1	4:d:1220:TYR:CD1	2.56	0.40
4:d:1242:LYS:HG2	4:d:1243:LEU:H	1.85	0.40
5:e:847:VAL:HG21	5:e:1131:LYS:NZ	2.36	0.40
5:e:863:MET:O	5:e:865:THR:N	2.55	0.40
5:e:869:VAL:HB	5:e:880:ILE:CG1	2.51	0.40
5:e:913:TRP:HZ3	5:e:919:GLU:HA	1.86	0.40
5:e:1077:TYR:HH	5:e:1103:TRP:HZ3	1.65	0.40
5:e:1177:GLU:HA	5:e:1180:GLU:HG3	2.03	0.40
9:I:29:ASP:O	9:I:92:ASN:HA	2.20	0.40
12:L:22:ARG:HD2	12:L:95:PHE:HE2	1.84	0.40
12:L:37:GLN:HG3	12:L:60:PHE:CE2	2.56	0.40
15:O:51:ILE:HD11	15:O:71:ALA:HB2	2.03	0.40
15:O:101:TYR:CZ	15:O:103:ILE:HD11	2.57	0.40
16:P:69:VAL:HG12	16:P:74:VAL:O	2.21	0.40
17:T:175:MET:SD	17:T:176:TYR:N	2.94	0.40
2:B:11:GLU:HB3	2:B:33:LEU:CD1	2.51	0.40
2:B:429:LEU:HD13	2:B:470:PHE:CD2	2.57	0.40
2:B:522:LYS:HD2	5:e:1074:ARG:HG3	2.04	0.40
2:B:875:ILE:HD12	2:B:962:PHE:CZ	2.57	0.40
3:C:36:LYS:HA	3:C:39:ASN:HD22	1.87	0.40
3:C:215:GLU:HA	3:C:218:ASN:HD22	1.87	0.40
3:C:663:ILE:O	3:C:667:LYS:HG3	2.21	0.40
3:C:715:ILE:HD12	3:C:715:ILE:HA	1.75	0.40
4:d:75:LEU:HD23	4:d:77:PRO:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:129:ILE:HA	4:d:132:THR:HG22	2.03	0.40
4:d:187:THR:HG23	10:J:79:PHE:HZ	1.85	0.40
4:d:976:PRO:HB2	4:d:1265:LYS:HE3	2.04	0.40
4:d:995:LEU:HD21	4:d:997:CYS:SG	2.62	0.40
5:e:35:VAL:HB	15:O:29:ASP:OD2	2.21	0.40
5:e:824:LYS:CD	5:e:1154:THR:HB	2.32	0.40
5:e:1072:ILE:HG21	5:e:1181:ARG:HG2	2.03	0.40
7:G:105:LEU:HA	7:G:108:LYS:HE2	2.04	0.40
8:H:48:ASP:O	8:H:52:ARG:HG2	2.21	0.40
13:M:77:ILE:HG13	13:M:77:ILE:O	2.22	0.40
15:O:17:ILE:O	15:O:20:SER:OG	2.35	0.40
16:P:30:ALA:HB2	16:P:77:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3371/4168 (81%)	2907 (86%)	454 (14%)	10 (0%)	36	72
2	B	4229/4595 (92%)	3790 (90%)	429 (10%)	10 (0%)	43	78
3	C	4232/4620 (92%)	3885 (92%)	337 (8%)	10 (0%)	43	78
4	d	445/667 (67%)	400 (90%)	45 (10%)	0	100	100
5	e	529/670 (79%)	459 (87%)	69 (13%)	1 (0%)	43	78
6	F	96/133 (72%)	82 (85%)	14 (15%)	0	100	100
7	G	93/159 (58%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	81 (98%)	2 (2%)	0	100	100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100	100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	93/111 (84%)	81 (87%)	12 (13%)	0	100	100
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
14	N	107/132 (81%)	99 (92%)	8 (8%)	0	100	100
15	O	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
16	P	101/110 (92%)	94 (93%)	7 (7%)	0	100	100
17	T	127/309 (41%)	109 (86%)	16 (13%)	2 (2%)	7	38
All	All	13963/16284 (86%)	12499 (90%)	1431 (10%)	33 (0%)	44	78

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO
2	B	4008	PRO
2	B	4432	PRO
3	C	2978	PRO
3	C	2979	PRO
3	C	3203	PRO
3	C	3379	GLN
3	C	4182	PRO
3	C	4188	PRO
3	C	4546	PRO
5	e	142	VAL
1	A	1351	ASP
1	A	4084	ILE
2	B	4556	THR
3	C	3204	ALA
2	B	3923	PRO
3	C	3378	ALA
17	T	188	PRO
1	A	982	ILE
1	A	3108	ASN
17	T	129	ASP
2	B	4557	TYR
1	A	1040	VAL

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Mol	Chain	Res	Type
1	A	3665	PRO
2	B	3922	MET
3	C	4121	VAL
1	A	1824	GLY
1	A	3593	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/3691 (8%)	291 (100%)	0	100	100
2	B	1215/4145 (29%)	1214 (100%)	1 (0%)	88	89
3	C	1094/4196 (26%)	1094 (100%)	0	100	100
4	d	386/609 (63%)	386 (100%)	0	100	100
5	e	364/597 (61%)	363 (100%)	1 (0%)	86	86
6	F	87/109 (80%)	87 (100%)	0	100	100
7	G	86/149 (58%)	86 (100%)	0	100	100
8	H	76/83 (92%)	76 (100%)	0	100	100
9	I	76/95 (80%)	76 (100%)	0	100	100
10	J	74/82 (90%)	74 (100%)	0	100	100
11	K	81/97 (84%)	81 (100%)	0	100	100
12	L	86/99 (87%)	86 (100%)	0	100	100
13	M	77/78 (99%)	77 (100%)	0	100	100
14	N	96/119 (81%)	96 (100%)	0	100	100
15	O	98/104 (94%)	97 (99%)	1 (1%)	68	78
16	P	97/104 (93%)	97 (100%)	0	100	100
17	T	118/271 (44%)	118 (100%)	0	100	100
All	All	4402/14628 (30%)	4399 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1315	ILE
5	e	1123	SER
15	O	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	44	ASN
1	A	55	ASN
1	A	56	GLN
1	A	184	ASN
1	A	284	ASN
1	A	343	ASN
2	B	36	GLN
2	B	45	ASN
2	B	54	GLN
2	B	60	ASN
2	B	77	GLN
2	B	134	GLN
2	B	138	ASN
2	B	156	ASN
2	B	160	GLN
2	B	167	GLN
2	B	179	HIS
2	B	209	ASN
2	B	223	ASN
2	B	236	ASN
2	B	322	HIS
2	B	404	ASN
2	B	437	ASN
2	B	553	GLN
2	B	666	ASN
2	B	724	HIS
2	B	788	GLN
2	B	864	ASN
2	B	894	ASN
2	B	922	ASN
2	B	935	ASN
2	B	945	GLN
2	B	1034	ASN
2	B	1061	GLN
2	B	1104	ASN

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Mol	Chain	Res	Type
2	B	1112	ASN
2	B	1175	ASN
2	B	1189	GLN
2	B	1258	ASN
2	B	1259	ASN
2	B	1323	ASN
2	B	1332	GLN
3	C	33	GLN
3	C	39	ASN
3	C	51	ASN
3	C	62	GLN
3	C	89	GLN
3	C	111	GLN
3	C	116	ASN
3	C	126	ASN
3	C	166	GLN
3	C	218	ASN
3	C	278	HIS
3	C	329	ASN
3	C	357	ASN
3	C	424	ASN
3	C	575	ASN
3	C	678	HIS
3	C	741	ASN
3	C	786	GLN
3	C	808	ASN
3	C	809	ASN
3	C	864	GLN
3	C	896	GLN
3	C	945	ASN
3	C	971	ASN
3	C	974	GLN
3	C	975	GLN
3	C	1032	GLN
3	C	1095	GLN
3	C	1098	GLN
3	C	1114	GLN
3	C	1186	ASN
3	C	1203	HIS
3	C	1214	GLN
4	d	164	ASN
4	d	1003	ASN

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Mol	Chain	Res	Type
4	d	1012	ASN
4	d	1078	ASN
4	d	1132	ASN
4	d	1158	GLN
4	d	1202	GLN
4	d	1254	GLN
5	e	52	ASN
5	e	59	HIS
5	e	876	ASN
5	e	1141	ASN
5	e	1168	GLN
5	e	1188	ASN
6	F	72	ASN
7	G	70	HIS
7	G	80	ASN
7	G	129	GLN
8	H	36	ASN
9	I	48	ASN
9	I	49	ASN
9	I	76	GLN
9	I	91	ASN
10	J	23	ASN
10	J	40	ASN
10	J	45	HIS
10	J	59	HIS
10	J	65	HIS
11	K	91	ASN
11	K	93	ASN
12	L	28	GLN
12	L	29	HIS
12	L	37	GLN
12	L	81	ASN
13	M	26	ASN
13	M	33	GLN
13	M	36	GLN
13	M	54	ASN
13	M	60	ASN
14	N	57	ASN
15	O	39	ASN
15	O	44	ASN
15	O	48	GLN
15	O	78	HIS

