



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 AM UTC

PDB ID : 3VKG / pdb_00003vkg
Title : X-ray structure of an MTBD truncation mutant of dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 2.81 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

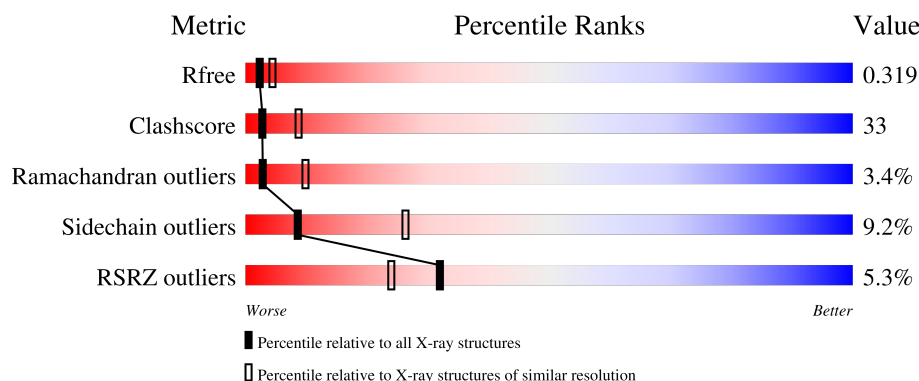
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

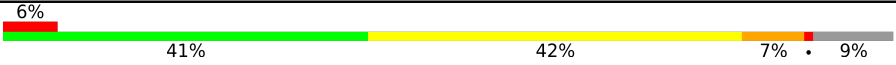
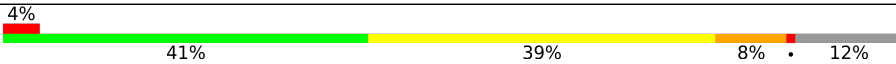
The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	3245	
1	B	3245	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 45284 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	2954	Total	C	N	O	S	0	0	0
			22821	14585	3870	4270	96			
1	B	2853	Total	C	N	O	S	0	0	0
			22146	14131	3745	4174	96			

There are 52 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
A	3494	THR	-	linker	UNP P34036

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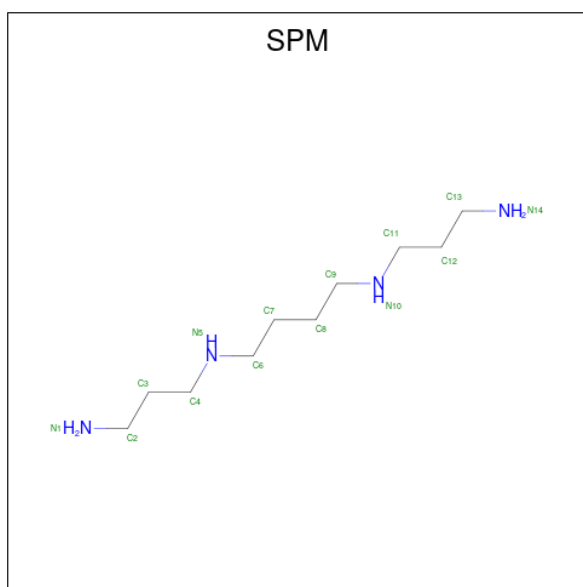
Chain	Residue	Modelled	Actual	Comment	Reference
A	3495	GLY	-	linker	UNP P34036
B	1364	MET	-	expression tag	UNP P34036
B	1365	THR	-	expression tag	UNP P34036
B	1366	ARG	-	expression tag	UNP P34036
B	1367	HIS	-	expression tag	UNP P34036
B	1368	HIS	-	expression tag	UNP P34036
B	1369	HIS	-	expression tag	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
B	3494	THR	-	linker	UNP P34036
B	3495	GLY	-	linker	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 3 is SPERMINE (CCD ID: SPM) (formula: $\text{C}_{10}\text{H}_{26}\text{N}_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	10	4		
3	A	1	Total	C	N	0	0
			14	10	4		
3	B	1	Total	C	N	0	0
			14	10	4		
3	B	1	Total	C	N	0	0
			14	10	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		

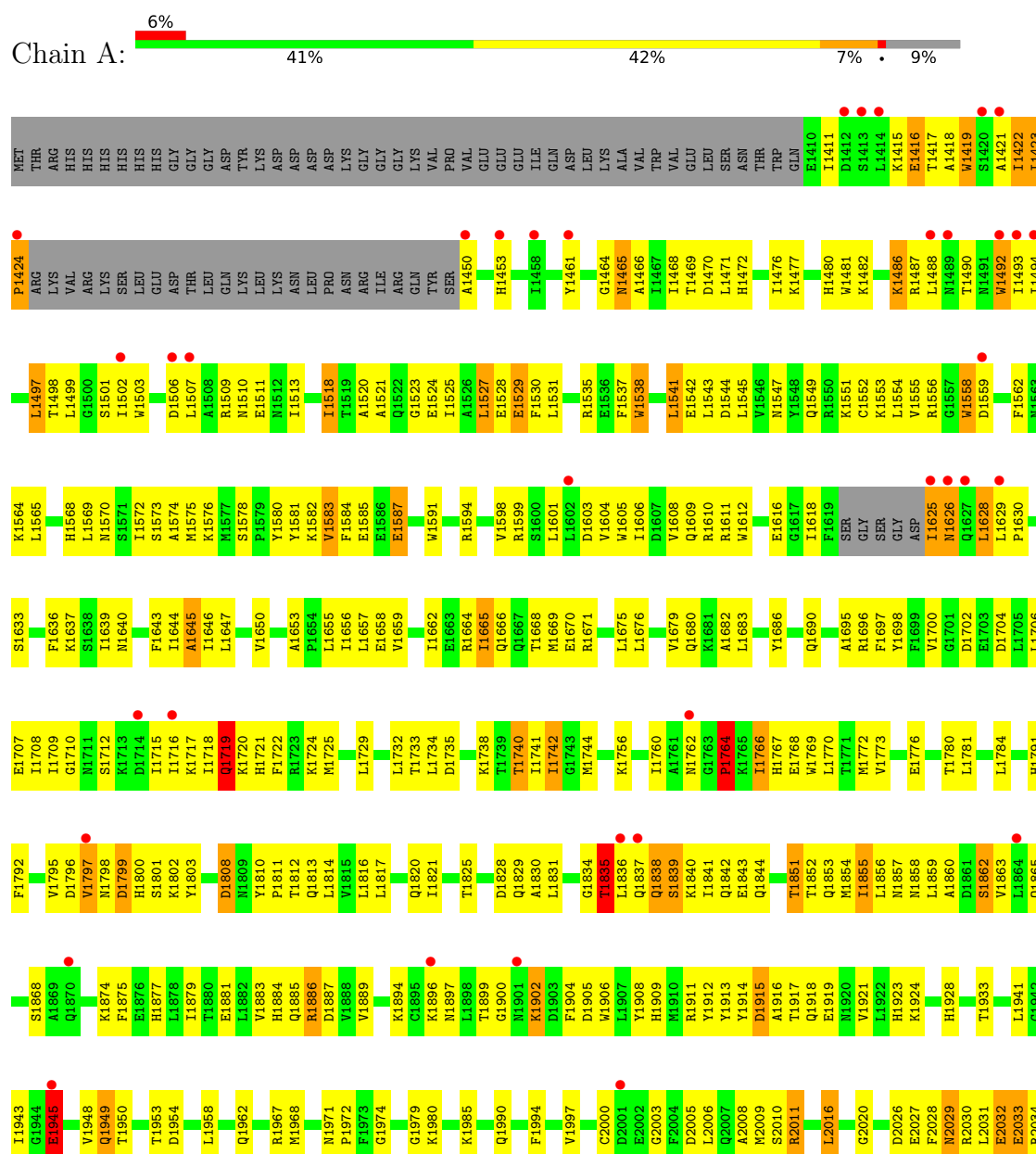
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	19	Total	O	0	0
			19	19		

3 Residue-property plots

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

- Molecule 1: Dynein heavy chain, cytoplasmic

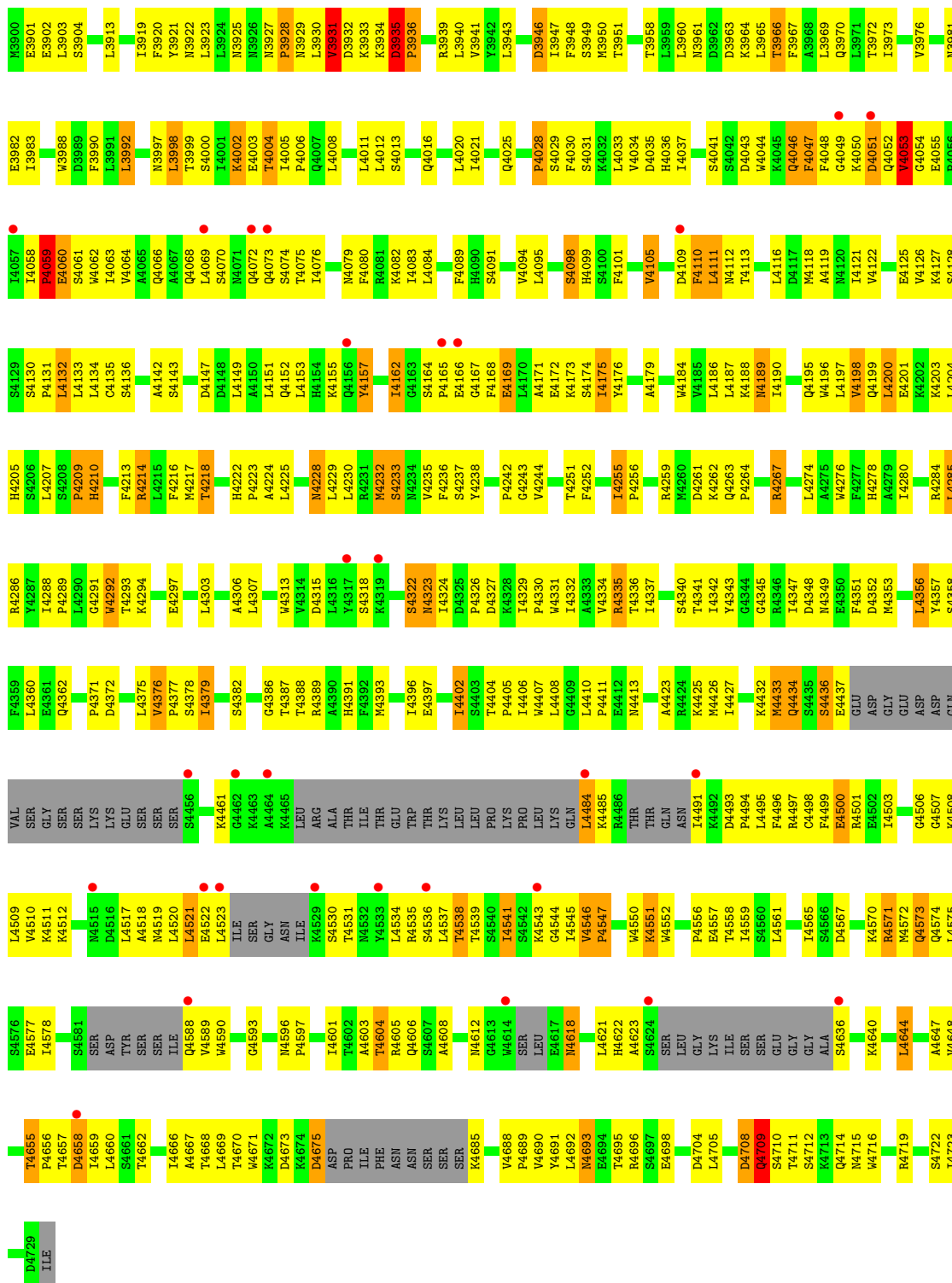




Q4017	D3935	K3860	S3779	L3719	K3647	K3554	V3360	K3290	ASN	M3147	I3069	I3001
K4018	P3936	E3861	R3750	V3720	H3648	N3555	K3561	K3291	L3216	M3148	C3070	V3004
V4019	N3937	T3862	T3781	Q3721			K3562		M3217	P3149	D3074	F3005
L4020	E3938	T3863	T3782	D3722			V3363	T3295	A3218	A3150	E3075	Q3007
I4021	R3939	E3864	F3783	V3723	S3651	R3559	V3364		I3219	P3151	R3076	Q3008
	L3940	I3865		E3724	E3656	L3564	D3365	Q3298	P3220	S3152	N3077	Q3009
V4027	V3943	A3866	V3788	ASN			L3366	V3299	S3221	F3154	V3078	
L4033	Y3942	L3867	T3789	ILE	E3660	L3567	GLU	K3300	H3223	H3155	E3080	L3013
V4034	N3943	T3868	P3790	ASP	N3661	L3568	LYS	D3301	S3222	F3154		
D4035	V3869	S3791	PRO	PRO			GLU	K3302	H3223	N3156		
H4036	I3947	E3870	S3792	VAL	M3664	R3571	ALA	Q3303	A3226	ARG		
I4037	F3948	E3871		ASN	L3665	V3574	THR	A3307	V3227	THR	F3083	L3014
Q4038	T3951	E3872	R3806	ASN	L3666	E3575	THR	Q3308	V3228	ALA	G3016	G3016
Q4039	T3874	E3873	P3807	PRO	K3667		GLY	K3309	Y3233	P3161	E3085	V3017
N4040	V3875	T3874	D3808	VAL	F3668	S3578	L3497	R3310	I3234	S3162	R3086	S3018
	K3876	K3877	T3809	LEU	N3669		R3498	R3311	I3234	A3163	K3088	G3019
D4043	K3877	K3878	H3810	ASN	V3670	F3581	E3500	E3312	T3237	L3164	T3089	K3022
K4044	K3878	K3879		LYS	V3671	N3582	V3501		I3238	R3167	L3090	S3023
K4045	I3879	S3814		ILE	L3672	T3583	E3502	V3315	Q3249	E3175	L3091	V3024
Q4046	D3815	D3816		ARG	L3673	Q3584	V3501	K3316	A3241	L3170	E3095	L3025
F4047	S3880	L3816		LYS	V3674	Q3585	E3502	R3317	N3242	D3171	R3026	R3026
F4048	V3881	L3817		LYS	D3676	S3586	Q3504	E3318	L3246	W3172	P3097	R3027
G4049	V3882	L3817		GLY	F3677	T3587	E3505	Q3319	L3246		G3097	V3028
K4050	K3883	K3818		GLY	S3677	V3588	N3506	A3320	Q3249		G3098	V3029
D4051	L3884	L3819		GLY	S3678		E3507	N3321	G3250	E3175	L3099	A3030
Q4052	L3885	Q3820		ARG		V3592	A3508	Q3322	G3250			W3031
V4053	Y3886	G3821		LEU	M3682	V3592	N3509		G3250	P3178	F3105	M3032
G4054	N3887	E3822		ILE	E3683	V3593	A3509	K3326	Q3252	E3179	T3106	
V3976	F3888	F3823		ILE	F3684		E3510	Q3327	Q3252	A3180	A3107	I3037
K3977	K3889	Q3824		ARG	S3596	S3596	L3511	R3327	N3253	K3181	L3108	Y3038
		K3825		LEU	A3597	A3597	K3512	V3328	Y3254	F3182	N3109	T3039
N3881	S3894	K3826		GLY	N3687	F3598	L3513	R3329	V3255	Q3183		
E3982	K3895	L3827		ASP	Q3688		K3514	D3330	T3256	V3184	K3113	K3041
I3983	V3896			GLN	A3689	Y3601	Q3515	Q3331	R3257	G3185	E3114	VAL
E3987	F3897	L3830		ASP	F3689	L3602	E3517	A3333	R3258	S3186	T3115	ASN
S4061	F3898	E3831		VAL	A3690	G3603	E3517	A3334	H3259	E3187	A3116	ASN
D3983	A3899			VAL	D3691	F3604	F3518	E3335	Y3260	F3188	Q3117	ASN
F3990	K3900	L3834		PHE	I3694	F3605	F3519	E3336	F3263	T3189	R3118	Y3046
D3992	E3901	L3835		SER	T3695	F3609	A3520	I3336	I3264		N3119	K3047
L3992	E3902	N3836		PRO	K3696	R3610	T3521	K3337	N3265	L3192	G3120	S3048
G3994	A3907	A3837			T3697		T3522	Q3338		L3192	L3121	S3049
G3995	K3907	L3838		M3761	S3698	V3624	T3523	A3341	V3268	L3194	I3122	D3050
D3996	L3908	Q3840		T3762	LEU		L3525	R3342	L3269	F3051	I3123	F3051
N3997	Y3909	A3841		F3763	ASP	F3628	E3526	Q3345	L3270	N3196	D3124	D3052
Q4072	F3911			L3764	SER	K3629	K3527	V3346	R3275	Q3198	S3125	D3054
S4074	S3912	I3845		F3765	SER	S3630	S3528	Q3347	D3276	Y3199	E3126	
	L3913	L3846		T3766	F3704	D3631	I3529	D3349	R3275	I3200	F3133	R3056
S4000	S4000	D3847		R3767	K3705	L3632	A3530	V3350	R3275	A3201		
I3919	I3919	D3848		D3768	K3706	S3633	T3531	V3350	E3279	P3202		
K4002	K4002	D3849		P3769	N3707	V3634	Y3532	V3351	E3280	P3203	V3137	L3059
E4003	N3926	S3850		T3770	L3708	P3635	Y3536	R3351	E3281	V3204	R3138	K3060
L4005	N3927	V3851		A3771		S3636	A3537	K3352	Q3282		R3139	R3061
F4006	P3928	L3852		F3772			T3538	K3353	L3283	Q3207	N3140	A3062
Q4007	S3929	T3854		T3773	E3714	P3641	L3539	E3354	H3284		L3141	G3063
	L3930	S3854		T3774	F3642	E3643	L3540	R3355	L3285		H3142	G3064
V4105	V3931	G3715		G3715	G3715	E3643	I3540	A3356	N3286	I3211	V3143	K3065
F4106	D3932	C3716		C3716	C3716	R3644		V3357	I3287	MEI	F3144	E3066
G4107	K3933	L3777		L3777	L3777	L3645	I3546	Q3358	T3288	GLY	F3145	G3067
E4108	K3934	C3778		C3778	L3718	N3646		K3359	L3289	ASN	T3146	K3068







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	204.26Å 221.81Å 192.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.45 – 2.81 96.45 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (96.45-2.81) 98.3 (96.45-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.82Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.262 , 0.319 0.263 , 0.319	Depositor DCC
R_{free} test set	10425 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	45284	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.62	1/23297 (0.0%)	1.06	132/31692 (0.4%)
1	B	0.60	2/22599 (0.0%)	1.05	135/30724 (0.4%)
All	All	0.61	3/45896 (0.0%)	1.06	267/62416 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2129	VAL	CA-CB	7.69	1.58	1.54
1	A	3862	THR	CA-CB	5.60	1.60	1.53
1	B	3109	MET	SD-CE	5.24	1.92	1.79

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2744	ASP	N-CA-C	11.20	123.49	111.28
1	A	4027	VAL	N-CA-C	8.68	116.15	107.55
1	A	2310	ALA	N-CA-C	-8.66	102.15	112.89
1	B	3030	ALA	N-CA-C	-8.44	102.16	111.36
1	B	4436	SER	N-CA-C	-8.43	102.93	113.55
1	A	2609	THR	N-CA-C	-8.38	102.10	111.07
1	B	3605	PHE	N-CA-C	8.37	121.90	110.35
1	B	2042	GLN	N-CA-C	-8.24	102.38	111.36
1	A	4496	PHE	N-CA-C	-8.06	102.49	111.28
1	A	3767	ARG	N-CA-C	-7.99	101.11	113.02
1	A	2354	ILE	N-CA-C	7.85	119.16	108.17
1	A	4681	ASN	N-CA-C	-7.83	103.80	112.72
1	B	3109	MET	N-CA-C	-7.81	105.71	114.62
1	B	2775	THR	N-CA-C	7.79	122.21	112.87
1	B	2354	ILE	N-CA-C	7.78	119.06	108.17
1	B	2938	PHE	CA-C-N	7.74	128.44	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2938	PHE	C-N-CA	7.74	128.44	119.47
1	A	3846	LEU	N-CA-C	7.64	122.04	112.87
1	A	2016	LEU	N-CA-C	-7.64	103.03	111.36
1	B	1695	ALA	N-CA-C	7.62	120.47	111.71
1	B	2691	PHE	CA-C-N	7.60	129.34	119.84
1	B	2691	PHE	C-N-CA	7.60	129.34	119.84
1	A	3605	PHE	N-CA-C	7.60	119.76	110.41
1	B	4127	LYS	N-CA-C	-7.57	99.91	110.35
1	A	3909	TYR	N-CA-C	7.44	120.03	110.65
1	A	4655	THR	CA-C-N	7.44	129.13	119.84
1	A	4655	THR	C-N-CA	7.44	129.13	119.84
1	B	4589	VAL	N-CA-C	7.38	118.92	108.36
1	A	1626	ASN	N-CA-C	-7.37	103.19	111.07
1	B	3331	GLN	N-CA-C	-7.33	101.78	111.24
1	B	2439	PHE	N-CA-C	-7.33	103.29	111.28
1	A	2966	SER	N-CA-C	7.31	119.24	111.28
1	B	1565	LEU	N-CA-C	-7.30	105.23	112.97
1	B	3051	PHE	N-CA-C	7.22	119.05	111.03
1	A	3151	SER	CA-C-N	7.21	126.73	119.24
1	A	3151	SER	C-N-CA	7.21	126.73	119.24
1	B	3351	ARG	N-CA-C	-7.18	102.56	111.75
1	A	2653	THR	N-CA-C	7.15	118.77	110.97
1	B	3588	VAL	N-CA-C	7.11	117.21	110.53
1	B	1564	LYS	N-CA-C	-7.02	104.19	112.89
1	B	4055	GLU	CA-C-N	-7.01	112.77	119.85
1	B	4055	GLU	C-N-CA	-7.01	112.77	119.85
1	A	3708	LEU	N-CA-C	-7.00	103.58	111.07
1	A	2285	SER	N-CA-C	6.94	118.54	110.97
1	A	3873	GLU	N-CA-C	-6.92	103.82	111.36
1	A	2834	ALA	N-CA-C	-6.90	104.86	113.55
1	B	4712	SER	N-CA-C	6.86	119.38	110.53
1	A	4261	ASP	N-CA-C	6.77	121.25	113.19
1	B	4292	TRP	N-CA-C	-6.76	98.89	108.96
1	B	4658	ASP	N-CA-C	-6.76	103.41	112.94
1	B	3848	ASP	N-CA-C	6.69	119.14	111.11
1	B	1845	LEU	N-CA-C	-6.61	104.16	111.36
1	A	2638	THR	N-CA-C	6.61	119.08	111.02
1	A	2488	ILE	CA-C-N	-6.59	113.88	120.21
1	A	2488	ILE	C-N-CA	-6.59	113.88	120.21
1	B	2647	VAL	N-CA-C	6.58	116.35	106.42
1	A	3831	GLU	N-CA-C	-6.56	104.05	111.14
1	B	1995	VAL	N-CA-C	6.54	117.25	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3332	GLN	N-CA-C	-6.53	104.24	111.82
1	B	2412	GLY	N-CA-C	-6.53	102.52	112.51
1	B	4719	ARG	N-CA-C	-6.52	105.15	113.23
1	B	3919	ILE	N-CA-C	-6.51	104.17	110.42
1	A	4573	GLN	N-CA-C	-6.47	104.15	111.14
1	A	4169	GLU	N-CA-C	6.44	119.26	111.40
1	B	1561	LEU	N-CA-C	-6.43	102.94	111.24
1	A	2941	VAL	N-CA-C	6.43	117.84	108.58
1	B	2186	ILE	N-CA-C	-6.43	106.03	111.56
1	B	2242	GLU	N-CA-C	-6.36	104.42	111.36
1	A	3851	VAL	N-CA-C	-6.36	104.84	111.58
1	A	4414	ALA	N-CA-C	-6.35	104.46	111.82
1	B	3580	ASN	N-CA-C	6.29	117.82	110.97
1	B	4054	GLY	N-CA-C	-6.28	98.30	113.18
1	A	4680	ASN	N-CA-C	-6.27	107.47	114.62
1	B	2548	VAL	N-CA-C	-6.27	105.03	110.74
1	A	3875	VAL	N-CA-C	-6.25	104.95	111.58
1	B	3767	ARG	N-CA-C	-6.23	105.62	113.72
1	A	1980	LYS	N-CA-C	6.23	117.76	110.97
1	B	2368	ASN	N-CA-C	6.22	117.73	111.07
1	B	3049	SER	N-CA-C	-6.22	106.01	113.97
1	A	3601	TYR	N-CA-C	6.21	121.19	112.93
1	A	1810	TYR	CA-C-N	6.21	126.16	119.76
1	A	1810	TYR	C-N-CA	6.21	126.16	119.76
1	B	2000	CYS	N-CA-C	6.18	118.09	111.36
1	B	4655	THR	CA-C-N	6.17	126.13	119.78
1	B	4655	THR	C-N-CA	6.17	126.13	119.78
1	B	3670	ARG	N-CA-C	-6.16	102.40	110.53
1	B	1668	THR	N-CA-C	-6.15	104.50	111.14
1	A	2813	ILE	N-CA-C	6.13	116.75	108.17
1	B	3730	LEU	N-CA-C	-6.13	107.03	114.75
1	A	3765	PHE	N-CA-C	6.12	119.46	109.06
1	A	4358	SER	N-CA-C	-6.11	104.53	111.07
1	A	2811	ALA	CA-C-N	-6.10	113.66	119.76
1	A	2811	ALA	C-N-CA	-6.10	113.66	119.76
1	A	4168	PHE	N-CA-C	6.08	117.90	111.28
1	B	3899	ALA	N-CA-C	-6.05	104.76	111.36
1	B	3597	ALA	N-CA-C	-6.05	104.61	112.23
1	B	3674	VAL	N-CA-C	6.04	117.28	108.58
1	B	1756	LYS	CA-C-N	6.03	127.37	119.84
1	B	1756	LYS	C-N-CA	6.03	127.37	119.84
1	A	1868	SER	N-CA-C	6.02	118.07	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2003	GLY	N-CA-C	-6.02	101.58	110.97
1	B	4402	ILE	N-CA-C	6.00	116.00	106.88
1	A	1497	LEU	N-CA-C	5.96	118.16	108.26
1	B	1939	GLU	N-CA-C	-5.95	100.30	109.76
1	B	4198	VAL	N-CA-C	-5.95	104.04	110.23
1	B	2608	ASN	N-CA-C	-5.94	105.12	113.20
1	A	2370	LEU	N-CA-C	-5.94	106.00	113.72
1	B	3076	SER	N-CA-C	-5.94	105.53	112.89
1	B	3309	LYS	N-CA-C	-5.94	104.94	111.82
1	A	1541	LEU	N-CA-C	5.92	119.40	110.64
1	B	2767	VAL	N-CA-C	5.91	117.44	111.00
1	B	2986	VAL	CA-C-N	5.91	126.83	119.98
1	B	2986	VAL	C-N-CA	5.91	126.83	119.98
1	A	2896	CYS	N-CA-C	5.90	119.10	108.48
1	A	2507	GLU	CA-C-N	5.90	127.21	119.84
1	A	2507	GLU	C-N-CA	5.90	127.21	119.84
1	B	1648	LYS	N-CA-C	-5.89	106.22	113.41
1	A	2376	LEU	N-CA-C	5.89	118.50	108.02
1	A	4719	ARG	N-CA-C	-5.88	104.82	112.23
1	B	4501	ARG	N-CA-C	-5.88	104.95	111.71
1	A	3520	ALA	N-CA-C	-5.87	104.30	112.45
1	A	3674	VAL	N-CA-C	5.87	117.20	108.23
1	A	1945	GLU	N-CA-C	5.86	118.61	109.52
1	B	4210	HIS	CA-C-N	5.86	126.26	119.47
1	B	4210	HIS	C-N-CA	5.86	126.26	119.47
1	B	3836	ASN	N-CA-C	-5.84	104.99	111.36
1	B	4255	ILE	CA-C-N	5.83	125.74	119.85
1	B	4255	ILE	C-N-CA	5.83	125.74	119.85
1	B	3913	LEU	N-CA-C	-5.82	105.01	111.36
1	B	1737	GLU	N-CA-C	-5.82	105.94	113.16
1	A	4352	ASP	N-CA-C	-5.80	104.92	112.23
1	B	3765	PHE	N-CA-C	5.80	118.52	109.52
1	B	3863	THR	N-CA-C	-5.80	106.20	113.28
1	B	2564	ASN	N-CA-C	5.80	117.47	111.03
1	B	2558	PHE	CA-C-N	5.79	127.08	119.84
1	B	2558	PHE	C-N-CA	5.79	127.08	119.84
1	B	3788	VAL	N-CA-C	5.79	117.05	109.58
1	B	3759	SER	N-CA-C	-5.77	106.28	113.15
1	A	2129	VAL	CA-C-N	-5.77	113.08	119.19
1	A	2129	VAL	C-N-CA	-5.77	113.08	119.19
1	A	4222	HIS	CA-C-N	5.77	127.05	119.84
1	A	4222	HIS	C-N-CA	5.77	127.05	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2437	GLU	CA-C-N	5.76	127.04	119.84
1	B	2437	GLU	C-N-CA	5.76	127.04	119.84
1	A	2602	ILE	N-CA-C	-5.73	107.19	113.43
1	B	3824	GLN	N-CA-C	-5.72	106.34	113.38
1	A	2605	VAL	CA-C-N	5.71	126.98	119.84
1	A	2605	VAL	C-N-CA	5.71	126.98	119.84
1	A	2593	PHE	N-CA-C	-5.71	105.20	111.82
1	B	3860	LYS	N-CA-C	-5.71	104.98	111.14
1	A	3766	THR	N-CA-C	-5.70	100.74	109.41
1	A	3342	ARG	N-CA-C	-5.69	104.69	111.69
1	A	1894	LYS	N-CA-C	-5.69	106.11	113.16
1	A	1810	TYR	N-CA-C	5.68	117.42	108.55
1	B	3882	VAL	N-CA-C	5.68	117.09	110.62
1	A	2687	THR	N-CA-C	-5.67	105.09	112.23
1	A	3307	ALA	N-CA-C	-5.67	105.09	112.23
1	B	2925	TRP	N-CA-C	-5.67	105.01	111.07
1	A	2574	LEU	N-CA-C	-5.65	105.27	111.82
1	A	4375	LEU	N-CA-C	-5.64	105.50	112.72
1	A	2620	ASP	N-CA-C	5.60	117.25	111.03
1	B	1971	ASN	N-CA-C	5.59	118.78	108.94
1	A	2368	ASN	N-CA-C	5.59	117.83	111.02
1	B	3946	ASP	N-CA-C	5.58	118.90	111.75
1	B	2360	ASP	CA-C-N	5.58	125.94	119.47
1	B	2360	ASP	C-N-CA	5.58	125.94	119.47
1	B	4358	SER	N-CA-C	-5.58	105.29	111.71
1	B	2305	VAL	N-CA-C	5.57	116.33	108.36
1	B	1653	ALA	CA-C-N	5.56	125.26	119.64
1	B	1653	ALA	C-N-CA	5.56	125.26	119.64
1	A	2275	VAL	N-CA-C	5.56	117.82	108.81
1	A	3287	ILE	N-CA-C	-5.54	103.91	111.89
1	B	3935	ASP	CA-C-N	5.54	126.77	119.84
1	B	3935	ASP	C-N-CA	5.54	126.77	119.84
1	B	2746	ILE	CB-CA-C	-5.54	104.89	111.81
1	B	2955	TRP	N-CA-C	5.54	120.31	113.50
1	B	4049	GLY	N-CA-C	5.54	117.84	111.36
1	A	3675	ILE	CB-CA-C	-5.54	105.93	111.80
1	A	2906	ALA	N-CA-C	5.53	117.39	111.36
1	A	3983	ILE	N-CA-C	5.53	116.14	108.84
1	A	3330	ASP	N-CA-C	-5.53	107.79	114.75
1	A	3050	ASP	N-CA-C	-5.51	104.79	112.45
1	A	3107	ALA	N-CA-C	-5.50	106.25	113.12
1	A	3818	LYS	N-CA-C	-5.49	106.08	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4376	VAL	CA-C-N	5.49	126.70	119.84
1	B	4376	VAL	C-N-CA	5.49	126.70	119.84
1	A	2030	ARG	N-CA-C	-5.49	103.05	110.68
1	A	2048	VAL	N-CA-C	-5.48	104.10	111.44
1	B	3131	LYS	N-CA-C	-5.47	105.40	111.36
1	B	1556	ARG	N-CA-C	5.46	118.31	108.48
1	B	2401	LYS	N-CA-C	5.46	117.66	111.11
1	B	2983	GLU	N-CA-C	5.45	122.41	110.80
1	A	1482	LYS	N-CA-C	-5.43	105.26	111.07
1	A	3167	ARG	N-CA-C	-5.43	107.20	113.88
1	B	1716	ILE	N-CA-C	-5.42	105.56	110.82
1	B	3781	VAL	N-CA-C	5.42	117.90	108.95
1	B	3047	LYS	N-CA-C	5.40	118.47	110.48
1	B	4244	VAL	N-CA-C	-5.39	105.12	111.00
1	A	4605	ARG	N-CA-C	-5.39	105.10	110.97
1	A	1538	TRP	N-CA-C	5.38	118.06	111.82
1	A	4457	SER	N-CA-C	5.37	116.82	111.07
1	B	4322	SER	N-CA-C	-5.37	105.50	111.36
1	A	3878	GLU	N-CA-C	-5.37	104.67	111.11
1	A	2829	GLY	N-CA-C	-5.36	106.01	112.49
1	B	4695	THR	N-CA-C	-5.35	106.59	113.01
1	A	4657	THR	N-CA-C	5.34	116.39	108.60
1	A	3716	CYS	CA-C-N	5.30	125.24	119.78
1	A	3716	CYS	C-N-CA	5.30	125.24	119.78
1	B	2999	LEU	N-CA-C	-5.30	106.14	113.18
1	A	1902	LYS	N-CA-C	5.28	120.37	113.30
1	A	3938	GLU	N-CA-C	-5.28	105.66	112.68
1	A	2761	THR	N-CA-C	-5.26	105.71	111.82
1	B	4345	GLY	N-CA-C	-5.26	106.41	112.83
1	A	4225	LEU	CA-C-N	-5.26	114.56	120.14
1	A	4225	LEU	C-N-CA	-5.26	114.56	120.14
1	B	4285	LEU	N-CA-C	-5.26	105.61	112.23
1	A	3052	ASP	N-CA-C	-5.25	105.73	111.82
1	A	2873	ILE	N-CA-C	-5.25	101.07	109.20
1	B	2113	LEU	N-CA-C	-5.23	105.66	111.36
1	A	3310	ASN	N-CA-C	-5.22	105.76	111.82
1	B	3879	ILE	N-CA-C	-5.22	105.52	110.42
1	B	2088	PRO	N-CA-C	-5.21	103.09	111.38
1	A	4664	ILE	N-CA-C	-5.20	100.89	108.17
1	A	2671	ILE	N-CA-C	5.19	115.38	108.11
1	B	2640	LYS	N-CA-C	-5.19	106.53	112.92
1	B	3136	GLN	N-CA-C	-5.18	104.56	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3631	ASP	N-CA-C	-5.18	106.71	112.57
1	A	4554	SER	N-CA-C	5.18	118.06	109.46
1	B	4243	GLY	N-CA-C	5.17	118.50	111.72
1	A	2101	ILE	N-CA-C	5.17	116.26	111.81
1	A	3830	LEU	N-CA-C	-5.17	106.23	112.54
1	A	4181	SER	N-CA-C	-5.17	104.91	111.11
1	A	2499	ALA	N-CA-C	-5.17	104.91	111.11
1	A	2412	GLY	N-CA-C	-5.17	105.48	112.14
1	A	1416	GLU	N-CA-C	5.15	117.63	111.71
1	A	2898	LEU	N-CA-C	-5.14	107.03	113.15
1	A	1587	GLU	N-CA-C	-5.14	105.13	111.40
1	A	3290	LYS	N-CA-C	-5.13	105.33	111.03
1	B	3503	GLN	N-CA-C	-5.13	106.11	112.93
1	A	4049	GLY	N-CA-C	5.13	121.72	112.54
1	A	4666	ILE	N-CA-C	5.11	113.94	107.70
1	B	2630	LYS	N-CA-C	5.11	118.40	110.17
1	A	3161	SER	CA-C-N	5.09	126.20	119.84
1	A	3161	SER	C-N-CA	5.09	126.20	119.84
1	A	3884	ALA	N-CA-C	-5.09	107.20	113.41
1	A	2994	VAL	N-CA-C	-5.08	105.44	110.62
1	B	2718	CYS	N-CA-C	5.07	117.57	109.81
1	B	3676	ASP	CA-C-N	5.07	124.68	119.05
1	B	3676	ASP	C-N-CA	5.07	124.68	119.05
1	A	2110	GLN	N-CA-C	5.07	116.50	111.07
1	A	4564	TRP	N-CA-C	-5.07	105.64	111.07
1	B	3258	ARG	N-CA-C	-5.06	105.85	112.23
1	B	2294	GLU	N-CA-C	-5.06	105.47	111.69
1	B	2838	LEU	N-CA-C	-5.06	107.06	113.18
1	B	3093	GLY	N-CA-C	5.06	125.17	113.18
1	A	3207	GLN	N-CA-C	-5.05	105.46	110.97
1	A	3502	GLU	N-CA-C	-5.05	105.77	111.28
1	B	2571	ASN	N-CA-C	-5.05	105.48	111.69
1	B	4110	PHE	N-CA-C	-5.05	103.81	111.34
1	A	2557	ASP	N-CA-C	-5.04	106.65	112.89
1	B	2139	LEU	N-CA-C	-5.04	102.31	110.32
1	A	2614	ASP	N-CA-C	5.03	119.05	113.01
1	B	3604	PHE	N-CA-C	5.03	116.76	111.28
1	B	3110	HIS	N-CA-C	-5.02	105.88	111.36
1	A	2767	VAL	N-CA-C	5.02	115.24	110.42
1	B	3270	LEU	N-CA-C	5.02	117.49	111.71
1	B	3103	GLU	N-CA-C	-5.00	105.54	111.69

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	22821	0	21998	1468	0
1	B	22146	0	21438	1492	0
2	A	108	0	48	14	0
2	B	108	0	48	9	0
3	A	28	0	52	2	0
3	B	28	0	52	5	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	0	1	0
5	B	19	0	0	1	0
All	All	45284	0	43636	2954	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 33.

