



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:43 pm BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

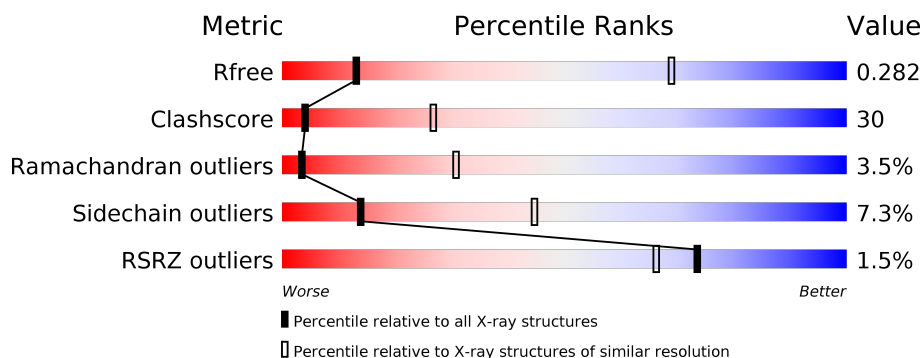
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	3367	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>42%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	3367	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>

## 2 Entry composition

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

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

- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

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

There are 48 discrepancies between the modelled and reference sequences:

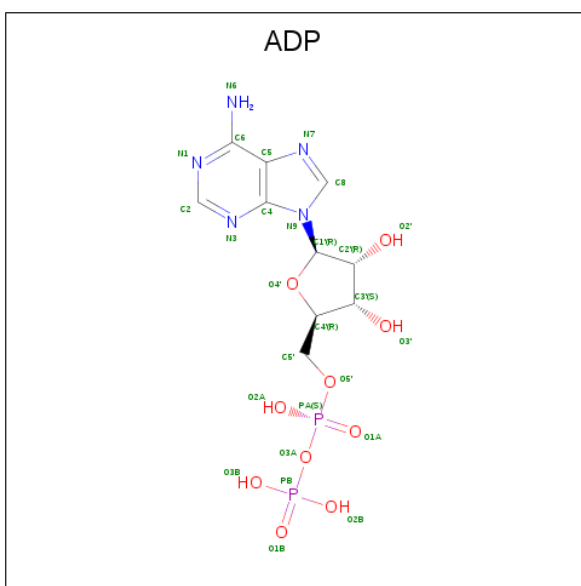
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION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

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

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

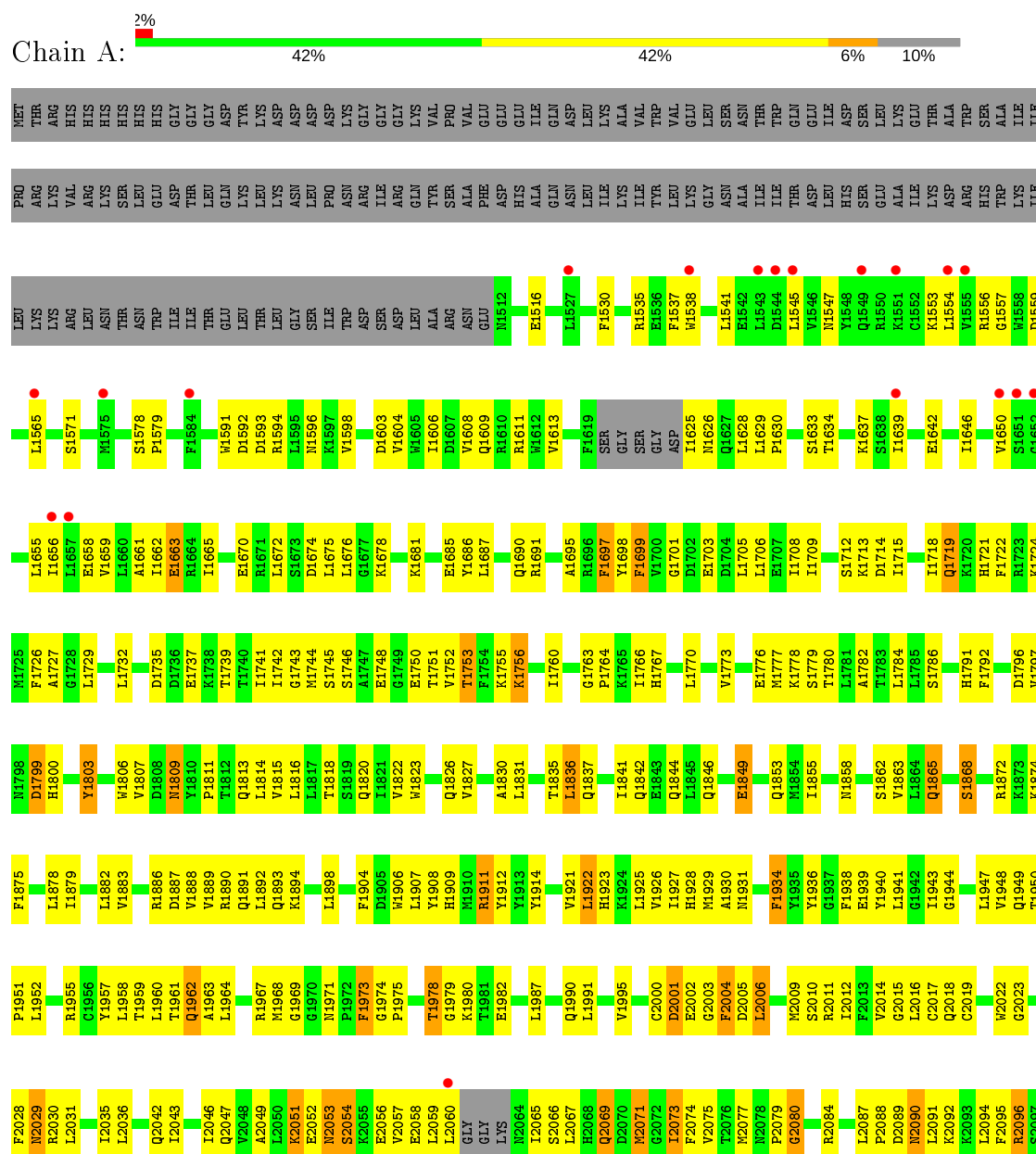


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

### 3 Residue-property plots

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

- Molecule 1: Dynein heavy chain, cytoplasmic





G4054	E4120	L3991	F3911	N3836	R3767	F3911	F3704	F3628	S3551	T3482	E3418	R3342	H3259	E3187
E4055	I4121	L3992	S3912	A3837	D3768	S3912	F3704	A3837	K3552	A3837	K3419	R3342	Y3260	
P4056	E4122	K3993	L3913	A3841	A3771	L3913	N3707	S3630	V3553	Q3484		Q3345	D3262	R3190
I4057	E4123	G3994	L3914	A3841	A3771	L3914	N3707	S3630	K3554	T3485	T3422	V3346	L3261	
P4059	E4124	G3995	A3915	G3842	T3774	A3915	A3711	V3634	N3555	Y3486	K3424	D3349	L3264	L3192
E4060	V4126	N3997	F3916	N3844	P3775	F3916	L3712	P3635	G3556	Y3487	K3425	V3350	N3265	E3195
S4061	E4127	L3998	L3917	L3845	D3776	L3917	G3715	L3638	D3558	S3488	K3426	K3353	Q3266	R3196
W4062	S4128	L3999	D3918	L3846	S3779	D3918	C3715	S3639	R3559	L3489	K3427	F3357	V3197	
W4063	S4129	F3920	L3919	D3847	S3780	F3920	C3716	E3643	P3560	ASP	E3428	V3357	Q3268	R3197
V4064	L4001	F3921	F3920	D3848	V3781	F3921	P3717	E3643	K3561	ARG	K3430	K3358	Q3198	
A4065	K4002	N3922	N3921	D3849	V3782	N3922	L3719	K3647	A3562	ILE	K3431	K3359	L3270	I3200
Q4066	E4003	L3923	L3922	S3850	T3782	L3923	L3719	E3647	L3563	LYS	K3431	V3360	L3271	K3201
A4067	T4004	L3924	L3924	V3851	F3783	L3924	V3720	E3648	L3564		L3432	K3361	P3202	
Q4068	L4005	N3925	N3925	T3854	N3784	N3925	Q3721	L3652	D3565	PRD	T3433	K3361	F3205	
L4069	P4006	N3926	N3926	L3855	F3786	N3926	F3722	P3653	N3566	LEU	S3434	K3274	R3206	
S4070	Q4007	N3927	N3927	L3855	F3786	N3927	F3722	S3654	K3567	ARG	K3435	K3275	I3206	
N4071	L4008	N3927	N3927	L3855	F3786	N3927	F3722	S3654	K3567	ARG	K3435	K3275	I3206	
Q4072	L4008	N3927	N3927	L3855	F3786	N3927	F3722	S3654	K3567	ARG	K3435	K3275	I3206	
Q4073	L4008	N3927	N3927	L3855	F3786	N3927	F3722	S3654	K3567	ARG	K3435	K3275	I3206	
S4074	L4011	L4011	L4011	L3858	K3859	L4011	L3858	L3652	N3568	GLU	K3436	L3278	A3209	
Q4075	L4012	L4012	L4012	L3859	K3859	L4012	L3859	L3652	N3568	GLU	K3436	L3278	A3209	
T4076	S4013	S4013	S4013	T3862	K3862	S4013	T3862	P3653	K3568	GLU	K3436	L3278	A3209	
V4077	T4014	T4014	T4014	T3862	K3862	T4014	T3862	S3654	K3568	GLU	K3436	L3278	A3209	
S4078	T4015	T4015	T4015	T3862	K3862	T4015	T3862	S3654	K3568	GLU	K3436	L3278	A3209	
W4079	Q4016	Q4016	Q4016	T3862	K3862	Q4016	Q4016	S3654	K3568	GLU	K3436	L3278	A3209	
F4080	Q4017	Q4017	Q4017	T3862	K3862	Q4017	Q4017	S3654	K3568	GLU	K3436	L3278	A3209	
R4081	Q4018	Q4018	Q4018	T3862	K3862	Q4018	Q4018	S3654	K3568	GLU	K3436	L3278	A3209	
K4082	L4020	L4020	L4020	T3862	K3862	L4020	L4020	S3654	K3568	GLU	K3436	L3278	A3209	
I4083	I4021	I4021	I4021	T3862	K3862	I4021	I4021	S3654	K3568	GLU	K3436	L3278	A3209	
L4084	C4022	C4022	C4022	T3862	K3862	L4084	L4084	S3654	K3568	GLU	K3436	L3278	A3209	
L4085	L4023	L4023	L4023	T3862	K3862	L4085	L4085	S3654	K3568	GLU	K3436	L3278	A3209	
M4086	R4024	R4024	R4024	T3862	K3862	M4086	M4086	S3654	K3568	GLU	K3436	L3278	A3209	
K4087	Q4025	Q4025	Q4025	T3862	K3862	K4087	K4087	S3654	K3568	GLU	K3436	L3278	A3209	
H4090	Q4026	Q4026	Q4026	T3862	K3862	H4090	H4090	S3654	K3568	GLU	K3436	L3278	A3209	
S4091	V4027	V4027	V4027	T3862	K3862	S4091	S4091	S3654	K3568	GLU	K3436	L3278	A3209	
D4092	P4028	P4028	P4028	T3862	K3862	D4092	D4092	S3654	K3568	GLU	K3436	L3278	A3209	
R4093	F4030	F4030	F4030	T3862	K3862	R4093	R4093	S3654	K3568	GLU	K3436	L3278	A3209	
V4094	S4031	S4031	S4031	T3862	K3862	V4094	V4094	S3654	K3568	GLU	K3436	L3278	A3209	
L4095	K4032	K4032	K4032	T3862	K3862	L4095	L4095	S3654	K3568	GLU	K3436	L3278	A3209	
S4098	L4034	L4034	L4034	T3862	K3862	S4098	S4098	S3654	K3568	GLU	K3436	L3278	A3209	
H4099	D4035	D4035	D4035	T3862	K3862	H4099	H4099	S3654	K3568	GLU	K3436	L3278	A3209	
S4100	H4036	H4036	H4036	T3862	K3862	S4100	S4100	S3654	K3568	GLU	K3436	L3278	A3209	
C4103	Q4039	Q4039	Q4039	T3862	K3862	C4103	C4103	S3654	K3568	GLU	K3436	L3278	A3209	
S4104	N4040	N4040	N4040	T3862	K3862	S4104	S4104	S3654	K3568	GLU	K3436	L3278	A3209	
V4105	D4043	D4043	D4043	T3862	K3862	V4105	V4105	S3654	K3568	GLU	K3436	L3278	A3209	
E4108	W4044	W4044	W4044	T3862	K3862	E4108	E4108	S3654	K3568	GLU	K3436	L3278	A3209	
D4109	R4045	R4045	R4045	T3862	K3862	D4109	D4109	S3654	K3568	GLU	K3436	L3278	A3209	
F4110	Q4046	Q4046	Q4046	T3862	K3862	F4110	F4110	S3654	K3568	GLU	K3436	L3278	A3209	
L4111	F4047	F4047	F4047	T3862	K3862	L4111	L4111	S3654	K3568	GLU	K3436	L3278	A3209	
N4112	F4048	F4048	F4048	T3862	K3862	N4112	N4112	S3654	K3568	GLU	K3436	L3278	A3209	
Q4049	G4049	G4049	G4049	T3862	K3862	Q4049	Q4049	S3654	K3568	GLU	K3436	L3278	A3209	
K4050	H3907	H3907	H3907	T3862	K3862	K4050	K4050	S3654	K3568	GLU	K3436	L3278	A3209	
D4051	R3988	R3988	R3988	T3862	K3862	D4051	D4051	S3654	K3568	GLU	K3436	L3278	A3209	
Q4052	L3909	L3909	L3909	T3862	K3862	Q4052	Q4052	S3654	K3568	GLU	K3436	L3278	A3209	
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E4122	L4162	L4162	L4162	T3862	K3862	E4122	E4122	S3654	K3568	GLU	K3436	L3278	A3209	
L4123	D4117	D4117	D4117	T3862	K3862	L4123	L4123	S3654	K3568	GLU	K3436	L3278	A3209	
S4206	S4206	S4206	S4206	T3862	K3862	S4206	S4206	S3654	K3568	GLU	K3436	L3278	A3209	
L4207	L4207	L4207	L4207	T3862	K3862	L4207	L4207	S3654	K3568	GLU	K3436	L3278	A3209	
E4129	L4182	L4182	L4182	T3862	K3862	E4129	E4129	S3654	K3568	GLU	K3436	L3278	A3209	
L4183	T4183	T4183	T4183	T3862	K3862	L4183	L4183	S3654	K3568	GLU	K3436	L3278	A3209	
W4184	W4184	W4184	W4184	T3862	K3862	W4184	W4184	S3654	K3568	GLU	K3436	L3278	A3209	
V4185	V4185	V4185	V4185	T3862	K3862	V4185	V4185	S3654	K3568	GLU	K3436	L3278	A3209	
L4186	L4186	L4186	L4186	T3862	K3862	L4186	L4186	S3654	K3568	GLU	K3436	L3278	A3209	
L4187	L4187	L4187	L4187	T3862	K3862	L4187	L4187	S3654	K3568	GLU	K3436	L3278	A3209	
K4188	K4188	K4188	K4188	T3862	K3862	K4188	K4188	S3654	K3568	GLU	K3436	L3278	A3209	
N4189	N4189	N4189	N4189	T3862	K3862	N4189	N4189	S3654	K3568	GLU	K3436	L3278	A3209	
L4190	L4190	L4190	L4190	T3862	K3862	L4190	L4190	S3654	K3568	GLU	K3436	L3278	A3209	
H4191	H4191	H4191	H4191	T3862	K3862	H4191	H4191	S3654	K3568	GLU	K3436	L3278	A3209	
L4192	L4192	L4192	L4192	T3862	K3862	L4192	L4192	S3654	K3568	GLU	K3436	L3278	A3209	
A4193	A4193	A4193	A4193	T3862	K3862	A4193	A4193	S3654	K3568	GLU	K3436	L3278	A3209	
E4197	E4197	E4197	E4197	T3862	K3862	E4197	E4197	S3654	K3568	GLU	K3436	L3278	A3209	
L4200	L4200	L4200	L4200	T3862	K3862	L4200	L4200	S3654	K3568	GLU	K3436	L3278	A3209	
E4201	E4201	E4201	E4201	T3862	K3862	E4201	E4201	S3654	K3568	GLU	K3436	L3278	A3209	
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H4205	H4205	H4205	H4205	T3862	K3862	H4205	H4205	S3654	K3568	GLU	K3436	L3278	A3209	
S4206	S4206	S4206	S4206	T3862	K3862	S4206	S4206	S3654	K3568	GLU	K3436	L3278	A3209	
L4207	L4207	L4207	L4207	T3862	K3862	L4207	L4207	S3654	K3568	GLU	K3436	L3278	A3209	
E4197	E4197	E4197	E4197	T3862	K3862	E4197	E4197	S3654	K3568	GLU	K3436	L3278	A3209	
L4200	L4200	L4200	L4200	T3862	K3862	L4200	L4200	S3654	K3568	GLU	K3436	L3278	A3209	
E4201	E4201	E4201	E4201	T3862	K3862	E4201	E4201	S3654	K3568	GLU	K3436	L3278	A3209	
L4204	L4204	L4204	L4204	T3862	K3862	L4204	L4204	S3654	K3568	GLU	K3436	L3278	A3209	
H4205	H4205	H4205	H4205	T3862	K3862	H4205	H4205	S3654	K3568	GLU	K3436	L3278	A3209	
S4206	S4206	S4206	S4206	T3862	K3862	S4206	S4206	S3654	K3568	GLU	K3436	L3278	A3209	
L4207	L4207	L4207	L4207	T3862	K3862	L4207	L4207	S3654	K3568	GLU	K3436	L3278	A3209	
E4197	E4197	E4197	E4197	T3862	K3862	E4197	E4197	S3654	K3568	GLU	K3436	L3278	A3209	
L4200	L4200	L4200	L4200	T3862	K3862	L4200	L4200	S3654	K3568	GLU	K3436	L3278	A3209	
E4201	E4201	E4201	E4201	T3862	K3862	E4201	E4201	S3654	K3568	GLU	K3436	L3278	A3209	
L4204	L4204	L4204	L4204	T3862	K3862	L4204	L4204	S3654	K3568	GLU	K3436	L3278	A3209	
H4205	H4205	H4205	H4205	T3862	K3862	H4205	H4205	S3654	K3568	GLU	K3436	L3278	A3209	
S4206	S4206	S4206	S4206	T3862	K3862	S4206	S4206	S3654	K3568					





V2759	H2667	P2596	Q2520	P2380	K2300	G2225	R2150	P1972	G1900	M1809	K1720
R2764	R2668	I2597	Q2521	M2381	S2301	SER	A2151	P1975	N1901	Y1810	H1721
M2766	Q2765	Q2598	R2522	G2382	H2304	L2228	L2152	P1976	D1902	P1811	F1722
	L2671	I2600	I2525	E2383	V2305	Q2229	S2154	G1978	W1906	Q1813	M1725
	L2672		M2526	R2384	V2308	P2230	V2155	G1979	L1907	F1726	F1727
			D2527	L2387	P2308	I2231	L2156	K1980	L1907	A1727	
			P2527		R2309	Q2235	K2163	T1981	Y1908	V1815	
			P2528	V2391	A2310	R2236	R2164	K1982	H1909	L1816	
			R2529	R2392	T2311	R2237	K2165	T1983	H1909	L1817	
			R2530	V2393	T2312	R2237	R2165	T1984	H1911	L1818	
			R2531	M2394	T2313	R2238	R2166	T1985		S1819	
			R2532	F2395	T2314	K2239	GLN	K1985	Y1914	L1734	
			R2533	E2396	Q2315	I2240	PRO			D1735	
					Q2315	I2241	PRO	Q1990	Y1914	D1736	
					L2320	Q2241	PRO	L1991	E1919	T1739	
					L2320	E2242	GLN	L1992	N1920	T1740	
					T2323	I2243	LEU	R1993	Y1921	I1741	
						A2244	PRO		L1922	V1827	
							PRO		H1923	D1828	
							ILE	V1997	K1924	L1831	
							THR		L1925	I1841	
							ASP	C2000	H1928		
							ALA	E2002	Y1926		
							GLU		L1927		
							THR	C2017	M1929	V1752	
							LYS	A2021	A1930	F1753	
							THR		N1931	F1754	
							LYS		F1938		
							ALA		F1939	S1759	
							ALA		Y1940	I1760	
							Q2185		L1941	I1848	
							Q2185		Y1935	E1849	
							Q2185		Y1936	A1761	
							Q2185		G1942	N1762	
							Q2185		G1942	G1763	
							Q2185		G1942	P1764	
							Q2185		G1942	I1765	
							Q2185		G1942	H1767	
							Q2185		G1942	V1769	
							Q2185		G1942	L1770	
							Q2185		G1942	V1773	
							Q2185		G1942	M1777	
							Q2185		G1942	T1780	
							Q2185		G1942	L1781	
							Q2185		G1942	A1782	
							Q2185		G1942	I1879	
							Q2185		G1942	V1883	
							Q2185		G1942	H1884	
							Q2185		G1942	Q1885	
							Q2185		G1942	S1788	
							Q2185		G1942	L1789	
							Q2185		G1942	V1889	
							Q2185		G1942	N1793	
							Q2185		G1942	L1892	
							Q2185		G1942	D1799	
							Q2185		G1942	H1800	
							Q2185		G1942	S1801	
							Q2185		G1942	T1899	

K4032	L3947	K3859	D876	M585	LEU	PHE	PRO	V3268	L3170	S3082	L2999	P2913	L2838
L4033	F3943	I3865	F3677	S586	ASP	ILE	ALA	I3271	D3171	F3083	R3000	Q2914	L2839
V4034	S3949	I3866		T3587	ARG	THR	ILE	T3272	M3172	L3084	I3001	R2915	P2840
H4036	R3954	L3867	A3681	V3588	ILE	SER	ILE	F3173	F3173	E3085	D3002	R2916	I2841
	V3955	K3868	M3682	V3592	PRO	ILE	ALA	K3273	G3174	R3086	R3003	L2917	L2842
S4041		V3869	F3684		LEU	ASN	GLN	K3274	E3175	M3087	V3004	V2918	R2843
S4042	L3764		L3685	A3595	ARG	THR	GLU	H2844	L3181	I3088	G3040	E2921	
L3958	F3765	L3872	L3686	F3598	GLU	ASP	ALA		F3182	F3089	H3011		L2849
L4043	L3766		L3687	F3598	GLU	THR	VAL		Q3183	L3090	A3012	W2925	T2850
N3960	R3767		Q3688		VAL	THR	SER		V3184	L3091	L3013	W2926	
N3961	D3768	K3876	Q3688	Y3601	GLU	LYS	THR		G3185	G3093	L3014	D2927	W2853
D3962	D3769	Q3877	Q3689	K3690	GLN	MET	ILE		S3186	G3094	L3015	K2928	W2854
D3963	F3769	E3878	G3603	G3603	LEU	MET	LYS		E3187	E3095	G3016	K2929	E2855
F4047	I3770	L3879	D3691		GLU	THR	LYS			VAL	I3017	K2930	F2856
D4051	L3965	E3880	K3692	F3604	ASN	THR	LYS		L3192	PRO	S3018	D2931	
Q4052	L3966	E3881	K3693	F3605	GLN	THR	LYS			GLY	S3019	E2932	Q2861
V4053	F3967	V3882	L3694	D3606	ALA	ILE	HIS		E3195	LEU	S3023	V2933	K2862
				Q3607	ALA	LYS	LEU		N3196	PHE	V3024	A2934	R2863
P4056	L3973	V3886	K3695	Q3607	ASN	ARG	ASP			GLU	L3025	L2935	F2864
I4057		N3887	K3696	F3609	GLU	GLU	GLU		Y3199	GLY	S3026	K2936	T2865
L4058	V3976	P3888	T3697	R3610	LEU	ILE	ILE		P3202	E3103	R3027	H2937	D2866
P4059	K3977	S3889	F3699	M3614	K3512	ILE	LYS			E3104	F3028	P2938	P2867
E4060	G3978	A3890	L3700	M3614		THR	SER			F3105	V3029	P2939	T2868
	T3979	L3891	D3701		L3525	LYS	LEU		K3212		A3030	S2940	T2869
I4063		S3892		K3617		PRO	PRO		GLY	M3109		V2941	
V4064		C3893	G3715	K3618	Y3536	THR	LYS		ASN	C3112	L3035	L2946	Y2872
		S3894	L3719	I3619		LEU	PRO		ASN		S3036	L2946	T2873
A4067	F3990	R3895	L3719	R3620	L3539	GLU	PRO		ASN		L3037	K2947	T2874
Q4068	N3785	N3785	D3722	S3623	R3541	ASP	THR		M3217	R3118	V3038	L2950	S2875
L4069	F3786	F3786	E3723	E3542	E3542	GLY	VAL		A3218	ASN	T3039		P2876
S4070	T3787	T3787	E3724	F3628	T3543	PHE	LYS		I3219	GLY	L3040	W2955	R2877
N4071	K3788	K3788	N3725		E3545	ASP	LYS		P3220	LEU	K3041	W2955	
Q4072	T3789	T3789		V3634	Q3545	THR	ALA		P3221	ILE	R3042	N2964	S2880
Q4073	P3790	P3790		P3635	T3546	GLY	MET			LEU	R3043	R2965	W2882
S4074	S3791	S3791	V3729	S3636		THR	GLU		V3228	ASP	Y3046	S2966	D2883
T4075	S3792	S3792	N3730	F3637	S3550	VAL	ALA		S3229	S3125		L2968	
I4076	L3793	L3793	N3731	L3638	S3551	ASN	VAL		S3230	L3129	D3050	V2972	L2886
			P3732	L3638	S3552	ANG	CYS		L3231	S3135	K3057	L2976	L2887
M4079	T3809	T3809	V3733	S3639	V3553	ALA	LEU		V3232	Q3136	L3058	K2977	
F4080	R3813	R3813	L3734	W3647		LEU	MET		V3233	V3137	L3059	L2976	Q2891
K4082	L3817	L3817	K3736		V3557	LYS	GLY		H3235	R3138	K3060	L2977	C2896
L4083			GLU	N3650	D3558	ALA	GLY		Q3236	R3139	R3061	I2984	T2897
L4084	ILE	ILE	ANG	S3651	R3559	CYS	LYS		T3237		A3062	D2985	L2898
L4085	LYS	LYS	LYS	L3652	S3560	GLY	LYS		I3238	M3140	G3063	V2986	E2899
M4086	LYS	LYS	LYS	P3653		PHO	LYS			F3145	K3065	P2987	G2900
	GLY	GLY	GLY	L3657	L3563	VAL	LEU		R3248		G3064	L2983	L2901
S4091	GLY	GLY	GLY	L3657	L3564	LYS	TRP			S3151	E3066	V2989	V2902
D4092	A3641		ARG	I3663	D3565	LYS	ALA		Y3254		E3067	V2990	K2903
R4093	S3842		ILE	M3664	N3566	THR	ASP		V3255	A3159	K3068	V2991	L2904
L4022	G3843		ILE		L3567	ALA	ASP		T3256	T3160	I3069	N2992	W2905
L4023	ILE	ILE	ILE	R3667		ARG	ILE		P3257	S3161		N2992	A2906
L4095	N3844		ILE	F3668	G3572	GLN	LYS		R3258			E2993	V2907
Q4096	L3846		ARG		K3571	THR	LYS		Q3259	P3162	Y3072	V2994	H2907
Q4025	D3847		LEU		K3573	THR	LYS		Y3260	A3163		L2995	E2908
Q4026	D3848		GLY	Y3671	K3574	THR	ILE			L3164		D2996	A2909
S4098	D3849		ASP	F3672	E3575	THR	MET					H2997	L2910
			GLN	L3673		SER	GLU		F3263		V3078		
F4101			GLN	V3674	T3583	GLU	PRO			M3166	L3079		
V4102			VAL	Q3584		ILE	ASN		V3267		S3081		

S4710	E4645	M4572	GLN	R4424	T4341	T4270	V4105	
	A4646	Q4573	ASN	R4425	I4342	I4271	A4193	
	G4647	Q4574	ILE	N4426	I4343	F4272	D4109	
	V4648	L4575	V4492	I4427	I4273	L4273	F4110	
	N4649	D4576	D4493	N4428	R4346	L4274	L4111	
	N4650	S4576	P4494	D4429			N4112	
	Q4653	S4581						T4113
		SER				N4349	F4277	L4200
		ASP	F4499	Q4430	L4431	E4350	R4278	E4201
		TYR	E4500	R4432	N4433	A4279		
S4721	D4658	SER	R4501	R4433	D4352	I4280	S4206	
	I4659	SER	E4502	Q4434		T4281	A4119	
	L4660	SER	T4503		L4355	Q4282	N4120	
	S4661	ILE		E4437	L4356	E4283	I4121	
	T4662	Q4588	GLU	L4430	I4357	R4284	E4123	
	A4663	N4590	GLY	ASP	S4358	L4285	K4124	
	L4664	L4509	GLY	GLY	F4359		E4125	
	S4665	L4510	GLU	L4360	L4360	T4288		
	L4666	G4592	ASP	ASP	E4361	P4289		
	A4667	G4593	ASP	GLN	Q4362			
S4728	T4668	N4596	L4517	VAL	F4364	T4293	P4131	
	L4669	P4597		SER	T4365	F4295	L4132	
	T4670	I4601	L4523	GLY		P4295	L4133	
	L4671	SER	ILE	SER	F4369	F4296	L4134	
	K4672	SER	SER	SER	N4370	E4297	A4135	
	D4673	GLY	D4371	LYS	I4371	A4224	S4136	
	S4674	ASN	ASN	LYS	D4372	L4225	F4137	
	D4675	LEU	ILE	GLU	F4373	R4304	P4138	
	ASP	E4617	F4529	SER	P4374	G4305		
	P4676	L4611	S4530	SER		A4306	D4141	
S4729	ILE		T4531	S4456	P4377	L4307	A4142	
	PHE	M4614		SER	S4378	D4308	S4143	
	ASN	SER	R4535		I4379	S4140	S4144	
	ASN	LEU	S4536	ARG	G4380	R4231	K4145	
	SER	E4617	L4537	ALA	H4391	T4310	V4146	
	SER	M4618		THR	L4381	D4311	D4147	
			S4540	ILE		I4312	D4148	
	K4685	L4621	L4541	LEU	T4388	N4313	F4149	
	L4686	H4622	S4542	THR	R4389	F4236	L4140	
	S4687	A4623	L4543	THR	I4390	S4237	L4162	
S4702	V4688	S4624	G4544	ALA	H4391	D4315	G4163	
	P4689	SER	T4545	THR		S4318		
	V4690	LEU	L4545	ILE	P4400		V4244	
	V4691	GLY	R4548	THR	E4401	S4322		
	L4692	LYS	E4549	GLU	L4402	N4323	T4251	
	N4693	ILE	N4550	THR	S4403	I4324	F4252	
		SER	K4551	LYS	T4404		I4253	
	L4696	SER	H4552	LEU	P4405	D4327	G4254	
	S4697	GLU	V4553	LEU	L4406	K4328	I4255	
	E4698	GLY	S4554	PRO	W4407	I4329	P4256	
S4703	S4702	ALA	V4555	LYS	G4408	A4330	A4257	
	I4703	S4636	P4556	PRO	L4410	N4331	T4258	
	D4704	F4637	L4557	LEU	I4411	T4332	R4259	
	L4705	N4638	T4558	LYS	P4411	A4333	M4260	
	P4706	V4639	GLN	LEU	E4412	V4334		
	V4707		L4561	LYS	M4413	T4336		
	D4708	M4642	F4568	ARG	E4415	I4337	Q4263	
	S4709	L4643	T4571	THR	K4422	L4338	P4264	
						G4339	A4265	
	D4710					S4340	E4266	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.78 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.0 (48.78-3.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.292 0.211 , 0.282	Depositor DCC
$R_{free}$ test set	4469 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 112.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/23866	0.44	1/32482 (0.0%)
1	B	0.24	0/22846	0.43	0/31076
All	All	0.24	0/46712	0.44	1/63558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3371	PRO	N-CA-CB	5.32	109.68	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23374	0	22545	1559	0
1	B	22384	0	21550	1149	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2704	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 30.