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Mol	Chain	Res	Type
16	P	73	ASN
16	P	79	HIS
16	P	91	GLN
16	P	95	ASN
17	T	165	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	ADP	C	4703	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	10 (23%)
19	ADP	C	4702	-	28,29,29	1.32	4 (14%)	43,45,45	1.99	10 (23%)
19	ADP	C	4701	-	28,29,29	1.33	4 (14%)	43,45,45	1.89	10 (23%)
20	ATP	C	4704	-	32,33,33	1.24	5 (15%)	48,52,52	1.80	9 (18%)

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
19	ADP	C	4703	-	-	1/16/32/32	0/3/3/3
19	ADP	C	4702	-	-	3/16/32/32	0/3/3/3
19	ADP	C	4701	-	-	3/16/32/32	0/3/3/3
20	ATP	C	4704	-	-	4/22/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	4701	ADP	C5-C4	4.30	1.46	1.39
19	C	4702	ADP	C5-C4	4.21	1.46	1.39
19	C	4703	ADP	C5-C4	4.21	1.46	1.39
20	C	4704	ATP	C5-C4	4.09	1.46	1.39
20	C	4704	ATP	C5-N7	-2.60	1.34	1.39
19	C	4701	ADP	C5-C6	2.54	1.48	1.41
19	C	4702	ADP	C5-N7	-2.53	1.34	1.39
19	C	4703	ADP	C5-C6	2.47	1.47	1.41
19	C	4701	ADP	C5-N7	-2.37	1.34	1.39
19	C	4703	ADP	C5-N7	-2.35	1.34	1.39
20	C	4704	ATP	C5-C6	2.33	1.47	1.41
19	C	4702	ADP	C5-C6	2.29	1.47	1.41
19	C	4701	ADP	C8-N7	2.29	1.36	1.31
19	C	4703	ADP	C8-N7	2.29	1.36	1.31
19	C	4703	ADP	C4-N9	-2.20	1.33	1.37
19	C	4702	ADP	C8-N7	2.08	1.35	1.31
20	C	4704	ATP	C4-N9	-2.04	1.33	1.37
20	C	4704	ATP	C8-N7	2.00	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4702	ADP	C5-C4-N3	-6.28	118.06	126.72
19	C	4701	ADP	C5-C4-N3	-6.04	118.41	126.72
20	C	4704	ATP	C5-C4-N3	-5.88	118.61	126.72
19	C	4703	ADP	C5-C4-N3	-5.51	119.12	126.72
19	C	4702	ADP	N3-C4-N9	5.29	136.17	127.17
20	C	4704	ATP	N3-C4-N9	4.98	135.63	127.17
19	C	4701	ADP	N3-C4-N9	4.84	135.41	127.17
19	C	4703	ADP	N3-C4-N9	4.30	134.49	127.17
19	C	4702	ADP	C2-N3-C4	3.96	121.50	111.83
20	C	4704	ATP	C2-N3-C4	3.92	121.40	111.83
19	C	4701	ADP	C2-N3-C4	3.90	121.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4703	ADP	C4-C5-N7	-3.70	106.36	110.58
19	C	4702	ADP	N3-C2-N1	-3.64	123.08	128.58
20	C	4704	ATP	N3-C2-N1	-3.63	123.08	128.58
19	C	4701	ADP	N3-C2-N1	-3.60	123.13	128.58
19	C	4703	ADP	C2-N3-C4	3.57	120.55	111.83
19	C	4701	ADP	C4-C5-N7	-3.37	106.73	110.58
19	C	4703	ADP	N3-C2-N1	-3.25	123.66	128.58
19	C	4703	ADP	C4-N9-C8	3.16	109.06	105.74
20	C	4704	ATP	C4-N9-C8	3.14	109.03	105.74
20	C	4704	ATP	C4-C5-N7	-3.01	107.14	110.58
19	C	4702	ADP	C4-C5-N7	-3.01	107.14	110.58
19	C	4702	ADP	C4-N9-C8	2.99	108.88	105.74
19	C	4701	ADP	C4-N9-C8	2.84	108.72	105.74
19	C	4703	ADP	C5-N7-C8	2.72	107.73	103.45
19	C	4701	ADP	C5-N7-C8	2.58	107.51	103.45
19	C	4702	ADP	C2'-C1'-N9	-2.58	106.90	113.30
20	C	4704	ATP	C5-N7-C8	2.54	107.45	103.45
19	C	4702	ADP	C5-N7-C8	2.44	107.29	103.45
19	C	4703	ADP	N9-C8-N7	-2.44	110.47	113.94
20	C	4704	ATP	N9-C8-N7	-2.33	110.62	113.94
19	C	4702	ADP	C3'-C2'-C1'	2.28	105.77	101.46
19	C	4701	ADP	N9-C8-N7	-2.17	110.86	113.94
19	C	4702	ADP	N9-C8-N7	-2.13	110.91	113.94
20	C	4704	ATP	N6-C6-N1	2.09	123.04	118.38
19	C	4701	ADP	O3B-PB-O2B	2.09	115.64	107.80
19	C	4703	ADP	C6-C5-N7	2.09	136.11	132.09
19	C	4703	ADP	O4'-C1'-N9	2.08	112.08	108.09
19	C	4701	ADP	O2A-PA-O1A	2.04	121.94	112.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	4701	ADP	C5'-O5'-PA-O1A
19	C	4701	ADP	C5'-O5'-PA-O3A
19	C	4702	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	C5'-O5'-PA-O2A
19	C	4702	ADP	C5'-O5'-PA-O3A
20	C	4704	ATP	C5'-O5'-PA-O1A
20	C	4704	ATP	C5'-O5'-PA-O3A
20	C	4704	ATP	O4'-C4'-C5'-O5'
20	C	4704	ATP	C3'-C4'-C5'-O5'