All (2954) 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:3330:ASP:HB3	1:A:3532:TYR:HE2	1.12	1.12
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.31	1.12
1:A:3766:THR:HG22	1:A:3768:ASP:H	1.14	1.09
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.20	1.06
1:B:1655:LEU:H	1:B:1655:LEU:HD22	1.20	1.05
1:A:2000:CYS:HB3	1:A:2031:LEU:HD13	1.34	1.04
1:A:2641:VAL:HG12	1:A:2642:ALA:H	1.14	1.04
1:B:3700:LEU:HD13	1:B:3701:ASP:N	1.72	1.03
1:B:2129:VAL:HG22	1:B:2130:PRO:HD3	1.38	1.03
1:B:4136:SER:HB3	1:B:4238:TYR:HB2	1.40	1.03
1:B:4318:SER:HB3	1:B:4324:ILE:HD11	1.38	1.02
1:B:2381:ASN:HD21	1:B:2383:GLU:HB2	1.17	1.01
1:B:2603:THR:HG22	1:B:2604:PRO:HD2	1.41	1.01
1:A:2688:LEU:HD13	1:A:2696:VAL:HG11	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2011:ARG:HB3	1:A:2011:ARG:HH11	1.27	0.99
1:B:4091:SER:H	3:B:9022:SPM:H132	1.25	0.99
1:A:3571:ARG:NH1	1:A:3571:ARG:HB3	1.78	0.99
1:B:4013:SER:H	1:B:4016:GLN:HE21	1.07	0.98
1:B:1653:ALA:HB1	1:B:1655:LEU:HD23	1.43	0.98
1:B:1813:GLN:HE22	1:B:1941:LEU:H	0.99	0.98
1:B:4222:HIS:CD2	1:B:4224:ALA:H	1.81	0.98
1:B:2582:GLY:HA2	1:B:2585:MET:HE3	1.45	0.97
1:A:4349:ASN:ND2	1:A:4352:ASP:H	1.62	0.97
1:A:3817:LEU:HA	1:A:3820:GLN:HE21	1.26	0.97
1:B:2746:ILE:O	1:B:2749:PRO:HD2	1.64	0.97
1:B:3139:ARG:HG3	1:B:3139:ARG:HH11	1.30	0.97
1:B:1886:ARG:HH11	1:B:1890:ARG:NH1	1.61	0.97
1:B:4222:HIS:HD2	1:B:4224:ALA:H	0.97	0.96
1:A:3109:MET:SD	1:A:3126:GLU:HG2	2.05	0.96
1:B:1640:ASN:HD21	1:B:1644:ILE:HD11	1.31	0.95
1:B:4618:ASN:H	1:B:4618:ASN:HD22	1.11	0.95
1:A:4349:ASN:HD22	1:A:4352:ASP:H	0.98	0.94
1:A:2370:LEU:HD21	1:A:2387:LEU:HB2	1.50	0.94
1:B:4322:SER:C	1:B:4323:ASN:HD22	1.75	0.94
1:A:1555:VAL:H	1:A:1609:GLN:HE22	1.16	0.94
1:A:1477:LYS:H	1:A:1480:HIS:HD2	0.94	0.94
1:A:4188:LYS:HA	1:A:4218:THR:HG22	1.47	0.93
1:B:4164:SER:HB3	1:B:4165:PRO:HD2	1.50	0.93
1:A:1477:LYS:H	1:A:1480:HIS:CD2	1.86	0.93
1:B:1605:TRP:HH2	1:B:1650:VAL:HG21	1.35	0.92
1:B:2000:CYS:HB3	1:B:2031:LEU:HD13	1.51	0.92
1:A:3330:ASP:HB3	1:A:3532:TYR:CE2	2.05	0.92
1:B:2515:VAL:HG11	1:B:2577:LEU:HD13	1.52	0.92
1:B:3965:LEU:HD23	1:B:4426:MET:HE1	1.52	0.91
1:B:4484:LEU:HD21	1:B:4496:PHE:CE1	2.06	0.91
1:A:1859:LEU:HB3	1:A:1879:ILE:HD11	1.51	0.91
1:B:3724:GLU:OE2	1:B:3766:THR:HG23	1.70	0.91
1:A:1813:GLN:HE22	1:A:1941:LEU:H	1.17	0.91
1:B:4618:ASN:H	1:B:4618:ASN:ND2	1.69	0.91
1:A:3806:ARG:HG3	1:A:3882:VAL:HG11	1.52	0.91
1:B:3043:ASN:ND2	1:B:3046:TYR:HB2	1.84	0.90
1:B:4693:ASN:HD22	1:B:4693:ASN:H	1.19	0.90
1:A:1415:LYS:O	1:A:1498:THR:HB	1.70	0.90
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.52	0.90
1:B:4709:GLN:HE21	1:B:4709:GLN:N	1.67	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1560:ASP:HA	1:B:1563:ASN:HB2	1.53	0.90
1:A:1611:ARG:HD3	1:A:1680:GLN:OE1	1.71	0.89
1:B:4657:THR:HG22	1:B:4658:ASP:H	1.35	0.89
1:A:2641:VAL:CG1	1:A:2642:ALA:H	1.86	0.89
1:B:1813:GLN:NE2	1:B:1941:LEU:H	1.69	0.89
1:B:4709:GLN:HE21	1:B:4709:GLN:H	0.89	0.89
1:A:2247:ARG:HH22	1:A:2287:GLU:HB3	1.37	0.89
1:B:4251:THR:HG23	1:B:4303:LEU:HD21	1.54	0.89
1:A:3935:ASP:OD1	1:A:3936:PRO:HD2	1.72	0.88
1:A:2059:LEU:HG	1:A:2060:LEU:HD12	1.55	0.88
1:A:3936:PRO:HG2	1:A:3937:ASN:H	1.38	0.88
1:B:3105:PHE:O	1:B:3109:MET:HG3	1.74	0.88
1:B:1740:THR:HB	1:B:1759:SER:HA	1.56	0.88
1:A:3673:LEU:HD13	1:A:3783:PHE:CE1	2.08	0.88
1:A:2044:GLN:NE2	1:A:2090:ASN:HB2	1.88	0.88
1:B:3785:ASN:HD21	1:B:3787:THR:HG23	1.39	0.88
1:A:4210:HIS:ND1	1:A:4211:PRO:HD2	1.89	0.87
1:B:3512:LYS:HA	1:B:3515:GLN:HE21	1.37	0.87
1:A:2582:GLY:HA2	1:A:2585:MET:HE3	1.55	0.87
1:A:3636:SER:HA	1:A:3644:ARG:NH2	1.88	0.87
1:A:1547:ASN:HA	1:A:1553:LYS:HG2	1.57	0.87
1:A:4210:HIS:HD1	1:A:4211:PRO:HD2	1.40	0.87
1:A:3661:ASN:HA	1:A:3664:MET:HE3	1.54	0.86
1:B:1831:LEU:HD21	1:B:1892:LEU:HD23	1.57	0.86
1:A:1573:SER:HA	1:A:1576:LYS:HE2	1.57	0.86
1:B:4604:THR:HG23	1:B:4671:TRP:HE1	1.38	0.86
1:B:2638:THR:HG21	1:B:2838:LEU:HD21	1.56	0.85
1:B:3970:GLN:HE22	1:B:4433:MET:HE2	1.39	0.85
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.57	0.85
1:B:2841:ASN:HD22	1:B:2841:ASN:H	1.25	0.85
1:A:3139:ARG:HH11	1:A:3139:ARG:HG3	1.42	0.85
1:A:3007:GLN:NE2	1:A:3008:PRO:HD2	1.92	0.84
1:B:1562:PHE:HA	1:B:1565:LEU:HB3	1.59	0.84
1:B:3700:LEU:HD13	1:B:3701:ASP:H	1.39	0.84
1:A:2405:LEU:HA	1:A:2408:ILE:HD11	1.58	0.84
1:A:3362:ALA:HB1	1:A:3497:LEU:HD11	1.59	0.84
1:A:3074:ASP:H	1:A:3077:ASN:ND2	1.74	0.84
1:A:2162:ILE:HD13	1:A:2197:ASN:HD22	1.40	0.83
1:A:2274:MET:HE1	1:A:2286:TRP:HB3	1.59	0.83
1:A:2929:LYS:O	1:A:2933:VAL:HG23	1.76	0.83
1:A:3317:ASN:HB2	1:A:3546:ILE:HG21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3043:ASN:HD22	1:B:3046:TYR:HB2	1.40	0.83
1:B:4189:ASN:H	1:B:4218:THR:HG22	1.43	0.83
1:A:3864:GLU:HG3	1:A:3865:ILE:N	1.94	0.83
1:B:4111:LEU:H	1:B:4111:LEU:HD12	1.43	0.83
1:B:4709:GLN:H	1:B:4709:GLN:NE2	1.74	0.83
1:B:2938:PHE:O	1:B:2941:VAL:HG12	1.78	0.83
1:B:3139:ARG:HG3	1:B:3139:ARG:NH1	1.89	0.83
1:B:2598:GLN:HG3	1:B:2612:LEU:HB2	1.60	0.83
1:B:3708:LEU:HD21	1:B:3730:LEU:HD21	1.60	0.83
1:B:3729:VAL:O	1:B:3729:VAL:HG22	1.77	0.82
1:A:4193:ALA:HB1	1:A:4196:TRP:HB3	1.61	0.82
1:A:2381:ASN:HD21	1:A:2383:GLU:HB2	1.44	0.82
1:A:3673:LEU:HD13	1:A:3783:PHE:HE1	1.44	0.82
1:B:3766:THR:HG22	1:B:3768:ASP:H	1.43	0.82
1:B:2233:MET:HA	1:B:2233:MET:HE3	1.60	0.82
1:A:2439:PHE:H	1:A:2495:GLN:HE22	1.24	0.82
1:A:4636:SER:HB3	1:A:4669:LEU:O	1.79	0.82
1:B:4640:LYS:HB3	1:B:4666:ILE:HD12	1.60	0.82
1:A:1690:GLN:HE22	1:A:1766:ILE:HG21	1.42	0.82
1:A:2286:TRP:O	1:A:2290:LEU:HB2	1.79	0.82
1:A:2142:GLN:N	1:A:2142:GLN:HE21	1.77	0.81
1:B:3256:THR:H	1:B:3259:HIS:CD2	1.98	0.81
1:B:3990:PHE:HD2	1:B:4084:LEU:HD22	1.45	0.81
1:B:1555:VAL:HG22	1:B:1609:GLN:HE21	1.44	0.81
1:B:2112:MET:O	1:B:2116:GLN:HG2	1.80	0.81
1:B:4119:ALA:HA	1:B:4149:LEU:HD11	1.62	0.81
1:A:3200:ILE:O	1:A:3202:PRO:HD3	1.80	0.81
1:B:1655:LEU:H	1:B:1655:LEU:CD2	1.92	0.81
1:A:3024:VAL:HG23	2:A:9004:ADP:O2A	1.79	0.81
1:A:3670:ARG:HD2	5:A:38:HOH:O	1.80	0.81
1:B:2375:LYS:HB3	1:B:2387:LEU:HB3	1.60	0.81
1:A:3665:LEU:HD13	1:A:3685:LEU:HD21	1.60	0.81
1:B:4604:THR:CG2	1:B:4671:TRP:HE1	1.94	0.81
1:B:2498:CYS:HA	1:B:2501:ILE:HD12	1.62	0.81
1:A:2552:ASN:ND2	1:A:2560:MET:H	1.78	0.81
1:B:2657:VAL:HG13	1:B:2687:THR:HG23	1.62	0.81
1:A:4349:ASN:ND2	1:A:4351:PHE:H	1.79	0.80
1:B:3126:GLU:O	1:B:3129:LEU:HB3	1.82	0.80
1:A:1477:LYS:N	1:A:1480:HIS:HD2	1.79	0.80
1:A:1813:GLN:NE2	1:A:1941:LEU:H	1.80	0.80
1:B:3686:MET:HE1	1:B:3696:LYS:HB2	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2552:ASN:HD21	1:A:2560:MET:H	1.25	0.80
1:B:2533:VAL:HB	1:B:2581:LEU:HD22	1.62	0.80
1:A:1766:ILE:HG23	1:A:1767:HIS:H	1.47	0.80
1:A:2391:VAL:O	1:A:2392:ARG:HD2	1.82	0.80
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	1.95	0.80
1:B:3130:TYR:O	1:B:3134:THR:HG23	1.81	0.80
1:B:3972:THR:HG23	1:B:4105:VAL:HG21	1.63	0.79
1:B:1739:THR:O	1:B:1760:ILE:HG12	1.82	0.79
1:B:3355:ILE:HD12	1:B:3511:LEU:HD22	1.64	0.79
1:B:4013:SER:H	1:B:4016:GLN:NE2	1.79	0.79
1:A:4109:ASP:HA	1:A:4112:ASN:ND2	1.97	0.79
1:B:3017:VAL:HG23	1:B:3174:GLY:O	1.82	0.79
1:B:3930:LEU:HD11	1:B:3943:LEU:HD21	1.65	0.79
1:B:4574:GLN:HE22	1:B:4590:TRP:H	1.30	0.79
1:A:3352:ASN:ND2	1:A:3515:GLN:OE1	2.15	0.79
1:B:1553:LYS:O	1:B:1647:LEU:HD13	1.82	0.79
1:B:3139:ARG:HH11	1:B:3139:ARG:CG	1.96	0.79
1:B:3903:LEU:HD23	1:B:4433:MET:HE1	1.64	0.79
1:B:3785:ASN:ND2	1:B:3787:THR:HG23	1.97	0.79
1:B:1735:ASP:OD2	1:B:1740:THR:HG23	1.84	0.78
1:B:3947:ILE:HG13	1:B:3948:PHE:H	1.45	0.78
1:A:3929:ASN:ND2	1:A:3942:TYR:HD1	1.81	0.78
1:B:4484:LEU:HD23	1:B:4484:LEU:C	2.09	0.78
1:B:2379:LEU:HD12	1:B:2383:GLU:HG2	1.64	0.78
1:A:2312:THR:OG1	1:A:2315:GLN:HG3	1.83	0.78
1:B:2706:THR:HA	1:B:2759:VAL:HG22	1.65	0.78
1:B:2835:LEU:HD11	1:B:2890:ILE:HD12	1.65	0.78
1:B:1813:GLN:HE22	1:B:1941:LEU:N	1.81	0.78
1:A:2684:LEU:HD22	1:A:2789:VAL:HG11	1.64	0.78
1:B:1886:ARG:NH1	1:B:1890:ARG:NH1	2.30	0.78
1:B:3768:ASP:HB3	1:B:3771:ALA:HB2	1.64	0.78
1:A:2044:GLN:O	1:A:2048:VAL:HG23	1.83	0.78
1:B:1851:THR:O	1:B:1854:MET:HB3	1.84	0.78
1:A:4306:ALA:O	1:A:4310:ILE:HG12	1.83	0.78
1:A:3281:GLU:HB3	1:A:3581:PHE:HE1	1.48	0.77
1:B:1556:ARG:HD2	1:B:1556:ARG:O	1.84	0.77
1:A:2526:MET:HE1	1:A:2803:LEU:HD12	1.66	0.77
1:A:2641:VAL:HG12	1:A:2642:ALA:N	1.94	0.77
1:B:4690:VAL:HG22	1:B:4723:ILE:HB	1.67	0.77
1:A:3075:GLU:O	1:A:3078:VAL:HG12	1.84	0.77
1:B:4020:LEU:HG	1:B:4034:VAL:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2836:MET:HE1	1:B:2839:LEU:HD12	1.67	0.77
1:A:3074:ASP:H	1:A:3077:ASN:HD22	1.31	0.77
1:A:1465:ASN:HA	1:A:1468:ILE:HD12	1.67	0.77
1:A:1842:GLN:OE1	1:A:1842:GLN:HA	1.85	0.77
1:A:3817:LEU:HA	1:A:3820:GLN:NE2	2.00	0.77
1:B:2238:LYS:HA	1:B:2241:GLN:HE21	1.50	0.77
1:B:3966:THR:HG22	1:B:4426:MET:HG3	1.66	0.77
1:B:3074:ASP:O	1:B:3077:ASN:HB2	1.85	0.76
1:A:3326:GLN:O	1:A:3330:ASP:HB2	1.84	0.76
1:A:4605:ARG:O	1:A:4609:SER:HB3	1.85	0.76
1:B:4188:LYS:HA	1:B:4218:THR:HG22	1.65	0.76
1:A:1797:VAL:HG12	1:A:1854:MET:HE1	1.68	0.76
1:A:1875:PHE:O	1:A:1879:ILE:HG12	1.86	0.76
1:B:1565:LEU:HD23	1:B:1565:LEU:O	1.85	0.76
1:B:2745:GLU:HG3	1:B:2748:LEU:HG	1.66	0.76
1:B:4484:LEU:HD21	1:B:4496:PHE:HE1	1.46	0.76
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.48	0.76
1:B:2144:HIS:HB2	1:B:2413:MET:HE3	1.64	0.76
1:B:2937:HIS:C	1:B:2939:PRO:HD3	2.11	0.76
1:B:1863:VAL:HG22	1:B:1872:ARG:HH11	1.49	0.76
1:A:2011:ARG:HB3	1:A:2011:ARG:NH1	2.00	0.75
1:A:2266:LEU:HD22	1:A:2392:ARG:HG2	1.67	0.75
1:A:3862:THR:HG23	1:A:3863:THR:N	2.01	0.75
1:A:2793:ASN:HD22	1:A:2800:ARG:HE	1.33	0.75
1:A:2886:LEU:O	1:A:2890:ILE:HG12	1.87	0.75
1:B:3602:ILE:HD12	1:B:3610:ARG:HG2	1.66	0.75
1:B:1655:LEU:HB2	1:B:1658:GLU:HB2	1.68	0.75
1:B:4323:ASN:HD22	1:B:4323:ASN:N	1.84	0.75
1:A:3723:VAL:HG22	1:A:3723:VAL:O	1.87	0.74
1:A:3862:THR:CG2	1:A:3863:THR:H	2.00	0.74
1:B:1546:VAL:HG11	1:B:1556:ARG:NH1	2.01	0.74
1:B:4313:TRP:HB3	1:B:4330:PRO:CG	2.17	0.74
1:B:2766:MET:HE2	1:B:2783:LEU:HD11	1.69	0.74
1:B:3037:ILE:HD13	1:B:3070:CYS:HB3	1.70	0.74
1:B:4379:ILE:O	1:B:4379:ILE:HG12	1.86	0.74
1:A:3342:ARG:HH11	1:A:3345:GLN:HE22	1.36	0.74
1:A:3834:LEU:HA	1:A:3854:THR:HG21	1.67	0.74
1:A:4213:PHE:O	1:A:4214:ARG:HG2	1.86	0.74
1:A:4220:GLU:O	1:A:4222:HIS:N	2.21	0.74
1:B:1899:THR:HB	1:B:1903:ASP:HB2	1.68	0.74
1:B:3219:ILE:CB	1:B:3220:PRO:HD3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3139:ARG:HG3	1:B:3139:ARG:O	1.87	0.74
1:B:1777:MET:CE	1:B:1939:GLU:HA	2.17	0.74
1:B:4060:GLU:O	1:B:4064:VAL:HG23	1.87	0.74
1:B:2104:ASP:O	1:B:2108:ILE:HG13	1.87	0.74
1:B:3973:ILE:HG13	1:B:3988:TRP:CZ3	2.22	0.74
1:A:2525:ILE:HG12	1:A:2815:LEU:HD12	1.70	0.74
1:B:4693:ASN:H	1:B:4693:ASN:ND2	1.85	0.74
1:B:4657:THR:HG22	1:B:4658:ASP:N	2.02	0.73
1:A:2426:ILE:HD12	1:A:2530:ARG:NH1	2.02	0.73
1:B:2793:ASN:HD22	1:B:2800:ARG:NH2	1.86	0.73
1:B:3700:LEU:CD1	1:B:3701:ASP:N	2.50	0.73
1:A:4569:SER:O	1:A:4573:GLN:HG3	1.87	0.73
1:A:1967:ARG:NH2	1:A:2069:GLN:O	2.21	0.73
1:A:3364:ALA:C	1:A:3366:LEU:H	1.95	0.73
1:A:4405:PRO:HG2	1:A:4412:GLU:HA	1.69	0.73
1:A:4572:MET:O	1:A:4575:LEU:HB2	1.87	0.73
1:A:1766:ILE:HG23	1:A:1767:HIS:N	2.02	0.73
1:B:3278:LEU:HD12	1:B:3585:MET:HE3	1.69	0.73
1:A:3253:ASN:HB2	1:A:3604:PHE:CE2	2.24	0.73
1:B:4657:THR:HG22	1:B:4659:ILE:H	1.53	0.73
1:B:2294:GLU:HG3	1:B:2299:ILE:O	1.88	0.73
1:B:3239:GLY:O	1:B:3242:ASN:HB2	1.88	0.73
1:B:3700:LEU:CD1	1:B:3701:ASP:H	2.02	0.73
1:A:3219:ILE:CB	1:A:3220:PRO:CD	2.67	0.73
1:A:4349:ASN:ND2	1:A:4352:ASP:N	2.36	0.73
1:B:3966:THR:CG2	1:B:4426:MET:HG3	2.19	0.73
1:B:4294:LYS:NZ	1:B:4348:ASP:OD1	2.22	0.72
1:A:2877:ARG:O	1:A:2881:ARG:HG3	1.89	0.72
1:A:3199:TYR:O	1:A:3200:ILE:HG13	1.89	0.72
1:A:3335:GLU:HG3	1:A:3529:ILE:HD11	1.71	0.72
1:B:2606:PRO:HD3	1:B:2624:TRP:CD1	2.24	0.72
1:B:2887:LEU:O	1:B:2891:GLN:HG3	1.89	0.72
1:B:4213:PHE:O	1:B:4214:ARG:HG2	1.89	0.72
1:A:1797:VAL:HG13	1:A:1855:ILE:HD11	1.69	0.72
1:A:3087:MET:HA	1:A:3087:MET:HE2	1.71	0.72
1:B:2642:ALA:HB3	1:B:2884:ARG:CG	2.19	0.72
1:A:1666:GLN:O	1:A:1670:GLU:HG3	1.89	0.72
1:A:3789:THR:HG22	1:A:3792:SER:H	1.55	0.72
1:A:4657:THR:H	1:A:4719:ARG:HH22	1.38	0.72
1:B:4189:ASN:H	1:B:4218:THR:CG2	2.02	0.72
1:A:1811:PRO:HD2	1:A:1814:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4197:LEU:HD22	1:A:4197:LEU:H	1.55	0.72
1:A:1972:PRO:HG2	1:A:2076:THR:HG22	1.72	0.72
1:A:4316:LEU:HD23	1:A:4317:TYR:HE2	1.55	0.72
1:B:3686:MET:CE	1:B:3696:LYS:HB2	2.19	0.72
1:B:3767:ARG:HD3	1:B:4205:HIS:CE1	2.24	0.72
1:B:4337:ILE:O	1:B:4341:THR:HB	1.89	0.72
1:A:1719:GLN:HA	1:A:1722:PHE:CD2	2.25	0.72
1:B:2717:HIS:O	1:B:2733:THR:HG22	1.89	0.72
1:A:3256:THR:H	1:A:3259:HIS:HD2	1.37	0.72
1:B:2438:PRO:HA	1:B:2495:GLN:HE22	1.55	0.72
1:B:3540:ILE:O	1:B:3544:GLU:HG3	1.88	0.72
1:B:4618:ASN:HD22	1:B:4618:ASN:N	1.85	0.72
1:A:2048:VAL:O	1:A:2052:GLU:HG3	1.90	0.71
1:B:1605:TRP:CH2	1:B:1650:VAL:HG21	2.22	0.71
1:A:1604:VAL:O	1:A:1608:VAL:HG23	1.90	0.71
1:A:2641:VAL:HB	1:A:2887:LEU:HD22	1.71	0.71
1:B:3112:CYS:SG	1:B:3133:PHE:HB2	2.29	0.71
1:B:4601:ILE:O	1:B:4604:THR:HG22	1.90	0.71
1:A:1704:ASP:HB3	1:A:1721:HIS:CE1	2.24	0.71
1:A:2607:ALA:C	1:A:2609:THR:H	1.97	0.71
1:A:3015:ILE:HG22	1:A:3149:PRO:HG3	1.70	0.71
1:B:1630:PRO:HG2	1:B:1631:ALA:H	1.56	0.71
1:B:2642:ALA:HB3	1:B:2884:ARG:HG2	1.72	0.71
1:B:3695:THR:HB	1:B:3718:LEU:HD12	1.71	0.71
1:A:1817:LEU:O	1:A:1821:ILE:HG13	1.90	0.71
1:B:2611:PRO:HD2	1:B:2614:ASP:OD2	1.89	0.71
1:A:2422:THR:HG22	1:A:2424:GLN:H	1.56	0.71
1:A:3331:GLN:HG3	1:A:3532:TYR:CB	2.21	0.71
1:A:3766:THR:HG22	1:A:3768:ASP:N	1.97	0.71
1:A:2327:TRP:CZ3	1:A:2380:PRO:HD2	2.26	0.71
1:B:3059:LEU:HD23	1:B:3137:VAL:HG21	1.71	0.71
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	1.72	0.71
1:A:2877:ARG:HG3	2:A:9003:ADP:H4'	1.71	0.71
1:B:2370:LEU:HD12	1:B:2377:LEU:HB2	1.72	0.71
1:A:2199:ILE:O	1:A:2203:MET:HB2	1.91	0.71
1:B:1711:ASN:ND2	1:B:1717:LYS:HD3	2.06	0.71
1:B:1886:ARG:HD3	1:B:1890:ARG:CZ	2.20	0.71
1:A:2011:ARG:HH11	1:A:2011:ARG:CB	2.03	0.70
1:B:3207:GLN:HA	1:B:3210:GLU:HG3	1.74	0.70
1:B:4393:MET:HE2	1:B:4396:ILE:HD12	1.73	0.70
1:B:1886:ARG:NH1	1:B:1890:ARG:HH12	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1640:ASN:O	1:A:1644:ILE:HG12	1.91	0.70
1:B:2174:ILE:HD13	1:B:2180:LYS:HD2	1.73	0.70
1:B:2187:TYR:O	1:B:2190:TYR:HB3	1.92	0.70
1:A:2350:ARG:HG2	1:A:2350:ARG:HH11	1.56	0.70
1:A:2940:SER:HB3	1:B:4000:SER:O	1.91	0.70
1:B:4313:TRP:HB3	1:B:4330:PRO:HG2	1.73	0.70
1:B:4711:THR:OG1	1:B:4716:TRP:NE1	2.24	0.70
1:A:3118:ARG:C	1:A:3120:GLY:H	1.98	0.70
1:A:3862:THR:HG23	1:A:3863:THR:H	1.57	0.70
1:A:4242:PRO:HA	1:A:4286:ARG:NH1	2.07	0.70
1:B:2603:THR:CG2	1:B:2604:PRO:HD2	2.21	0.70
1:B:3351:ARG:O	1:B:3355:ILE:HG13	1.92	0.70
1:A:3038:TYR:OH	1:A:3054:ASP:HB3	1.92	0.70
1:A:3335:GLU:HG3	1:A:3529:ILE:CD1	2.22	0.70
1:B:1803:TYR:OH	1:B:1878:LEU:HD21	1.92	0.70
1:B:4596:ASN:C	1:B:4596:ASN:HD22	1.98	0.70
1:B:4685:LYS:HD3	1:B:4704:ASP:HB3	1.71	0.70
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.27	0.70
1:A:2338:ARG:HH11	1:A:2338:ARG:HG2	1.56	0.70
1:A:3333:ALA:HA	1:A:3336:ILE:HD12	1.74	0.70
1:A:4185:VAL:HB	1:A:4215:LEU:HD12	1.73	0.70
1:B:1671:ARG:O	1:B:1675:LEU:HG	1.92	0.70
1:B:4167:GLY:O	1:B:4171:ALA:HB2	1.92	0.70
1:B:4318:SER:CB	1:B:4324:ILE:HD11	2.20	0.70
1:A:2708:GLU:HA	1:A:2711:LEU:HD12	1.74	0.69
1:B:2863:ARG:HG3	1:B:2925:TRP:CE2	2.27	0.69
1:A:2203:MET:H	1:A:2205:PRO:HD2	1.55	0.69
1:B:2361:PRO:HD3	1:B:2402:TYR:O	1.91	0.69
1:B:2641:VAL:HG12	1:B:2642:ALA:N	2.05	0.69
1:A:3636:SER:HA	1:A:3644:ARG:HH21	1.55	0.69
1:B:2714:PHE:CE2	1:B:2766:MET:HE1	2.26	0.69
1:B:3080:GLU:O	1:B:3083:PHE:HB2	1.91	0.69
1:B:4222:HIS:HD2	1:B:4224:ALA:N	1.81	0.69
1:B:4011:LEU:HD11	1:B:4041:SER:HB2	1.73	0.69
1:B:4169:GLU:C	1:B:4171:ALA:H	2.00	0.69
1:B:3256:THR:H	1:B:3259:HIS:HD2	1.40	0.69
1:B:3886:TYR:O	1:B:3889:MET:HG3	1.92	0.69
1:B:1832:GLY:HA3	1:B:1836:LEU:HD13	1.75	0.69
1:B:3664:MET:O	1:B:3668:PHE:HB3	1.93	0.69
1:B:4389:ARG:HG2	1:B:4389:ARG:HH11	1.56	0.69
1:A:1851:THR:O	1:A:1854:MET:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2441:PRO:C	1:B:2443:GLU:H	1.99	0.69
1:B:4331:TRP:O	1:B:4335:ARG:HB2	1.93	0.69
1:A:2725:SER:HB3	1:A:2727:GLU:HG3	1.75	0.68
1:A:4259:ARG:NH1	1:A:4311:ASP:OD2	2.26	0.68
1:B:1548:TYR:HE2	1:B:1613:VAL:HG22	1.59	0.68
1:A:2918:VAL:O	1:A:2918:VAL:HG12	1.94	0.68
1:A:3139:ARG:HG3	1:A:3139:ARG:NH1	2.07	0.68
1:B:3602:ILE:HG23	1:B:3610:ARG:HG2	1.72	0.68
1:B:4506:GLY:O	1:B:4510:VAL:HG23	1.92	0.68
1:B:4556:PRO:O	1:B:4559:ILE:HG22	1.92	0.68
1:A:2127:LYS:HE3	1:A:2222:VAL:O	1.93	0.68
1:B:3689:TYR:HB2	1:B:3694:ILE:HD12	1.76	0.68
1:B:4189:ASN:N	1:B:4189:ASN:HD22	1.90	0.68
1:A:2524:HIS:HE1	1:A:2585:MET:HE2	1.56	0.68
1:A:3929:ASN:HD21	1:A:3942:TYR:HD1	1.42	0.68
1:B:3108:LEU:HD11	1:B:3133:PHE:CE2	2.28	0.68
1:B:4225:LEU:HD23	1:B:4230:LEU:HD21	1.76	0.68
1:B:4604:THR:HG23	1:B:4604:THR:O	1.92	0.68
1:A:3000:ARG:HD2	1:A:3171:ASP:OD2	1.94	0.68
1:B:3338:GLN:HA	1:B:3338:GLN:HE21	1.57	0.68
1:A:3180:ALA:O	1:A:3184:VAL:HG23	1.93	0.68
1:A:4368:ALA:HA	1:A:4373:PHE:CE1	2.28	0.68
1:B:2381:ASN:ND2	1:B:2383:GLU:HB2	2.00	0.68
1:B:2358:ASP:OD2	1:B:2756:THR:HB	1.93	0.68
1:A:1417:THR:HB	1:A:1422:ILE:HG22	1.76	0.68
1:A:1857:ASN:O	1:A:1860:ALA:HB3	1.93	0.68
1:A:1735:ASP:N	1:A:1742:ILE:HD11	2.08	0.68
1:A:2036:LEU:O	1:A:2040:SER:HB3	1.93	0.67
1:B:2308:PRO:HG3	1:B:2355:PHE:HB3	1.76	0.67
1:B:2591:GLU:HA	1:B:2613:LEU:HD12	1.76	0.67
1:A:2128:ILE:HD12	1:A:2131:LEU:HD23	1.77	0.67
1:A:2142:GLN:HE21	1:A:2142:GLN:CA	2.06	0.67
1:A:2381:ASN:ND2	1:A:2383:GLU:HB2	2.09	0.67
1:A:2501:ILE:HD13	1:A:2566:SER:HA	1.74	0.67
1:A:1859:LEU:HB3	1:A:1879:ILE:CD1	2.24	0.67
1:A:4293:THR:HB	1:A:4352:ASP:OD1	1.93	0.67
1:B:1653:ALA:HB1	1:B:1655:LEU:CD2	2.22	0.67
1:A:3965:LEU:HD23	1:A:4426:MET:HE1	1.76	0.67
1:A:4200:LEU:HD22	1:A:4204:LEU:CD1	2.25	0.67
1:B:2129:VAL:HG22	1:B:2130:PRO:CD	2.21	0.67
1:B:2332:PHE:CE1	1:B:2353:ILE:HG21	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3690:ALA:O	1:B:3693:LYS:N	2.27	0.67
1:B:4351:PHE:CD2	1:B:4689:PRO:HG3	2.29	0.67
1:A:3197:PRO:O	1:A:3198:GLN:HG3	1.94	0.67
1:A:3973:ILE:HG13	1:A:3988:TRP:CZ3	2.29	0.67
1:B:3602:ILE:HG22	1:B:3664:MET:HE1	1.77	0.67
1:A:2911:ARG:HD3	1:A:2915:ASP:OD2	1.95	0.67
1:B:3512:LYS:HA	1:B:3515:GLN:NE2	2.09	0.67
1:A:3153:ASP:OD1	1:A:3156:ASN:ND2	2.28	0.67
1:A:3853:SER:OG	1:A:3854:THR:N	2.28	0.67
1:A:4121:ILE:O	1:A:4126:VAL:HG12	1.94	0.67
1:B:4133:LEU:HD23	1:B:4230:LEU:HD23	1.75	0.67
1:A:1554:LEU:HD22	1:A:1609:GLN:HG3	1.76	0.67
1:A:2290:LEU:HD11	1:A:2352:TRP:CD2	2.30	0.67
1:A:2378:THR:O	1:A:2378:THR:HG23	1.95	0.67
1:A:3163:ALA:HB1	1:A:3167:ARG:HG3	1.76	0.67
1:B:2793:ASN:ND2	1:B:2800:ARG:NH2	2.41	0.67
1:B:3827:LEU:HD12	1:B:3827:LEU:O	1.95	0.67
1:B:4294:LYS:HZ1	1:B:4348:ASP:CG	2.01	0.67
1:A:2284:THR:O	1:A:2288:VAL:HG23	1.94	0.67
1:A:2598:GLN:HG3	1:A:2612:LEU:HB2	1.76	0.67
1:A:3839:SER:C	1:A:3841:ALA:H	2.03	0.67
1:A:4599:ALA:HA	1:A:4602:THR:HG22	1.76	0.67
1:B:1906:TRP:CZ2	1:B:1911:ARG:HG2	2.30	0.67
1:A:1704:ASP:O	1:A:1708:ILE:HG13	1.94	0.66
1:A:2247:ARG:NH2	1:A:2287:GLU:HB3	2.09	0.66
1:B:1811:PRO:O	1:B:1815:VAL:HG23	1.95	0.66
1:B:2375:LYS:HD3	1:B:2387:LEU:HD23	1.77	0.66
1:B:2612:LEU:HD11	1:B:2624:TRP:CH2	2.28	0.66
1:B:2797:ASP:HB2	1:B:2800:ARG:HG3	1.77	0.66
1:B:3042:VAL:HG11	1:B:3079:LEU:HG	1.76	0.66
1:B:4060:GLU:HA	1:B:4063:ILE:HD13	1.76	0.66
1:B:1546:VAL:CG1	1:B:1556:ARG:NH1	2.58	0.66
1:B:1554:LEU:HD22	1:B:1609:GLN:NE2	2.09	0.66
1:B:4494:PRO:HB3	1:B:4606:GLN:HB2	1.77	0.66
1:A:3919:ILE:HD13	1:A:3951:THR:HA	1.75	0.66
1:A:4384:PRO:HB3	1:A:4395:TRP:CD1	2.29	0.66
1:A:2372:ASP:OD1	1:A:2373:ASP:N	2.25	0.66
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	1.77	0.66
1:A:3115:THR:HA	1:A:3118:ARG:NH1	2.10	0.66
1:A:3647:TRP:HD1	1:A:3688:GLN:OE1	1.79	0.66
1:B:2839:LEU:HD13	1:B:2842:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1968:MET:HE3	1:A:2051:LYS:NZ	2.11	0.66
1:B:2547:ASN:HB2	1:B:2568:TYR:OH	1.95	0.66
1:B:2564:ASN:C	1:B:2566:SER:H	2.04	0.66
1:A:2504:GLN:O	1:A:2507:GLU:HG2	1.95	0.66
1:A:2610:ILE:HD12	1:A:2615:TYR:OH	1.96	0.66
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	1.78	0.66
1:A:1555:VAL:H	1:A:1609:GLN:NE2	1.91	0.66
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.30	0.66
1:A:4005:ILE:H	1:A:4017:GLN:NE2	1.93	0.66
1:A:4623:ALA:HB2	1:A:4703:ILE:HD11	1.78	0.66
1:B:3514:LYS:HA	1:B:3517:GLU:HG3	1.77	0.66
1:B:4005:ILE:HG21	1:B:4008:LEU:HD12	1.78	0.66
1:B:1551:LYS:HE2	1:B:1616:GLU:OE1	1.95	0.66
1:B:1791:HIS:O	1:B:1795:VAL:HG23	1.95	0.66
1:A:3689:TYR:HB2	1:A:3694:ILE:HD11	1.78	0.66
1:B:3682:MET:O	1:B:3686:MET:HG2	1.95	0.66
1:A:2090:ASN:HD22	1:A:2091:LEU:N	1.94	0.65
1:A:2200:ASN:HD22	1:A:2228:LEU:HD22	1.61	0.65
1:A:2405:LEU:HA	1:A:2408:ILE:CD1	2.26	0.65
1:B:2758:ARG:O	1:B:2761:THR:HG22	1.96	0.65
1:B:4169:GLU:HG3	1:B:4173:LYS:HZ2	1.60	0.65
1:A:3817:LEU:O	1:A:3820:GLN:HG2	1.96	0.65
1:A:4136:SER:O	1:A:4220:GLU:HA	1.96	0.65
1:B:1789:LEU:HD23	1:B:1818:THR:HG23	1.78	0.65
1:B:1915:ASP:OD1	1:B:1917:THR:HG23	1.96	0.65
1:A:1962:GLN:CB	1:A:4341:THR:HG21	2.26	0.65
1:A:4693:ASN:C	1:A:4693:ASN:HD22	2.04	0.65
1:B:2714:PHE:C	1:B:2716:HIS:H	2.04	0.65
1:B:4135:CYS:O	1:B:4237:SER:HA	1.94	0.65
1:A:1628:LEU:HD22	1:A:1686:TYR:OH	1.96	0.65
1:B:2388:PRO:HB2	1:B:2390:ASN:OD1	1.97	0.65
1:A:2339:ILE:HA	1:A:2346:GLU:HG2	1.78	0.65
1:A:2488:ILE:O	1:A:2488:ILE:HG22	1.95	0.65
1:A:3062:ALA:HB2	1:A:3069:ILE:HD13	1.78	0.65
1:A:3203:PRO:HG2	1:B:3619:ILE:HD11	1.79	0.65
1:A:3256:THR:H	1:A:3259:HIS:CD2	2.14	0.65
1:B:1610:ARG:HH11	1:B:1610:ARG:HG3	1.60	0.65
1:B:4168:PHE:O	1:B:4171:ALA:HB3	1.97	0.65
1:A:2977:LYS:C	1:A:2979:PHE:H	2.04	0.65
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	1.77	0.65
1:B:4013:SER:N	1:B:4016:GLN:HE21	1.87	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4534:LEU:O	1:B:4538:THR:HG23	1.96	0.65
1:A:2823:SER:O	1:A:2827:ILE:HG13	1.96	0.65
1:B:2311:ILE:HB	1:B:2315:GLN:HE21	1.60	0.65
1:B:3579:GLU:HA	1:B:3579:GLU:OE2	1.96	0.65
1:A:3086:ARG:HH11	1:A:3096:VAL:HG12	1.61	0.65
1:B:1605:TRP:CZ3	1:B:1669:MET:HE3	2.32	0.65
1:A:2617:VAL:HG13	1:A:2617:VAL:O	1.97	0.65
1:A:2684:LEU:CD2	1:A:2789:VAL:HG11	2.27	0.65
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.59	0.65
1:A:2026:ASP:OD2	1:A:2027:GLU:HG3	1.97	0.65
1:A:2542:ASN:O	1:A:2546:VAL:HG23	1.97	0.65
1:A:4572:MET:HA	1:A:4575:LEU:HD12	1.77	0.65
1:B:4618:ASN:ND2	1:B:4618:ASN:N	2.41	0.65
1:A:4217:MET:HE1	1:A:4229:LEU:HD11	1.78	0.64
1:B:4572:MET:O	1:B:4575:LEU:HB2	1.97	0.64
1:B:2651:VAL:O	1:B:2655:ARG:HG2	1.97	0.64
1:B:4386:GLY:HA3	1:B:4391:HIS:HB3	1.78	0.64
1:A:2641:VAL:CG1	1:A:2642:ALA:N	2.52	0.64
1:A:4660:LEU:HD12	1:A:4660:LEU:N	2.13	0.64
1:B:1788:SER:HA	1:B:1810:TYR:CZ	2.33	0.64
1:B:3038:TYR:OH	1:B:3054:ASP:HB3	1.97	0.64
1:B:4332:ILE:HD12	1:B:4332:ILE:H	1.60	0.64
1:B:4621:LEU:HD13	1:B:4671:TRP:CE2	2.32	0.64
1:A:2653:THR:O	1:A:2657:VAL:HG23	1.97	0.64
1:A:3023:SER:O	1:A:3027:ARG:HG3	1.96	0.64
1:A:3342:ARG:NH1	1:A:3345:GLN:HE22	1.94	0.64
1:A:4494:PRO:HD2	1:A:4610:GLN:HE22	1.62	0.64
1:B:2498:CYS:HA	1:B:2501:ILE:CD1	2.27	0.64
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.79	0.64
1:B:3947:ILE:HG13	1:B:3948:PHE:N	2.12	0.64
1:B:3981:ASN:ND2	1:B:4074:SER:OG	2.29	0.64
1:A:3056:ARG:HH11	1:A:3099:LEU:HD12	1.63	0.64
1:B:2029:ASN:HD22	1:B:2029:ASN:N	1.94	0.64
1:B:3219:ILE:CB	1:B:3220:PRO:CD	2.74	0.64
1:B:4323:ASN:N	1:B:4323:ASN:ND2	2.46	0.64
1:A:3352:ASN:O	1:A:3356:ALA:HB2	1.97	0.64
1:A:3862:THR:CG2	1:A:3863:THR:N	2.58	0.64
1:A:3872:THR:O	1:A:3876:MET:HG2	1.98	0.64
1:B:4043:ASP:HB3	1:B:4059:PRO:HB3	1.78	0.64
1:B:4169:GLU:HG3	1:B:4173:LYS:NZ	2.13	0.64
1:A:2533:VAL:HB	1:A:2581:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4147:ASP:OD2	1:A:4157:TYR:HE2	1.81	0.64
1:A:4572:MET:HE2	1:A:4575:LEU:HD12	1.79	0.64
1:B:2501:ILE:HD13	1:B:2565:GLN:O	1.98	0.64
1:A:2052:GLU:O	1:A:2053:ASN:HB2	1.97	0.64
1:A:3359:LYS:HZ1	1:A:3505:GLU:HA	1.63	0.64
1:A:3834:LEU:CA	1:A:3854:THR:HG21	2.27	0.64
1:A:4574:GLN:O	1:A:4578:ILE:HG13	1.98	0.64
1:B:2129:VAL:CG2	1:B:2130:PRO:HD3	2.22	0.64
1:B:3603:GLY:HA3	1:B:3783:PHE:O	1.98	0.64
1:A:2359:VAL:HA	1:A:2363:TRP:HE1	1.63	0.64
1:A:3022:LYS:O	1:A:3026:SER:HB2	1.98	0.64
1:A:3061:ARG:NH1	1:A:3067:GLU:OE1	2.31	0.64
1:A:3724:GLU:OE2	1:A:3766:THR:HG23	1.98	0.64
1:A:4146:VAL:CG1	1:A:4157:TYR:OH	2.45	0.64
1:A:4623:ALA:CB	1:A:4703:ILE:HD11	2.28	0.64
1:B:2494:VAL:HG11	1:B:2548:VAL:HG11	1.79	0.64
1:B:2638:THR:O	1:B:2641:VAL:HG23	1.98	0.64
1:B:3701:ASP:OD1	1:B:3702:SER:N	2.30	0.64
1:B:4546:VAL:HA	1:B:4561:LEU:HD21	1.79	0.64
1:B:4648:VAL:HA	1:B:4662:THR:HG21	1.80	0.64
1:B:1601:LEU:HA	1:B:1666:GLN:OE1	1.99	0.63
1:B:1788:SER:HA	1:B:1810:TYR:CE2	2.32	0.63
1:B:2212:ILE:O	1:B:2215:ILE:HG22	1.97	0.63
1:A:1605:TRP:CD2	1:A:1669:MET:HE2	2.33	0.63
1:A:2447:GLN:HE22	1:A:2492:LEU:CD2	2.11	0.63
1:B:1781:LEU:HG	1:B:1814:LEU:HD11	1.80	0.63
1:B:2668:ARG:HG2	1:B:2668:ARG:HH11	1.63	0.63
1:A:4277:PHE:CE1	1:A:4360:LEU:HD13	2.33	0.63
1:B:3344:LEU:HB3	1:B:3518:ILE:CD1	2.29	0.63
1:B:4267:ARG:HG2	1:B:4267:ARG:HH11	1.64	0.63
1:A:1551:LYS:NZ	1:A:1616:GLU:OE2	2.31	0.63
1:A:4620:ARG:HD3	1:A:4679:PHE:CD2	2.33	0.63
1:B:2841:ASN:HD22	1:B:2841:ASN:N	1.94	0.63
1:B:4132:LEU:HD13	1:B:4216:PHE:CE1	2.33	0.63
1:A:2044:GLN:HE22	1:A:2090:ASN:HB2	1.60	0.63
1:A:3584:GLN:O	1:A:3588:VAL:HG23	1.98	0.63
1:B:1655:LEU:HD22	1:B:1655:LEU:N	2.02	0.63
1:B:1763:GLY:H	1:B:1764:PRO:CD	2.12	0.63
1:B:2996:ASP:O	1:B:3000:ARG:HG3	1.98	0.63
1:A:2527:ASP:O	1:A:2532:ARG:NH1	2.30	0.63
1:A:4186:LEU:HA	1:A:4216:PHE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1792:PHE:O	1:B:1795:VAL:HB	1.99	0.63
1:A:2243:ILE:HD12	1:A:2292:ALA:HB2	1.80	0.63
1:A:2340:ILE:HD11	1:A:2386:ALA:O	1.99	0.63
1:A:3145:PHE:CD1	1:A:3164:LEU:HD11	2.33	0.63
1:A:3074:ASP:N	1:A:3077:ASN:HD22	1.96	0.63
1:A:4621:LEU:HD13	1:A:4671:TRP:CE2	2.33	0.63
1:B:1558:TRP:HZ3	1:B:1602:LEU:HB3	1.63	0.63
1:B:2231:ILE:HG23	1:B:2257:GLU:OE2	1.98	0.63
1:B:2999:LEU:O	1:B:3003:ARG:HG3	1.99	0.63
1:B:3976:VAL:HG23	1:B:3982:GLU:HA	1.79	0.63
1:A:3015:ILE:CG2	1:A:3149:PRO:HG3	2.28	0.63
1:A:3673:LEU:HA	1:A:3764:LEU:HB2	1.80	0.63
1:B:1640:ASN:ND2	1:B:1644:ILE:HD11	2.10	0.63
1:B:2598:GLN:CG	1:B:2612:LEU:HB2	2.29	0.63
1:B:2984:LEU:HD13	1:B:2986:VAL:CG2	2.28	0.63
1:B:3708:LEU:CD2	1:B:3730:LEU:HD21	2.29	0.63
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.34	0.63
1:A:2548:VAL:HG11	1:A:2565:GLN:NE2	2.03	0.62
1:B:4091:SER:N	3:B:9022:SPM:H132	2.06	0.62
1:A:1862:SER:O	1:A:1865:GLN:HG2	1.98	0.62
1:A:2415:TRP:CD1	1:A:2417:SER:HG	2.17	0.62
1:A:2839:LEU:HD22	1:A:2896:CYS:HB2	1.79	0.62
1:A:3928:PRO:C	1:A:3930:LEU:H	2.06	0.62
1:B:3324:LEU:HD11	1:B:3539:LEU:HG	1.80	0.62
1:B:3963:ASP:HA	1:B:3966:THR:HG23	1.80	0.62
1:A:1464:GLY:O	1:A:1466:ALA:N	2.32	0.62
1:A:1537:PHE:CE2	1:A:1541:LEU:HD22	2.35	0.62
1:A:2239:LYS:HE2	1:A:2295:GLN:HB3	1.81	0.62
1:A:2890:ILE:HA	1:A:2893:MET:CE	2.28	0.62
1:B:1646:ILE:HG21	1:B:1669:MET:HE1	1.81	0.62
1:B:3934:LYS:O	1:B:3936:PRO:HD3	1.99	0.62
1:A:3285:LEU:HD13	1:A:3578:SER:HA	1.81	0.62
1:B:3035:LEU:HD22	1:B:3068:LYS:HB3	1.79	0.62
1:B:4131:PRO:HD2	1:B:4233:SER:HB3	1.79	0.62
1:A:1418:ALA:O	1:A:1422:ILE:HG23	2.00	0.62
1:A:1525:ILE:O	1:A:1529:GLU:HB2	1.99	0.62
1:B:1611:ARG:O	1:B:1612:TRP:C	2.43	0.62
1:B:2861:GLN:HG3	1:B:2874:TYR:HB2	1.81	0.62
1:B:4484:LEU:HD21	1:B:4496:PHE:CZ	2.34	0.62
1:A:2439:PHE:H	1:A:2495:GLN:NE2	1.97	0.62
1:A:2968:LEU:O	1:A:2972:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3673:LEU:HB2	1:A:3781:VAL:HG21	1.82	0.62
1:A:3928:PRO:HG2	1:A:3929:ASN:H	1.63	0.62
1:A:4648:VAL:HG12	1:A:4662:THR:HG21	1.80	0.62
1:B:4076:ILE:HD13	1:B:4105:VAL:HG12	1.81	0.62
1:A:2525:ILE:HD11	1:A:2813:ILE:HG21	1.81	0.62
1:A:3643:GLU:OE2	1:A:3666:LYS:HE2	1.99	0.62
1:A:4171:ALA:C	1:A:4173:LYS:H	2.05	0.62
1:B:1777:MET:HE3	1:B:1939:GLU:HA	1.81	0.62
1:B:3849:ASP:HA	1:B:3852:ILE:HG22	1.81	0.62
1:A:1417:THR:C	1:A:1498:THR:HG22	2.24	0.62
1:A:1564:LYS:HD2	1:A:1568:HIS:CE1	2.34	0.62
1:A:1655:LEU:HB2	1:A:1658:GLU:HB2	1.82	0.62
1:A:2898:LEU:O	1:A:2898:LEU:HD22	2.00	0.62
1:A:3061:ARG:HG2	1:A:3061:ARG:HH11	1.64	0.62
1:A:4599:ALA:HA	1:A:4602:THR:CG2	2.29	0.62
1:B:3278:LEU:CD1	1:B:3585:MET:HE3	2.28	0.62
1:A:2350:ARG:HG2	1:A:2350:ARG:NH1	2.13	0.62
1:A:4660:LEU:HD12	1:A:4660:LEU:H	1.63	0.62
1:B:1785:LEU:HA	1:B:1814:LEU:HD23	1.82	0.62
1:B:4294:LYS:NZ	1:B:4348:ASP:CG	2.58	0.62
1:A:3817:LEU:HD21	1:A:3872:THR:HG21	1.82	0.62
1:B:2237:ARG:HH21	1:B:2260:LEU:HD23	1.65	0.62
1:B:3053:ASP:OD2	1:B:3053:ASP:N	2.32	0.62
1:A:2331:LEU:HD21	1:A:2773:TRP:CG	2.34	0.61
1:A:1543:LEU:O	1:A:1545:LEU:HD13	2.01	0.61
1:A:1834:GLY:O	1:A:1835:THR:HG23	2.00	0.61
1:A:2202:THR:O	1:A:2203:MET:HG3	2.01	0.61
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.99	0.61
1:A:2966:SER:HA	1:A:2969:ARG:HG2	1.82	0.61
1:A:3327:MET:HE3	1:A:3536:TYR:HA	1.82	0.61
1:A:4179:ALA:HA	1:A:4213:PHE:CD1	2.34	0.61
1:A:4519:ASN:O	1:A:4520:LEU:C	2.42	0.61
1:B:2439:PHE:HA	3:B:9018:SPM:H111	1.81	0.61
1:B:3030:ALA:CB	1:B:3037:ILE:HD11	2.31	0.61
1:B:4189:ASN:N	1:B:4189:ASN:ND2	2.47	0.61
1:A:3497:LEU:O	1:A:3501:VAL:HG23	2.00	0.61
1:B:2339:ILE:HG12	1:B:2346:GLU:HG2	1.82	0.61
1:B:2942:ASN:ND2	1:B:2944:ASP:HB2	2.15	0.61
1:B:3104:GLU:O	1:B:3106:THR:N	2.34	0.61
1:B:3344:LEU:HB3	1:B:3518:ILE:HD13	1.82	0.61
1:A:2028:PHE:HB2	1:A:2075:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3359:LYS:HE3	1:A:3505:GLU:OE1	1.99	0.61
1:A:3848:ASP:O	1:A:3851:VAL:HG12	2.00	0.61
1:A:4606:GLN:O	1:A:4610:GLN:N	2.30	0.61
1:B:1863:VAL:HG22	1:B:1872:ARG:NH1	2.15	0.61
1:B:2071:MET:HG3	1:B:2072:GLY:N	2.15	0.61
1:B:4484:LEU:HD22	1:B:4500:GLU:HG3	1.83	0.61
1:A:3253:ASN:HB2	1:A:3604:PHE:CD2	2.36	0.61
1:A:4153:LEU:O	1:A:4154:HIS:HB2	2.01	0.61
1:A:4259:ARG:HD3	1:A:4271:TYR:OH	2.01	0.61
1:B:2441:PRO:O	1:B:2443:GLU:N	2.33	0.61
1:B:2969:ARG:O	1:B:2973:LYS:HB2	2.01	0.61
1:B:2971:TYR:CE2	1:B:2975:ARG:HG3	2.35	0.61
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.01	0.61
1:A:3860:LYS:O	1:A:3862:THR:N	2.34	0.61
1:B:1554:LEU:HD22	1:B:1609:GLN:HE22	1.65	0.61
1:B:2609:THR:O	1:B:2610:ILE:HG13	2.00	0.61
1:B:4122:VAL:HG21	1:B:4149:LEU:HD21	1.83	0.61
1:A:4349:ASN:ND2	1:A:4351:PHE:N	2.49	0.61
1:B:2016:LEU:HB3	1:B:2071:MET:HE3	1.83	0.61
1:B:3253:ASN:HB2	1:B:3604:PHE:CE2	2.34	0.61
1:B:4318:SER:HB3	1:B:4324:ILE:CD1	2.24	0.61
1:A:3179:GLU:OE1	1:A:3179:GLU:N	2.33	0.61
1:A:3342:ARG:HH11	1:A:3345:GLN:NE2	1.99	0.61
1:B:2342:ASN:ND2	1:B:2347:SER:H	1.99	0.61
1:B:3686:MET:HE2	1:B:3696:LYS:HD2	1.83	0.61
1:A:2907:HIS:CE1	1:A:2911:ARG:HE	2.18	0.61
1:A:3864:GLU:CG	1:A:3865:ILE:N	2.63	0.61
1:B:2960:TYR:O	1:B:2961:GLN:HG3	2.00	0.61
1:B:4004:THR:OG1	1:B:4006:PRO:HD3	2.00	0.61
1:B:4389:ARG:HG2	1:B:4389:ARG:NH1	2.16	0.61
1:B:4636:SER:HA	1:B:4670:THR:HG22	1.82	0.61
1:A:2905:TRP:HZ3	1:A:2930:ILE:HG23	1.66	0.60
1:B:2254:GLU:HB2	1:B:2420:ILE:HG22	1.83	0.60
1:A:1877:HIS:HE1	1:A:1943:ILE:O	1.84	0.60
1:A:4091:SER:H	3:A:9016:SPM:H132	1.66	0.60
1:B:1821:ILE:HG23	1:B:1912:TYR:O	2.00	0.60
1:B:2309:LYS:HZ3	1:B:2756:THR:HG21	1.63	0.60
1:A:2551:TYR:CD1	1:A:2619:ILE:HG13	2.36	0.60
1:A:4036:HIS:HD2	1:A:4044:TRP:HE1	1.49	0.60
1:B:3335:GLU:O	1:B:3338:GLN:HB3	2.01	0.60
1:A:1486:LYS:HG2	1:A:1487:ARG:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2377:LEU:O	1:A:2384:ARG:HA	2.01	0.60
1:A:3086:ARG:HD2	1:A:3096:VAL:HG11	1.84	0.60
1:A:3969:LEU:O	1:A:3973:ILE:HG12	2.02	0.60
1:A:4644:LEU:HD23	1:A:4647:ALA:C	2.27	0.60
1:B:1624:ASP:OD2	1:B:1624:ASP:N	2.34	0.60
1:B:1819:SER:O	1:B:1822:VAL:HG12	2.00	0.60
1:A:1886:ARG:HG3	1:A:1887:ASP:N	2.14	0.60
1:A:3678:SER:HB2	1:A:3913:LEU:HD23	1.82	0.60
1:A:4374:PRO:HB2	1:A:4377:PRO:HG3	1.83	0.60
1:B:1655:LEU:HG	1:B:1658:GLU:OE2	2.02	0.60
1:B:1962:GLN:HB3	1:B:4341:THR:HG21	1.84	0.60
1:B:2206:LYS:HE2	1:B:2413:MET:HB3	1.83	0.60
1:B:2344:ARG:O	1:B:2344:ARG:HG2	1.99	0.60
1:A:4242:PRO:HA	1:A:4286:ARG:HH11	1.66	0.60
1:B:2525:ILE:HD12	1:B:2525:ILE:N	2.16	0.60
1:B:3063:GLY:HA2	1:B:3136:GLN:HB2	1.83	0.60
1:B:3700:LEU:CG	1:B:3701:ASP:H	2.14	0.60
1:A:2200:ASN:HA	1:A:2204:ILE:CG2	2.32	0.60
1:B:3766:THR:HG22	1:B:3768:ASP:N	2.15	0.60
1:B:4053:VAL:O	1:B:4053:VAL:HG22	2.01	0.60
1:A:1470:ASP:HB3	1:A:1518:ILE:HD12	1.84	0.60
1:A:1612:TRP:CZ2	1:A:1616:GLU:HG3	2.36	0.60
1:A:1732:LEU:HB3	1:A:1741:ILE:HG23	1.83	0.60
1:A:2142:GLN:N	1:A:2142:GLN:NE2	2.50	0.60
1:A:2978:VAL:O	1:A:2978:VAL:HG12	2.02	0.60
1:B:3326:GLN:HG3	1:B:3326:GLN:O	2.01	0.60
1:B:4168:PHE:O	1:B:4172:GLU:HG3	2.02	0.60
1:A:1766:ILE:CG2	1:A:1767:HIS:H	2.15	0.60
1:B:2291:GLU:O	1:B:2295:GLN:HG2	2.01	0.60
1:B:2379:LEU:O	1:B:2381:ASN:N	2.35	0.60
1:A:1531:LEU:O	1:A:1535:ARG:HB2	2.02	0.59
1:A:2905:TRP:CZ3	1:A:2930:ILE:HG23	2.37	0.59
1:A:4033:LEU:HD13	1:A:4062:TRP:CZ2	2.36	0.59
1:B:2200:ASN:HD22	1:B:2204:ILE:HG13	1.66	0.59
1:B:2231:ILE:HG13	1:B:2231:ILE:O	2.01	0.59
1:B:3928:PRO:O	1:B:3931:VAL:HG23	2.02	0.59
1:A:2068:HIS:CE1	1:A:2070:ASP:HB2	2.37	0.59
1:A:2856:PHE:CE1	1:A:2930:ILE:HG13	2.37	0.59
1:A:3192:LEU:HD22	1:A:3268:VAL:HG22	1.83	0.59
1:A:3204:VAL:O	1:A:3207:GLN:HB3	2.02	0.59
1:A:3281:GLU:HB3	1:A:3581:PHE:CE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3351:ARG:HG3	1:B:3355:ILE:CD1	2.33	0.59
1:A:1962:GLN:HB3	1:A:4341:THR:HG21	1.84	0.59
1:A:4122:VAL:HG21	1:A:4216:PHE:HZ	1.67	0.59
1:A:4349:ASN:HD22	1:A:4352:ASP:N	1.83	0.59
1:A:3279:GLU:HG3	1:A:3585:MET:HE3	1.84	0.59
1:A:3355:ILE:HG21	1:A:3508:ALA:HB2	1.83	0.59
1:A:3721:GLN:HE22	1:A:4205:HIS:CD2	2.20	0.59
1:A:3789:THR:HG23	1:A:3791:SER:H	1.68	0.59
1:A:4187:LEU:N	1:A:4187:LEU:HD12	2.17	0.59
1:B:1777:MET:HE1	1:B:1939:GLU:HA	1.84	0.59
1:B:3289:LEU:HD22	1:B:3293:ARG:NH2	2.17	0.59
1:B:3563:LEU:HD11	1:B:3845:ILE:HG13	1.85	0.59
1:B:3903:LEU:HD23	1:B:4433:MET:CE	2.31	0.59
1:A:1797:VAL:HG12	1:A:1854:MET:CE	2.32	0.59
1:A:4193:ALA:HB1	1:A:4196:TRP:CB	2.33	0.59