All (2704) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00
1:A:3373:ILE:HD13	1:A:3373:ILE:H	1.29	0.98
1:A:3673:LEU:HB2	1:A:3781:VAL:HG11	1.45	0.97
1:B:1959:THR:HG22	1:B:4341:THR:HA	1.46	0.96
1:B:1554:LEU:HB3	1:B:1609:GLN:HE22	1.29	0.95
1:B:4251:THR:HG23	1:B:4303:LEU:HD21	1.46	0.95
1:B:1928:HIS:CD2	1:B:1933:THR:HG22	2.02	0.95
1:A:4375:LEU:HD11	1:A:4383:VAL:HG23	1.48	0.95
1:B:3673:LEU:HB2	1:B:3781:VAL:HG11	1.44	0.95
1:A:3425:LYS:HD2	1:A:3428:GLU:HG3	1.49	0.94
1:B:2533:VAL:HB	1:B:2581:LEU:HD22	1.51	0.93
1:B:1655:LEU:HB2	1:B:1658:GLU:HB2	1.45	0.93
1:B:4574:GLN:HE22	1:B:4590:TRP:H	1.15	0.93
1:B:4121:ILE:HA	1:B:4125:GLU:HG3	1.48	0.93
1:A:2274:MET:HE3	1:A:2286:TRP:HB3	1.50	0.92
1:B:1972:PRO:HG2	1:B:2076:THR:HG22	1.52	0.92
1:A:4270:ILE:HA	1:A:4273:LEU:HD12	1.52	0.90
1:B:1789:LEU:HD23	1:B:1818:THR:HG23	1.50	0.90
1:A:3837:ALA:HB1	1:A:3850:SER:HB3	1.53	0.89
1:A:1639:ILE:HG23	1:A:1672:LEU:HD22	1.53	0.89
1:A:2313:LYS:HE3	1:A:2366:ASN:HD21	1.36	0.89
1:A:3018:SER:HB2	1:A:3256:THR:HG21	1.52	0.89
1:A:4495:LEU:H	1:A:4495:LEU:HD12	1.38	0.89
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.55	0.89
1:B:3930:LEU:HB3	1:B:3939:ARG:HH21	1.37	0.89
1:A:2200:ASN:HD22	1:A:2228:LEU:HD13	1.36	0.88
1:B:1813:GLN:HE22	1:B:1940:TYR:HA	1.37	0.88
1:B:2603:THR:HG22	1:B:2604:PRO:HD2	1.54	0.88
1:A:1690:GLN:HE22	1:A:1766:ILE:HG21	1.38	0.88
1:A:4046:GLN:HE22	1:A:4057:ILE:H	1.19	0.88
1:A:2447:GLN:HA	1:A:2450:ASN:HD22	1.39	0.88
1:B:4270:ILE:HG22	1:B:4310:ILE:HD13	1.55	0.88
1:B:1524:GLU:HG2	1:B:1580:TYR:HB3	1.57	0.87
1:A:3552:LYS:HA	1:A:3555:ASN:HD22	1.40	0.87
1:A:2570:THR:HG21	1:A:2603:THR:HG21	1.57	0.86
1:A:2914:GLN:HB2	1:A:2926:THR:HG21	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2381:ASN:HD21	1:B:2383:GLU:HB2	1.40	0.86
1:A:2200:ASN:HB2	1:A:2228:LEU:HD22	1.56	0.86
1:B:4604:THR:HG23	1:B:4671:TRP:HE1	1.40	0.86
1:A:4621:LEU:HD21	1:A:4669:LEU:HD23	1.55	0.86
1:B:3271:ILE:HG13	1:B:3592:VAL:HG11	1.57	0.86
1:A:2293:ILE:HG22	1:A:2350:ARG:HH22	1.41	0.85
1:B:4109:ASP:HA	1:B:4112:ASN:ND2	1.92	0.85
1:A:4686:LEU:HD21	1:A:4721:VAL:HG11	1.59	0.85
1:A:3809:THR:HA	1:A:3812:LYS:HE2	1.59	0.84
1:A:2560:MET:HG3	1:A:2561:SER:H	1.42	0.84
1:A:4251:THR:HG23	1:A:4303:LEU:HD21	1.58	0.84
1:B:2525:ILE:HD11	1:B:2815:LEU:HB2	1.58	0.84
1:A:4648:VAL:HG12	1:A:4662:THR:HG21	1.60	0.83
1:B:2841:ASN:ND2	1:B:2842:LEU:H	1.75	0.83
1:A:2910:LEU:HD23	1:A:2930:ILE:HD12	1.59	0.83
1:B:3930:LEU:HD11	1:B:3943:LEU:HD21	1.59	0.83
1:B:4548:LYS:HD2	1:B:4549:GLU:N	1.93	0.83
1:A:3718:LEU:HG	1:A:3719:LEU:H	1.42	0.83
1:B:4402:ILE:HD12	1:B:4402:ILE:H	1.42	0.83
1:A:4109:ASP:HA	1:A:4112:ASN:ND2	1.95	0.82
1:A:4190:ILE:HG12	1:A:4219:SER:HB3	1.61	0.82
1:A:3981:ASN:HD22	1:A:4076:ILE:HB	1.44	0.82
1:B:3785:ASN:HD21	1:B:3787:THR:HG23	1.43	0.82
1:B:2250:VAL:HB	1:B:2425:MET:HG3	1.60	0.82
1:B:1926:VAL:HG22	1:B:1935:TYR:CE2	2.15	0.82
1:A:3652:LEU:HD12	1:A:3653:PRO:HD2	1.62	0.82
1:B:1781:LEU:HG	1:B:1814:LEU:HD11	1.61	0.81
1:A:2651:VAL:HG13	1:A:2652:ASP:H	1.44	0.81
1:B:4657:THR:HG22	1:B:4659:ILE:H	1.45	0.81
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	1.61	0.81
1:A:4185:VAL:HG12	1:A:4186:LEU:H	1.44	0.81
1:B:2129:VAL:HG22	1:B:2130:PRO:HD3	1.62	0.81
1:B:4335:ARG:HH21	1:B:4365:THR:HG22	1.46	0.81
1:A:2371:LEU:CB	1:A:2410:ARG:HG3	2.10	0.81
1:A:3238:ILE:HG12	1:A:3601:TYR:CD2	2.16	0.81
1:A:3700:LEU:HD22	1:A:3701:ASP:H	1.43	0.80
1:A:3789:THR:HB	1:A:3790:PRO:HD2	1.63	0.80
1:A:2140:SER:HB2	1:A:2142:GLN:HE22	1.45	0.80
1:A:2857:TYR:HA	1:A:2913:PHE:HE1	1.46	0.80
1:A:2370:LEU:HD21	1:A:2387:LEU:HD13	1.64	0.80
1:A:4654:LEU:HD11	1:A:4705:LEU:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1660:LEU:HA	1:B:1665:ILE:HD11	1.63	0.80
1:A:2236:LEU:HD21	1:A:2293:ILE:HD13	1.63	0.80
1:A:3694:ILE:HG12	1:A:3717:PRO:HB2	1.63	0.80
1:A:4654:LEU:HD13	1:A:4686:LEU:HD23	1.62	0.79
1:A:2110:GLN:HG3	1:A:2122:GLU:HA	1.64	0.79
1:B:3607:GLN:HG2	1:B:3657:LEU:HD22	1.65	0.79
1:B:4270:ILE:HD11	1:B:4329:ILE:HD13	1.65	0.79
1:A:4086:MET:HG3	1:A:4093:ARG:HB2	1.65	0.79
1:A:4349:ASN:HD21	1:A:4351:PHE:HB2	1.46	0.79
1:A:2300:LYS:O	1:A:2349:LYS:HB2	1.81	0.79
1:B:4189:ASN:H	1:B:4218:THR:HG22	1.47	0.79
1:B:3844:ASN:O	1:B:3848:ASP:HB3	1.81	0.79
1:A:4353:MET:HE3	1:A:4356:LEU:HD23	1.64	0.78
1:A:2283:THR:HA	1:A:2286:TRP:HE1	1.48	0.78
1:A:2706:THR:HB	1:A:2707:PRO:HD2	1.65	0.78
1:A:2886:LEU:O	1:A:2890:ILE:HG12	1.84	0.78
1:B:2106:GLU:OE1	1:B:2129:VAL:HG21	1.82	0.78
1:B:4264:PRO:HB3	1:B:4323:ASN:HA	1.64	0.78
1:A:3673:LEU:HB2	1:A:3781:VAL:CG1	2.14	0.78
1:B:2657:VAL:HG13	1:B:2687:THR:HG23	1.64	0.78
1:B:3338:GLN:HG2	1:B:3525:LEU:HD13	1.65	0.78
1:A:1823:TRP:O	1:A:1827:VAL:HG23	1.84	0.78
1:A:2204:ILE:HA	1:A:2207:LEU:HD12	1.65	0.78
1:A:2705:THR:HA	1:A:2709:LEU:HD12	1.66	0.78
1:A:1796:ASP:HB3	1:A:1799:ASP:HB3	1.65	0.77
1:A:4575:LEU:H	1:A:4575:LEU:HD12	1.49	0.77
1:B:2578:MET:HB3	1:B:2597:ILE:HD12	1.65	0.77
1:B:4332:ILE:HD12	1:B:4332:ILE:H	1.48	0.77
1:B:4121:ILE:O	1:B:4125:GLU:HB2	1.85	0.77
1:B:3219:ILE:CB	1:B:3220:PRO:HD3	2.15	0.77
1:A:2766:MET:HB3	1:A:2783:LEU:HD11	1.67	0.76
1:A:4318:SER:HA	1:A:4321:ARG:HH21	1.50	0.76
1:A:3058:LEU:HD21	1:A:3141:LEU:HD11	1.67	0.76
1:A:3384:LYS:HD3	1:A:3386:LYS:HD3	1.66	0.76
1:B:3230:SER:HA	1:B:3620:ARG:HE	1.51	0.76
1:B:3313:LEU:HD13	1:B:3550:SER:HA	1.65	0.76
1:A:2505:TYR:O	1:A:2512:VAL:HG23	1.85	0.76
1:A:1959:THR:HA	1:A:4341:THR:OG1	1.85	0.76
1:B:3671:TYR:O	1:B:3781:VAL:HG13	1.86	0.76
1:B:4046:GLN:HG3	1:B:4047:PHE:N	2.00	0.76
1:B:4531:THR:O	1:B:4535:ARG:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.84	0.76
1:B:4067:ALA:HB1	1:B:4073:GLN:HG3	1.65	0.76
1:B:3639:SER:HB3	1:B:3663:ILE:HD11	1.68	0.76
1:A:1813:GLN:HE22	1:A:1940:TYR:HA	1.50	0.75
1:A:3927:ASN:HB3	1:A:3930:LEU:HB2	1.68	0.75
1:B:1822:VAL:HG22	1:B:1826:GLN:HE21	1.50	0.75
1:A:3731:ASN:H	1:A:3731:ASN:HD22	1.35	0.75
1:A:4122:VAL:HG21	1:A:4216:PHE:CZ	2.20	0.75
1:B:4011:LEU:HD11	1:B:4041:SER:HB2	1.68	0.75
1:A:2273:MET:HB2	1:A:2395:PHE:HB2	1.68	0.75
1:B:3027:ARG:HA	1:B:3037:ILE:HD11	1.68	0.75
1:B:3966:THR:HG22	1:B:4426:MET:HG3	1.68	0.75
1:B:2426:ILE:HD12	1:B:2426:ILE:H	1.51	0.75
1:A:3358:GLN:HA	1:A:3361:LYS:HE2	1.69	0.75
1:A:3443:MET:HG3	1:A:3449:ARG:HG3	1.68	0.75
1:A:3039:THR:HG22	1:A:3040:ILE:H	1.50	0.75
1:A:4622:HIS:HE2	1:A:4678:ILE:HG21	1.50	0.75
1:A:4648:VAL:HG13	1:A:4657:THR:HG21	1.68	0.75
1:B:3766:THR:HG22	1:B:3768:ASP:H	1.52	0.75
1:B:3035:LEU:HD22	1:B:3068:LYS:HB3	1.68	0.75
1:A:2586:GLY:HA2	1:A:2815:LEU:HD13	1.67	0.75
1:B:1950:THR:HB	1:B:1951:PRO:HD2	1.68	0.75
1:A:3015:ILE:HD13	1:A:3147:MET:HG3	1.68	0.74
1:B:2315:GLN:HB3	1:B:2775:THR:HG21	1.69	0.74
1:A:2397:VAL:HG21	1:A:2400:LEU:HD21	1.68	0.74
1:A:3696:LYS:HZ2	1:A:4206:SER:HB3	1.52	0.74
1:B:2638:THR:HG21	1:B:2838:LEU:HD21	1.68	0.74
1:A:1547:ASN:HA	1:A:1553:LYS:HG2	1.70	0.74
1:B:1476:ILE:HG23	1:B:1480:HIS:HB2	1.68	0.74
1:A:2105:ARG:HG2	1:A:2105:ARG:HH11	1.53	0.74
1:A:3774:THR:HB	1:A:3775:PRO:HD2	1.70	0.73
1:A:4122:VAL:HG21	1:A:4216:PHE:HZ	1.53	0.73
1:B:4278:HIS:HD2	1:B:4343:TYR:OH	1.71	0.73
1:A:2309:LYS:HE2	1:A:2756:THR:HG21	1.68	0.73
1:A:4053:VAL:O	1:A:4053:VAL:HG12	1.86	0.73
1:A:3388:LEU:HD23	1:A:3473:ALA:HB1	1.68	0.73
1:A:2793:ASN:HD22	1:A:2793:ASN:N	1.85	0.73
1:A:3725:ASN:HD22	1:A:3725:ASN:H	1.35	0.73
1:A:3281:GLU:HB3	1:A:3581:PHE:HE1	1.54	0.73
1:A:1886:ARG:HG3	1:A:1887:ASP:N	2.04	0.73
1:B:3700:LEU:HD13	1:B:3701:ASP:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3202:PRO:HD2	1:A:3624:VAL:O	1.88	0.73
1:B:3602:ILE:HG23	1:B:3610:ARG:HG2	1.70	0.73
1:A:2675:PRO:HD2	1:A:2816:VAL:O	1.88	0.73
1:A:3453:THR:HA	1:A:3457:LEU:HB2	1.70	0.73
1:B:2572:ARG:HG2	1:B:2617:VAL:HG11	1.69	0.73
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	2.04	0.73
1:B:4157:TYR:HB3	1:B:4184:TRP:HB2	1.71	0.73
1:A:2080:GLY:HA3	1:A:2084:ARG:O	1.89	0.73
1:B:3789:THR:HB	1:B:3790:PRO:HD2	1.70	0.73
1:B:4189:ASN:HD22	1:B:4189:ASN:N	1.85	0.73
1:A:3475:GLY:O	1:A:3478:VAL:HG12	1.88	0.73
1:A:4024:ARG:HD3	1:A:4034:VAL:HG21	1.71	0.73
1:B:3584:GLN:O	1:B:3588:VAL:HG23	1.87	0.73
1:B:2514:LYS:HE2	1:B:2600:ILE:HD11	1.71	0.72
1:A:1655:LEU:HB2	1:A:1658:GLU:HB2	1.69	0.72
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	1.70	0.72
1:A:3281:GLU:HB3	1:A:3581:PHE:CE1	2.24	0.72
1:A:3724:GLU:OE2	1:A:3766:THR:HG23	1.88	0.72
1:B:4136:SER:HB3	1:B:4238:TYR:HB2	1.72	0.72
1:B:1899:THR:HB	1:B:1903:ASP:HB2	1.72	0.72
1:B:2938:PHE:O	1:B:2941:VAL:HG12	1.88	0.72
1:B:4005:ILE:HD13	1:B:4020:LEU:HD23	1.70	0.72
1:A:2042:GLN:HE21	1:A:2059:LEU:HD11	1.54	0.72
1:B:2841:ASN:HD22	1:B:2842:LEU:H	1.37	0.72
1:A:1763:GLY:N	1:A:1764:PRO:HD3	2.04	0.72
1:A:2626:LEU:HD12	1:A:2626:LEU:H	1.55	0.71
1:A:2587:LEU:HG	1:A:2817:ASP:HB2	1.72	0.71
1:A:3700:LEU:HD13	1:A:3701:ASP:N	2.04	0.71
1:B:3292:LEU:HD13	1:B:3571:ARG:HA	1.72	0.71
1:B:4601:ILE:O	1:B:4604:THR:HG22	1.90	0.71
1:A:2042:GLN:NE2	1:A:2059:LEU:HD11	2.06	0.71
1:A:1742:ILE:HG22	1:A:1753:THR:HG22	1.71	0.71
1:A:3555:ASN:HB3	1:A:3559:ARG:NH1	2.04	0.71
1:A:4347:ILE:HG21	1:A:4353:MET:HG2	1.72	0.71
1:B:2839:LEU:HD13	1:B:2842:LEU:HD12	1.70	0.71
1:B:4506:GLY:O	1:B:4510:VAL:HG23	1.91	0.71
1:A:2371:LEU:HB3	1:A:2410:ARG:HG3	1.71	0.71
1:B:3700:LEU:HD22	1:B:3701:ASP:H	1.54	0.71
1:A:1807:VAL:HG13	1:A:1815:VAL:HG11	1.73	0.71
1:A:2208:VAL:HA	1:A:2415:TRP:CD1	2.24	0.71
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3674:VAL:HG22	1:B:3784:VAL:HB	1.71	0.71
1:A:4242:PRO:HA	1:A:4286:ARG:NH1	2.01	0.71
1:A:4553:TYR:H	1:A:4553:TYR:HD1	1.38	0.71
1:B:3234:ILE:HG23	1:B:3617:TRP:NE1	2.06	0.71
1:A:2176:ASP:N	1:A:2179:SER:HG	1.87	0.71
1:A:2258:LYS:HA	1:A:2261:GLN:HG3	1.71	0.71
1:A:3859:LYS:O	1:A:3862:THR:HG22	1.90	0.71
1:A:4533:TYR:O	1:A:4537:LEU:HG	1.90	0.71
1:B:4157:TYR:CB	1:B:4184:TRP:HB2	2.21	0.71
1:A:3037:ILE:H	1:A:3037:ILE:HD13	1.56	0.71
1:A:4591:LEU:HD21	1:A:4601:ILE:HD11	1.72	0.71
1:A:2942:ASN:O	1:A:2944:ASP:N	2.24	0.71
1:A:4029:SER:HB2	1:A:4081:ARG:HH12	1.56	0.71
1:B:4703:ILE:HD12	1:B:4705:LEU:HD21	1.71	0.71
1:B:2282:LYS:HA	1:B:2416:PHE:CD1	2.26	0.71
1:A:4494:PRO:HG2	1:A:4607:SER:HA	1.73	0.70
1:B:2124:LEU:HD22	1:B:2195:LEU:HD22	1.71	0.70
1:B:4574:GLN:HE22	1:B:4590:TRP:N	1.89	0.70
1:B:1823:TRP:CD1	1:B:1885:GLN:HB3	2.26	0.70
1:A:1879:ILE:O	1:A:1883:VAL:HG23	1.91	0.70
1:A:2006:LEU:HD23	1:A:2035:ILE:HG23	1.73	0.70
1:A:2371:LEU:HB2	1:A:2410:ARG:HG3	1.71	0.70
1:A:4540:SER:HB2	1:A:4545:ILE:O	1.91	0.70
1:B:1879:ILE:O	1:B:1883:VAL:HG23	1.91	0.70
1:B:3238:ILE:CG2	1:B:3255:VAL:HG11	2.20	0.70
1:A:2113:LEU:HD21	1:A:2156:LEU:HD22	1.74	0.70
1:A:2788:PHE:O	1:A:2789:VAL:HG23	1.90	0.70
1:A:3153:ASP:HA	1:A:3156:ASN:ND2	2.06	0.70
1:A:3677:PRO:HG3	1:A:3787:THR:HG22	1.72	0.70
1:A:4095:LEU:HD11	1:A:4422:LYS:HB3	1.73	0.70
1:A:4649:TRP:HA	1:A:4649:TRP:CE3	2.27	0.70
1:A:2106:GLU:CD	1:A:2106:GLU:H	1.95	0.70
1:A:2954:ASN:HD22	1:A:2954:ASN:H	1.39	0.70
1:A:2308:PRO:HD2	1:A:2357:GLY:HA3	1.74	0.70
1:A:4179:ALA:HB1	1:A:4209:PRO:HB3	1.73	0.70
1:A:3380:VAL:HG11	1:A:3435:ILE:HG21	1.72	0.70
1:A:3812:LYS:O	1:A:3816:LEU:HB3	1.91	0.70
1:B:1928:HIS:NE2	1:B:1933:THR:HG22	2.06	0.70
1:A:3331:GLN:HE22	1:A:3533:LYS:HG3	1.56	0.69
1:A:4086:MET:CG	1:A:4093:ARG:HB2	2.21	0.69
1:B:2850:THR:O	1:B:2854:VAL:HG23	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3433:THR:HG22	1:A:3437:ASN:ND2	2.06	0.69
1:B:1687:LEU:HD21	1:B:1706:LEU:HD23	1.74	0.69
1:B:2540:LEU:HD23	1:B:2576:SER:HA	1.72	0.69
1:A:1846:GLN:HA	1:A:1893:GLN:NE2	2.08	0.69
1:A:4128:SER:HB2	1:A:4213:PHE:HB3	1.74	0.69
1:B:1739:THR:HB	1:B:1761:ALA:HB2	1.74	0.69
1:B:3700:LEU:HD12	1:B:3700:LEU:H	1.58	0.69
1:B:2235:GLN:NE2	1:B:2296:VAL:HG13	2.06	0.69
1:A:3912:SER:HB3	1:A:4231:ARG:HG2	1.75	0.69
1:B:1846:GLN:O	1:B:1850:GLN:HG2	1.92	0.69
1:B:3238:ILE:HG12	1:B:3601:TYR:CG	2.28	0.69
1:A:2028:PHE:HB3	1:A:2075:VAL:HG13	1.72	0.69
1:B:1534:VAL:HG13	1:B:1568:HIS:HD2	1.58	0.69
1:B:3238:ILE:HG21	1:B:3255:VAL:HG11	1.73	0.69
1:B:3256:THR:HB	1:B:3257:PRO:HD2	1.74	0.69
1:B:3768:ASP:HB3	1:B:3771:ALA:HB2	1.73	0.69
1:A:1746:SER:OG	1:A:1750:GLU:HB3	1.93	0.69
1:A:2202:THR:HG22	1:A:2265:ILE:HG12	1.74	0.69
1:B:2200:ASN:HB2	1:B:2228:LEU:HD22	1.75	0.69
1:B:2282:LYS:HA	1:B:2416:PHE:HD1	1.57	0.69
1:A:4623:ALA:HB2	1:A:4703:ILE:HD11	1.75	0.69
1:A:1770:LEU:O	1:A:1773:VAL:HG22	1.93	0.69
1:B:4005:ILE:CD1	1:B:4020:LEU:HD23	2.24	0.68
1:A:2748:LEU:HD21	1:A:2800:ARG:NH1	2.09	0.68
1:B:3724:GLU:OE2	1:B:3766:THR:HG23	1.93	0.68
1:B:4362:GLN:HB2	1:B:4714:GLN:NE2	2.08	0.68
1:B:2865:THR:H	1:B:2868:ILE:HD12	1.58	0.68
1:B:4574:GLN:NE2	1:B:4590:TRP:H	1.87	0.68
1:A:1886:ARG:NH1	1:A:1890:ARG:HH22	1.91	0.68
1:B:3652:LEU:HD12	1:B:3653:PRO:HD2	1.74	0.68
1:A:3210:GLU:HG3	1:A:3211:ILE:H	1.57	0.68
1:B:1545:LEU:H	1:B:1545:LEU:HD12	1.57	0.68
1:B:3043:ASN:ND2	1:B:3046:TYR:HB2	2.07	0.68
1:A:1554:LEU:HB3	1:A:1609:GLN:HE21	1.59	0.68
1:A:2010:SER:HB3	1:A:2060:LEU:HD21	1.75	0.68
1:B:1743:GLY:HA2	1:B:1754:PHE:CD1	2.29	0.68
1:B:2320:LEU:HD23	1:B:2320:LEU:O	1.93	0.68
1:A:4200:LEU:HD22	1:A:4204:LEU:HD11	1.75	0.68
1:A:1715:ILE:HD11	1:A:1760:ILE:HD13	1.74	0.68
1:A:1931:ASN:OD1	1:A:1962:GLN:NE2	2.25	0.68
1:A:2293:ILE:CG2	1:A:2350:ARG:HH22	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2400:LEU:HD13	1:B:2408:ILE:HD11	1.76	0.68
1:A:1846:GLN:HA	1:A:1893:GLN:HE22	1.59	0.67
1:A:2742:PHE:HA	1:A:2789:VAL:O	1.94	0.67
1:A:3961:ASN:O	1:A:3964:LYS:HB2	1.94	0.67
1:A:2699:LEU:HD11	1:A:2713:THR:HG21	1.77	0.67
1:A:3013:LEU:HD12	1:A:3145:PHE:HB3	1.74	0.67
1:B:2231:ILE:HG21	1:B:2264:GLN:NE2	2.09	0.67
1:A:2212:ILE:HG22	1:A:2213:PRO:HD3	1.77	0.67
1:B:4251:THR:HG23	1:B:4303:LEU:CD2	2.23	0.67
1:A:3563:LEU:HD11	1:A:3851:VAL:HG22	1.77	0.67
1:B:2793:ASN:HB3	1:B:2794:PRO:HD2	1.76	0.67
1:A:1963:ALA:HB1	1:A:2096:ARG:HG3	1.76	0.67
1:A:2447:GLN:HE22	1:A:2492:LEU:HD23	1.58	0.67
1:A:3397:PRO:HG2	1:A:3419:TRP:CZ2	2.29	0.67
1:B:4189:ASN:H	1:B:4218:THR:CG2	2.08	0.67
1:B:2815:LEU:HD23	1:B:2816:VAL:N	2.09	0.67
1:B:4189:ASN:H	1:B:4189:ASN:HD22	1.40	0.67
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.30	0.67
1:A:4210:HIS:ND1	1:A:4211:PRO:HD2	2.09	0.67
1:A:4259:ARG:HD3	1:A:4271:TYR:OH	1.95	0.67
1:A:2014:VAL:HG13	1:A:2065:ILE:HG21	1.78	0.66
1:A:4548:LYS:HG3	1:A:4549:GLU:H	1.60	0.66
1:B:1719:GLN:HA	1:B:1722:PHE:CD2	2.29	0.66
1:B:3078:VAL:HG23	1:B:3083:PHE:HB2	1.76	0.66
1:B:3958:THR:HG23	1:B:4235:VAL:HB	1.76	0.66
1:B:2297:ASP:O	1:B:2299:ILE:HG13	1.94	0.66
1:B:2361:PRO:HD3	1:B:2402:TYR:O	1.96	0.66
1:A:2595:LYS:HE3	1:A:2611:PRO:HG3	1.75	0.66
1:A:4270:ILE:HD13	1:A:4314:VAL:HG21	1.78	0.66
1:B:2423:THR:HG23	1:B:2530:ARG:HD2	1.76	0.66
1:B:2766:MET:HB3	1:B:2783:LEU:HD11	1.75	0.66
1:A:2108:ILE:O	1:A:2112:MET:HB2	1.96	0.66
1:A:3875:VAL:O	1:A:3879:ILE:HG12	1.95	0.66
1:A:3925:ASN:N	1:A:3925:ASN:HD22	1.93	0.66
1:B:2861:GLN:HG3	1:B:2874:TYR:HB2	1.75	0.66
1:A:3245:LEU:HD12	1:A:3249:GLN:HB2	1.78	0.66
1:A:4572:MET:HE1	1:A:4575:LEU:HD11	1.77	0.66
1:A:2124:LEU:HD22	1:A:2195:LEU:HD22	1.78	0.66
1:A:2125:ALA:HA	1:A:2128:ILE:HG22	1.78	0.66
1:B:2113:LEU:HD21	1:B:2156:LEU:HD22	1.78	0.66
1:A:2315:GLN:HB3	1:A:2775:THR:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2910:LEU:CD2	1:A:2930:ILE:HD12	2.25	0.66
1:A:3309:LYS:O	1:A:3313:LEU:HG	1.96	0.66
1:B:1769:TRP:O	1:B:1773:VAL:HG23	1.96	0.66
1:B:2984:LEU:HD22	1:B:2986:VAL:HG22	1.78	0.66
1:A:3989:ASP:O	1:A:3993:LYS:HB2	1.96	0.66
1:B:1885:GLN:O	1:B:1889:VAL:HG23	1.96	0.66
1:B:3785:ASN:ND2	1:B:3787:THR:HG23	2.11	0.66
1:A:3410:LEU:HD22	1:A:3452:ILE:HD11	1.78	0.65
1:A:3647:TRP:HB3	1:A:3652:LEU:HD23	1.78	0.65
1:A:3965:LEU:HG	1:A:4426:MET:HE3	1.77	0.65
1:A:4230:LEU:H	1:A:4230:LEU:HD12	1.61	0.65
1:A:2289:TYR:O	1:A:2293:ILE:HG12	1.95	0.65
1:A:3285:LEU:HD13	1:A:3578:SER:HA	1.78	0.65
1:A:2535:ASN:HD22	1:A:2668:ARG:HH12	1.45	0.65
1:A:3271:ILE:HG13	1:A:3592:VAL:HG11	1.78	0.65
1:A:4186:LEU:C	1:A:4187:LEU:HD12	2.17	0.65
1:B:1901:ASN:HD22	1:B:1901:ASN:H	1.43	0.65
1:B:2498:CYS:HA	1:B:2501:ILE:HD12	1.77	0.65
1:B:3639:SER:HB3	1:B:3663:ILE:CD1	2.25	0.65
1:A:2552:ASN:HD21	1:A:2560:MET:HB2	1.59	0.65
1:A:3700:LEU:CD2	1:A:3701:ASP:H	2.09	0.65
1:A:4054:GLY:O	1:A:4055:GLU:C	2.34	0.65
1:B:2359:VAL:HG13	1:B:2364:VAL:HG21	1.79	0.65
1:B:3813:ARG:O	1:B:3817:LEU:HD13	1.97	0.65
1:A:2975:ARG:HE	1:A:2975:ARG:HA	1.61	0.65
1:B:2339:ILE:HA	1:B:2346:GLU:HG2	1.76	0.65
1:A:1537:PHE:O	1:A:1541:LEU:HB2	1.97	0.65
1:A:2948:ARG:HG2	1:A:2948:ARG:HH11	1.62	0.65
1:A:3015:ILE:HG22	1:A:3149:PRO:HG3	1.77	0.65
1:A:3242:ASN:OD1	1:A:3253:ASN:HB3	1.96	0.65
1:A:4024:ARG:HG3	1:A:4031:SER:HA	1.78	0.65
1:A:4622:HIS:ND1	1:A:4623:ALA:N	2.45	0.65
1:A:2120:THR:O	1:A:2121:ALA:C	2.33	0.65
1:A:3255:VAL:HA	1:A:3259:HIS:HD2	1.61	0.65
1:B:1920:ASN:HD22	1:B:1921:VAL:H	1.44	0.65
1:B:3949:SER:HA	1:B:4110:PHE:HE1	1.62	0.65
1:A:1748:GLU:HG2	1:A:1943:ILE:HB	1.79	0.65
1:A:2305:VAL:HG21	1:A:2769:LYS:HE2	1.79	0.65
1:A:4553:TYR:HB3	1:A:4595:LEU:HD23	1.79	0.65
1:A:4649:TRP:HA	1:A:4649:TRP:HE3	1.60	0.65
1:B:3109:MET:HB3	1:B:3129:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4389:ARG:HG2	1:B:4389:ARG:HH11	1.62	0.65
1:A:2127:LYS:C	1:A:2130:PRO:HD2	2.17	0.64
1:A:2129:VAL:HB	1:A:2130:PRO:HD3	1.78	0.64
1:A:2968:LEU:O	1:A:2972:VAL:HG23	1.97	0.64
1:A:3270:LEU:HB2	1:A:3592:VAL:HG13	1.77	0.64
1:A:4221:ILE:H	1:A:4221:ILE:HD12	1.62	0.64
1:B:3063:GLY:HA2	1:B:3136:GLN:HB3	1.78	0.64
1:B:4063:ILE:H	1:B:4063:ILE:HD12	1.62	0.64
1:B:1931:ASN:HB2	1:B:4312:TYR:CZ	2.32	0.64
1:A:2704:ALA:HB3	1:A:3085:GLU:HG3	1.77	0.64
1:B:4288:ILE:HG23	1:B:4292:TRP:O	1.97	0.64
1:A:2606:PRO:HD3	1:A:2624:TRP:CD1	2.32	0.64
1:A:3700:LEU:H	1:A:3700:LEU:HD12	1.62	0.64
1:A:1921:VAL:HG23	1:A:1922:LEU:HD22	1.79	0.64
1:A:2525:ILE:HG13	1:A:2584:SER:O	1.98	0.64
1:A:2651:VAL:HG13	1:A:2652:ASP:N	2.12	0.64
1:A:3387:HIS:CB	1:A:3473:ALA:HB2	2.27	0.64
1:B:1811:PRO:O	1:B:1815:VAL:HG23	1.98	0.64
1:B:2866:PRO:HG3	1:B:2873:ILE:HG22	1.78	0.64
1:A:1811:PRO:HD2	1:A:1814:LEU:HD12	1.78	0.64
1:A:3528:SER:O	1:A:3531:THR:HG22	1.98	0.64
1:B:4188:LYS:HA	1:B:4218:THR:HG22	1.80	0.64
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.80	0.64
1:A:4349:ASN:HD22	1:A:4352:ASP:N	1.95	0.64
1:A:2199:ILE:O	1:A:2203:MET:HB2	1.98	0.64
1:A:2273:MET:CB	1:A:2395:PHE:HB2	2.27	0.64
1:A:2506:PHE:CD1	1:A:2512:VAL:HG21	2.33	0.64
1:A:4050:LYS:O	1:A:4052:GLN:N	2.30	0.64
1:B:3991:LEU:O	1:B:4427:ILE:HD12	1.98	0.64
1:A:1545:LEU:HB3	1:A:1553:LYS:HE2	1.80	0.64
1:A:2979:PHE:CE2	1:A:3028:PHE:HA	2.33	0.64
1:A:3696:LYS:NZ	1:A:4206:SER:HB3	2.13	0.64
1:A:3897:TYR:HE1	1:A:3913:LEU:HA	1.63	0.64
1:A:4296:PHE:CE2	1:A:4347:ILE:HD13	2.33	0.64
1:B:3299:VAL:HG11	1:B:3564:LEU:HG	1.78	0.64
1:A:3114:GLU:HG2	1:A:3118:ARG:NH1	2.13	0.64
1:A:4693:ASN:N	1:A:4693:ASN:HD22	1.95	0.64
1:B:1694:PHE:HB3	1:B:1697:PHE:CD2	2.33	0.64
1:B:1554:LEU:HD12	1:B:2323:THR:HG22	1.79	0.64
1:B:4548:LYS:HD2	1:B:4549:GLU:H	1.59	0.64
1:A:1611:ARG:HH11	1:A:1611:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2051:LYS:O	1:A:2051:LYS:HD3	1.96	0.64
1:A:2163:LYS:HB2	1:A:2194:VAL:HG11	1.79	0.64
1:A:2207:LEU:HD13	1:A:2215:ILE:HG21	1.79	0.64
1:A:3293:ARG:HG3	1:A:3293:ARG:HH11	1.63	0.64
1:A:3785:ASN:HD22	1:A:3786:PHE:N	1.95	0.64
1:A:3804:THR:O	1:A:3807:PRO:HD3	1.98	0.64
1:A:4362:GLN:HG3	1:A:4714:GLN:OE1	1.97	0.64
1:B:1557:GLY:O	1:B:1561:LEU:HD23	1.98	0.64
1:B:4351:PHE:CE2	1:B:4689:PRO:HG3	2.32	0.64
1:A:2490:ALA:O	1:A:2494:VAL:HG23	1.97	0.63
1:A:4296:PHE:CE2	1:A:4347:ILE:HA	2.33	0.63
1:A:4396:ILE:O	1:A:4399:LEU:HB2	1.98	0.63
1:B:3043:ASN:HD22	1:B:3046:TYR:HB2	1.63	0.63
1:B:3087:MET:CE	1:B:3090:LEU:HD23	2.28	0.63
1:A:3387:HIS:HB3	1:A:3473:ALA:HB2	1.80	0.63
1:B:4607:SER:O	1:B:4611:LEU:HG	1.98	0.63
1:A:1811:PRO:O	1:A:1815:VAL:HG23	1.98	0.63
1:A:3416:LYS:HE3	1:A:3418:GLU:HB3	1.80	0.63
1:A:3711:ALA:HA	1:A:3716:CYS:SG	2.39	0.63
1:A:4277:PHE:HB2	1:A:4363:LEU:HD12	1.79	0.63
1:B:1525:ILE:HA	1:B:1528:GLU:HB3	1.80	0.63
1:B:1607:ASP:O	1:B:1611:ARG:HG2	1.97	0.63
1:B:1780:THR:HG22	1:B:1784:LEU:HD12	1.80	0.63
1:B:3563:LEU:HD11	1:B:3845:ILE:HD11	1.79	0.63
1:A:3985:GLU:O	1:A:3989:ASP:HB2	1.97	0.63
1:A:4571:ARG:HA	1:A:4590:TRP:HZ3	1.63	0.63
1:A:2995:LEU:HA	1:A:2998:ILE:HD11	1.80	0.63
1:B:1523:GLY:HA3	1:B:1580:TYR:CE2	2.33	0.63
1:B:3238:ILE:HD11	1:B:3617:TRP:HZ2	1.63	0.63
1:A:2938:PHE:HB3	1:A:2941:VAL:HG23	1.80	0.63
1:A:2972:VAL:O	1:A:2976:LEU:HB2	1.98	0.63
1:A:3482:THR:O	1:A:3486:TYR:HB2	1.99	0.63
1:A:3994:GLY:HA3	1:A:4087:LYS:CE	2.29	0.63
1:A:4310:ILE:O	1:A:4314:VAL:HB	1.99	0.63
1:A:2995:LEU:HD23	1:A:2998:ILE:HD11	1.80	0.63
1:A:3063:GLY:HA2	1:A:3136:GLN:HB3	1.81	0.63
1:B:3841:ALA:O	1:B:3842:SER:CB	2.35	0.63
1:A:2000:CYS:SG	1:A:2031:LEU:HD11	2.37	0.63
1:A:3255:VAL:HA	1:A:3259:HIS:CD2	2.33	0.63
1:A:3445:THR:HG23	1:A:3449:ARG:NH1	2.14	0.63
1:A:4269:ARG:CZ	1:A:4383:VAL:HG11	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1592:ASP:O	1:B:1596:ASN:HB2	1.99	0.63
1:B:3035:LEU:CD2	1:B:3068:LYS:HB3	2.28	0.63
1:B:4133:LEU:HD23	1:B:4230:LEU:HD23	1.79	0.63
1:B:2711:LEU:HD12	1:B:2714:PHE:HD2	1.63	0.63
1:B:2751:THR:HB	1:B:2756:THR:H	1.63	0.63
1:A:2250:VAL:HB	1:A:2425:MET:HE2	1.80	0.62
1:A:3300:LYS:HA	1:A:3564:LEU:HD11	1.81	0.62
1:A:3647:TRP:CH2	1:A:3663:ILE:HD12	2.34	0.62
1:A:3725:ASN:H	1:A:3725:ASN:ND2	1.96	0.62
1:A:4049:GLY:O	1:A:4050:LYS:O	2.17	0.62
1:B:2841:ASN:HD22	1:B:2841:ASN:N	1.97	0.62
1:A:1922:LEU:HD13	1:A:1938:PHE:HD1	1.63	0.62
1:B:3865:ILE:O	1:B:3869:VAL:HG23	1.98	0.62
1:B:4194:PRO:O	1:B:4197:LEU:HB2	1.99	0.62
1:A:2247:ARG:HB2	1:A:2249:LEU:HG	1.81	0.62
1:A:2542:ASN:O	1:A:2546:VAL:HG23	1.99	0.62
1:A:3599:LEU:HD11	1:A:3638:LEU:HD13	1.80	0.62
1:B:2877:ARG:HB3	1:B:2881:ARG:HH12	1.63	0.62
1:A:1695:ALA:HB1	1:A:2019:CYS:SG	2.39	0.62
1:A:2205:PRO:HG2	1:A:2265:ILE:HD11	1.81	0.62
1:A:1743:GLY:HA3	1:A:1753:THR:HA	1.81	0.62
1:A:1975:PRO:HD2	1:A:2101:ILE:HA	1.80	0.62
1:A:2546:VAL:HA	1:A:2549:ILE:HD12	1.80	0.62
1:A:2793:ASN:ND2	1:A:2793:ASN:N	2.44	0.62
1:B:2080:GLY:HA2	1:B:2086:ASN:ND2	2.14	0.62
1:A:1927:ILE:HD13	1:A:1991:LEU:HD22	1.79	0.62
1:A:3011:HIS:ND1	1:A:3143:VAL:HG23	2.15	0.62
1:B:2277:PRO:HA	1:B:2398:GLN:HG3	1.81	0.62
1:B:3844:ASN:O	1:B:3848:ASP:CB	2.47	0.62
1:B:2584:SER:HB3	1:B:2813:ILE:HB	1.82	0.62
1:A:1957:TYR:CD2	1:A:1987:LEU:HD13	2.35	0.62
1:A:2645:ASP:O	1:A:2647:VAL:HG23	1.98	0.62
1:A:3557:VAL:O	1:A:3561:ILE:HG13	2.00	0.62
1:B:2199:ILE:HG23	1:B:2203:MET:HG3	1.81	0.62
1:B:2206:LYS:HB3	1:B:2413:MET:HB3	1.81	0.62
1:A:3408:VAL:HG11	1:A:3477:LEU:HG	1.82	0.62
1:A:3452:ILE:HG21	1:A:3485:THR:HG21	1.82	0.62
1:A:3634:VAL:HB	1:A:3635:PRO:HD3	1.82	0.62
1:A:3812:LYS:HB3	1:A:3875:VAL:HG22	1.81	0.62
1:A:4389:ARG:HG2	1:A:4389:ARG:HH11	1.65	0.62
1:A:3566:ASN:HB3	1:A:3855:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4568:PHE:O	1:A:4572:MET:HG2	2.00	0.62
1:B:1726:PHE:CD2	1:B:1729:LEU:HD22	2.35	0.62
1:B:4410:LEU:HD22	1:B:4411:PRO:HD2	1.81	0.62
1:A:1967:ARG:HH22	1:A:2069:GLN:HG3	1.63	0.61
1:A:2151:ALA:O	1:A:2155:VAL:HG12	1.99	0.61
1:A:4402:ILE:HD12	1:A:4402:ILE:H	1.65	0.61
1:A:2357:GLY:O	1:A:2397:VAL:HG12	2.00	0.61
1:A:2954:ASN:H	1:A:2954:ASN:ND2	1.97	0.61
1:A:3445:THR:N	1:A:3446:PRO:HD2	2.16	0.61
1:B:2275:VAL:HG13	1:B:2397:VAL:HG13	1.82	0.61
1:A:2090:ASN:HD22	1:A:2090:ASN:C	2.02	0.61
1:A:2912:LEU:C	1:A:2913:PHE:HD2	2.04	0.61
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.35	0.61
1:B:2212:ILE:N	1:B:2213:PRO:HD2	2.15	0.61
1:A:2239:LYS:HA	1:A:2239:LYS:HE3	1.81	0.61
1:A:2243:ILE:HD12	1:A:2292:ALA:HB2	1.82	0.61
1:A:2670:LEU:HG	1:A:2789:VAL:HG22	1.83	0.61
1:A:3271:ILE:O	1:A:3275:ARG:HB2	2.00	0.61
1:B:2208:VAL:HG23	1:B:2211:ASP:HB2	1.81	0.61
1:B:2704:ALA:HB2	1:B:3085:GLU:OE2	1.98	0.61
1:B:3664:MET:O	1:B:3668:PHE:HB3	1.99	0.61
1:B:4402:ILE:HD12	1:B:4402:ILE:N	2.14	0.61
1:A:3260:TYR:O	1:A:3264:ILE:HG12	2.01	0.61
1:A:3731:ASN:N	1:A:3731:ASN:HD22	1.97	0.61
1:A:2258:LYS:HD3	1:A:2261:GLN:HG3	1.83	0.61
1:A:2262:LEU:HD11	1:A:2274:MET:HE2	1.81	0.61
1:A:2272:VAL:O	1:A:2394:MET:HA	2.00	0.61
1:A:2791:ALA:O	1:A:2792:CYS:HB3	2.00	0.61
1:A:2869:GLN:HB3	1:A:2872:TYR:CD1	2.36	0.61
1:A:4329:ILE:HD12	1:A:4331:TRP:CZ2	2.35	0.61
1:B:2140:SER:O	1:B:2142:GLN:HG2	1.99	0.61
1:B:3673:LEU:HB2	1:B:3781:VAL:CG1	2.26	0.61
1:A:2948:ARG:HD3	1:A:2950:ILE:HG13	1.82	0.61
1:A:4076:ILE:HD11	1:A:4104:SER:O	2.00	0.61
1:A:4589:VAL:HG12	1:A:4638:ASN:O	2.01	0.61
1:A:2088:PRO:HB2	1:A:2090:ASN:ND2	2.15	0.61
1:A:3474:CYS:HA	1:A:3477:LEU:HD22	1.83	0.61
1:A:3686:MET:HE2	1:A:3696:LYS:HD2	1.81	0.61
1:A:4600:TYR:O	1:A:4604:THR:HG23	2.01	0.61
1:B:2305:VAL:HG22	1:B:2354:ILE:HB	1.83	0.61
1:B:2732:PRO:HG3	1:B:2739:LEU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3587:THR:HB	1:A:3628:PHE:HA	1.82	0.61
1:B:2586:GLY:HA2	1:B:2815:LEU:HD13	1.81	0.61
1:B:3291:LYS:HD2	1:B:3835:LEU:HG	1.81	0.61
1:B:4189:ASN:N	1:B:4218:THR:HG22	2.14	0.61
1:A:2190:TYR:O	1:A:2194:VAL:HG23	2.01	0.61
1:A:2985:ASP:O	1:A:2987:PRO:HD3	2.01	0.61
1:A:4624:SER:HB2	1:A:4668:THR:HB	1.83	0.61
1:B:3650:ASN:OD1	1:B:3688:GLN:HA	2.00	0.61
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.01	0.60
1:A:3385:LYS:O	1:A:3389:ASP:HB2	2.00	0.60
1:A:4396:ILE:HA	1:A:4399:LEU:HD12	1.83	0.60
1:A:4503:ILE:HG23	1:A:4575:LEU:HB3	1.82	0.60
1:B:2582:GLY:HA2	1:B:2585:MET:HE3	1.81	0.60
1:B:2869:GLN:HB2	1:B:2872:TYR:CG	2.36	0.60
1:B:4135:CYS:HA	1:B:4219:SER:O	2.00	0.60
1:A:1687:LEU:HD22	1:A:1705:LEU:HD23	1.83	0.60
1:A:3137:VAL:HG13	1:A:3141:LEU:HD23	1.82	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:HE2	1.83	0.60
1:A:4590:TRP:CE3	1:A:4593:GLY:HA3	2.36	0.60
1:B:3559:ARG:NE	1:B:3846:LEU:O	2.35	0.60
1:A:3239:GLY:O	1:A:3243:ILE:HG13	2.00	0.60
1:A:4536:SER:HB2	1:A:4548:LYS:NZ	2.16	0.60
1:A:4636:SER:HB3	1:A:4670:THR:HA	1.83	0.60
1:A:2144:HIS:HB2	1:A:2413:MET:SD	2.40	0.60
1:A:2408:ILE:O	1:A:2409:SER:C	2.38	0.60
1:A:2903:ARG:NH2	1:A:2950:ILE:HA	2.16	0.60
1:B:2231:ILE:HG21	1:B:2264:GLN:HE22	1.64	0.60
1:B:2364:VAL:HB	1:B:2407:THR:HG21	1.82	0.60
1:B:3219:ILE:O	1:B:3221:PRO:HD3	2.00	0.60
1:A:2118:PHE:CE1	1:A:2163:LYS:HD2	2.37	0.60
1:A:2309:LYS:HG3	1:A:2358:ASP:HB2	1.84	0.60
1:A:3345:GLN:O	1:A:3349:ASP:HB2	2.01	0.60
1:A:4690:VAL:O	1:A:4700:LEU:HB2	2.01	0.60
1:A:1763:GLY:H	1:A:1764:PRO:HD3	1.65	0.60
1:A:2250:VAL:HB	1:A:2425:MET:CE	2.31	0.60
1:A:2532:ARG:HG3	1:A:2808:LEU:O	2.01	0.60
1:A:2917:LEU:HD12	1:A:2923:LYS:HA	1.84	0.60
1:A:3075:GLU:O	1:A:3078:VAL:HG12	2.01	0.60
1:A:3562:ALA:O	1:A:3566:ASN:HB2	2.02	0.60
1:A:3718:LEU:HD23	1:A:3762:ILE:HG13	1.84	0.60
1:A:4092:ASP:OD2	1:A:4093:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4182:GLY:HA3	1:A:4212:SER:OG	2.02	0.60
1:B:1820:GLN:HE22	1:B:1990:GLN:NE2	1.99	0.60
1:B:2976:LEU:HD12	1:B:2990:LEU:HD11	1.84	0.60
1:B:3813:ARG:HB3	1:B:3879:ILE:HD13	1.83	0.60
1:A:3598:PHE:CD2	1:A:3634:VAL:HG11	2.36	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:NZ	2.17	0.60
1:A:4503:ILE:HA	1:A:4575:LEU:HD23	1.84	0.60
1:B:1752:VAL:HG22	1:B:1811:PRO:HG3	1.84	0.60
1:B:1908:TYR:CE1	1:B:1958:LEU:HD22	2.37	0.60
1:A:2239:LYS:HD3	1:A:2295:GLN:NE2	2.16	0.60
1:A:2730:LEU:HD23	1:A:2783:LEU:HD23	1.83	0.60
1:A:4574:GLN:NE2	1:A:4590:TRP:HB3	2.17	0.60
1:B:2129:VAL:HG22	1:B:2130:PRO:CD	2.30	0.60
1:B:2522:ARG:HD3	1:B:2585:MET:SD	2.42	0.60
1:B:4153:LEU:HB2	1:B:4155:LYS:HG2	1.83	0.60
1:B:4541:ILE:HA	1:B:4561:LEU:HD11	1.83	0.60
1:A:1921:VAL:HG23	1:A:1922:LEU:CD2	2.32	0.60
1:A:3040:ILE:HG22	1:A:3042:VAL:HG13	1.82	0.60
1:A:3803:LYS:HE3	1:A:3810:HIS:NE2	2.17	0.60
1:B:1608:VAL:HG21	1:B:1669:MET:HG3	1.83	0.60
1:B:3559:ARG:O	1:B:3563:LEU:HB2	2.02	0.60
1:B:4060:GLU:O	1:B:4064:VAL:HG23	2.02	0.60
1:A:2091:LEU:HD22	1:A:2095:PHE:CE1	2.37	0.60
1:A:2439:PHE:H	1:A:2495:GLN:HE22	1.48	0.60
1:A:3262:ASP:HB2	1:A:3670:ARG:HE	1.67	0.60
1:A:1604:VAL:HG11	1:A:1670:GLU:HA	1.84	0.59
1:A:3922:ASN:HD22	1:A:3922:ASN:N	2.00	0.59
1:A:4004:THR:OG1	1:A:4006:PRO:HD3	2.01	0.59
1:A:3969:LEU:HD12	1:A:4426:MET:HE2	1.82	0.59
1:B:3017:VAL:HG13	1:B:3174:GLY:O	2.02	0.59
1:A:4691:TYR:CD2	1:A:4696:ARG:HG2	2.36	0.59
1:B:1948:VAL:O	1:B:1950:THR:HG23	2.02	0.59
1:B:3671:TYR:HD2	1:B:3734:LEU:HA	1.67	0.59
1:B:4499:PHE:O	1:B:4503:ILE:HB	2.01	0.59
1:A:2864:PHE:HB3	1:A:2872:TYR:CD2	2.38	0.59
1:A:3785:ASN:HD22	1:A:3786:PHE:H	1.49	0.59
1:A:4644:LEU:HD12	1:A:4723:ILE:HG12	1.85	0.59
1:B:2494:VAL:HG11	1:B:2548:VAL:HB	1.84	0.59
1:A:2273:MET:SD	1:A:2408:ILE:HG22	2.42	0.59
1:A:3923:LEU:HD22	1:A:3947:ILE:HG12	1.83	0.59
1:A:4545:ILE:O	1:A:4561:LEU:HD21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4715:ASN:O	1:A:4719:ARG:HB2	2.02	0.59
1:B:2377:LEU:O	1:B:2384:ARG:HA	2.02	0.59
1:B:2616:SER:HB3	1:B:2627:TRP:CE2	2.37	0.59
1:B:3673:LEU:HD22	1:B:3783:PHE:HE1	1.66	0.59
1:B:4124:LYS:O	1:B:4125:GLU:HG2	2.01	0.59
1:B:4137:VAL:HB	1:B:4138:PRO:HD2	1.85	0.59
1:B:4131:PRO:HD2	1:B:4232:MET:O	2.03	0.59
1:A:3672:PRO:HA	1:A:3782:THR:HG23	1.84	0.59
1:A:4190:ILE:HB	1:A:4197:LEU:HD11	1.83	0.59
1:A:4371:PRO:HA	1:A:4385:GLU:OE1	2.03	0.59
1:B:1612:TRP:O	1:B:1616:GLU:HB2	2.02	0.59
1:B:2000:CYS:HB3	1:B:2031:LEU:HD13	1.83	0.59
1:A:2528:PHE:CE1	1:A:2533:VAL:HG11	2.38	0.59
1:A:3730:LEU:HD11	1:A:3762:ILE:CD1	2.33	0.59
1:A:3731:ASN:HB2	1:A:3732:PRO:HD3	1.84	0.59
1:A:4157:TYR:OH	1:A:4186:LEU:HD22	2.03	0.59
1:A:4597:PRO:HB2	1:A:4700:LEU:HD21	1.85	0.59
1:B:3809:THR:HG21	1:B:3882:VAL:HG11	1.84	0.59
1:B:3897:TYR:HE1	1:B:3913:LEU:HA	1.67	0.59
1:B:4273:LEU:HD13	1:B:4363:LEU:O	2.02	0.59
1:B:3024:VAL:HG11	2:B:9010:ADP:H3'	1.83	0.59
1:A:2293:ILE:HG22	1:A:2350:ARG:NH2	2.12	0.59
1:A:2648:ILE:HG21	1:A:2827:ILE:HA	1.84	0.59
1:A:2938:PHE:HB3	1:A:2941:VAL:CG2	2.33	0.59
1:A:3924:LEU:HD23	1:A:3943:LEU:CD2	2.32	0.59
1:A:3951:THR:O	1:A:3955:VAL:HG23	2.02	0.59
1:B:1625:ILE:HD12	1:B:1628:LEU:HB2	1.83	0.59
1:B:2863:ARG:O	1:B:2863:ARG:HD3	2.02	0.59
1:A:3190:ARG:HA	1:A:3224:ARG:HH12	1.66	0.59
1:A:4494:PRO:HD3	1:A:4610:GLN:HE22	1.67	0.59
1:B:1546:VAL:HG22	1:B:1556:ARG:CZ	2.33	0.59
1:B:4207:LEU:O	1:B:4209:PRO:HD3	2.02	0.59
1:B:4424:ARG:NH2	1:B:4558:THR:HG21	2.17	0.59
1:A:2863:ARG:HD2	1:A:2864:PHE:CE1	2.36	0.59
1:A:3313:LEU:HD13	1:A:3550:SER:OG	2.03	0.59
1:A:4136:SER:O	1:A:4221:ILE:HD12	2.03	0.59
1:B:1477:LYS:H	1:B:1480:HIS:HD2	1.50	0.59
1:B:2273:MET:HG2	1:B:2395:PHE:HB2	1.84	0.59
1:B:2598:GLN:HG2	1:B:2612:LEU:HD23	1.85	0.59
1:B:4332:ILE:O	1:B:4336:THR:HG23	2.02	0.59
1:A:1538:TRP:HZ3	1:A:1656:ILE:HD13	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:THR:CG2	1:A:2103:PRO:HD3	2.33	0.59
1:A:2598:GLN:CG	1:A:2612:LEU:HB2	2.33	0.59
1:A:2991:PHE:HE1	1:A:2993:GLU:HB2	1.67	0.59
1:A:4572:MET:HA	1:A:4575:LEU:HD13	1.85	0.59
1:B:3788:VAL:HG11	1:B:3913:LEU:HD22	1.85	0.59
1:A:1763:GLY:N	1:A:1764:PRO:CD	2.65	0.58
1:A:1797:VAL:CG1	1:A:1855:ILE:HD11	2.33	0.58
1:A:1973:PHE:CE1	1:A:2099:ALA:HA	2.38	0.58
1:A:2278:SER:HA	1:A:2806:ARG:HH11	1.68	0.58
1:A:4066:GLN:NE2	1:A:4081:ARG:HD3	2.18	0.58
1:B:3233:TYR:CD2	1:B:3620:ARG:HG3	2.38	0.58
1:B:4109:ASP:HA	1:B:4112:ASN:HD22	1.67	0.58
1:A:1735:ASP:OD2	1:A:1737:GLU:HB2	2.03	0.58
1:B:2375:LYS:HB3	1:B:2387:LEU:HB3	1.84	0.58
1:B:4349:ASN:HB3	1:B:4352:ASP:OD2	2.03	0.58
1:B:4351:PHE:CD2	1:B:4689:PRO:HG3	2.38	0.58
1:A:2043:ILE:HG23	1:A:2073:ILE:HD12	1.84	0.58
1:A:3331:GLN:NE2	1:A:3533:LYS:HG3	2.18	0.58
1:A:3723:VAL:HG12	1:A:3766:THR:OG1	2.03	0.58
1:A:4193:ALA:O	1:A:4197:LEU:HD23	2.03	0.58
1:B:3027:ARG:HG2	1:B:3037:ILE:HD12	1.85	0.58
1:B:3170:LEU:HD21	1:B:3172:TRP:HE3	1.67	0.58
1:B:4030:PHE:HD1	1:B:4033:LEU:HD22	1.68	0.58
1:A:2153:LYS:O	1:A:2157:VAL:HG23	2.03	0.58
1:A:3830:LEU:HB3	1:A:3858:LEU:HD13	1.86	0.58
1:A:4251:THR:HG23	1:A:4303:LEU:CD2	2.30	0.58
1:A:4349:ASN:HD22	1:A:4352:ASP:H	1.51	0.58
1:A:4368:ALA:HA	1:A:4373:PHE:CE1	2.38	0.58
1:B:1901:ASN:HD22	1:B:1901:ASN:N	2.01	0.58
1:B:2166:CYS:HA	1:B:2190:TYR:OH	2.03	0.58
1:B:3182:PHE:O	1:B:3186:SER:HB2	2.03	0.58
1:A:2087:LEU:HB2	1:A:2092:LYS:HG3	1.86	0.58
1:A:2361:PRO:HD3	1:A:2402:TYR:O	2.03	0.58
1:A:3803:LYS:HG3	1:A:3810:HIS:CD2	2.39	0.58
1:A:4003:GLU:HG3	1:B:2842:LEU:CD2	2.34	0.58
1:A:4032:LYS:HG3	1:A:4069:LEU:HD11	1.83	0.58
1:B:1884:HIS:O	1:B:1888:VAL:HG23	2.03	0.58
1:B:3620:ARG:HH11	1:B:3620:ARG:HG2	1.69	0.58
1:A:1950:THR:HB	1:A:1951:PRO:HD2	1.84	0.58
1:A:2212:ILE:N	1:A:2213:PRO:HD2	2.18	0.58
1:B:1821:ILE:HG21	1:B:1914:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2338:ARG:HD2	1:B:2346:GLU:OE1	2.04	0.58
1:A:1849:GLU:HG3	1:A:1893:GLN:OE1	2.03	0.58
1:B:1719:GLN:HA	1:B:1722:PHE:CE2	2.38	0.58
1:B:2997:HIS:O	1:B:3001:ILE:HG13	2.03	0.58
1:B:3013:LEU:HD22	1:B:3164:LEU:HD12	1.85	0.58
1:B:4388:THR:HG23	1:B:4391:HIS:HD2	1.68	0.58
1:A:3615:ARG:O	1:A:3619:ILE:HG13	2.03	0.58
1:A:4572:MET:HA	1:A:4575:LEU:CD1	2.34	0.58
1:B:1855:ILE:HG22	1:B:1859:LEU:HD12	1.85	0.58
1:B:3923:LEU:HD22	1:B:3947:ILE:HG23	1.85	0.58
1:A:1863:VAL:HG21	1:A:2115:SER:O	2.04	0.58
1:A:2135:CYS:HB3	1:A:2147:PHE:CZ	2.38	0.58
1:B:1748:GLU:HB3	1:B:1943:ILE:HD12	1.85	0.58
1:A:1995:VAL:HA	1:A:2022:TRP:HB2	1.84	0.58
1:B:1643:PHE:CE2	1:B:1647:LEU:HD11	2.39	0.58
1:B:1926:VAL:HG12	1:B:1928:HIS:CD2	2.39	0.58
1:B:3192:LEU:HD11	1:B:3268:VAL:HA	1.84	0.58
1:B:3263:PHE:O	1:B:3267:VAL:HG23	2.03	0.58
1:B:4648:VAL:HA	1:B:4662:THR:HG21	1.85	0.58
1:A:2838:LEU:O	1:A:2839:LEU:HD23	2.04	0.57
1:A:3255:VAL:O	1:A:3255:VAL:HG13	2.03	0.57
1:A:3337:LYS:HA	1:A:3341:ALA:HB3	1.86	0.57
1:A:3595:ALA:HB1	1:A:3638:LEU:HD11	1.85	0.57
1:A:4559:ILE:HG23	1:A:4559:ILE:O	2.04	0.57
1:B:1939:GLU:O	1:B:1941:LEU:HG	2.03	0.57
1:B:1813:GLN:NE2	1:B:1941:LEU:H	2.02	0.57
1:B:2863:ARG:HG3	1:B:2925:TRP:CE2	2.39	0.57
1:B:3785:ASN:HD21	1:B:3787:THR:CG2	2.16	0.57
1:A:3274:LYS:O	1:A:3278:LEU:HD23	2.04	0.57
1:A:3487:TYR:O	1:A:3490:ILE:HG12	2.04	0.57
1:A:4284:ARG:HG3	1:A:4408:LEU:HB3	1.86	0.57
1:A:1982:GLU:HG3	2:A:9001:ADP:H3'	1.86	0.57
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.03	0.57
1:B:4189:ASN:ND2	1:B:4189:ASN:N	2.53	0.57
1:A:2739:LEU:HD23	1:A:2740:VAL:N	2.19	0.57
1:B:2869:GLN:HB2	1:B:2872:TYR:CD2	2.39	0.57
1:B:3674:VAL:HG13	1:B:3786:PHE:HD2	1.68	0.57
1:B:3897:TYR:CE1	1:B:3913:LEU:HA	2.38	0.57
1:B:4255:ILE:HD11	1:B:4307:LEU:HD11	1.85	0.57
1:A:2560:MET:HG3	1:A:2561:SER:N	2.16	0.57
1:A:2839:LEU:HD11	1:A:2890:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3668:PHE:CD1	1:A:3672:PRO:HD3	2.39	0.57
1:A:4277:PHE:HB2	1:A:4363:LEU:CD1	2.34	0.57
1:B:1888:VAL:O	1:B:1892:LEU:HD12	2.04	0.57
1:B:2533:VAL:HB	1:B:2581:LEU:CD2	2.30	0.57
1:A:3909:TYR:OH	1:A:3960:LEU:HG	2.04	0.57
1:A:4313:TRP:HB3	1:A:4330:PRO:HG2	1.86	0.57
1:B:1687:LEU:HD21	1:B:1706:LEU:CD2	2.33	0.57
1:B:1889:VAL:HA	1:B:1892:LEU:HD13	1.86	0.57
1:B:2219:LEU:CD1	1:B:2228:LEU:HD11	2.35	0.57
1:B:2235:GLN:HE22	1:B:2296:VAL:HG13	1.68	0.57
1:B:2417:SER:O	1:B:2420:ILE:HG12	2.03	0.57
1:B:2578:MET:HE1	1:B:2612:LEU:HD12	1.86	0.57
1:B:4379:ILE:O	1:B:4379:ILE:HG13	2.05	0.57
1:A:2053:ASN:O	1:A:2054:SER:C	2.42	0.57
1:A:2195:LEU:O	1:A:2199:ILE:HG12	2.04	0.57
1:A:2252:LYS:O	1:A:2256:VAL:HG23	2.05	0.57
1:A:2873:ILE:HD12	1:A:2873:ILE:H	1.68	0.57
1:A:3863:THR:O	1:A:3867:LEU:HB3	2.04	0.57
1:B:2835:LEU:HD11	1:B:2890:ILE:HD12	1.85	0.57
1:B:2841:ASN:HD22	1:B:2842:LEU:N	2.02	0.57
1:B:3638:LEU:HD12	1:B:3663:ILE:HG21	1.86	0.57
1:B:4318:SER:HB3	1:B:4324:ILE:HD11	1.85	0.57
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.40	0.57
1:A:4288:ILE:HG23	1:A:4292:TRP:O	2.04	0.57
1:B:2270:HIS:HA	1:B:2392:ARG:HH11	1.70	0.57
1:B:1591:TRP:O	1:B:1595:LEU:HB2	2.05	0.57
1:A:1718:ILE:HG22	1:A:1722:PHE:CE2	2.40	0.57
1:A:4245:LYS:HD2	1:A:4399:LEU:O	2.04	0.57
1:B:2540:LEU:HD12	1:B:2662:ALA:HB3	1.85	0.57
1:B:3238:ILE:HG12	1:B:3601:TYR:CD2	2.40	0.57
1:B:3793:LEU:HD23	1:B:3894:SER:HA	1.86	0.57
1:A:1681:LYS:O	1:A:1685:GLU:HG3	2.04	0.57
1:A:1978:THR:HG22	1:A:2103:PRO:HD3	1.87	0.57
1:A:4050:LYS:O	1:A:4051:ASP:C	2.42	0.57
1:A:4415:GLU:OE2	1:A:4415:GLU:HA	2.05	0.57
1:B:2586:GLY:HA2	1:B:2815:LEU:CD1	2.34	0.57
1:B:3912:SER:HB3	1:B:4231:ARG:HG2	1.86	0.57
1:B:4313:TRP:HB3	1:B:4330:PRO:HG2	1.87	0.57
1:A:2989:VAL:HG13	1:A:3187:GLU:CD	2.25	0.56
1:A:3266:GLN:HE21	1:A:3270:LEU:CD2	2.18	0.56
1:A:3439:ASP:HB3	1:A:3442:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.69	0.56
1:A:3291:LYS:HG3	1:A:3835:LEU:HD22	1.86	0.56
1:A:4132:LEU:HD23	1:A:4236:PHE:HE2	1.70	0.56
1:A:4375:LEU:HD11	1:A:4383:VAL:CG2	2.30	0.56
1:B:1537:PHE:O	1:B:1541:LEU:HB2	2.05	0.56
1:B:3274:LYS:HE3	1:B:3637:PHE:CE2	2.39	0.56
1:B:3614:MET:O	1:B:3618:MET:HG3	2.04	0.56
1:B:4043:ASP:HB3	1:B:4059:PRO:HB3	1.87	0.56
1:B:4543:LYS:HD2	1:B:4545:ILE:HD13	1.87	0.56
1:A:1978:THR:HG21	1:A:2101:ILE:O	2.05	0.56
1:A:1927:ILE:HD13	1:A:1991:LEU:CD2	2.35	0.56
1:A:2121:ALA:O	1:A:2122:GLU:C	2.43	0.56
1:A:4132:LEU:HD13	1:A:4216:PHE:CE1	2.40	0.56
1:A:4432:LYS:C	1:A:4434:GLN:H	2.08	0.56
1:B:4618:ASN:N	1:B:4618:ASN:HD22	2.02	0.56
1:A:2675:PRO:HG2	1:A:2678:SER:HB3	1.88	0.56
1:A:2979:PHE:HE2	1:A:3028:PHE:HA	1.70	0.56
1:A:3195:GLU:OE1	1:A:3224:ARG:HB2	2.04	0.56
1:B:1554:LEU:HB3	1:B:1609:GLN:NE2	2.09	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.44	0.56
1:A:2560:MET:CE	1:A:2564:ASN:HD22	2.18	0.56
1:A:3299:VAL:HG21	1:A:3563:LEU:HD23	1.87	0.56
1:A:3567:LEU:CD2	1:A:3855:LEU:HD11	2.36	0.56
1:A:3813:ARG:HB2	1:A:3813:ARG:CZ	2.34	0.56
1:A:3813:ARG:HB3	1:A:3879:ILE:HD11	1.88	0.56
1:B:1531:LEU:HD13	1:B:1587:GLU:OE2	2.05	0.56
1:B:1956:CYS:SG	1:B:1983:THR:HG21	2.45	0.56
1:A:2229:GLN:HB3	1:A:2230:PRO:HD2	1.86	0.56
1:A:3584:GLN:O	1:A:3588:VAL:HG23	2.06	0.56
1:A:3598:PHE:HA	1:A:3602:ILE:HG12	1.88	0.56
1:A:3682:MET:SD	1:A:3696:LYS:HE2	2.46	0.56
1:A:4277:PHE:O	1:A:4281:ILE:HG12	2.06	0.56
1:A:2806:ARG:HH12	2:A:9002:ADP:PB	2.28	0.56
1:B:2660:LEU:HD21	1:B:2672:LEU:HD21	1.87	0.56
1:B:4213:PHE:CZ	1:B:4215:LEU:HB2	2.40	0.56
1:A:1752:VAL:HG22	1:A:1811:PRO:HG3	1.86	0.56
1:A:1947:LEU:HD11	1:A:1982:GLU:HB3	1.87	0.56
1:A:4117:ASP:OD1	1:A:4119:ALA:HB3	2.06	0.56
1:B:2144:HIS:HB3	1:B:2400:LEU:HD12	1.86	0.56
1:B:2739:LEU:HB3	1:B:2786:ILE:HG12	1.87	0.56
1:A:2087:LEU:O	1:A:2092:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1948:VAL:O	1:A:1950:THR:HG23	2.06	0.56
1:A:2284:THR:O	1:A:2288:VAL:HG23	2.06	0.56
1:A:4534:LEU:HA	1:A:4537:LEU:HD12	1.88	0.56
1:B:2560:MET:HG3	1:B:2564:ASN:HB2	1.88	0.56
1:B:2670:LEU:HD11	1:B:2789:VAL:HG13	1.88	0.56
1:B:2841:ASN:ND2	1:B:2841:ASN:N	2.54	0.56
1:A:2954:ASN:N	1:A:2954:ASN:ND2	2.53	0.56
1:A:3445:THR:HA	1:A:3449:ARG:HD3	1.87	0.56
1:A:3848:ASP:HB3	1:A:3851:VAL:HG12	1.88	0.56
1:A:3887:ASN:HB3	1:A:3888:PRO:HD3	1.88	0.56
1:B:2841:ASN:ND2	1:B:2842:LEU:N	2.52	0.56
1:B:3043:ASN:H	1:B:3043:ASN:HD22	1.54	0.56
1:B:3758:PRO:HG2	1:B:3759:SER:H	1.71	0.56
1:A:1687:LEU:HD21	1:A:1706:LEU:HD23	1.88	0.56
1:A:1862:SER:O	1:A:1865:GLN:HG2	2.06	0.56
1:A:2748:LEU:N	1:A:2749:PRO:CD	2.69	0.56
1:A:2906:ALA:O	1:A:2910:LEU:HG	2.05	0.56
1:A:2941:VAL:HG12	1:A:2942:ASN:N	2.20	0.56
1:A:3376:ALA:O	1:A:3380:VAL:HG23	2.06	0.56
1:A:3813:ARG:HH22	1:A:3817:LEU:CD1	2.18	0.56
1:A:4622:HIS:HE2	1:A:4678:ILE:CG2	2.16	0.56
1:B:1479:ARG:HB2	1:B:1479:ARG:CZ	2.35	0.56
1:B:2081:TYR:O	1:B:2084:ARG:HD2	2.06	0.56
1:B:2163:LYS:HB2	1:B:2194:VAL:HG11	1.87	0.56
1:A:2381:ASN:OD1	1:A:2383:GLU:HB2	2.06	0.56
1:A:3404:ALA:HA	1:A:3462:PHE:HE1	1.71	0.56
1:A:4589:VAL:HG12	1:A:4639:VAL:HA	1.88	0.56
1:B:2276:GLY:O	1:B:2398:GLN:HA	2.06	0.56
1:B:3729:VAL:HG22	1:B:3729:VAL:O	2.05	0.56
1:A:1957:TYR:O	1:A:1961:THR:HG23	2.07	0.55
1:A:3292:LEU:HD22	1:A:3567:LEU:HD22	1.89	0.55
1:B:3908:LEU:HD22	1:B:4221:ILE:HG23	1.87	0.55
1:B:4147:ASP:HA	1:B:4157:TYR:OH	2.06	0.55
1:B:4190:ILE:HG12	1:B:4219:SER:HB2	1.86	0.55
1:B:4389:ARG:HG2	1:B:4389:ARG:NH1	2.21	0.55
1:B:4535:ARG:HG2	1:B:4535:ARG:HH11	1.71	0.55
1:A:1800:HIS:HB2	1:A:1858:ASN:HD22	1.71	0.55
1:A:2910:LEU:HD23	1:A:2930:ILE:CD1	2.33	0.55
1:A:3673:LEU:HD13	1:A:3783:PHE:CE1	2.40	0.55
1:A:4005:ILE:HG22	1:A:4008:LEU:HB2	1.87	0.55
1:B:2829:GLY:HA2	1:B:2850:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3700:LEU:CD2	1:B:3701:ASP:H	2.18	0.55
1:B:4388:THR:O	1:B:4391:HIS:HB2	2.07	0.55
1:A:1699:PHE:HE1	1:A:2015:GLY:HA3	1.71	0.55
1:A:1926:VAL:HG12	1:A:1928:HIS:CD2	2.41	0.55
1:A:2615:TYR:HD1	1:A:2624:TRP:HB3	1.72	0.55
1:A:2650:THR:H	1:A:2653:THR:HB	1.71	0.55
1:A:2991:PHE:CE1	1:A:2993:GLU:HB2	2.40	0.55
1:A:4590:TRP:CD2	1:A:4593:GLY:HA3	2.42	0.55
1:B:2101:ILE:O	1:B:2103:PRO:HD3	2.07	0.55
1:B:2440:ASP:OD1	1:B:2441:PRO:HD2	2.06	0.55
1:B:2603:THR:O	1:B:2605:VAL:HG13	2.06	0.55
1:A:3066:GLU:HG2	1:A:3136:GLN:HE21	1.71	0.55
1:A:3368:LYS:C	1:A:3374:ILE:HD11	2.26	0.55
1:A:3419:TRP:CE3	1:A:3422:ILE:HD11	2.42	0.55
1:B:2369:SER:HA	1:B:2372:ASP:OD2	2.07	0.55
1:A:1625:ILE:HG23	1:A:1626:ASN:H	1.70	0.55
1:A:2606:PRO:HG2	1:A:2615:TYR:CE1	2.42	0.55
1:A:3555:ASN:HB3	1:A:3559:ARG:HH11	1.71	0.55
1:B:2774:ARG:HB2	1:B:2781:ILE:CD1	2.37	0.55
1:A:1763:GLY:H	1:A:1764:PRO:CD	2.19	0.55
1:A:1875:PHE:O	1:A:1879:ILE:HG12	2.07	0.55
1:A:3471:SER:HB3	1:A:3474:CYS:SG	2.47	0.55
1:A:3930:LEU:HG	1:A:3939:ARG:NH1	2.21	0.55
1:A:3991:LEU:O	1:A:3991:LEU:HD12	2.07	0.55
1:A:4094:VAL:HB	1:A:4423:ALA:HB1	1.88	0.55
1:B:1872:ARG:HH12	1:B:2164:ARG:HD3	1.71	0.55
1:A:1608:VAL:HG13	1:A:1676:LEU:CD1	2.37	0.55
1:A:1797:VAL:HG13	1:A:1855:ILE:HD11	1.89	0.55
1:A:2274:MET:CE	1:A:2286:TRP:HB3	2.30	0.55
1:A:2765:GLN:O	1:A:2769:LYS:HB2	2.07	0.55
1:A:3453:THR:O	1:A:3458:GLU:HG2	2.06	0.55
1:A:4319:LYS:H	1:A:4321:ARG:NH2	2.04	0.55
1:B:1555:VAL:HG23	1:B:1609:GLN:HE21	1.70	0.55
1:B:3018:SER:O	1:B:3256:THR:HB	2.06	0.55
1:B:3306:LEU:HD22	1:B:3553:VAL:HG13	1.89	0.55
1:B:4132:LEU:HD13	1:B:4216:PHE:CE1	2.42	0.55
1:B:4644:LEU:HG	1:B:4664:ILE:HD11	1.88	0.55
1:B:4624:SER:HB2	1:B:4668:THR:HB	1.87	0.55
1:B:4685:LYS:HE2	1:B:4706:PRO:HD3	1.88	0.55
1:A:2262:LEU:HD11	1:A:2274:MET:CE	2.37	0.55