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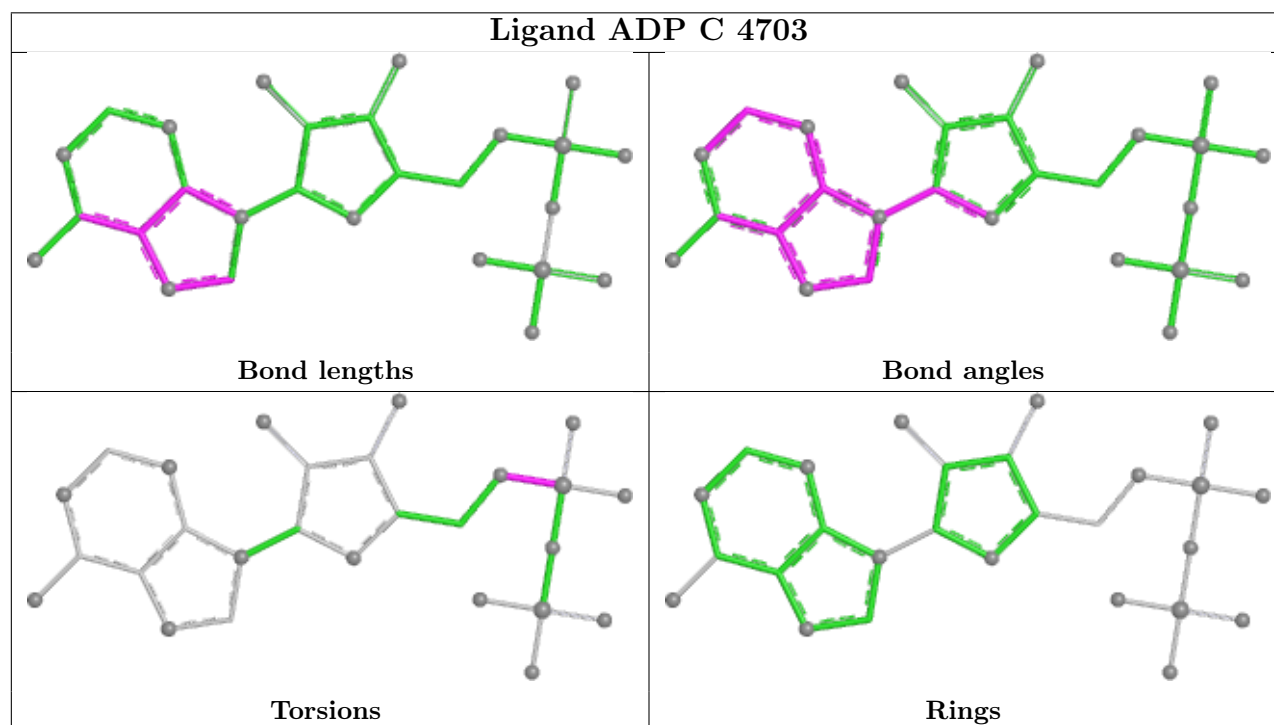
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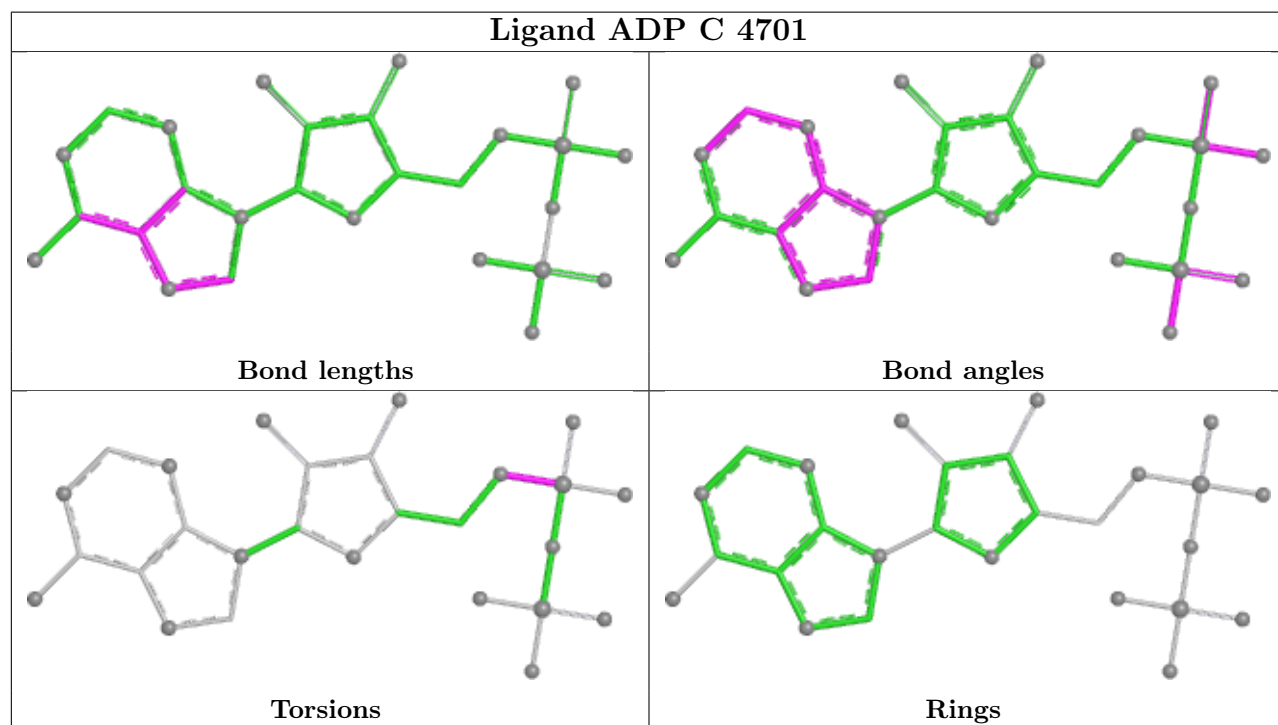
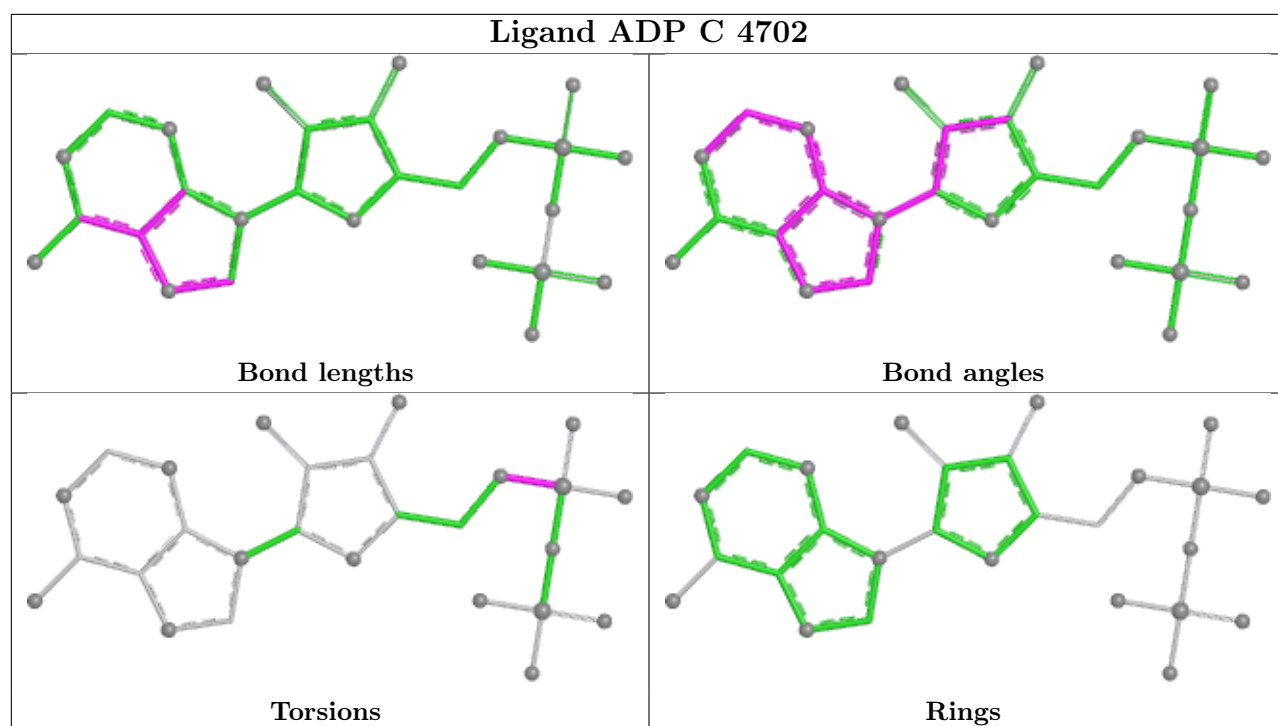
Mol	Chain	Res	Type	Atoms
19	C	4701	ADP	C5'-O5'-PA-O2A
19	C	4703	ADP	C5'-O5'-PA-O1A