1:A:4329:ILE:HG23	1:A:4330:PRO:HD2	1.85	0.59
1:B:1608:VAL:O	1:B:1609:GLN:C	2.46	0.59
1:B:2578:MET:HB3	1:B:2597:ILE:HD12	1.82	0.59
1:B:2668:ARG:HG2	1:B:2668:ARG:NH1	2.16	0.59
1:B:2695:GLU:O	1:B:2739:LEU:HD12	2.02	0.59
1:B:3194:LEU:O	1:B:3223:HIS:HD2	1.84	0.59
1:A:2275:VAL:HG13	1:A:2397:VAL:HG23	1.84	0.59
1:A:3015:ILE:HG21	1:A:3172:TRP:CZ3	2.37	0.59
1:A:3588:VAL:O	1:A:3592:VAL:HG23	2.03	0.59
1:A:3641:PRO:HA	1:A:3644:ARG:NH1	2.16	0.59
1:A:3780:ARG:NH1	1:A:3780:ARG:HB2	2.17	0.59
1:B:2237:ARG:O	1:B:2241:GLN:NE2	2.35	0.59
1:B:2541:MET:O	1:B:2544:SER:HB2	2.02	0.59
1:B:3059:LEU:HD11	1:B:3090:LEU:HD22	1.85	0.59
1:B:4133:LEU:CD2	1:B:4230:LEU:HD23	2.32	0.59
1:A:2643:SER:O	1:A:2646:VAL:HG12	2.03	0.59
1:A:4121:ILE:HA	1:A:4125:GLU:HB3	1.84	0.59
1:B:2370:LEU:CD1	1:B:2377:LEU:HB2	2.32	0.59
1:B:2863:ARG:O	1:B:2863:ARG:HD3	2.02	0.59
1:B:2921:GLU:CD	1:B:2921:GLU:H	2.10	0.59
1:A:2440:ASP:HB3	1:A:2443:GLU:HG3	1.85	0.59
1:A:3298:GLN:O	1:A:3301:ASP:HB2	2.03	0.59
1:A:3780:ARG:CB	1:A:3780:ARG:HH11	2.15	0.59
1:B:3023:SER:HB2	2:B:9010:ADP:O1A	2.03	0.59
1:B:3966:THR:CB	1:B:4426:MET:HG3	2.32	0.59
1:B:4608:ALA:O	1:B:4612:ASN:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1605:TRP:HH2	1:A:1650:VAL:HG21	1.68	0.59
1:A:1696:ARG:HD3	1:A:1725:MET:O	2.02	0.59
1:A:2270:HIS:HA	1:A:2392:ARG:HE	1.67	0.59
1:A:2525:ILE:HD12	1:A:2526:MET:N	2.17	0.59
1:A:3525:LEU:O	1:A:3529:ILE:HG22	2.02	0.59
1:B:2554:LEU:C	1:B:2556:SER:H	2.10	0.59
1:B:3049:SER:O	1:B:3053:ASP:OD2	2.21	0.59
1:B:3170:LEU:HD23	1:B:3170:LEU:C	2.28	0.59
1:B:4165:PRO:HG2	1:B:4166:GLU:H	1.68	0.59
1:B:4294:LYS:NZ	1:B:4348:ASP:OD2	2.36	0.59
1:A:3086:ARG:HH11	1:A:3096:VAL:CG1	2.15	0.59
1:B:3923:LEU:HD22	1:B:3947:ILE:HG23	1.85	0.59
1:B:4657:THR:CG2	1:B:4658:ASP:H	2.13	0.59
1:A:1780:THR:O	1:A:1784:LEU:HB2	2.03	0.58
1:A:2338:ARG:HH11	1:A:2338:ARG:CG	2.15	0.58
1:A:2660:LEU:HD21	1:A:2672:LEU:HD21	1.85	0.58
1:A:3500:GLU:O	1:A:3503:GLN:HB3	2.03	0.58
1:B:3324:LEU:CD1	1:B:3539:LEU:HG	2.33	0.58
1:A:1742:ILE:HD13	1:A:1742:ILE:N	2.18	0.58
1:A:2065:ILE:HG22	1:A:2066:SER:N	2.18	0.58
1:A:2607:ALA:C	1:A:2609:THR:N	2.61	0.58
1:A:3817:LEU:HD21	1:A:3872:THR:CG2	2.33	0.58
1:B:1548:TYR:HD1	1:B:1548:TYR:O	1.85	0.58
1:B:1840:LYS:O	1:B:1844:GLN:HG3	2.04	0.58
1:B:1890:ARG:O	1:B:1893:GLN:N	2.35	0.58
1:B:2381:ASN:HD22	1:B:2381:ASN:C	2.10	0.58
1:B:3073:PHE:CE1	1:B:3077:ASN:HB3	2.38	0.58
1:B:3299:VAL:HB	1:B:3564:LEU:HD21	1.85	0.58
1:B:3825:VAL:O	1:B:3829:ILE:HG12	2.03	0.58
1:A:1662:ILE:HB	1:A:1665:ILE:HG12	1.85	0.58
1:A:2200:ASN:ND2	1:A:2228:LEU:HD22	2.17	0.58
1:A:3322:GLN:C	1:A:3322:GLN:HE21	2.10	0.58
1:A:3571:ARG:HB3	1:A:3571:ARG:CZ	2.33	0.58
1:B:1547:ASN:HD22	1:B:1547:ASN:C	2.11	0.58
1:B:1912:TYR:CD2	1:B:1912:TYR:N	2.71	0.58
1:B:3095:GLU:HG3	1:B:3134:THR:HB	1.84	0.58
1:B:3348:LEU:HD12	1:B:3518:ILE:HD12	1.85	0.58
1:B:3715:GLY:HA2	1:B:3760:PHE:HB2	1.84	0.58
1:A:3069:ILE:O	1:A:3141:LEU:O	2.20	0.58
1:A:4603:ALA:O	1:A:4606:GLN:HG2	2.02	0.58
1:B:2613:LEU:HD22	1:B:2655:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3351:ARG:HG3	1:B:3355:ILE:HD11	1.84	0.58
1:B:3927:ASN:HB3	1:B:3930:LEU:HD12	1.84	0.58
1:A:1523:GLY:HA3	1:A:1580:TYR:CE2	2.38	0.58
1:A:1968:MET:HE3	1:A:2051:LYS:HZ1	1.67	0.58
1:A:4337:ILE:O	1:A:4341:THR:HB	2.04	0.58
1:B:2823:SER:O	1:B:2827:ILE:HG13	2.03	0.58
1:B:4171:ALA:O	1:B:4175:ILE:HG13	2.03	0.58
1:A:1422:ILE:HG21	1:A:1499:LEU:HG	1.84	0.58
1:A:1884:HIS:HE1	1:A:1954:ASP:OD2	1.86	0.58
1:A:4046:GLN:NE2	1:A:4056:PRO:HA	2.19	0.58
1:A:3672:PRO:HG2	1:A:3763:PHE:HD1	1.67	0.58
1:A:4164:SER:HB2	1:A:4165:PRO:HD2	1.85	0.58
1:B:2836:MET:HE2	1:B:2836:MET:HA	1.85	0.58
1:B:2984:LEU:HD13	1:B:2986:VAL:HG21	1.86	0.58
1:B:4134:LEU:HD23	1:B:4142:ALA:HB1	1.85	0.58
1:A:1908:TYR:CE1	1:A:1958:LEU:HD22	2.39	0.58
1:A:4221:ILE:H	1:A:4221:ILE:HD12	1.69	0.58
1:A:4316:LEU:HD23	1:A:4317:TYR:CE2	2.35	0.58
1:A:4575:LEU:HA	1:A:4578:ILE:HD12	1.86	0.58
1:B:1562:PHE:HD2	1:B:1565:LEU:HD22	1.68	0.58
1:B:4313:TRP:HB3	1:B:4330:PRO:HG3	1.84	0.58
1:A:1733:THR:O	1:A:1742:ILE:HG12	2.04	0.58
1:A:2195:LEU:O	1:A:2199:ILE:HG12	2.04	0.58
1:A:3064:CYS:O	1:A:3066:GLU:HG3	2.03	0.58
1:A:3665:LEU:CD1	1:A:3685:LEU:HD21	2.32	0.58
1:A:4063:ILE:HG22	1:A:4063:ILE:O	2.03	0.58
1:B:1592:ASP:O	1:B:1595:LEU:N	2.37	0.58
1:B:3990:PHE:CD2	1:B:4084:LEU:HD22	2.33	0.58
1:A:1916:ALA:O	1:A:1918:GLN:N	2.31	0.58
1:A:3226:ALA:HB1	1:A:3624:VAL:HG13	1.85	0.58
1:A:3776:ASP:OD2	1:A:3780:ARG:NH2	2.36	0.58
1:A:4193:ALA:O	1:A:4197:LEU:HD22	2.03	0.58
1:B:3094:GLY:O	1:B:3137:VAL:HG11	2.04	0.58
1:B:3901:GLU:O	1:B:3901:GLU:HG2	2.02	0.58
1:B:4322:SER:HB2	1:B:4323:ASN:ND2	2.18	0.58
1:B:4543:LYS:HD2	1:B:4545:ILE:CD1	2.33	0.58
1:A:1628:LEU:C	1:A:1630:PRO:HD3	2.29	0.57
1:A:1812:THR:HG21	1:A:1943:ILE:HG23	1.87	0.57
1:A:3318:GLU:O	1:A:3322:GLN:HB2	2.04	0.57
1:B:1668:THR:O	1:B:1672:LEU:HG	2.04	0.57
1:B:1886:ARG:HD3	1:B:1890:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2723:THR:HG22	1:B:2727:GLU:N	2.18	0.57
1:A:3242:ASN:OD1	1:A:3253:ASN:HB3	2.03	0.57
1:A:3288:GLY:HA3	1:A:3574:TRP:CZ3	2.39	0.57
1:A:3814:SER:O	1:A:3815:ASP:C	2.46	0.57
1:B:1872:ARG:HH12	1:B:2164:ARG:HD3	1.70	0.57
1:B:2720:TYR:CE1	1:B:2730:LEU:HD13	2.39	0.57
1:B:4186:LEU:HD12	1:B:4187:LEU:N	2.20	0.57
1:B:3095:GLU:HG3	1:B:3134:THR:CG2	2.34	0.57
1:B:3350:VAL:C	1:B:3352:ASN:N	2.59	0.57
1:B:4076:ILE:HD13	1:B:4105:VAL:CG1	2.33	0.57
1:B:4673:ASP:C	1:B:4675:ASP:H	2.11	0.57
1:A:1792:PHE:HE1	1:A:1803:TYR:HE1	1.49	0.57
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.86	0.57
1:A:3807:PRO:O	1:A:3808:ASP:C	2.48	0.57
1:B:3061:ARG:HB2	1:B:3069:ILE:HD11	1.86	0.57
1:B:4349:ASN:OD1	1:B:4351:PHE:N	2.37	0.57
1:A:1558:TRP:HH2	1:A:1605:TRP:CD1	2.23	0.57
1:A:2258:LYS:HD3	1:A:2261:GLN:OE1	2.04	0.57
1:A:3039:THR:HG22	1:A:3040:ILE:N	2.18	0.57
1:A:3219:ILE:CB	1:A:3220:PRO:HD3	2.35	0.57
1:A:3315:VAL:O	1:A:3319:GLN:HG3	2.03	0.57
1:A:3674:VAL:HG12	1:A:3676:ASP:HB2	1.86	0.57
1:B:1562:PHE:O	1:B:1565:LEU:C	2.48	0.57
1:B:2729:VAL:HG12	1:B:2782:LYS:HB3	1.86	0.57
1:B:3923:LEU:HD22	1:B:3947:ILE:CG2	2.34	0.57
1:A:1594:ARG:O	1:A:1598:VAL:HG23	2.04	0.57
1:A:2123:VAL:HG12	1:A:2127:LYS:HD2	1.87	0.57
1:A:2262:LEU:HD11	1:A:2416:PHE:HZ	1.70	0.57
1:A:2405:LEU:HA	1:A:2408:ILE:CG1	2.35	0.57
1:A:2573:LEU:HD23	1:A:2573:LEU:C	2.30	0.57
1:B:1614:TYR:CD2	1:B:1615:LEU:HD22	2.40	0.57
1:B:3115:THR:C	1:B:3117:GLN:N	2.60	0.57
1:B:4169:GLU:C	1:B:4171:ALA:N	2.61	0.57
1:A:2212:ILE:H	1:A:2213:PRO:HD2	1.70	0.57
1:A:2284:THR:HG21	2:A:9002:ADP:N7	2.20	0.57
1:A:3806:ARG:HG3	1:A:3882:VAL:CG1	2.31	0.57
1:A:4183:THR:C	1:A:4184:TRP:HD1	2.12	0.57
1:B:1739:THR:HB	1:B:1761:ALA:HB2	1.87	0.57
1:B:1925:LEU:HD12	1:B:1926:VAL:H	1.70	0.57
1:B:2564:ASN:O	1:B:2566:SER:N	2.36	0.57
1:B:3340:ASP:O	1:B:3343:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3727:ASP:CB	1:B:3729:VAL:HG12	2.34	0.57
1:A:2440:ASP:OD1	1:A:2442:GLN:HB2	2.04	0.57
1:A:2902:VAL:CG2	1:A:2941:VAL:HG21	2.20	0.57
1:A:3695:THR:HB	1:A:3718:LEU:CD1	2.34	0.57
1:B:1886:ARG:HH11	1:B:1890:ARG:CZ	2.17	0.57
1:B:4261:ASP:OD1	1:B:4388:THR:HB	2.05	0.57
1:A:2375:LYS:HB3	1:A:2387:LEU:HB3	1.87	0.57
1:A:3682:MET:SD	1:A:3696:LYS:HD2	2.45	0.57
1:A:4339:GLY:O	1:A:4344:GLY:HA3	2.04	0.57
1:A:4657:THR:H	1:A:4719:ARG:NH2	2.01	0.57
1:B:1889:VAL:O	1:B:1893:GLN:HG3	2.05	0.57
1:A:2898:LEU:HD22	1:A:2941:VAL:CG2	2.35	0.57
1:A:3246:LEU:O	1:A:3249:GLN:O	2.21	0.57
1:A:3337:LYS:O	1:A:3341:ALA:N	2.35	0.57
1:B:1558:TRP:CZ3	1:B:1602:LEU:HB3	2.38	0.57
1:B:1980:LYS:O	1:B:1984:VAL:HG23	2.05	0.57
1:B:2128:ILE:HG23	1:B:2129:VAL:N	2.20	0.57
1:A:1770:LEU:O	1:A:1773:VAL:HG22	2.04	0.56
1:A:3817:LEU:CD2	1:A:3817:LEU:N	2.68	0.56
1:A:1796:ASP:O	1:A:1798:ASN:N	2.37	0.56
1:A:1799:ASP:OD1	1:A:1802:LYS:N	2.37	0.56
1:A:1853:GLN:HA	1:A:1856:LEU:HD12	1.87	0.56
1:A:2422:THR:HB	1:A:2425:MET:HG3	1.87	0.56
1:A:2439:PHE:N	1:A:2495:GLN:HE22	1.99	0.56
1:A:3936:PRO:HG2	1:A:3937:ASN:N	2.16	0.56
1:A:4050:LYS:O	1:A:4051:ASP:C	2.48	0.56
1:A:4146:VAL:HG12	1:A:4157:TYR:OH	2.04	0.56
1:B:1729:LEU:HD11	1:B:1732:LEU:HD21	1.88	0.56
1:B:2611:PRO:C	1:B:2613:LEU:N	2.62	0.56
1:B:3061:ARG:HB3	1:B:3067:GLU:OE2	2.04	0.56
1:B:4362:GLN:HB2	1:B:4714:GLN:NE2	2.19	0.56
1:B:4570:LYS:O	1:B:4573:GLN:HB2	2.04	0.56
1:B:4657:THR:HG21	1:B:4659:ILE:HB	1.86	0.56
1:A:2140:SER:HB3	1:A:2142:GLN:HE22	1.70	0.56
1:A:2192:ILE:HG23	1:A:2223:PHE:CD1	2.40	0.56
1:A:2898:LEU:HD13	1:A:2941:VAL:HG23	1.86	0.56
1:A:3515:GLN:C	1:A:3517:GLU:N	2.61	0.56
1:A:3866:ALA:O	1:A:3869:VAL:HB	2.04	0.56
1:A:3928:PRO:O	1:A:3930:LEU:N	2.39	0.56
1:A:4368:ALA:HA	1:A:4373:PHE:CD1	2.39	0.56
1:A:4621:LEU:HD21	1:A:4669:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2309:LYS:O	1:B:2758:ARG:HD2	2.05	0.56
1:B:2427:PHE:CE1	1:B:2534:LEU:HD21	2.40	0.56
1:B:2491:GLY:C	1:B:2493:LYS:N	2.62	0.56
1:B:2494:VAL:HG11	1:B:2548:VAL:CG1	2.35	0.56
1:B:3135:SER:HA	1:B:3138:ARG:HG2	1.88	0.56
1:B:3315:VAL:O	1:B:3316:LYS:C	2.48	0.56
1:B:3776:ASP:O	1:B:3780:ARG:HG2	2.05	0.56
1:B:4119:ALA:CA	1:B:4149:LEU:HD11	2.34	0.56
1:B:4121:ILE:HA	1:B:4125:GLU:HG3	1.86	0.56
1:B:4276:TRP:CE2	1:B:4375:LEU:HD22	2.41	0.56
1:B:4322:SER:CB	1:B:4323:ASN:HD22	2.19	0.56
1:A:1671:ARG:O	1:A:1675:LEU:HD13	2.05	0.56
1:A:1928:HIS:CD2	1:A:1933:THR:HG22	2.40	0.56
1:A:2864:PHE:O	1:A:2872:TYR:HB3	2.05	0.56
1:A:4137:VAL:CG2	1:A:4138:PRO:HD2	2.36	0.56
1:A:4278:HIS:HD2	1:A:4343:TYR:OH	1.88	0.56
1:B:2379:LEU:C	1:B:2381:ASN:H	2.13	0.56
1:B:3921:TYR:CE2	1:B:3925:ASN:ND2	2.72	0.56
1:A:1419:TRP:C	1:A:1421:ALA:N	2.61	0.56
1:A:1800:HIS:HB2	1:A:1858:ASN:HD22	1.71	0.56
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.51	0.56
1:B:1837:GLN:O	1:B:1838:GLN:C	2.48	0.56
1:B:3047:LYS:C	1:B:3049:SER:H	2.13	0.56
1:B:3091:LEU:HD11	1:B:3145:PHE:CE2	2.40	0.56
1:B:3635:PRO:HA	1:B:3663:ILE:HG13	1.86	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.45	0.56
1:B:4278:HIS:HD2	1:B:4343:TYR:OH	1.88	0.56
1:A:2257:GLU:O	1:A:2261:GLN:HG3	2.06	0.56
1:A:2574:LEU:HD22	1:A:2597:ILE:HG22	1.88	0.56
1:A:4188:LYS:HA	1:A:4218:THR:CG2	2.28	0.56
1:A:4190:ILE:HB	1:A:4197:LEU:HD11	1.88	0.56
1:B:3207:GLN:O	1:B:3210:GLU:HB2	2.06	0.56
1:B:3827:LEU:O	1:B:3831:GLU:HG3	2.05	0.56
1:B:4147:ASP:OD1	1:B:4157:TYR:OH	2.24	0.56
1:B:4264:PRO:HB3	1:B:4323:ASN:HA	1.87	0.56
1:B:4693:ASN:ND2	1:B:4693:ASN:N	2.47	0.56
1:A:2059:LEU:HG	1:A:2060:LEU:CD1	2.32	0.56
1:A:2528:PHE:CE1	1:A:2533:VAL:HG11	2.41	0.56
1:A:2536:SER:HB2	1:A:2580:GLY:O	2.06	0.56
1:A:3287:ILE:O	1:A:3291:LYS:HG2	2.06	0.56
1:A:4263:GLN:O	1:A:4267:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2237:ARG:HE	1:B:2260:LEU:CD2	2.18	0.56
1:B:2265:ILE:HD12	1:B:2414:VAL:HG22	1.88	0.56
1:B:4537:LEU:O	1:B:4541:ILE:HG13	2.05	0.56
1:A:2380:PRO:C	1:A:2382:GLY:H	2.14	0.56
1:A:2571:ASN:OD1	1:A:2624:TRP:NE1	2.38	0.56
1:A:3331:GLN:HG3	1:A:3532:TYR:HB3	1.87	0.56
1:A:3721:GLN:O	1:A:3722:ASP:C	2.49	0.56
1:A:4600:TYR:O	1:A:4604:THR:HG23	2.06	0.56
1:B:2965:ARG:HD3	1:B:2995:LEU:HD12	1.87	0.56
1:B:3966:THR:HG22	1:B:4426:MET:HE2	1.87	0.56
1:A:4188:LYS:CA	1:A:4218:THR:HG22	2.28	0.56
1:B:1875:PHE:O	1:B:1879:ILE:HG13	2.05	0.56
1:B:2332:PHE:HE1	1:B:2353:ILE:HG21	1.71	0.56
1:B:2379:LEU:HD12	1:B:2383:GLU:CG	2.33	0.56
1:B:4423:ALA:O	1:B:4427:ILE:HG12	2.05	0.56
1:A:1531:LEU:HD11	1:A:1584:PHE:HB3	1.88	0.56
1:A:2612:LEU:HD11	1:A:2624:TRP:CH2	2.41	0.56
1:A:3268:VAL:HG12	1:A:3269:LEU:HD23	1.87	0.56
1:A:3270:LEU:HB3	1:A:3592:VAL:HG13	1.88	0.56
1:A:3664:MET:O	1:A:3668:PHE:HB3	2.05	0.56
1:B:3289:LEU:HD13	1:B:3293:ARG:HH21	1.71	0.56
1:B:4214:ARG:CG	1:B:4214:ARG:HH11	2.18	0.56
1:A:1554:LEU:HB3	1:A:1609:GLN:CD	2.31	0.55
1:A:2855:GLU:O	1:A:2859:GLU:HG2	2.06	0.55
1:A:4121:ILE:HG21	1:A:4236:PHE:HZ	1.71	0.55
1:A:4166:GLU:O	1:A:4170:LEU:HG	2.06	0.55
1:A:4711:THR:CG2	1:A:4715:ASN:HB3	2.36	0.55
1:B:3019:GLY:HA2	2:B:9010:ADP:H5'2	1.89	0.55
1:B:3568:ASN:ND2	1:B:3571:ARG:HH12	2.04	0.55
1:B:4184:TRP:NE1	1:B:4214:ARG:HG3	2.20	0.55
1:A:2262:LEU:HG	1:A:2414:VAL:HG21	1.89	0.55
1:A:3788:VAL:HG21	1:A:3913:LEU:CD2	2.36	0.55
1:A:4620:ARG:NH1	1:A:4679:PHE:HB3	2.22	0.55
1:B:1863:VAL:HG21	1:B:2115:SER:O	2.05	0.55
1:B:2597:ILE:O	1:B:2600:ILE:HG22	2.05	0.55
1:B:3278:LEU:HD12	1:B:3585:MET:CE	2.36	0.55
1:A:1639:ILE:HG21	1:A:1676:LEU:HD21	1.87	0.55
1:A:2641:VAL:O	1:A:2643:SER:N	2.39	0.55
1:A:2856:PHE:HZ	1:A:2926:THR:HG23	1.72	0.55
1:A:3194:LEU:O	1:A:3223:HIS:HD2	1.89	0.55
1:B:2714:PHE:C	1:B:2716:HIS:N	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4186:LEU:HA	1:B:4216:PHE:O	2.06	0.55
1:B:4280:ILE:CD1	1:B:4408:LEU:HD23	2.36	0.55
1:A:3118:ARG:C	1:A:3120:GLY:N	2.64	0.55
1:B:1831:LEU:HA	1:B:1841:ILE:HG23	1.88	0.55
1:B:2636:VAL:HG12	1:B:2637:GLU:N	2.22	0.55
1:B:3708:LEU:HD21	1:B:3730:LEU:CD2	2.35	0.55
1:B:4523:LEU:O	1:B:4523:LEU:HD23	2.06	0.55
1:A:2028:PHE:CB	1:A:2075:VAL:HG13	2.36	0.55
1:A:2595:LYS:HA	1:A:2598:GLN:HB2	1.89	0.55
1:A:2677:GLY:O	2:A:9003:ADP:H5'2	2.06	0.55
1:A:3109:MET:HA	1:A:3109:MET:HE2	1.88	0.55
1:A:3528:SER:O	1:A:3532:TYR:HD1	1.90	0.55
1:B:1920:ASN:HD22	1:B:1921:VAL:N	2.04	0.55
1:B:1947:LEU:HD21	1:B:1982:GLU:HG2	1.88	0.55
1:B:2607:ALA:C	1:B:2609:THR:H	2.13	0.55
1:A:1709:ILE:O	1:A:1712:SER:HB2	2.06	0.55
1:A:2949:PRO:HG2	1:A:2951:LEU:HD13	1.89	0.55
1:A:3001:ILE:O	1:A:3004:VAL:HB	2.06	0.55
1:A:3046:TYR:CD2	1:A:3079:LEU:HD12	2.42	0.55
1:A:3929:ASN:ND2	1:A:3942:TYR:CD1	2.70	0.55
1:A:4551:LYS:C	1:A:4553:TYR:H	2.14	0.55
1:B:1555:VAL:HG22	1:B:1609:GLN:NE2	2.19	0.55
1:B:2044:GLN:O	1:B:2048:VAL:HG23	2.06	0.55
1:B:2250:VAL:HB	1:B:2425:MET:CG	2.36	0.55
1:B:2250:VAL:HB	1:B:2425:MET:HG2	1.88	0.55
1:B:3211:ILE:O	1:B:3212:MET:HB2	2.07	0.55
1:B:4189:ASN:N	1:B:4218:THR:HG22	2.17	0.55
1:A:1662:ILE:HB	1:A:1665:ILE:CG1	2.36	0.55
1:A:1856:LEU:HD22	1:A:2114:TYR:HE2	1.71	0.55
1:A:2314:ASP:OD1	1:A:2319:SER:HB3	2.06	0.55
1:A:3359:LYS:NZ	1:A:3505:GLU:HA	2.22	0.55
1:B:1719:GLN:HA	1:B:1722:PHE:CD2	2.41	0.55
1:B:1766:ILE:HG23	1:B:1767:HIS:N	2.21	0.55
1:B:3966:THR:HB	1:B:4426:MET:HG3	1.87	0.55
1:B:4289:PRO:HA	1:B:4292:TRP:O	2.07	0.55
1:A:2090:ASN:ND2	1:A:2091:LEU:HG	2.22	0.55
1:A:3860:LYS:C	1:A:3862:THR:N	2.64	0.55
1:A:3864:GLU:HG3	1:A:3865:ILE:H	1.70	0.55
1:A:4143:SER:HB2	1:A:4188:LYS:HD2	1.89	0.55
1:A:4157:TYR:OH	1:A:4186:LEU:HD22	2.07	0.55
1:B:1662:ILE:CG2	1:B:1663:GLU:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2000:CYS:C	1:B:2002:GLU:H	2.14	0.55
1:B:2515:VAL:HG11	1:B:2577:LEU:CD1	2.33	0.55
1:B:2627:TRP:CE2	1:B:2655:ARG:HB3	2.40	0.55
1:B:3584:GLN:O	1:B:3588:VAL:HG23	2.06	0.55
1:B:3612:ASP:O	1:B:3616:LYS:HG3	2.07	0.55
1:B:4036:HIS:HD2	1:B:4044:TRP:HE1	1.54	0.55
1:A:2000:CYS:CB	1:A:2031:LEU:HD13	2.22	0.55
1:A:4693:ASN:ND2	1:A:4695:THR:OG1	2.40	0.55
1:B:1611:ARG:O	1:B:1614:TYR:N	2.40	0.55
1:B:1624:ASP:OD2	1:B:1710:GLY:O	2.25	0.55
1:B:1785:LEU:CA	1:B:1814:LEU:HD23	2.36	0.55
1:B:2128:ILE:O	1:B:2131:LEU:HB3	2.07	0.55
1:B:2506:PHE:HE1	1:B:2573:LEU:HD11	1.71	0.55
1:B:2669:PRO:HA	1:B:2788:PHE:O	2.06	0.55
1:B:3232:VAL:O	1:B:3236:GLN:HG3	2.06	0.55
1:A:3197:PRO:C	1:A:3198:GLN:HG3	2.32	0.55
1:A:3816:LEU:HB3	1:A:3817:LEU:HD23	1.87	0.55
1:A:4436:SER:C	1:A:4438:GLU:H	2.15	0.55
1:B:2197:ASN:O	1:B:2197:ASN:ND2	2.39	0.55
1:B:3104:GLU:C	1:B:3106:THR:H	2.15	0.55
1:B:3238:ILE:HG12	1:B:3601:TYR:CG	2.42	0.55
1:B:4351:PHE:CE2	1:B:4689:PRO:HG3	2.42	0.55
1:A:1565:LEU:O	1:A:1569:LEU:HB2	2.06	0.54
1:A:3571:ARG:HH11	1:A:3571:ARG:CB	2.19	0.54
1:A:4118:MET:O	1:A:4122:VAL:HG12	2.08	0.54
1:B:2163:LYS:C	1:B:2165:LYS:H	2.16	0.54
1:B:2599:THR:O	1:B:2599:THR:HG22	2.06	0.54
1:B:3315:VAL:HG12	1:B:3316:LYS:N	2.21	0.54
1:B:3575:GLU:C	1:B:3577:GLN:H	2.15	0.54
1:B:4176:TYR:OH	1:B:4203:LYS:HG3	2.06	0.54
1:A:2204:ILE:HG23	1:A:2205:PRO:HD3	1.89	0.54
1:A:4134:LEU:HB3	1:A:4238:TYR:CE2	2.42	0.54
1:B:2714:PHE:O	1:B:2716:HIS:N	2.40	0.54
1:B:3704:PHE:CD2	1:B:3705:MET:N	2.75	0.54
1:B:4711:THR:HG1	1:B:4716:TRP:CD1	2.25	0.54
1:A:2863:ARG:HG3	1:A:2925:TRP:CZ2	2.42	0.54
1:A:3511:LEU:O	1:A:3514:LYS:N	2.40	0.54
1:A:3981:ASN:HB3	1:A:4074:SER:OG	2.07	0.54
1:A:4134:LEU:HD23	1:A:4238:TYR:OH	2.07	0.54
1:B:1548:TYR:CD1	1:B:1548:TYR:C	2.86	0.54
1:B:1640:ASN:O	1:B:1644:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2223:PHE:C	1:B:2225:GLY:N	2.63	0.54
1:B:2502:ILE:CG2	1:B:2573:LEU:HD13	2.38	0.54
1:B:2525:ILE:HD12	1:B:2525:ILE:H	1.72	0.54
1:B:3028:PHE:O	1:B:3032:MET:HG2	2.06	0.54
1:B:3577:GLN:O	1:B:3580:ASN:HB2	2.06	0.54
1:A:1764:PRO:CG	1:A:1772:MET:HE1	2.38	0.54
1:A:2026:ASP:OD2	1:A:2026:ASP:C	2.50	0.54
1:A:2212:ILE:N	1:A:2213:PRO:HD2	2.22	0.54
1:A:2998:ILE:HG22	1:A:3029:VAL:CG2	2.38	0.54
1:A:3331:GLN:HG3	1:A:3532:TYR:HB2	1.89	0.54
1:A:3563:LEU:HD21	1:A:3845:ILE:HG22	1.89	0.54
1:B:4688:VAL:HG13	1:B:4722:SER:HA	1.89	0.54
1:A:2398:GLN:HE22	1:A:2805:HIS:HB2	1.72	0.54
1:A:2426:ILE:HD12	1:A:2530:ARG:HH11	1.71	0.54
1:A:2898:LEU:HD13	1:A:2941:VAL:CG2	2.38	0.54
1:A:3238:ILE:N	1:A:3238:ILE:HD12	2.23	0.54
1:A:3825:VAL:C	1:A:3827:LEU:H	2.15	0.54
1:B:2381:ASN:ND2	1:B:2381:ASN:C	2.66	0.54
1:B:4157:TYR:HB3	1:B:4184:TRP:HB2	1.90	0.54
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.22	0.54
1:A:2187:TYR:O	1:A:2190:TYR:HB3	2.06	0.54
1:A:2498:CYS:O	1:A:2502:ILE:HG12	2.07	0.54
1:A:2819:PRO:HD2	1:A:2876:PRO:HG2	1.89	0.54
1:A:3238:ILE:HG12	1:A:3601:TYR:CG	2.43	0.54
1:A:3308:GLN:O	1:A:3311:ARG:N	2.36	0.54
1:A:4494:PRO:HD2	1:A:4610:GLN:NE2	2.22	0.54
1:A:4678:ILE:O	1:A:4680:ASN:N	2.39	0.54
1:B:2556:SER:O	1:B:2559:PRO:HD3	2.08	0.54
1:B:4200:LEU:O	1:B:4204:LEU:HB2	2.06	0.54
1:B:4657:THR:HG22	1:B:4659:ILE:N	2.22	0.54
1:B:3052:ASP:HA	1:B:3055:LEU:HB2	1.88	0.54
1:B:4089:PHE:C	3:B:9022:SPM:H131	2.33	0.54
1:A:1836:LEU:O	1:A:1837:GLN:C	2.50	0.54
1:A:2667:HIS:HB2	3:A:9012:SPM:H121	1.90	0.54
1:A:3039:THR:CG2	1:A:3040:ILE:N	2.69	0.54
1:B:2372:ASP:HB3	1:B:2410:ARG:HD3	1.90	0.54
1:B:2611:PRO:C	1:B:2613:LEU:H	2.15	0.54
1:B:2642:ALA:HB3	1:B:2884:ARG:HG3	1.89	0.54
1:B:3298:GLN:O	1:B:3302:LEU:HB2	2.08	0.54
1:B:4099:HIS:CD2	1:B:4099:HIS:C	2.85	0.54
1:B:4604:THR:CG2	1:B:4604:THR:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2266:LEU:O	1:A:2392:ARG:NH1	2.41	0.54
1:B:1945:GLU:OE1	1:B:1945:GLU:HA	2.08	0.54
1:B:2572:ARG:NH1	1:B:2575:TYR:CE2	2.76	0.54
1:B:4332:ILE:O	1:B:4336:THR:HG23	2.08	0.54
1:A:2259:ILE:CG2	1:A:2289:TYR:HB2	2.38	0.54
1:A:2313:LYS:HE3	1:A:2366:ASN:ND2	2.22	0.54
1:A:4572:MET:HE2	1:A:4575:LEU:CD1	2.37	0.54
1:B:1996:LEU:HD13	1:B:2016:LEU:HD21	1.89	0.54
1:A:1527:LEU:O	1:A:1530:PHE:HB3	2.08	0.53
1:A:2204:ILE:N	1:A:2205:PRO:CD	2.72	0.53
1:A:2525:ILE:HD12	1:A:2526:MET:H	1.73	0.53
1:A:3312:GLU:O	1:A:3316:LYS:HB2	2.08	0.53
1:B:1554:LEU:HD22	1:B:1609:GLN:CD	2.34	0.53
1:B:1606:ILE:HG23	1:B:1607:ASP:N	2.23	0.53
1:B:2273:MET:HG2	1:B:2395:PHE:HB2	1.90	0.53
1:B:3108:LEU:HD11	1:B:3133:PHE:CZ	2.43	0.53
1:B:4622:HIS:O	1:B:4669:LEU:HA	2.07	0.53
1:A:1949:GLN:NE2	1:A:1953:THR:HG21	2.23	0.53
1:A:3774:THR:O	1:A:3775:PRO:C	2.49	0.53
1:A:3987:GLU:OE1	1:A:4081:ARG:NE	2.38	0.53
1:B:2401:LYS:HD3	1:B:2402:TYR:CE2	2.43	0.53
1:B:3973:ILE:HG13	1:B:3988:TRP:CE3	2.43	0.53
1:A:1702:ASP:O	1:A:1706:LEU:HG	2.07	0.53
1:A:1734:LEU:C	1:A:1742:ILE:HD11	2.33	0.53
1:A:2215:ILE:HG23	1:A:2216:GLN:N	2.24	0.53
1:A:2828:TYR:CZ	1:A:2879:LEU:HB3	2.44	0.53
1:A:3069:ILE:HG22	1:A:3070:CYS:N	2.23	0.53
1:A:3086:ARG:NH1	1:A:3096:VAL:HG12	2.23	0.53
1:B:2282:LYS:HB2	2:B:9008:ADP:O3B	2.07	0.53
1:B:2720:TYR:HA	1:B:2729:VAL:O	2.09	0.53
1:B:3185:GLY:HA2	1:B:3264:ILE:CD1	2.37	0.53
1:A:1572:ILE:O	1:A:1575:MET:HG2	2.07	0.53
1:A:3056:ARG:NH1	1:A:3099:LEU:HD12	2.23	0.53
1:A:3338:GLN:HE21	1:A:3338:GLN:HA	1.72	0.53
1:A:3605:PHE:CD1	1:A:3605:PHE:N	2.74	0.53
1:A:4553:TYR:HD2	1:A:4595:LEU:HD22	1.73	0.53
1:B:2942:ASN:HD21	1:B:2944:ASP:HB2	1.71	0.53
1:B:3316:LYS:O	1:B:3317:ASN:C	2.52	0.53
1:B:3324:LEU:O	1:B:3328:VAL:HG12	2.08	0.53
1:B:4118:MET:O	1:B:4122:VAL:HG22	2.09	0.53
1:A:1419:TRP:NE1	1:A:1481:TRP:HZ2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1520:ALA:O	1:A:1524:GLU:HG3	2.09	0.53
1:A:2227:GLN:O	1:A:2229:GLN:NE2	2.37	0.53
1:A:2357:GLY:O	1:A:2397:VAL:HG12	2.08	0.53
1:A:2699:LEU:HD22	1:A:2741:VAL:CG1	2.38	0.53
1:A:3808:ASP:OD2	1:A:3809:THR:HG23	2.09	0.53
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	1.90	0.53
1:A:4418:LEU:HD11	1:A:4422:LYS:NZ	2.24	0.53
1:A:4621:LEU:CD2	1:A:4669:LEU:HD23	2.38	0.53
1:B:1691:ARG:NH2	1:B:1702:ASP:OD2	2.38	0.53
1:B:1755:LYS:O	1:B:1757:PRO:HD3	2.08	0.53
1:B:2339:ILE:HA	1:B:2346:GLU:HG2	1.90	0.53
1:B:3689:TYR:O	1:B:3690:ALA:C	2.51	0.53
1:B:4229:LEU:O	1:B:4233:SER:OG	2.27	0.53
1:A:3780:ARG:HB2	1:A:3780:ARG:HH11	1.73	0.53
1:A:3960:LEU:HA	1:A:4239:GLU:OE2	2.09	0.53
1:B:2602:ILE:O	1:B:2603:THR:O	2.27	0.53
1:B:2714:PHE:CZ	1:B:2766:MET:HE1	2.44	0.53
1:B:4432:LYS:C	1:B:4434:GLN:H	2.17	0.53
1:A:1840:LYS:O	1:A:1843:GLU:HB3	2.08	0.53
1:A:2918:VAL:HG22	1:A:3172:TRP:CE2	2.43	0.53
1:A:3027:ARG:O	1:A:3030:ALA:HB3	2.09	0.53
1:A:3069:ILE:N	1:A:3069:ILE:HD12	2.22	0.53
1:A:3335:GLU:CG	1:A:3529:ILE:HD11	2.38	0.53
1:A:3789:THR:HG22	1:A:3792:SER:OG	2.08	0.53
1:A:4040:ASN:N	1:A:4040:ASN:ND2	2.55	0.53
1:A:4067:ALA:O	1:A:4073:GLN:NE2	2.42	0.53
1:A:4137:VAL:HG23	1:A:4138:PRO:HD2	1.91	0.53
1:B:2295:GLN:O	1:B:2296:VAL:C	2.51	0.53
1:B:2617:VAL:HG22	1:B:2624:TRP:CZ3	2.44	0.53
1:B:3289:LEU:HD13	1:B:3293:ARG:NH2	2.23	0.53
1:B:3690:ALA:O	1:B:3691:ASP:C	2.52	0.53
1:B:4640:LYS:HB3	1:B:4666:ILE:CD1	2.37	0.53
1:A:1916:ALA:C	1:A:1918:GLN:H	2.16	0.53
1:A:2937:HIS:C	1:A:2939:PRO:HD3	2.34	0.53
1:A:3234:ILE:O	1:A:3238:ILE:HD13	2.09	0.53
1:B:2554:LEU:O	1:B:2556:SER:N	2.40	0.53
1:B:3677:PRO:CD	1:B:3787:THR:HG22	2.39	0.53
1:A:1734:LEU:CD2	1:A:1741:ILE:HD13	2.39	0.53
1:A:3252:GLN:HE21	1:A:3253:ASN:H	1.57	0.53
1:A:3525:LEU:O	1:A:3526:GLU:C	2.51	0.53
1:A:3605:PHE:HB3	1:A:3609:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2491:GLY:C	1:B:2493:LYS:H	2.16	0.53
1:B:2793:ASN:ND2	1:B:2800:ARG:HH21	2.07	0.53
1:B:4603:ALA:C	1:B:4605:ARG:H	2.16	0.53
1:A:1879:ILE:O	1:A:1883:VAL:HG23	2.08	0.53
1:A:4501:ARG:O	1:A:4505:THR:OG1	2.17	0.53
1:B:2738:TRP:CH2	1:B:2785:LYS:HA	2.43	0.53
1:B:3529:ILE:O	1:B:3533:LYS:HB2	2.08	0.53
1:B:4647:ALA:O	1:B:4662:THR:CG2	2.56	0.53
1:A:1490:THR:HG21	1:A:1492:TRP:NE1	2.24	0.52
1:A:1506:ASP:CB	1:A:1509:ARG:HB3	2.40	0.52
1:A:1710:GLY:C	1:A:1712:SER:H	2.17	0.52
1:A:2140:SER:HB3	1:A:2142:GLN:NE2	2.23	0.52
1:A:2206:LYS:HG2	1:A:2413:MET:O	2.10	0.52
1:A:2748:LEU:N	1:A:2749:PRO:CD	2.73	0.52
1:A:3928:PRO:C	1:A:3930:LEU:N	2.66	0.52
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.40	0.52
1:B:3047:LYS:O	1:B:3050:ASP:HB2	2.09	0.52
1:B:4252:PHE:CG	1:B:4393:MET:HE3	2.44	0.52
1:B:4657:THR:CG2	1:B:4659:ILE:H	2.22	0.52
1:A:2524:HIS:CD2	1:A:2528:PHE:HB2	2.44	0.52
1:A:2798:ALA:O	1:A:2800:ARG:NH1	2.42	0.52
1:A:3334:ALA:O	1:A:3335:GLU:C	2.52	0.52
1:B:2128:ILE:HD13	1:B:2195:LEU:HD21	1.91	0.52
1:A:3117:GLN:HG2	1:A:3118:ARG:N	2.24	0.52
1:A:3346:VAL:O	1:A:3349:ASP:HB2	2.10	0.52
1:A:4170:LEU:N	1:A:4170:LEU:HD23	2.24	0.52
1:A:4605:ARG:HG2	1:A:4605:ARG:HH11	1.74	0.52
1:B:1695:ALA:C	1:B:1697:PHE:H	2.17	0.52
1:B:1925:LEU:HD12	1:B:1926:VAL:N	2.23	0.52
1:B:2432:ASP:O	1:B:2434:LEU:N	2.42	0.52
1:B:4484:LEU:C	1:B:4484:LEU:CD2	2.81	0.52
1:A:1424:PRO:HB3	1:A:1469:THR:OG1	2.09	0.52
1:A:2378:THR:HA	1:A:2384:ARG:HA	1.91	0.52
1:A:2568:TYR:HB2	1:A:2622:ALA:HB1	1.90	0.52
1:A:3571:ARG:HH11	1:A:3571:ARG:C	2.18	0.52
1:A:3766:THR:HG22	1:A:3767:ARG:N	2.24	0.52
1:A:4580:GLU:O	1:A:4581:SER:C	2.51	0.52
1:B:1816:LEU:O	1:B:1820:GLN:HG3	2.10	0.52
1:B:1904:PHE:C	1:B:1906:TRP:N	2.66	0.52
1:B:2223:PHE:O	1:B:2225:GLY:N	2.43	0.52
1:B:4189:ASN:H	1:B:4189:ASN:HD22	1.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4349:ASN:OD1	1:B:4352:ASP:N	2.30	0.52
1:B:4522:GLU:O	1:B:4523:LEU:C	2.51	0.52
1:A:2359:VAL:HG23	1:A:2397:VAL:HG11	1.90	0.52
1:A:2408:ILE:HG13	1:A:2409:SER:H	1.74	0.52
1:A:3064:CYS:C	1:A:3066:GLU:H	2.17	0.52
1:A:3337:LYS:H	1:A:3337:LYS:HD2	1.75	0.52
1:A:3896:VAL:O	1:A:3899:ALA:HB3	2.10	0.52
1:B:2165:LYS:O	1:B:2166:CYS:HB2	2.09	0.52
1:B:2976:LEU:HD11	1:B:2990:LEU:HD21	1.91	0.52
1:B:3313:LEU:HD13	1:B:3550:SER:HA	1.91	0.52
1:A:2591:GLU:HG2	1:A:2613:LEU:HD22	1.91	0.52
1:A:2746:ILE:O	1:A:2749:PRO:HD2	2.10	0.52
1:A:2918:VAL:O	1:A:2919:GLU:HG2	2.10	0.52
1:A:3695:THR:HB	1:A:3718:LEU:HD11	1.92	0.52
1:B:1817:LEU:O	1:B:1821:ILE:HG13	2.10	0.52
1:B:3103:GLU:O	1:B:3106:THR:HG23	2.10	0.52
1:A:3063:GLY:HA3	1:A:3133:PHE:CE1	2.44	0.52
1:B:1828:ASP:OD2	1:B:1901:ASN:HB2	2.09	0.52
1:B:1901:ASN:H	1:B:1901:ASN:HD22	1.57	0.52
1:B:4052:GLN:O	1:B:4053:VAL:C	2.51	0.52
1:B:4094:VAL:O	1:B:4098:SER:OG	2.27	0.52
1:B:4186:LEU:HD12	1:B:4187:LEU:H	1.74	0.52
1:B:4688:VAL:HG11	1:B:4723:ILE:HG13	1.91	0.52
1:A:2273:MET:O	1:A:2413:MET:HG3	2.10	0.52
1:A:2511:LEU:CD2	1:A:2515:VAL:HG23	2.39	0.52
1:A:2522:ARG:NH1	1:A:2589:GLU:OE2	2.42	0.52
1:A:2700:ASN:HD22	1:A:3089:THR:HG22	1.75	0.52
1:A:4134:LEU:HD12	1:A:4217:MET:O	2.10	0.52
1:A:4669:LEU:N	1:A:4669:LEU:HD12	2.24	0.52
1:B:3806:ARG:HD2	1:B:3882:VAL:HG11	1.91	0.52
1:B:4293:THR:HG22	1:B:4696:ARG:HD2	1.91	0.52
1:A:2179:SER:O	1:A:2180:LYS:C	2.52	0.52
1:A:3998:LEU:CD1	1:A:4018:LYS:HD3	2.40	0.52
1:A:4285:LEU:O	1:A:4288:ILE:HG13	2.10	0.52
1:B:1802:LYS:O	1:B:1805:GLU:HB3	2.09	0.52
1:B:2231:ILE:HD11	1:B:2233:MET:HB2	1.92	0.52
1:B:2997:HIS:C	1:B:2999:LEU:H	2.18	0.52
1:B:3324:LEU:HD11	1:B:3539:LEU:HB3	1.91	0.52
1:A:2378:THR:O	1:A:2378:THR:CG2	2.57	0.52
1:A:2697:VAL:HG23	1:A:2739:LEU:HD21	1.92	0.52
1:A:2845:PHE:CZ	1:B:4002:LYS:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2994:VAL:O	1:A:2998:ILE:HG12	2.10	0.52
1:A:3860:LYS:C	1:A:3862:THR:H	2.18	0.52
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.45	0.52
1:A:4381:LEU:HD11	1:A:4395:TRP:CZ2	2.45	0.52
1:B:2314:ASP:O	1:B:2316:LEU:N	2.42	0.52
1:B:2991:PHE:HA	1:B:3183:GLN:NE2	2.25	0.52
1:B:3161:SER:N	1:B:3162:PRO:HD3	2.25	0.52
1:A:1606:ILE:O	1:A:1610:ARG:HG3	2.10	0.51
1:A:1770:LEU:HA	1:A:1773:VAL:HG22	1.92	0.51
1:A:2672:LEU:O	1:A:2791:ALA:HA	2.10	0.51
1:A:3060:LYS:O	1:A:3064:CYS:HB2	2.10	0.51
1:A:3078:VAL:O	1:A:3078:VAL:HG13	2.11	0.51
1:B:1562:PHE:O	1:B:1566:ALA:N	2.43	0.51
1:B:3107:ALA:C	1:B:3109:MET:H	2.18	0.51
1:B:3317:ASN:O	1:B:3318:GLU:C	2.52	0.51
1:A:1719:GLN:HA	1:A:1722:PHE:CE2	2.45	0.51
1:A:2239:LYS:CE	1:A:2295:GLN:HE21	2.24	0.51
1:A:2988:LEU:HD21	1:A:3024:VAL:HG11	1.91	0.51
1:A:3506:ASN:O	1:A:3509:ASN:HB2	2.09	0.51
1:A:3947:ILE:HG23	1:A:3948:PHE:N	2.24	0.51
1:B:1607:ASP:O	1:B:1611:ARG:HD3	2.11	0.51
1:B:1846:GLN:HA	1:B:1893:GLN:NE2	2.25	0.51
1:B:2144:HIS:CB	1:B:2413:MET:HE3	2.37	0.51
1:B:3598:PHE:O	1:B:3602:ILE:HB	2.10	0.51
1:A:1720:LYS:HE2	1:A:2384:ARG:CZ	2.41	0.51
1:A:2112:MET:O	1:A:2116:GLN:HG2	2.10	0.51
1:B:1971:ASN:HD22	1:B:2097:SER:HB3	1.76	0.51
1:B:2506:PHE:CD1	1:B:2512:VAL:HG21	2.45	0.51
1:B:4050:LYS:O	1:B:4051:ASP:C	2.52	0.51
1:B:4648:VAL:HG23	1:B:4655:THR:HB	1.92	0.51
1:A:1656:ILE:O	1:A:1659:VAL:HG22	2.10	0.51
1:A:2873:ILE:HD12	1:A:2873:ILE:C	2.36	0.51
1:A:2885:ALA:HB1	1:A:2908:GLU:OE1	2.10	0.51
1:B:2278:SER:H	1:B:2398:GLN:HE21	1.57	0.51
1:B:3328:VAL:O	1:B:3332:GLN:HG3	2.09	0.51
1:B:4214:ARG:HH11	1:B:4214:ARG:HG3	1.75	0.51
1:A:1549:GLN:HE21	1:A:1551:LYS:NZ	2.08	0.51
1:A:2568:TYR:HB2	1:A:2622:ALA:CB	2.40	0.51
1:A:2935:LEU:HD21	1:A:2943:LEU:HD23	1.91	0.51
1:A:3182:PHE:CE1	1:A:3217:MET:HE2	2.45	0.51
1:A:3880:SER:O	1:A:3881:GLU:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3930:LEU:HD11	1:A:3939:ARG:HG2	1.93	0.51
1:A:4507:GLY:HA2	1:A:4510:VAL:HG23	1.93	0.51
1:B:2574:LEU:HD11	1:B:2601:ALA:HB1	1.91	0.51
1:B:4079:ASN:O	1:B:4082:LYS:HB2	2.10	0.51
1:A:1528:GLU:HB2	1:A:1584:PHE:CE1	2.45	0.51
1:A:1722:PHE:C	1:A:1724:LYS:N	2.68	0.51
1:A:2405:LEU:CD2	1:A:2408:ILE:HD11	2.41	0.51
1:A:3251:ARG:HH12	1:A:3675:ILE:HD13	1.74	0.51
1:A:3515:GLN:C	1:A:3517:GLU:H	2.18	0.51
1:A:3634:VAL:N	1:A:3635:PRO:CD	2.74	0.51
1:A:3697:THR:HG21	1:A:3718:LEU:HD21	1.92	0.51
1:A:4046:GLN:HE22	1:A:4056:PRO:HA	1.75	0.51
1:A:4134:LEU:HD23	1:A:4238:TYR:CZ	2.46	0.51
1:A:4432:LYS:C	1:A:4434:GLN:H	2.17	0.51
1:A:4499:PHE:O	1:A:4503:ILE:HG13	2.11	0.51
1:B:2874:TYR:CE1	1:B:2916:ARG:CZ	2.94	0.51
1:B:4128:SER:OG	1:B:4209:PRO:HG2	2.11	0.51
1:B:4263:GLN:HA	1:B:4264:PRO:C	2.35	0.51
1:A:1722:PHE:C	1:A:1724:LYS:H	2.18	0.51
1:A:2575:TYR:HA	1:A:2578:MET:HE2	1.93	0.51
1:A:4622:HIS:O	1:A:4669:LEU:HA	2.10	0.51
1:B:1606:ILE:C	1:B:1608:VAL:N	2.68	0.51
1:B:1904:PHE:C	1:B:1906:TRP:H	2.19	0.51
1:B:2745:GLU:N	1:B:2791:ALA:O	2.44	0.51
1:B:3327:MET:SD	1:B:3535:GLU:HB3	2.50	0.51
1:B:3961:ASN:HA	1:B:3964:LYS:HE2	1.93	0.51
1:B:3981:ASN:OD1	1:B:4076:ILE:HD12	2.10	0.51
1:A:1820:GLN:NE2	1:A:1881:GLU:OE1	2.44	0.51
1:A:2640:LYS:O	1:A:2641:VAL:O	2.29	0.51
1:A:3598:PHE:HZ	1:A:3660:GLU:HB3	1.76	0.51
1:A:4556:PRO:O	1:A:4559:ILE:HG22	2.11	0.51
1:A:4646:GLY:O	1:A:4719:ARG:NH1	2.44	0.51
1:A:4659:ILE:HG22	1:A:4661:SER:N	2.26	0.51
1:B:2315:GLN:HB3	1:B:2775:THR:HG21	1.93	0.51
1:B:2379:LEU:HD12	1:B:2383:GLU:CB	2.40	0.51
1:B:2540:LEU:HD12	1:B:2662:ALA:CB	2.41	0.51
1:B:2615:TYR:HD1	1:B:2625:SER:O	1.94	0.51
1:B:3101:GLU:O	1:B:3104:GLU:HB2	2.11	0.51
1:B:3343:GLU:HG3	1:B:3347:GLN:HE22	1.75	0.51
1:B:3544:GLU:O	1:B:3545:GLN:C	2.54	0.51
1:B:3970:GLN:NE2	1:B:4433:MET:HE2	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4068:GLN:C	1:B:4070:SER:H	2.19	0.51
1:A:1769:TRP:HA	1:A:1772:MET:HE3	1.92	0.51
1:A:1831:LEU:HB3	1:A:1900:GLY:C	2.36	0.51
1:A:3056:ARG:HG3	1:A:3099:LEU:HD11	1.91	0.51
1:A:3196:ASN:HB3	1:A:3223:HIS:CG	2.45	0.51
1:A:3302:LEU:HD12	1:A:3302:LEU:O	2.11	0.51
1:B:1639:ILE:HG21	1:B:1676:LEU:HD21	1.92	0.51
1:B:1958:LEU:O	1:B:1962:GLN:HB2	2.11	0.51
1:B:2522:ARG:HB3	1:B:2589:GLU:OE1	2.11	0.51
1:A:1554:LEU:HD22	1:A:1609:GLN:CG	2.41	0.51
1:A:1719:GLN:HA	1:A:1722:PHE:HD2	1.72	0.51
1:A:2005:ASP:HB3	1:A:2008:ALA:HB3	1.93	0.51
1:A:2306:MET:HE2	1:A:2316:LEU:CD1	2.41	0.51
1:A:2404:THR:O	1:A:2408:ILE:HG12	2.11	0.51
1:A:2541:MET:HE3	1:A:2541:MET:O	2.11	0.51
1:A:3241:ALA:HB1	1:A:3605:PHE:CE2	2.46	0.51
1:A:4649:TRP:C	1:A:4650:ASN:HD22	2.18	0.51
1:B:1813:GLN:HG3	1:B:1814:LEU:HD12	1.94	0.51
1:B:3348:LEU:HD22	1:B:3511:LEU:HD11	1.93	0.51
1:B:4155:LYS:HE2	1:B:4184:TRP:CZ2	2.46	0.51
1:B:4280:ILE:HD13	1:B:4408:LEU:HD23	1.92	0.51
1:A:2705:THR:O	1:A:2705:THR:HG22	2.09	0.50
1:A:3105:PHE:O	1:A:3109:MET:HG2	2.10	0.50
1:A:4196:TRP:CE3	1:A:4197:LEU:HD13	2.46	0.50
1:A:4576:SER:O	1:A:4578:ILE:N	2.44	0.50
1:B:1592:ASP:OD2	1:B:1592:ASP:C	2.54	0.50
1:B:3348:LEU:HD12	1:B:3518:ILE:CD1	2.41	0.50
1:B:3729:VAL:O	1:B:3729:VAL:CG2	2.49	0.50
1:B:4376:VAL:HG12	1:B:4379:ILE:HG22	1.93	0.50
1:B:4571:ARG:HD3	1:B:4593:GLY:O	2.11	0.50
1:A:2638:THR:O	1:A:2641:VAL:HG23	2.11	0.50
1:A:2989:VAL:O	1:A:2991:PHE:N	2.44	0.50
1:A:3186:SER:HA	1:A:3228:VAL:HG21	1.92	0.50
1:A:3694:ILE:HG22	1:A:3695:THR:H	1.76	0.50
1:A:3849:ASP:O	1:A:3853:SER:HB3	2.11	0.50
1:A:4117:ASP:OD1	1:A:4119:ALA:HB3	2.11	0.50
1:A:4157:TYR:HH	1:A:4186:LEU:HD22	1.76	0.50
1:B:2029:ASN:HD22	1:B:2029:ASN:H	1.59	0.50
1:B:2541:MET:SD	1:B:2573:LEU:HD12	2.51	0.50
1:B:2690:ALA:O	1:B:2691:PHE:CD1	2.64	0.50
1:B:2984:LEU:HD13	1:B:2986:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3598:PHE:HZ	1:B:3660:GLU:HG2	1.76	0.50
1:B:4590:TRP:CE3	1:B:4593:GLY:HA3	2.46	0.50
1:A:2337:ARG:HH12	1:A:2383:GLU:CD	2.18	0.50
1:A:2438:PRO:HA	1:A:2495:GLN:HE22	1.76	0.50
1:A:2747:ASN:HD22	1:A:2747:ASN:N	2.09	0.50
1:A:2832:ASN:HA	1:A:2835:LEU:HB3	1.92	0.50
1:A:3364:ALA:O	1:A:3366:LEU:N	2.45	0.50
1:A:3864:GLU:HG3	1:A:3865:ILE:HG13	1.92	0.50
1:A:4020:LEU:HD21	1:A:4037:ILE:HD12	1.94	0.50
1:A:4573:GLN:O	1:A:4574:GLN:C	2.54	0.50
1:B:3292:LEU:HD13	1:B:3571:ARG:HA	1.93	0.50
1:B:3879:ILE:O	1:B:3881:GLU:N	2.44	0.50
1:B:4200:LEU:O	1:B:4200:LEU:HD23	2.11	0.50
1:B:4596:ASN:C	1:B:4596:ASN:ND2	2.66	0.50
1:A:3342:ARG:HD3	1:A:3522:ILE:HD11	1.93	0.50
1:A:3682:MET:O	1:A:3686:MET:HB2	2.12	0.50
1:A:4117:ASP:OD2	1:A:4119:ALA:HB3	2.12	0.50
1:A:4146:VAL:CG1	1:A:4157:TYR:HH	2.24	0.50
1:A:4645:GLU:O	1:A:4721:VAL:HG23	2.11	0.50
1:A:4654:LEU:HD11	1:A:4688:VAL:HG21	1.93	0.50
1:B:2010:SER:HA	1:B:2042:GLN:HE22	1.77	0.50
1:B:2497:GLU:O	1:B:2501:ILE:HG13	2.12	0.50
1:B:2793:ASN:HD22	1:B:2800:ARG:CZ	2.23	0.50
1:B:3319:GLN:O	1:B:3320:ALA:C	2.55	0.50
1:B:3352:ASN:HA	1:B:3511:LEU:CD2	2.41	0.50
1:B:4169:GLU:OE1	1:B:4169:GLU:HA	2.11	0.50
1:B:4251:THR:CG2	1:B:4303:LEU:HD21	2.34	0.50
1:B:4341:THR:HG22	1:B:4342:ILE:HG13	1.93	0.50
1:B:4509:LEU:HD13	1:B:4552:TRP:CE2	2.46	0.50
1:A:1419:TRP:HZ2	1:A:1471:LEU:O	1.94	0.50
1:A:3199:TYR:C	1:A:3200:ILE:HG13	2.36	0.50
1:A:3260:TYR:O	1:A:3263:PHE:HB3	2.11	0.50
1:A:3511:LEU:O	1:A:3512:LYS:C	2.54	0.50
1:A:3697:THR:OG1	1:A:3698:SER:N	2.44	0.50
1:A:3894:SER:O	1:A:3898:PHE:HD2	1.95	0.50
1:B:1863:VAL:HG23	1:B:1872:ARG:HD3	1.94	0.50
1:B:1907:LEU:O	1:B:1911:ARG:NH1	2.44	0.50
1:B:2422:THR:OG1	1:B:2424:GLN:HB2	2.11	0.50
1:B:3157:ARG:O	1:B:3160:THR:HB	2.11	0.50
1:B:3238:ILE:HD12	1:B:3238:ILE:N	2.27	0.50
1:B:3602:ILE:CD1	1:B:3610:ARG:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4190:ILE:HB	1:B:4197:LEU:HD21	1.94	0.50
1:B:4573:GLN:O	1:B:4577:GLU:HG3	2.12	0.50
1:A:1525:ILE:HA	1:A:1528:GLU:HB3	1.94	0.50
1:B:2233:MET:HA	1:B:2233:MET:CE	2.37	0.50
1:B:2677:GLY:O	2:B:9009:ADP:H5'2	2.11	0.50
1:B:3871:GLU:O	1:B:3875:VAL:HG23	2.11	0.50
1:A:1985:LYS:HD2	1:A:1997:VAL:HG21	1.93	0.50
1:A:2338:ARG:CG	1:A:2338:ARG:NH1	2.71	0.50
1:A:2918:VAL:HG22	1:A:3172:TRP:CD2	2.46	0.50
1:A:3582:ASN:O	1:A:3586:SER:HB3	2.12	0.50
1:A:3775:PRO:O	1:A:3778:CYS:HB2	2.12	0.50
1:B:3192:LEU:HD11	1:B:3268:VAL:HA	1.93	0.50
1:B:3536:TYR:O	1:B:3540:ILE:HD13	2.12	0.50
1:B:4122:VAL:HG11	1:B:4216:PHE:HZ	1.77	0.50
1:B:4259:ARG:NH2	1:B:4307:LEU:HB3	2.26	0.50
1:A:2421:LEU:HD11	2:A:9002:ADP:C5	2.46	0.50
1:A:3817:LEU:N	1:A:3817:LEU:HD22	2.27	0.50
1:B:1727:ALA:HB2	1:B:1994:PHE:CD1	2.46	0.50