1:A:2446:GLN:O	1:A:2450:ASN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4571:ARG:O	1:A:4574:GLN:HB3	2.07	0.55
1:A:1907:LEU:HA	1:A:1911:ARG:NH1	2.21	0.55
1:A:2439:PHE:H	1:A:2495:GLN:NE2	2.05	0.55
1:A:3647:TRP:HH2	1:A:3663:ILE:HD12	1.71	0.55
1:B:2000:CYS:C	1:B:2002:GLU:H	2.10	0.55
1:B:2612:LEU:HD11	1:B:2624:TRP:CH2	2.42	0.55
1:B:2779:THR:O	1:B:2781:ILE:HD12	2.06	0.55
1:B:2863:ARG:HD2	1:B:2864:PHE:CE1	2.42	0.55
1:B:2918:VAL:HG13	1:B:3172:TRP:NE1	2.22	0.55
1:B:4095:LEU:HD11	1:B:4422:LYS:CB	2.37	0.55
1:A:3965:LEU:HG	1:A:4426:MET:CE	2.37	0.55
1:A:4495:LEU:CD1	1:A:4495:LEU:H	2.16	0.55
1:B:4024:ARG:HA	1:B:4030:PHE:O	2.07	0.55
1:A:1755:LYS:HG2	1:A:1780:THR:HG23	1.89	0.54
1:A:2648:ILE:HD13	1:A:2831:PHE:CZ	2.42	0.54
1:A:3253:ASN:HB2	1:A:3604:PHE:CE2	2.42	0.54
1:A:3373:ILE:CD1	1:A:3373:ILE:H	2.06	0.54
1:B:2898:LEU:O	1:B:2902:VAL:HG23	2.06	0.54
1:B:4101:PHE:O	1:B:4105:VAL:HG23	2.07	0.54
1:B:4571:ARG:HD3	1:B:4593:GLY:O	2.06	0.54
1:A:1908:TYR:CE1	1:A:1958:LEU:HD13	2.42	0.54
1:A:2204:ILE:N	1:A:2205:PRO:CD	2.69	0.54
1:A:2196:LEU:HD21	1:A:2219:LEU:HD22	1.89	0.54
1:A:2275:VAL:HG13	1:A:2415:TRP:CE3	2.42	0.54
1:A:3266:GLN:HE21	1:A:3270:LEU:HD21	1.71	0.54
1:A:3390:GLU:O	1:A:3394:LEU:HG	2.07	0.54
1:A:4413:ASN:ND2	1:A:4660:LEU:HG	2.22	0.54
1:B:1694:PHE:CE1	1:B:1770:LEU:HD13	2.42	0.54
1:B:2832:ASN:HA	1:B:2835:LEU:HB3	1.89	0.54
1:B:3652:LEU:HB2	1:B:3684:PHE:CD1	2.43	0.54
1:A:1890:ARG:O	1:A:1894:LYS:HG3	2.07	0.54
1:A:2431:LEU:HD11	1:A:2506:PHE:CD2	2.42	0.54
1:A:3647:TRP:HB3	1:A:3652:LEU:CD2	2.37	0.54
1:A:3830:LEU:HB3	1:A:3858:LEU:CD1	2.37	0.54
1:B:2200:ASN:HA	1:B:2204:ILE:HG12	1.89	0.54
1:B:2968:LEU:O	1:B:2972:VAL:HG23	2.07	0.54
1:A:3086:ARG:HH11	1:A:3096:VAL:CG1	2.20	0.54
1:A:4319:LYS:N	1:A:4321:ARG:NH2	2.55	0.54
1:B:2283:THR:HA	1:B:2286:TRP:NE1	2.22	0.54
1:B:2331:LEU:HD21	1:B:2773:TRP:CD1	2.43	0.54
1:B:4013:SER:H	1:B:4016:GLN:HE21	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1691:ARG:HD3	1:A:1698:TYR:CD1	2.41	0.54
1:A:3336:ILE:O	1:A:3340:ASP:HB3	2.08	0.54
1:A:3700:LEU:CG	1:A:3701:ASP:H	2.20	0.54
1:A:4121:ILE:O	1:A:4126:VAL:HG12	2.06	0.54
1:A:4553:TYR:CD1	1:A:4553:TYR:N	2.75	0.54
1:B:1548:TYR:CD1	1:B:1549:GLN:HG2	2.43	0.54
1:B:1655:LEU:HD22	1:B:1655:LEU:H	1.72	0.54
1:B:2024:CYS:HA	1:B:2074:PHE:O	2.06	0.54
1:B:2498:CYS:SG	1:B:2569:ILE:HG13	2.47	0.54
1:B:2803:LEU:HD12	1:B:2808:LEU:HD21	1.90	0.54
1:B:2990:LEU:HD23	1:B:2994:VAL:HG11	1.90	0.54
1:B:4323:ASN:ND2	1:B:4323:ASN:N	2.54	0.54
1:A:1951:PRO:HG2	1:A:2104:ASP:OD1	2.08	0.54
1:A:2014:VAL:HG22	1:A:2065:ILE:HD13	1.90	0.54
1:A:2766:MET:HB3	1:A:2783:LEU:CD1	2.36	0.54
1:A:3602:ILE:O	1:A:3604:PHE:N	2.40	0.54
1:A:4122:VAL:HG23	1:A:4214:ARG:HD2	1.89	0.54
1:B:1782:ALA:HA	1:B:1938:PHE:CE1	2.42	0.54
1:B:2603:THR:CG2	1:B:2604:PRO:HD2	2.31	0.54
1:B:2874:TYR:OH	1:B:2916:ARG:HD2	2.08	0.54
1:A:2121:ALA:O	1:A:2124:LEU:N	2.41	0.54
1:A:3423:ARG:O	1:A:3426:ILE:HG22	2.07	0.54
1:A:4254:GLY:O	1:A:4256:PRO:HD3	2.07	0.54
1:B:2519:ALA:HB2	1:B:2593:PHE:CZ	2.43	0.54
1:B:2516:LEU:HD12	1:B:2581:LEU:HD13	1.90	0.54
1:B:4080:PHE:HB2	1:B:4101:PHE:CE1	2.43	0.54
1:A:2031:LEU:HD23	1:A:2035:ILE:HG22	1.89	0.54
1:A:2751:THR:HB	1:A:2755:GLY:HA2	1.90	0.54
1:A:3263:PHE:O	1:A:3267:VAL:HG23	2.07	0.54
1:A:3399:THR:N	1:A:3400:PRO:HD2	2.23	0.54
1:A:4013:SER:H	1:A:4016:GLN:HB3	1.73	0.54
1:A:4348:ASP:OD2	1:A:4349:ASN:N	2.40	0.54
1:B:2641:VAL:HG12	1:B:2642:ALA:N	2.23	0.54
1:B:4058:ILE:HD12	1:B:4082:LYS:HG2	1.89	0.54
1:A:1724:LYS:HD3	1:A:2382:GLY:O	2.07	0.54
1:A:2266:LEU:HD21	1:A:2394:MET:HE3	1.89	0.54
1:A:2447:GLN:HE22	1:A:2492:LEU:CD2	2.21	0.54
1:A:3043:ASN:N	1:A:3043:ASN:HD22	2.05	0.54
1:A:4547:PRO:HB2	1:A:4550:TRP:CE3	2.43	0.54
1:B:1982:GLU:HA	1:B:1982:GLU:OE1	2.08	0.54
1:B:1975:PRO:HD2	1:B:2100:MET:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2500:ALA:HA	1:B:2503:SER:OG	2.08	0.54
1:B:2636:VAL:HG21	1:B:2648:ILE:HD11	1.89	0.54
1:B:2929:LYS:O	1:B:2933:VAL:HG23	2.07	0.54
1:B:4336:THR:O	1:B:4340:SER:HB3	2.08	0.54
1:A:1822:VAL:HG12	1:A:1826:GLN:OE1	2.07	0.54
1:A:2128:ILE:HG13	1:A:2152:LEU:HD21	1.90	0.54
1:A:2689:ARG:C	1:A:2691:PHE:H	2.12	0.54
1:A:2819:PRO:HD2	1:A:2876:PRO:HG2	1.89	0.54
1:A:3109:MET:O	1:A:3112:CYS:HB2	2.08	0.54
1:A:3373:ILE:HD13	1:A:3373:ILE:N	2.12	0.54
1:A:3760:PHE:CG	1:A:3761:MET:N	2.75	0.54
1:A:3827:LEU:O	1:A:3831:GLU:HG3	2.08	0.54
1:A:4318:SER:CA	1:A:4321:ARG:HH21	2.19	0.54
1:B:2653:THR:O	1:B:2657:VAL:HG23	2.08	0.54
1:B:3255:VAL:HA	1:B:3259:HIS:CD2	2.43	0.54
1:B:3677:PRO:CD	1:B:3787:THR:HG22	2.38	0.54
1:B:4257:ALA:HB2	1:B:4389:ARG:HD3	1.90	0.54
1:A:2653:THR:O	1:A:2657:VAL:HG23	2.07	0.53
1:B:1910:MET:CA	1:B:1929:MET:HG3	2.39	0.53
1:B:4639:VAL:O	1:B:4666:ILE:HD12	2.08	0.53
1:A:2969:ARG:HG3	1:A:2970:GLU:N	2.23	0.53
1:A:3218:ALA:O	1:A:3219:ILE:C	2.47	0.53
1:A:3698:SER:HB2	1:A:3721:GLN:HB2	1.90	0.53
1:A:4375:LEU:CD1	1:A:4383:VAL:HG23	2.32	0.53
1:A:4553:TYR:N	1:A:4553:TYR:HD1	2.05	0.53
1:B:1581:TYR:O	1:B:1585:GLU:HB2	2.08	0.53
1:B:1646:ILE:O	1:B:1650:VAL:HG23	2.08	0.53
1:B:1831:LEU:HD13	1:B:1900:GLY:O	2.07	0.53
1:B:2863:ARG:HG3	1:B:2925:TRP:CZ2	2.44	0.53
1:B:3342:ARG:O	1:B:3345:GLN:HB3	2.07	0.53
1:A:2825:THR:O	1:A:2829:GLY:HA3	2.08	0.53
1:A:3418:GLU:O	1:A:3422:ILE:HG23	2.08	0.53
1:A:4012:LEU:N	1:A:4012:LEU:HD12	2.23	0.53
1:B:1655:LEU:HB2	1:B:1658:GLU:CB	2.31	0.53
1:B:1920:ASN:HD22	1:B:1921:VAL:N	2.06	0.53
1:B:2050:LEU:HG	1:B:2067:LEU:HD21	1.89	0.53
1:A:1699:PHE:HD1	1:A:1699:PHE:N	2.06	0.53
1:A:1803:TYR:HE1	1:A:1855:ILE:HD13	1.74	0.53
1:A:1827:VAL:O	1:A:1831:LEU:HG	2.08	0.53
1:A:4376:VAL:HG12	1:A:4379:ILE:HG22	1.90	0.53
1:A:4596:ASN:C	1:A:4596:ASN:HD22	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2118:PHE:CE1	1:B:2163:LYS:HG3	2.44	0.53
1:B:2309:LYS:CE	1:B:2756:THR:HG21	2.39	0.53
1:B:3677:PRO:HG3	1:B:3787:THR:HG22	1.89	0.53
1:B:3700:LEU:HD13	1:B:3701:ASP:H	1.71	0.53
1:A:1650:VAL:HG13	1:A:1659:VAL:HG11	1.91	0.53
1:A:2704:ALA:O	1:A:2706:THR:HG23	2.08	0.53
1:A:2994:VAL:O	1:A:2998:ILE:HG12	2.08	0.53
1:B:4671:TRP:C	1:B:4672:LYS:HG2	2.29	0.53
1:A:2016:LEU:HD21	1:A:2023:GLY:HA3	1.89	0.53
1:A:2274:MET:HE1	1:A:2286:TRP:HD1	1.73	0.53
1:A:2341:ASP:O	1:A:2343:VAL:N	2.40	0.53
1:B:2515:VAL:HG11	1:B:2577:LEU:HD13	1.90	0.53
1:B:2540:LEU:HD12	1:B:2662:ALA:CB	2.39	0.53
1:B:3067:GLU:O	1:B:3069:ILE:HG13	2.08	0.53
1:B:3109:MET:O	1:B:3129:LEU:HD21	2.09	0.53
1:B:4098:SER:O	1:B:4102:VAL:HG23	2.09	0.53
1:A:1709:ILE:HA	1:A:1766:ILE:HG12	1.90	0.53
1:A:1820:GLN:HB3	1:A:1912:TYR:CD2	2.44	0.53
1:A:2397:VAL:HG21	1:A:2400:LEU:CD2	2.38	0.53
1:A:2745:GLU:HB3	1:A:2748:LEU:HD12	1.91	0.53
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.29	0.53
1:B:1948:VAL:O	1:B:1950:THR:N	2.41	0.53
1:B:4260:MET:HG3	1:B:4271:TYR:CD1	2.43	0.53
1:B:4693:ASN:ND2	1:B:4693:ASN:H	2.06	0.53
1:A:2274:MET:HE1	1:A:2286:TRP:CD1	2.44	0.53
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.73	0.53
1:A:3700:LEU:HD13	1:A:3701:ASP:H	1.73	0.53
1:A:4036:HIS:HD2	1:A:4044:TRP:HE1	1.56	0.53
1:B:1558:TRP:CZ3	1:B:1606:ILE:HB	2.44	0.53
1:B:1541:LEU:HD23	1:B:1656:ILE:HG21	1.91	0.53
1:B:1932:ALA:HB1	1:B:1934:PHE:CE2	2.44	0.53
1:B:4278:HIS:CD2	1:B:4303:LEU:HB2	2.44	0.53
1:B:4597:PRO:HG2	1:B:4692:LEU:HD13	1.90	0.53
1:A:2701:PHE:CG	1:A:2705:THR:HG21	2.43	0.53
1:A:3821:GLY:O	1:A:3825:VAL:HG23	2.08	0.53
1:A:4207:LEU:O	1:A:4209:PRO:HD3	2.08	0.53
1:B:2280:GLY:O	1:B:2420:ILE:HD11	2.08	0.53
1:B:2497:GLU:O	1:B:2501:ILE:HG13	2.08	0.53
1:A:1538:TRP:CH2	1:A:1565:LEU:HG	2.44	0.53
1:A:2142:GLN:HE21	1:A:2208:VAL:HG11	1.75	0.53
1:A:2359:VAL:CG2	1:A:2397:VAL:HG11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3802:LEU:CD2	1:A:3882:VAL:HG12	2.39	0.53
1:A:4122:VAL:HG22	1:A:4122:VAL:O	2.08	0.53
1:A:4188:LYS:HA	1:A:4218:THR:HB	1.90	0.53
1:B:1538:TRP:HZ3	1:B:1656:ILE:HD13	1.73	0.53
1:B:3895:ARG:HH12	1:B:3977:LYS:HG2	1.73	0.53
1:A:2598:GLN:HG2	1:A:2612:LEU:HD22	1.90	0.52
1:A:3956:THR:OG1	1:A:3964:LYS:HE3	2.08	0.52
1:A:2017:CYS:HB3	1:A:2067:LEU:HD12	1.90	0.52
1:A:3555:ASN:O	1:A:3559:ARG:HD3	2.09	0.52
1:A:3776:ASP:O	1:A:3780:ARG:HG2	2.09	0.52
1:A:3927:ASN:HB3	1:A:3930:LEU:CB	2.39	0.52
1:B:1525:ILE:HG13	1:B:1529:GLU:HG2	1.91	0.52
1:B:1612:TRP:CZ2	1:B:1644:ILE:HD11	2.44	0.52
1:B:1863:VAL:HG21	1:B:2115:SER:O	2.09	0.52
1:B:2205:PRO:HA	1:B:2261:GLN:OE1	2.09	0.52
1:B:2661:HIS:O	1:B:2665:SER:HB3	2.09	0.52
1:B:2818:PHE:HD1	1:B:2876:PRO:HD3	1.74	0.52
1:B:2704:ALA:HB2	1:B:3085:GLU:CD	2.29	0.52
1:A:2142:GLN:HE21	1:A:2208:VAL:CG1	2.22	0.52
1:A:2297:ASP:C	1:A:2299:ILE:H	2.12	0.52
1:A:2275:VAL:HB	1:A:2413:MET:HE2	1.90	0.52
1:A:2431:LEU:HD21	1:A:2506:PHE:CE2	2.44	0.52
1:A:2578:MET:CE	1:A:2613:LEU:HA	2.39	0.52
1:A:3233:TYR:O	1:A:3237:THR:HG23	2.10	0.52
1:A:3878:GLU:O	1:A:3882:VAL:HG23	2.10	0.52
1:A:4693:ASN:N	1:A:4693:ASN:ND2	2.57	0.52
1:B:3023:SER:HB2	2:B:9010:ADP:O1A	2.09	0.52
1:B:3059:LEU:HD23	1:B:3137:VAL:HG11	1.92	0.52
1:B:4118:MET:O	1:B:4122:VAL:HG22	2.08	0.52
1:A:2956:LEU:HD21	1:A:2971:TYR:CG	2.44	0.52
1:B:2838:LEU:O	1:B:2840:PRO:HD3	2.10	0.52
1:A:3439:ASP:C	1:A:3441:LYS:H	2.13	0.52
1:A:4048:PHE:HD1	1:A:4048:PHE:H	1.58	0.52
1:B:1930:ALA:HB2	1:B:1958:LEU:HD11	1.91	0.52
1:B:2036:LEU:HD23	1:B:2040:SER:HB3	1.90	0.52
1:B:2532:ARG:HH11	1:B:2532:ARG:HG2	1.74	0.52
1:B:3017:VAL:HG11	1:B:3175:GLU:CD	2.30	0.52
1:B:3082:SER:HA	1:B:3085:GLU:OE1	2.09	0.52
1:B:3681:ALA:HB2	1:B:3786:PHE:CG	2.45	0.52
1:A:1690:GLN:HE22	1:A:1766:ILE:CG2	2.17	0.52
1:A:2258:LYS:HE3	1:A:2415:TRP:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2857:TYR:HA	1:A:2913:PHE:CE1	2.36	0.52
1:A:3225:ASP:O	1:A:3229:SER:HB3	2.08	0.52
1:A:3415:LYS:O	1:A:3417:LEU:HD12	2.09	0.52
1:A:4103:CYS:SG	1:A:4108:GLU:HA	2.50	0.52
1:A:4371:PRO:O	1:A:4372:ASP:HB2	2.09	0.52
1:B:2144:HIS:HB3	1:B:2400:LEU:CD1	2.40	0.52
1:B:2907:HIS:HA	1:B:2910:LEU:HD12	1.92	0.52
1:B:4323:ASN:HD22	1:B:4323:ASN:N	2.06	0.52
1:A:2139:LEU:O	1:A:2140:SER:C	2.48	0.52
1:A:2142:GLN:HG2	1:A:2208:VAL:HG11	1.91	0.52
1:A:2531:LEU:HD12	1:A:2809:ARG:HD2	1.91	0.52
1:A:2708:GLU:O	1:A:2711:LEU:HB2	2.10	0.52
1:A:2793:ASN:HD22	1:A:2793:ASN:H	1.57	0.52
1:A:4006:PRO:C	1:A:4008:LEU:H	2.11	0.52
1:A:4413:ASN:HD21	1:A:4660:LEU:HG	1.74	0.52
1:B:1600:SER:O	1:B:1604:VAL:HG23	2.10	0.52
1:B:2282:LYS:NZ	1:B:2282:LYS:HB2	2.25	0.52
1:B:2748:LEU:N	1:B:2749:PRO:CD	2.73	0.52
1:B:4156:GLN:O	1:B:4183:THR:HB	2.10	0.52
1:A:1629:LEU:HD11	1:A:1686:TYR:CD2	2.44	0.52
1:A:2003:GLY:O	1:A:2004:PHE:C	2.49	0.52
1:A:2105:ARG:HG2	1:A:2105:ARG:NH1	2.23	0.52
1:A:2528:PHE:HE1	1:A:2533:VAL:HG11	1.73	0.52
1:A:3373:ILE:HG12	1:A:3374:ILE:H	1.74	0.52
1:A:3653:PRO:HB2	1:A:3658:CYS:SG	2.50	0.52
1:A:4288:ILE:CG2	1:A:4289:PRO:HA	2.40	0.52
1:B:1565:LEU:HD23	1:B:1595:LEU:CD1	2.39	0.52
1:B:1873:LYS:HB3	1:B:1943:ILE:HG21	1.90	0.52
1:B:2231:ILE:HD11	1:B:2260:LEU:HG	1.91	0.52
1:B:2506:PHE:CE1	1:B:2512:VAL:HG21	2.43	0.52
1:B:2531:LEU:HD13	1:B:2809:ARG:NH2	2.24	0.52
1:B:3233:TYR:O	1:B:3237:THR:HG23	2.09	0.52
1:B:4270:ILE:CG2	1:B:4310:ILE:HD13	2.34	0.52
1:A:2408:ILE:O	1:A:2410:ARG:N	2.43	0.52
1:A:3698:SER:C	1:A:3700:LEU:H	2.13	0.52
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.09	0.52
1:A:3924:LEU:HD23	1:A:3943:LEU:HD21	1.91	0.52
1:A:3988:TRP:NE1	1:A:3992:LEU:HD11	2.25	0.52
1:B:2741:VAL:HB	1:B:2788:PHE:CD2	2.44	0.52
1:B:2906:ALA:O	1:B:2909:ALA:HB3	2.10	0.52
1:B:4157:TYR:HB2	1:B:4184:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1964:LEU:HD12	1:A:2074:PHE:HZ	1.75	0.52
1:A:2641:VAL:HG12	1:A:2831:PHE:HB3	1.92	0.52
1:A:2893:MET:HE3	1:A:2896:CYS:HB2	1.92	0.52
1:A:3813:ARG:HG3	1:A:3814:SER:N	2.24	0.52
1:A:4033:LEU:HD13	1:A:4062:TRP:CE2	2.45	0.52
1:B:4423:ALA:O	1:B:4427:ILE:HG12	2.10	0.52
1:A:1715:ILE:HD11	1:A:1760:ILE:HG21	1.92	0.51
1:A:2561:SER:OG	1:A:2564:ASN:HB3	2.09	0.51
1:B:1957:TYR:O	1:B:1961:THR:HG23	2.10	0.51
1:B:2820:SER:OG	1:B:2823:SER:HB2	2.09	0.51
1:B:2910:LEU:O	1:B:2914:GLN:HB3	2.10	0.51
1:B:3843:GLY:O	1:B:3845:ILE:N	2.35	0.51
1:B:3563:LEU:HD11	1:B:3845:ILE:CD1	2.40	0.51
1:A:2898:LEU:CD1	1:A:2941:VAL:HG22	2.40	0.51
1:A:4213:PHE:CZ	1:A:4215:LEU:HB2	2.45	0.51
1:A:4269:ARG:HG2	1:A:4369:PHE:CE1	2.45	0.51
1:B:1817:LEU:O	1:B:1821:ILE:HG13	2.10	0.51
1:B:2764:ARG:HD2	1:B:2806:ARG:O	2.10	0.51
1:B:4690:VAL:HG21	1:B:4701:PHE:CE1	2.45	0.51
1:A:2271:GLY:O	1:A:2411:CYS:HA	2.10	0.51
1:A:2535:ASN:ND2	1:A:2668:ARG:HH12	2.08	0.51
1:A:3567:LEU:HD23	1:A:3855:LEU:HD11	1.92	0.51
1:A:4136:SER:O	1:A:4220:GLU:HA	2.10	0.51
1:B:1937:GLY:HA3	1:B:1992:GLY:O	2.10	0.51
1:B:1975:PRO:HG2	1:B:1978:THR:HG21	1.91	0.51
1:B:2549:ILE:O	1:B:2553:GLN:HB2	2.09	0.51
1:B:3595:ALA:O	1:B:3598:PHE:HB3	2.11	0.51
1:B:3682:MET:SD	1:B:3696:LYS:HE2	2.49	0.51
1:B:4671:TRP:O	1:B:4672:LYS:HG2	2.11	0.51
1:B:4690:VAL:HG11	1:B:4701:PHE:CZ	2.44	0.51
1:A:1959:THR:HG21	1:A:2098:MET:HB2	1.92	0.51
1:A:2144:HIS:O	1:A:2413:MET:HG2	2.10	0.51
1:A:2732:PRO:CG	1:A:2739:LEU:HB2	2.40	0.51
1:A:2918:VAL:HG13	1:A:3172:TRP:NE1	2.26	0.51
1:A:3366:LEU:O	1:A:3366:LEU:HD12	2.10	0.51
1:A:3730:LEU:HD13	1:A:3734:LEU:HD21	1.91	0.51
1:A:3969:LEU:HD12	1:A:4426:MET:CE	2.41	0.51
1:B:2311:ILE:HB	1:B:2315:GLN:HE21	1.76	0.51
1:B:3902:GLU:C	1:B:3904:SER:H	2.13	0.51
1:B:4636:SER:HA	1:B:4670:THR:HG22	1.91	0.51
1:B:4592:GLY:HA3	1:B:4725:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1611:ARG:NH1	1:A:1611:ARG:HG3	2.23	0.51
1:A:2370:LEU:HD12	1:A:2377:LEU:CB	2.41	0.51
1:A:2586:GLY:HA2	1:A:2815:LEU:CD1	2.37	0.51
1:A:3114:GLU:HG2	1:A:3118:ARG:HH12	1.74	0.51
1:A:3353:LYS:O	1:A:3357:VAL:HG23	2.10	0.51
1:A:3452:ILE:CG2	1:A:3485:THR:HG21	2.39	0.51
1:A:3670:ARG:O	1:A:3782:THR:HG22	2.10	0.51
1:A:3768:ASP:HB3	1:A:3771:ALA:HB2	1.93	0.51
1:A:4025:GLN:HG3	1:B:2899:GLU:OE2	2.10	0.51
1:A:4240:ASN:OD1	1:A:4240:ASN:N	2.38	0.51
1:B:1920:ASN:ND2	1:B:1921:VAL:H	2.09	0.51
1:B:2238:LYS:HA	1:B:2241:GLN:HE21	1.74	0.51
1:B:3843:GLY:C	1:B:3845:ILE:H	2.13	0.51
1:A:1625:ILE:HG23	1:A:1626:ASN:OD1	2.11	0.51
1:A:2738:TRP:CE2	1:A:2785:LYS:HG2	2.46	0.51
1:A:4200:LEU:HD22	1:A:4204:LEU:CD1	2.41	0.51
1:B:1662:ILE:HB	1:B:1665:ILE:CG2	2.40	0.51
1:B:1971:ASN:O	1:B:2097:SER:HA	2.11	0.51
1:B:2815:LEU:HD23	1:B:2815:LEU:C	2.31	0.51
1:B:3889:MET:CE	1:B:3943:LEU:HB3	2.41	0.51
1:B:4086:MET:HG3	1:B:4097:TYR:CD2	2.45	0.51
1:B:4222:HIS:CG	1:B:4223:PRO:HD2	2.45	0.51
1:B:4340:SER:HB2	1:B:4357:TYR:OH	2.10	0.51
1:B:2638:THR:O	1:B:2641:VAL:HG23	2.10	0.51
1:B:3306:LEU:HD13	1:B:3557:VAL:HG22	1.92	0.51
1:A:2732:PRO:HG3	1:A:2739:LEU:HB2	1.93	0.51
1:A:3289:LEU:HD13	1:A:3293:ARG:NH2	2.25	0.51
1:A:3721:GLN:NE2	1:A:4205:HIS:NE2	2.58	0.51
1:A:4384:PRO:HB3	1:A:4395:TRP:CD1	2.45	0.51
1:B:1556:ARG:HG2	1:B:1557:GLY:N	2.25	0.51
1:B:2219:LEU:HD13	1:B:2228:LEU:HD11	1.93	0.51
1:B:2643:SER:HB3	1:B:2646:VAL:HG23	1.93	0.51
1:B:2801:VAL:HG12	1:B:2802:GLN:N	2.25	0.51
1:B:2877:ARG:HB3	1:B:2881:ARG:NH1	2.26	0.51
1:B:2931:ASP:O	1:B:2935:LEU:HG	2.11	0.51
1:B:3063:GLY:HA2	1:B:3136:GLN:CB	2.41	0.51
1:B:3566:ASN:ND2	1:B:3859:LYS:NZ	2.59	0.51
1:B:4121:ILE:HA	1:B:4125:GLU:CG	2.32	0.51
1:B:4550:TRP:O	1:B:4552:TRP:N	2.40	0.51
1:A:1713:LYS:O	1:A:1715:ILE:N	2.44	0.51
1:A:2138:GLN:NE2	1:A:2218:LEU:HD21	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2327:TRP:CZ3	1:A:2380:PRO:HD2	2.46	0.51
1:A:2619:ILE:O	1:A:2619:ILE:HG13	2.11	0.51
1:A:2540:LEU:HD23	1:A:2662:ALA:HB3	1.92	0.51
1:A:4299:ASN:OD1	1:A:4301:ALA:HB3	2.11	0.51
1:A:4389:ARG:HH12	1:A:4393:MET:CE	2.24	0.51
1:A:4428:ASN:O	1:A:4432:LYS:HG2	2.10	0.51
1:B:1520:ALA:HA	1:B:1580:TYR:CE1	2.46	0.51
1:B:1639:ILE:HG21	1:B:1676:LEU:HG	1.93	0.51
1:B:2283:THR:HA	1:B:2286:TRP:HE1	1.76	0.51
1:B:2542:ASN:O	1:B:2546:VAL:HG23	2.10	0.51
1:B:2849:LEU:HD21	1:B:2886:LEU:HD13	1.93	0.51
1:B:2921:GLU:H	1:B:2921:GLU:CD	2.13	0.51
1:B:2968:LEU:CD2	1:B:2999:LEU:HD11	2.41	0.51
1:B:3219:ILE:CB	1:B:3220:PRO:CD	2.89	0.51
1:A:2204:ILE:HG13	1:A:2205:PRO:HD3	1.92	0.51
1:A:3032:MET:C	1:A:3034:GLY:H	2.15	0.51
1:A:3425:LYS:HA	1:A:3428:GLU:CG	2.41	0.51
1:A:4222:HIS:ND1	1:A:4223:PRO:HD2	2.26	0.51
1:B:1578:SER:C	1:B:1580:TYR:H	2.14	0.51
1:B:1823:TRP:O	1:B:1827:VAL:HG23	2.10	0.51
1:B:1892:LEU:HA	1:B:1895:CYS:SG	2.51	0.51
1:B:2199:ILE:O	1:B:2203:MET:HB2	2.11	0.51
1:B:3583:THR:O	1:B:3587:THR:HG23	2.11	0.51
1:B:3618:MET:HB3	1:B:3628:PHE:CZ	2.46	0.51
1:B:3790:PRO:HA	1:B:3898:PHE:CE2	2.46	0.51
1:A:2582:GLY:O	1:A:2585:MET:HB2	2.11	0.50
1:A:2839:LEU:HD22	1:A:2896:CYS:HB3	1.93	0.50
1:A:3116:ALA:HB1	1:A:3121:LEU:O	2.12	0.50
1:B:1573:SER:HA	1:B:1576:LYS:HE2	1.93	0.50
1:B:1527:LEU:HD22	1:B:1575:MET:HB2	1.92	0.50
1:B:1687:LEU:HD11	1:B:1706:LEU:HD21	1.93	0.50
1:B:4288:ILE:HG23	1:B:4289:PRO:HA	1.92	0.50
1:B:4644:LEU:HD13	1:B:4647:ALA:HB3	1.92	0.50
1:A:1776:GLU:HA	1:A:1779:SER:HB3	1.93	0.50
1:A:1963:ALA:HB1	1:A:2096:ARG:CG	2.41	0.50
1:A:2212:ILE:N	1:A:2213:PRO:CD	2.75	0.50
1:A:2856:PHE:CE1	1:A:2930:ILE:HG12	2.46	0.50
1:A:3923:LEU:HD11	1:A:3943:LEU:HA	1.94	0.50
1:B:1479:ARG:O	1:B:1483:ILE:HG13	2.11	0.50
1:B:1534:VAL:HG13	1:B:1568:HIS:CD2	2.42	0.50
1:B:2729:VAL:HG12	1:B:2782:LYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3038:TYR:CD2	1:B:3058:LEU:HD13	2.46	0.50
1:B:4267:ARG:NH2	1:B:4315:ASP:OD1	2.43	0.50
1:A:1719:GLN:HA	1:A:1722:PHE:CD2	2.46	0.50
1:A:4285:LEU:O	1:A:4288:ILE:HG13	2.10	0.50
1:B:1951:PRO:HG2	1:B:2104:ASP:OD2	2.10	0.50
1:B:4170:LEU:HD12	1:B:4171:ALA:N	2.26	0.50
1:B:4686:LEU:HD12	1:B:4687:SER:N	2.27	0.50
1:A:2049:ALA:O	1:A:2054:SER:HB3	2.12	0.50
1:A:2586:GLY:O	1:A:2590:ARG:HB2	2.10	0.50
1:A:3067:GLU:O	1:A:3069:ILE:HD12	2.12	0.50
1:A:4044:TRP:CE3	1:A:4048:PHE:HE1	2.29	0.50
1:A:4122:VAL:HA	1:A:4126:VAL:HG11	1.91	0.50
1:A:4326:PRO:HB3	1:A:4369:PHE:CD2	2.46	0.50
1:B:1907:LEU:HA	1:B:1911:ARG:NH1	2.26	0.50
1:B:1967:ARG:HG2	1:B:1967:ARG:HH11	1.75	0.50
1:B:2135:CYS:HB3	1:B:2139:LEU:HD12	1.92	0.50
1:B:2142:GLN:HB2	1:B:2145:TYR:CD1	2.46	0.50
1:A:2533:VAL:HB	1:A:2581:LEU:HA	1.94	0.50
1:A:2954:ASN:HD22	1:A:2954:ASN:N	2.02	0.50
1:A:3380:VAL:HG11	1:A:3435:ILE:CG2	2.41	0.50
1:A:3834:LEU:HA	1:A:3854:THR:HG21	1.93	0.50
1:A:4028:PRO:C	1:A:4030:PHE:H	2.15	0.50
1:A:4118:MET:HB3	1:A:4149:LEU:HD22	1.94	0.50
1:B:2865:THR:N	1:B:2868:ILE:HD12	2.26	0.50
1:A:2720:TYR:HE1	1:A:2781:ILE:HG21	1.76	0.50
1:A:4052:GLN:C	1:A:4054:GLY:H	2.14	0.50
1:B:1862:SER:O	1:B:1867:LEU:HD21	2.12	0.50
1:B:1926:VAL:HG22	1:B:1935:TYR:HE2	1.75	0.50
1:B:2367:LEU:HD12	1:B:2367:LEU:N	2.26	0.50
1:B:3691:ASP:C	1:B:3693:LYS:H	2.15	0.50
1:B:4111:LEU:N	1:B:4111:LEU:HD12	2.26	0.50
1:A:1971:ASN:ND2	1:A:2087:LEU:HD11	2.26	0.50
1:A:2197:ASN:O	1:A:2201:ASP:HB2	2.12	0.50
1:A:2627:TRP:O	1:A:2629:ASN:N	2.45	0.50
1:A:2913:PHE:CD2	1:A:2913:PHE:N	2.79	0.50
1:A:4388:THR:O	1:A:4391:HIS:HB2	2.12	0.50
1:A:4518:ALA:C	1:A:4520:LEU:H	2.15	0.50
1:B:1662:ILE:HB	1:B:1665:ILE:HG23	1.93	0.50
1:B:2723:THR:CG2	1:B:2727:GLU:HB2	2.42	0.50
1:B:4020:LEU:HD11	1:B:4033:LEU:HG	1.93	0.50
1:B:3105:PHE:O	1:B:3109:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2918:VAL:HG22	1:B:3172:TRP:CD2	2.47	0.50
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.94	0.50
1:A:1889:VAL:HA	1:A:1892:LEU:HD12	1.94	0.50
1:A:3410:LEU:HA	1:A:3414:GLY:O	2.12	0.50
1:A:3433:THR:HG22	1:A:3437:ASN:HD22	1.75	0.50
1:A:3583:THR:O	1:A:3587:THR:HG23	2.11	0.50
1:A:3977:LYS:O	1:A:3979:THR:HG23	2.12	0.50
1:A:4078:SER:HA	1:A:4081:ARG:HD2	1.94	0.50
1:A:4185:VAL:HG12	1:A:4186:LEU:N	2.19	0.50
1:B:2989:VAL:HG13	1:B:3187:GLU:OE2	2.12	0.50
1:B:4644:LEU:O	1:B:4661:SER:HB2	2.11	0.50
1:A:1926:VAL:HG12	1:A:1928:HIS:NE2	2.26	0.49
1:A:2798:ALA:C	1:A:2800:ARG:H	2.14	0.49
1:A:4278:HIS:CD2	1:A:4343:TYR:OH	2.64	0.49
1:A:3992:LEU:HD22	1:A:4430:LEU:CB	2.41	0.49
1:B:1522:GLN:O	1:B:1525:ILE:HG22	2.11	0.49
1:B:1781:LEU:O	1:B:1814:LEU:HD21	2.12	0.49
1:B:2504:GLN:HA	1:B:2507:GLU:OE2	2.12	0.49
1:B:2976:LEU:HD11	1:B:2990:LEU:HD21	1.94	0.49
1:B:3061:ARG:HB3	1:B:3067:GLU:OE2	2.12	0.49
1:B:3181:LEU:CB	1:B:3232:VAL:HG13	2.42	0.49
1:B:4132:LEU:HD13	1:B:4216:PHE:CZ	2.47	0.49
1:B:4259:ARG:NH2	1:B:4307:LEU:HB3	2.27	0.49
1:B:4339:GLY:HA3	1:B:4360:LEU:HD11	1.93	0.49
1:A:2511:LEU:HD11	1:A:2574:LEU:HD21	1.94	0.49
1:A:3011:HIS:CE1	1:A:3143:VAL:HG23	2.47	0.49
1:A:3059:LEU:HD21	1:A:3090:LEU:HD13	1.94	0.49
1:A:3337:LYS:CB	1:A:3525:LEU:HD13	2.24	0.49
1:A:3919:ILE:HG21	1:A:3951:THR:HA	1.94	0.49
1:A:4055:GLU:HG3	1:A:4093:ARG:NH1	2.27	0.49
1:A:4054:GLY:O	1:A:4055:GLU:O	2.30	0.49
1:B:1494:ILE:HA	1:B:1497:LEU:HD12	1.93	0.49
1:B:3935:ASP:O	1:B:3939:ARG:HG3	2.12	0.49
1:B:4060:GLU:HA	1:B:4063:ILE:HD13	1.94	0.49
1:B:4402:ILE:CD1	1:B:4402:ILE:H	2.21	0.49
1:B:4596:ASN:HD22	1:B:4596:ASN:C	2.15	0.49
1:B:4642:MET:HG2	1:B:4725:SER:HA	1.94	0.49
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.94	0.49
1:A:1739:THR:O	1:A:1760:ILE:HG12	2.12	0.49
1:A:2057:VAL:HG22	1:A:2058:GLU:H	1.78	0.49
1:A:2018:GLN:HE21	1:A:2066:SER:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2133:LYS:HD3	1:A:2133:LYS:O	2.12	0.49
1:A:2869:GLN:HG2	1:A:2871:HIS:CE1	2.47	0.49
1:A:3192:LEU:O	1:A:3224:ARG:NH2	2.46	0.49
1:A:3398:PRO:C	1:A:3400:PRO:HD2	2.33	0.49
1:A:3723:VAL:HG23	1:A:3764:LEU:HD22	1.94	0.49
1:A:4068:GLN:C	1:A:4070:SER:H	2.15	0.49
1:A:4365:THR:HB	1:A:4366:PRO:HD2	1.93	0.49
1:A:4574:GLN:HE22	1:A:4590:TRP:H	1.60	0.49
1:B:3135:SER:HA	1:B:3138:ARG:HG2	1.95	0.49
1:B:3700:LEU:CG	1:B:3701:ASP:H	2.23	0.49
1:A:1887:ASP:O	1:A:1891:GLN:HG3	2.12	0.49
1:A:2029:ASN:HD22	1:A:2030:ARG:N	2.11	0.49
1:A:2302:GLU:HG2	1:A:2304:HIS:CE1	2.46	0.49
1:A:2374:ASN:O	1:A:2375:LYS:HB2	2.11	0.49
1:A:3338:GLN:HA	1:A:3342:ARG:CB	2.42	0.49
1:A:3725:ASN:N	1:A:3725:ASN:ND2	2.58	0.49
1:A:4075:THR:HG23	1:A:4076:ILE:N	2.27	0.49
1:A:4122:VAL:HA	1:A:4126:VAL:CG1	2.42	0.49
1:A:4244:VAL:HG23	1:A:4403:SER:CB	2.42	0.49
1:B:3192:LEU:HD11	1:B:3268:VAL:HG22	1.94	0.49
1:A:1934:PHE:N	1:A:1934:PHE:CD2	2.81	0.49
1:A:2370:LEU:HD23	1:A:2387:LEU:HD22	1.95	0.49
1:A:3116:ALA:HB1	1:A:3123:LEU:HD12	1.94	0.49
1:A:3947:ILE:CG2	1:A:3948:PHE:N	2.76	0.49
1:B:2021:ALA:O	1:B:2071:MET:HA	2.13	0.49
1:B:3316:LYS:HD2	1:B:3546:ILE:HD12	1.94	0.49
1:A:1629:LEU:N	1:A:1630:PRO:HD3	2.28	0.49
1:A:1699:PHE:N	1:A:1699:PHE:CD1	2.77	0.49
1:A:1907:LEU:HA	1:A:1911:ARG:HH11	1.77	0.49
1:A:2029:ASN:HD22	1:A:2029:ASN:N	2.10	0.49
1:A:3217:MET:O	1:A:3218:ALA:C	2.50	0.49
1:A:3655:ASP:O	1:A:3659:ILE:HG13	2.13	0.49
1:A:3674:VAL:HG13	1:A:3786:PHE:HD2	1.78	0.49
1:B:2315:GLN:HB3	1:B:2775:THR:CG2	2.41	0.49
1:B:2832:ASN:HD22	1:B:2835:LEU:HD23	1.77	0.49
1:B:2839:LEU:HD22	1:B:2896:CYS:HB3	1.95	0.49
1:B:4012:LEU:N	1:B:4012:LEU:HD23	2.27	0.49
1:B:4313:TRP:HB3	1:B:4330:PRO:CG	2.42	0.49
1:A:2272:VAL:HA	1:A:2412:GLY:H	1.77	0.49
1:A:2848:ASN:HB3	1:A:2938:PHE:HE1	1.77	0.49
1:A:3039:THR:HG22	1:A:3040:ILE:N	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2612:LEU:HD11	1:B:2624:TRP:CZ3	2.48	0.49
1:B:4167:GLY:HA2	1:B:4170:LEU:HD11	1.93	0.49
1:A:2941:VAL:CG1	1:A:2942:ASN:N	2.76	0.49
1:A:2948:ARG:NH1	1:A:2948:ARG:HG2	2.28	0.49
1:A:3262:ASP:CB	1:A:3670:ARG:HE	2.25	0.49
1:A:3997:ASN:HD21	1:A:4001:ILE:HD11	1.77	0.49
1:A:4068:GLN:N	1:A:4073:GLN:HE21	2.11	0.49
1:A:4072:GLN:OE1	1:A:4077:VAL:HG21	2.11	0.49
1:A:4295:PHE:C	1:A:4295:PHE:CD2	2.86	0.49
1:B:2000:CYS:CB	1:B:2031:LEU:HD13	2.42	0.49
1:B:2517:GLU:O	1:B:2521:GLN:HG2	2.13	0.49
1:B:2677:GLY:HA3	1:B:2875:SER:OG	2.12	0.49
1:B:3991:LEU:HG	1:B:3992:LEU:HD23	1.94	0.49
1:B:4109:ASP:HA	1:B:4112:ASN:HD21	1.72	0.49
1:A:2208:VAL:HG22	1:A:2211:ASP:HB2	1.95	0.49
1:A:2610:ILE:HD12	1:A:2615:TYR:OH	2.13	0.49
1:A:3069:ILE:O	1:A:3141:LEU:O	2.30	0.49
1:A:3981:ASN:HD22	1:A:4076:ILE:CB	2.20	0.49
1:A:4230:LEU:HB3	1:A:4235:VAL:HG21	1.94	0.49
1:A:4536:SER:HB2	1:A:4548:LYS:HZ1	1.77	0.49
1:A:4548:LYS:O	1:A:4550:TRP:N	2.46	0.49
1:A:4596:ASN:ND2	1:A:4599:ALA:H	2.11	0.49
1:B:2723:THR:OG1	1:B:2724:PRO:HD2	2.13	0.49
1:B:4618:ASN:H	1:B:4618:ASN:ND2	2.11	0.49
1:A:1565:LEU:HD11	1:A:1598:VAL:HG12	1.94	0.49
1:A:1603:ASP:O	1:A:1606:ILE:HG22	2.13	0.49
1:A:1639:ILE:HG21	1:A:1676:LEU:HG	1.94	0.49
1:A:1800:HIS:HB2	1:A:1858:ASN:ND2	2.28	0.49
1:A:3180:ALA:O	1:A:3184:VAL:HG23	2.12	0.49
1:A:3370:GLU:O	1:A:3372:ALA:N	2.46	0.49
1:A:3689:TYR:CB	1:A:3694:ILE:HD11	2.21	0.49
1:A:4402:ILE:HD12	1:A:4402:ILE:N	2.26	0.49
1:B:1823:TRP:NE1	1:B:1885:GLN:HB3	2.27	0.49
1:B:1934:PHE:CD2	1:B:1934:PHE:N	2.81	0.49
1:B:1959:THR:HG21	1:B:2098:MET:SD	2.53	0.49
1:B:2241:GLN:HA	1:B:2244:ALA:HB3	1.93	0.49
1:B:2655:ARG:O	1:B:2659:VAL:HG23	2.13	0.49
1:B:3929:ASN:HB3	1:B:3942:TYR:CD1	2.47	0.49
1:B:4693:ASN:HD22	1:B:4693:ASN:N	2.09	0.49
1:A:1820:GLN:HE22	1:A:1990:GLN:HE22	1.60	0.48
1:A:2572:ARG:O	1:A:2575:TYR:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3017:VAL:HG22	1:A:3018:SER:N	2.27	0.48
1:A:3048:SER:HB2	1:A:3080:GLU:OE1	2.13	0.48
1:A:3457:LEU:HD11	1:A:3482:THR:HA	1.95	0.48
1:A:3598:PHE:O	1:A:3602:ILE:HB	2.11	0.48
1:B:1926:VAL:HG12	1:B:1928:HIS:NE2	2.28	0.48
1:B:2616:SER:HB3	1:B:2627:TRP:CD2	2.47	0.48
1:B:3540:ILE:O	1:B:3544:GLU:HG3	2.13	0.48
1:A:2720:TYR:CE1	1:A:2781:ILE:HG21	2.48	0.48
1:A:3150:ALA:O	1:A:3151:SER:C	2.51	0.48
1:A:3238:ILE:HG12	1:A:3601:TYR:HD2	1.69	0.48
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	1.95	0.48
1:A:4083:ILE:HD11	1:A:4098:SER:HA	1.94	0.48
1:A:4589:VAL:CG1	1:A:4639:VAL:HA	2.43	0.48
1:B:1934:PHE:HB3	1:B:1993:ARG:HH22	1.78	0.48
1:B:1813:GLN:NE2	1:B:1940:TYR:HA	2.17	0.48
1:B:2229:GLN:O	1:B:2230:PRO:O	2.30	0.48
1:B:2276:GLY:O	1:B:2282:LYS:HE2	2.13	0.48
1:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.95	0.48
1:B:2968:LEU:HG	1:B:2995:LEU:HD22	1.95	0.48
1:B:3295:THR:O	1:B:3299:VAL:HG23	2.12	0.48
1:B:4263:GLN:HA	1:B:4264:PRO:C	2.34	0.48
1:B:4513:ILE:HD12	1:B:4568:PHE:CE2	2.47	0.48
1:A:2088:PRO:C	1:A:2090:ASN:H	2.16	0.48
1:A:3007:GLN:NE2	1:A:3008:PRO:HD2	2.29	0.48
1:A:4133:LEU:HD21	1:A:4225:LEU:HD13	1.94	0.48
1:A:4604:THR:OG1	1:A:4671:TRP:HZ3	1.96	0.48
1:B:2604:PRO:O	1:B:2624:TRP:NE1	2.46	0.48
1:B:2720:TYR:CE1	1:B:2730:LEU:HD13	2.48	0.48
1:B:4306:ALA:HB1	1:B:4338:LEU:HD13	1.94	0.48
1:A:3145:PHE:CE2	1:A:3164:LEU:HD21	2.48	0.48
1:A:3920:PHE:O	1:A:3923:LEU:HB3	2.13	0.48
1:A:4133:LEU:HA	1:A:4217:MET:HB2	1.94	0.48
1:A:4335:ARG:HD3	1:A:4361:GLU:HA	1.96	0.48
1:B:1910:MET:HA	1:B:1929:MET:HG3	1.95	0.48
1:B:2080:GLY:HA3	1:B:2084:ARG:O	2.13	0.48
1:B:2621:ASP:C	1:B:2623:ASN:H	2.16	0.48
1:B:2782:LYS:HB2	1:B:2782:LYS:NZ	2.28	0.48
1:B:3673:LEU:HD13	1:B:3783:PHE:CE1	2.48	0.48
1:A:2273:MET:HG3	1:A:2413:MET:CE	2.44	0.48
1:A:2752:ASP:C	1:A:2754:TYR:H	2.17	0.48
1:A:3042:VAL:HB	1:A:3079:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3289:LEU:HD13	1:A:3293:ARG:HH22	1.77	0.48
1:A:3425:LYS:HA	1:A:3428:GLU:HG2	1.95	0.48
1:A:4047:PHE:HD2	1:A:4048:PHE:CD1	2.32	0.48
1:A:4190:ILE:HB	1:A:4197:LEU:HD21	1.94	0.48
1:A:4684:SER:O	1:A:4707:TYR:CE2	2.67	0.48
1:B:2025:PHE:HB2	1:B:2075:VAL:HG22	1.94	0.48
1:B:2641:VAL:CG2	1:B:2887:LEU:HD22	2.43	0.48
1:B:2774:ARG:HB2	1:B:2781:ILE:HD13	1.94	0.48
1:B:3677:PRO:HG3	1:B:3769:PRO:HB3	1.94	0.48
1:B:4024:ARG:HG3	1:B:4031:SER:O	2.14	0.48
1:A:2204:ILE:CG1	1:A:2205:PRO:HD3	2.44	0.48
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.95	0.48
1:A:2952:TYR:CE1	1:A:2962:PRO:HG3	2.48	0.48
1:A:3238:ILE:HD12	1:A:3238:ILE:N	2.28	0.48
1:A:3371:PRO:O	1:A:3372:ALA:C	2.52	0.48
1:A:3408:VAL:HG11	1:A:3477:LEU:CG	2.43	0.48
1:A:3487:TYR:O	1:A:3489:GLU:N	2.47	0.48
1:A:3664:MET:O	1:A:3668:PHE:HB3	2.13	0.48
1:A:3924:LEU:C	1:A:3925:ASN:HD22	2.15	0.48
1:A:4029:SER:CB	1:A:4081:ARG:HH12	2.25	0.48
1:A:4384:PRO:HB3	1:A:4395:TRP:CG	2.48	0.48
1:B:3196:ASN:ND2	1:B:3199:TYR:HB2	2.28	0.48
1:B:3911:PHE:CZ	1:B:3955:VAL:HG13	2.49	0.48
1:B:3990:PHE:CE2	1:B:4023:LEU:HD13	2.48	0.48
1:B:4410:LEU:CD2	1:B:4411:PRO:HD2	2.43	0.48
1:B:4653:GLN:OE1	1:B:4708:ASP:HA	2.14	0.48
1:A:1960:LEU:O	1:A:1964:LEU:N	2.39	0.48
1:A:1974:GLY:C	1:A:2079:PRO:HD3	2.34	0.48
1:A:1973:PHE:HE1	1:A:2099:ALA:CB	2.27	0.48
1:A:3323:LYS:HE3	1:A:3539:LEU:HG	1.95	0.48
1:A:3865:ILE:HA	1:A:3869:VAL:HG23	1.94	0.48
1:A:3891:LEU:HD21	1:A:3895:ARG:NH2	2.28	0.48
1:B:1525:ILE:HD12	1:B:1528:GLU:HB3	1.96	0.48
1:B:1694:PHE:CE1	1:B:1770:LEU:HB3	2.48	0.48
1:B:3011:HIS:ND1	1:B:3091:LEU:HD22	2.28	0.48
1:B:3677:PRO:HB3	1:B:3769:PRO:HD3	1.94	0.48
1:B:3887:ASN:N	1:B:3888:PRO:CD	2.77	0.48
1:B:4400:PRO:HG2	1:B:4407:TRP:CH2	2.49	0.48
1:B:4540:SER:HB2	1:B:4545:ILE:O	2.13	0.48
1:A:1974:GLY:CA	1:A:2079:PRO:HD3	2.44	0.48
1:A:3863:THR:O	1:A:3863:THR:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3987:GLU:HG3	1:A:4027:VAL:CG1	2.44	0.48
1:A:4184:TRP:CD1	1:A:4184:TRP:N	2.82	0.48
1:A:4406:ILE:HB	1:A:4412:GLU:OE2	2.14	0.48
1:A:4591:LEU:CD2	1:A:4601:ILE:HD11	2.42	0.48
1:B:2084:ARG:HH11	1:B:2084:ARG:HG2	1.79	0.48
1:B:3955:VAL:HG12	1:B:3959:LEU:HG	1.96	0.48
1:B:4070:SER:O	1:B:4071:ASN:C	2.52	0.48
1:A:1800:HIS:CB	1:A:1858:ASN:HD22	2.26	0.48
1:A:1701:GLY:HA2	1:A:2011:ARG:NH1	2.29	0.48
1:A:3397:PRO:HG2	1:A:3419:TRP:CE2	2.48	0.48
1:A:3473:ALA:O	1:A:3476:PRO:HD2	2.13	0.48
1:A:4132:LEU:HB2	1:A:4216:PHE:HD1	1.79	0.48
1:A:4655:THR:HG22	1:A:4708:ASP:HB2	1.96	0.48
1:B:3273:GLU:OE1	1:B:3667:ARG:NH2	2.47	0.48
1:B:3585:MET:HA	1:B:3588:VAL:HG23	1.96	0.48
1:B:3638:LEU:HB2	1:B:3663:ILE:HD12	1.96	0.48
1:B:3731:ASN:HB2	1:B:3732:PRO:HD3	1.94	0.48
1:B:1962:GLN:HB3	1:B:4341:THR:HG21	1.96	0.48
1:B:4407:TRP:CD1	1:B:4407:TRP:N	2.82	0.48
1:A:1535:ARG:HA	1:A:1591:TRP:CZ2	2.49	0.48
1:A:2299:ILE:CG2	1:A:2349:LYS:HA	2.44	0.48
1:A:2375:LYS:HG2	1:A:2387:LEU:HD23	1.95	0.48
1:A:2208:VAL:HA	1:A:2415:TRP:HD1	1.74	0.48
1:A:2704:ALA:HB3	1:A:3085:GLU:CG	2.44	0.48
1:A:2813:ILE:HG22	1:A:2814:LEU:N	2.28	0.48
1:A:3145:PHE:CD1	1:A:3164:LEU:HD11	2.48	0.48
1:A:3695:THR:HG21	1:A:3707:ASN:OD1	2.14	0.48
1:A:4201:GLU:HG3	1:A:4228:ASN:HB2	1.94	0.48
1:B:2532:ARG:NH1	1:B:2532:ARG:HG2	2.29	0.48
1:B:3232:VAL:O	1:B:3236:GLN:HG3	2.14	0.48
1:B:3350:VAL:HG12	1:B:3354:GLU:OE2	2.13	0.48
1:B:4083:ILE:CD1	1:B:4098:SER:HA	2.44	0.48
1:B:4288:ILE:CG2	1:B:4289:PRO:HA	2.44	0.48
1:B:4360:LEU:C	1:B:4362:GLN:H	2.17	0.48
1:A:3078:VAL:O	1:A:3078:VAL:HG13	2.13	0.47
1:A:3699:PHE:CZ	1:A:3726:ILE:HG13	2.49	0.47
1:A:4048:PHE:N	1:A:4048:PHE:CD1	2.82	0.47
1:A:4296:PHE:CZ	1:A:4347:ILE:HD13	2.49	0.47
1:B:2397:VAL:HG22	1:B:2398:GLN:N	2.29	0.47
1:B:2613:LEU:HD22	1:B:2655:ARG:NH1	2.29	0.47
1:B:2886:LEU:HD23	1:B:2904:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3960:LEU:HD23	1:B:4237:SER:HB2	1.96	0.47
1:A:2128:ILE:HG23	1:A:2129:VAL:N	2.29	0.47
1:A:2207:LEU:CD1	1:A:2215:ILE:HG21	2.43	0.47
1:A:2497:GLU:O	1:A:2501:ILE:HG13	2.13	0.47
1:A:3074:ASP:H	1:A:3077:ASN:HD22	1.62	0.47
1:A:3408:VAL:HG23	1:A:3409:CYS:H	1.80	0.47
1:A:3930:LEU:HD11	1:A:3939:ARG:HG2	1.95	0.47
1:A:4268:SER:OG	1:A:4387:THR:HA	2.14	0.47
1:A:4335:ARG:HD3	1:A:4360:LEU:C	2.35	0.47
1:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.96	0.47
1:A:3903:LEU:HD23	1:A:4433:MET:SD	2.54	0.47
1:B:1568:HIS:O	1:B:1572:ILE:HG13	2.14	0.47
1:B:1910:MET:HB2	1:B:1929:MET:HG3	1.95	0.47
1:B:2212:ILE:N	1:B:2213:PRO:CD	2.77	0.47
1:B:2918:VAL:HG22	1:B:3172:TRP:CE2	2.49	0.47
1:B:4568:PHE:O	1:B:4572:MET:HG2	2.14	0.47
1:A:1639:ILE:CD1	1:A:1675:LEU:HB3	2.44	0.47
1:A:1934:PHE:HE1	1:A:1964:LEU:HD22	1.78	0.47
1:A:2313:LYS:CE	1:A:2366:ASN:HD21	2.17	0.47
1:A:3781:VAL:HG12	1:A:3782:THR:N	2.29	0.47
1:A:3897:TYR:CE1	1:A:3913:LEU:HA	2.47	0.47
1:A:3997:ASN:O	1:A:3999:THR:N	2.47	0.47
1:A:3997:ASN:ND2	1:A:4001:ILE:HD11	2.27	0.47
1:B:1628:LEU:HD13	1:B:1709:ILE:HG22	1.95	0.47
1:B:1659:VAL:C	1:B:1661:ALA:H	2.18	0.47
1:B:3013:LEU:O	1:B:3013:LEU:HG	2.13	0.47
1:A:2368:ASN:HB3	1:A:2410:ARG:NH1	2.29	0.47
1:A:2598:GLN:HG3	1:A:2612:LEU:HB2	1.96	0.47
1:A:2616:SER:OG	1:A:2617:VAL:N	2.47	0.47
1:A:3219:ILE:CB	1:A:3220:PRO:CD	2.93	0.47
1:A:3480:TRP:HE1	1:A:3484:GLN:HE21	1.62	0.47
1:A:3338:GLN:HG3	1:A:3529:ILE:HD12	1.96	0.47
1:A:3804:THR:C	1:A:3806:ARG:H	2.18	0.47
1:B:1591:TRP:HA	1:B:1591:TRP:CE3	2.49	0.47
1:B:1811:PRO:HB2	1:B:1814:LEU:HD12	1.95	0.47
1:B:1971:ASN:HA	1:B:2075:VAL:O	2.14	0.47
1:B:2309:LYS:O	1:B:2758:ARG:HD2	2.14	0.47
1:B:2363:TRP:CH2	1:B:2395:PHE:HE1	2.32	0.47
1:B:2427:PHE:O	1:B:2431:LEU:HG	2.14	0.47
1:B:2595:LYS:HE3	1:B:2611:PRO:HG3	1.96	0.47
1:B:2754:TYR:O	1:B:2755:GLY:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3966:THR:N	1:B:4426:MET:HE2	2.29	0.47
1:A:1592:ASP:O	1:A:1596:ASN:HB2	2.14	0.47
1:A:1628:LEU:C	1:A:1630:PRO:HD3	2.35	0.47
1:A:2010:SER:O	1:A:2060:LEU:HD11	2.14	0.47
1:A:2282:LYS:HB2	2:A:9002:ADP:O3B	2.15	0.47
1:A:3648:HIS:CE1	1:A:3654:SER:HA	2.49	0.47
1:A:3730:LEU:CD2	1:A:3733:VAL:HB	2.44	0.47
1:A:4200:LEU:HD22	1:A:4204:LEU:CG	2.45	0.47
1:A:4313:TRP:HB3	1:A:4330:PRO:CG	2.45	0.47
1:B:1603:ASP:O	1:B:1606:ILE:HG22	2.15	0.47
1:B:1920:ASN:ND2	1:B:1921:VAL:N	2.62	0.47
1:B:3605:PHE:HB3	1:B:3609:PHE:HB3	1.95	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:CG2	2.45	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:HG23	1.96	0.47
1:A:2204:ILE:HA	1:A:2207:LEU:CD1	2.42	0.47
1:A:2250:VAL:HG21	1:A:2425:MET:HA	1.97	0.47
1:A:3794:GLN:HG3	1:A:3891:LEU:HA	1.96	0.47
1:A:4326:PRO:HB3	1:A:4369:PHE:HD2	1.79	0.47
1:B:1766:ILE:HG23	1:B:1767:HIS:N	2.30	0.47
1:B:2667:HIS:HA	1:B:2787:GLN:OE1	2.14	0.47
1:B:2532:ARG:CZ	1:B:2813:ILE:HD12	2.45	0.47
1:B:4596:ASN:ND2	1:B:4596:ASN:C	2.68	0.47
1:B:4618:ASN:H	1:B:4618:ASN:HD22	1.60	0.47
1:A:3032:MET:O	1:A:3034:GLY:N	2.47	0.47
1:A:3036:SER:N	1:A:3068:LYS:O	2.48	0.47
1:A:3370:GLU:O	1:A:3371:PRO:C	2.51	0.47
1:A:4043:ASP:N	1:A:4043:ASP:OD2	2.45	0.47
1:A:4430:LEU:O	1:A:4434:GLN:HB2	2.15	0.47
1:B:1611:ARG:O	1:B:1615:LEU:HD23	2.14	0.47
1:B:2125:ALA:O	1:B:2129:VAL:HG13	2.14	0.47
1:B:2540:LEU:HB3	1:B:2576:SER:OG	2.14	0.47
1:B:2676:PRO:HG3	1:B:2873:ILE:HD12	1.96	0.47
1:B:4119:ALA:HA	1:B:4149:LEU:HD11	1.96	0.47
1:B:4359:PHE:O	1:B:4362:GLN:HB3	2.15	0.47
1:A:1927:ILE:C	1:A:1928:HIS:HD2	2.18	0.47
1:A:2088:PRO:HB2	1:A:2090:ASN:HD21	1.80	0.47
1:A:2196:LEU:HA	1:A:2199:ILE:HG12	1.97	0.47
1:A:2273:MET:HB3	1:A:2395:PHE:CD1	2.50	0.47
1:A:2990:LEU:HD23	1:A:2994:VAL:HG11	1.97	0.47
1:A:3074:ASP:H	1:A:3077:ASN:ND2	2.13	0.47
1:A:4109:ASP:O	1:A:4112:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4344:GLY:HA2	1:A:4347:ILE:HG13	1.95	0.47
1:A:4690:VAL:HG21	1:A:4701:PHE:CE1	2.50	0.47
1:B:1547:ASN:HD21	1:B:1550:ARG:H	1.63	0.47
1:B:1782:ALA:HB2	1:B:1922:LEU:HD23	1.96	0.47
1:B:2231:ILE:HG12	1:B:2260:LEU:HD23	1.96	0.47
1:B:2335:THR:O	1:B:2339:ILE:HG13	2.14	0.47
1:B:2512:VAL:HA	1:B:2515:VAL:HG12	1.95	0.47
1:B:2882:TRP:CZ2	1:B:2909:ALA:HB2	2.48	0.47
1:B:3650:ASN:O	1:B:3651:SER:HB2	2.15	0.47
1:B:3698:SER:HB3	1:B:3700:LEU:CD1	2.44	0.47
1:B:4059:PRO:O	1:B:4063:ILE:HD12	2.15	0.47
1:B:4429:ASP:O	1:B:4433:MET:HG3	2.15	0.47
1:B:4673:ASP:C	1:B:4675:ASP:H	2.18	0.47
1:A:2127:LYS:HB3	1:A:2222:VAL:HG13	1.97	0.47
1:A:2641:VAL:O	1:A:2646:VAL:HG11	2.15	0.47
1:A:2766:MET:CB	1:A:2783:LEU:HD11	2.42	0.47
1:A:3563:LEU:O	1:A:3567:LEU:HG	2.14	0.47
1:A:3988:TRP:O	1:A:3992:LEU:HG	2.14	0.47
1:A:4162:ILE:HG13	1:A:4187:LEU:HD23	1.97	0.47
1:A:4244:VAL:HG23	1:A:4403:SER:HB3	1.96	0.47
1:A:4269:ARG:HA	1:A:4392:PHE:CZ	2.50	0.47
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.49	0.47
1:B:3043:ASN:HD22	1:B:3043:ASN:N	2.10	0.47
1:B:3849:ASP:HA	1:B:3852:ILE:HG22	1.97	0.47
1:A:1868:SER:O	1:A:1872:ARG:HB2	2.15	0.47
1:A:2370:LEU:CD2	1:A:2387:LEU:HD22	2.45	0.47
1:A:3776:ASP:HB3	1:A:3780:ARG:HH12	1.80	0.47
1:A:4295:PHE:C	1:A:4295:PHE:HD2	2.18	0.47
1:B:2252:LYS:HE2	1:B:2254:GLU:HG2	1.96	0.47
1:B:2556:SER:C	1:B:2558:PHE:H	2.17	0.47
1:B:2587:LEU:HD12	1:B:2817:ASP:HB3	1.96	0.47
1:B:3601:TYR:O	1:B:3602:ILE:C	2.53	0.47
1:B:4005:ILE:HG21	1:B:4008:LEU:HD12	1.96	0.47
1:A:2316:LEU:HD23	1:A:2363:TRP:HB2	1.97	0.47
1:A:2424:GLN:HG3	1:A:2508:PRO:HG3	1.97	0.47
1:A:2905:TRP:CZ3	1:A:2934:ALA:HB2	2.50	0.47
1:A:4376:VAL:HB	1:A:4381:LEU:HB2	1.97	0.47
1:B:2660:LEU:O	1:B:2664:LEU:HB2	2.15	0.47
1:B:2669:PRO:HG2	1:B:2810:HIS:O	2.14	0.47
1:B:2701:PHE:CE2	1:B:2759:VAL:HG11	2.50	0.47
1:B:2309:LYS:HE2	1:B:2756:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3677:PRO:CG	1:B:3787:THR:HG22	2.45	0.47
1:B:3930:LEU:O	1:B:3931:VAL:C	2.53	0.47
1:B:4157:TYR:HB2	1:B:4184:TRP:C	2.35	0.47
1:B:4136:SER:O	1:B:4220:GLU:HA	2.15	0.47
1:B:4650:ASN:O	1:B:4653:GLN:HG3	2.15	0.47
1:A:2065:ILE:HG22	1:A:2066:SER:N	2.30	0.46
1:A:2651:VAL:CG1	1:A:2652:ASP:H	2.23	0.46
1:A:3040:ILE:HG22	1:A:3040:ILE:O	2.14	0.46
1:A:3285:LEU:HD22	1:A:3578:SER:HB2	1.97	0.46
1:A:3452:ILE:O	1:A:3457:LEU:HD23	2.15	0.46
1:A:3270:LEU:CB	1:A:3592:VAL:HG13	2.44	0.46
1:A:3639:SER:HB2	1:A:3643:GLU:OE1	2.15	0.46
1:A:4099:HIS:ND1	1:A:4111:LEU:HD12	2.30	0.46
1:A:4537:LEU:HD23	1:A:4548:LYS:HE3	1.97	0.46
1:A:4599:ALA:O	1:A:4602:THR:HG22	2.15	0.46
1:B:1576:LYS:HG2	1:B:1585:GLU:OE2	2.14	0.46
1:B:1642:GLU:O	1:B:1646:ILE:HG12	2.16	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CZ	2.49	0.46
1:B:2270:HIS:HB3	1:B:2392:ARG:NH1	2.29	0.46
1:B:2774:ARG:HG2	1:B:2776:SER:OG	2.15	0.46
1:B:3973:ILE:HG13	1:B:3988:TRP:CZ3	2.50	0.46
1:A:1886:ARG:CZ	1:A:1890:ARG:HH22	2.28	0.46
1:A:1969:GLY:N	1:A:2047:GLN:NE2	2.64	0.46
1:A:2101:ILE:HD13	1:A:2101:ILE:N	2.30	0.46
1:A:4067:ALA:C	1:A:4073:GLN:HE21	2.19	0.46
1:B:1555:VAL:H	1:B:1609:GLN:NE2	2.12	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CE2	2.50	0.46
1:B:2532:ARG:HG3	1:B:2808:LEU:O	2.14	0.46
1:B:3027:ARG:HA	1:B:3037:ILE:CD1	2.43	0.46
1:B:4128:SER:HB2	1:B:4213:PHE:HB3	1.96	0.46
1:B:4604:THR:HG23	1:B:4671:TRP:NE1	2.21	0.46
1:A:1809:ASN:HD22	1:A:1809:ASN:HA	1.60	0.46
1:A:2415:TRP:HA	1:A:2415:TRP:CE3	2.51	0.46
1:A:2720:TYR:CE1	1:A:2730:LEU:HD13	2.50	0.46
1:A:2956:LEU:HD21	1:A:2971:TYR:CD2	2.50	0.46
1:A:3021:GLY:O	1:A:3025:LEU:HB2	2.14	0.46
1:A:3283:LEU:C	1:A:3283:LEU:HD23	2.36	0.46
1:A:3975:SER:C	1:A:3977:LYS:H	2.18	0.46
1:A:4220:GLU:O	1:A:4222:HIS:N	2.49	0.46
1:B:1601:LEU:HA	1:B:1666:GLN:OE1	2.16	0.46
1:B:4030:PHE:HE1	1:B:4085:LEU:HG	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4190:ILE:HG12	1:B:4219:SER:CB	2.44	0.46
1:A:1630:PRO:O	1:A:1634:THR:HG23	2.15	0.46
1:A:2492:LEU:HG	1:A:2496:LYS:NZ	2.31	0.46
1:A:2882:TRP:CZ2	1:A:2905:TRP:NE1	2.83	0.46
1:A:2903:ARG:HB2	1:A:2945:ALA:O	2.15	0.46
1:A:3071:PHE:HE2	1:A:3087:MET:HE3	1.79	0.46
1:A:3219:ILE:CB	1:A:3220:PRO:HD3	2.46	0.46
1:A:4087:LYS:HG2	1:A:4087:LYS:O	2.15	0.46
1:A:4589:VAL:HG22	1:A:4590:TRP:N	2.29	0.46
1:B:2191:GLU:HA	1:B:2194:VAL:HG23	1.98	0.46
1:B:2529:THR:OG1	1:B:2532:ARG:HB2	2.15	0.46
1:B:2937:HIS:C	1:B:2939:PRO:HD3	2.35	0.46
1:B:3288:GLY:HA3	1:B:3574:TRP:CZ3	2.49	0.46
1:B:3773:PHE:HB3	1:B:3777:LEU:HD23	1.98	0.46
1:A:1948:VAL:O	1:A:1950:THR:N	2.49	0.46
1:A:2257:GLU:O	1:A:2261:GLN:HG2	2.16	0.46
1:A:2856:PHE:CZ	1:A:2930:ILE:HG12	2.49	0.46
1:A:3324:LEU:HD12	1:A:3539:LEU:CD2	2.46	0.46
1:A:3733:VAL:C	1:A:3735:ASN:H	2.19	0.46
1:A:3998:LEU:O	1:A:3998:LEU:HD13	2.15	0.46
1:B:1555:VAL:H	1:B:1609:GLN:HE22	1.64	0.46
1:B:1846:GLN:O	1:B:1849:GLU:HB3	2.16	0.46
1:B:2127:LYS:C	1:B:2130:PRO:HD2	2.35	0.46
1:B:2907:HIS:HB2	1:B:2950:ILE:HG21	1.96	0.46
1:A:1786:SER:HB2	1:A:1914:TYR:OH	2.16	0.46
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	1.98	0.46
1:A:2376:LEU:HA	1:A:2385:LEU:O	2.15	0.46
1:A:2435:SER:HB3	1:A:2496:LYS:HG2	1.97	0.46
1:A:2832:ASN:ND2	1:A:2883:ASP:OD2	2.49	0.46
1:A:3113:LYS:HG3	1:A:3123:LEU:O	2.15	0.46
1:A:3007:GLN:O	1:A:3142:HIS:HE1	1.99	0.46
1:A:3387:HIS:HB2	1:A:3473:ALA:HB2	1.95	0.46
1:A:3725:ASN:N	1:A:3725:ASN:HD22	1.99	0.46
1:A:4044:TRP:HE3	1:A:4048:PHE:HE1	1.62	0.46
1:A:4044:TRP:CE2	1:A:4059:PRO:HG3	2.51	0.46
1:B:1721:HIS:C	1:B:1725:MET:HE2	2.36	0.46
1:B:1799:ASP:OD1	1:B:1801:SER:HB3	2.15	0.46
1:B:2748:LEU:HD11	1:B:3162:PRO:HG2	1.97	0.46
1:B:3891:LEU:HD21	1:B:3895:ARG:NH2	2.31	0.46
1:B:4296:PHE:HB3	1:B:4346:ARG:HD2	1.98	0.46
1:A:2243:ILE:HG21	1:A:2288:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2578:MET:HE1	1:A:2613:LEU:HA	1.96	0.46
1:A:3830:LEU:HD12	1:A:3858:LEU:HD13	1.96	0.46
1:A:3990:PHE:HD2	1:A:4084:LEU:HD22	1.81	0.46
1:A:4318:SER:HA	1:A:4321:ARG:NH2	2.23	0.46
1:B:2749:PRO:O	1:B:2757:GLN:HG2	2.16	0.46
1:B:2532:ARG:NH1	1:B:2813:ILE:HD12	2.31	0.46
1:B:2841:ASN:ND2	1:B:2842:LEU:HG	2.31	0.46
1:B:3788:VAL:HG11	1:B:3913:LEU:CD2	2.46	0.46
1:B:4020:LEU:HG	1:B:4034:VAL:HG22	1.98	0.46
1:B:4222:HIS:ND1	1:B:4223:PRO:HD2	2.31	0.46
1:B:4281:ILE:HG13	1:B:4282:GLN:N	2.31	0.46
1:B:1962:GLN:CB	1:B:4341:THR:HG21	2.46	0.46
1:B:4645:GLU:HG3	1:B:4722:SER:OG	2.15	0.46
1:A:1904:PHE:C	1:A:1906:TRP:H	2.17	0.46
1:A:2059:LEU:HG	1:A:2060:LEU:HG	1.97	0.46
1:A:2205:PRO:HG3	1:A:2261:GLN:OE1	2.16	0.46
1:A:2360:ASP:HB2	1:A:2361:PRO:HD2	1.96	0.46
1:A:2443:GLU:OE2	1:A:2489:PRO:HB2	2.15	0.46
1:A:2603:THR:HG22	1:A:2604:PRO:HD2	1.97	0.46
1:A:2829:GLY:HA2	1:A:2850:THR:OG1	2.16	0.46
1:A:4022:CYS:O	1:A:4026:GLN:HB2	2.16	0.46
1:A:4681:ASN:ND2	1:A:4685:LYS:HE3	2.30	0.46
1:A:4719:ARG:HG3	1:A:4719:ARG:HH11	1.81	0.46
1:B:3993:LYS:O	1:B:3994:GLY:C	2.54	0.46
1:B:4597:PRO:HG2	1:B:4692:LEU:CD1	2.46	0.46
1:A:1530:PHE:CZ	1:A:1571:SER:HB2	2.51	0.46
1:A:1745:SER:OG	1:A:1751:THR:HG22	2.16	0.46
1:A:3925:ASN:N	1:A:3925:ASN:ND2	2.63	0.46
1:A:4395:TRP:CZ3	1:A:4399:LEU:HD11	2.51	0.46
1:A:4596:ASN:ND2	1:A:4596:ASN:C	2.69	0.46
1:B:1683:LEU:O	1:B:1683:LEU:HD12	2.16	0.46
1:B:3715:GLY:HA3	1:B:3758:PRO:HG2	1.98	0.46
1:B:4331:TRP:CZ2	1:B:4369:PHE:HE2	2.34	0.46
1:B:4284:ARG:NH2	1:B:4355:LEU:HD21	2.31	0.46
1:A:1662:ILE:HG22	1:A:1663:GLU:N	2.32	0.46
1:A:1911:ARG:HD3	1:A:1911:ARG:H	1.81	0.46
1:A:2641:VAL:O	1:A:2643:SER:N	2.49	0.46
1:A:2864:PHE:HB3	1:A:2872:TYR:HD2	1.81	0.46
1:A:2952:TYR:CZ	1:A:2962:PRO:HG3	2.51	0.46
1:A:3017:VAL:HG21	1:A:3257:PRO:HD3	1.98	0.46