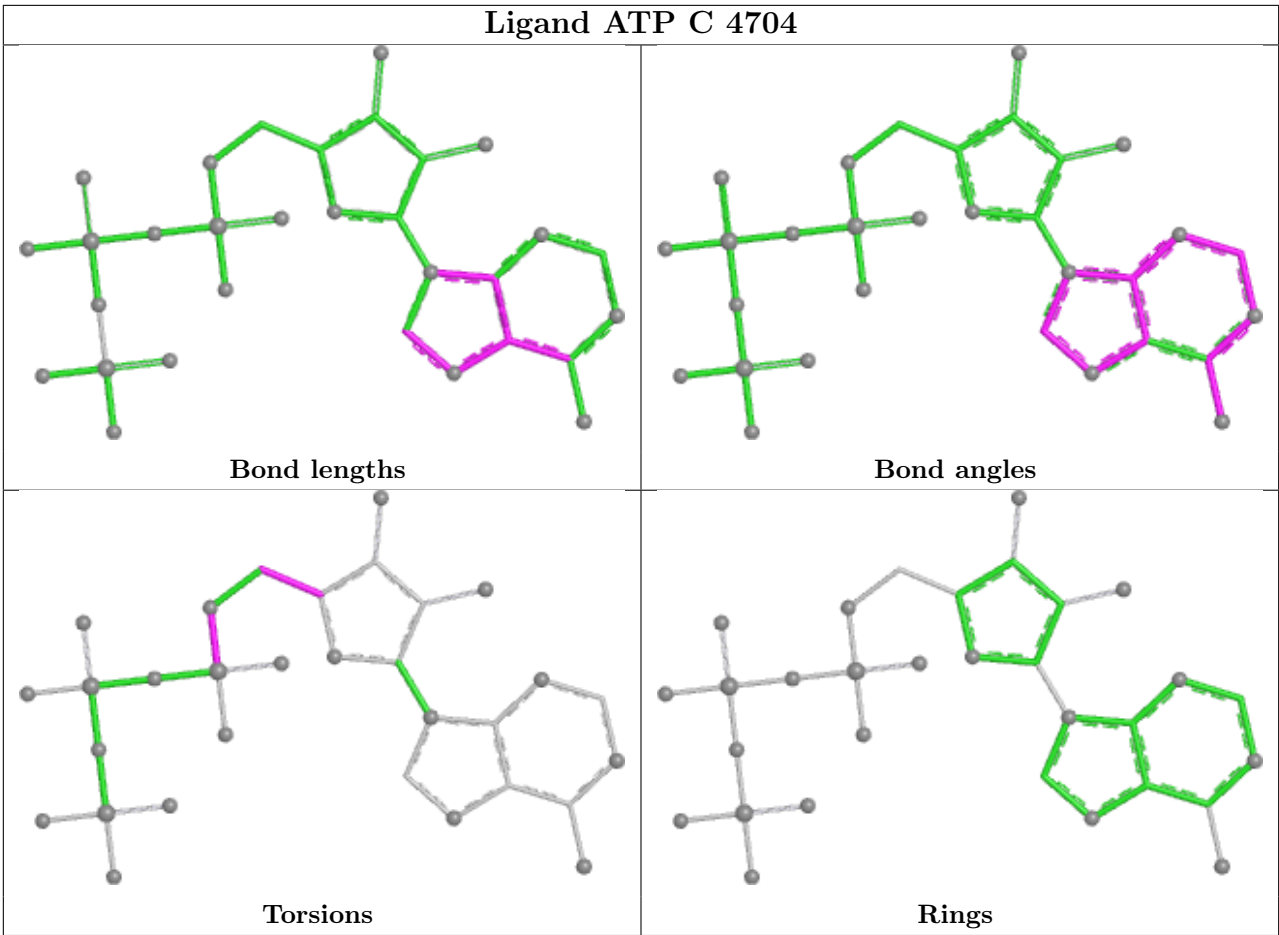
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	22
2	B	13
3	C	9
5	e	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	389:ASP	C	390:THR	N	29.62
1	e	1233:LEU	C	1234:ALA	N	29.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	1201:ARG	C	1202:GLN	N	19.87
1	A	1299:VAL	C	1300:GLN	N	17.01
1	e	1251:GLU	C	1252:LYS	N	15.83
1	A	2300:SER	C	2301:ASP	N	13.90
1	A	2232:GLU	C	2233:PRO	N	13.47
1	B	4440:MET	C	4441:ILE	N	12.83
1	A	1507:PRO	C	1508:GLY	N	12.62
1	B	2495:LYS	C	2496:VAL	N	12.29
1	A	2533:PRO	C	2534:VAL	N	10.44
1	A	4018:CYS	C	4019:ILE	N	10.38
1	B	2583:MET	C	2584:VAL	N	9.42
1	A	2296:ALA	C	2297:GLY	N	9.01
1	A	4109:ASN	C	4110:ALA	N	8.24
1	A	2058:THR	C	2059:LEU	N	8.10
1	A	2897:GLN	C	2898:ARG	N	6.96
1	A	1972:PHE	C	1973:ASP	N	6.76
1	B	1775:VAL	C	1776:ARG	N	6.38
1	A	2132:ALA	C	2133:GLY	N	5.82
1	A	3472:THR	C	3473:ILE	N	5.79
1	A	3921:LYS	C	3922:THR	N	5.38
1	B	2658:SER	C	2659:GLY	N	5.09
1	A	2630:GLU	C	2631:ALA	N	4.86
1	B	2091:ARG	C	2092:GLY	N	4.86
1	B	3793:ASP	C	3794:GLU	N	4.34
1	A	1725:GLY	C	1726:TYR	N	4.16
1	A	2000:LEU	C	2001:MET	N	3.91
1	A	2612:GLU	C	2613:THR	N	3.44
1	B	4123:ASP	C	4124:PRO	N	3.30
1	B	2229:LYS	C	2230:THR	N	3.20
1	B	3552:ASN	C	3553:LEU	N	3.19
1	A	2495:ASP	C	2496:MET	N	3.16
1	B	2702:LYS	C	2703:ALA	N	3.15
1	B	2006:PRO	C	2007:GLY	N	3.09
1	A	1592:ARG	C	1593:SER	N	3.08
1	A	2176:THR	C	2177:ILE	N	3.05
1	B	1212:ILE	C	1213:PRO	N	2.70
1	C	3218:LYS	C	3219:ASP	N	1.19
1	C	3227:LYS	C	3228:LYS	N	1.19
1	C	3311:ASN	C	3312:GLN	N	1.19
1	C	3216:GLU	C	3217:SER	N	1.18
1	C	3225:ALA	C	3226:ASN	N	1.18
1	C	3234:LYS	C	3235:TYR	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3272:SER	C	3273:TYR	N	1.18
1	C	3304:GLU	C	3305:LEU	N	1.18
1	C	3334:LYS	C	3335:TRP	N	1.18

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16304. These allow visual inspection of the internal detail of the map and identification of artifacts.

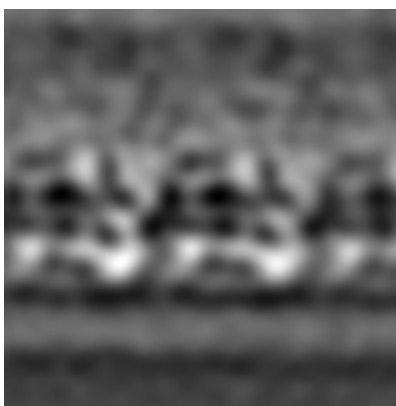
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

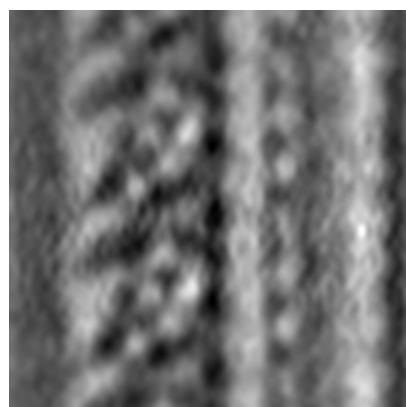


Y

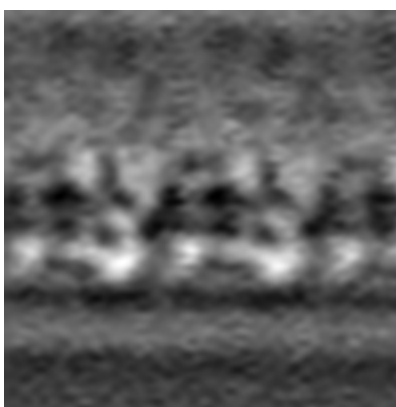


Z

6.1.2 Raw map



X



Y



Z

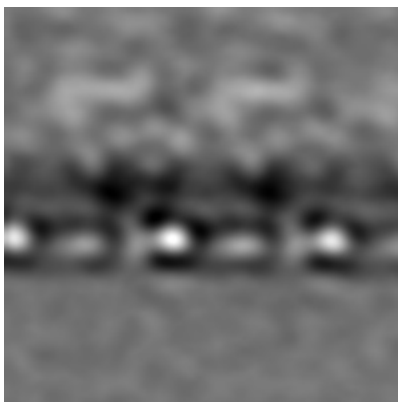
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 37

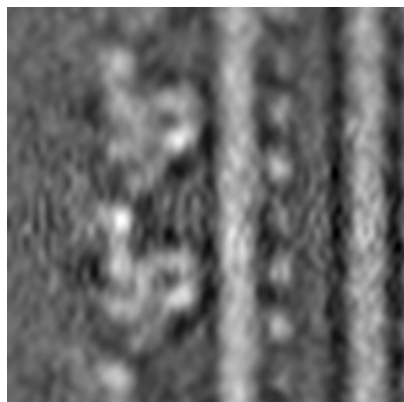


Y Index: 37

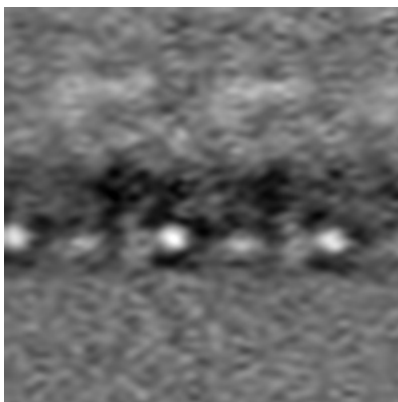


Z Index: 37

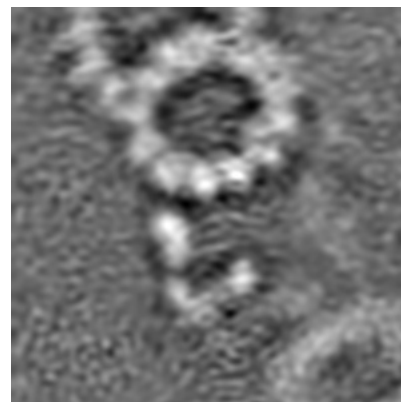
6.2.2 Raw map



X Index: 37



Y Index: 37



Z Index: 37

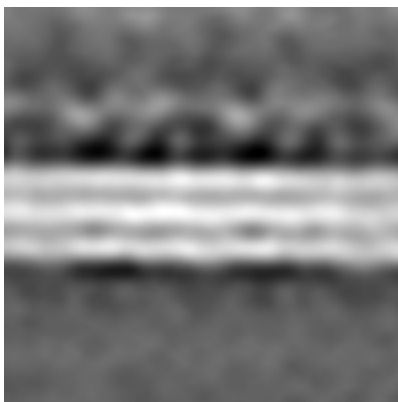
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 29