1:B:2564:ASN:C	1:B:2566:SER:N	2.66	0.50
1:B:2612:LEU:O	1:B:2612:LEU:HD13	2.12	0.50
1:B:3902:GLU:C	1:B:4433:MET:HE3	2.37	0.50
1:B:4176:TYR:O	1:B:4179:ALA:HB3	2.12	0.50
1:B:4217:MET:HE1	1:B:4229:LEU:HD11	1.91	0.50
1:B:4274:LEU:HD12	1:B:4274:LEU:O	2.11	0.50
1:B:4673:ASP:C	1:B:4675:ASP:N	2.70	0.50
1:A:1605:TRP:CE3	1:A:1669:MET:HE2	2.47	0.50
1:A:1885:GLN:O	1:A:1889:VAL:HG23	2.11	0.50
1:A:2046:ILE:O	1:A:2049:ALA:HB3	2.12	0.50
1:A:2273:MET:HG2	1:A:2395:PHE:CD1	2.47	0.50
1:A:2361:PRO:HD3	1:A:2402:TYR:O	2.12	0.50
1:A:3233:TYR:O	1:A:3237:THR:HG23	2.12	0.50
1:A:4168:PHE:O	1:A:4172:GLU:HG2	2.12	0.50
1:B:2427:PHE:HE1	1:B:2534:LEU:HD21	1.77	0.50
1:B:4132:LEU:HD23	1:B:4236:PHE:CE2	2.47	0.50
1:B:4536:SER:O	1:B:4537:LEU:C	2.55	0.50
1:A:2274:MET:HE1	1:A:2286:TRP:CB	2.37	0.49
1:A:3074:ASP:O	1:A:3077:ASN:HB2	2.12	0.49
1:A:3359:LYS:CE	1:A:3505:GLU:HA	2.42	0.49
1:A:3694:ILE:HA	1:A:3717:PRO:O	2.12	0.49
1:A:4131:PRO:HB2	1:A:4233:SER:HB3	1.94	0.49
1:B:1560:ASP:CA	1:B:1563:ASN:HB2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1592:ASP:CG	1:B:1593:ASP:N	2.65	0.49
1:B:1729:LEU:HD23	1:B:1729:LEU:C	2.36	0.49
1:B:1739:THR:O	1:B:1760:ILE:CG1	2.56	0.49
1:B:3046:TYR:OH	1:B:3054:ASP:OD2	2.29	0.49
1:B:3109:MET:HA	1:B:3112:CYS:HB2	1.93	0.49
1:B:3805:GLU:HB3	1:B:3886:TYR:OH	2.12	0.49
1:B:3930:LEU:HD11	1:B:3943:LEU:CD2	2.39	0.49
1:B:4126:VAL:HG23	1:B:4214:ARG:HE	1.77	0.49
1:B:4693:ASN:HD22	1:B:4693:ASN:N	1.89	0.49
1:A:2056:GLU:HA	1:A:2065:ILE:O	2.12	0.49
1:A:2162:ILE:HG22	1:A:2194:VAL:HG13	1.94	0.49
1:A:2307:ASP:HB3	1:A:2310:ALA:CB	2.41	0.49
1:A:2688:LEU:CD1	1:A:2696:VAL:HG11	2.30	0.49
1:A:3091:LEU:HD21	1:A:3143:VAL:HB	1.94	0.49
1:A:4517:LEU:O	1:A:4518:ALA:C	2.55	0.49
1:A:4708:ASP:C	1:A:4708:ASP:OD1	2.54	0.49
1:B:1614:TYR:HD2	1:B:1615:LEU:HD22	1.78	0.49
1:B:1695:ALA:C	1:B:1697:PHE:N	2.70	0.49
1:B:1701:GLY:HA2	1:B:2011:ARG:NH1	2.27	0.49
1:B:3696:LYS:HZ1	1:B:3721:GLN:HE22	1.60	0.49
1:B:3696:LYS:NZ	1:B:3721:GLN:HE22	2.10	0.49
1:A:1690:GLN:HE22	1:A:1766:ILE:CG2	2.17	0.49
1:A:2751:THR:HG22	1:A:2757:GLN:HG3	1.94	0.49
1:A:4146:VAL:HG11	1:A:4157:TYR:OH	2.11	0.49
1:A:4349:ASN:HD21	1:A:4351:PHE:HB2	1.77	0.49
1:A:4436:SER:C	1:A:4438:GLU:N	2.68	0.49
1:B:1655:LEU:HB2	1:B:1658:GLU:CB	2.41	0.49
1:B:2189:GLN:HE22	1:B:2225:GLY:HA3	1.77	0.49
1:B:3848:ASP:O	1:B:3849:ASP:HB2	2.12	0.49
1:B:3879:ILE:C	1:B:3881:GLU:N	2.67	0.49
1:A:1837:GLN:O	1:A:1838:GLN:C	2.54	0.49
1:A:2088:PRO:O	1:A:2089:ASP:C	2.55	0.49
1:A:2372:ASP:CG	1:A:2373:ASP:H	2.18	0.49
1:A:2903:ARG:NH1	1:A:2950:ILE:HG23	2.27	0.49
1:A:4690:VAL:HG21	1:A:4701:PHE:CE1	2.47	0.49
1:B:2128:ILE:CG2	1:B:2129:VAL:N	2.75	0.49
1:B:2546:VAL:O	1:B:2550:GLU:HB2	2.12	0.49
1:B:3350:VAL:O	1:B:3351:ARG:C	2.54	0.49
1:B:3866:ALA:O	1:B:3869:VAL:HB	2.12	0.49
1:A:2020:GLY:HA2	1:A:2071:MET:HB3	1.95	0.49
1:A:2551:TYR:CE1	1:A:2619:ILE:HG23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3285:LEU:O	1:A:3289:LEU:HD12	2.12	0.49
1:A:3673:LEU:HD11	1:A:3773:PHE:CE2	2.47	0.49
1:A:3823:PHE:HA	1:A:3865:ILE:HD11	1.94	0.49
1:B:1859:LEU:O	1:B:1862:SER:HB2	2.13	0.49
1:B:1973:PHE:HA	1:B:2077:MET:O	2.11	0.49
1:B:2075:VAL:CG1	1:B:2077:MET:HE3	2.42	0.49
1:B:2241:GLN:HA	1:B:2244:ALA:HB3	1.93	0.49
1:B:2493:LYS:O	1:B:2497:GLU:HG3	2.12	0.49
1:B:2525:ILE:H	1:B:2525:ILE:CD1	2.25	0.49
1:B:2863:ARG:O	1:B:2863:ARG:CD	2.60	0.49
1:B:3187:GLU:O	1:B:3190:ARG:HG2	2.12	0.49
1:B:3288:GLY:HA3	1:B:3574:TRP:CZ3	2.47	0.49
1:B:3545:GLN:O	1:B:3548:THR:HB	2.11	0.49
1:B:4322:SER:C	1:B:4323:ASN:ND2	2.57	0.49
1:B:4411:PRO:HB2	1:B:4413:ASN:OD1	2.11	0.49
1:A:2524:HIS:HD2	1:A:2528:PHE:HB2	1.77	0.49
1:A:3815:ASP:O	1:A:3816:LEU:C	2.55	0.49
1:A:3823:PHE:CB	1:A:3865:ILE:HG12	2.42	0.49
1:A:4576:SER:O	1:A:4579:SER:N	2.45	0.49
1:A:4597:PRO:HG2	1:A:4692:LEU:HD11	1.93	0.49
1:B:2430:TYR:O	1:B:2431:LEU:C	2.54	0.49
1:B:2525:ILE:HD11	1:B:2584:SER:HB2	1.95	0.49
1:B:3068:LYS:HA	1:B:3140:ASN:O	2.13	0.49
1:B:3343:GLU:C	1:B:3345:GLN:N	2.70	0.49
1:B:3598:PHE:CZ	1:B:3660:GLU:HG2	2.47	0.49
1:B:4091:SER:HA	1:B:4094:VAL:HG23	1.95	0.49
1:B:4109:ASP:CB	1:B:4112:ASN:HD22	2.25	0.49
1:A:2380:PRO:C	1:A:2382:GLY:N	2.69	0.49
1:A:4623:ALA:HB2	1:A:4703:ILE:CD1	2.43	0.49
1:B:1671:ARG:HG2	1:B:1675:LEU:HD11	1.94	0.49
1:B:2369:SER:HA	1:B:2372:ASP:OD2	2.12	0.49
1:B:3164:LEU:C	1:B:3166:ASN:H	2.20	0.49
1:B:3343:GLU:C	1:B:3345:GLN:H	2.21	0.49
1:B:3903:LEU:HD21	1:B:3967:PHE:CD1	2.48	0.49
1:B:4322:SER:CB	1:B:4323:ASN:ND2	2.75	0.49
1:A:2551:TYR:CD1	1:A:2619:ILE:CG1	2.95	0.49
1:A:2598:GLN:OE1	1:A:2611:PRO:HA	2.13	0.49
1:A:2669:PRO:HA	1:A:2788:PHE:O	2.13	0.49
1:A:2865:THR:C	1:A:2867:ASP:H	2.20	0.49
1:A:2876:PRO:HB2	2:A:9003:ADP:O4'	2.12	0.49
1:A:3009:GLN:N	1:A:3138:ARG:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3069:ILE:O	1:A:3142:HIS:HB2	2.13	0.49
1:A:3252:GLN:HE21	1:A:3253:ASN:N	2.10	0.49
1:A:3354:GLU:O	1:A:3356:ALA:N	2.46	0.49
1:A:3691:ASP:C	1:A:3691:ASP:OD1	2.56	0.49
1:A:3768:ASP:C	1:A:3768:ASP:OD2	2.56	0.49
1:B:1918:GLN:O	1:B:1924:LYS:HE2	2.13	0.49
1:B:2011:ARG:HH21	1:B:2012:ILE:HD11	1.77	0.49
1:B:3785:ASN:HD21	1:B:3787:THR:CG2	2.20	0.49
1:A:2243:ILE:HD13	1:A:2291:GLU:OE2	2.13	0.49
1:A:2839:LEU:CD2	1:A:2896:CYS:HB2	2.42	0.49
1:B:2205:PRO:HG3	1:B:2261:GLN:HG2	1.95	0.49
1:B:2866:PRO:HG3	1:B:2873:ILE:HG23	1.93	0.49
1:B:3635:PRO:C	1:B:3637:PHE:H	2.21	0.49
1:B:3697:THR:O	1:B:3720:VAL:HA	2.13	0.49
1:B:3819:ILE:HG23	1:B:3823:PHE:CE2	2.47	0.49
1:B:4315:ASP:HA	1:B:4318:SER:OG	2.13	0.49
1:B:4597:PRO:HG2	1:B:4692:LEU:HD11	1.94	0.49
1:A:1813:GLN:HE22	1:A:1941:LEU:N	1.99	0.49
1:A:2090:ASN:HD22	1:A:2091:LEU:H	1.61	0.49
1:A:2607:ALA:O	1:A:2609:THR:N	2.45	0.49
1:A:2998:ILE:HG22	1:A:3029:VAL:HG23	1.94	0.49
1:A:3656:GLU:O	1:A:3660:GLU:HG3	2.13	0.49
1:A:3864:GLU:CG	1:A:3865:ILE:H	2.24	0.49
1:A:4128:SER:HB3	1:A:4211:PRO:O	2.13	0.49
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.12	0.49
1:B:1608:VAL:HG22	1:B:1676:LEU:HD12	1.95	0.49
1:B:1642:GLU:OE1	1:B:1668:THR:HG23	2.13	0.49
1:B:1694:PHE:O	1:B:1697:PHE:HB2	2.12	0.49
1:B:1763:GLY:N	1:B:1764:PRO:CD	2.74	0.49
1:B:1842:GLN:HA	1:B:1842:GLN:NE2	2.28	0.49
1:B:2263:HIS:HB2	1:B:2289:TYR:CE1	2.47	0.49
1:B:2300:LYS:CB	1:B:2349:LYS:HG2	2.43	0.49
1:B:4644:LEU:HB2	1:B:4662:THR:HG23	1.95	0.49
1:A:1564:LYS:HD2	1:A:1568:HIS:NE2	2.28	0.48
1:A:2544:SER:OG	1:A:2572:ARG:NH1	2.46	0.48
1:A:4011:LEU:C	1:A:4012:LEU:HD12	2.38	0.48
1:B:1777:MET:HE3	1:B:1940:TYR:H	1.78	0.48
1:B:1783:THR:O	1:B:1784:LEU:C	2.55	0.48
1:B:2723:THR:HG21	1:B:2727:GLU:HB2	1.95	0.48
1:B:3091:LEU:HD11	1:B:3145:PHE:HE2	1.77	0.48
1:B:3947:ILE:HD11	1:B:3948:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3972:THR:CG2	1:B:4105:VAL:HG21	2.38	0.48
1:B:4005:ILE:O	1:B:4005:ILE:HG22	2.13	0.48
1:A:1578:SER:C	1:A:1580:TYR:H	2.21	0.48
1:A:1646:ILE:HD11	1:A:1668:THR:HG21	1.95	0.48
1:A:3141:LEU:O	1:A:3142:HIS:HB2	2.13	0.48
1:A:3689:TYR:HB2	1:A:3694:ILE:CD1	2.42	0.48
1:A:3976:VAL:HB	1:A:3981:ASN:O	2.12	0.48
1:A:4507:GLY:HA2	1:A:4510:VAL:CG2	2.43	0.48
1:A:4592:GLY:HA3	1:A:4725:SER:O	2.13	0.48
1:B:3188:PHE:HB3	1:B:3264:ILE:HG21	1.94	0.48
1:B:4011:LEU:O	1:B:4012:LEU:HD23	2.13	0.48
1:B:4322:SER:HB2	1:B:4323:ASN:HD22	1.78	0.48
1:A:1419:TRP:C	1:A:1421:ALA:H	2.20	0.48
1:A:1629:LEU:HD11	1:A:1686:TYR:CG	2.49	0.48
1:A:1767:HIS:CG	1:A:1768:GLU:N	2.81	0.48
1:A:2169:PRO:HG2	1:A:2186:ILE:HG22	1.95	0.48
1:A:2586:GLY:HA2	1:A:2815:LEU:HD22	1.94	0.48
1:A:2643:SER:O	1:A:2645:ASP:N	2.47	0.48
1:A:3019:GLY:C	2:A:9004:ADP:H5'2	2.38	0.48
1:A:3634:VAL:HB	1:A:3635:PRO:HD3	1.93	0.48
1:B:2243:ILE:HD13	1:B:2291:GLU:HB2	1.95	0.48
1:B:2723:THR:CG2	1:B:2727:GLU:HB2	2.43	0.48
1:B:3017:VAL:HG22	1:B:3175:GLU:OE2	2.13	0.48
1:B:3781:VAL:CG1	1:B:3782:THR:N	2.76	0.48
1:B:4075:THR:HG23	1:B:4076:ILE:N	2.27	0.48
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	1.96	0.48
1:A:2359:VAL:HA	1:A:2363:TRP:NE1	2.26	0.48
1:A:3355:ILE:CG2	1:A:3508:ALA:HB2	2.43	0.48
1:A:3598:PHE:O	1:A:3602:ILE:HB	2.12	0.48
1:A:3902:GLU:HB3	1:A:4433:MET:HB3	1.95	0.48
1:A:4122:VAL:CG2	1:A:4216:PHE:HZ	2.26	0.48
1:B:1592:ASP:O	1:B:1593:ASP:C	2.55	0.48
1:B:1611:ARG:HH11	1:B:1611:ARG:HG3	1.78	0.48
1:B:1715:ILE:HD12	1:B:1734:LEU:HD21	1.95	0.48
1:B:2050:LEU:HG	1:B:2067:LEU:HD21	1.95	0.48
1:B:2374:ASN:O	1:B:2376:LEU:N	2.47	0.48
1:B:3545:GLN:O	1:B:3548:THR:N	2.47	0.48
1:B:4201:GLU:OE2	1:B:4232:MET:HE2	2.13	0.48
1:A:1796:ASP:C	1:A:1796:ASP:OD2	2.56	0.48
1:A:2853:MET:HE3	1:A:2882:TRP:HB3	1.95	0.48
1:A:4063:ILE:HD13	1:A:4082:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4157:TYR:OH	1:A:4186:LEU:HB2	2.12	0.48
1:A:4590:TRP:CD2	1:A:4593:GLY:HA3	2.48	0.48
1:B:2781:ILE:HD12	1:B:2781:ILE:N	2.28	0.48
1:B:2841:ASN:H	1:B:2841:ASN:ND2	2.03	0.48
1:B:3188:PHE:CB	1:B:3264:ILE:HG21	2.43	0.48
1:B:3774:THR:HB	1:B:3775:PRO:HD2	1.96	0.48
1:B:3939:ARG:O	1:B:3943:LEU:HG	2.13	0.48
1:B:4213:PHE:C	1:B:4214:ARG:HG2	2.37	0.48
1:A:1899:THR:HG22	1:A:1899:THR:O	2.14	0.48
1:A:3074:ASP:CB	1:A:3077:ASN:HD22	2.27	0.48
1:A:3825:VAL:C	1:A:3827:LEU:N	2.71	0.48
1:A:3858:LEU:O	1:A:3862:THR:HB	2.13	0.48
1:A:3965:LEU:CD2	1:A:4426:MET:HE1	2.43	0.48
1:A:4436:SER:O	1:A:4438:GLU:N	2.47	0.48
1:B:1908:TYR:CE1	1:B:1958:LEU:HD22	2.48	0.48
1:B:3539:LEU:O	1:B:3540:ILE:C	2.55	0.48
1:B:4012:LEU:HA	1:B:4016:GLN:NE2	2.28	0.48
1:B:4059:PRO:C	1:B:4061:SER:N	2.71	0.48
1:B:4176:TYR:OH	1:B:4203:LYS:CG	2.61	0.48
1:A:2275:VAL:HG22	1:A:2397:VAL:HG22	1.96	0.48
1:A:2359:VAL:CG2	1:A:2397:VAL:HG11	2.43	0.48
1:A:2935:LEU:HD21	1:A:2943:LEU:CD2	2.43	0.48
1:A:3185:GLY:O	1:A:3189:THR:HG23	2.13	0.48
1:A:3632:LEU:HD23	1:A:3632:LEU:C	2.39	0.48
1:B:1639:ILE:HG21	1:B:1676:LEU:CD2	2.44	0.48
1:B:2439:PHE:H	1:B:2495:GLN:HE22	1.61	0.48
1:B:2602:ILE:O	1:B:2603:THR:C	2.56	0.48
1:B:2688:LEU:HD13	1:B:2696:VAL:HB	1.95	0.48
1:B:3704:PHE:CG	1:B:3705:MET:N	2.82	0.48
1:B:4118:MET:O	1:B:4119:ALA:C	2.56	0.48
1:B:4669:LEU:HD12	1:B:4669:LEU:N	2.28	0.48
1:A:1679:VAL:O	1:A:1682:ALA:HB3	2.14	0.48
1:A:1974:GLY:O	1:A:2078:ASN:HA	2.14	0.48
1:A:2271:GLY:HA3	1:A:2371:LEU:HD22	1.96	0.48
1:A:2848:ASN:HD21	1:B:4002:LYS:HE3	1.79	0.48
1:A:2965:ARG:CZ	1:A:2992:ASN:ND2	2.76	0.48
1:A:4117:ASP:OD1	1:A:4117:ASP:C	2.56	0.48
1:A:4284:ARG:O	1:A:4291:GLY:HA3	2.13	0.48
1:B:1608:VAL:O	1:B:1611:ARG:N	2.47	0.48
1:B:1781:LEU:O	1:B:1814:LEU:HD21	2.14	0.48
1:B:1826:GLN:O	1:B:1827:VAL:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3226:ALA:HB1	1:B:3624:VAL:CG1	2.43	0.48
1:B:3256:THR:HG21	1:B:3779:SER:HB3	1.95	0.48
1:B:3328:VAL:O	1:B:3328:VAL:HG22	2.12	0.48
1:B:3559:ARG:O	1:B:3563:LEU:HB2	2.14	0.48
1:B:4668:THR:C	1:B:4669:LEU:HD12	2.39	0.48
1:A:1949:GLN:HE22	1:A:1953:THR:CG2	2.27	0.48
1:A:3332:GLN:O	1:A:3336:ILE:HG13	2.13	0.48
1:A:4062:TRP:C	1:A:4064:VAL:H	2.22	0.48
1:B:2205:PRO:CB	1:B:2265:ILE:HD11	2.43	0.48
1:B:2223:PHE:C	1:B:2225:GLY:H	2.20	0.48
1:B:2258:LYS:HD2	1:B:2414:VAL:CG1	2.44	0.48
1:B:2379:LEU:C	1:B:2381:ASN:N	2.71	0.48
1:B:2432:ASP:O	1:B:2433:THR:C	2.57	0.48
1:B:2439:PHE:H	1:B:2495:GLN:NE2	2.12	0.48
1:B:2542:ASN:O	1:B:2543:ARG:C	2.57	0.48
1:B:2751:THR:HB	1:B:2756:THR:H	1.79	0.48
1:B:3538:THR:O	1:B:3542:GLU:HG3	2.14	0.48
1:A:2977:LYS:C	1:A:2979:PHE:N	2.71	0.48
1:A:3283:LEU:HD23	1:A:3284:HIS:N	2.28	0.48
1:A:3809:THR:HB	1:A:3879:ILE:CD1	2.44	0.48
1:A:4251:THR:HG23	1:A:4303:LEU:HD22	1.95	0.48
1:A:4553:TYR:C	1:A:4553:TYR:CD1	2.92	0.48
1:A:4571:ARG:O	1:A:4574:GLN:HB3	2.14	0.48
1:B:1828:ASP:O	1:B:1830:ALA:N	2.46	0.48
1:B:1870:GLN:HG2	1:B:1943:ILE:CD1	2.44	0.48
1:B:1870:GLN:HG2	1:B:1943:ILE:HD11	1.95	0.48
1:B:2204:ILE:N	1:B:2205:PRO:CD	2.77	0.48
1:B:2621:ASP:O	1:B:2622:ALA:HB3	2.13	0.48
1:B:3033:ASN:HB2	1:B:3035:LEU:HG	1.94	0.48
1:B:3673:LEU:HB3	1:B:3781:VAL:HG11	1.94	0.48
1:A:1419:TRP:CE2	1:A:1481:TRP:HZ2	2.31	0.47
1:A:1800:HIS:CG	1:A:1858:ASN:HD22	2.32	0.47
1:A:2615:TYR:CE1	1:A:2626:LEU:HG	2.49	0.47
1:A:2976:LEU:HD22	1:A:2990:LEU:HD21	1.96	0.47
1:A:3815:ASP:O	1:A:3819:ILE:N	2.47	0.47
1:A:4070:SER:C	1:A:4072:GLN:H	2.22	0.47
1:B:1786:SER:O	1:B:1787:GLU:C	2.57	0.47
1:B:4267:ARG:HG2	1:B:4267:ARG:NH1	2.28	0.47
1:A:1945:GLU:OE1	1:A:1945:GLU:HA	2.13	0.47
1:A:3605:PHE:H	1:A:3605:PHE:HD1	1.58	0.47
1:B:1828:ASP:O	1:B:1831:LEU:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2869:GLN:HB2	1:B:2872:TYR:CD2	2.49	0.47
1:B:3892:SER:O	1:B:3896:VAL:HG23	2.14	0.47
1:A:1830:ALA:O	1:A:1841:ILE:HG23	2.14	0.47
1:A:2297:ASP:OD1	1:A:2297:ASP:N	2.46	0.47
1:A:2729:VAL:HB	1:A:2782:LYS:O	2.14	0.47
1:A:4044:TRP:HB3	1:A:4048:PHE:CE2	2.50	0.47
1:B:1547:ASN:HD21	1:B:1550:ARG:H	1.61	0.47
1:B:1841:ILE:O	1:B:1844:GLN:N	2.42	0.47
1:B:2295:GLN:O	1:B:2298:ASN:N	2.43	0.47
1:B:2360:ASP:C	1:B:2360:ASP:OD1	2.57	0.47
1:B:3095:GLU:HG3	1:B:3134:THR:CB	2.44	0.47
1:B:3132:TYR:O	1:B:3136:GLN:HG2	2.14	0.47
1:B:3160:THR:C	1:B:3162:PRO:HD3	2.39	0.47
1:B:3539:LEU:HA	1:B:3539:LEU:HD12	1.70	0.47
1:B:3719:LEU:HD23	1:B:3719:LEU:C	2.40	0.47
1:A:1643:PHE:O	1:A:1647:LEU:HB2	2.14	0.47
1:A:1735:ASP:O	1:A:1738:LYS:N	2.36	0.47
1:A:1854:MET:O	1:A:1857:ASN:N	2.46	0.47
1:A:2032:GLU:O	1:A:2034:ARG:N	2.47	0.47
1:A:2274:MET:CE	1:A:2286:TRP:HB3	2.39	0.47
1:A:2875:SER:C	1:A:2877:ARG:H	2.22	0.47
1:A:3851:VAL:CG1	1:A:3852:ILE:N	2.77	0.47
1:A:3853:SER:O	1:A:3854:THR:C	2.57	0.47
1:A:3865:ILE:O	1:A:3869:VAL:HG23	2.14	0.47
1:A:4225:LEU:HD13	1:A:4230:LEU:HD11	1.96	0.47
1:A:4293:THR:HG22	1:A:4294:LYS:HG3	1.95	0.47
1:A:4324:ILE:HD13	1:A:4329:ILE:HD11	1.95	0.47
1:A:4668:THR:C	1:A:4669:LEU:HD12	2.39	0.47
1:B:2359:VAL:HG13	1:B:2364:VAL:HG21	1.96	0.47
1:B:2377:LEU:O	1:B:2385:LEU:N	2.40	0.47
1:B:3067:GLU:O	1:B:3069:ILE:HG13	2.14	0.47
1:B:4184:TRP:HE1	1:B:4214:ARG:HG3	1.78	0.47
1:A:1558:TRP:O	1:A:1562:PHE:HD2	1.98	0.47
1:A:1797:VAL:O	1:A:1854:MET:HE1	2.14	0.47
1:A:2447:GLN:HE22	1:A:2492:LEU:HD22	1.79	0.47
1:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.14	0.47
1:A:3051:PHE:HZ	1:A:3087:MET:HE3	1.80	0.47
1:A:3347:GLN:O	1:A:3350:VAL:HG23	2.14	0.47
1:A:4117:ASP:OD1	1:A:4117:ASP:O	2.33	0.47
1:B:1555:VAL:HG23	1:B:1555:VAL:O	2.14	0.47
1:B:1630:PRO:O	1:B:1631:ALA:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4284:ARG:O	1:B:4291:GLY:HA3	2.15	0.47
1:B:4284:ARG:NH2	1:B:4410:LEU:HD21	2.29	0.47
1:B:4387:THR:H	1:B:4391:HIS:CD2	2.31	0.47
1:B:4484:LEU:HD23	1:B:4485:LYS:N	2.29	0.47
1:B:4636:SER:CA	1:B:4670:THR:HG22	2.44	0.47
1:A:1974:GLY:HA2	1:A:2079:PRO:HD3	1.96	0.47
1:A:2549:ILE:O	1:A:2553:GLN:HG3	2.15	0.47
1:A:3362:ALA:CB	1:A:3497:LEU:HD11	2.36	0.47
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.49	0.47
1:A:3936:PRO:C	1:A:3938:GLU:H	2.23	0.47
1:A:4153:LEU:O	1:A:4154:HIS:CB	2.62	0.47
1:B:1616:GLU:C	1:B:1616:GLU:CD	2.82	0.47
1:B:2713:THR:HG22	1:B:2713:THR:O	2.14	0.47
1:B:2975:ARG:HA	1:B:2975:ARG:HE	1.80	0.47
1:B:3205:PHE:CD1	1:B:3624:VAL:HG22	2.49	0.47
1:B:3768:ASP:CB	1:B:3771:ALA:HB2	2.39	0.47
1:B:4176:TYR:O	1:B:4179:ALA:N	2.47	0.47
1:B:4201:GLU:HG3	1:B:4228:ASN:HB3	1.96	0.47
1:B:4623:ALA:HA	1:B:4668:THR:O	2.15	0.47
1:A:1766:ILE:CG2	1:A:1767:HIS:N	2.71	0.47
1:A:2140:SER:HB2	1:A:2211:ASP:OD2	2.14	0.47
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.14	0.47
1:A:2272:VAL:O	1:A:2394:MET:HA	2.15	0.47
1:A:2283:THR:HB	2:A:9002:ADP:O1A	2.15	0.47
1:A:2433:THR:O	1:A:2437:GLU:HB2	2.14	0.47
1:A:2717:HIS:CB	1:A:2739:LEU:HD11	2.45	0.47
1:A:2873:ILE:HD12	1:A:2874:TYR:N	2.29	0.47
1:A:2893:MET:HE1	1:A:2896:CYS:SG	2.54	0.47
1:A:3201:ALA:HB1	1:A:3221:PRO:HD2	1.97	0.47
1:A:3694:ILE:HG23	1:A:3717:PRO:HB2	1.95	0.47
1:A:3711:ALA:O	1:A:3715:GLY:N	2.48	0.47
1:A:3839:SER:C	1:A:3841:ALA:N	2.70	0.47
1:A:3972:THR:HG23	1:A:4105:VAL:HG21	1.96	0.47
1:A:4003:GLU:HB3	1:A:4021:ILE:HD13	1.97	0.47
1:A:4351:PHE:CZ	1:A:4689:PRO:HB3	2.49	0.47
1:A:4639:VAL:HG12	1:A:4640:LYS:N	2.29	0.47
1:B:1610:ARG:HG3	1:B:1610:ARG:NH1	2.28	0.47
1:B:1643:PHE:CZ	1:B:1647:LEU:HD11	2.49	0.47
1:B:1662:ILE:HG22	1:B:1663:GLU:N	2.28	0.47
1:B:1777:MET:HE3	1:B:1940:TYR:N	2.30	0.47
1:B:1888:VAL:O	1:B:1891:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2101:ILE:O	1:B:2103:PRO:HD3	2.14	0.47
1:B:2212:ILE:N	1:B:2213:PRO:HD2	2.29	0.47
1:B:2229:GLN:C	1:B:2230:PRO:O	2.57	0.47
1:B:2441:PRO:C	1:B:2443:GLU:N	2.68	0.47
1:B:3042:VAL:HG11	1:B:3079:LEU:CG	2.44	0.47
1:B:3935:ASP:O	1:B:3939:ARG:HG3	2.15	0.47
1:B:4386:GLY:CA	1:B:4391:HIS:HB3	2.44	0.47
1:B:4571:ARG:O	1:B:4572:MET:C	2.58	0.47
1:A:1909:HIS:O	1:A:1911:ARG:HD3	2.15	0.47
1:A:2836:MET:HG3	1:A:2846:ALA:HA	1.97	0.47
1:A:2863:ARG:HG3	1:A:2925:TRP:CE2	2.50	0.47
1:A:2917:LEU:HD12	1:A:2923:LYS:HA	1.97	0.47
1:A:3689:TYR:CB	1:A:3694:ILE:HD11	2.44	0.47
1:A:3859:LYS:C	1:A:3862:THR:HG22	2.39	0.47
1:A:4020:LEU:CD1	1:A:4033:LEU:HD23	2.45	0.47
1:A:4060:GLU:O	1:A:4064:VAL:HG23	2.14	0.47
1:A:4418:LEU:HD11	1:A:4422:LYS:HZ1	1.79	0.47
1:B:1920:ASN:HD22	1:B:1920:ASN:C	2.21	0.47
1:B:2969:ARG:HG3	1:B:2995:LEU:HD11	1.97	0.47
1:B:3030:ALA:HB3	1:B:3037:ILE:HD11	1.97	0.47
1:B:3247:LYS:O	1:B:3247:LYS:HG2	2.15	0.47
1:B:3677:PRO:HD3	1:B:3787:THR:HG22	1.97	0.47
1:B:4008:LEU:HD11	1:B:4034:VAL:HG13	1.95	0.47
1:B:4547:PRO:HG2	1:B:4550:TRP:CZ3	2.49	0.47
1:A:2865:THR:C	1:A:2867:ASP:N	2.70	0.47
1:A:2898:LEU:O	1:A:2941:VAL:HG22	2.14	0.47
1:A:3022:LYS:HB2	2:A:9004:ADP:O3B	2.15	0.47
1:A:3258:ARG:HG2	1:A:3779:SER:HB2	1.95	0.47
1:A:4117:ASP:CG	1:A:4119:ALA:HB3	2.40	0.47
1:B:2425:MET:HB3	2:B:9008:ADP:C2	2.50	0.47
1:B:2843:ARG:HH11	1:B:2843:ARG:HG3	1.79	0.47
1:B:3095:GLU:CG	1:B:3134:THR:CG2	2.92	0.47
1:B:3104:GLU:C	1:B:3106:THR:N	2.73	0.47
1:B:3237:THR:OG1	1:B:3238:ILE:HD12	2.15	0.47
1:A:1706:LEU:O	1:A:1707:GLU:C	2.58	0.47
1:A:2262:LEU:HD21	1:A:2274:MET:HE3	1.97	0.47
1:A:2575:TYR:HA	1:A:2578:MET:CE	2.45	0.47
1:A:2728:THR:CG2	1:A:2779:THR:HG21	2.45	0.47
1:A:2991:PHE:CE1	1:A:2993:GLU:HB2	2.50	0.47
1:A:4589:VAL:O	1:A:4589:VAL:HG13	2.14	0.47
1:B:1606:ILE:C	1:B:1608:VAL:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1792:PHE:CE2	1:B:1822:VAL:HG21	2.50	0.47
1:B:2201:ASP:O	1:B:2205:PRO:HG2	2.15	0.47
1:B:3348:LEU:HD23	1:B:3348:LEU:HA	1.78	0.47
1:B:3602:ILE:HD12	1:B:3610:ARG:HA	1.97	0.47
1:B:3782:THR:O	1:B:3782:THR:HG22	2.14	0.47
1:B:4590:TRP:HA	1:B:4640:LYS:O	2.15	0.47
1:A:1797:VAL:C	1:A:1854:MET:HE1	2.40	0.46
1:A:2204:ILE:HA	1:A:2207:LEU:HG	1.96	0.46
1:A:2548:VAL:HG13	1:A:2560:MET:CE	2.45	0.46
1:A:3521:THR:O	1:A:3524:ALA:HB3	2.15	0.46
1:A:3602:ILE:HD12	1:A:3610:ARG:HA	1.96	0.46
1:A:4502:GLU:O	1:A:4503:ILE:C	2.58	0.46
1:A:4507:GLY:O	1:A:4510:VAL:N	2.48	0.46
1:B:2533:VAL:HB	1:B:2581:LEU:CD2	2.39	0.46
1:B:2638:THR:HG21	1:B:2838:LEU:CD2	2.37	0.46
1:B:2907:HIS:CE1	1:B:2911:ARG:HE	2.33	0.46
1:B:3087:MET:O	1:B:3091:LEU:N	2.47	0.46
1:B:4371:PRO:O	1:B:4372:ASP:HB2	2.16	0.46
1:A:1948:VAL:O	1:A:1950:THR:N	2.49	0.46
1:A:2262:LEU:CD2	1:A:2274:MET:HE3	2.46	0.46
1:A:2446:GLN:HA	1:A:2449:ARG:NH2	2.30	0.46
1:A:2511:LEU:HD23	1:A:2515:VAL:HG23	1.96	0.46
1:A:2706:THR:HB	1:A:2707:PRO:HD2	1.96	0.46
1:A:4221:ILE:HG22	1:A:4221:ILE:O	2.14	0.46
1:B:2360:ASP:HB2	1:B:2361:PRO:HD2	1.97	0.46
1:B:2863:ARG:HG3	1:B:2925:TRP:CZ2	2.49	0.46
1:B:3108:LEU:C	1:B:3109:MET:HG2	2.39	0.46
1:B:3275:ARG:HA	1:B:3585:MET:HE1	1.96	0.46
1:B:3673:LEU:HD23	1:B:3673:LEU:C	2.41	0.46
1:B:4210:HIS:O	1:B:4213:PHE:HB3	2.16	0.46
1:B:4347:ILE:CG2	1:B:4353:MET:HG2	2.45	0.46
1:A:1967:ARG:HD3	1:A:2050:LEU:O	2.15	0.46
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.29	0.46
1:A:2525:ILE:HG21	1:A:2815:LEU:CD1	2.45	0.46
1:A:2551:TYR:HE1	1:A:2619:ILE:HG23	1.80	0.46
1:A:2723:THR:HB	1:A:2724:PRO:HD2	1.97	0.46
1:A:2911:ARG:NH1	1:A:2915:ASP:OD1	2.48	0.46
1:A:2948:ARG:HG2	1:A:2948:ARG:HH11	1.80	0.46
1:A:2989:VAL:HG23	2:A:9004:ADP:N1	2.30	0.46
1:B:1665:ILE:C	1:B:1667:GLN:H	2.23	0.46
1:B:3038:TYR:CD2	1:B:3058:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3603:GLY:N	1:B:3664:MET:HE1	2.30	0.46
1:B:3605:PHE:HB3	1:B:3609:PHE:CB	2.45	0.46
1:B:3840:GLN:O	1:B:3841:ALA:C	2.57	0.46
1:B:4130:SER:OG	1:B:4233:SER:HA	2.15	0.46
1:B:4690:VAL:HG22	1:B:4723:ILE:CB	2.43	0.46
1:A:1422:ILE:HD12	1:A:1423:ILE:N	2.30	0.46
1:A:2548:VAL:HG13	1:A:2560:MET:HE3	1.96	0.46
1:A:2717:HIS:HB2	1:A:2739:LEU:HD11	1.97	0.46
1:A:3279:GLU:HG3	1:A:3585:MET:CE	2.44	0.46
1:A:3335:GLU:O	1:A:3338:GLN:HB2	2.14	0.46
1:A:3354:GLU:C	1:A:3356:ALA:N	2.72	0.46
1:A:4210:HIS:ND1	1:A:4211:PRO:CD	2.71	0.46
1:B:2093:LYS:HB2	1:B:2093:LYS:NZ	2.30	0.46
1:B:3725:ASN:N	1:B:3725:ASN:ND2	2.61	0.46
1:A:3265:ASN:O	1:A:3269:LEU:HG	2.15	0.46
1:A:4515:ASN:O	1:A:4516:ASP:C	2.57	0.46
1:B:1559:ASP:C	1:B:1561:LEU:H	2.24	0.46
1:B:1691:ARG:HD3	1:B:1698:TYR:HA	1.98	0.46
1:B:1828:ASP:C	1:B:1830:ALA:N	2.73	0.46
1:B:1901:ASN:HD22	1:B:1901:ASN:N	2.13	0.46
1:B:2108:ILE:HD12	1:B:2149:LEU:HD11	1.97	0.46
1:B:2606:PRO:HB2	1:B:2615:TYR:CE2	2.51	0.46
1:B:3065:LYS:O	1:B:3066:GLU:HB2	2.16	0.46
1:B:3161:SER:O	1:B:3163:ALA:N	2.49	0.46
1:B:4636:SER:CB	1:B:4670:THR:HG22	2.46	0.46
1:A:1690:GLN:NE2	1:A:1766:ILE:HG21	2.20	0.46
1:A:2309:LYS:HE3	1:A:2756:THR:HG21	1.97	0.46
1:A:3083:PHE:CD2	1:A:3083:PHE:N	2.83	0.46
1:A:3854:THR:O	1:A:3857:THR:HB	2.15	0.46
1:B:1683:LEU:O	1:B:1686:TYR:HB3	2.16	0.46
1:B:2231:ILE:CD1	1:B:2233:MET:HB2	2.46	0.46
1:B:2381:ASN:ND2	1:B:2383:GLU:H	2.13	0.46
1:B:2620:ASP:O	1:B:2621:ASP:C	2.59	0.46
1:B:2705:THR:HB	1:B:2749:PRO:HG3	1.97	0.46
1:B:2938:PHE:N	1:B:2939:PRO:HD3	2.24	0.46
1:B:4327:ASP:OD1	1:B:4327:ASP:N	2.48	0.46
1:A:1528:GLU:HB2	1:A:1584:PHE:CZ	2.51	0.46
1:A:3338:GLN:O	1:A:3342:ARG:HG2	2.15	0.46
1:A:4576:SER:C	1:A:4578:ILE:N	2.71	0.46
1:B:2948:ARG:HD2	1:B:2950:ILE:HG13	1.97	0.46
1:B:3136:GLN:O	1:B:3137:VAL:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3674:VAL:HG13	1:B:3786:PHE:HD2	1.81	0.46
1:B:3902:GLU:C	1:B:3904:SER:N	2.72	0.46
1:A:1653:ALA:HB1	1:A:1658:GLU:OE1	2.16	0.46
1:A:2610:ILE:HD13	1:A:2626:LEU:HD21	1.98	0.46
1:A:2689:ARG:C	1:A:2691:PHE:H	2.23	0.46
1:A:2969:ARG:HB3	1:A:2995:LEU:HD11	1.97	0.46
1:A:4639:VAL:O	1:A:4666:ILE:HA	2.16	0.46
1:B:1831:LEU:HA	1:B:1841:ILE:CG2	2.45	0.46
1:B:1872:ARG:NH1	1:B:2164:ARG:HD3	2.29	0.46
1:B:2239:LYS:O	1:B:2243:ILE:HG13	2.16	0.46
1:B:2332:PHE:CD1	1:B:2353:ILE:HG21	2.51	0.46
1:B:3061:ARG:NH2	1:B:3067:GLU:OE1	2.49	0.46
1:B:3275:ARG:HG2	1:B:3585:MET:CE	2.46	0.46
1:B:3701:ASP:OD1	1:B:3701:ASP:C	2.58	0.46
1:B:4073:GLN:HG2	1:B:4073:GLN:O	2.14	0.46
1:A:1510:ASN:O	1:A:1511:GLU:C	2.57	0.46
1:A:1921:VAL:HA	1:A:1924:LYS:HD2	1.98	0.46
1:A:2032:GLU:O	1:A:2033:GLU:C	2.59	0.46
1:A:2147:PHE:HE1	1:A:2203:MET:HE3	1.79	0.46
1:A:2432:ASP:O	1:A:2436:ASN:HB2	2.15	0.46
1:A:4117:ASP:OD1	1:A:4120:ASN:N	2.42	0.46
1:A:4171:ALA:C	1:A:4173:LYS:N	2.73	0.46
1:A:4335:ARG:NH2	1:A:4365:THR:HG22	2.31	0.46
1:B:1615:LEU:HD22	1:B:1615:LEU:N	2.31	0.46
1:B:1803:TYR:O	1:B:1806:TRP:HB3	2.15	0.46
1:B:2311:ILE:HB	1:B:2315:GLN:NE2	2.30	0.46
1:B:2611:PRO:O	1:B:2613:LEU:N	2.49	0.46
1:B:2745:GLU:HG2	1:B:2748:LEU:CD1	2.46	0.46
1:B:4588:GLN:O	1:B:4640:LYS:NZ	2.47	0.46
1:A:2053:ASN:N	1:A:2053:ASN:HD22	2.14	0.46
1:A:2223:PHE:N	1:A:2224:PRO:HD3	2.31	0.46
1:A:3790:PRO:HA	1:A:3898:PHE:CE2	2.51	0.46
1:A:4200:LEU:HD22	1:A:4204:LEU:HD12	1.98	0.46
1:B:3063:GLY:HA2	1:B:3136:GLN:CB	2.46	0.46
1:B:3344:LEU:HB3	1:B:3518:ILE:HD11	1.98	0.46
1:B:3946:ASP:O	1:B:3950:MET:HG3	2.16	0.46
1:B:4214:ARG:CG	1:B:4214:ARG:NH1	2.78	0.46
1:B:4535:ARG:O	1:B:4536:SER:C	2.59	0.46
1:A:1690:GLN:NE2	1:A:1709:ILE:HG12	2.31	0.45
1:A:1715:ILE:O	1:A:1716:ILE:C	2.58	0.45
1:A:1796:ASP:O	1:A:1799:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1820:GLN:HE22	1:A:1990:GLN:HE22	1.64	0.45
1:A:2202:THR:O	1:A:2203:MET:CG	2.63	0.45
1:A:3069:ILE:HG22	1:A:3070:CYS:H	1.80	0.45
1:A:3270:LEU:HB3	1:A:3592:VAL:CG1	2.46	0.45
1:B:1693:ALA:HB1	1:B:1767:HIS:CD2	2.50	0.45
1:B:1962:GLN:CB	1:B:4341:THR:HG21	2.46	0.45
1:B:2426:ILE:H	1:B:2426:ILE:HD12	1.81	0.45
1:B:2706:THR:HB	1:B:2707:PRO:HD2	1.96	0.45
1:B:2718:CYS:HA	1:B:2733:THR:H	1.81	0.45
1:B:2798:ALA:HB3	1:B:3159:ALA:HB2	1.98	0.45
1:B:3922:ASN:O	1:B:3923:LEU:C	2.58	0.45
1:A:1857:ASN:HA	1:A:1860:ALA:HB3	1.97	0.45
1:A:2028:PHE:O	1:A:2031:LEU:HB2	2.17	0.45
1:A:2372:ASP:O	1:A:2373:ASP:CG	2.59	0.45
1:A:2648:ILE:HD11	1:A:2831:PHE:CE1	2.50	0.45
1:A:3074:ASP:N	1:A:3077:ASN:ND2	2.54	0.45
1:A:3720:VAL:O	1:A:3765:PHE:HB2	2.16	0.45
1:A:3858:LEU:C	1:A:3860:LYS:N	2.73	0.45
1:A:4175:ILE:O	1:A:4178:ALA:HB3	2.16	0.45
1:A:4284:ARG:NH2	1:A:4410:LEU:HD21	2.31	0.45
1:A:4657:THR:OG1	1:A:4658:ASP:N	2.50	0.45
1:B:2714:PHE:HE2	1:B:2766:MET:HE1	1.76	0.45
1:B:2869:GLN:O	1:B:2870:ALA:C	2.57	0.45
1:B:2918:VAL:HG22	1:B:3172:TRP:CE2	2.50	0.45
1:B:3111:ALA:O	1:B:3112:CYS:C	2.60	0.45
1:B:3588:VAL:O	1:B:3592:VAL:HG23	2.16	0.45
1:B:4011:LEU:C	1:B:4012:LEU:HD23	2.41	0.45
1:B:4329:ILE:HD12	1:B:4331:TRP:CZ2	2.51	0.45
1:B:4494:PRO:CB	1:B:4606:GLN:HB2	2.46	0.45
1:A:1770:LEU:O	1:A:1773:VAL:CG2	2.64	0.45
1:A:1912:TYR:CD2	1:A:1912:TYR:N	2.83	0.45
1:A:2263:HIS:ND1	1:A:2289:TYR:OH	2.43	0.45
1:A:2273:MET:HE2	1:A:2413:MET:HE2	1.98	0.45
1:A:2440:ASP:HB3	1:A:2443:GLU:CG	2.46	0.45
1:A:3836:ASN:O	1:A:3839:SER:HB2	2.16	0.45
1:A:3936:PRO:CG	1:A:3937:ASN:H	2.16	0.45
1:A:3961:ASN:N	1:A:4239:GLU:OE2	2.44	0.45
1:A:4277:PHE:CZ	1:A:4360:LEU:HD13	2.51	0.45
1:B:1606:ILE:CG2	1:B:1607:ASP:N	2.79	0.45
1:B:2738:TRP:CZ3	1:B:2785:LYS:HA	2.52	0.45
1:B:2800:ARG:HG2	1:B:2800:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3598:PHE:CD2	1:B:3634:VAL:HG11	2.51	0.45
1:B:3629:LYS:NZ	1:B:3632:LEU:HD13	2.31	0.45
1:B:3665:LEU:HD13	1:B:3685:LEU:HD21	1.98	0.45
1:B:3876:MET:O	1:B:3880:SER:HB2	2.16	0.45
1:B:3882:VAL:HG23	1:B:3883:SER:N	2.31	0.45
1:B:4110:PHE:C	1:B:4112:ASN:H	2.23	0.45
1:B:4329:ILE:CG2	1:B:4330:PRO:HD2	2.46	0.45
1:A:1417:THR:O	1:A:1498:THR:HA	2.16	0.45
1:A:1499:LEU:HD13	1:A:1503:TRP:CH2	2.52	0.45
1:A:3567:LEU:O	1:A:3571:ARG:HB2	2.16	0.45
1:A:3723:VAL:O	1:A:3723:VAL:CG2	2.59	0.45
1:A:4134:LEU:HB3	1:A:4238:TYR:HE2	1.81	0.45
1:A:4165:PRO:HG2	1:A:4166:GLU:H	1.81	0.45
1:A:4557:GLU:O	1:A:4559:ILE:HG22	2.17	0.45
1:B:1793:ASN:C	1:B:1795:VAL:H	2.23	0.45
1:B:2312:THR:OG1	1:B:2315:GLN:HG3	2.17	0.45
1:B:2331:LEU:HD21	1:B:2773:TRP:CD1	2.51	0.45
1:B:2794:PRO:C	1:B:2796:THR:H	2.25	0.45
1:B:3185:GLY:HA2	1:B:3264:ILE:HD11	1.97	0.45
1:B:4046:GLN:O	1:B:4047:PHE:C	2.59	0.45
1:B:4413:ASN:ND2	1:B:4660:LEU:CD2	2.79	0.45
1:A:1578:SER:C	1:A:1580:TYR:N	2.72	0.45
1:A:1656:ILE:HG23	1:A:1657:LEU:N	2.32	0.45
1:A:1863:VAL:HG21	1:A:2115:SER:O	2.17	0.45
1:A:2307:ASP:CG	1:A:2310:ALA:HB2	2.42	0.45
1:A:2367:LEU:HD22	1:A:2371:LEU:HG	1.99	0.45
1:A:3004:VAL:O	1:A:3006:ARG:N	2.50	0.45
1:A:4134:LEU:HD23	1:A:4238:TYR:CE2	2.51	0.45
1:B:1665:ILE:C	1:B:1667:GLN:N	2.73	0.45
1:B:2294:GLU:OE2	1:B:2300:LYS:HA	2.17	0.45
1:B:2766:MET:CE	1:B:2783:LEU:HD11	2.43	0.45
1:B:3511:LEU:O	1:B:3515:GLN:NE2	2.49	0.45
1:B:4335:ARG:HG2	1:B:4360:LEU:HB3	1.98	0.45
1:B:4356:LEU:HD23	1:B:4356:LEU:HA	1.77	0.45
1:A:1808:ASP:OD2	1:A:1808:ASP:N	2.46	0.45
1:A:2090:ASN:HD21	1:A:2091:LEU:HG	1.81	0.45
1:A:2142:GLN:CA	1:A:2142:GLN:NE2	2.78	0.45
1:A:2189:GLN:NE2	1:A:2192:ILE:HD12	2.32	0.45
1:A:2283:THR:OG1	1:A:2396:GLU:OE1	2.29	0.45
1:A:2331:LEU:HD11	1:A:2773:TRP:CE3	2.51	0.45
1:A:2360:ASP:HB2	1:A:2361:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2976:LEU:O	1:A:2980:TYR:CD1	2.70	0.45
1:B:2192:ILE:HG23	1:B:2223:PHE:CD1	2.52	0.45
1:B:2986:VAL:O	1:B:2986:VAL:HG23	2.17	0.45
1:A:1781:LEU:HD23	1:A:1814:LEU:HD11	1.98	0.45
1:A:2307:ASP:HB3	1:A:2310:ALA:HB3	1.99	0.45
1:A:2879:LEU:HD23	1:A:2879:LEU:HA	1.86	0.45
1:A:2918:VAL:O	1:A:2918:VAL:CG1	2.64	0.45
1:A:3300:LYS:O	1:A:3303:GLN:HB2	2.17	0.45
1:A:4184:TRP:N	1:A:4184:TRP:CD1	2.84	0.45
1:B:1640:ASN:HD21	1:B:1644:ILE:CD1	2.16	0.45
1:B:2229:GLN:O	1:B:2230:PRO:O	2.34	0.45
1:B:2676:PRO:HD3	1:B:2793:ASN:OD1	2.16	0.45
1:B:3078:VAL:HG22	1:B:3078:VAL:O	2.16	0.45
1:B:3671:TYR:CD2	1:B:3734:LEU:HA	2.52	0.45
1:B:4499:PHE:CD1	1:B:4578:ILE:HD13	2.51	0.45
1:B:4636:SER:HB3	1:B:4670:THR:HG22	1.98	0.45
1:B:4647:ALA:O	1:B:4662:THR:HG21	2.16	0.45
1:B:4692:LEU:HD22	1:B:4698:GLU:OE1	2.16	0.45
1:A:1569:LEU:HD23	1:A:1569:LEU:HA	1.76	0.45
1:A:2266:LEU:CD2	1:A:2392:ARG:HG2	2.42	0.45
1:A:2567:ASN:O	1:A:2571:ASN:ND2	2.50	0.45
1:A:2651:VAL:O	1:A:2655:ARG:CB	2.65	0.45
1:A:3015:ILE:HD13	1:A:3147:MET:HG3	1.99	0.45
1:A:3024:VAL:HG23	2:A:9004:ADP:PA	2.56	0.45
1:A:3064:CYS:C	1:A:3066:GLU:N	2.75	0.45
1:A:3114:GLU:HG2	1:A:3118:ARG:NH2	2.31	0.45
1:A:3761:MET:HE2	1:A:3763:PHE:CZ	2.52	0.45
1:A:3887:ASN:HB3	1:A:3888:PRO:HD3	1.98	0.45
1:A:4507:GLY:O	1:A:4508:LYS:C	2.59	0.45
1:A:4624:SER:HB2	1:A:4668:THR:HB	1.99	0.45
1:B:1784:LEU:O	1:B:1785:LEU:C	2.59	0.45
1:B:2494:VAL:HG12	1:B:2498:CYS:SG	2.57	0.45
1:B:2669:PRO:HD2	1:B:2810:HIS:O	2.17	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:H	1.80	0.45
1:B:3091:LEU:HD12	1:B:3164:LEU:HD22	1.99	0.45
1:B:3326:GLN:O	1:B:3330:ASP:HB2	2.15	0.45
1:B:4058:ILE:O	1:B:4059:PRO:C	2.60	0.45
1:A:2200:ASN:HA	1:A:2204:ILE:HG22	1.97	0.45
1:A:3064:CYS:O	1:A:3066:GLU:N	2.50	0.45
1:A:3335:GLU:CD	1:A:3529:ILE:HD11	2.41	0.45
1:A:3527:LYS:O	1:A:3528:SER:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4551:LYS:O	1:A:4553:TYR:N	2.49	0.45
1:B:1777:MET:HE3	1:B:1939:GLU:CA	2.46	0.45
1:B:2998:ILE:O	1:B:2998:ILE:HG13	2.17	0.45
1:B:3698:SER:C	1:B:3700:LEU:H	2.24	0.45
1:B:3702:SER:C	1:B:3704:PHE:N	2.74	0.45
1:B:3760:PHE:CD1	1:B:3761:MET:N	2.85	0.45
1:A:1572:ILE:O	1:A:1576:LYS:HG3	2.16	0.45
1:A:1729:LEU:HD12	1:A:1744:MET:SD	2.57	0.45
1:A:1796:ASP:O	1:A:1797:VAL:C	2.60	0.45
1:A:1816:LEU:O	1:A:1820:GLN:HG3	2.16	0.45
1:A:2651:VAL:O	1:A:2655:ARG:HB2	2.17	0.45
1:A:4605:ARG:HA	1:A:4671:TRP:CE3	2.52	0.45
1:A:4707:TYR:OH	1:A:4713:LYS:HE2	2.18	0.45
1:B:1555:VAL:CG2	1:B:1609:GLN:HE21	2.21	0.45
1:B:1837:GLN:C	1:B:1839:SER:N	2.71	0.45
1:B:2057:VAL:HG23	1:B:2057:VAL:O	2.17	0.45
1:B:2238:LYS:O	1:B:2241:GLN:HG2	2.17	0.45
1:B:2309:LYS:HZ1	1:B:2756:THR:HG21	1.77	0.45
1:B:2340:ILE:HD11	1:B:2386:ALA:O	2.17	0.45
1:B:2427:PHE:CE2	1:B:2513:HIS:CE1	3.05	0.45
1:B:2845:PHE:O	1:B:2848:ASN:HB2	2.17	0.45
1:B:3325:LYS:HA	1:B:3328:VAL:HG12	1.98	0.45
1:B:3343:GLU:OE1	1:B:3343:GLU:HA	2.16	0.45
1:B:3928:PRO:C	1:B:3930:LEU:H	2.24	0.45
1:B:4020:LEU:HD21	1:B:4037:ILE:HD12	1.98	0.45
1:A:1915:ASP:O	1:A:1915:ASP:CG	2.60	0.44
1:A:3251:ARG:NH2	1:A:3604:PHE:O	2.50	0.44
1:A:3861:GLU:O	1:A:3864:GLU:HG2	2.17	0.44
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.52	0.44
1:A:4135:CYS:SG	1:A:4225:LEU:CD1	3.05	0.44
1:A:4551:LYS:C	1:A:4553:TYR:N	2.74	0.44
1:A:4601:ILE:HD13	1:A:4701:PHE:HD2	1.82	0.44
1:B:1715:ILE:O	1:B:1715:ILE:HG22	2.16	0.44
1:B:2320:LEU:HD23	1:B:2321:ASP:O	2.18	0.44
1:B:2416:PHE:N	1:B:2416:PHE:CD2	2.85	0.44
1:B:2617:VAL:HG22	1:B:2624:TRP:CE3	2.52	0.44
1:B:2745:GLU:HG2	1:B:2748:LEU:HD12	1.99	0.44
1:B:3251:ARG:NH2	1:B:3604:PHE:CZ	2.85	0.44
1:B:3594:LEU:HD11	1:B:3618:MET:HG2	1.99	0.44
1:B:4021:ILE:O	1:B:4025:GLN:HB3	2.17	0.44
1:B:4546:VAL:CG1	1:B:4551:LYS:HG3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:ALA:O	1:A:1453:HIS:HB2	2.16	0.44
1:A:2338:ARG:O	1:A:2346:GLU:OE2	2.34	0.44
1:A:2382:GLY:O	1:A:2384:ARG:HG3	2.17	0.44
1:A:2669:PRO:HG3	1:A:2767:VAL:HG21	2.00	0.44
1:A:2771:GLY:HA3	1:A:2781:ILE:O	2.17	0.44
1:A:3724:GLU:N	1:A:3724:GLU:CD	2.75	0.44
1:A:4318:SER:O	1:A:4321:ARG:HD3	2.17	0.44
1:A:4604:THR:OG1	1:A:4671:TRP:HZ3	2.00	0.44
1:B:2050:LEU:HD11	1:B:2071:MET:HG2	1.98	0.44
1:B:2314:ASP:C	1:B:2316:LEU:N	2.75	0.44
1:B:2729:VAL:HB	1:B:2782:LYS:O	2.17	0.44
1:A:1856:LEU:O	1:A:1860:ALA:N	2.50	0.44
1:A:3315:VAL:O	1:A:3316:LYS:C	2.60	0.44
1:A:3632:LEU:HD23	1:A:3632:LEU:O	2.17	0.44
1:A:3901:GLU:O	1:A:3901:GLU:HG2	2.17	0.44
1:A:4107:GLY:C	1:A:4109:ASP:N	2.75	0.44
1:A:4659:ILE:HG22	1:A:4661:SER:H	1.82	0.44
1:A:4694:GLU:OE2	1:A:4727:LYS:NZ	2.50	0.44
1:B:2036:LEU:O	1:B:2036:LEU:HD23	2.16	0.44
1:B:2259:ILE:HG23	1:B:2289:TYR:HB2	1.98	0.44
1:B:2522:ARG:HD3	1:B:2585:MET:SD	2.57	0.44
1:B:3093:GLY:O	1:B:3138:ARG:HB3	2.17	0.44
1:B:3151:SER:C	1:B:3153:ASP:H	2.25	0.44
1:B:3194:LEU:H	1:B:3224:ARG:NH2	2.15	0.44
1:B:3563:LEU:O	1:B:3567:LEU:HG	2.18	0.44
1:B:3903:LEU:N	1:B:4433:MET:HE3	2.32	0.44
1:B:4025:GLN:O	1:B:4025:GLN:HG2	2.17	0.44
1:B:4109:ASP:HA	1:B:4112:ASN:ND2	2.32	0.44
1:B:4499:PHE:CE1	1:B:4578:ILE:HD13	2.52	0.44
1:B:4521:LEU:O	1:B:4522:GLU:C	2.61	0.44
1:A:1645:ALA:O	1:A:1646:ILE:C	2.59	0.44
1:A:1715:ILE:C	1:A:1717:LYS:N	2.75	0.44
1:A:3118:ARG:O	1:A:3120:GLY:N	2.50	0.44
1:A:3270:LEU:HD12	1:A:3270:LEU:HA	1.76	0.44
1:A:3331:GLN:HE21	1:A:3532:TYR:HB3	1.82	0.44
1:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.99	0.44
1:A:4201:GLU:HG3	1:A:4228:ASN:HB2	1.98	0.44
1:A:4575:LEU:O	1:A:4578:ILE:HB	2.17	0.44
1:B:1630:PRO:HG2	1:B:1631:ALA:N	2.29	0.44
1:B:1719:GLN:C	1:B:1721:HIS:H	2.26	0.44
1:B:1904:PHE:O	1:B:1906:TRP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2492:LEU:HD12	1:B:2495:GLN:HB2	1.99	0.44
1:B:2501:ILE:HG21	1:B:2566:SER:HA	1.98	0.44
1:B:2606:PRO:HB3	1:B:2615:TYR:CZ	2.52	0.44
1:B:2641:VAL:O	1:B:2831:PHE:CE2	2.71	0.44
1:B:3352:ASN:CA	1:B:3511:LEU:HD21	2.47	0.44
1:B:3690:ALA:O	1:B:3692:LYS:N	2.50	0.44
1:B:3879:ILE:C	1:B:3881:GLU:H	2.25	0.44
1:B:4044:TRP:HB3	1:B:4048:PHE:CE2	2.52	0.44
1:B:4164:SER:HB3	1:B:4165:PRO:CD	2.33	0.44
1:A:2313:LYS:HE3	1:A:2366:ASN:HD21	1.81	0.44
1:A:2763:ILE:HG22	1:A:2807:PHE:HE2	1.82	0.44
1:A:3686:MET:CE	1:A:3719:LEU:HD13	2.48	0.44
1:A:4373:PHE:O	1:A:4382:SER:HB2	2.17	0.44
1:B:1782:ALA:HB2	1:B:1922:LEU:CD2	2.48	0.44
1:B:2265:ILE:CD1	1:B:2414:VAL:HG22	2.47	0.44
1:B:2399:ASP:C	1:B:2399:ASP:OD2	2.60	0.44
1:B:2732:PRO:O	1:B:2734:GLN:N	2.50	0.44
1:B:2937:HIS:O	1:B:2939:PRO:HD3	2.17	0.44
1:B:3073:PHE:CD2	1:B:3145:PHE:CE1	3.06	0.44
1:B:3563:LEU:HD22	1:B:3567:LEU:HD11	1.99	0.44
1:B:3717:PRO:HA	1:B:3761:MET:O	2.17	0.44
1:B:4517:LEU:O	1:B:4521:LEU:HB2	2.17	0.44
1:B:4572:MET:O	1:B:4573:GLN:C	2.59	0.44
1:A:1468:ILE:HD11	1:A:1503:TRP:HE1	1.83	0.44