1:A:4263:GLN:NE2	1:A:4322:SER:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4278:HIS:HD2	1:A:4343:TYR:OH	1.99	0.46
1:A:4402:ILE:CD1	1:A:4402:ILE:H	2.28	0.46
1:B:2044:GLN:O	1:B:2048:VAL:HG23	2.16	0.46
1:B:3789:THR:H	1:B:3792:SER:HB3	1.81	0.46
1:B:4095:LEU:HD11	1:B:4422:LYS:HB3	1.97	0.46
1:B:4274:LEU:HD11	1:B:4306:ALA:HB1	1.98	0.46
1:B:4400:PRO:HG2	1:B:4407:TRP:HH2	1.81	0.46
1:A:1642:GLU:O	1:A:1646:ILE:HG13	2.16	0.45
1:A:2338:ARG:HH11	1:A:2338:ARG:HG2	1.81	0.45
1:A:2851:ASP:HB3	1:A:2937:HIS:CE1	2.51	0.45
1:A:2980:TYR:OH	1:A:2987:PRO:HA	2.15	0.45
1:A:4726:TRP:CH2	1:A:4728:SER:HB2	2.51	0.45
1:A:2249:LEU:HB3	2:A:9002:ADP:N6	2.30	0.45
1:B:1534:VAL:HG22	1:B:1568:HIS:CD2	2.50	0.45
1:B:1604:VAL:O	1:B:1608:VAL:HG23	2.16	0.45
1:B:1822:VAL:HG13	1:B:1823:TRP:N	2.31	0.45
1:B:1985:LYS:HD3	1:B:1997:VAL:HG21	1.98	0.45
1:B:2275:VAL:HG11	1:B:2400:LEU:HG	1.97	0.45
1:B:2873:ILE:O	1:B:2873:ILE:HG13	2.14	0.45
1:B:3912:SER:HB3	1:B:4231:ARG:CG	2.45	0.45
1:B:4122:VAL:HG11	1:B:4216:PHE:HZ	1.81	0.45
1:B:4434:GLN:HE21	1:B:4434:GLN:HB3	1.55	0.45
1:B:4574:GLN:NE2	1:B:4590:TRP:HB3	2.31	0.45
1:A:3015:ILE:CG2	1:A:3149:PRO:HG3	2.45	0.45
1:A:3271:ILE:HG12	1:A:3592:VAL:HG21	1.97	0.45
1:A:3551:SER:O	1:A:3554:LYS:HB2	2.16	0.45
1:A:4039:GLN:HB3	1:A:4040:ASN:H	1.57	0.45
1:A:4309:SER:O	1:A:4312:TYR:HB3	2.16	0.45
1:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.16	0.45
1:B:1931:ASN:HD21	1:B:1962:GLN:HE22	1.64	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:O	2.16	0.45
1:B:2309:LYS:HZ3	1:B:2756:THR:HG21	1.77	0.45
1:B:2331:LEU:HD21	1:B:2773:TRP:CG	2.51	0.45
1:B:4379:ILE:HG23	1:B:4381:LEU:HG	1.98	0.45
1:A:3190:ARG:C	1:A:3192:LEU:H	2.20	0.45
1:A:3481:ALA:O	1:A:3485:THR:HG23	2.16	0.45
1:A:3798:LEU:O	1:A:3802:LEU:HG	2.17	0.45
1:A:3814:SER:C	1:A:3818:LYS:HD3	2.37	0.45
1:A:4026:GLN:HB3	1:A:4027:VAL:H	1.60	0.45
1:A:4281:ILE:HG13	1:A:4282:GLN:N	2.31	0.45
1:A:4337:ILE:O	1:A:4341:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4653:GLN:O	1:A:4655:THR:HG23	2.17	0.45
1:B:2745:GLU:HG2	1:B:2748:LEU:HD11	1.98	0.45
1:B:4431:GLN:HG2	1:B:4431:GLN:O	2.16	0.45
1:A:2323:THR:O	1:A:2324:THR:HG23	2.16	0.45
1:A:2738:TRP:CZ3	1:A:2785:LYS:HA	2.51	0.45
1:A:2398:GLN:NE2	1:A:2806:ARG:HG2	2.31	0.45
1:A:2845:PHE:O	1:A:2848:ASN:HB2	2.16	0.45
1:A:2896:CYS:SG	1:A:2897:THR:N	2.90	0.45
1:A:2976:LEU:HD12	1:A:3028:PHE:CE1	2.51	0.45
1:A:3792:SER:OG	1:A:3793:LEU:N	2.50	0.45
1:A:3893:CYS:HB3	1:A:3916:PHE:HZ	1.81	0.45
1:B:2849:LEU:HD13	1:B:2901:LEU:HD11	1.99	0.45
1:B:3015:ILE:HD12	1:B:3170:LEU:HD11	1.98	0.45
1:B:3536:TYR:O	1:B:3540:ILE:HD13	2.16	0.45
1:B:3306:LEU:HD13	1:B:3557:VAL:CG2	2.46	0.45
1:B:3990:PHE:HD2	1:B:4084:LEU:HD22	1.82	0.45
1:B:4047:PHE:HE1	1:B:4086:MET:HE1	1.81	0.45
1:B:4335:ARG:NH2	1:B:4365:THR:HG22	2.22	0.45
1:A:3459:ASP:HB3	1:A:3462:PHE:CB	2.47	0.45
1:A:3549:GLU:O	1:A:3553:VAL:HG23	2.17	0.45
1:A:3686:MET:CE	1:A:3696:LYS:HB2	2.46	0.45
1:A:4279:ALA:O	1:A:4283:GLU:HB2	2.17	0.45
1:A:4349:ASN:O	1:A:4352:ASP:HB2	2.16	0.45
1:A:4648:VAL:HG23	1:A:4655:THR:OG1	2.16	0.45
1:B:2630:LYS:CB	1:B:2654:THR:HG21	2.47	0.45
1:B:3930:LEU:HD22	1:B:3939:ARG:HE	1.81	0.45
1:B:4012:LEU:HA	1:B:4016:GLN:NE2	2.31	0.45
1:A:1726:PHE:HB2	1:A:1729:LEU:HB3	1.98	0.45
1:A:1784:LEU:HB3	1:A:1814:LEU:HD13	1.99	0.45
1:A:1842:GLN:OE1	1:A:1893:GLN:HG2	2.17	0.45
1:A:1968:MET:HB3	1:A:2094:LEU:O	2.16	0.45
1:A:1973:PHE:C	1:A:1973:PHE:CD1	2.89	0.45
1:A:1964:LEU:HD12	1:A:2074:PHE:CZ	2.51	0.45
1:A:2603:THR:CB	1:A:2604:PRO:HD2	2.46	0.45
1:A:3011:HIS:C	1:A:3168:CYS:HB3	2.36	0.45
1:A:3350:VAL:O	1:A:3350:VAL:HG12	2.15	0.45
1:A:3897:TYR:HD2	1:A:3898:PHE:CD2	2.34	0.45
1:A:3919:ILE:HD13	1:A:3951:THR:HA	1.98	0.45
1:B:2819:PRO:HB2	1:B:2824:LEU:CD2	2.46	0.45
1:B:3673:LEU:HD22	1:B:3783:PHE:CE1	2.48	0.45
1:B:4404:THR:HB	1:B:4405:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4693:ASN:ND2	1:B:4693:ASN:N	2.64	0.45
1:B:4714:GLN:O	1:B:4718:GLN:HG3	2.16	0.45
1:A:1907:LEU:HD22	1:A:1911:ARG:NH1	2.31	0.45
1:A:2124:LEU:HD22	1:A:2195:LEU:CD2	2.46	0.45
1:A:2435:SER:CB	1:A:2496:LYS:HG2	2.47	0.45
1:A:3022:LYS:HA	1:A:3173:PHE:CE1	2.52	0.45
1:A:3234:ILE:O	1:A:3238:ILE:HD13	2.17	0.45
1:A:3463:ASP:O	1:A:3467:VAL:HG23	2.17	0.45
1:A:3388:LEU:CD2	1:A:3473:ALA:HB1	2.44	0.45
1:A:4249:LEU:O	1:A:4253:ILE:HG13	2.17	0.45
1:B:2825:THR:HG23	1:B:2854:VAL:HG21	1.98	0.45
1:B:3004:VAL:O	1:B:3010:GLY:HA3	2.17	0.45
1:B:3542:GLU:O	1:B:3546:ILE:HG12	2.16	0.45
1:B:3696:LYS:HG3	1:B:3719:LEU:HD23	1.99	0.45
1:B:4666:ILE:HG13	1:B:4667:ALA:N	2.32	0.45
1:A:1800:HIS:CD2	1:A:1858:ASN:HB3	2.52	0.45
1:A:1922:LEU:HD13	1:A:1938:PHE:CD1	2.48	0.45
1:A:2902:VAL:HG21	1:A:2941:VAL:CG2	2.47	0.45
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.52	0.45
1:A:4329:ILE:HB	1:A:4331:TRP:CE2	2.51	0.45
1:A:4384:PRO:HG2	1:A:4392:PHE:CD1	2.51	0.45
1:A:4668:THR:C	1:A:4669:LEU:HD12	2.37	0.45
1:B:1618:ILE:HD13	1:B:1683:LEU:HD21	1.99	0.45
1:B:1740:THR:HG22	1:B:1759:SER:HA	1.98	0.45
1:B:2091:LEU:HD22	1:B:2095:PHE:CE2	2.51	0.45
1:B:3990:PHE:CZ	1:B:4023:LEU:HD13	2.52	0.45
1:B:4197:LEU:HB3	1:B:4226:PRO:HG2	1.98	0.45
1:B:4618:ASN:N	1:B:4618:ASN:ND2	2.65	0.45
1:A:1925:LEU:HD23	1:A:1936:TYR:HB2	1.98	0.45
1:A:2052:GLU:O	1:A:2053:ASN:CB	2.64	0.45
1:A:2140:SER:HB2	1:A:2211:ASP:OD2	2.15	0.45
1:A:2196:LEU:HA	1:A:2199:ILE:CG1	2.46	0.45
1:A:2526:MET:O	1:A:2527:ASP:C	2.55	0.45
1:A:3145:PHE:CG	1:A:3164:LEU:HD11	2.52	0.45
1:A:3218:ALA:O	1:A:3220:PRO:N	2.49	0.45
1:A:3602:ILE:O	1:A:3603:GLY:C	2.54	0.45
1:A:3639:SER:OG	1:A:3663:ILE:HD11	2.17	0.45
1:A:4032:LYS:HA	1:A:4032:LYS:HE2	1.97	0.45
1:A:4046:GLN:NE2	1:A:4057:ILE:HG22	2.32	0.45
1:A:4311:ASP:O	1:A:4315:ASP:HB3	2.17	0.45
1:A:4347:ILE:CG2	1:A:4353:MET:HG2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2204:ILE:N	1:B:2205:PRO:CD	2.80	0.45
1:B:2270:HIS:HB3	1:B:2392:ARG:HH11	1.82	0.45
1:B:3254:TYR:CD2	1:B:3775:PRO:HA	2.52	0.45
1:B:4095:LEU:HD11	1:B:4422:LYS:HB2	1.99	0.45
1:B:3992:LEU:HD12	1:B:4434:GLN:NE2	2.31	0.45
1:B:4621:LEU:HG	1:B:4622:HIS:H	1.82	0.45
1:B:4657:THR:HG22	1:B:4658:ASP:N	2.32	0.45
1:A:2272:VAL:HB	1:A:2394:MET:HE2	1.97	0.45
1:A:3027:ARG:HH11	1:A:3027:ARG:HB2	1.81	0.45
1:A:3540:ILE:N	1:A:3540:ILE:HD12	2.32	0.45
1:A:3542:GLU:O	1:A:3546:ILE:HG13	2.17	0.45
1:A:3696:LYS:HZ3	1:A:3721:GLN:CD	2.21	0.45
1:A:3813:ARG:HA	1:A:3875:VAL:HG11	1.99	0.45
1:A:3908:LEU:HD21	1:A:4237:SER:OG	2.16	0.45
1:A:3912:SER:HB3	1:A:4231:ARG:CG	2.45	0.45
1:A:3903:LEU:HD13	1:A:3959:LEU:HD21	1.99	0.45
1:A:4116:LEU:HB3	1:A:4117:ASP:H	1.52	0.45
1:A:4455:SER:C	1:A:4457:SER:H	2.20	0.45
1:B:1548:TYR:HD2	1:B:1554:LEU:HD11	1.82	0.45
1:B:1764:PRO:HB2	1:B:1768:GLU:CB	2.47	0.45
1:B:2641:VAL:HG13	1:B:2831:PHE:HB3	1.98	0.45
1:B:2998:ILE:CG2	1:B:3025:LEU:HD22	2.47	0.45
1:B:3078:VAL:O	1:B:3078:VAL:HG13	2.16	0.45
1:B:4220:GLU:O	1:B:4222:HIS:N	2.50	0.45
1:B:4197:LEU:HD13	1:B:4226:PRO:HD3	1.99	0.45
1:B:4253:ILE:HG22	1:B:4253:ILE:O	2.17	0.45
1:A:1777:MET:CE	1:A:1939:GLU:HA	2.48	0.44
1:A:1958:LEU:O	1:A:1962:GLN:HB2	2.16	0.44
1:A:2730:LEU:HD22	1:A:2772:PHE:CZ	2.52	0.44
1:A:3682:MET:CE	1:A:3721:GLN:HE21	2.31	0.44
1:A:3776:ASP:HB3	1:A:3780:ARG:NH1	2.31	0.44
1:A:3825:VAL:HA	1:A:3828:ARG:HD3	1.99	0.44
1:A:4076:ILE:HD12	1:A:4105:VAL:HG22	1.99	0.44
1:B:1629:LEU:HD22	1:B:1632:GLU:HG2	1.98	0.44
1:B:1869:ALA:HA	1:B:1872:ARG:HB3	1.99	0.44
1:B:2381:ASN:ND2	1:B:2383:GLU:HB2	2.20	0.44
1:B:2705:THR:HG22	1:B:2759:VAL:HG21	1.98	0.44
1:B:2774:ARG:C	1:B:2776:SER:H	2.20	0.44
1:A:1609:GLN:O	1:A:1613:VAL:HG23	2.17	0.44
1:A:1748:GLU:HB3	1:A:1943:ILE:HD12	1.99	0.44
1:A:2142:GLN:NE2	1:A:2208:VAL:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2302:GLU:HG2	1:A:2304:HIS:HE1	1.81	0.44
1:A:2359:VAL:HG11	1:A:2400:LEU:HD22	1.99	0.44
1:A:2433:THR:HG23	1:A:2437:GLU:HG3	1.99	0.44
1:A:2898:LEU:HD13	1:A:2898:LEU:O	2.17	0.44
1:A:3408:VAL:HG23	1:A:3409:CYS:N	2.32	0.44
1:A:3490:ILE:O	1:A:3490:ILE:HG13	2.18	0.44
1:A:3974:ILE:O	1:A:3977:LYS:HB2	2.17	0.44
1:A:4121:ILE:HG22	1:A:4122:VAL:N	2.32	0.44
1:B:2263:HIS:HB2	1:B:2289:TYR:CE1	2.52	0.44
1:B:2955:TRP:HZ2	1:B:3002:ASP:OD1	2.00	0.44
1:B:3088:ASN:OD1	1:B:3163:ALA:HB3	2.17	0.44
1:B:3233:TYR:CG	1:B:3620:ARG:HG3	2.52	0.44
1:B:4192:LEU:C	1:B:4194:PRO:HD3	2.38	0.44
1:A:2016:LEU:HD21	1:A:2023:GLY:CA	2.47	0.44
1:A:2056:GLU:O	1:A:2056:GLU:HG3	2.17	0.44
1:A:2340:ILE:HD11	1:A:2386:ALA:O	2.17	0.44
1:A:2502:ILE:HD12	1:A:2506:PHE:HE2	1.82	0.44
1:A:3055:LEU:O	1:A:3059:LEU:HD23	2.17	0.44
1:A:3361:LYS:HE2	1:A:3361:LYS:HB3	1.84	0.44
1:A:3809:THR:HG22	1:A:3812:LYS:NZ	2.32	0.44
1:A:4691:TYR:HA	1:A:4699:LEU:HA	1.99	0.44
1:B:2660:LEU:HD21	1:B:2672:LEU:CD2	2.48	0.44
1:B:4266:GLU:HG3	1:B:4369:PHE:CE1	2.52	0.44
1:B:4686:LEU:HD12	1:B:4687:SER:H	1.83	0.44
1:A:2046:ILE:HD11	1:A:2059:LEU:HD22	2.00	0.44
1:A:2399:ASP:O	1:A:2400:LEU:HD23	2.16	0.44
1:A:2641:VAL:HG21	1:A:2887:LEU:HD13	1.99	0.44
1:A:2742:PHE:HD1	1:A:2789:VAL:HG12	1.83	0.44
1:A:2902:VAL:HG22	1:A:2938:PHE:CD2	2.53	0.44
1:A:3670:ARG:NH1	1:A:3781:VAL:O	2.51	0.44
1:A:3675:ILE:O	1:A:3675:ILE:HG22	2.17	0.44
1:A:3731:ASN:H	1:A:3731:ASN:ND2	2.09	0.44
1:A:3805:GLU:HB3	1:A:3886:TYR:OH	2.17	0.44
1:B:1640:ASN:ND2	1:B:1644:ILE:HG12	2.32	0.44
1:B:2381:ASN:ND2	1:B:2381:ASN:C	2.71	0.44
1:B:3011:HIS:CE1	1:B:3091:LEU:HA	2.53	0.44
1:B:3316:LYS:HD2	1:B:3546:ILE:CD1	2.47	0.44
1:B:3601:TYR:O	1:B:3603:GLY:N	2.50	0.44
1:B:4087:LYS:HG2	1:B:4087:LYS:O	2.17	0.44
1:B:3958:THR:CG2	1:B:4235:VAL:HB	2.47	0.44
1:B:4244:VAL:HG23	1:B:4403:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4405:PRO:HD3	1:B:4415:GLU:HG2	1.98	0.44
1:B:4693:ASN:HD22	1:B:4693:ASN:H	1.64	0.44
1:A:1719:GLN:OE1	1:A:1732:LEU:N	2.50	0.44
1:A:2200:ASN:O	1:A:2204:ILE:HG12	2.18	0.44
1:A:2200:ASN:ND2	1:A:2228:LEU:HD13	2.18	0.44
1:A:2339:ILE:HG21	1:A:2391:VAL:CG2	2.48	0.44
1:A:3154:PHE:C	1:A:3156:ASN:H	2.21	0.44
1:A:3274:LYS:HD3	1:A:3274:LYS:HA	1.77	0.44
1:A:3293:ARG:HG3	1:A:3293:ARG:NH1	2.27	0.44
1:A:3338:GLN:NE2	1:A:3525:LEU:HB2	2.32	0.44
1:A:3727:ASP:CB	1:A:3729:VAL:HG12	2.48	0.44
1:A:3902:GLU:O	1:A:3905:GLN:HG2	2.17	0.44
1:A:4513:ILE:HA	1:A:4550:TRP:HE1	1.82	0.44
1:A:4673:ASP:O	1:A:4677:PRO:HD2	2.18	0.44
1:B:1828:ASP:OD2	1:B:1901:ASN:HB2	2.17	0.44
1:B:2301:SER:HA	1:B:2350:ARG:O	2.18	0.44
1:B:2886:LEU:O	1:B:2890:ILE:HG13	2.18	0.44
1:B:2976:LEU:CD1	1:B:2990:LEU:HD11	2.48	0.44
1:B:3602:ILE:HG23	1:B:3610:ARG:CG	2.43	0.44
1:A:1628:LEU:HD23	1:A:1628:LEU:O	2.18	0.44
1:A:2125:ALA:HA	1:A:2128:ILE:CG2	2.46	0.44
1:A:2152:LEU:O	1:A:2152:LEU:HD13	2.18	0.44
1:A:3410:LEU:HD23	1:A:3410:LEU:C	2.38	0.44
1:A:4075:THR:HG23	1:A:4076:ILE:H	1.82	0.44
1:A:4296:PHE:HE2	1:A:4347:ILE:HA	1.77	0.44
1:B:2986:VAL:O	1:B:2988:LEU:HG	2.17	0.44
1:B:4304:ARG:HA	1:B:4307:LEU:HD12	1.99	0.44
1:B:4265:ALA:H	1:B:4323:ASN:HB3	1.83	0.44
1:B:4330:PRO:O	1:B:4333:ALA:HB3	2.17	0.44
1:A:1674:ASP:OD1	1:A:1678:LYS:HE2	2.17	0.44
1:A:1904:PHE:C	1:A:1906:TRP:N	2.71	0.44
1:A:2056:GLU:HB2	1:A:2065:ILE:O	2.18	0.44
1:A:2077:MET:HE2	1:A:2077:MET:HB3	1.81	0.44
1:A:2991:PHE:O	1:A:2992:ASN:C	2.55	0.44
1:A:3521:THR:O	1:A:3525:LEU:HD12	2.18	0.44
1:A:3603:GLY:HA2	1:A:3664:MET:CE	2.48	0.44
1:B:1530:PHE:CZ	1:B:1571:SER:HB2	2.53	0.44
1:B:2694:PHE:HA	1:B:2738:TRP:O	2.18	0.44
1:B:3013:LEU:HD13	1:B:3145:PHE:HB3	2.00	0.44
1:B:3164:LEU:C	1:B:3166:ASN:H	2.22	0.44
1:B:3715:GLY:HA2	1:B:3760:PHE:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4374:PRO:HB3	1:B:4377:PRO:HG3	1.98	0.44
1:B:4686:LEU:HD22	1:B:4716:TRP:HB3	2.00	0.44
1:A:1535:ARG:HA	1:A:1591:TRP:HZ2	1.83	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HA	1.81	0.44
1:A:1695:ALA:CB	1:A:2019:CYS:SG	3.06	0.44
1:A:2289:TYR:CE1	1:A:2293:ILE:HD11	2.53	0.44
1:A:2376:LEU:HD12	1:A:2385:LEU:C	2.38	0.44
1:A:2903:ARG:HD2	1:A:2945:ALA:O	2.18	0.44
1:A:2926:THR:O	1:A:2930:ILE:HG13	2.18	0.44
1:A:3205:PHE:CE2	1:A:3221:PRO:HB3	2.52	0.44
1:A:3812:LYS:HB3	1:A:3875:VAL:CG2	2.47	0.44
1:A:3813:ARG:HH22	1:A:3817:LEU:HD13	1.83	0.44
1:A:3869:VAL:O	1:A:3869:VAL:HG12	2.18	0.44
1:B:2612:LEU:O	1:B:2612:LEU:HD13	2.18	0.44
1:B:2766:MET:HB3	1:B:2783:LEU:CD1	2.43	0.44
1:B:2828:TYR:HE1	1:B:2880:SER:HA	1.83	0.44
1:B:3552:LYS:NZ	1:B:3552:LYS:HB2	2.33	0.44
1:B:3553:VAL:O	1:B:3557:VAL:HG23	2.18	0.44
1:B:3872:THR:O	1:B:3876:MET:HG2	2.18	0.44
1:B:4289:PRO:HB2	1:B:4696:ARG:HD2	2.00	0.44
1:B:4689:PRO:HD2	1:B:4721:VAL:O	2.18	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HB2	1.83	0.44
1:A:2361:PRO:HD2	1:A:2754:TYR:CE1	2.53	0.44
1:A:2913:PHE:HD2	1:A:2913:PHE:N	2.15	0.44
1:A:2903:ARG:HH22	1:A:2950:ILE:HA	1.82	0.44
1:A:3190:ARG:HA	1:A:3224:ARG:NH1	2.32	0.44
1:A:3700:LEU:CD1	1:A:3701:ASP:H	2.31	0.44
1:A:4257:ALA:C	1:A:4259:ARG:H	2.21	0.44
1:B:1869:ALA:O	1:B:1872:ARG:HB3	2.17	0.44
1:B:2112:MET:O	1:B:2116:GLN:HG2	2.17	0.44
1:B:2839:LEU:CD2	1:B:2896:CYS:HB3	2.48	0.44
1:B:2965:ARG:HG3	1:B:2965:ARG:HH11	1.82	0.44
1:B:3903:LEU:HD11	1:B:3967:PHE:CD1	2.53	0.44
1:A:1591:TRP:CE3	1:A:1591:TRP:HA	2.53	0.43
1:A:1756:LYS:HB2	1:A:1756:LYS:NZ	2.32	0.43
1:A:2091:LEU:HD22	1:A:2095:PHE:HE1	1.80	0.43
1:A:2255:TRP:CH2	1:A:2259:ILE:HD11	2.53	0.43
1:A:2560:MET:HE3	1:A:2564:ASN:HD22	1.81	0.43
1:A:2617:VAL:HG13	1:A:2617:VAL:O	2.18	0.43
1:A:3585:MET:HA	1:A:3588:VAL:HG23	2.00	0.43
1:A:3652:LEU:HD12	1:A:3653:PRO:CD	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4690:VAL:HG11	1:A:4701:PHE:CE2	2.53	0.43
1:A:2249:LEU:HD22	2:A:9002:ADP:C5	2.53	0.43
1:B:2426:ILE:H	1:B:2426:ILE:CD1	2.27	0.43
1:B:2714:PHE:HE1	1:B:2741:VAL:HG21	1.83	0.43
1:B:2902:VAL:HG21	1:B:2941:VAL:HG21	2.00	0.43
1:B:3046:TYR:CE1	1:B:3050:ASP:HB2	2.53	0.43
1:B:3038:TYR:HE2	1:B:3058:LEU:HD22	1.82	0.43
1:B:3961:ASN:HA	1:B:3964:LYS:HE2	2.00	0.43
1:A:2547:ASN:O	1:A:2551:TYR:HB2	2.17	0.43
1:A:2650:THR:OG1	1:A:2651:VAL:N	2.50	0.43
1:A:3462:PHE:CE2	1:A:3478:VAL:HG23	2.53	0.43
1:B:1674:ASP:O	1:B:1678:LYS:HG3	2.18	0.43
1:B:2265:ILE:HD12	1:B:2414:VAL:HG22	1.99	0.43
1:B:2522:ARG:NH1	1:B:2593:PHE:HD1	2.16	0.43
1:B:4024:ARG:O	1:B:4024:ARG:HG2	2.17	0.43
1:B:4153:LEU:HB2	1:B:4155:LYS:CG	2.46	0.43
1:B:4691:TYR:HA	1:B:4698:GLU:O	2.18	0.43
1:A:1755:LYS:HA	1:A:1755:LYS:HD2	1.80	0.43
1:A:1922:LEU:CD1	1:A:1938:PHE:HD1	2.31	0.43
1:A:2053:ASN:N	1:A:2053:ASN:ND2	2.65	0.43
1:A:2400:LEU:HB3	1:A:2403:ALA:HB3	2.00	0.43
1:A:2408:ILE:HG13	1:A:2409:SER:H	1.83	0.43
1:A:3019:GLY:HA2	2:A:9004:ADP:H5'2	2.00	0.43
1:A:3470:ALA:O	1:A:3471:SER:HB2	2.17	0.43
1:A:4319:LYS:O	1:A:4321:ARG:NH1	2.52	0.43
1:A:1958:LEU:HD23	1:A:4341:THR:HB	1.99	0.43
1:A:4091:SER:O	1:A:4420:SER:HA	2.18	0.43
1:B:1497:LEU:HD22	1:B:1501:SER:HB2	1.99	0.43
1:B:2282:LYS:HZ2	1:B:2282:LYS:HB2	1.83	0.43
1:B:2773:TRP:CZ3	1:B:2780:TRP:HB2	2.53	0.43
1:B:3686:MET:HA	1:B:3694:ILE:HG21	2.00	0.43
1:B:4225:LEU:HD23	1:B:4230:LEU:HD21	2.00	0.43
1:A:1604:VAL:O	1:A:1608:VAL:HG23	2.18	0.43
1:A:1835:THR:O	1:A:1836:LEU:CB	2.67	0.43
1:A:2359:VAL:HB	1:A:2397:VAL:HG11	2.00	0.43
1:A:3062:ALA:HB2	1:A:3069:ILE:HD13	1.99	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CD2	2.53	0.43
1:A:3933:LYS:HB3	1:A:3933:LYS:HZ3	1.84	0.43
1:A:3990:PHE:CE2	1:A:4023:LEU:HG	2.54	0.43
1:A:4052:GLN:O	1:A:4054:GLY:N	2.43	0.43
1:A:4182:GLY:HA3	1:A:4212:SER:HG	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1831:LEU:HA	1:B:1841:ILE:HG23	1.99	0.43
1:B:1975:PRO:HG2	1:B:1978:THR:CG2	2.48	0.43
1:B:2964:ASN:HD21	1:B:2967:ASP:CG	2.22	0.43
1:B:3041:LYS:N	1:B:3041:LYS:HD2	2.33	0.43
1:B:3192:LEU:HD22	1:B:3271:ILE:HG21	2.00	0.43
1:B:3635:PRO:C	1:B:3637:PHE:H	2.21	0.43
1:B:3634:VAL:HB	1:B:3635:PRO:HD3	1.99	0.43
1:B:4012:LEU:HD11	1:B:4020:LEU:HD22	2.01	0.43
1:B:4022:CYS:HB3	1:B:4026:GLN:HE21	1.84	0.43
1:A:1830:ALA:O	1:A:1841:ILE:HG23	2.18	0.43
1:A:3096:VAL:HB	1:A:3099:LEU:HB2	2.00	0.43
1:A:3445:THR:HA	1:A:3449:ARG:HB2	2.00	0.43
1:A:4132:LEU:HB2	1:A:4216:PHE:CD1	2.52	0.43
1:B:1639:ILE:HG23	1:B:1672:LEU:HD22	2.01	0.43
1:B:2352:TRP:CD1	1:B:2392:ARG:HB2	2.54	0.43
1:B:3234:ILE:HG23	1:B:3617:TRP:CD1	2.54	0.43
1:B:3289:LEU:HA	1:B:3292:LEU:HD12	1.99	0.43
1:B:4574:GLN:HE22	1:B:4590:TRP:HB3	1.82	0.43
1:A:1955:ARG:HB2	1:A:1955:ARG:NH1	2.33	0.43
1:A:2012:ILE:HG22	1:A:2016:LEU:CD1	2.49	0.43
1:A:2057:VAL:HG22	1:A:2058:GLU:N	2.34	0.43
1:A:2200:ASN:ND2	1:A:2228:LEU:HB3	2.33	0.43
1:A:3015:ILE:HG21	1:A:3172:TRP:CH2	2.54	0.43
1:A:3078:VAL:O	1:A:3078:VAL:HG22	2.19	0.43
1:A:3357:VAL:O	1:A:3357:VAL:HG12	2.18	0.43
1:A:3638:LEU:HD22	1:A:3667:ARG:HD3	2.01	0.43
1:A:4066:GLN:HE22	1:A:4081:ARG:HD3	1.81	0.43
1:A:4337:ILE:HG22	1:A:4338:LEU:HD12	1.99	0.43
1:B:1653:ALA:HB1	1:B:1658:GLU:HG2	2.01	0.43
1:B:1744:MET:SD	1:B:1777:MET:HG3	2.59	0.43
1:B:2882:TRP:O	1:B:2886:LEU:HG	2.18	0.43
1:B:3160:THR:O	1:B:3162:PRO:HD3	2.18	0.43
1:B:3181:LEU:HB3	1:B:3232:VAL:HG13	2.00	0.43
1:B:3902:GLU:C	1:B:3904:SER:N	2.71	0.43
1:B:4407:TRP:H	1:B:4407:TRP:HD1	1.64	0.43
1:B:3993:LYS:HG3	1:B:4431:GLN:HG3	1.99	0.43
1:B:4728:SER:OG	1:B:4729:ASP:N	2.51	0.43
1:A:1906:TRP:CZ2	1:A:1911:ARG:HG2	2.54	0.43
1:A:2145:TYR:OH	1:A:2207:LEU:HA	2.18	0.43
1:A:2270:HIS:ND1	1:A:2270:HIS:N	2.66	0.43
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2678:SER:HB2	1:A:2817:ASP:O	2.18	0.43
1:A:2748:LEU:HD21	1:A:2800:ARG:CZ	2.48	0.43
1:A:3451:ALA:O	1:A:3455:GLY:N	2.51	0.43
1:A:4179:ALA:HA	1:A:4213:PHE:CD1	2.53	0.43
1:A:4280:ILE:HG21	1:A:4359:PHE:CE1	2.53	0.43
1:A:4288:ILE:HG23	1:A:4289:PRO:HA	2.01	0.43
1:A:4389:ARG:NH1	1:A:4389:ARG:HG2	2.32	0.43
1:A:4648:VAL:HG13	1:A:4657:THR:CG2	2.44	0.43
1:B:1546:VAL:O	1:B:1553:LYS:HA	2.19	0.43
1:B:1766:ILE:HD12	1:B:1769:TRP:HE1	1.84	0.43
1:B:2968:LEU:HD22	1:B:2999:LEU:HD11	2.00	0.43
1:B:3238:ILE:HD11	1:B:3617:TRP:CZ2	2.48	0.43
1:B:4293:THR:HG23	1:B:4352:ASP:OD1	2.19	0.43
1:A:1658:GLU:O	1:A:1661:ALA:HB3	2.19	0.43
1:A:2290:LEU:HD23	1:A:2301:SER:O	2.19	0.43
1:A:2327:TRP:CZ2	1:A:2379:LEU:HD22	2.54	0.43
1:A:2304:HIS:N	1:A:2352:TRP:O	2.51	0.43
1:A:3197:PRO:HG2	1:A:3198:GLN:OE1	2.18	0.43
1:A:3324:LEU:HD12	1:A:3539:LEU:HD23	2.00	0.43
1:A:3416:LYS:HE3	1:A:3418:GLU:CB	2.48	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CG	2.54	0.43
1:A:3862:THR:C	1:A:3864:GLU:H	2.22	0.43
1:A:4379:ILE:HG23	1:A:4381:LEU:HD13	2.00	0.43
1:B:1606:ILE:HG23	1:B:1607:ASP:N	2.33	0.43
1:B:1780:THR:HG22	1:B:1784:LEU:CD1	2.48	0.43
1:B:2840:PRO:O	1:B:2843:ARG:HB2	2.19	0.43
1:B:3065:LYS:O	1:B:3066:GLU:C	2.57	0.43
1:B:3139:ARG:HH11	1:B:3139:ARG:HG3	1.84	0.43
1:B:3289:LEU:O	1:B:3293:ARG:HG3	2.19	0.43
1:B:3675:ILE:HG22	1:B:3675:ILE:O	2.19	0.43
1:B:3725:ASN:ND2	1:B:3725:ASN:N	2.67	0.43
1:B:4028:PRO:O	1:B:4031:SER:N	2.52	0.43
1:B:4058:ILE:CD1	1:B:4082:LYS:HG2	2.48	0.43
1:B:4331:TRP:HZ2	1:B:4369:PHE:CE2	2.37	0.43
1:A:1578:SER:HA	1:A:1579:PRO:HD3	1.92	0.43
1:A:1892:LEU:C	1:A:1894:LYS:H	2.22	0.43
1:A:2269:ASN:O	1:A:2272:VAL:HG23	2.19	0.43
1:A:2645:ASP:O	1:A:2646:VAL:C	2.57	0.43
1:A:2774:ARG:CZ	1:A:2781:ILE:HD11	2.48	0.43
1:A:3588:VAL:O	1:A:3592:VAL:HG23	2.18	0.43
1:A:3859:LYS:C	1:A:3859:LYS:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3902:GLU:HB3	1:A:4433:MET:HG2	2.00	0.43
1:A:4565:ILE:HG22	1:A:4566:SER:N	2.34	0.43
1:B:2304:HIS:NE2	1:B:2351:HIS:HD2	2.17	0.43
1:B:2339:ILE:HG21	1:B:2391:VAL:CG2	2.49	0.43
1:B:3202:PRO:HG3	1:B:3623:SER:O	2.19	0.43
1:B:3272:ASN:HD22	1:B:3272:ASN:HA	1.61	0.43
1:B:3620:ARG:NH1	1:B:3620:ARG:HG2	2.34	0.43
1:B:3895:ARG:NH1	1:B:3977:LYS:HG2	2.34	0.43
1:B:4023:LEU:O	1:B:4027:VAL:HB	2.18	0.43
1:B:4079:ASN:O	1:B:4082:LYS:HB2	2.18	0.43
1:B:4185:VAL:O	1:B:4215:LEU:HD12	2.19	0.43
1:B:4282:GLN:O	1:B:4285:LEU:HB2	2.19	0.43
1:A:1927:ILE:O	1:A:1928:HIS:HD2	2.01	0.43
1:A:2211:ASP:C	1:A:2213:PRO:HD2	2.38	0.43
1:A:2362:GLU:C	1:A:2364:VAL:H	2.22	0.43
1:A:3391:ILE:HD11	1:A:3471:SER:OG	2.19	0.43
1:A:3953:ASN:O	1:A:3956:THR:HG22	2.19	0.43
1:A:4335:ARG:HG2	1:A:4360:LEU:HG	2.01	0.43
1:A:4432:LYS:C	1:A:4434:GLN:N	2.72	0.43
1:A:4659:ILE:HD12	1:A:4659:ILE:N	2.34	0.43
1:A:4708:ASP:C	1:A:4710:SER:H	2.22	0.43
1:B:4075:THR:HG23	1:B:4076:ILE:N	2.34	0.43
1:B:4324:ILE:HG13	1:B:4324:ILE:H	1.52	0.43
1:B:4617:GLU:HG2	1:B:4618:ASN:N	2.34	0.43
1:B:4638:ASN:HB3	1:B:4666:ILE:HD11	2.00	0.43
1:A:1963:ALA:HA	1:A:2096:ARG:HH11	1.83	0.42
1:A:1967:ARG:NH1	1:A:2053:ASN:HA	2.34	0.42
1:A:3716:CYS:H	1:A:3760:PHE:HB2	1.84	0.42
1:A:4024:ARG:HA	1:A:4030:PHE:O	2.19	0.42
1:A:4354:ARG:HD3	1:A:4717:TYR:CD2	2.53	0.42
1:B:2196:LEU:HD11	1:B:2223:PHE:CD2	2.54	0.42
1:B:2368:ASN:O	1:B:2410:ARG:NH1	2.52	0.42
1:B:2271:GLY:HA2	1:B:2393:VAL:O	2.19	0.42
1:B:2849:LEU:CD1	1:B:2901:LEU:HD11	2.49	0.42
1:B:3722:ASP:HA	1:B:3724:GLU:OE1	2.19	0.42
1:B:3723:VAL:HG23	1:B:3764:LEU:HD22	2.01	0.42
1:A:1554:LEU:HD22	1:A:1609:GLN:HG3	2.00	0.42
1:A:1907:LEU:HD22	1:A:1911:ARG:CZ	2.49	0.42
1:A:2425:MET:HE2	1:A:2425:MET:HB3	1.81	0.42
1:A:2560:MET:CG	1:A:2565:GLN:HB2	2.49	0.42
1:A:3782:THR:HG23	1:A:3782:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4358:SER:O	1:A:4362:GLN:HB2	2.19	0.42
1:A:3992:LEU:CD1	1:A:4434:GLN:HG3	2.48	0.42
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.18	0.42
1:A:4678:ILE:O	1:A:4678:ILE:HG22	2.19	0.42
1:B:2109:ALA:HA	1:B:2156:LEU:CD1	2.49	0.42
1:B:2423:THR:HA	1:B:2426:ILE:HD13	2.00	0.42
1:B:2886:LEU:HD23	1:B:2904:LEU:HD22	2.01	0.42
1:B:2991:PHE:CE1	1:B:2993:GLU:HB2	2.54	0.42
1:B:3234:ILE:HG23	1:B:3617:TRP:CE2	2.54	0.42
1:B:3598:PHE:CD2	1:B:3634:VAL:HG11	2.55	0.42
1:B:3647:TRP:HB3	1:B:3652:LEU:CD2	2.49	0.42
1:B:3676:ASP:CB	1:B:3681:ALA:HB3	2.49	0.42
1:B:4673:ASP:OD1	1:B:4674:LYS:N	2.52	0.42
1:A:1816:LEU:HD23	1:A:1878:LEU:CD1	2.49	0.42
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	2.02	0.42
1:A:2525:ILE:HD12	1:A:2526:MET:N	2.33	0.42
1:A:2832:ASN:CG	1:A:2849:LEU:HD23	2.39	0.42
1:A:2870:ALA:C	1:A:2872:TYR:H	2.21	0.42
1:A:3067:GLU:HG2	1:A:3068:LYS:N	2.34	0.42
1:A:3096:VAL:HB	1:A:3099:LEU:HD22	2.01	0.42
1:A:3156:ASN:C	1:A:3158:SER:H	2.21	0.42
1:A:3718:LEU:HG	1:A:3719:LEU:N	2.21	0.42
1:B:1505:SER:O	1:B:1506:ASP:C	2.57	0.42
1:B:1960:LEU:HD13	1:B:2074:PHE:CE1	2.54	0.42
1:B:2017:CYS:SG	1:B:2046:ILE:HD13	2.59	0.42
1:B:2129:VAL:N	1:B:2130:PRO:CD	2.82	0.42
1:B:2669:PRO:HA	1:B:2788:PHE:O	2.19	0.42
1:A:4000:SER:O	1:B:2940:SER:HB3	2.19	0.42
1:B:3030:ALA:HB3	1:B:3037:ILE:HD11	2.00	0.42
1:B:3078:VAL:O	1:B:3078:VAL:HG22	2.18	0.42
1:B:3698:SER:HB3	1:B:3700:LEU:HD12	2.00	0.42
1:B:3962:ASP:C	1:B:3964:LYS:H	2.23	0.42
1:A:1639:ILE:HG12	1:A:1675:LEU:HD23	2.01	0.42
1:A:1732:LEU:HD13	1:A:1741:ILE:HD12	2.01	0.42
1:A:1752:VAL:CG2	1:A:1811:PRO:HG3	2.48	0.42
1:A:1816:LEU:O	1:A:1820:GLN:HG3	2.19	0.42
1:A:1973:PHE:HD1	1:A:1973:PHE:O	2.02	0.42
1:A:2142:GLN:HB2	1:A:2145:TYR:CD1	2.54	0.42
1:A:2266:LEU:HD21	1:A:2394:MET:CE	2.49	0.42
1:A:2615:TYR:CD2	1:A:2615:TYR:N	2.87	0.42
1:A:2819:PRO:HB2	1:A:2824:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3018:SER:O	1:A:3257:PRO:HD2	2.18	0.42
1:A:3209:ALA:CB	1:A:3221:PRO:HG3	2.49	0.42
1:A:3700:LEU:CD1	1:A:3701:ASP:N	2.80	0.42
1:A:3993:LYS:O	1:A:3995:GLY:N	2.53	0.42
1:A:4109:ASP:CA	1:A:4112:ASN:HD22	2.11	0.42
1:A:4134:LEU:HD23	1:A:4236:PHE:HB2	2.01	0.42
1:A:4168:PHE:O	1:A:4172:GLU:HG3	2.19	0.42
1:A:4289:PRO:HA	1:A:4292:TRP:O	2.20	0.42
1:B:1811:PRO:HB2	1:B:1814:LEU:CD1	2.49	0.42
1:B:2125:ALA:C	1:B:2127:LYS:H	2.21	0.42
1:B:2272:VAL:HG12	1:B:2273:MET:N	2.34	0.42
1:B:2591:GLU:HA	1:B:2613:LEU:HD12	2.01	0.42
1:B:3057:MET:O	1:B:3061:ARG:HG3	2.19	0.42
1:B:3039:THR:HG22	1:B:3072:ILE:HB	2.01	0.42
1:B:3181:LEU:HB2	1:B:3232:VAL:HG13	2.01	0.42
1:B:3960:LEU:CD2	1:B:4237:SER:HB2	2.50	0.42
1:A:1708:ILE:HD11	1:A:1721:HIS:HB3	2.01	0.42
1:A:2051:LYS:C	1:A:2051:LYS:HD3	2.39	0.42
1:A:1967:ARG:CB	1:A:2051:LYS:HA	2.50	0.42
1:A:2408:ILE:O	1:A:2411:CYS:HB2	2.20	0.42
1:A:2502:ILE:CG2	1:A:2573:LEU:HD12	2.48	0.42
1:A:2534:LEU:HB3	1:A:2538:PHE:CE2	2.55	0.42
1:A:2587:LEU:CG	1:A:2817:ASP:HB2	2.45	0.42
1:A:2905:TRP:HZ3	1:A:2934:ALA:HB2	1.83	0.42
1:A:3262:ASP:OD2	1:A:3670:ARG:NE	2.52	0.42
1:A:3192:LEU:HD11	1:A:3271:ILE:HG22	2.01	0.42
1:A:3536:TYR:O	1:A:3540:ILE:HD13	2.20	0.42
1:A:4373:PHE:CD1	1:A:4374:PRO:HD2	2.54	0.42
1:B:2112:MET:SD	1:B:2153:LYS:HG2	2.59	0.42
1:B:2528:PHE:HE1	1:B:2533:VAL:HG11	1.85	0.42
1:B:2706:THR:HA	1:B:2759:VAL:HG22	2.01	0.42
1:B:3084:LEU:O	1:B:3087:MET:N	2.52	0.42
1:B:3598:PHE:O	1:B:3602:ILE:HB	2.20	0.42
1:A:1766:ILE:HG23	1:A:1767:HIS:N	2.35	0.42
1:A:1777:MET:HE3	1:A:1939:GLU:HA	2.02	0.42
1:A:1979:GLY:O	1:A:1980:LYS:C	2.58	0.42
1:A:2106:GLU:CD	1:A:2106:GLU:N	2.69	0.42
1:A:2370:LEU:HD23	1:A:2370:LEU:O	2.19	0.42
1:A:2415:TRP:HA	1:A:2415:TRP:HE3	1.83	0.42
1:A:2910:LEU:HB3	1:A:2911:ARG:HH12	1.85	0.42
1:A:3009:GLN:HG2	1:A:3138:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3061:ARG:O	1:A:3067:GLU:HB3	2.18	0.42
1:A:3108:LEU:HD11	1:A:3133:PHE:CZ	2.54	0.42
1:A:3915:ALA:O	1:A:3918:ASP:HB2	2.19	0.42
1:A:3954:ARG:HD3	1:A:3954:ARG:O	2.19	0.42
1:A:4178:ALA:HA	1:A:4183:THR:OG1	2.20	0.42
1:A:4128:SER:CB	1:A:4213:PHE:HB3	2.48	0.42
1:B:1598:VAL:HG22	1:B:1660:LEU:HD22	2.01	0.42
1:B:1914:TYR:CZ	1:B:1924:LYS:HB3	2.54	0.42
1:B:2230:PRO:HB3	1:B:2237:ARG:HH22	1.84	0.42
1:B:2327:TRP:CH2	1:B:2380:PRO:HD2	2.55	0.42
1:B:2610:ILE:HD12	1:B:2615:TYR:OH	2.20	0.42
1:B:3043:ASN:N	1:B:3043:ASN:ND2	2.68	0.42
1:B:3160:THR:C	1:B:3162:PRO:HD3	2.40	0.42
1:A:2126:GLY:O	1:A:2130:PRO:HG2	2.19	0.42
1:A:2269:ASN:O	1:A:2271:GLY:N	2.53	0.42
1:A:2270:HIS:HB2	1:A:2392:ARG:HD2	2.02	0.42
1:A:2426:ILE:CD1	1:A:2530:ARG:HD3	2.50	0.42
1:A:2573:LEU:C	1:A:2573:LEU:HD23	2.40	0.42
1:A:2701:PHE:HB2	1:A:2745:GLU:O	2.20	0.42
1:A:3457:LEU:HD12	1:A:3486:TYR:CE1	2.55	0.42
1:B:2290:LEU:HD22	1:B:2352:TRP:CZ3	2.55	0.42
1:B:2588:VAL:HG23	1:B:2589:GLU:N	2.34	0.42
1:B:2773:TRP:CH2	1:B:2780:TRP:HB2	2.54	0.42
1:B:3061:ARG:O	1:B:3067:GLU:HB3	2.19	0.42
1:B:3990:PHE:CD2	1:B:4084:LEU:HD22	2.55	0.42
1:A:1791:HIS:HD2	1:A:1806:TRP:HD1	1.66	0.42
1:A:2057:VAL:HB	1:A:2067:LEU:HD13	2.01	0.42
1:A:1952:LEU:HD22	1:A:2103:PRO:HA	2.01	0.42
1:A:2561:SER:HA	1:A:2562:PRO:HD3	1.95	0.42
1:A:2849:LEU:HA	1:A:2938:PHE:HZ	1.85	0.42
1:A:3268:VAL:HG13	1:A:3269:LEU:N	2.35	0.42
1:A:3602:ILE:HG22	1:A:3603:GLY:N	2.34	0.42
1:A:4313:TRP:CD1	1:A:4334:VAL:HG22	2.55	0.42
1:B:1608:VAL:HG13	1:B:1676:LEU:CD1	2.50	0.42
1:B:1907:LEU:HD22	1:B:1911:ARG:NH2	2.34	0.42
1:B:2084:ARG:CZ	1:B:4295:PHE:CD2	3.03	0.42
1:B:2513:HIS:O	1:B:2517:GLU:HG3	2.19	0.42
1:B:2528:PHE:CE1	1:B:2533:VAL:HG11	2.54	0.42
1:B:2825:THR:CG2	1:B:2854:VAL:HG21	2.50	0.42
1:B:3259:HIS:NE2	1:B:3779:SER:HA	2.34	0.42
1:B:4036:HIS:CD2	1:B:4044:TRP:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4280:ILE:HG23	1:B:4408:LEU:HA	2.01	0.42
1:B:4284:ARG:CG	1:B:4408:LEU:HB3	2.49	0.42
1:A:1792:PHE:CD2	1:A:1792:PHE:C	2.92	0.42
1:A:2009:MET:HE3	1:A:2012:ILE:HB	2.02	0.42
1:A:2071:MET:HG3	1:A:2071:MET:O	2.20	0.42
1:A:2585:MET:O	1:A:2815:LEU:HD13	2.19	0.42
1:A:2842:LEU:HD11	1:A:2897:THR:C	2.40	0.42
1:A:2989:VAL:HG13	1:A:3187:GLU:OE2	2.20	0.42
1:A:3075:GLU:C	1:A:3077:ASN:H	2.23	0.42
1:A:3224:ARG:HB2	1:A:3224:ARG:HE	1.73	0.42
1:A:3449:ARG:NH1	1:A:3449:ARG:HB3	2.35	0.42
1:B:2540:LEU:HB3	1:B:2576:SER:CB	2.49	0.42
1:B:2856:PHE:HE2	1:B:2913:PHE:CD2	2.37	0.42
1:B:3039:THR:CG2	1:B:3072:ILE:HB	2.50	0.42
1:B:2989:VAL:HG21	1:B:3184:VAL:HA	2.02	0.42
1:B:3235:HIS:CE1	1:B:3260:TYR:HB2	2.55	0.42
1:B:3256:THR:CG2	1:B:3779:SER:HB3	2.50	0.42
1:B:3976:VAL:O	1:B:3979:THR:HG23	2.20	0.42
1:A:1556:ARG:HG2	1:A:1557:GLY:N	2.35	0.42
1:A:1746:SER:HB3	1:A:1940:TYR:CZ	2.55	0.42
1:A:1818:THR:O	1:A:1822:VAL:HG23	2.20	0.42
1:A:1929:MET:O	1:A:1930:ALA:HB3	2.20	0.42
1:A:1973:PHE:HE1	1:A:2099:ALA:CA	2.33	0.42
1:A:2833:ARG:HA	1:A:2846:ALA:HB1	2.02	0.42
1:A:3148:ASN:HA	1:A:3149:PRO:HD3	1.93	0.42
1:A:3315:VAL:O	1:A:3319:GLN:HB2	2.19	0.42
1:A:4065:ALA:O	1:A:4069:LEU:HB2	2.20	0.42
1:A:4070:SER:C	1:A:4072:GLN:N	2.72	0.42
1:A:4418:LEU:HD11	1:A:4422:LYS:HZ3	1.84	0.42
1:A:4575:LEU:H	1:A:4575:LEU:CD1	2.26	0.42
1:B:1615:LEU:HD13	1:B:1618:ILE:HD12	2.01	0.42
1:B:1952:LEU:HA	1:B:1955:ARG:NH2	2.35	0.42
1:B:2684:LEU:HD13	1:B:2684:LEU:C	2.40	0.42
1:B:3017:VAL:HG11	1:B:3175:GLU:HA	2.01	0.42
1:B:4070:SER:O	1:B:4072:GLN:N	2.53	0.42
1:B:4434:GLN:O	1:B:4434:GLN:HG2	2.19	0.42
1:A:2140:SER:HB2	1:A:2142:GLN:NE2	2.23	0.41
1:A:2204:ILE:HG13	1:A:2205:PRO:CD	2.50	0.41
1:A:2898:LEU:HD11	1:A:2941:VAL:HG22	2.01	0.41
1:A:3889:MET:SD	1:A:3889:MET:C	2.99	0.41
1:A:4370:ASN:N	1:A:4370:ASN:HD22	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1565:LEU:HD23	1:B:1595:LEU:HD12	2.00	0.41
1:B:2272:VAL:O	1:B:2394:MET:HA	2.20	0.41
1:B:2292:ALA:O	1:B:2296:VAL:HG23	2.20	0.41
1:B:2370:LEU:HD12	1:B:2377:LEU:HB2	2.02	0.41
1:B:2579:TRP:HZ2	1:B:2655:ARG:HD2	1.84	0.41
1:B:3923:LEU:HD22	1:B:3947:ILE:CG2	2.47	0.41
1:B:4191:HIS:CD2	1:B:4220:GLU:HG2	2.54	0.41
1:A:1831:LEU:HA	1:A:1841:ILE:HG12	2.02	0.41
1:A:1973:PHE:HD1	1:A:1973:PHE:C	2.23	0.41
1:A:2258:LYS:HA	1:A:2261:GLN:CG	2.44	0.41
1:A:2370:LEU:HA	1:A:2375:LYS:HA	2.02	0.41
1:A:2745:GLU:CB	1:A:2748:LEU:HD12	2.50	0.41
1:A:2783:LEU:HD22	1:A:2786:ILE:HB	2.01	0.41
1:A:3256:THR:HB	1:A:3257:PRO:HD2	2.01	0.41
1:A:3808:ASP:CG	1:A:3809:THR:N	2.73	0.41
1:A:3990:PHE:O	1:A:3994:GLY:HA2	2.20	0.41
1:A:4337:ILE:O	1:A:4341:THR:CG2	2.68	0.41
1:A:4623:ALA:HB2	1:A:4703:ILE:CD1	2.48	0.41
1:A:4684:SER:O	1:A:4707:TYR:HE2	2.02	0.41
1:B:1785:LEU:HB2	1:B:1814:LEU:HD23	2.00	0.41
1:B:1960:LEU:HD13	1:B:2074:PHE:HE1	1.85	0.41
1:B:3573:ARG:HH11	1:B:3573:ARG:HG2	1.84	0.41
1:B:3700:LEU:CD1	1:B:3701:ASP:H	2.30	0.41
1:B:3877:GLN:O	1:B:3881:GLU:HB2	2.20	0.41
1:B:4277:PHE:HZ	1:B:4356:LEU:HD21	1.84	0.41
1:A:1625:ILE:HG23	1:A:1626:ASN:N	2.33	0.41
1:A:1719:GLN:HA	1:A:1722:PHE:CE2	2.56	0.41
1:A:1959:THR:O	1:A:1963:ALA:CB	2.69	0.41
1:A:2893:MET:O	1:A:2895:GLY:N	2.46	0.41
1:A:3148:ASN:OD1	1:A:3150:ALA:N	2.45	0.41
1:A:3206:ILE:HA	1:A:3221:PRO:HG2	2.03	0.41
1:A:3443:MET:HE3	1:A:3449:ARG:HA	2.02	0.41
1:A:3994:GLY:O	1:A:3995:GLY:C	2.58	0.41
1:A:4278:HIS:O	1:A:4282:GLN:HB2	2.20	0.41
1:B:1590:HIS:NE2	1:B:1594:ARG:NH1	2.68	0.41
1:B:1872:ARG:NH2	1:B:2164:ARG:NE	2.68	0.41
1:B:2208:VAL:HG12	1:B:2415:TRP:NE1	2.36	0.41
1:B:2231:ILE:CG2	1:B:2264:GLN:HE22	2.31	0.41
1:B:2578:MET:O	1:B:2582:GLY:HA3	2.19	0.41
1:B:2670:LEU:HD12	1:B:2670:LEU:O	2.20	0.41
1:B:3563:LEU:CD1	1:B:3845:ILE:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3566:ASN:HD21	1:B:3859:LYS:HZ2	1.69	0.41
1:B:3910:GLN:HB3	1:B:4231:ARG:HD3	2.03	0.41
1:B:3886:TYR:CE2	1:B:3940:LEU:HD23	2.56	0.41
1:B:3960:LEU:HB3	1:B:4239:GLU:OE2	2.21	0.41
1:B:4201:GLU:HG3	1:B:4228:ASN:HB2	2.03	0.41
1:B:4284:ARG:HG2	1:B:4408:LEU:HB3	2.02	0.41
1:A:1697:PHE:CD2	1:A:1705:LEU:HD11	2.55	0.41
1:A:1701:GLY:HA2	1:A:2011:ARG:CZ	2.50	0.41
1:A:2127:LYS:O	1:A:2130:PRO:HD2	2.20	0.41
1:A:2376:LEU:HD12	1:A:2386:ALA:N	2.35	0.41
1:A:2612:LEU:HD12	1:A:2612:LEU:O	2.21	0.41
1:A:2749:PRO:HG2	1:A:2759:VAL:HG11	2.01	0.41
1:A:2774:ARG:HH21	1:A:2779:THR:HB	1.85	0.41
1:A:2586:GLY:CA	1:A:2815:LEU:HD13	2.43	0.41
1:A:2868:ILE:HG21	1:A:2922:GLU:OE2	2.21	0.41
1:A:3164:LEU:HA	1:A:3164:LEU:HD12	1.81	0.41
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	2.01	0.41
1:A:3553:VAL:O	1:A:3557:VAL:HG23	2.21	0.41
1:A:3652:LEU:HD21	1:A:3662:ALA:HB2	2.02	0.41
1:A:3819:ILE:C	1:A:3821:GLY:H	2.23	0.41
1:A:4012:LEU:H	1:A:4012:LEU:HD12	1.84	0.41
1:A:4270:ILE:HG22	1:A:4310:ILE:HD13	2.01	0.41
1:A:4314:VAL:O	1:A:4314:VAL:CG1	2.68	0.41
1:A:4349:ASN:ND2	1:A:4352:ASP:N	2.65	0.41
1:A:4648:VAL:CG1	1:A:4662:THR:HG21	2.41	0.41
1:A:4692:LEU:HD12	1:A:4700:LEU:HD21	2.02	0.41
1:B:2036:LEU:O	1:B:2036:LEU:HD23	2.20	0.41
1:B:2556:SER:C	1:B:2558:PHE:N	2.73	0.41
1:B:3602:ILE:O	1:B:3603:GLY:C	2.59	0.41
1:B:4068:GLN:C	1:B:4070:SER:H	2.24	0.41
1:B:4371:PRO:O	1:B:4372:ASP:HB2	2.20	0.41
1:A:1782:ALA:HA	1:A:1938:PHE:CZ	2.55	0.41
1:A:2204:ILE:CA	1:A:2207:LEU:HD12	2.44	0.41
1:A:2222:VAL:C	1:A:2224:PRO:HD3	2.40	0.41
1:A:2376:LEU:HD21	1:A:2384:ARG:HB3	2.02	0.41
1:A:2606:PRO:HG2	1:A:2615:TYR:CD1	2.56	0.41
1:A:2832:ASN:HA	1:A:2835:LEU:HB3	2.01	0.41
1:A:4012:LEU:HD21	1:A:4020:LEU:HD22	2.02	0.41
1:A:4283:GLU:OE2	1:A:4286:ARG:NH1	2.54	0.41
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	2.01	0.41
1:A:4401:GLU:HB2	1:A:4402:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1493:ILE:O	1:B:1497:LEU:HG	2.21	0.41
1:B:1817:LEU:HD11	1:B:1936:TYR:CD2	2.55	0.41
1:B:2223:PHE:C	1:B:2225:GLY:H	2.23	0.41
1:B:3606:ASP:O	1:B:3610:ARG:HG3	2.21	0.41
1:B:4006:PRO:C	1:B:4008:LEU:H	2.24	0.41
1:B:4553:TYR:O	1:B:4555:VAL:HG22	2.20	0.41
1:A:1766:ILE:HG23	1:A:1767:HIS:H	1.84	0.41
1:A:1888:VAL:HG22	1:A:1909:HIS:CE1	2.56	0.41
1:A:2275:VAL:HG23	1:A:2397:VAL:HG23	2.03	0.41
1:A:2579:TRP:HZ2	1:A:2655:ARG:HD2	1.85	0.41
1:A:2694:PHE:CD2	1:A:2738:TRP:HB2	2.56	0.41
1:A:2748:LEU:CD2	1:A:2800:ARG:HD3	2.51	0.41
1:A:3439:ASP:OD2	1:A:3442:LYS:HE2	2.21	0.41
1:A:3571:ARG:NH1	1:A:3571:ARG:HB3	2.35	0.41
1:A:4001:ILE:HB	1:A:4018:LYS:HD3	2.02	0.41
1:A:4006:PRO:O	1:A:4008:LEU:N	2.52	0.41
1:A:4240:ASN:HA	1:A:4241:PRO:HD2	1.89	0.41
1:A:4278:HIS:HD2	1:A:4343:TYR:CE1	2.39	0.41
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.67	0.41
1:A:4535:ARG:HG2	1:A:4535:ARG:HH11	1.84	0.41
1:A:4537:LEU:CD2	1:A:4548:LYS:HE3	2.50	0.41
1:A:4670:THR:HG22	1:A:4671:TRP:N	2.36	0.41
1:B:1910:MET:CB	1:B:1929:MET:HG3	2.50	0.41
1:B:2670:LEU:C	1:B:2670:LEU:HD12	2.41	0.41
1:B:2711:LEU:HD12	1:B:2711:LEU:HA	1.89	0.41
1:B:3087:MET:HE2	1:B:3090:LEU:HD23	2.03	0.41
1:B:4184:TRP:NE1	1:B:4214:ARG:HB2	2.35	0.41
1:A:2057:VAL:HG13	1:A:2059:LEU:H	1.86	0.41
1:A:2615:TYR:HD2	1:A:2615:TYR:N	2.18	0.41
1:A:2696:VAL:HG22	1:A:2697:VAL:N	2.36	0.41
1:A:2855:GLU:OE2	1:A:2933:VAL:HG22	2.21	0.41
1:B:1497:LEU:HB3	1:B:1501:SER:CB	2.51	0.41
1:B:1500:GLY:O	1:B:1504:ASP:N	2.50	0.41
1:B:1483:ILE:HG22	1:B:1517:VAL:HG22	2.02	0.41
1:B:2239:LYS:O	1:B:2243:ILE:HG13	2.21	0.41
1:B:2278:SER:H	1:B:2398:GLN:NE2	2.17	0.41
1:B:2363:TRP:C	1:B:2365:GLU:H	2.24	0.41
1:B:2400:LEU:HD13	1:B:2408:ILE:CD1	2.48	0.41
1:B:2853:MET:HA	1:B:2882:TRP:CZ3	2.56	0.41
1:B:3567:LEU:HD23	1:B:3567:LEU:HA	1.94	0.41
1:B:3903:LEU:O	1:B:3909:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4023:LEU:HG	1:B:4030:PHE:CD1	2.56	0.41
1:B:4509:LEU:HD23	1:B:4568:PHE:CE1	2.55	0.41
1:B:4535:ARG:HG2	1:B:4535:ARG:NH1	2.34	0.41
1:B:4644:LEU:HD23	1:B:4723:ILE:HG12	2.02	0.41
1:A:2000:CYS:O	1:A:2001:ASP:C	2.58	0.41
1:A:2028:PHE:CB	1:A:2075:VAL:HG13	2.44	0.41
1:A:2269:ASN:C	1:A:2271:GLY:H	2.24	0.41
1:A:2579:TRP:CE3	1:A:2659:VAL:HG21	2.56	0.41
1:A:3567:LEU:HD23	1:A:3567:LEU:HA	1.91	0.41
1:A:3652:LEU:HB2	1:A:3684:PHE:CD1	2.55	0.41
1:A:4033:LEU:HD13	1:A:4062:TRP:CZ2	2.55	0.41
1:A:4426:MET:O	1:A:4430:LEU:HG	2.21	0.41
1:B:3258:ARG:HD2	1:B:3779:SER:HB2	2.01	0.41
1:B:3781:VAL:HG12	1:B:3782:THR:N	2.34	0.41
1:B:3930:LEU:O	1:B:3932:ASP:N	2.54	0.41
1:A:1712:SER:HB3	1:A:1766:ILE:HB	2.03	0.41
1:A:1726:PHE:CD2	1:A:1729:LEU:HD22	2.55	0.41
1:A:2848:ASN:HB3	1:A:2938:PHE:CE1	2.55	0.41
1:A:2890:ILE:HD13	1:A:2893:MET:CE	2.51	0.41
1:A:3078:VAL:HG23	1:A:3083:PHE:HB2	2.02	0.41
1:A:3597:ALA:O	1:A:3601:TYR:HD1	2.04	0.41
1:A:4060:GLU:O	1:A:4064:VAL:HG23	2.21	0.41
1:A:4592:GLY:CA	1:A:4725:SER:HB2	2.50	0.41
1:B:1844:GLN:O	1:B:1847:SER:HB2	2.21	0.41
1:B:2029:ASN:N	1:B:2029:ASN:HD22	2.18	0.41
1:B:2151:ALA:O	1:B:2154:SER:N	2.52	0.41
1:B:2236:LEU:O	1:B:2240:ILE:HG13	2.21	0.41
1:B:2270:HIS:CA	1:B:2392:ARG:HH11	2.33	0.41
1:B:2420:ILE:HG13	1:B:2421:LEU:N	2.36	0.41
1:B:2492:LEU:O	1:B:2493:LYS:C	2.59	0.41
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.43	0.41
1:B:3228:VAL:HA	1:B:3231:LEU:HD12	2.03	0.41
1:B:3647:TRP:HB3	1:B:3652:LEU:HD22	2.02	0.41
1:B:4056:PRO:HD2	1:B:4093:ARG:NH2	2.36	0.41
1:B:4157:TYR:HB2	1:B:4184:TRP:CB	2.50	0.41
1:B:4162:ILE:HG22	1:B:4163:GLY:N	2.35	0.41
1:B:4306:ALA:HA	1:B:4338:LEU:HD22	2.03	0.41
1:B:4277:PHE:HB2	1:B:4363:LEU:HD12	2.03	0.41
1:B:4094:VAL:HB	1:B:4423:ALA:HB1	2.02	0.41
1:B:4503:ILE:HD11	1:B:4575:LEU:O	2.21	0.41
1:A:1886:ARG:HG3	1:A:1887:ASP:H	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:PRO:C	1:A:2090:ASN:N	2.75	0.41
1:A:3093:GLY:O	1:A:3095:GLU:N	2.54	0.41
1:A:3230:SER:HA	1:A:3620:ARG:HE	1.86	0.41
1:A:3844:ASN:O	1:A:3848:ASP:HB2	2.20	0.41
1:A:4024:ARG:CG	1:A:4031:SER:HA	2.49	0.41
1:B:1739:THR:O	1:B:1760:ILE:N	2.54	0.41
1:B:1734:LEU:HA	1:B:1742:ILE:HG12	2.03	0.41
1:B:1831:LEU:HB3	1:B:1900:GLY:HA2	2.02	0.41
1:B:2084:ARG:HG2	1:B:2084:ARG:NH1	2.36	0.41
1:B:2381:ASN:HD22	1:B:2381:ASN:C	2.25	0.41
1:B:2887:LEU:O	1:B:2891:GLN:HG3	2.21	0.41
1:B:3539:LEU:HA	1:B:3539:LEU:HD12	1.92	0.41
1:B:3571:ARG:O	1:B:3575:GLU:HG3	2.19	0.41
1:B:4022:CYS:HB3	1:B:4026:GLN:NE2	2.36	0.41
1:B:4141:ASP:OD2	1:B:4143:SER:HB2	2.21	0.41
1:B:4145:LYS:HE2	1:B:4238:TYR:CE1	2.55	0.41
1:B:4509:LEU:O	1:B:4513:ILE:HG13	2.20	0.41
1:B:4649:TRP:HA	1:B:4649:TRP:CE3	2.55	0.41
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.36	0.41
1:A:1939:GLU:O	1:A:1941:LEU:HG	2.21	0.41
1:A:2332:PHE:HA	1:A:2335:THR:OG1	2.20	0.41
1:A:2359:VAL:HG23	1:A:2397:VAL:HG11	2.03	0.41
1:A:3606:ASP:O	1:A:3610:ARG:HG3	2.21	0.41
1:A:3698:SER:C	1:A:3700:LEU:HD12	2.41	0.41
1:A:4063:ILE:HD13	1:A:4082:LYS:NZ	2.36	0.41
1:A:4122:VAL:HB	1:A:4132:LEU:CD2	2.51	0.41
1:A:4606:GLN:HA	1:A:4609:SER:OG	2.21	0.41
1:B:1909:HIS:O	1:B:1911:ARG:HD3	2.22	0.41
1:B:1947:LEU:HD21	1:B:1982:GLU:CG	2.51	0.41
1:B:2260:LEU:O	1:B:2263:HIS:HB3	2.21	0.41
1:B:3015:ILE:O	1:B:3173:PHE:N	2.51	0.41
1:B:3017:VAL:HG13	1:B:3174:GLY:C	2.41	0.41
1:B:3685:LEU:O	1:B:3689:TYR:HB2	2.20	0.41
1:B:4711:THR:OG1	1:B:4716:TRP:NE1	2.54	0.41
1:A:1633:SER:O	1:A:1637:LYS:HG2	2.21	0.40
1:A:2269:ASN:C	1:A:2271:GLY:N	2.74	0.40
1:A:2439:PHE:HZ	1:A:2542:ASN:OD1	2.03	0.40
1:A:2877:ARG:HD2	1:A:2881:ARG:NH2	2.36	0.40
1:A:2935:LEU:C	1:A:2935:LEU:HD23	2.41	0.40
1:A:3022:LYS:HB2	1:A:3022:LYS:NZ	2.36	0.40
1:A:3025:LEU:HD23	1:A:3025:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3199:TYR:OH	1:A:3226:ALA:HB2	2.21	0.40
1:A:3237:THR:OG1	1:A:3238:ILE:HD12	2.21	0.40
1:A:3720:VAL:HG21	1:A:3762:ILE:HD11	2.03	0.40
1:A:4090:HIS:C	1:A:4092:ASP:H	2.24	0.40
1:A:4086:MET:HG2	1:A:4093:ARG:HB2	1.99	0.40
1:A:4647:ALA:HA	1:A:4657:THR:HG22	2.02	0.40
1:B:2120:THR:HB	1:B:2124:LEU:HG	2.03	0.40
1:B:2754:TYR:O	1:B:2756:THR:HG22	2.21	0.40
1:B:3046:TYR:CZ	1:B:3050:ASP:HB2	2.55	0.40
1:B:3234:ILE:O	1:B:3238:ILE:HD13	2.21	0.40
1:B:3976:VAL:HG13	1:B:4105:VAL:HG11	2.01	0.40
1:B:4499:PHE:HA	1:B:4502:GLU:HB2	2.03	0.40
1:A:2005:ASP:OD1	1:A:2006:LEU:N	2.55	0.40
1:A:2212:ILE:O	1:A:2215:ILE:HG22	2.22	0.40
1:A:3225:ASP:O	1:A:3229:SER:CB	2.69	0.40
1:A:3698:SER:O	1:A:3704:PHE:HB2	2.22	0.40
1:A:3727:ASP:C	1:A:3729:VAL:H	2.25	0.40
1:A:3997:ASN:O	1:A:3998:LEU:C	2.60	0.40
1:A:4117:ASP:C	1:A:4119:ALA:H	2.25	0.40
1:B:1546:VAL:HG12	1:B:1547:ASN:N	2.36	0.40
1:B:1928:HIS:CG	1:B:1933:THR:HG22	2.52	0.40
1:B:1820:GLN:NE2	1:B:1990:GLN:NE2	2.66	0.40
1:B:2081:TYR:O	1:B:2082:ALA:HB3	2.21	0.40
1:B:3218:ALA:O	1:B:3219:ILE:C	2.60	0.40
1:B:4083:ILE:HD11	1:B:4098:SER:HA	2.03	0.40
1:B:4264:PRO:HA	1:B:4322:SER:O	2.21	0.40
1:B:4493:ASP:OD1	1:B:4494:PRO:HD2	2.21	0.40
1:A:1726:PHE:CB	1:A:1729:LEU:HB3	2.51	0.40
1:A:2793:ASN:HB3	1:A:2794:PRO:HD2	2.04	0.40
1:A:2986:VAL:O	1:A:2988:LEU:HG	2.20	0.40
1:A:2995:LEU:CD2	1:A:2998:ILE:HD11	2.48	0.40
1:A:3256:THR:HB	1:A:3257:PRO:CD	2.51	0.40
1:A:4130:SER:HA	1:A:4131:PRO:HD3	1.88	0.40
1:A:4189:ASN:HA	1:A:4191:HIS:CD2	2.57	0.40
1:A:4245:LYS:HE2	1:A:4249:LEU:HD11	2.03	0.40
1:A:4418:LEU:HD11	1:A:4422:LYS:NZ	2.36	0.40
1:B:1696:ARG:HH21	1:B:1726:PHE:HA	1.86	0.40
1:B:2379:LEU:HD12	1:B:2383:GLU:HG2	2.03	0.40
1:B:3256:THR:N	1:B:3259:HIS:HD2	2.19	0.40
1:B:3700:LEU:CD1	1:B:3701:ASP:N	2.80	0.40
1:B:4402:ILE:N	1:B:4402:ILE:CD1	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4403:SER:HB2	1:B:4407:TRP:CD2	2.56	0.40
1:B:3966:THR:HG23	1:B:4426:MET:HE3	2.02	0.40
1:B:4428:ASN:O	1:B:4432:LYS:HG3	2.21	0.40
1:B:4703:ILE:CD1	1:B:4705:LEU:HD21	2.45	0.40
1:A:1853:GLN:HE22	1:A:1886:ARG:HH11	1.68	0.40
1:A:1898:LEU:HA	1:A:1898:LEU:HD23	1.89	0.40
1:A:2529:THR:O	1:A:2530:ARG:C	2.60	0.40
1:A:2536:SER:HB2	1:A:2580:GLY:O	2.21	0.40
1:A:3947:ILE:O	1:A:3947:ILE:HD13	2.21	0.40
1:A:4247:ASN:HD21	1:A:4282:GLN:NE2	2.19	0.40
1:B:1867:LEU:H	1:B:1867:LEU:HD12	1.86	0.40
1:B:2029:ASN:HD22	1:B:2030:ARG:N	2.20	0.40
1:B:2135:CYS:O	1:B:2139:LEU:HB2	2.21	0.40
1:B:2258:LYS:HD3	1:B:2261:GLN:OE1	2.21	0.40
1:B:2688:LEU:HD13	1:B:2696:VAL:HB	2.04	0.40
1:B:3002:ASP:HA	1:B:3029:VAL:HG11	2.04	0.40
1:A:1778:LYS:HB3	1:A:1922:LEU:HD11	2.04	0.40
1:A:1831:LEU:HD22	1:A:1898:LEU:HD13	2.04	0.40
1:A:2036:LEU:HD12	1:A:2036:LEU:O	2.21	0.40
1:A:2236:LEU:HD21	1:A:2293:ILE:CD1	2.44	0.40
1:A:2591:GLU:OE1	1:A:2611:PRO:HG2	2.22	0.40
1:A:2710:LEU:HD23	1:A:2762:PHE:CE2	2.57	0.40
1:A:3066:GLU:HG2	1:A:3136:GLN:NE2	2.36	0.40
1:A:3459:ASP:HA	1:A:3460:PRO:HD3	1.97	0.40
1:A:3296:GLU:HG3	1:A:3567:LEU:HD13	2.04	0.40
1:A:3845:ILE:HG13	1:A:3845:ILE:H	1.57	0.40
1:A:4057:ILE:HD12	1:A:4057:ILE:HA	1.96	0.40
1:A:4284:ARG:CG	1:A:4408:LEU:HB3	2.49	0.40
1:B:1906:TRP:CZ2	1:B:1911:ARG:HG2	2.57	0.40
1:B:1928:HIS:NE2	1:B:1933:THR:CG2	2.81	0.40
1:B:1813:GLN:HE22	1:B:1941:LEU:H	1.69	0.40
1:B:2309:LYS:HG3	1:B:2358:ASP:HB2	2.02	0.40
1:B:2270:HIS:CB	1:B:2392:ARG:HH11	2.34	0.40
1:B:2519:ALA:HB2	1:B:2593:PHE:CE1	2.57	0.40
1:B:2645:ASP:OD2	1:B:2645:ASP:N	2.54	0.40
1:B:2745:GLU:HG2	1:B:2748:LEU:CD1	2.51	0.40
1:B:2799:GLY:HA3	1:B:3159:ALA:HB1	2.04	0.40
1:B:3271:ILE:HA	1:B:3592:VAL:HG21	2.03	0.40
1:B:3927:ASN:HB3	1:B:3930:LEU:HD12	2.02	0.40
1:B:4432:LYS:C	1:B:4434:GLN:H	2.25	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	2	24
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	6	38
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	3	31