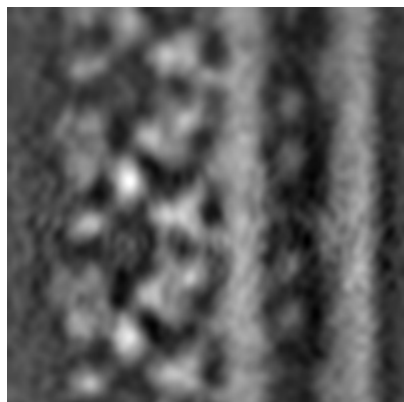


Y Index: 42

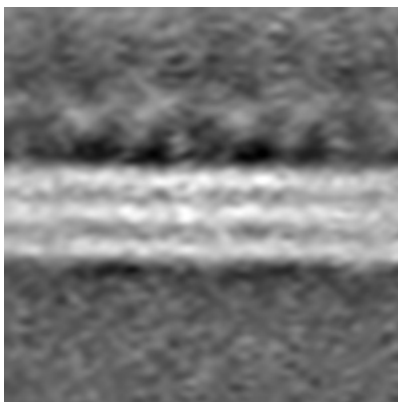


Z Index: 22

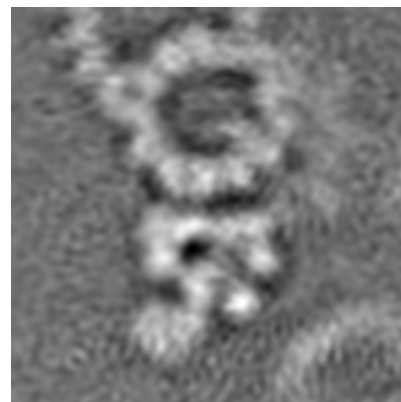
6.3.2 Raw map



X Index: 29



Y Index: 42

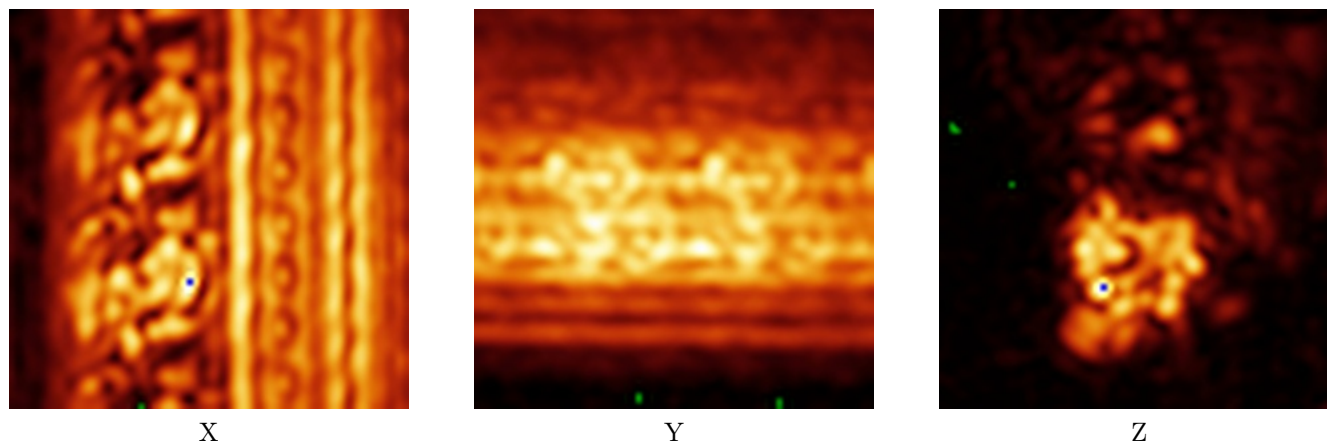


Z Index: 22

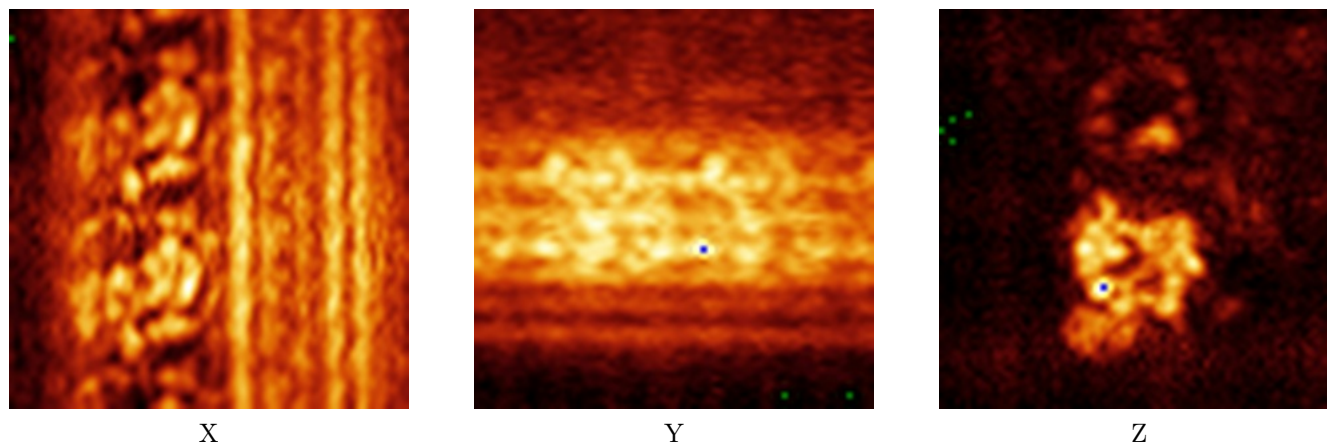
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



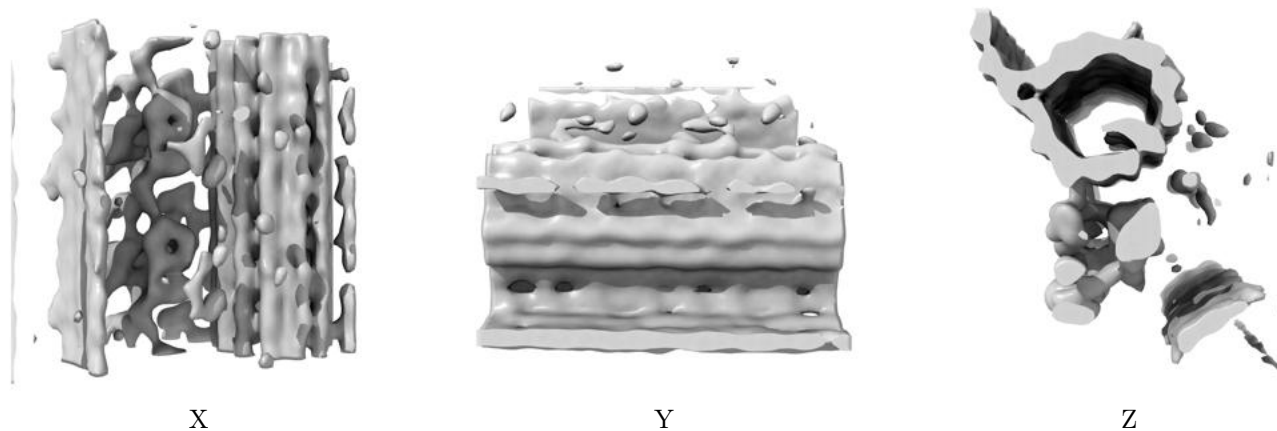
6.4.2 Raw map



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.