1:A:1538:TRP:HZ3	1:A:1656:ILE:HD13	1.82	0.44
1:A:1574:ALA:C	1:A:1576:LYS:H	2.25	0.44
1:A:2029:ASN:HD22	1:A:2029:ASN:N	2.14	0.44
1:A:2276:GLY:O	1:A:2398:GLN:HA	2.18	0.44
1:A:3017:VAL:HG21	1:A:3257:PRO:HD3	2.00	0.44
1:A:3056:ARG:HH11	1:A:3099:LEU:CD1	2.28	0.44
1:A:4110:PHE:CD1	1:A:4110:PHE:C	2.96	0.44
1:A:4174:SER:O	1:A:4178:ALA:HB2	2.17	0.44
1:A:4605:ARG:HA	1:A:4671:TRP:CZ3	2.53	0.44
1:B:1611:ARG:HH11	1:B:1611:ARG:CG	2.31	0.44
1:B:1655:LEU:CB	1:B:1658:GLU:HG3	2.47	0.44
1:B:2965:ARG:HG3	1:B:2965:ARG:HH11	1.82	0.44
1:B:4099:HIS:HD2	1:B:4099:HIS:O	2.01	0.44
1:A:1612:TRP:O	1:A:1616:GLU:HB2	2.17	0.44
1:A:3031:TRP:CZ3	1:A:3032:MET:HG2	2.52	0.44
1:A:3114:GLU:HG3	1:A:3117:GLN:NE2	2.33	0.44
1:A:3196:ASN:C	1:A:3198:GLN:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3301:ASP:C	1:A:3303:GLN:N	2.76	0.44
1:A:3977:LYS:HA	1:A:3982:GLU:HG3	1.99	0.44
1:A:4036:HIS:CD2	1:A:4044:TRP:HE1	2.34	0.44
1:A:4318:SER:O	1:A:4319:LYS:C	2.61	0.44
1:B:1548:TYR:O	1:B:1548:TYR:CD1	2.67	0.44
1:B:1665:ILE:O	1:B:1667:GLN:N	2.51	0.44
1:B:1681:LYS:HE3	1:B:1685:GLU:OE2	2.17	0.44
1:B:2236:LEU:HD22	1:B:2240:ILE:HD11	2.00	0.44
1:B:2364:VAL:HG11	1:B:2407:THR:HB	1.99	0.44
1:B:2704:ALA:HB2	1:B:3085:GLU:OE2	2.18	0.44
1:B:3234:ILE:O	1:B:3238:ILE:HD13	2.17	0.44
1:B:3324:LEU:HD11	1:B:3539:LEU:CG	2.44	0.44
1:A:2020:GLY:CA	1:A:2068:HIS:HB3	2.48	0.44
1:A:2282:LYS:O	1:A:2285:SER:HB2	2.17	0.44
1:A:2405:LEU:O	1:A:2408:ILE:HG13	2.18	0.44
1:A:2543:ARG:HD3	1:A:2661:HIS:CD2	2.53	0.44
1:A:2566:SER:O	1:A:2570:THR:OG1	2.28	0.44
1:A:4159:SER:OG	1:A:4160:PHE:N	2.51	0.44
1:A:4213:PHE:O	1:A:4214:ARG:CG	2.60	0.44
1:A:4556:PRO:O	1:A:4557:GLU:C	2.61	0.44
1:B:2359:VAL:HG23	1:B:2397:VAL:HG21	1.99	0.44
1:B:3605:PHE:HB3	1:B:3609:PHE:HB3	2.00	0.44
1:B:3767:ARG:HD3	1:B:4205:HIS:NE2	2.32	0.44
1:B:4597:PRO:HG2	1:B:4692:LEU:CD1	2.48	0.44
1:B:4708:ASP:C	1:B:4708:ASP:OD1	2.60	0.44
1:A:2531:LEU:HD13	1:A:2809:ARG:NE	2.33	0.44
1:A:3061:ARG:CZ	1:A:3067:GLU:OE1	2.66	0.44
1:A:3555:ASN:O	1:A:3559:ARG:HB2	2.17	0.44
1:A:3768:ASP:HA	1:A:3769:PRO:HD2	1.82	0.44
1:A:3936:PRO:O	1:A:3938:GLU:N	2.51	0.44
1:A:3998:LEU:C	1:A:4000:SER:H	2.26	0.44
1:A:3998:LEU:HD13	1:A:4018:LYS:HD3	2.00	0.44
1:A:4057:ILE:O	1:A:4057:ILE:CG2	2.65	0.44
1:A:4189:ASN:H	1:A:4218:THR:HG22	1.83	0.44
1:B:2189:GLN:NE2	1:B:2225:GLY:HA3	2.33	0.44
1:B:2797:ASP:HB2	1:B:2800:ARG:CG	2.47	0.44
1:B:3997:ASN:O	1:B:3998:LEU:C	2.61	0.44
1:B:4122:VAL:HG11	1:B:4216:PHE:CZ	2.53	0.44
1:A:1697:PHE:O	1:A:1700:VAL:HG22	2.18	0.43
1:A:2590:ARG:HG2	1:A:2613:LEU:HD13	1.99	0.43
1:A:3858:LEU:O	1:A:3860:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4392:PHE:O	1:A:4396:ILE:HG13	2.18	0.43
1:B:1557:GLY:O	1:B:1561:LEU:HB2	2.18	0.43
1:B:1700:VAL:CG1	1:B:1704:ASP:HB2	2.47	0.43
1:B:1748:GLU:O	1:B:1870:GLN:HG3	2.18	0.43
1:B:1788:SER:CA	1:B:1810:TYR:CZ	3.01	0.43
1:B:2236:LEU:HD22	1:B:2240:ILE:CD1	2.48	0.43
1:B:2549:ILE:O	1:B:2553:GLN:HB2	2.17	0.43
1:B:2641:VAL:HB	1:B:2887:LEU:HD22	1.98	0.43
1:B:2848:ASN:HD22	1:B:2848:ASN:HA	1.53	0.43
1:B:3644:ARG:O	1:B:3647:TRP:HB2	2.18	0.43
1:B:3949:SER:HA	1:B:4110:PHE:HE1	1.83	0.43
1:B:4256:PRO:HG2	1:B:4259:ARG:HB3	1.99	0.43
1:B:4507:GLY:O	1:B:4508:LYS:C	2.60	0.43
1:B:4572:MET:CE	1:B:4575:LEU:HD12	2.48	0.43
1:A:1490:THR:HG21	1:A:1492:TRP:CD1	2.53	0.43
1:A:1570:ASN:O	1:A:1573:SER:N	2.51	0.43
1:A:2057:VAL:CG1	1:A:2065:ILE:HB	2.48	0.43
1:A:2327:TRP:CH2	1:A:2380:PRO:HD2	2.52	0.43
1:A:3178:PRO:HB2	1:A:3179:GLU:OE1	2.18	0.43
1:A:3836:ASN:O	1:A:3839:SER:N	2.46	0.43
1:A:4140:TYR:C	1:A:4140:TYR:CD1	2.97	0.43
1:A:4644:LEU:HD23	1:A:4648:VAL:N	2.32	0.43
1:B:1605:TRP:CE3	1:B:1669:MET:HE3	2.53	0.43
1:B:1823:TRP:CD1	1:B:1885:GLN:HB3	2.53	0.43
1:B:2129:VAL:CG2	1:B:2130:PRO:CD	2.89	0.43
1:B:2781:ILE:N	1:B:2781:ILE:CD1	2.81	0.43
1:B:3084:LEU:HD22	1:B:3161:SER:CB	2.48	0.43
1:B:3351:ARG:O	1:B:3355:ILE:CG1	2.64	0.43
1:B:3545:GLN:O	1:B:3546:ILE:C	2.61	0.43
1:B:4493:ASP:O	1:B:4494:PRO:C	2.61	0.43
1:B:4644:LEU:HD13	1:B:4647:ALA:HB3	2.00	0.43
1:A:1472:HIS:CG	1:A:1472:HIS:O	2.70	0.43
1:A:1740:THR:O	1:A:1742:ILE:HD13	2.18	0.43
1:A:1838:GLN:O	1:A:1839:SER:C	2.61	0.43
1:A:2239:LYS:HE3	1:A:2295:GLN:HE21	1.83	0.43
1:A:3506:ASN:HA	1:A:3509:ASN:HD22	1.82	0.43
1:A:3689:TYR:CE1	1:A:3761:MET:SD	3.11	0.43
1:A:4112:ASN:O	1:A:4113:THR:C	2.61	0.43
1:A:4293:THR:HG22	1:A:4294:LYS:CG	2.48	0.43
1:B:1617:GLY:O	1:B:1618:ILE:C	2.60	0.43
1:B:1871:LYS:O	1:B:1875:PHE:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2540:LEU:O	1:B:2541:MET:C	2.62	0.43
1:B:2602:ILE:C	1:B:2603:THR:O	2.60	0.43
1:B:2606:PRO:CB	1:B:2615:TYR:CE2	3.00	0.43
1:B:3004:VAL:HG11	1:B:3012:ALA:HB2	2.00	0.43
1:B:3233:TYR:CD2	1:B:3620:ARG:HG3	2.53	0.43
1:B:3348:LEU:HD22	1:B:3511:LEU:CD1	2.48	0.43
1:B:3635:PRO:HA	1:B:3663:ILE:CD1	2.48	0.43
1:B:3972:THR:HG21	1:B:4101:PHE:CE2	2.53	0.43
1:B:4222:HIS:CD2	1:B:4223:PRO:N	2.86	0.43
1:B:4393:MET:O	1:B:4397:GLU:HG3	2.18	0.43
1:A:1419:TRP:CZ3	1:A:1502:ILE:HD12	2.54	0.43
1:A:1854:MET:O	1:A:1856:LEU:N	2.51	0.43
1:A:2490:ALA:O	1:A:2494:VAL:HG23	2.19	0.43
1:A:2525:ILE:HD13	1:A:2526:MET:HG3	2.00	0.43
1:A:2547:ASN:O	1:A:2551:TYR:HB2	2.18	0.43
1:A:2627:TRP:HB3	1:A:2651:VAL:HG23	2.01	0.43
1:A:3987:GLU:CD	1:A:4081:ARG:HE	2.26	0.43
1:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.99	0.43
1:A:4495:LEU:O	1:A:4498:CYS:HB3	2.18	0.43
1:A:4503:ILE:HG13	1:A:4503:ILE:H	1.70	0.43
1:A:4656:PRO:HA	1:A:4719:ARG:NH2	2.34	0.43
1:B:2439:PHE:HA	3:B:9018:SPM:C11	2.48	0.43
1:B:2491:GLY:O	1:B:2493:LYS:N	2.50	0.43
1:B:2952:TYR:CE1	1:B:2962:PRO:HD3	2.54	0.43
1:B:3813:ARG:CG	1:B:3814:SER:N	2.81	0.43
1:B:4404:THR:HB	1:B:4405:PRO:HD2	2.00	0.43
1:A:2212:ILE:N	1:A:2213:PRO:CD	2.80	0.43
1:A:2551:TYR:C	1:A:2551:TYR:CD2	2.96	0.43
1:A:3875:VAL:O	1:A:3879:ILE:HG12	2.18	0.43
1:A:4221:ILE:HD12	1:A:4221:ILE:N	2.34	0.43
1:A:4719:ARG:HH11	1:A:4719:ARG:CG	2.32	0.43
1:B:1639:ILE:HD11	1:B:1675:LEU:HB3	2.00	0.43
1:B:1835:THR:O	1:B:1835:THR:HG22	2.19	0.43
1:B:1907:LEU:HD23	1:B:1907:LEU:HA	1.85	0.43
1:B:2205:PRO:HB3	1:B:2265:ILE:HD11	2.00	0.43
1:B:2314:ASP:O	1:B:2317:PHE:N	2.52	0.43
1:B:2696:VAL:HA	1:B:2740:VAL:O	2.18	0.43
1:B:3022:LYS:HB2	2:B:9010:ADP:O3B	2.18	0.43
1:B:3038:TYR:C	1:B:3039:THR:CG2	2.92	0.43
1:B:3308:GLN:OE1	1:B:3311:ARG:NH2	2.38	0.43
1:B:3902:GLU:C	1:B:3904:SER:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4204:LEU:HB3	1:B:4232:MET:HE1	2.00	0.43
1:A:2275:VAL:HG12	1:A:2276:GLY:N	2.33	0.43
1:A:2427:PHE:O	1:A:2430:TYR:HB3	2.19	0.43
1:A:2679:GLY:O	1:A:2683:THR:OG1	2.34	0.43
1:A:3362:ALA:HA	1:A:3365:ASP:HB2	2.00	0.43
1:A:3672:PRO:HA	1:A:3782:THR:O	2.19	0.43
1:A:3993:LYS:O	1:A:3996:ASP:HB2	2.19	0.43
1:B:1736:ASP:OD2	1:B:1736:ASP:N	2.52	0.43
1:B:2187:TYR:O	1:B:2190:TYR:N	2.51	0.43
1:B:2536:SER:HB2	1:B:2580:GLY:O	2.19	0.43
1:B:3057:MET:HA	1:B:3060:LYS:CB	2.48	0.43
1:B:3696:LYS:NZ	1:B:3721:GLN:NE2	2.67	0.43
1:B:3723:VAL:O	1:B:3725:ASN:N	2.52	0.43
1:B:3798:LEU:HD12	1:B:3798:LEU:O	2.18	0.43
1:B:3940:LEU:O	1:B:3940:LEU:HD13	2.19	0.43
1:B:3973:ILE:HD13	1:B:3983:ILE:HG13	2.01	0.43
1:B:4028:PRO:O	1:B:4029:SER:C	2.62	0.43
1:B:4197:LEU:O	1:B:4198:VAL:C	2.61	0.43
1:A:1554:LEU:HD23	1:A:1647:LEU:HD21	2.00	0.43
1:A:1576:LYS:HG2	1:A:1581:TYR:CE1	2.53	0.43
1:A:1828:ASP:OD2	1:A:1913:TYR:HE1	2.01	0.43
1:A:2239:LYS:HA	1:A:2239:LYS:HD2	1.77	0.43
1:A:2447:GLN:HE22	1:A:2492:LEU:HD23	1.81	0.43
1:A:2910:LEU:O	1:A:2914:GLN:HB3	2.19	0.43
1:A:3936:PRO:CG	1:A:3937:ASN:N	2.78	0.43
1:A:4355:LEU:CD1	1:A:4718:GLN:HA	2.48	0.43
1:B:1769:TRP:O	1:B:1773:VAL:HG23	2.19	0.43
1:B:2092:LYS:HE2	1:B:4297:GLU:OE1	2.19	0.43
1:B:2723:THR:OG1	1:B:2724:PRO:HD2	2.18	0.43
1:B:4164:SER:CB	1:B:4165:PRO:HD2	2.33	0.43
1:B:4491:ILE:O	1:B:4491:ILE:CG1	2.67	0.43
1:B:4704:ASP:O	1:B:4705:LEU:HD23	2.18	0.43
1:A:1480:HIS:CE1	1:A:1521:ALA:HA	2.54	0.43
1:A:2090:ASN:ND2	1:A:2091:LEU:N	2.64	0.43
1:A:2158:SER:O	1:A:2159:ALA:C	2.61	0.43
1:A:2199:ILE:HG21	1:A:2219:LEU:HD11	2.01	0.43
1:A:3154:PHE:HD2	1:A:3155:HIS:NE2	2.17	0.43
1:A:3255:VAL:O	1:A:3255:VAL:HG13	2.18	0.43
1:A:3766:THR:HG22	1:A:3767:ARG:H	1.83	0.43
1:A:4192:LEU:O	1:A:4194:PRO:HD2	2.18	0.43
1:A:4719:ARG:HH11	1:A:4719:ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.18	0.43
1:B:1863:VAL:CG2	1:B:1872:ARG:HH11	2.26	0.43
1:B:2370:LEU:HD23	1:B:2370:LEU:C	2.44	0.43
1:B:2532:ARG:HG2	1:B:2532:ARG:HH11	1.83	0.43
1:B:2665:SER:O	1:B:2667:HIS:ND1	2.52	0.43
1:B:2706:THR:O	1:B:2707:PRO:C	2.60	0.43
1:B:2759:VAL:O	1:B:2763:ILE:HG13	2.19	0.43
1:B:2869:GLN:HB2	1:B:2872:TYR:CG	2.54	0.43
1:B:3352:ASN:HA	1:B:3511:LEU:HD21	2.01	0.43
1:B:4571:ARG:CD	1:B:4593:GLY:O	2.67	0.43
1:A:1422:ILE:HD12	1:A:1422:ILE:C	2.43	0.43
1:A:1575:MET:O	1:A:1575:MET:HG3	2.19	0.43
1:A:1904:PHE:C	1:A:1906:TRP:N	2.73	0.43
1:A:1974:GLY:CA	1:A:2079:PRO:HD3	2.49	0.43
1:A:1994:PHE:C	1:A:1994:PHE:CD1	2.97	0.43
1:A:2106:GLU:HA	1:A:2129:VAL:HG21	1.99	0.43
1:A:2262:LEU:HD21	1:A:2274:MET:HG2	2.00	0.43
1:A:2551:TYR:HD1	1:A:2619:ILE:CG1	2.32	0.43
1:A:3540:ILE:HD13	1:A:3540:ILE:HA	1.93	0.43
1:A:4222:HIS:HA	1:A:4223:PRO:HD2	1.78	0.43
1:B:1826:GLN:O	1:B:1828:ASP:N	2.52	0.43
1:B:2197:ASN:C	1:B:2197:ASN:HD22	2.25	0.43
1:B:2322:LEU:HD23	1:B:2322:LEU:HA	1.84	0.43
1:B:2626:LEU:HB3	1:B:2629:ASN:ND2	2.33	0.43
1:B:3602:ILE:HD13	1:B:3602:ILE:HA	1.86	0.43
1:B:3653:PRO:HB2	1:B:3655:ASP:OD1	2.18	0.43
1:B:4063:ILE:HD12	1:B:4063:ILE:H	1.83	0.43
1:B:4189:ASN:HD22	1:B:4218:THR:CG2	2.32	0.43
1:B:4590:TRP:CZ3	1:B:4593:GLY:HA3	2.54	0.43
1:A:1555:VAL:HB	1:A:1558:TRP:CZ2	2.54	0.43
1:A:1662:ILE:O	1:A:1665:ILE:HG13	2.19	0.43
1:A:2587:LEU:O	1:A:2591:GLU:HG3	2.18	0.43
1:A:3643:GLU:OE2	1:A:3666:LYS:CE	2.65	0.43
1:A:3648:HIS:O	1:A:3651:SER:N	2.51	0.43
1:A:4066:GLN:O	1:A:4066:GLN:HG2	2.19	0.43
1:A:4155:LYS:O	1:A:4156:GLN:C	2.62	0.43
1:A:4369:PHE:CD2	1:A:4369:PHE:N	2.87	0.43
1:A:4576:SER:O	1:A:4577:GLU:C	2.60	0.43
1:B:1737:GLU:HB2	1:B:1739:THR:HG23	2.01	0.43
1:B:1846:GLN:O	1:B:1850:GLN:HG2	2.19	0.43
1:B:1863:VAL:O	1:B:1872:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3139:ARG:CG	1:B:3139:ARG:O	2.62	0.43
1:B:4020:LEU:HD11	1:B:4033:LEU:HG	2.01	0.43
1:B:4167:GLY:O	1:B:4171:ALA:CB	2.66	0.43
1:A:2944:ASP:O	1:A:2945:ALA:C	2.61	0.42
1:A:3256:THR:O	1:A:3257:PRO:C	2.61	0.42
1:A:3358:GLN:HB3	1:A:3504:LEU:HD11	2.01	0.42
1:A:3858:LEU:HA	1:A:3858:LEU:HD12	1.54	0.42
1:B:1804:SER:O	1:B:1805:GLU:C	2.61	0.42
1:B:2135:CYS:C	1:B:2137:GLU:H	2.26	0.42
1:B:2636:VAL:CG1	1:B:2637:GLU:N	2.81	0.42
1:B:3073:PHE:CD2	1:B:3145:PHE:HE1	2.37	0.42
1:B:3671:TYR:HD2	1:B:3734:LEU:HA	1.83	0.42
1:B:3727:ASP:CB	1:B:3729:VAL:CG1	2.97	0.42
1:A:1481:TRP:HB3	1:A:1494:ILE:HG13	1.99	0.42
1:A:1581:TYR:O	1:A:1582:LYS:C	2.61	0.42
1:A:1756:LYS:HB2	1:A:1776:GLU:CD	2.44	0.42
1:A:2680:LYS:N	2:A:9003:ADP:O2B	2.50	0.42
1:A:2759:VAL:HG13	1:A:2760:ILE:HD13	2.01	0.42
1:A:2875:SER:C	1:A:2877:ARG:N	2.77	0.42
1:A:2902:VAL:HG22	1:A:2938:PHE:CD2	2.54	0.42
1:A:2903:ARG:NH2	1:A:2947:LYS:O	2.52	0.42
1:A:3061:ARG:NH1	1:A:3061:ARG:HG2	2.33	0.42
1:A:3083:PHE:N	1:A:3083:PHE:HD2	2.17	0.42
1:A:3644:ARG:O	1:A:3645:LEU:C	2.62	0.42
1:A:4020:LEU:CD2	1:A:4034:VAL:HG22	2.49	0.42
1:A:4062:TRP:C	1:A:4064:VAL:N	2.77	0.42
1:A:4568:PHE:CZ	1:A:4572:MET:SD	3.12	0.42
1:A:4694:GLU:O	1:A:4696:ARG:N	2.52	0.42
1:B:1655:LEU:HB2	1:B:1658:GLU:HG3	2.01	0.42
1:B:1871:LYS:O	1:B:1875:PHE:HD2	2.02	0.42
1:B:2502:ILE:HB	1:B:2573:LEU:HD13	2.01	0.42
1:B:2660:LEU:HD22	1:B:2670:LEU:HD13	2.01	0.42
1:B:3074:ASP:CG	1:B:3075:GLU:N	2.77	0.42
1:B:3238:ILE:HG22	1:B:3255:VAL:HG22	2.01	0.42
1:B:3324:LEU:HD12	1:B:3539:LEU:HD23	2.01	0.42
1:B:3354:GLU:C	1:B:3356:ALA:N	2.76	0.42
1:B:3730:LEU:O	1:B:3731:ASN:C	2.61	0.42
1:B:4174:SER:O	1:B:4175:ILE:C	2.62	0.42
1:A:1470:ASP:CB	1:A:1518:ILE:HD12	2.49	0.42
1:A:1576:LYS:HG2	1:A:1581:TYR:CZ	2.54	0.42
1:A:1601:LEU:HA	1:A:1666:GLN:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1914:TYR:OH	1:A:1924:LYS:HD3	2.19	0.42
1:A:1950:THR:HG21	1:A:2108:ILE:HG13	2.01	0.42
1:A:2346:GLU:O	1:A:2351:HIS:HE1	2.02	0.42
1:A:2405:LEU:HD23	1:A:2408:ILE:HD11	2.00	0.42
1:A:2689:ARG:C	1:A:2691:PHE:N	2.76	0.42
1:A:2911:ARG:HD3	1:A:2911:ARG:HA	1.86	0.42
1:A:3074:ASP:OD1	1:A:3146:THR:OG1	2.31	0.42
1:A:3074:ASP:CA	1:A:3077:ASN:HD22	2.32	0.42
1:A:3179:GLU:H	1:A:3179:GLU:CD	2.27	0.42
1:A:3295:THR:O	1:A:3299:VAL:HG23	2.19	0.42
1:A:4317:TYR:CD2	1:A:4317:TYR:N	2.88	0.42
1:B:1552:CYS:SG	1:B:1647:LEU:HD12	2.59	0.42
1:B:1558:TRP:CE2	1:B:1606:ILE:HG13	2.54	0.42
1:B:2863:ARG:HD2	1:B:2864:PHE:CE1	2.55	0.42
1:B:3628:PHE:CD1	1:B:3628:PHE:C	2.97	0.42
1:B:3949:SER:HA	1:B:4110:PHE:CE1	2.54	0.42
1:B:4070:SER:C	1:B:4072:GLN:N	2.76	0.42
1:B:4596:ASN:ND2	1:B:4596:ASN:O	2.52	0.42
1:B:4666:ILE:HG13	1:B:4667:ALA:H	1.84	0.42
1:B:4709:GLN:N	1:B:4709:GLN:NE2	2.49	0.42
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.20	0.42
1:A:1968:MET:CE	1:A:2051:LYS:NZ	2.81	0.42
1:A:2408:ILE:O	1:A:2409:SER:C	2.62	0.42
1:A:2728:THR:HG21	1:A:2779:THR:HG21	2.01	0.42
1:A:3023:SER:CB	1:A:3027:ARG:HH12	2.32	0.42
1:A:3686:MET:HE2	1:A:3719:LEU:HD13	2.00	0.42
1:A:4509:LEU:O	1:A:4510:VAL:C	2.62	0.42
1:B:1608:VAL:HG12	1:B:1609:GLN:N	2.33	0.42
1:B:1910:MET:HA	1:B:1929:MET:HB2	2.01	0.42
1:B:2000:CYS:C	1:B:2002:GLU:N	2.77	0.42
1:B:2197:ASN:ND2	1:B:2197:ASN:C	2.77	0.42
1:B:2607:ALA:C	1:B:2609:THR:N	2.76	0.42
1:B:2836:MET:CE	1:B:2839:LEU:HD12	2.41	0.42
1:B:4030:PHE:CD2	1:B:4030:PHE:N	2.88	0.42
1:B:4288:ILE:HG23	1:B:4289:PRO:HA	2.01	0.42
1:B:4404:THR:H	1:B:4407:TRP:CD1	2.37	0.42
1:B:4484:LEU:CD2	1:B:4500:GLU:HG3	2.49	0.42
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	2.01	0.42
1:A:2554:LEU:HD12	1:A:2554:LEU:HA	1.85	0.42
1:A:2718:CYS:HB3	1:A:2731:ARG:O	2.19	0.42
1:A:2997:HIS:O	1:A:3001:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3179:GLU:HG3	1:A:3216:LEU:HD11	2.01	0.42
1:A:3286:ASN:C	1:A:3288:GLY:N	2.74	0.42
1:A:3602:ILE:HG23	1:A:3610:ARG:CG	2.49	0.42
1:A:4355:LEU:O	1:A:4358:SER:HB3	2.20	0.42
1:A:4622:HIS:HB2	1:A:4679:PHE:HE1	1.84	0.42
1:B:1671:ARG:HG3	1:B:1671:ARG:HH11	1.85	0.42
1:B:1856:LEU:O	1:B:1860:ALA:N	2.48	0.42
1:B:1916:ALA:O	1:B:1917:THR:C	2.62	0.42
1:B:2496:LYS:O	1:B:2497:GLU:C	2.62	0.42
1:B:2552:ASN:O	1:B:2554:LEU:N	2.53	0.42
1:B:3506:ASN:OD1	1:B:3506:ASN:C	2.62	0.42
1:B:3700:LEU:HD13	1:B:3701:ASP:CA	2.48	0.42
1:B:3701:ASP:OD1	1:B:3703:SER:N	2.47	0.42
1:B:3789:THR:HB	1:B:3790:PRO:HD2	2.00	0.42
1:B:3981:ASN:O	1:B:3982:GLU:C	2.61	0.42
1:B:4621:LEU:HD13	1:B:4671:TRP:CD2	2.54	0.42
1:B:4711:THR:HG1	1:B:4716:TRP:NE1	2.17	0.42
1:A:1417:THR:CB	1:A:1422:ILE:HG22	2.48	0.42
1:A:2598:GLN:OE1	1:A:2612:LEU:N	2.52	0.42
1:A:3185:GLY:HA2	1:A:3264:ILE:HD13	2.00	0.42
1:A:3536:TYR:O	1:A:3539:LEU:N	2.53	0.42
1:A:4142:ALA:O	1:A:4143:SER:C	2.63	0.42
1:A:4604:THR:OG1	1:A:4671:TRP:CZ3	2.73	0.42
1:B:2051:LYS:C	1:B:2053:ASN:H	2.27	0.42
1:B:2252:LYS:HE2	1:B:2254:GLU:HG2	2.00	0.42
1:B:2909:ALA:O	1:B:2913:PHE:HB2	2.19	0.42
1:B:2918:VAL:HG22	1:B:3172:TRP:CZ2	2.55	0.42
1:B:3088:ASN:HD21	1:B:3163:ALA:HB2	1.84	0.42
1:B:3240:GLU:C	1:B:3242:ASN:N	2.77	0.42
1:B:3893:CYS:HG	1:B:3920:PHE:HE1	1.66	0.42
1:B:4165:PRO:HG2	1:B:4166:GLU:N	2.31	0.42
1:A:1549:GLN:HE21	1:A:1551:LYS:CE	2.33	0.42
1:A:1569:LEU:HD13	1:A:1599:ARG:NH2	2.34	0.42
1:A:2008:ALA:HA	1:A:2011:ARG:NH1	2.35	0.42
1:A:2972:VAL:O	1:A:2976:LEU:HB2	2.20	0.42
1:A:3864:GLU:CG	1:A:3865:ILE:HG13	2.50	0.42
1:A:4561:LEU:O	1:A:4565:ILE:HG13	2.19	0.42
1:A:4712:SER:OG	1:A:4715:ASN:HB2	2.19	0.42
1:B:1614:TYR:HD2	1:B:1615:LEU:CD2	2.33	0.42
1:B:1763:GLY:H	1:B:1764:PRO:HD3	1.85	0.42
1:B:1830:ALA:O	1:B:1841:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2540:LEU:HD12	1:B:2662:ALA:HB3	2.01	0.42
1:B:2963:VAL:HG12	1:B:2964:ASN:N	2.35	0.42
1:B:2972:VAL:HG12	1:B:2976:LEU:HD12	2.02	0.42
1:B:3127:GLU:O	1:B:3128:GLU:C	2.61	0.42
1:B:3338:GLN:O	1:B:3341:ALA:N	2.52	0.42
1:B:3795:SER:O	1:B:3796:GLN:C	2.63	0.42
1:B:3865:ILE:C	1:B:3867:LEU:N	2.77	0.42
1:B:4207:LEU:O	1:B:4209:PRO:HD3	2.19	0.42
1:B:4255:ILE:O	1:B:4389:ARG:NE	2.46	0.42
1:A:1715:ILE:CG2	1:A:1719:GLN:HE22	2.32	0.42
1:A:1735:ASP:OD2	1:A:1740:THR:HG23	2.19	0.42
1:A:1852:THR:C	1:A:1854:MET:N	2.78	0.42
1:A:1979:GLY:HA2	2:A:9001:ADP:O2A	2.20	0.42
1:A:2386:ALA:O	1:A:2388:PRO:HD3	2.19	0.42
1:A:2747:ASN:HD22	1:A:2747:ASN:H	1.68	0.42
1:A:2863:ARG:HG3	1:A:2925:TRP:CH2	2.54	0.42
1:A:3908:LEU:O	1:A:3908:LEU:HG	2.18	0.42
1:A:3990:PHE:O	1:A:3994:GLY:N	2.51	0.42
1:B:1655:LEU:CD2	1:B:1655:LEU:N	2.70	0.42
1:B:3113:LYS:O	1:B:3116:ALA:HB3	2.20	0.42
1:B:3930:LEU:O	1:B:3931:VAL:C	2.62	0.42
1:A:2423:THR:HA	1:A:2530:ARG:HH11	1.85	0.42
1:A:2914:GLN:O	1:A:2916:ARG:N	2.52	0.42
1:A:3059:LEU:HD13	1:A:3137:VAL:HG21	2.02	0.42
1:A:3330:ASP:C	1:A:3532:TYR:CE2	2.98	0.42
1:A:3886:TYR:CE2	1:A:3940:LEU:HD13	2.55	0.42
1:A:4134:LEU:HD23	1:A:4238:TYR:HH	1.84	0.42
1:A:4175:ILE:HA	1:A:4185:VAL:HG21	2.02	0.42
1:A:4609:SER:C	1:A:4611:LEU:H	2.28	0.42
1:B:1559:ASP:C	1:B:1561:LEU:N	2.75	0.42
1:B:1788:SER:HB2	1:B:1810:TYR:CD1	2.54	0.42
1:B:1929:MET:O	1:B:1930:ALA:HB3	2.20	0.42
1:B:2307:ASP:HA	1:B:2308:PRO:HD3	1.89	0.42
1:B:2423:THR:HA	1:B:2426:ILE:HD13	2.02	0.42
1:B:2511:LEU:O	1:B:2512:VAL:C	2.63	0.42
1:B:2711:LEU:O	1:B:2714:PHE:HB2	2.19	0.42
1:B:2965:ARG:HG3	1:B:2965:ARG:NH1	2.34	0.42
1:B:3193:ASP:C	1:B:3193:ASP:OD1	2.63	0.42
1:B:3503:GLN:O	1:B:3504:LEU:C	2.63	0.42
1:B:3668:PHE:CD1	1:B:3668:PHE:O	2.73	0.42
1:B:4122:VAL:HG12	1:B:4132:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4691:TYR:HA	1:B:4698:GLU:O	2.19	0.42
1:A:1416:GLU:O	1:A:1498:THR:HG21	2.20	0.42
1:A:1544:ASP:OD2	1:A:1556:ARG:NE	2.43	0.42
1:A:1545:LEU:HA	1:A:1554:LEU:O	2.19	0.42
1:A:1732:LEU:HD13	1:A:1741:ILE:HD12	2.02	0.42
1:A:2341:ASP:O	1:A:2343:VAL:N	2.52	0.42
1:A:2391:VAL:C	1:A:2392:ARG:HD2	2.44	0.42
1:A:3285:LEU:HD13	1:A:3578:SER:CA	2.49	0.42
1:A:3838:LEU:O	1:A:3841:ALA:HB3	2.20	0.42
1:A:4187:LEU:HD13	1:A:4217:MET:HG2	2.02	0.42
1:A:4200:LEU:CD2	1:A:4204:LEU:HG	2.50	0.42
1:A:4691:TYR:CD2	1:A:4696:ARG:HG2	2.54	0.42
1:B:1591:TRP:O	1:B:1595:LEU:HB2	2.19	0.42
1:B:1642:GLU:O	1:B:1646:ILE:HG12	2.20	0.42
1:B:1786:SER:O	1:B:1789:LEU:HB2	2.20	0.42
1:B:2616:SER:O	1:B:2624:TRP:HE3	2.03	0.42
1:B:3939:ARG:C	1:B:3941:VAL:H	2.27	0.42
1:B:4044:TRP:HZ2	1:B:4062:TRP:HB2	1.85	0.42
1:B:4285:LEU:O	1:B:4288:ILE:HG13	2.20	0.42
1:A:1603:ASP:O	1:A:1606:ILE:HG22	2.20	0.41
1:A:1825:THR:O	1:A:1829:GLN:HG3	2.20	0.41
1:A:1828:ASP:OD2	1:A:1913:TYR:CE1	2.73	0.41
1:A:2388:PRO:HB2	1:A:2390:ASN:OD1	2.20	0.41
1:A:3199:TYR:CG	1:A:3200:ILE:N	2.88	0.41
1:A:3536:TYR:O	1:A:3537:ALA:C	2.62	0.41
1:A:3767:ARG:NE	1:A:4205:HIS:CE1	2.88	0.41
1:A:4509:LEU:HD22	1:A:4552:TRP:HB2	2.02	0.41
1:A:4659:ILE:N	1:A:4659:ILE:HD12	2.35	0.41
1:A:4695:THR:O	1:A:4696:ARG:HB2	2.19	0.41
1:B:1547:ASN:HD22	1:B:1548:TYR:N	2.18	0.41
1:B:1711:ASN:ND2	1:B:1717:LYS:CD	2.80	0.41
1:B:1947:LEU:HB3	2:B:9007:ADP:N1	2.35	0.41
1:B:1947:LEU:HB3	2:B:9007:ADP:C6	2.55	0.41
1:B:1965:GLU:O	1:B:1967:ARG:NH1	2.52	0.41
1:B:2355:PHE:CE2	1:B:2367:LEU:HD21	2.55	0.41
1:B:2504:GLN:HE21	1:B:2504:GLN:HB2	1.65	0.41
1:B:2963:VAL:CG1	1:B:2968:LEU:HB2	2.49	0.41
1:B:3239:GLY:HA2	1:B:3255:VAL:HG21	2.02	0.41
1:B:3344:LEU:O	1:B:3348:LEU:HB2	2.19	0.41
1:B:3570:GLU:O	1:B:3573:ARG:N	2.53	0.41
1:B:3758:PRO:C	1:B:3760:PHE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4029:SER:HB2	1:B:4066:GLN:HE21	1.85	0.41
1:B:4043:ASP:O	1:B:4059:PRO:HG3	2.20	0.41
1:B:4143:SER:OG	1:B:4188:LYS:HE3	2.20	0.41
1:B:4162:ILE:HG13	1:B:4196:TRP:CZ3	2.55	0.41
1:B:4340:SER:OG	1:B:4357:TYR:OH	2.30	0.41
1:A:1604:VAL:HG11	1:A:1670:GLU:HA	2.02	0.41
1:A:1655:LEU:HD12	1:A:1658:GLU:OE1	2.20	0.41
1:A:2434:LEU:HD11	1:A:2545:ILE:HD13	2.03	0.41
1:A:2689:ARG:O	1:A:2691:PHE:N	2.53	0.41
1:A:2807:PHE:O	1:A:2809:ARG:N	2.54	0.41
1:A:2907:HIS:O	1:A:2911:ARG:HG2	2.20	0.41
1:A:3051:PHE:CZ	1:A:3087:MET:HE3	2.56	0.41
1:A:3202:PRO:HA	1:A:3203:PRO:HD3	1.93	0.41
1:A:3338:GLN:HE21	1:A:3338:GLN:CA	2.28	0.41
1:A:3689:TYR:O	1:A:3694:ILE:HG13	2.20	0.41
1:A:3721:GLN:HE21	1:A:3721:GLN:HB3	1.57	0.41
1:A:3889:MET:SD	1:A:3889:MET:C	3.03	0.41
1:A:4058:ILE:HD13	1:A:4085:LEU:HD12	2.02	0.41
1:B:1758:ILE:HD12	1:B:1773:VAL:HG22	2.02	0.41
1:B:1764:PRO:HB2	1:B:1768:GLU:CB	2.50	0.41
1:B:1926:VAL:HG12	1:B:1928:HIS:CD2	2.53	0.41
1:B:2016:LEU:HD23	1:B:2021:ALA:HB3	2.01	0.41
1:B:2085:SER:HB3	1:B:2092:LYS:CE	2.50	0.41
1:B:2112:MET:SD	1:B:2153:LYS:HG2	2.60	0.41
1:B:2359:VAL:HG12	1:B:2360:ASP:N	2.35	0.41
1:B:2540:LEU:HD12	1:B:2540:LEU:HA	1.95	0.41
1:B:2609:THR:O	1:B:2610:ILE:CG1	2.67	0.41
1:B:2748:LEU:O	1:B:2749:PRO:C	2.63	0.41
1:B:2841:ASN:N	1:B:2841:ASN:ND2	2.64	0.41
1:B:3773:PHE:CE2	1:B:3783:PHE:HE1	2.38	0.41
1:B:4262:LYS:CB	1:B:4267:ARG:HH12	2.33	0.41
1:B:4523:LEU:HD23	1:B:4523:LEU:C	2.46	0.41
1:B:4546:VAL:HG12	1:B:4551:LYS:HG3	2.02	0.41
1:A:1476:ILE:O	1:A:1476:ILE:HG22	2.19	0.41
1:A:2057:VAL:HG12	1:A:2065:ILE:HB	2.02	0.41
1:A:3017:VAL:HG22	1:A:3018:SER:N	2.35	0.41
1:A:3200:ILE:O	1:A:3202:PRO:CD	2.61	0.41
1:A:3351:ARG:HH11	1:A:3351:ARG:HG3	1.85	0.41
1:A:4219:SER:OG	1:A:4220:GLU:N	2.53	0.41
1:A:4609:SER:C	1:A:4611:LEU:N	2.78	0.41
1:B:1562:PHE:CD2	1:B:1565:LEU:HD22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1844:GLN:O	1:B:1848:ILE:HG13	2.20	0.41
1:B:1846:GLN:HA	1:B:1893:GLN:HE22	1.83	0.41
1:B:2572:ARG:HA	1:B:2572:ARG:HD2	1.77	0.41
1:B:2694:PHE:HE1	1:B:2787:GLN:HE22	1.68	0.41
1:B:2889:ALA:CB	1:B:2904:LEU:HD11	2.50	0.41
1:B:3088:ASN:ND2	1:B:3163:ALA:HB2	2.36	0.41
1:B:3342:ARG:O	1:B:3345:GLN:HB3	2.21	0.41
1:B:3549:GLU:O	1:B:3553:VAL:HG23	2.20	0.41
1:B:3923:LEU:CD1	1:B:3946:ASP:HB2	2.50	0.41
1:B:3958:THR:HG23	1:B:4235:VAL:HB	2.02	0.41
1:B:4068:GLN:C	1:B:4070:SER:N	2.78	0.41
1:A:1840:LYS:O	1:A:1843:GLU:N	2.52	0.41
1:A:1852:THR:O	1:A:1853:GLN:C	2.63	0.41
1:A:2748:LEU:HD21	1:A:2800:ARG:NH1	2.35	0.41
1:A:3809:THR:O	1:A:3810:HIS:C	2.61	0.41
1:A:4051:ASP:OD1	1:A:4658:ASP:CB	2.68	0.41
1:A:4315:ASP:O	1:A:4319:LYS:HB2	2.20	0.41
1:B:1719:GLN:C	1:B:1721:HIS:N	2.77	0.41
1:B:2506:PHE:CE1	1:B:2512:VAL:HG21	2.55	0.41
1:B:2561:SER:O	1:B:2562:PRO:C	2.63	0.41
1:B:2889:ALA:HB1	1:B:2904:LEU:HD11	2.02	0.41
1:B:2960:TYR:O	1:B:2961:GLN:CG	2.67	0.41
1:B:3011:HIS:CD2	1:B:3143:VAL:H	2.38	0.41
1:B:3296:GLU:OE1	1:B:3571:ARG:HD3	2.21	0.41
1:B:3324:LEU:O	1:B:3327:MET:HB3	2.20	0.41
1:B:3970:GLN:OE1	1:B:4433:MET:HE1	2.20	0.41
1:A:1949:GLN:NE2	1:A:1953:THR:CG2	2.82	0.41
1:A:2052:GLU:O	1:A:2053:ASN:CB	2.67	0.41
1:A:2273:MET:O	1:A:2275:VAL:HG23	2.20	0.41
1:A:2400:LEU:O	1:A:2402:TYR:N	2.53	0.41
1:A:3027:ARG:HA	1:A:3037:ILE:CD1	2.51	0.41
1:A:3337:LYS:HB3	1:A:3525:LEU:HD11	2.03	0.41
1:A:3522:ILE:CG2	1:A:3523:THR:N	2.84	0.41
1:A:4002:LYS:HB2	1:B:2845:PHE:CZ	2.56	0.41
1:A:4137:VAL:O	1:A:4138:PRO:C	2.63	0.41
1:B:1548:TYR:HD1	1:B:1548:TYR:C	2.25	0.41
1:B:1558:TRP:HH2	1:B:1605:TRP:HB3	1.85	0.41
1:B:2572:ARG:NH1	1:B:2575:TYR:CD2	2.88	0.41
1:B:2670:LEU:HB3	1:B:2812:PRO:HG2	2.03	0.41
1:B:2984:LEU:HD22	1:B:2986:VAL:HG13	2.02	0.41
1:B:3570:GLU:O	1:B:3571:ARG:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3602:ILE:HG12	1:B:3617:TRP:HH2	1.86	0.41
1:B:3780:ARG:HE	1:B:3780:ARG:HB3	1.58	0.41
1:B:3865:ILE:O	1:B:3866:ALA:C	2.64	0.41
1:B:4518:ALA:O	1:B:4519:ASN:C	2.64	0.41
1:B:4567:ASP:O	1:B:4571:ARG:HG2	2.20	0.41
1:B:4655:THR:HA	1:B:4656:PRO:HD3	1.89	0.41
1:A:1497:LEU:HD22	1:A:1501:SER:CB	2.50	0.41
1:A:1587:GLU:HG2	1:A:1591:TRP:CD1	2.56	0.41
1:A:1633:SER:O	1:A:1637:LYS:HG2	2.21	0.41
1:A:1916:ALA:C	1:A:1918:GLN:N	2.74	0.41
1:A:2090:ASN:HD22	1:A:2090:ASN:C	2.26	0.41
1:A:2376:LEU:HD11	1:A:2384:ARG:CB	2.50	0.41
1:A:2966:SER:HA	1:A:2969:ARG:CG	2.49	0.41
1:A:3023:SER:HB3	1:A:3027:ARG:NH1	2.34	0.41
1:A:3527:LYS:O	1:A:3530:ALA:N	2.53	0.41
1:A:3816:LEU:HB3	1:A:3817:LEU:CD2	2.50	0.41
1:A:4172:GLU:HG2	1:A:4172:GLU:H	1.60	0.41
1:A:4605:ARG:HG2	1:A:4605:ARG:NH1	2.35	0.41
1:B:1828:ASP:C	1:B:1830:ALA:H	2.29	0.41
1:B:1873:LYS:HA	1:B:1876:GLU:OE2	2.21	0.41
1:B:2379:LEU:HB2	1:B:2383:GLU:CB	2.50	0.41
1:B:2522:ARG:HH21	1:B:2592:ASN:CB	2.33	0.41
1:B:2560:MET:CG	1:B:2564:ASN:HB2	2.50	0.41
1:B:2665:SER:O	1:B:2667:HIS:CE1	2.73	0.41
1:B:2875:SER:C	1:B:2877:ARG:N	2.78	0.41
1:B:2897:THR:O	1:B:2898:LEU:C	2.63	0.41
1:B:3921:TYR:CD2	1:B:3925:ASN:ND2	2.85	0.41
1:B:3988:TRP:O	1:B:3992:LEU:HG	2.19	0.41
1:B:4030:PHE:HD1	1:B:4033:LEU:HD22	1.86	0.41
1:B:4242:PRO:HA	1:B:4286:ARG:NH2	2.36	0.41
1:B:4666:ILE:HG13	1:B:4667:ALA:N	2.35	0.41
1:A:1461:TYR:HE1	1:A:1503:TRP:HB3	1.86	0.41
1:A:1464:GLY:O	1:A:1465:ASN:C	2.63	0.41
1:A:2096:ARG:HH11	1:A:2096:ARG:HG3	1.84	0.41
1:A:2196:LEU:HD23	1:A:2196:LEU:HA	1.86	0.41
1:A:2364:VAL:C	1:A:2366:ASN:H	2.29	0.41
1:A:2525:ILE:CG2	1:A:2815:LEU:CD1	2.98	0.41
1:A:3338:GLN:HE22	1:A:3522:ILE:HG13	1.85	0.41
1:A:3554:LYS:HB3	1:A:3554:LYS:HE3	1.87	0.41
1:A:3564:LEU:HD23	1:A:3564:LEU:HA	1.82	0.41
1:A:3863:THR:O	1:A:3864:GLU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4149:LEU:HD12	1:A:4149:LEU:HA	1.73	0.41
1:A:4201:GLU:HG2	1:A:4232:MET:CE	2.51	0.41
1:B:1552:CYS:HB2	1:B:1647:LEU:HD12	2.02	0.41
1:B:1696:ARG:HD2	1:B:1774:GLU:HG3	2.02	0.41
1:B:2239:LYS:HE2	1:B:2295:GLN:HB3	2.02	0.41
1:B:3014:LEU:O	1:B:3146:THR:HA	2.20	0.41
1:B:3148:ASN:C	1:B:3150:ALA:H	2.28	0.41
1:B:3354:GLU:O	1:B:3356:ALA:N	2.54	0.41
1:B:3602:ILE:HG22	1:B:3664:MET:CE	2.46	0.41
1:B:3635:PRO:HA	1:B:3663:ILE:CG1	2.50	0.41
1:B:4376:VAL:HG13	1:B:4407:TRP:HA	2.02	0.41
1:A:1542:GLU:HG2	1:A:1655:LEU:HD23	2.02	0.41
1:A:1625:ILE:HA	1:A:1628:LEU:HB2	2.02	0.41
1:A:1854:MET:O	1:A:1855:ILE:C	2.63	0.41
1:A:1971:ASN:HA	1:A:2075:VAL:O	2.21	0.41
1:A:2424:GLN:HG2	1:A:2513:HIS:NE2	2.35	0.41
1:A:2617:VAL:O	1:A:2617:VAL:CG1	2.67	0.41
1:A:2699:LEU:HD22	1:A:2741:VAL:HG13	2.02	0.41
1:A:2884:ARG:O	1:A:2888:GLU:HG3	2.20	0.41
1:A:3194:LEU:O	1:A:3223:HIS:CD2	2.72	0.41
1:A:4130:SER:OG	1:A:4233:SER:HA	2.21	0.41
1:A:4136:SER:OG	1:A:4238:TYR:HB2	2.21	0.41
1:A:4553:TYR:CD2	1:A:4595:LEU:HD22	2.55	0.41
1:B:2320:LEU:HD23	1:B:2320:LEU:C	2.46	0.41
1:B:2555:HIS:C	1:B:2557:ASP:N	2.78	0.41
1:B:2998:ILE:CG2	1:B:3025:LEU:HD22	2.50	0.41
1:B:3127:GLU:O	1:B:3130:TYR:N	2.51	0.41
1:B:4195:GLN:OE1	1:B:4195:GLN:HA	2.20	0.41
1:B:4484:LEU:HD22	1:B:4500:GLU:CG	2.50	0.41
1:B:4495:LEU:HA	1:B:4495:LEU:HD23	1.83	0.41
1:A:1411:ILE:HD13	1:A:1411:ILE:HA	1.92	0.41
1:A:1582:LYS:O	1:A:1583:VAL:C	2.64	0.41
1:A:1715:ILE:O	1:A:1717:LYS:N	2.54	0.41
1:A:1718:ILE:O	1:A:1719:GLN:C	2.64	0.41
1:A:2405:LEU:HD22	1:A:2408:ILE:HD11	2.03	0.41
1:A:2605:VAL:HG13	1:A:2606:PRO:HD2	2.03	0.41
1:A:2723:THR:N	1:A:2727:GLU:O	2.39	0.41
1:A:2952:TYR:O	1:A:2953:SER:HB2	2.20	0.41
1:A:3238:ILE:HG12	1:A:3601:TYR:HB3	2.03	0.41
1:A:3839:SER:O	1:A:3841:ALA:N	2.53	0.41
1:A:3969:LEU:HD23	1:A:3969:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4186:LEU:HD12	1:A:4187:LEU:N	2.36	0.41
1:A:4704:ASP:O	1:A:4705:LEU:HD23	2.21	0.41
1:B:2127:LYS:HB3	1:B:2222:VAL:HG13	2.02	0.41
1:B:2142:GLN:HG3	1:B:2145:TYR:CZ	2.56	0.41
1:B:2178:GLU:HA	1:B:2178:GLU:OE1	2.20	0.41
1:B:2563:GLU:O	1:B:2567:ASN:ND2	2.54	0.41
1:B:2591:GLU:OE1	1:B:2611:PRO:HG2	2.20	0.41
1:B:2766:MET:HB3	1:B:2783:LEU:HD11	2.03	0.41
1:B:2768:GLU:HB2	1:B:2810:HIS:CE1	2.56	0.41
1:B:3185:GLY:HA2	1:B:3264:ILE:HD13	2.02	0.41
1:B:3238:ILE:HG22	1:B:3255:VAL:CG2	2.51	0.41
1:B:3246:LEU:HD22	1:B:3252:GLN:OE1	2.21	0.41
1:B:3320:ALA:O	1:B:3324:LEU:HD13	2.21	0.41
1:B:3324:LEU:CD1	1:B:3539:LEU:CG	2.98	0.41
1:B:3515:GLN:HE21	1:B:3515:GLN:HB2	1.49	0.41
1:B:3879:ILE:O	1:B:3880:SER:C	2.63	0.41
1:B:4003:GLU:CG	1:B:4004:THR:N	2.84	0.41
1:B:4036:HIS:CD2	1:B:4044:TRP:HE1	2.36	0.41
1:B:4122:VAL:HG12	1:B:4132:LEU:CD1	2.50	0.41
1:B:4274:LEU:HD21	1:B:4306:ALA:HB3	2.03	0.41
1:B:4347:ILE:HG21	1:B:4353:MET:HG2	2.02	0.41
1:B:4402:ILE:O	1:B:4402:ILE:HG22	2.20	0.41
1:B:4434:GLN:HE21	1:B:4434:GLN:HB3	1.72	0.41
1:B:4520:LEU:O	1:B:4523:LEU:HB3	2.20	0.41
1:B:4536:SER:O	1:B:4539:THR:N	2.54	0.41
1:A:1636:PHE:O	1:A:1637:LYS:C	2.64	0.41
1:A:1900:GLY:C	1:A:1902:LYS:N	2.77	0.41
1:A:2865:THR:O	1:A:2867:ASP:N	2.54	0.41
1:A:3017:VAL:HB	1:A:3175:GLU:OE2	2.21	0.41
1:A:3062:ALA:HB2	1:A:3069:ILE:CD1	2.48	0.41
1:A:3338:GLN:O	1:A:3342:ARG:N	2.54	0.41
1:A:3587:THR:HB	1:A:3628:PHE:HA	2.02	0.41
1:A:4055:GLU:HA	1:A:4056:PRO:HD3	1.96	0.41
1:B:1558:TRP:CZ3	1:B:1606:ILE:HB	2.56	0.41
1:B:1590:HIS:C	1:B:1592:ASP:N	2.79	0.41
1:B:2264:GLN:O	1:B:2267:ASN:HB3	2.21	0.41
1:B:2732:PRO:C	1:B:2734:GLN:N	2.78	0.41
1:B:2747:ASN:HB2	1:B:2801:VAL:O	2.21	0.41
1:B:3091:LEU:HA	1:B:3091:LEU:HD23	1.52	0.41
1:B:3108:LEU:HG	1:B:3108:LEU:O	2.21	0.41
1:B:3234:ILE:HG23	1:B:3617:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3253:ASN:HB2	1:B:3604:PHE:CD2	2.56	0.41
1:B:3781:VAL:HG13	1:B:3782:THR:N	2.36	0.41
1:B:3969:LEU:HD23	1:B:3969:LEU:HA	1.91	0.41
1:B:4068:GLN:O	1:B:4070:SER:N	2.54	0.41
1:B:4080:PHE:HB2	1:B:4101:PHE:CE1	2.56	0.41
1:B:4461:LYS:CB	1:B:4565:ILE:HD13	2.51	0.41
1:B:4603:ALA:C	1:B:4605:ARG:N	2.79	0.41
1:B:4688:VAL:HA	1:B:4689:PRO:HD3	1.89	0.41
1:A:1715:ILE:HD12	1:A:1760:ILE:HD13	2.03	0.40
1:A:1879:ILE:HG21	1:A:2115:SER:HA	2.02	0.40
1:A:1967:ARG:HH22	1:A:2069:GLN:HA	1.86	0.40
1:A:2282:LYS:HG2	1:A:2416:PHE:CD2	2.56	0.40
1:A:2582:GLY:CA	1:A:2585:MET:HE3	2.40	0.40
1:A:2915:ASP:OD2	1:A:3000:ARG:HD3	2.21	0.40
1:A:3005:PHE:N	1:A:3005:PHE:CD1	2.89	0.40
1:A:3251:ARG:HH12	1:A:3675:ILE:CD1	2.33	0.40
1:A:3275:ARG:O	1:A:3276:ASP:C	2.63	0.40
1:A:3629:LYS:HB2	1:A:3632:LEU:HB2	2.04	0.40
1:A:3878:GLU:O	1:A:3882:VAL:HG23	2.21	0.40
1:A:3912:SER:HB3	1:A:4231:ARG:HG3	2.02	0.40
1:A:4689:PRO:HB2	1:A:4699:LEU:CD1	2.51	0.40
1:B:2075:VAL:O	1:B:2075:VAL:HG12	2.20	0.40
1:B:3091:LEU:CD1	1:B:3164:LEU:HD22	2.51	0.40
1:B:3697:THR:HG23	1:B:3720:VAL:HG13	2.03	0.40
1:B:4222:HIS:CD2	1:B:4222:HIS:C	2.99	0.40
1:A:2376:LEU:HD11	1:A:2384:ARG:HB3	2.03	0.40
1:A:2690:ALA:C	1:A:2692:PRO:HD3	2.45	0.40
1:A:2897:THR:C	1:A:2899:GLU:H	2.27	0.40
1:A:3139:ARG:HH11	1:A:3139:ARG:CG	2.19	0.40
1:A:3936:PRO:C	1:A:3938:GLU:N	2.78	0.40
1:A:4053:VAL:HG12	1:A:4054:GLY:N	2.36	0.40
1:A:4145:LYS:HE3	1:A:4238:TYR:CD1	2.57	0.40
1:A:4309:SER:O	1:A:4313:TRP:CD1	2.74	0.40
1:B:1739:THR:OG1	1:B:1740:THR:HG22	2.21	0.40
1:B:2223:PHE:O	1:B:2224:PRO:C	2.64	0.40
1:B:2528:PHE:HE1	1:B:2533:VAL:HG11	1.86	0.40
1:B:3008:PRO:O	1:B:3009:GLN:C	2.64	0.40
1:B:3112:CYS:HB3	1:B:3129:LEU:HD11	2.03	0.40
1:B:3865:ILE:O	1:B:3867:LEU:N	2.54	0.40
1:B:3921:TYR:CZ	1:B:3925:ASN:ND2	2.89	0.40
1:B:4033:LEU:HD13	1:B:4062:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4332:ILE:HA	1:B:4335:ARG:HH12	1.86	0.40
1:B:4511:LYS:O	1:B:4512:LYS:C	2.64	0.40
1:B:4541:ILE:O	1:B:4544:GLY:N	2.55	0.40
1:A:1554:LEU:HB3	1:A:1609:GLN:NE2	2.37	0.40
1:A:2116:GLN:HE21	1:A:2157:VAL:HA	1.86	0.40
1:A:2252:LYS:HB2	1:A:2425:MET:HE3	2.03	0.40
1:A:2515:VAL:HG12	1:A:2581:LEU:HD12	2.04	0.40
1:A:2590:ARG:CD	1:A:2613:LEU:HD11	2.51	0.40
1:A:3351:ARG:HG3	1:A:3351:ARG:NH1	2.36	0.40
1:A:3602:ILE:HG23	1:A:3610:ARG:CD	2.52	0.40
1:A:3686:MET:C	1:A:3687:ASN:HD22	2.28	0.40
1:B:1640:ASN:ND2	1:B:1644:ILE:CD1	2.82	0.40
1:B:1705:LEU:O	1:B:1709:ILE:HG13	2.21	0.40
1:B:1821:ILE:HG21	1:B:1914:TYR:HB2	2.03	0.40
1:B:2031:LEU:O	1:B:2032:GLU:C	2.64	0.40
1:B:2202:THR:O	1:B:2203:MET:HE2	2.22	0.40
1:B:2241:GLN:HB2	1:B:2251:THR:HG21	2.04	0.40
1:B:2260:LEU:HD12	1:B:2260:LEU:HA	1.77	0.40
1:B:2344:ARG:O	1:B:2344:ARG:CG	2.67	0.40
1:B:2578:MET:HA	1:B:2593:PHE:HE2	1.86	0.40
1:B:2766:MET:HE2	1:B:2783:LEU:CD1	2.46	0.40
1:B:3559:ARG:NE	1:B:3849:ASP:OD1	2.54	0.40
1:B:3700:LEU:HD22	1:B:3701:ASP:H	1.87	0.40
1:B:4189:ASN:HD22	1:B:4218:THR:HG23	1.87	0.40
1:B:4436:SER:O	1:B:4437:GLU:O	2.39	0.40
1:A:1507:LEU:O	1:A:1511:GLU:N	2.55	0.40
1:A:1800:HIS:HB2	1:A:1858:ASN:ND2	2.34	0.40
1:A:1812:THR:HA	1:A:1874:LYS:HD2	2.03	0.40
1:A:2105:ARG:O	1:A:2106:GLU:C	2.62	0.40
1:A:2544:SER:O	1:A:2548:VAL:HG23	2.21	0.40
1:A:3592:VAL:O	1:A:3593:VAL:C	2.63	0.40
1:A:4173:LYS:O	1:A:4174:SER:C	2.64	0.40
1:B:1681:LYS:O	1:B:1685:GLU:HG3	2.21	0.40
1:B:1850:GLN:O	1:B:1851:THR:C	2.63	0.40
1:B:2054:SER:OG	1:B:2056:GLU:O	2.40	0.40
1:B:2275:VAL:HG12	1:B:2276:GLY:N	2.35	0.40
1:B:2547:ASN:O	1:B:2619:ILE:HD11	2.21	0.40
1:B:3687:ASN:O	1:B:3689:TYR:N	2.55	0.40
1:B:3887:ASN:N	1:B:3888:PRO:CD	2.84	0.40
1:B:4083:ILE:CD1	1:B:4098:SER:HA	2.52	0.40
1:B:4153:LEU:HB3	1:B:4155:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4517:LEU:HD23	1:B:4517:LEU:HA	1.92	0.40
1:A:1618:ILE:CD1	1:A:1683:LEU:HD21	2.52	0.40
1:A:1698:TYR:O	1:A:2011:ARG:HG2	2.22	0.40
1:A:1710:GLY:C	1:A:1712:SER:N	2.80	0.40
1:A:2009:MET:O	1:A:2010:SER:C	2.64	0.40
1:A:2273:MET:HG2	1:A:2395:PHE:CG	2.56	0.40
1:A:2364:VAL:O	1:A:2367:LEU:N	2.48	0.40
1:A:3571:ARG:O	1:A:3575:GLU:HG3	2.22	0.40
1:A:3596:SER:O	1:A:3597:ALA:C	2.65	0.40
1:A:4044:TRP:HZ2	1:A:4062:TRP:CG	2.40	0.40
1:A:4187:LEU:HD11	1:A:4215:LEU:HD11	2.04	0.40
1:A:4349:ASN:HD21	1:A:4351:PHE:H	1.61	0.40
1:A:4357:TYR:HA	1:A:4360:LEU:HB2	2.03	0.40
1:A:4589:VAL:CG1	1:A:4638:ASN:O	2.69	0.40
1:B:1606:ILE:O	1:B:1608:VAL:N	2.54	0.40
1:B:1800:HIS:CE1	1:B:1858:ASN:CB	3.05	0.40
1:B:1916:ALA:HA	1:B:1924:LYS:CD	2.51	0.40
1:B:1985:LYS:HD3	1:B:1997:VAL:HG21	2.04	0.40
1:B:2241:GLN:CB	1:B:2251:THR:HG21	2.51	0.40
1:B:2552:ASN:O	1:B:2556:SER:N	2.54	0.40
1:B:2642:ALA:HB2	1:B:2883:ASP:HB3	2.03	0.40
1:B:3047:LYS:C	1:B:3049:SER:N	2.79	0.40
1:B:3191:ASN:HB2	5:B:26:HOH:O	2.20	0.40
1:B:3328:VAL:O	1:B:3332:GLN:CG	2.69	0.40
1:B:3834:LEU:HD22	1:B:3858:LEU:CD1	2.52	0.40
1:B:3960:LEU:O	1:B:3961:ASN:C	2.65	0.40
1:B:4497:ARG:HG3	1:B:4497:ARG:HH11	1.87	0.40
1:B:4604:THR:O	1:B:4671:TRP:NE1	2.55	0.40
1:B:4708:ASP:OD1	1:B:4710:SER:OG	2.38	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	2908/3245 (90%)	2474 (85%)	332 (11%)	102 (4%)	3	9
1	B	2813/3245 (87%)	2376 (84%)	347 (12%)	90 (3%)	3	10
All	All	5721/6490 (88%)	4850 (85%)	679 (12%)	192 (3%)	3	10