All (205) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	B	1980	LYS
1	B	2071	MET
1	B	3602	ILE
1	B	3931	VAL
1	B	4207	LEU
1	A	1714	ASP
1	A	1949	GLN
1	A	2004	PHE
1	A	2080	GLY
1	A	2101	ILE
1	A	2342	ASN
1	A	2527	ASP
1	A	2530	ARG
1	A	2628	LYS
1	A	2642	ALA
1	A	2645	ASP
1	A	2727	GLU
1	A	2776	SER
1	A	2789	VAL
1	A	2792	CYS
1	A	3218	ALA
1	A	3430	ASN
1	A	3440	THR
1	A	3488	SER
1	A	3715	GLY
1	A	3719	LEU
1	A	3841	ALA
1	A	3926	ASN
1	A	3994	GLY
1	A	3998	LEU
1	A	4000	SER
1	A	4014	THR
1	A	4053	VAL
1	A	4116	LEU
1	A	4123	GLU
1	A	4125	GLU
1	A	4158	LYS
1	A	4221	ILE
1	A	4342	ILE
1	A	4594	LEU
1	A	4666	ILE
1	A	4672	LYS

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Mol	Chain	Res	Type
1	A	4709	GLN
1	B	1919	GLU
1	B	2141	ALA
1	B	2230	PRO
1	B	2384	ARG
1	B	2600	ILE
1	B	2641	VAL
1	B	2755	GLY
1	B	2775	THR
1	B	3092	ALA
1	B	3603	GLY
1	B	3842	SER
1	B	3844	ASN
1	B	4113	THR
1	B	4221	ILE
1	B	4297	GLU
1	B	4340	SER
1	B	4464	ALA
1	B	4551	LYS
1	A	1663	GLU
1	A	1697	PHE
1	A	1703	GLU
1	A	1727	ALA
1	A	1923	HIS
1	A	2001	ASP
1	A	2089	ASP
1	A	2140	SER
1	A	2282	LYS
1	A	2329	ASP
1	A	2374	ASN
1	A	2705	THR
1	A	2871	HIS
1	A	2990	LEU
1	A	3082	SER
1	A	3671	TYR
1	A	3693	LYS
1	A	3843	GLY
1	A	3933	LYS
1	A	4007	GLN
1	A	4055	GLU
1	A	4118	MET
1	A	4131	PRO