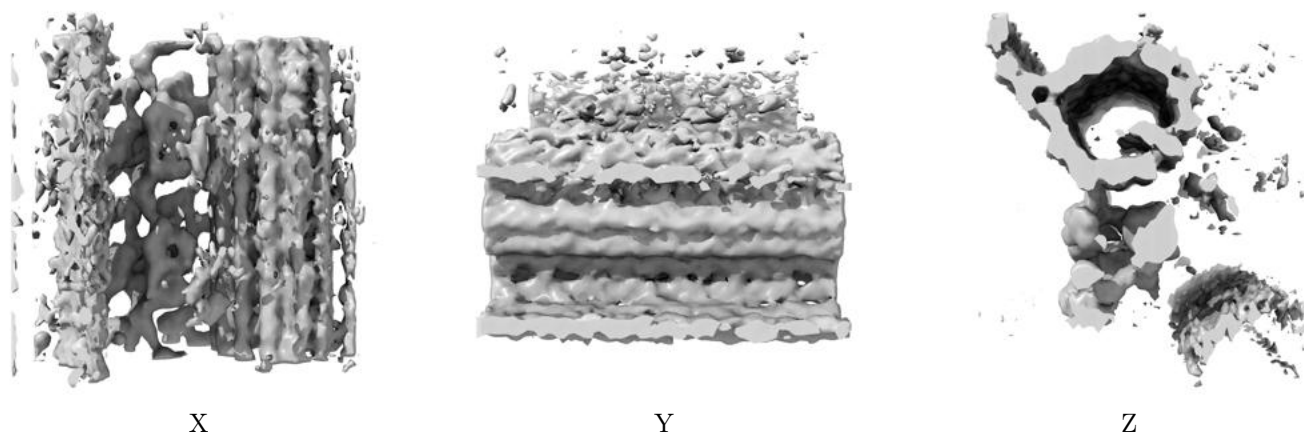
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

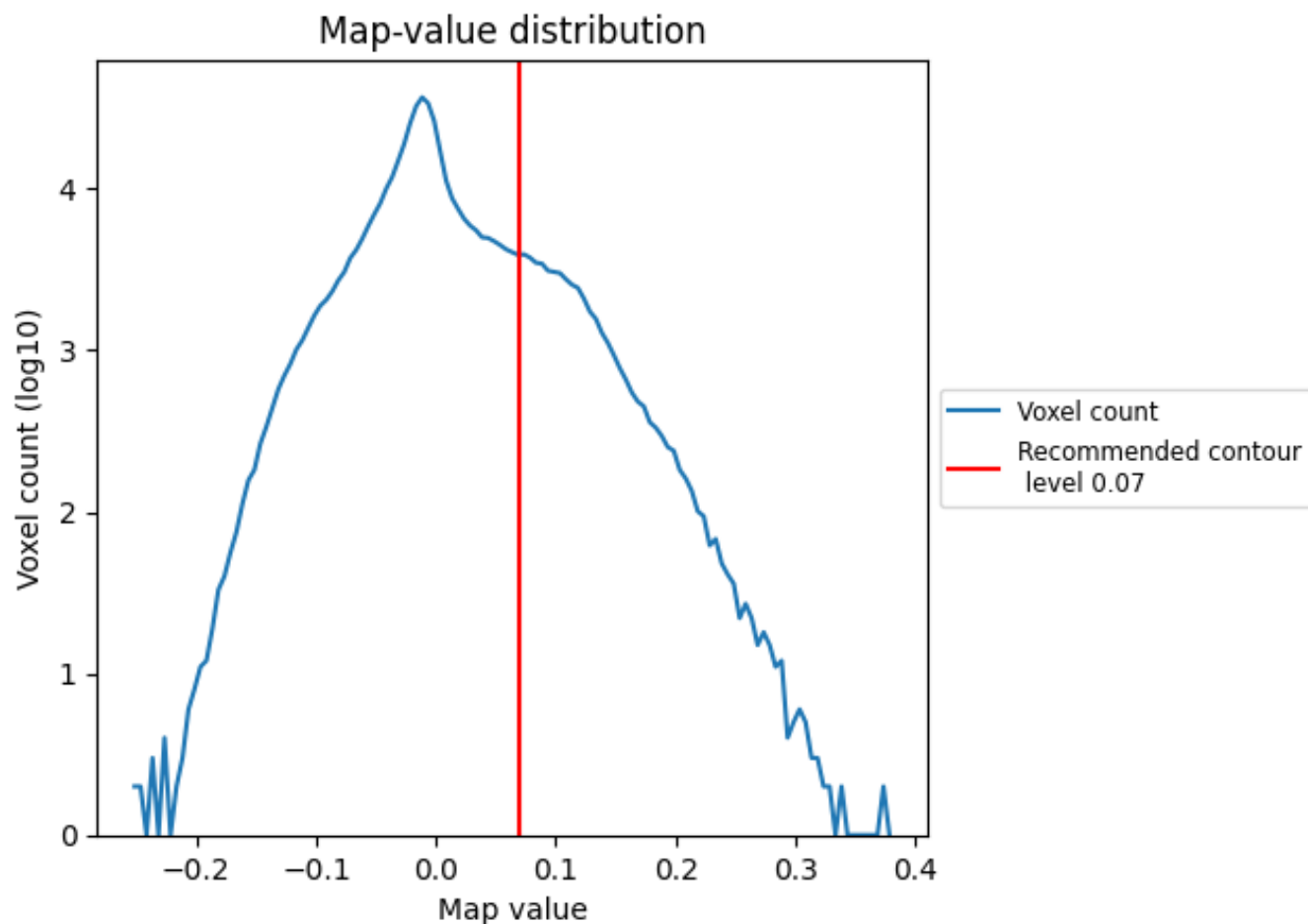
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

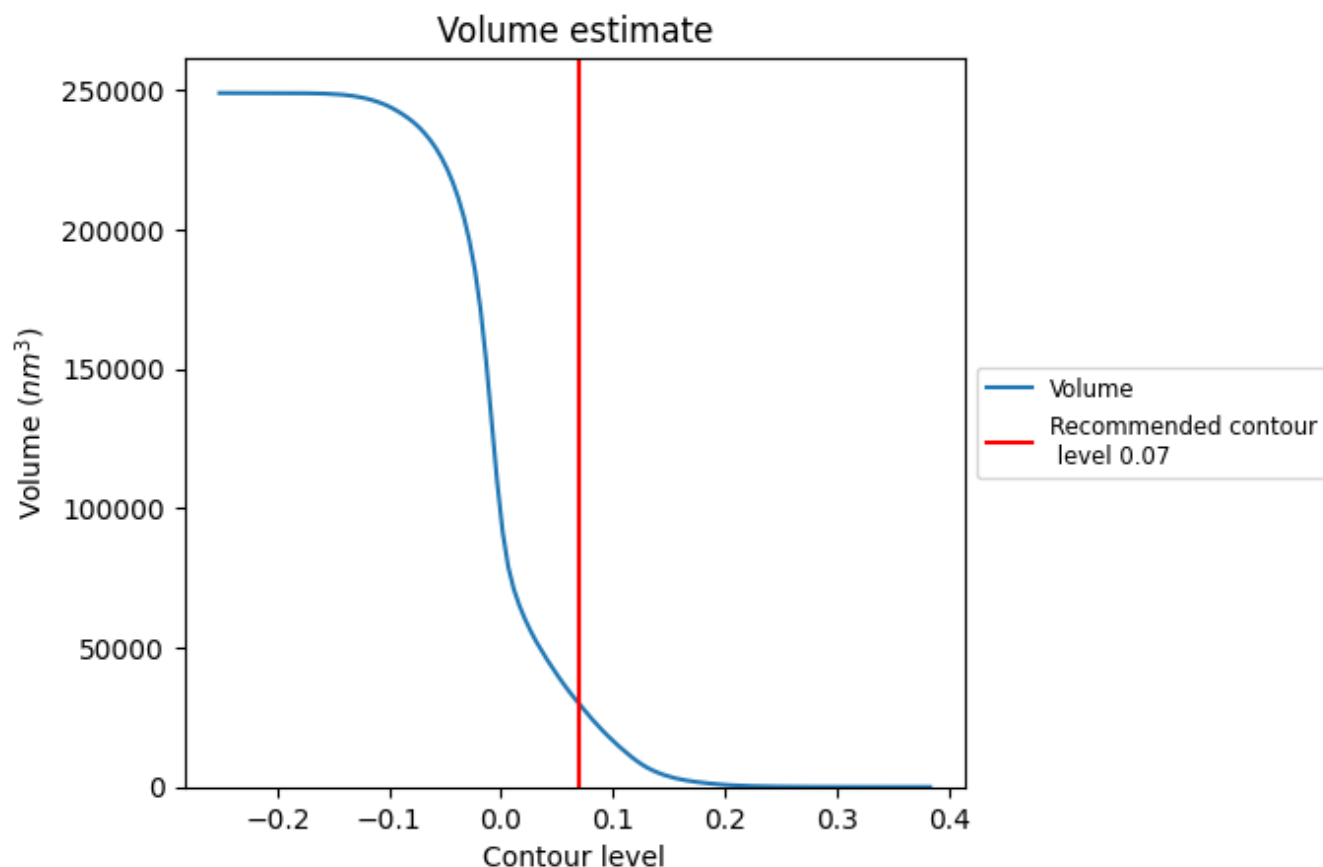
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