All (192) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1465	ASN
1	A	1583	VAL
1	A	1797	VAL
1	A	1835	THR
1	A	1839	SER
1	A	1919	GLU
1	A	2641	VAL
1	A	3697	THR
1	A	3722	ASP
1	A	3814	SER
1	A	3815	ASP
1	A	4045	LYS
1	A	4051	ASP
1	A	4221	ILE
1	A	4520	LEU
1	A	4557	GLU
1	B	1592	ASP
1	B	2296	VAL
1	B	2432	ASP
1	B	2442	GLN
1	B	2555	HIS
1	B	2559	PRO
1	B	2641	VAL
1	B	2982	GLU
1	B	2983	GLU
1	B	3105	PHE
1	B	3162	PRO
1	B	3220	PRO
1	B	4051	ASP
1	B	4053	VAL
1	B	4530	SER
1	A	1762	ASN
1	A	1764	PRO
1	A	1838	GLN
1	A	2033	GLU

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Mol	Chain	Res	Type
1	A	2203	MET
1	A	2384	ARG
1	A	2401	LYS
1	A	2608	ASN
1	A	2642	ALA
1	A	2871	HIS
1	A	2992	ASN
1	A	3005	PHE
1	A	3365	ASP
1	A	3816	LEU
1	A	3861	GLU
1	A	3866	ALA
1	A	3929	ASN
1	A	3937	ASN
1	A	4145	LYS
1	A	4209	PRO
1	A	4510	VAL
1	A	4519	ASN
1	A	4552	TRP
1	A	4559	ILE
1	A	4577	GLU
1	A	4679	PHE
1	A	4695	THR
1	B	1559	ASP
1	B	1611	ARG
1	B	1826	GLN
1	B	1829	GLN
1	B	2315	GLN
1	B	2433	THR
1	B	2553	GLN
1	B	2565	GLN
1	B	2600	ILE
1	B	2715	ASP
1	B	3164	LEU
1	B	3688	GLN
1	B	3691	ASP
1	B	3724	GLU
1	B	3729	VAL
1	B	3841	ALA
1	B	3932	ASP
1	B	3933	LYS
1	B	3999	THR