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Mol	Chain	Res	Type
1	A	4163	GLY
1	A	4168	PHE
1	A	4318	SER
1	A	4401	GLU
1	A	4412	GLU
1	B	1663	GLU
1	B	2001	ASP
1	B	2527	ASP
1	B	2915	ASP
1	B	3080	GLU
1	B	3094	GLY
1	B	3248	ARG
1	B	3692	LYS
1	B	4071	ASN
1	B	4692	LEU
1	A	1799	ASP
1	A	1837	GLN
1	A	2002	GLU
1	A	2054	SER
1	A	2122	GLU
1	A	2177	ALA
1	A	2270	HIS
1	A	2370	LEU
1	A	2653	THR
1	A	2690	ALA
1	A	2744	ASP
1	A	2891	GLN
1	A	3094	GLY
1	A	3166	ASN
1	A	3444	MET
1	A	3699	PHE
1	A	3907	HIS
1	A	4026	GLN
1	A	4029	SER
1	A	4259	ARG
1	A	4519	ASN
1	B	1506	ASP
1	B	2165	LYS
1	B	2308	PRO
1	B	2401	LYS
1	B	2749	PRO
1	B	2947	LYS

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Mol	Chain	Res	Type
1	B	3932	ASP
1	B	4003	GLU
1	B	4051	ASP
1	B	4053	VAL
1	B	4189	ASN
1	B	4674	LYS
1	A	2363	TRP
1	A	2601	ALA
1	A	2987	PRO
1	A	3140	ASN
1	A	3142	HIS
1	A	3471	SER
1	A	3712	LEU
1	A	3999	THR
1	A	4011	LEU
1	A	4169	GLU
1	A	4579	SER
1	A	4691	TYR
1	A	4712	SER
1	B	1498	THR
1	B	2069	GLN
1	B	2140	SER
1	B	2210	ASP
1	B	2558	PHE
1	B	3693	LYS
1	B	3849	ASP
1	B	3963	ASP
1	B	4412	GLU
1	A	1868	SER
1	A	1944	GLY
1	A	2966	SER
1	A	3164	LEU
1	A	3716	CYS
1	A	3845	ILE
1	B	1582	LYS
1	B	1630	PRO
1	B	1727	ALA
1	B	4459	GLU
1	B	4621	LEU
1	A	3395	PRO
1	A	3806	ARG
1	A	3976	VAL