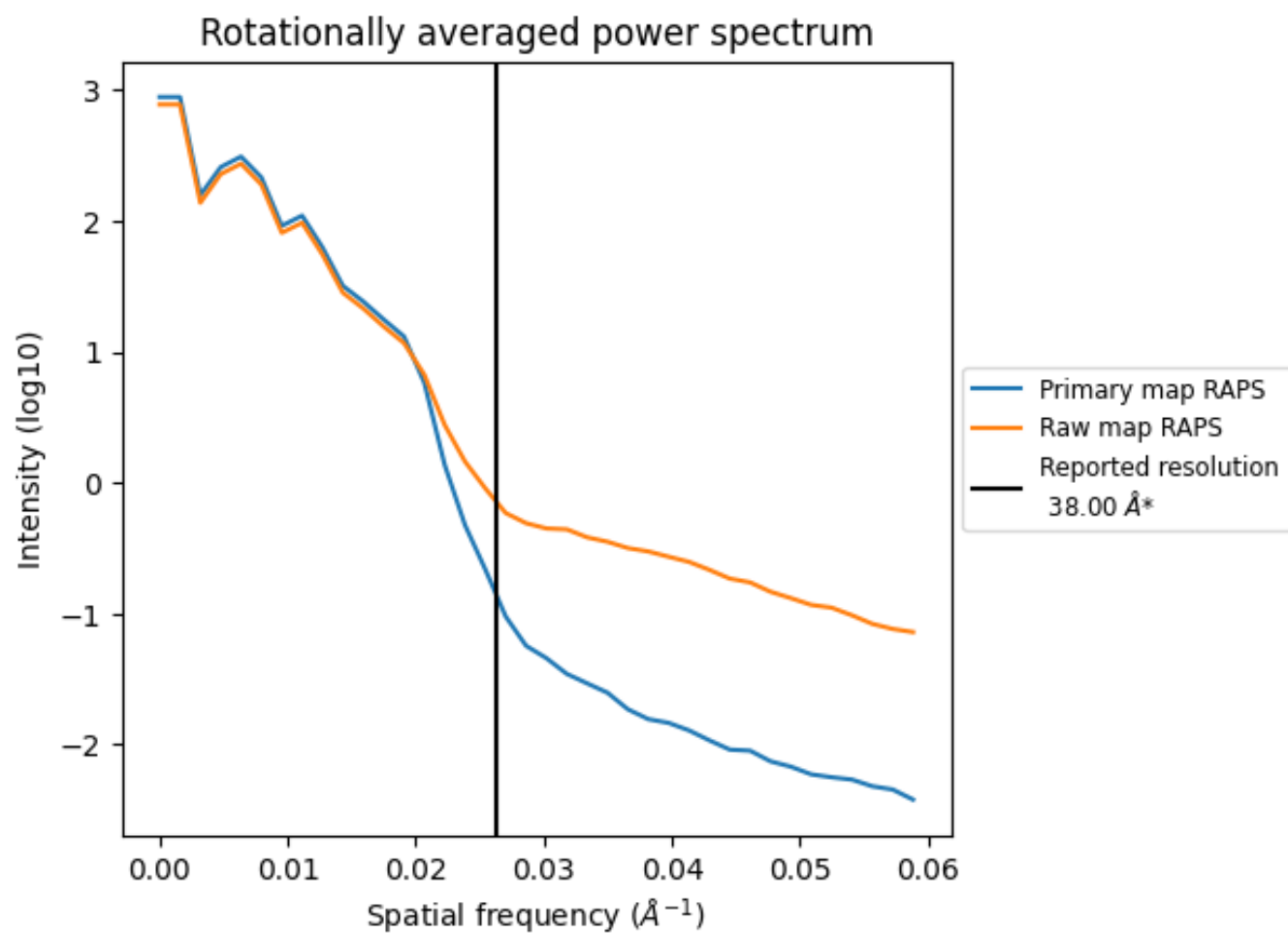
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29745 nm^3 ; this corresponds to an approximate mass of 26870 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 ⓘ

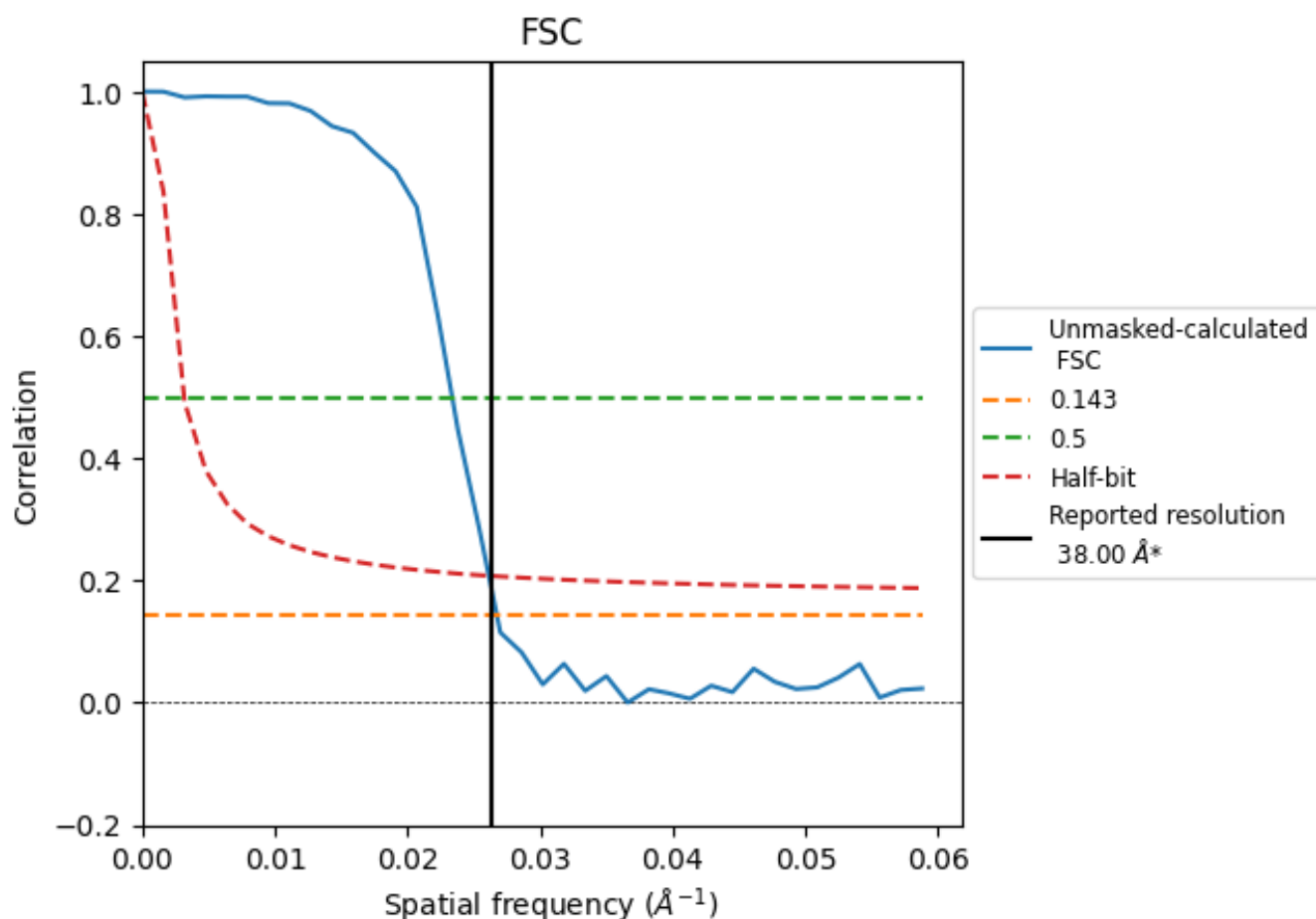


*Reported resolution corresponds to spatial frequency of 0.026 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.026 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

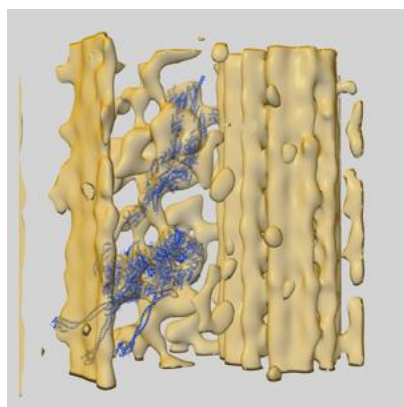
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	38.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	37.31	42.74	38.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

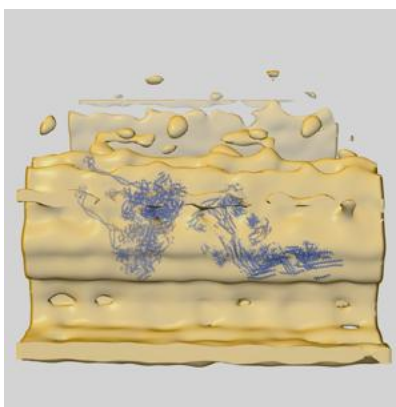
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16304 and PDB model 8BWY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