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Mol	Chain	Res	Type
1	B	4069	LEU
1	B	4378	SER
1	B	4541	ILE
1	B	4551	LYS
1	B	4708	ASP
1	B	4709	GLN
1	A	1585	GLU
1	A	1896	LYS
1	A	1917	THR
1	A	2373	ASP
1	A	2644	PRO
1	A	2690	ALA
1	A	2808	LEU
1	A	2915	ASP
1	A	2990	LEU
1	A	3065	LYS
1	A	3119	ASN
1	A	3355	ILE
1	A	3361	LYS
1	A	3865	ILE
1	A	3998	LEU
1	A	4223	PRO
1	A	4579	SER
1	B	1664	ARG
1	B	1827	VAL
1	B	1828	ASP
1	B	2230	PRO
1	B	2233	MET
1	B	2295	GLN
1	B	2343	VAL
1	B	2380	PRO
1	B	2733	THR
1	B	2747	ASN
1	B	2871	HIS
1	B	3044	ASN
1	B	3048	SER
1	B	3700	LEU
1	B	3704	PHE
1	B	3929	ASN
1	B	4047	PHE
1	B	4175	ILE
1	B	4498	CYS

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Mol	Chain	Res	Type
1	B	4571	ARG
1	A	1552	CYS
1	A	1558	TRP
1	A	1664	ARG
1	A	1695	ALA
1	A	1897	ASN
1	A	1949	GLN
1	A	2178	GLU
1	A	2209	ALA
1	A	2224	PRO
1	A	2365	GLU
1	A	3164	LEU
1	A	3840	GLN
1	A	3859	LYS
1	A	3863	THR
1	A	3936	PRO
1	A	4007	GLN
1	A	4138	PRO
1	A	4172	GLU
1	A	4437	GLU
1	B	1593	ASP
1	B	1612	TRP
1	B	1786	SER
1	B	1922	LEU
1	B	1929	MET
1	B	2164	ARG
1	B	2638	THR
1	B	3009	GLN
1	B	3684	PHE
1	B	3880	SER
1	B	4433	MET
1	A	1645	ALA
1	A	1855	ILE
1	A	1923	HIS
1	A	2843	ARG
1	A	2870	ALA
1	A	2978	VAL
1	A	3078	VAL
1	A	3162	PRO
1	A	3512	LYS
1	A	3526	GLU
1	A	3705	MET