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Mol	Chain	Res	Type
1	B	4131	PRO
1	A	4056	PRO
1	B	3093	GLY
1	B	4556	PRO
1	A	2644	PRO
1	A	2755	GLY
1	A	3602	ILE
1	A	3677	PRO
1	B	1579	PRO
1	B	2380	PRO
1	A	2208	VAL
1	B	4094	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2457/3028 (81%)	2249 (92%)	208 (8%)	10	40
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	18	50
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	14	45

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1516	GLU
1	A	1559	ASP
1	A	1593	ASP
1	A	1594	ARG
1	A	1665	ILE
1	A	1699	PHE
1	A	1719	GLN
1	A	1744	MET
1	A	1753	THR
1	A	1756	LYS
1	A	1803	TYR

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Mol	Chain	Res	Type
1	A	1809	ASN
1	A	1844	GLN
1	A	1849	GLU
1	A	1865	GLN
1	A	1874	LYS
1	A	1882	LEU
1	A	1911	ARG
1	A	1922	LEU
1	A	1934	PHE
1	A	1962	GLN
1	A	1973	PHE
1	A	1978	THR
1	A	2006	LEU
1	A	2029	ASN
1	A	2051	LYS
1	A	2053	ASN
1	A	2069	GLN
1	A	2071	MET
1	A	2073	ILE
1	A	2090	ASN
1	A	2096	ARG
1	A	2105	ARG
1	A	2107	MET
1	A	2120	THR
1	A	2136	GLN
1	A	2142	GLN
1	A	2149	LEU
1	A	2152	LEU
1	A	2221	ASP
1	A	2234	ASP
1	A	2239	LYS
1	A	2274	MET
1	A	2297	ASP
1	A	2324	THR
1	A	2329	ASP
1	A	2346	GLU
1	A	2350	ARG
1	A	2359	VAL
1	A	2369	SER
1	A	2384	ARG
1	A	2392	ARG
1	A	2408	ILE

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Mol	Chain	Res	Type
1	A	2409	SER
1	A	2415	TRP
1	A	2424	GLN
1	A	2435	SER
1	A	2442	GLN
1	A	2450	ASN
1	A	2511	LEU
1	A	2512	VAL
1	A	2527	ASP
1	A	2529	THR
1	A	2572	ARG
1	A	2587	LEU
1	A	2603	THR
1	A	2613	LEU
1	A	2614	ASP
1	A	2615	TYR
1	A	2626	LEU
1	A	2645	ASP
1	A	2650	THR
1	A	2685	THR
1	A	2694	PHE
1	A	2728	THR
1	A	2747	ASN
1	A	2761	THR
1	A	2793	ASN
1	A	2809	ARG
1	A	2817	ASP
1	A	2863	ARG
1	A	2873	ILE
1	A	2880	SER
1	A	2883	ASP
1	A	2897	THR
1	A	2926	THR
1	A	2944	ASP
1	A	2954	ASN
1	A	2998	ILE
1	A	3007	GLN
1	A	3026	SER
1	A	3027	ARG
1	A	3037	ILE
1	A	3043	ASN
1	A	3052	ASP

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Mol	Chain	Res	Type
1	A	3084	LEU
1	A	3123	LEU
1	A	3141	LEU
1	A	3143	VAL
1	A	3145	PHE
1	A	3158	SER
1	A	3168	CYS
1	A	3175	GLU
1	A	3179	GLU
1	A	3186	SER
1	A	3195	GLU
1	A	3200	ILE
1	A	3216	LEU
1	A	3240	GLU
1	A	3269	LEU
1	A	3278	LEU
1	A	3330	ASP
1	A	3337	LYS
1	A	3365	ASP
1	A	3366	LEU
1	A	3373	ILE
1	A	3381	SER
1	A	3399	THR
1	A	3405	MET
1	A	3432	ILE
1	A	3457	LEU
1	A	3468	ASN
1	A	3516	ASP
1	A	3536	TYR
1	A	3564	LEU
1	A	3566	ASN
1	A	3569	SER
1	A	3571	ARG
1	A	3583	THR
1	A	3584	GLN
1	A	3612	ASP
1	A	3623	SER
1	A	3630	SER
1	A	3663	ILE
1	A	3676	ASP
1	A	3678	SER
1	A	3691	ASP

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Mol	Chain	Res	Type
1	A	3695	THR
1	A	3700	LEU
1	A	3707	ASN
1	A	3719	LEU
1	A	3725	ASN
1	A	3730	LEU
1	A	3731	ASN
1	A	3759	SER
1	A	3760	PHE
1	A	3776	ASP
1	A	3785	ASN
1	A	3791	SER
1	A	3799	HIS
1	A	3806	ARG
1	A	3813	ARG
1	A	3817	LEU
1	A	3830	LEU
1	A	3865	ILE
1	A	3867	LEU
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3947	ILE
1	A	3974	ILE
1	A	3998	LEU
1	A	4007	GLN
1	A	4023	LEU
1	A	4026	GLN
1	A	4034	VAL
1	A	4039	GLN
1	A	4043	ASP
1	A	4048	PHE
1	A	4055	GLU
1	A	4069	LEU
1	A	4079	ASN
1	A	4100	SER
1	A	4200	LEU
1	A	4206	SER
1	A	4232	MET
1	A	4240	ASN
1	A	4259	ARG
1	A	4267	ARG

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Mol	Chain	Res	Type
1	A	4282	GLN
1	A	4286	ARG
1	A	4290	LEU
1	A	4295	PHE
1	A	4321	ARG
1	A	4337	ILE
1	A	4353	MET
1	A	4360	LEU
1	A	4362	GLN
1	A	4385	GLU
1	A	4388	THR
1	A	4404	THR
1	A	4428	ASN
1	A	4434	GLN
1	A	4503	ILE
1	A	4550	TRP
1	A	4553	TYR
1	A	4565	ILE
1	A	4566	SER
1	A	4596	ASN
1	A	4606	GLN
1	A	4638	ASN
1	A	4649	TRP
1	A	4671	TRP
1	A	4692	LEU
1	A	4693	ASN
1	A	4694	GLU
1	A	4711	THR
1	A	4714	GLN
1	B	1479	ARG
1	B	1490	THR
1	B	1545	LEU
1	B	1547	ASN
1	B	1555	VAL
1	B	1596	ASN
1	B	1629	LEU
1	B	1640	ASN
1	B	1658	GLU
1	B	1671	ARG
1	B	1712	SER
1	B	1734	LEU
1	B	1736	ASP

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Mol	Chain	Res	Type
1	B	1762	ASN
1	B	1793	ASN
1	B	1809	ASN
1	B	1817	LEU
1	B	1828	ASP
1	B	1867	LEU
1	B	1901	ASN
1	B	1911	ARG
1	B	1920	ASN
1	B	1946	ARG
1	B	2029	ASN
1	B	2071	MET
1	B	2106	GLU
1	B	2129	VAL
1	B	2149	LEU
1	B	2166	CYS
1	B	2185	GLN
1	B	2189	GLN
1	B	2197	ASN
1	B	2211	ASP
1	B	2235	GLN
1	B	2236	LEU
1	B	2239	LYS
1	B	2253	GLN
1	B	2254	GLU
1	B	2260	LEU
1	B	2290	LEU
1	B	2313	LYS
1	B	2320	LEU
1	B	2342	ASN
1	B	2352	TRP
1	B	2374	ASN
1	B	2381	ASN
1	B	2423	THR
1	B	2425	MET
1	B	2432	ASP
1	B	2504	GLN
1	B	2541	MET
1	B	2550	GLU
1	B	2581	LEU
1	B	2587	LEU
1	B	2603	THR

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Mol	Chain	Res	Type
1	B	2612	LEU
1	B	2613	LEU
1	B	2699	LEU
1	B	2745	GLU
1	B	2797	ASP
1	B	2821	THR
1	B	2825	THR
1	B	2841	ASN
1	B	2843	ARG
1	B	2883	ASP
1	B	2897	THR
1	B	2899	GLU
1	B	2927	ASP
1	B	2928	LYS
1	B	2929	LYS
1	B	2946	LEU
1	B	2966	SER
1	B	2977	LYS
1	B	2984	LEU
1	B	2996	ASP
1	B	3018	SER
1	B	3026	SER
1	B	3043	ASN
1	B	3050	ASP
1	B	3059	LEU
1	B	3087	MET
1	B	3140	ASN
1	B	3151	SER
1	B	3164	LEU
1	B	3195	GLU
1	B	3284	HIS
1	B	3302	LEU
1	B	3322	GLN
1	B	3560	SER
1	B	3563	LEU
1	B	3566	ASN
1	B	3619	ILE
1	B	3620	ARG
1	B	3623	SER
1	B	3676	ASP
1	B	3700	LEU
1	B	3725	ASN

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Mol	Chain	Res	Type
1	B	3780	ARG
1	B	3833	SER
1	B	3867	LEU
1	B	3954	ARG
1	B	3998	LEU
1	B	4005	ILE
1	B	4012	LEU
1	B	4029	SER
1	B	4046	GLN
1	B	4091	SER
1	B	4105	VAL
1	B	4157	TYR
1	B	4185	VAL
1	B	4189	ASN
1	B	4200	LEU
1	B	4206	SER
1	B	4218	THR
1	B	4219	SER
1	B	4232	MET
1	B	4258	THR
1	B	4309	SER
1	B	4318	SER
1	B	4323	ASN
1	B	4324	ILE
1	B	4327	ASP
1	B	4334	VAL
1	B	4356	LEU
1	B	4402	ILE
1	B	4413	ASN
1	B	4425	LYS
1	B	4434	GLN
1	B	4500	GLU
1	B	4503	ILE
1	B	4548	LYS
1	B	4555	VAL
1	B	4558	THR
1	B	4573	GLN
1	B	4576	SER
1	B	4596	ASN
1	B	4607	SER
1	B	4618	ASN
1	B	4644	LEU

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Mol	Chain	Res	Type
1	B	4693	ASN
1	B	4698	GLU
1	B	4709	GLN
1	B	4715	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1512	ASN
1	A	1522	GLN
1	A	1549	GLN
1	A	1563	ASN
1	A	1609	GLN
1	A	1690	GLN
1	A	1791	HIS
1	A	1798	ASN
1	A	1809	ASN
1	A	1813	GLN
1	A	1844	GLN
1	A	1853	GLN
1	A	1857	ASN
1	A	1858	ASN
1	A	1865	GLN
1	A	1877	HIS
1	A	1971	ASN
1	A	1990	GLN
1	A	2018	GLN
1	A	2029	ASN
1	A	2042	GLN
1	A	2044	GLN
1	A	2047	GLN
1	A	2053	ASN
1	A	2086	ASN
1	A	2090	ASN
1	A	2136	GLN
1	A	2138	GLN
1	A	2142	GLN
1	A	2167	GLN
1	A	2197	ASN
1	A	2200	ASN
1	A	2295	GLN
1	A	2351	HIS

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Mol	Chain	Res	Type
1	A	2366	ASN
1	A	2368	ASN
1	A	2428	GLN
1	A	2436	ASN
1	A	2447	GLN
1	A	2450	ASN
1	A	2495	GLN
1	A	2535	ASN
1	A	2552	ASN
1	A	2553	GLN
1	A	2564	ASN
1	A	2565	GLN
1	A	2598	GLN
1	A	2656	HIS
1	A	2747	ASN
1	A	2787	GLN
1	A	2793	ASN
1	A	2810	HIS
1	A	2826	GLN
1	A	2869	GLN
1	A	2907	HIS
1	A	2942	ASN
1	A	2954	ASN
1	A	2961	GLN
1	A	3007	GLN
1	A	3009	GLN
1	A	3033	ASN
1	A	3043	ASN
1	A	3077	ASN
1	A	3156	ASN
1	A	3223	HIS
1	A	3253	ASN
1	A	3266	GLN
1	A	3277	GLN
1	A	3286	ASN
1	A	3331	GLN
1	A	3338	GLN
1	A	3377	GLN
1	A	3437	ASN
1	A	3555	ASN
1	A	3566	ASN
1	A	3607	GLN

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Mol	Chain	Res	Type
1	A	3646	ASN
1	A	3687	ASN
1	A	3721	GLN
1	A	3725	ASN
1	A	3731	ASN
1	A	3785	ASN
1	A	3794	GLN
1	A	3820	GLN
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3981	ASN
1	A	4017	GLN
1	A	4046	GLN
1	A	4066	GLN
1	A	4073	GLN
1	A	4079	ASN
1	A	4112	ASN
1	A	4191	HIS
1	A	4210	HIS
1	A	4234	ASN
1	A	4263	GLN
1	A	4278	HIS
1	A	4282	GLN
1	A	4349	ASN
1	A	4362	GLN
1	A	4370	ASN
1	A	4413	ASN
1	A	4573	GLN
1	A	4574	GLN
1	A	4596	ASN
1	A	4610	GLN
1	A	4653	GLN
1	A	4693	ASN
1	A	4715	ASN
1	A	4718	GLN
1	B	1480	HIS
1	B	1522	GLN
1	B	1547	ASN
1	B	1568	HIS
1	B	1589	ASN
1	B	1609	GLN

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Mol	Chain	Res	Type
1	B	1640	ASN
1	B	1690	GLN
1	B	1793	ASN
1	B	1813	GLN
1	B	1820	GLN
1	B	1826	GLN
1	B	1857	ASN
1	B	1891	GLN
1	B	1901	ASN
1	B	1920	ASN
1	B	1931	ASN
1	B	1990	GLN
1	B	2029	ASN
1	B	2044	GLN
1	B	2086	ASN
1	B	2110	GLN
1	B	2235	GLN
1	B	2241	GLN
1	B	2264	GLN
1	B	2315	GLN
1	B	2342	ASN
1	B	2351	HIS
1	B	2368	ASN
1	B	2381	ASN
1	B	2398	GLN
1	B	2504	GLN
1	B	2542	ASN
1	B	2547	ASN
1	B	2564	ASN
1	B	2571	ASN
1	B	2793	ASN
1	B	2826	GLN
1	B	2832	ASN
1	B	2841	ASN
1	B	2861	GLN
1	B	2937	HIS
1	B	2992	ASN
1	B	3043	ASN
1	B	3196	ASN
1	B	3223	HIS
1	B	3235	HIS
1	B	3272	ASN

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Mol	Chain	Res	Type
1	B	3322	GLN
1	B	3338	GLN
1	B	3555	ASN
1	B	3566	ASN
1	B	3577	GLN
1	B	3687	ASN
1	B	3725	ASN
1	B	3731	ASN
1	B	3785	ASN
1	B	3794	GLN
1	B	3799	HIS
1	B	3925	ASN
1	B	3926	ASN
1	B	3953	ASN
1	B	3981	ASN
1	B	4016	GLN
1	B	4026	GLN
1	B	4036	HIS
1	B	4038	GLN
1	B	4040	ASN
1	B	4052	GLN
1	B	4112	ASN
1	B	4152	GLN
1	B	4189	ASN
1	B	4199	GLN
1	B	4263	GLN
1	B	4278	HIS
1	B	4323	ASN
1	B	4391	HIS
1	B	4413	ASN
1	B	4434	GLN
1	B	4573	GLN
1	B	4574	GLN
1	B	4596	ASN
1	B	4618	ASN
1	B	4651	ASN
1	B	4693	ASN
1	B	4709	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ADP	B	9009	-	24,29,29	1.25	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	B	9007	-	24,29,29	1.23	3 (12%)	29,45,45	1.54	5 (17%)
2	ADP	A	9001	-	24,29,29	1.26	3 (12%)	29,45,45	1.57	5 (17%)
2	ADP	B	9010	-	24,29,29	1.24	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	B	9008	-	24,29,29	1.23	3 (12%)	29,45,45	1.55	5 (17%)
2	ADP	A	9004	-	24,29,29	1.23	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9002	-	24,29,29	1.23	2 (8%)	29,45,45	1.56	5 (17%)
2	ADP	A	9003	-	24,29,29	1.26	3 (12%)	29,45,45	1.56	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9009	-	-	5/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	4/12/32/32	0/3/3/3
2	ADP	A	9001	-	-	5/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9008	-	-	2/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	3/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	5/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	2.99	1.48	1.40
2	B	9008	ADP	C5-C4	2.95	1.48	1.40
2	B	9009	ADP	C5-C4	2.93	1.48	1.40
2	A	9003	ADP	C5-C4	2.93	1.48	1.40
2	B	9010	ADP	C5-C4	2.91	1.48	1.40
2	A	9004	ADP	C5-C4	2.91	1.48	1.40
2	B	9007	ADP	C5-C4	2.90	1.48	1.40
2	A	9001	ADP	C5-C4	2.90	1.48	1.40
2	A	9001	ADP	C2-N3	2.85	1.36	1.32
2	B	9008	ADP	C2-N3	2.79	1.36	1.32
2	A	9002	ADP	C2-N3	2.78	1.36	1.32
2	B	9010	ADP	C2-N3	2.78	1.36	1.32
2	B	9009	ADP	C2-N3	2.78	1.36	1.32
2	A	9003	ADP	C2-N3	2.77	1.36	1.32
2	B	9007	ADP	C2-N3	2.74	1.36	1.32
2	A	9004	ADP	C2-N3	2.71	1.36	1.32
2	A	9001	ADP	O4'-C1'	2.34	1.44	1.41
2	A	9003	ADP	O4'-C1'	2.25	1.44	1.41
2	B	9009	ADP	O4'-C1'	2.22	1.44	1.41
2	B	9010	ADP	O4'-C1'	2.11	1.44	1.41
2	A	9004	ADP	O4'-C1'	2.06	1.44	1.41
2	B	9007	ADP	O4'-C1'	2.03	1.43	1.41
2	B	9008	ADP	O4'-C1'	2.00	1.43	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9004	ADP	N3-C2-N1	-4.33	121.91	128.68
2	A	9003	ADP	N3-C2-N1	-4.30	121.96	128.68
2	B	9007	ADP	N3-C2-N1	-4.29	121.97	128.68
2	B	9010	ADP	N3-C2-N1	-4.27	122.00	128.68
2	A	9001	ADP	N3-C2-N1	-4.27	122.00	128.68
2	B	9009	ADP	N3-C2-N1	-4.25	122.03	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9002	ADP	N3-C2-N1	-4.20	122.11	128.68
2	B	9008	ADP	N3-C2-N1	-4.18	122.14	128.68
2	A	9003	ADP	C3'-C2'-C1'	3.70	106.55	100.98
2	A	9001	ADP	C3'-C2'-C1'	3.68	106.52	100.98
2	B	9009	ADP	C3'-C2'-C1'	3.67	106.50	100.98
2	B	9007	ADP	C3'-C2'-C1'	3.60	106.40	100.98
2	B	9008	ADP	C3'-C2'-C1'	3.57	106.36	100.98
2	A	9002	ADP	C3'-C2'-C1'	3.54	106.31	100.98
2	B	9010	ADP	C3'-C2'-C1'	3.54	106.31	100.98
2	A	9004	ADP	C3'-C2'-C1'	3.52	106.28	100.98
2	A	9002	ADP	PA-O3A-PB	-3.22	121.77	132.83
2	B	9008	ADP	PA-O3A-PB	-3.15	122.01	132.83
2	A	9001	ADP	PA-O3A-PB	-3.12	122.11	132.83
2	B	9009	ADP	PA-O3A-PB	-3.01	122.49	132.83
2	A	9003	ADP	PA-O3A-PB	-2.98	122.61	132.83
2	B	9010	ADP	PA-O3A-PB	-2.98	122.61	132.83
2	A	9004	ADP	PA-O3A-PB	-2.94	122.73	132.83
2	B	9007	ADP	PA-O3A-PB	-2.84	123.08	132.83
2	B	9007	ADP	C4-C5-N7	-2.61	106.68	109.40
2	B	9010	ADP	C4-C5-N7	-2.60	106.69	109.40
2	A	9001	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	9004	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	9002	ADP	C4-C5-N7	-2.58	106.71	109.40
2	B	9009	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	9003	ADP	C4-C5-N7	-2.57	106.72	109.40
2	B	9008	ADP	C4-C5-N7	-2.57	106.72	109.40
2	A	9004	ADP	C2-N1-C6	2.28	122.66	118.75
2	B	9007	ADP	C2-N1-C6	2.24	122.58	118.75
2	A	9001	ADP	C2-N1-C6	2.23	122.57	118.75
2	A	9003	ADP	C2-N1-C6	2.22	122.56	118.75
2	B	9010	ADP	C2-N1-C6	2.22	122.56	118.75
2	B	9009	ADP	C2-N1-C6	2.21	122.54	118.75
2	B	9008	ADP	C2-N1-C6	2.21	122.53	118.75
2	A	9002	ADP	C2-N1-C6	2.18	122.49	118.75

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9007	ADP	C5'-O5'-PA-O3A
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A

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

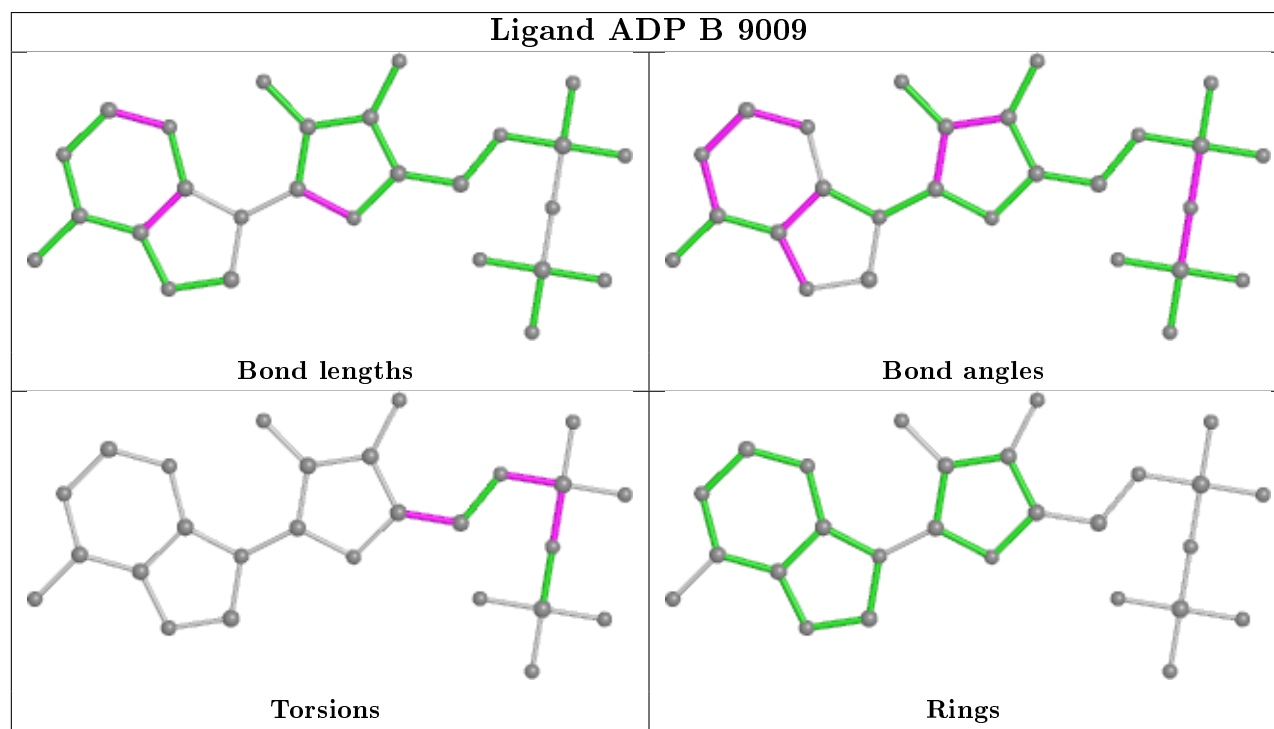
There are no ring outliers.