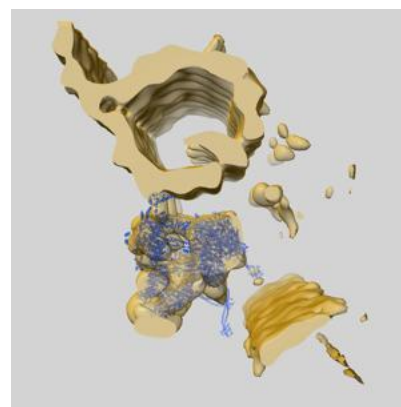
9.1 Map-model overlay [i](#)



X



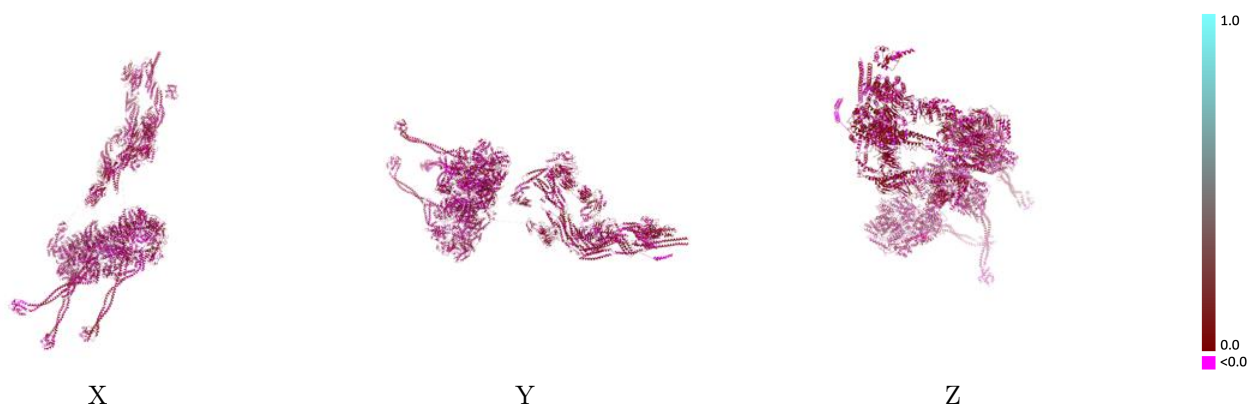
Y



Z

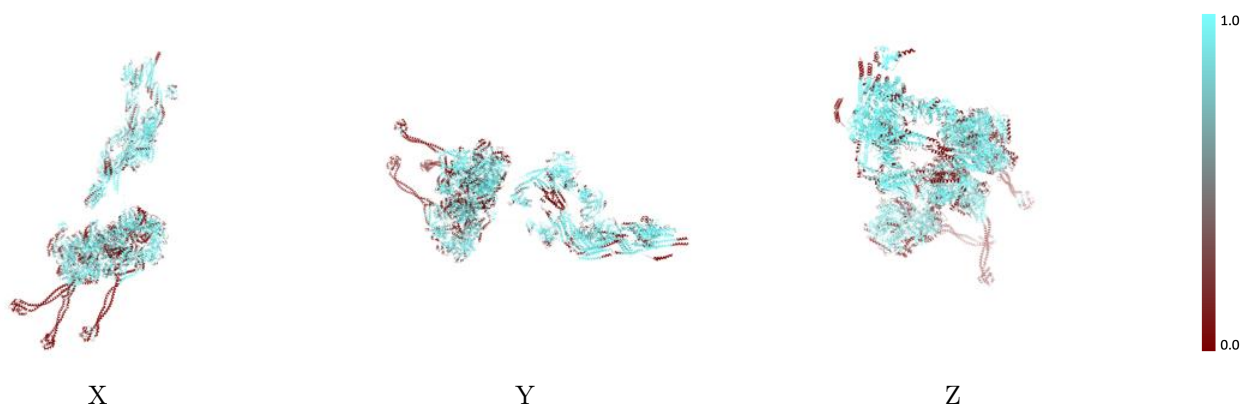
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



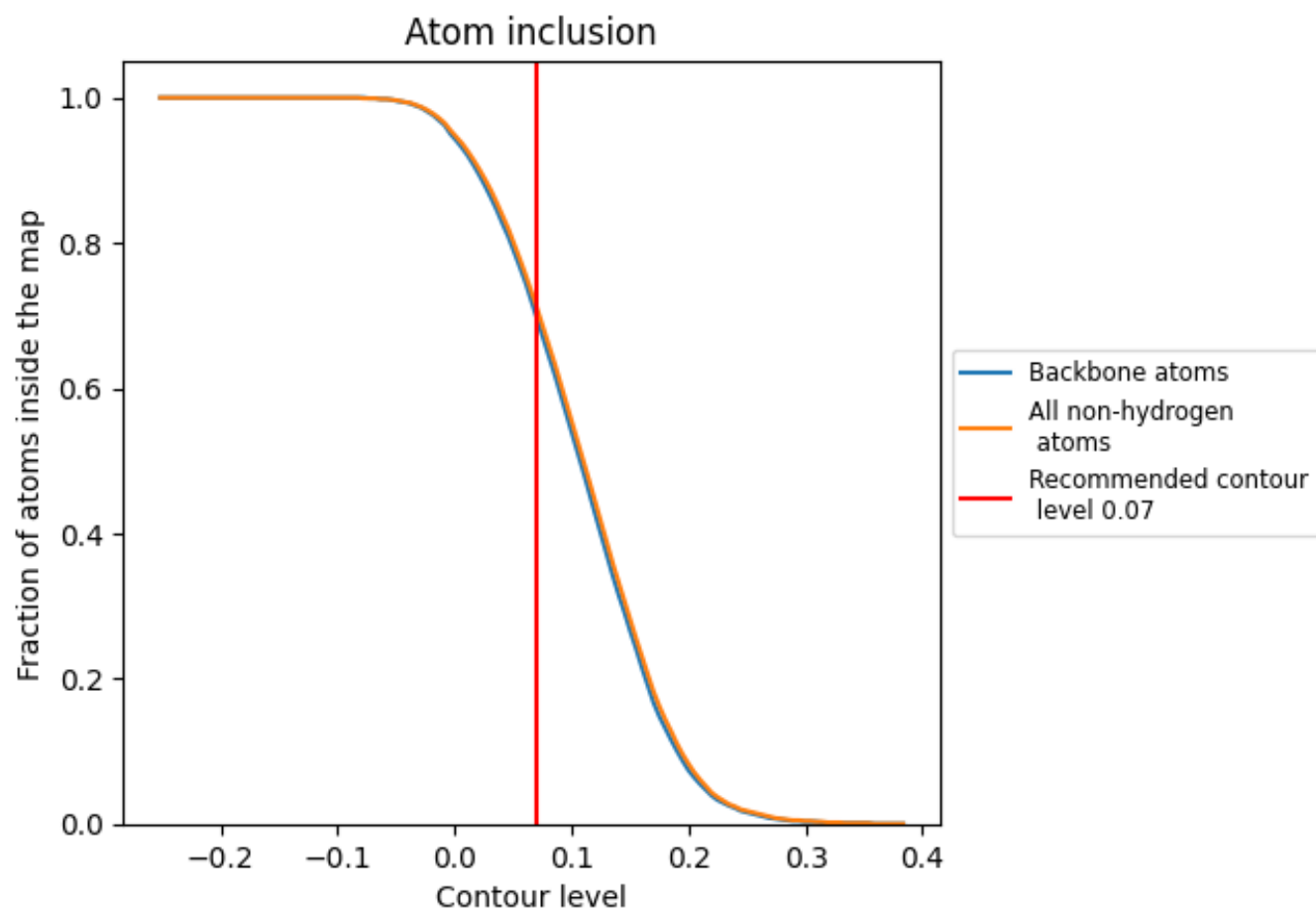
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 71% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.0360
A	 0.6750	 0.0350
B	 0.6630	 0.0350
C	 0.7000	 0.0370
F	 0.8470	 0.0450
G	 0.8310	 0.0380
H	 0.9050	 0.0430
I	 0.8240	 0.0520
J	 0.9210	 0.0580
K	 0.7370	 0.0360
L	 0.7260	 0.0130
M	 0.9820	 0.0690
N	 0.9300	 0.0400
O	 0.8320	 0.0260
P	 0.9330	 0.0590
T	 0.6940	 0.0350
V	 0.7880	 0.0490
d	 0.9190	 0.0420
e	 0.7580	 0.0250
x	 0.6910	 0.0490