5 monomers are involved in 10 short contacts:

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

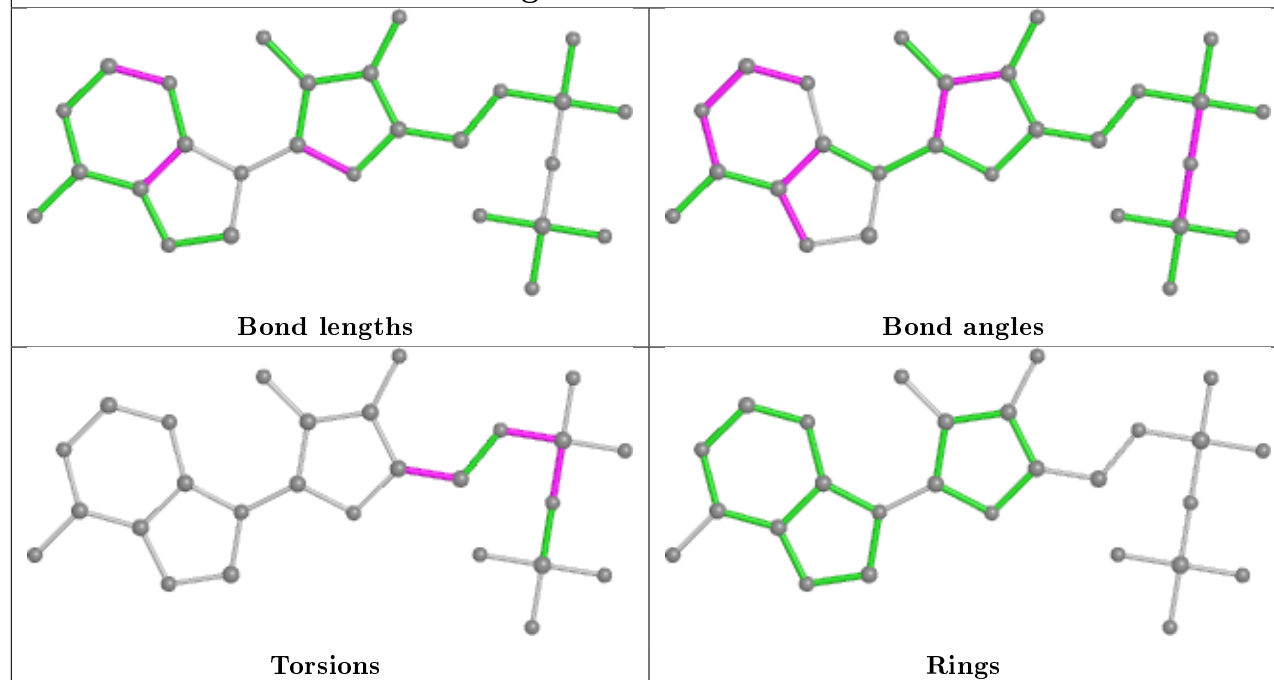
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

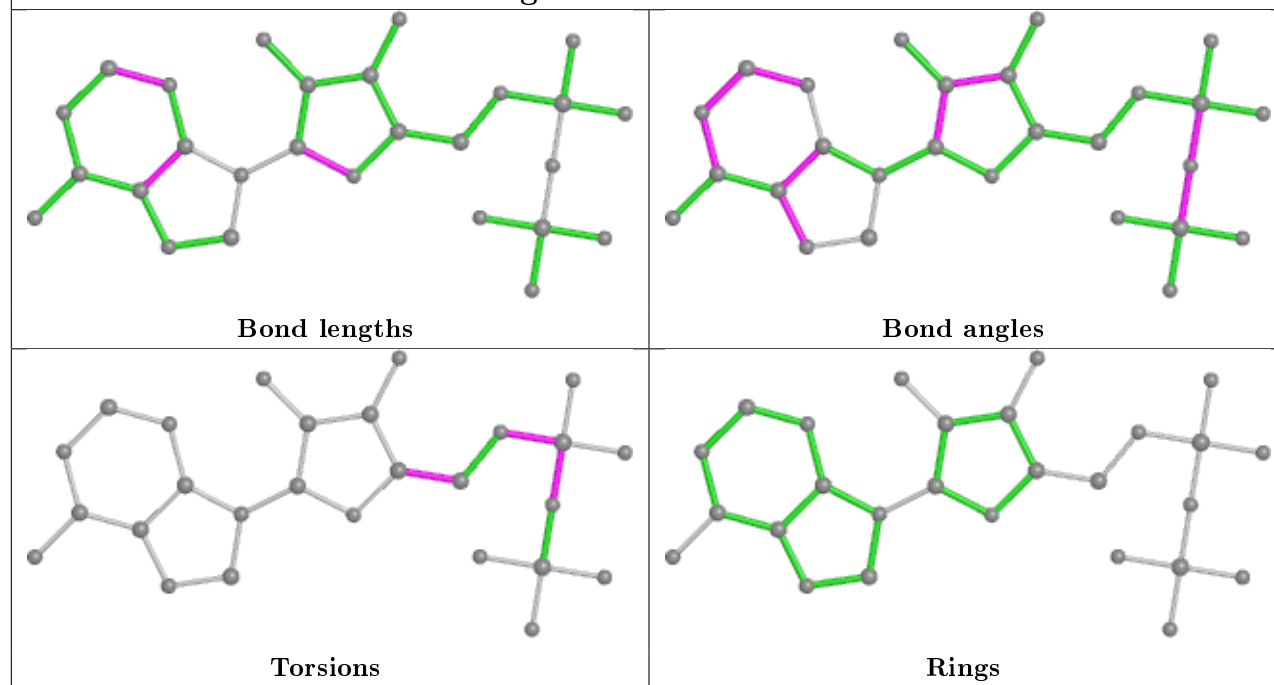




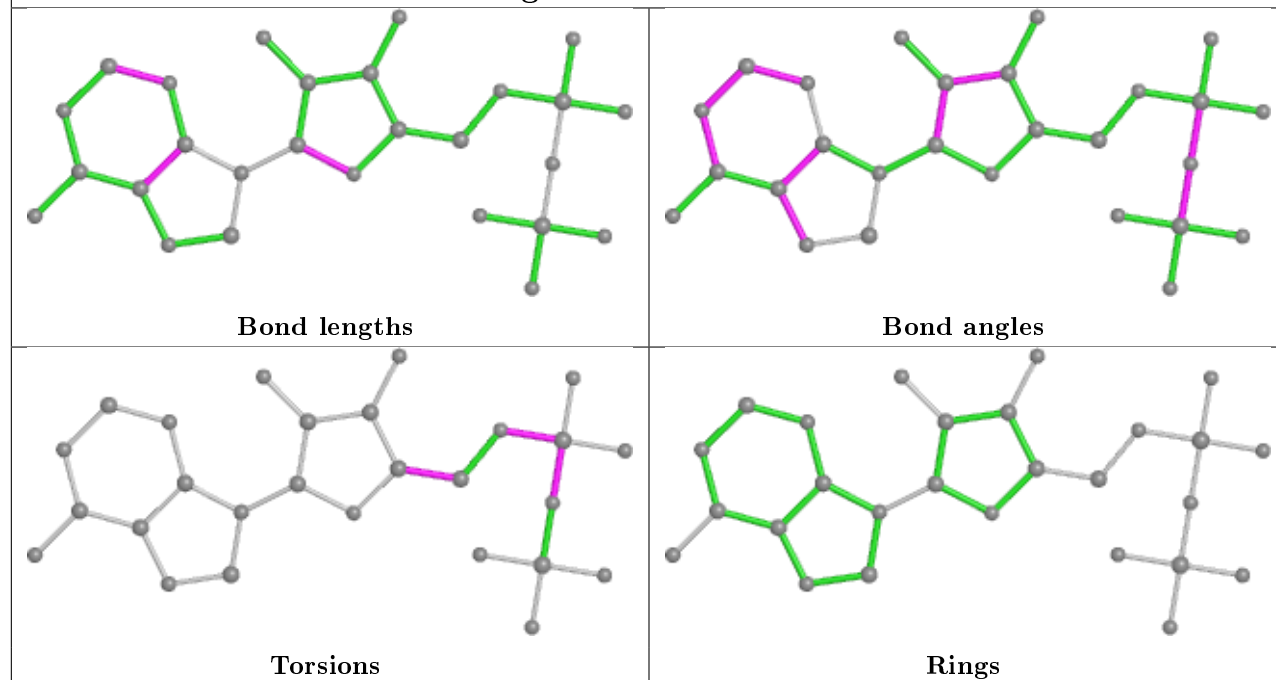
## Ligand ADP B 9007



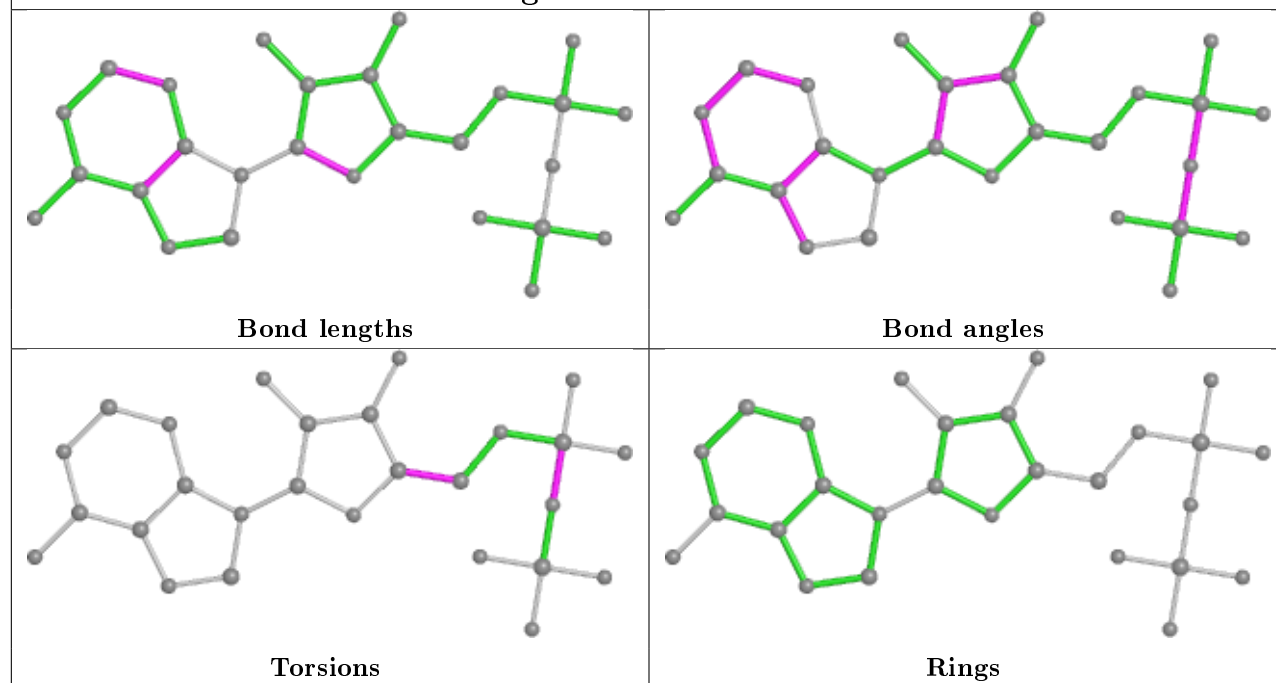
## Ligand ADP A 9001



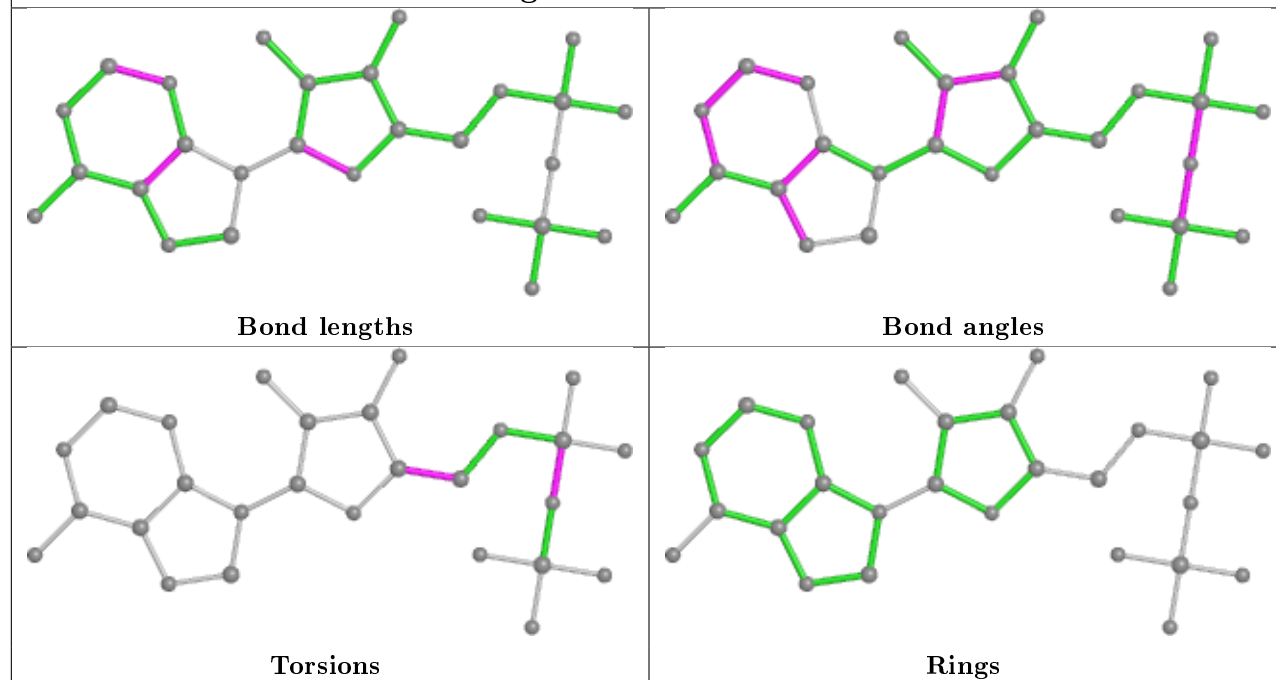
## Ligand ADP B 9010



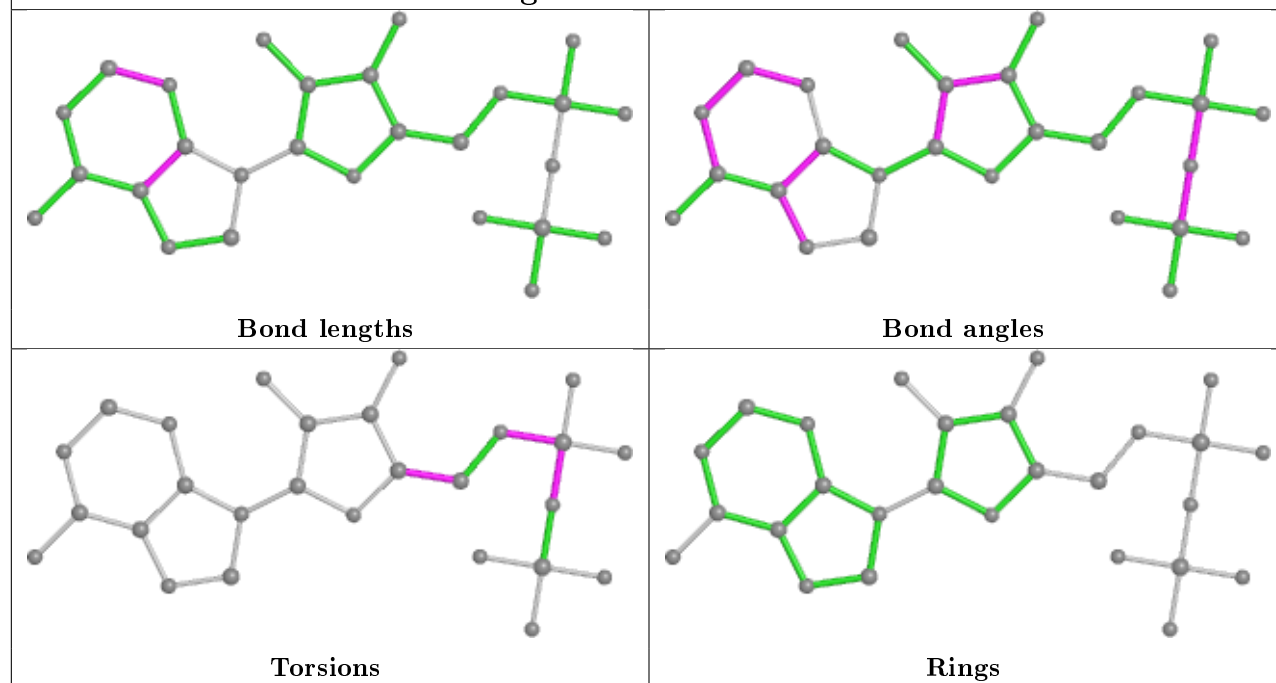
## Ligand ADP B 9008

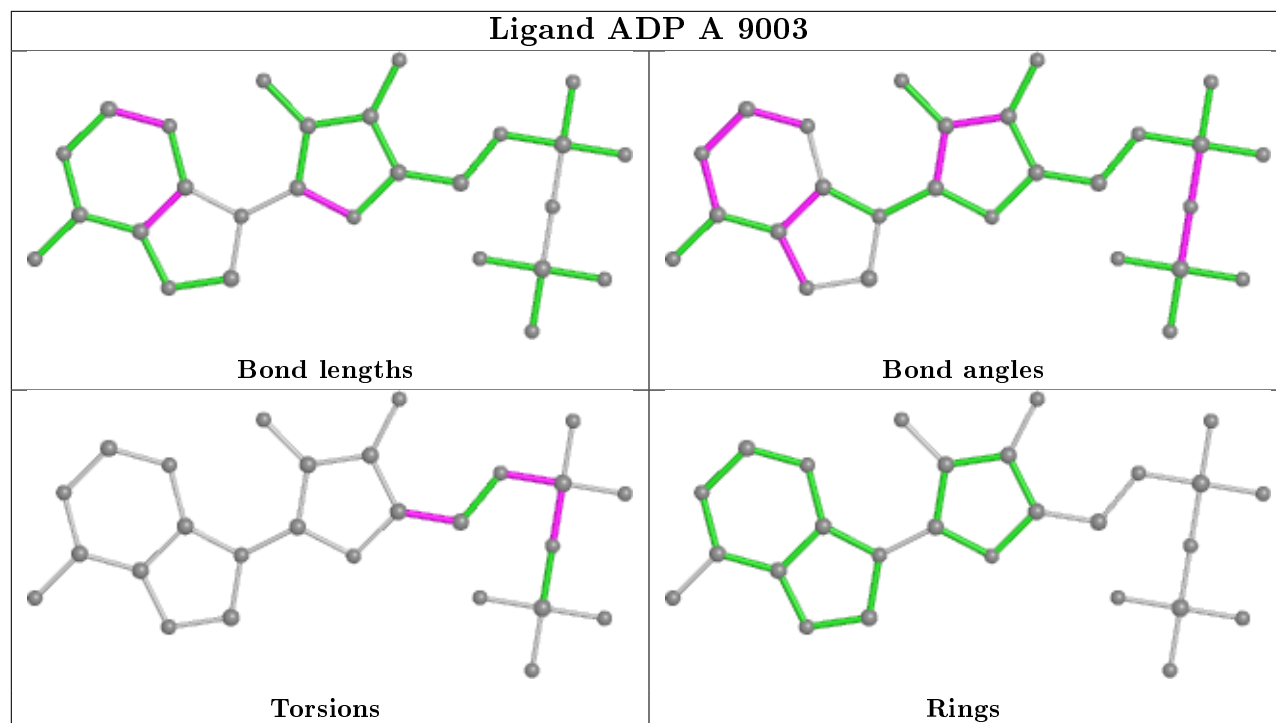


## Ligand ADP A 9004



## Ligand ADP A 9002





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	3042/3367 (90%)	-0.14	61 (2%) 65 58	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.18	29 (0%) 82 76	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.16	90 (1%) 73 66	64, 133, 209, 335	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.7
1	B	1517	VAL	4.8
1	A	1652	GLY	4.7
1	A	4187	LEU	4.5
1	A	1651	SER	4.1
1	A	3516	ASP	4.0
1	A	1555	VAL	4.0
1	A	3718	LEU	3.8
1	A	4122	VAL	3.8
1	A	4550	TRP	3.7
1	A	1545	LEU	3.6
1	B	1484	LEU	3.6
1	A	1650	VAL	3.6
1	A	4165	PRO	3.4
1	A	4509	LEU	3.4
1	A	3512	LYS	3.4
1	A	4217	MET	3.4
1	A	4162	ILE	3.3
1	A	3842	SER	3.3
1	A	3515	GLN	3.2
1	A	3518	ILE	3.2
1	A	1657	LEU	3.1
1	B	3356	ALA	3.0
1	A	3328	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	3334	ALA	3.0
1	B	2304	HIS	3.0
1	B	2720	TYR	2.9
1	B	2335	THR	2.9
1	A	4215	LEU	2.9
1	B	4517	LEU	2.9
1	A	4185	VAL	2.9
1	A	4168	PHE	2.9
1	A	3513	LEU	2.8
1	A	1575	MET	2.8
1	A	3846	LEU	2.8
1	A	1554	LEU	2.8
1	A	1656	ILE	2.7
1	A	1538	TRP	2.7
1	B	4541	ILE	2.7
1	A	1584	PHE	2.7
1	A	3866	ALA	2.6
1	B	1495	THR	2.6
1	A	3536	TYR	2.6
1	A	3360	VAL	2.6
1	A	1639	ILE	2.5
1	B	1575	MET	2.5
1	A	4118	MET	2.5
1	A	3359	LYS	2.5
1	B	2620	ASP	2.4
1	B	1543	LEU	2.4
1	B	2574	LEU	2.4
1	A	1527	LEU	2.4
1	A	3330	ASP	2.4
1	A	4131	PRO	2.3
1	A	1565	LEU	2.3
1	A	3762	ILE	2.3
1	A	3764	LEU	2.3
1	B	1656	ILE	2.3
1	A	4186	LEU	2.3
1	A	2060	LEU	2.3
1	B	1511	GLU	2.3
1	A	4192	LEU	2.3
1	A	1549	GLN	2.3
1	B	1514	TYR	2.3
1	A	1551	LYS	2.3
1	A	2353	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	4635	ALA	2.2
1	A	1544	ASP	2.2
1	A	3341	ALA	2.2
1	A	4142	ALA	2.2
1	B	3112	CYS	2.2
1	B	4550	TRP	2.2
1	A	2452	ASN	2.2
1	B	4215	LEU	2.2
1	B	1497	LEU	2.2
1	A	3319	GLN	2.2
1	A	3346	VAL	2.2
1	A	3533	LYS	2.2
1	B	1515	ARG	2.1
1	B	3341	ALA	2.1
1	A	3388	LEU	2.1
1	B	3544	GLU	2.1
1	B	3324	LEU	2.1
1	B	3842	SER	2.1
1	B	1510	ASN	2.1
1	A	3763	PHE	2.0
1	B	4537	LEU	2.0
1	B	3309	LYS	2.0
1	A	4183	THR	2.0
1	B	2597	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

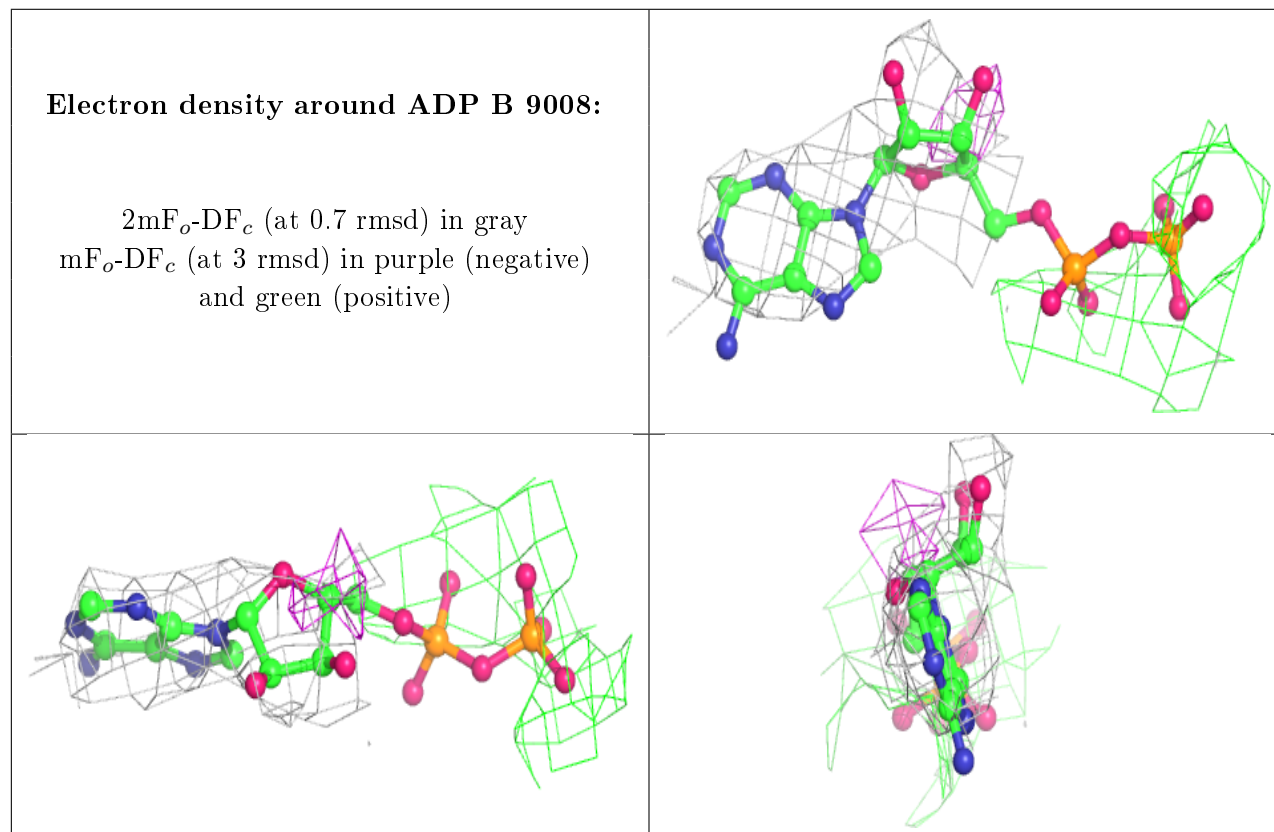
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	9008	27/27	0.85	0.40	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.31	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	129,129,129,129	0
2	ADP	A	9001	27/27	0.94	0.38	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	129,129,129,129	0

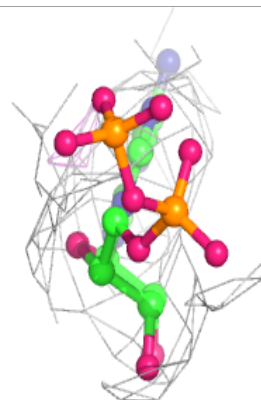
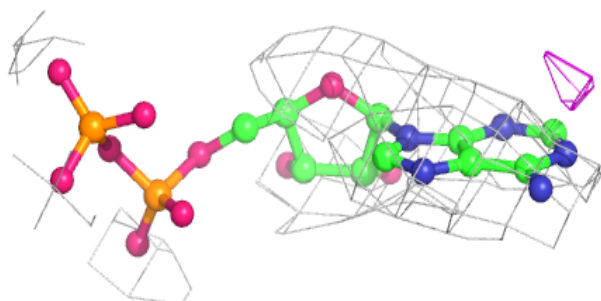
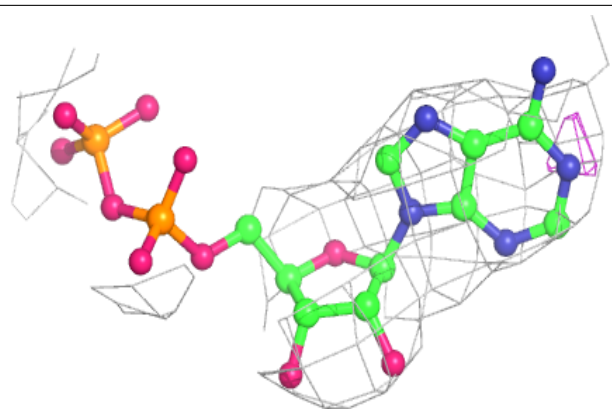
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



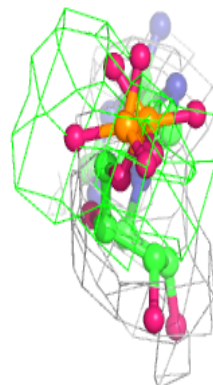
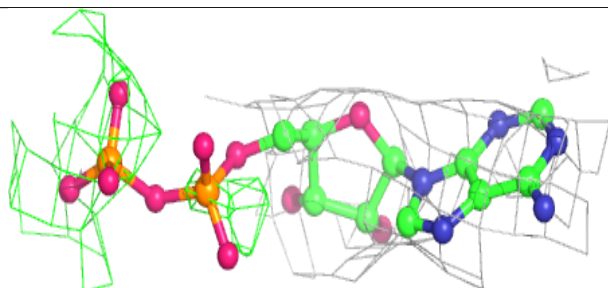
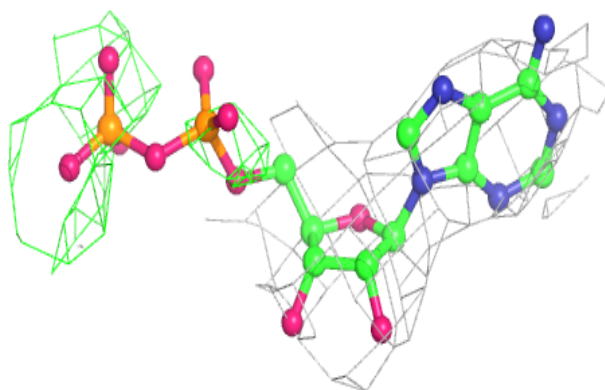


**Electron density around ADP B 9010:**

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

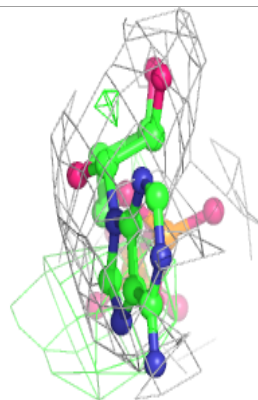
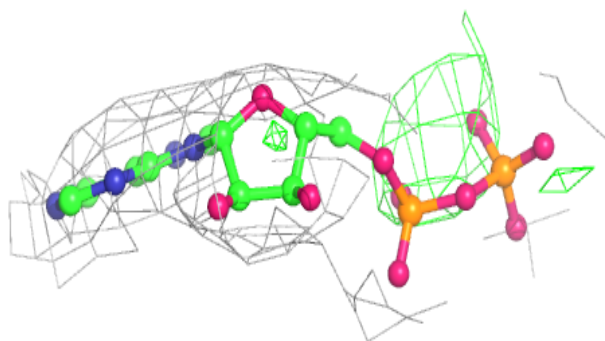
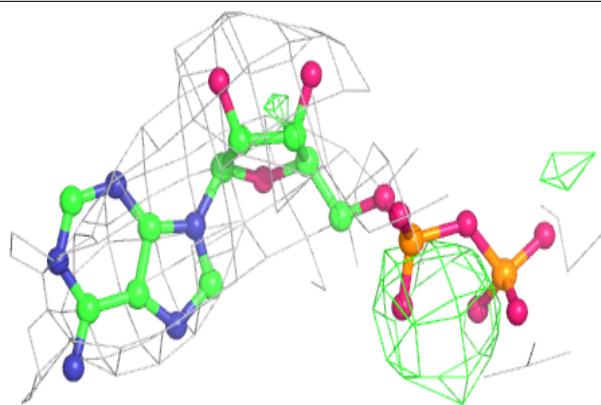
**Electron density around ADP A 9002:**

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

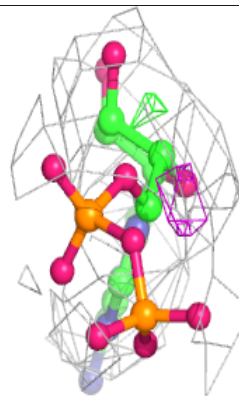
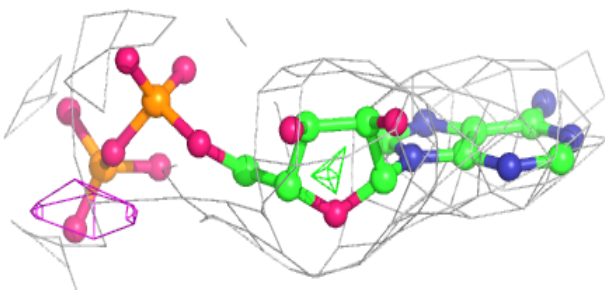
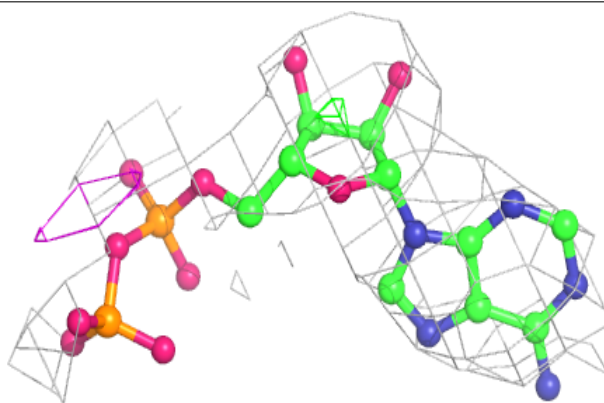


**Electron density around ADP B 9007:**

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

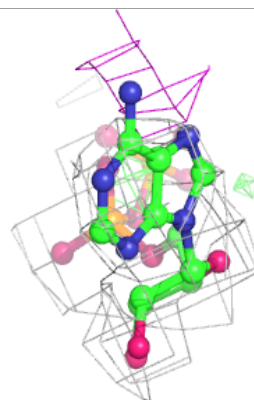
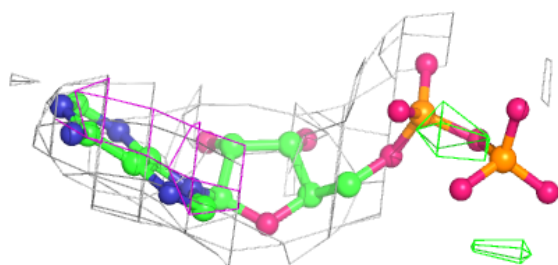
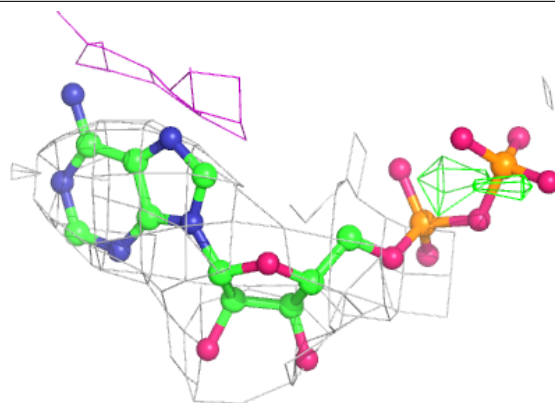
**Electron density around ADP A 9004:**

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

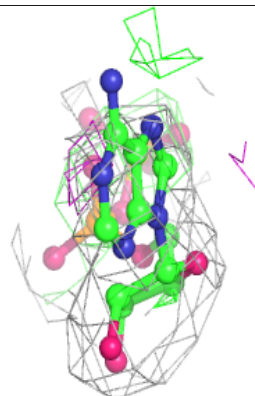
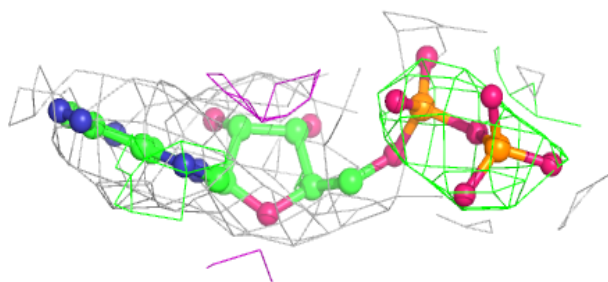
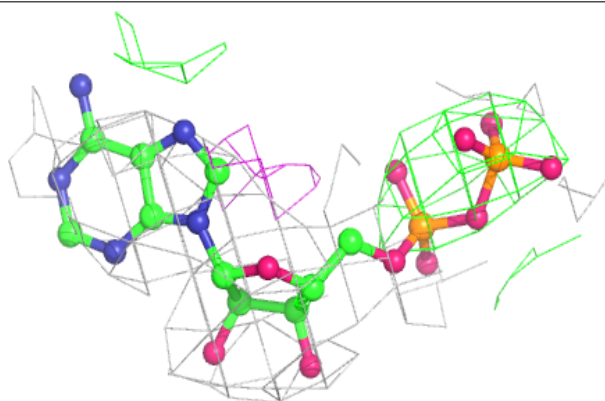


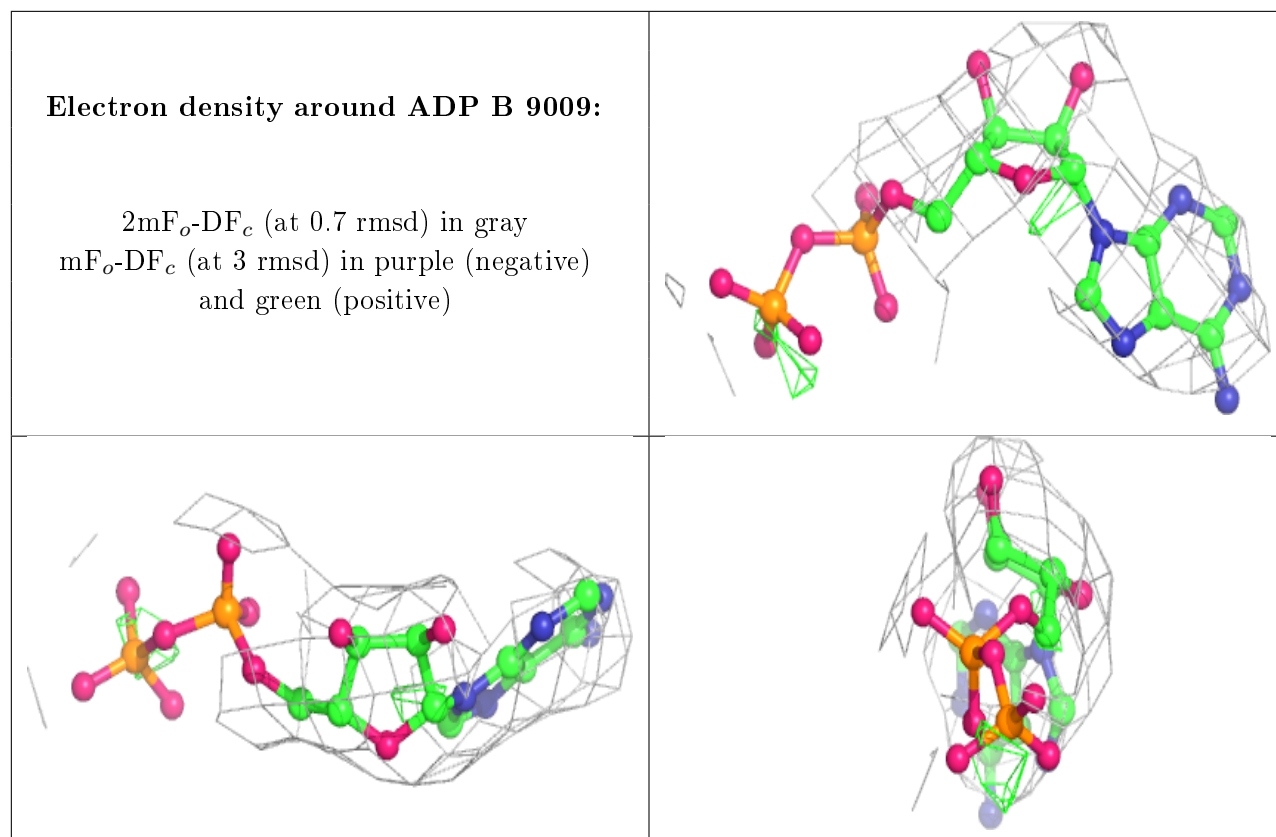
**Electron density around ADP A 9003:**

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

**Electron density around ADP A 9001:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.