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Mol	Chain	Res	Type
1	A	3826	LYS
1	A	3926	ASN
1	A	3999	THR
1	B	1655	LEU
1	B	1663	GLU
1	B	1666	GLN
1	B	2492	LEU
1	B	2603	THR
1	B	2692	PRO
1	B	3320	ALA
1	B	3576	GLN
1	B	4531	THR
1	A	1719	GLN
1	A	4143	SER
1	A	4144	SER
1	A	4708	ASP
1	B	1630	PRO
1	B	2511	LEU
1	B	2998	ILE
1	B	4059	PRO
1	B	4151	LEU
1	A	2606	PRO
1	B	3152	PRO
1	B	3931	VAL
1	B	3928	PRO
1	A	3219	ILE
1	A	4678	ILE
1	B	4377	PRO
1	A	1766	ILE
1	A	3197	PRO
1	B	2669	PRO

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2408/2921 (82%)	2199 (91%)	209 (9%)	9 29
1	B	2369/2921 (81%)	2140 (90%)	229 (10%)	8 24
All	All	4777/5842 (82%)	4339 (91%)	438 (9%)	8 26

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1419	TRP
1	A	1422	ILE
1	A	1423	ILE
1	A	1424	PRO
1	A	1486	LYS
1	A	1488	LEU
1	A	1492	TRP
1	A	1493	ILE
1	A	1513	ILE
1	A	1518	ILE
1	A	1527	LEU
1	A	1529	GLU
1	A	1559	ASP
1	A	1625	ILE
1	A	1626	ASN
1	A	1628	LEU
1	A	1665	ILE
1	A	1719	GLN
1	A	1740	THR
1	A	1742	ILE
1	A	1764	PRO
1	A	1799	ASP
1	A	1801	SER
1	A	1808	ASP
1	A	1835	THR
1	A	1844	GLN
1	A	1851	THR
1	A	1862	SER
1	A	1886	ARG
1	A	1905	ASP
1	A	1915	ASP
1	A	1945	GLU

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Mol	Chain	Res	Type
1	A	2006	LEU
1	A	2011	ARG
1	A	2016	LEU
1	A	2029	ASN
1	A	2032	GLU
1	A	2050	LEU
1	A	2051	LYS
1	A	2053	ASN
1	A	2066	SER
1	A	2069	GLN
1	A	2090	ASN
1	A	2106	GLU
1	A	2107	MET
1	A	2112	MET
1	A	2122	GLU
1	A	2137	GLU
1	A	2142	GLN
1	A	2155	VAL
1	A	2180	LYS
1	A	2204	ILE
1	A	2226	SER
1	A	2227	GLN
1	A	2236	LEU
1	A	2251	THR
1	A	2252	LYS
1	A	2262	LEU
1	A	2284	THR
1	A	2305	VAL
1	A	2328	THR
1	A	2338	ARG
1	A	2346	GLU
1	A	2362	GLU
1	A	2367	LEU
1	A	2370	LEU
1	A	2392	ARG
1	A	2404	THR
1	A	2424	GLN
1	A	2442	GLN
1	A	2503	SER
1	A	2511	LEU
1	A	2525	ILE
1	A	2567	ASN

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Mol	Chain	Res	Type
1	A	2572	ARG
1	A	2606	PRO
1	A	2637	GLU
1	A	2641	VAL
1	A	2659	VAL
1	A	2683	THR
1	A	2696	VAL
1	A	2699	LEU
1	A	2702	SER
1	A	2709	LEU
1	A	2710	LEU
1	A	2728	THR
1	A	2739	LEU
1	A	2747	ASN
1	A	2796	THR
1	A	2804	THR
1	A	2847	ASP
1	A	2865	THR
1	A	2866	PRO
1	A	2873	ILE
1	A	2878	GLU
1	A	2894	ASP
1	A	2896	CYS
1	A	2898	LEU
1	A	2904	LEU
1	A	2956	LEU
1	A	2957	THR
1	A	2975	ARG
1	A	2998	ILE
1	A	2999	LEU
1	A	3026	SER
1	A	3048	SER
1	A	3053	ASP
1	A	3059	LEU
1	A	3080	GLU
1	A	3089	THR
1	A	3095	GLU
1	A	3113	LYS
1	A	3117	GLN
1	A	3139	ARG
1	A	3141	LEU
1	A	3179	GLU

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Mol	Chain	Res	Type
1	A	3187	GLU
1	A	3195	GLU
1	A	3204	VAL
1	A	3268	VAL
1	A	3308	GLN
1	A	3310	ASN
1	A	3312	GLU
1	A	3316	LYS
1	A	3322	GLN
1	A	3327	MET
1	A	3328	VAL
1	A	3330	ASP
1	A	3335	GLU
1	A	3338	GLN
1	A	3349	ASP
1	A	3365	ASP
1	A	3505	GLU
1	A	3513	LEU
1	A	3515	GLN
1	A	3531	THR
1	A	3554	LYS
1	A	3571	ARG
1	A	3586	SER
1	A	3605	PHE
1	A	3624	VAL
1	A	3630	SER
1	A	3670	ARG
1	A	3673	LEU
1	A	3694	ILE
1	A	3695	THR
1	A	3696	LYS
1	A	3707	ASN
1	A	3708	LEU
1	A	3721	GLN
1	A	3770	THR
1	A	3788	VAL
1	A	3789	THR
1	A	3817	LEU
1	A	3845	ILE
1	A	3857	THR
1	A	3858	LEU
1	A	3863	THR

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Mol	Chain	Res	Type
1	A	3874	THR
1	A	3885	LEU
1	A	3933	LYS
1	A	3943	LEU
1	A	3947	ILE
1	A	3977	LYS
1	A	3989	ASP
1	A	3998	LEU
1	A	4007	GLN
1	A	4039	GLN
1	A	4040	ASN
1	A	4046	GLN
1	A	4057	ILE
1	A	4061	SER
1	A	4066	GLN
1	A	4072	GLN
1	A	4091	SER
1	A	4117	ASP
1	A	4129	SER
1	A	4133	LEU
1	A	4136	SER
1	A	4170	LEU
1	A	4195	GLN
1	A	4198	VAL
1	A	4200	LEU
1	A	4209	PRO
1	A	4211	PRO
1	A	4218	THR
1	A	4233	SER
1	A	4237	SER
1	A	4259	ARG
1	A	4286	ARG
1	A	4293	THR
1	A	4309	SER
1	A	4319	LYS
1	A	4321	ARG
1	A	4353	MET
1	A	4360	LEU
1	A	4559	ILE
1	A	4572	MET
1	A	4606	GLN
1	A	4607	SER

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Mol	Chain	Res	Type
1	A	4609	SER
1	A	4610	GLN
1	A	4645	GLU
1	A	4655	THR
1	A	4671	TRP
1	A	4693	ASN
1	A	4703	ILE
1	A	4719	ARG
1	A	4729	ASP
1	B	1547	ASN
1	B	1561	LEU
1	B	1563	ASN
1	B	1573	SER
1	B	1594	ARG
1	B	1610	ARG
1	B	1611	ARG
1	B	1624	ASP
1	B	1655	LEU
1	B	1665	ILE
1	B	1672	LEU
1	B	1690	GLN
1	B	1697	PHE
1	B	1737	GLU
1	B	1740	THR
1	B	1774	GLU
1	B	1781	LEU
1	B	1822	VAL
1	B	1840	LYS
1	B	1849	GLU
1	B	1867	LEU
1	B	1872	ARG
1	B	1887	ASP
1	B	1894	LYS
1	B	1901	ASN
1	B	1912	TYR
1	B	1917	THR
1	B	1921	VAL
1	B	1946	ARG
1	B	1959	THR
1	B	1982	GLU
1	B	2002	GLU
1	B	2007	GLN

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Mol	Chain	Res	Type
1	B	2029	ASN
1	B	2031	LEU
1	B	2036	LEU
1	B	2041	GLN
1	B	2071	MET
1	B	2075	VAL
1	B	2093	LYS
1	B	2104	ASP
1	B	2106	GLU
1	B	2120	THR
1	B	2129	VAL
1	B	2149	LEU
1	B	2231	ILE
1	B	2236	LEU
1	B	2239	LYS
1	B	2252	LYS
1	B	2253	GLN
1	B	2254	GLU
1	B	2260	LEU
1	B	2360	ASP
1	B	2374	ASN
1	B	2381	ASN
1	B	2397	VAL
1	B	2404	THR
1	B	2420	ILE
1	B	2425	MET
1	B	2429	ASN
1	B	2432	ASP
1	B	2440	ASP
1	B	2492	LEU
1	B	2494	VAL
1	B	2504	GLN
1	B	2508	PRO
1	B	2525	ILE
1	B	2540	LEU
1	B	2550	GLU
1	B	2587	LEU
1	B	2591	GLU
1	B	2603	THR
1	B	2613	LEU
1	B	2617	VAL
1	B	2620	ASP

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Mol	Chain	Res	Type
1	B	2621	ASP
1	B	2651	VAL
1	B	2670	LEU
1	B	2696	VAL
1	B	2699	LEU
1	B	2700	ASN
1	B	2715	ASP
1	B	2721	LYS
1	B	2725	SER
1	B	2746	ILE
1	B	2749	PRO
1	B	2756	THR
1	B	2758	ARG
1	B	2759	VAL
1	B	2835	LEU
1	B	2841	ASN
1	B	2843	ARG
1	B	2848	ASN
1	B	2876	PRO
1	B	2883	ASP
1	B	2904	LEU
1	B	2942	ASN
1	B	2946	LEU
1	B	2977	LYS
1	B	2984	LEU
1	B	3017	VAL
1	B	3043	ASN
1	B	3053	ASP
1	B	3059	LEU
1	B	3068	LYS
1	B	3078	VAL
1	B	3087	MET
1	B	3088	ASN
1	B	3095	GLU
1	B	3109	MET
1	B	3112	CYS
1	B	3126	GLU
1	B	3139	ARG
1	B	3140	ASN
1	B	3162	PRO
1	B	3164	LEU
1	B	3195	GLU

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Mol	Chain	Res	Type
1	B	3210	GLU
1	B	3255	VAL
1	B	3280	GLU
1	B	3282	GLN
1	B	3283	LEU
1	B	3315	VAL
1	B	3319	GLN
1	B	3326	GLN
1	B	3327	MET
1	B	3330	ASP
1	B	3332	GLN
1	B	3335	GLU
1	B	3338	GLN
1	B	3343	GLU
1	B	3506	ASN
1	B	3515	GLN
1	B	3517	GLU
1	B	3523	THR
1	B	3528	SER
1	B	3533	LYS
1	B	3535	GLU
1	B	3539	LEU
1	B	3547	LYS
1	B	3555	ASN
1	B	3563	LEU
1	B	3585	MET
1	B	3602	ILE
1	B	3620	ARG
1	B	3624	VAL
1	B	3642	GLU
1	B	3645	LEU
1	B	3691	ASP
1	B	3695	THR
1	B	3700	LEU
1	B	3712	LEU
1	B	3725	ASN
1	B	3726	ILE
1	B	3780	ARG
1	B	3781	VAL
1	B	3787	THR
1	B	3800	GLU
1	B	3827	LEU

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Mol	Chain	Res	Type
1	B	3838	LEU
1	B	3840	GLN
1	B	3867	LEU
1	B	3877	GLN
1	B	3878	GLU
1	B	3880	SER
1	B	3931	VAL
1	B	3935	ASP
1	B	3936	PRO
1	B	3951	THR
1	B	3966	THR
1	B	3992	LEU
1	B	3998	LEU
1	B	4002	LYS
1	B	4004	THR
1	B	4028	PRO
1	B	4031	SER
1	B	4035	ASP
1	B	4046	GLN
1	B	4053	VAL
1	B	4059	PRO
1	B	4060	GLU
1	B	4095	LEU
1	B	4098	SER
1	B	4105	VAL
1	B	4111	LEU
1	B	4113	THR
1	B	4116	LEU
1	B	4132	LEU
1	B	4152	GLN
1	B	4157	TYR
1	B	4162	ILE
1	B	4169	GLU
1	B	4189	ASN
1	B	4199	GLN
1	B	4200	LEU
1	B	4209	PRO
1	B	4214	ARG
1	B	4218	THR
1	B	4228	ASN
1	B	4232	MET
1	B	4233	SER

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Mol	Chain	Res	Type
1	B	4267	ARG
1	B	4323	ASN
1	B	4326	PRO
1	B	4334	VAL
1	B	4335	ARG
1	B	4356	LEU
1	B	4379	ILE
1	B	4382	SER
1	B	4406	ILE
1	B	4425	LYS
1	B	4434	GLN
1	B	4484	LEU
1	B	4500	GLU
1	B	4503	ILE
1	B	4521	LEU
1	B	4538	THR
1	B	4546	VAL
1	B	4547	PRO
1	B	4557	GLU
1	B	4558	THR
1	B	4573	GLN
1	B	4604	THR
1	B	4618	ASN
1	B	4644	LEU
1	B	4675	ASP
1	B	4693	ASN
1	B	4709	GLN
1	B	4715	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (224) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1480	HIS
1	A	1522	GLN
1	A	1547	ASN
1	A	1549	GLN
1	A	1563	ASN
1	A	1609	GLN
1	A	1690	GLN
1	A	1798	ASN
1	A	1809	ASN
1	A	1813	GLN

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Mol	Chain	Res	Type
1	A	1820	GLN
1	A	1844	GLN
1	A	1857	ASN
1	A	1858	ASN
1	A	1865	GLN
1	A	1877	HIS
1	A	1884	HIS
1	A	1893	GLN
1	A	1918	GLN
1	A	1923	HIS
1	A	1928	HIS
1	A	1949	GLN
1	A	1971	ASN
1	A	2018	GLN
1	A	2029	ASN
1	A	2044	GLN
1	A	2047	GLN
1	A	2053	ASN
1	A	2090	ASN
1	A	2116	GLN
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	2267	ASN
1	A	2295	GLN
1	A	2342	ASN
1	A	2351	HIS
1	A	2368	ASN
1	A	2424	GLN
1	A	2428	GLN
1	A	2429	ASN
1	A	2447	GLN
1	A	2495	GLN
1	A	2535	ASN
1	A	2552	ASN
1	A	2553	GLN
1	A	2555	HIS
1	A	2565	GLN
1	A	2700	ASN

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Mol	Chain	Res	Type
1	A	2716	HIS
1	A	2747	ASN
1	A	2757	GLN
1	A	2778	HIS
1	A	2793	ASN
1	A	2826	GLN
1	A	2832	ASN
1	A	2848	ASN
1	A	2907	HIS
1	A	2954	ASN
1	A	2997	HIS
1	A	3007	GLN
1	A	3033	ASN
1	A	3077	ASN
1	A	3117	GLN
1	A	3198	GLN
1	A	3223	HIS
1	A	3236	GLN
1	A	3249	GLN
1	A	3252	GLN
1	A	3259	HIS
1	A	3277	GLN
1	A	3286	ASN
1	A	3303	GLN
1	A	3322	GLN
1	A	3331	GLN
1	A	3338	GLN
1	A	3345	GLN
1	A	3509	ASN
1	A	3555	ASN
1	A	3582	ASN
1	A	3646	ASN
1	A	3687	ASN
1	A	3794	GLN
1	A	3820	GLN
1	A	3887	ASN
1	A	3929	ASN
1	A	3970	GLN
1	A	3981	ASN
1	A	4017	GLN
1	A	4025	GLN
1	A	4036	HIS

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Mol	Chain	Res	Type
1	A	4038	GLN
1	A	4039	GLN
1	A	4040	ASN
1	A	4066	GLN
1	A	4079	ASN
1	A	4112	ASN
1	A	4154	HIS
1	A	4205	HIS
1	A	4234	ASN
1	A	4263	GLN
1	A	4278	HIS
1	A	4282	GLN
1	A	4323	ASN
1	A	4349	ASN
1	A	4362	GLN
1	A	4370	ASN
1	A	4573	GLN
1	A	4606	GLN
1	A	4610	GLN
1	A	4622	HIS
1	A	4638	ASN
1	A	4650	ASN
1	A	4693	ASN
1	A	4718	GLN
1	B	1547	ASN
1	B	1549	GLN
1	B	1609	GLN
1	B	1640	ASN
1	B	1690	GLN
1	B	1767	HIS
1	B	1793	ASN
1	B	1813	GLN
1	B	1842	GLN
1	B	1850	GLN
1	B	1857	ASN
1	B	1865	GLN
1	B	1870	GLN
1	B	1893	GLN
1	B	1901	ASN
1	B	1920	ASN
1	B	1949	GLN
1	B	1962	GLN

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Mol	Chain	Res	Type
1	B	1971	ASN
1	B	1990	GLN
1	B	2029	ASN
1	B	2042	GLN
1	B	2044	GLN
1	B	2047	GLN
1	B	2068	HIS
1	B	2110	GLN
1	B	2116	GLN
1	B	2189	GLN
1	B	2200	ASN
1	B	2241	GLN
1	B	2264	GLN
1	B	2295	GLN
1	B	2315	GLN
1	B	2342	ASN
1	B	2368	ASN
1	B	2381	ASN
1	B	2398	GLN
1	B	2495	GLN
1	B	2504	GLN
1	B	2567	ASN
1	B	2571	ASN
1	B	2629	ASN
1	B	2787	GLN
1	B	2793	ASN
1	B	2832	ASN
1	B	2841	ASN
1	B	2861	GLN
1	B	2907	HIS
1	B	2914	GLN
1	B	2964	ASN
1	B	2992	ASN
1	B	3009	GLN
1	B	3011	HIS
1	B	3043	ASN
1	B	3140	ASN
1	B	3183	GLN
1	B	3223	HIS
1	B	3236	GLN
1	B	3259	HIS
1	B	3265	ASN

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Mol	Chain	Res	Type
1	B	3272	ASN
1	B	3282	GLN
1	B	3303	GLN
1	B	3338	GLN
1	B	3515	GLN
1	B	3555	ASN
1	B	3566	ASN
1	B	3568	ASN
1	B	3577	GLN
1	B	3721	GLN
1	B	3725	ASN
1	B	3731	ASN
1	B	3785	ASN
1	B	3794	GLN
1	B	3820	GLN
1	B	3840	GLN
1	B	3907	HIS
1	B	3926	ASN
1	B	3953	ASN
1	B	3981	ASN
1	B	4016	GLN
1	B	4025	GLN
1	B	4036	HIS
1	B	4052	GLN
1	B	4066	GLN
1	B	4090	HIS
1	B	4112	ASN
1	B	4189	ASN
1	B	4222	HIS
1	B	4228	ASN
1	B	4250	HIS
1	B	4263	GLN
1	B	4278	HIS
1	B	4323	ASN
1	B	4362	GLN
1	B	4391	HIS
1	B	4431	GLN
1	B	4573	GLN
1	B	4574	GLN
1	B	4596	ASN
1	B	4606	GLN
1	B	4618	ASN

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Mol	Chain	Res	Type
1	B	4650	ASN
1	B	4651	ASN
1	B	4693	ASN
1	B	4709	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	B	9007	4	28,29,29	1.58	3 (10%)	43,45,45	1.87	11 (25%)
2	ADP	A	9004	-	28,29,29	1.72	6 (21%)	43,45,45	1.85	10 (23%)
2	ADP	B	9008	4	28,29,29	1.85	6 (21%)	43,45,45	1.87	11 (25%)
3	SPM	B	9018	-	13,13,13	0.56	0	12,12,12	0.86	0
2	ADP	B	9010	-	28,29,29	1.71	5 (17%)	43,45,45	1.87	11 (25%)
2	ADP	B	9009	-	28,29,29	1.80	5 (17%)	43,45,45	1.86	11 (25%)
3	SPM	A	9016	-	13,13,13	0.52	0	12,12,12	0.88	0
2	ADP	A	9003	-	28,29,29	1.78	6 (21%)	43,45,45	2.03	13 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	9001	-	28,29,29	1.64	5 (17%)	43,45,45	1.88	12 (27%)
2	ADP	A	9002	4	28,29,29	1.73	5 (17%)	43,45,45	1.95	10 (23%)
3	SPM	A	9012	-	13,13,13	0.59	0	12,12,12	0.81	0
3	SPM	B	9022	-	13,13,13	0.40	0	12,12,12	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9007	4	-	6/16/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/16/32/32	0/3/3/3
2	ADP	B	9008	4	-	5/16/32/32	0/3/3/3
3	SPM	B	9018	-	-	7/11/11/11	-
2	ADP	B	9010	-	-	6/16/32/32	0/3/3/3
2	ADP	B	9009	-	-	6/16/32/32	0/3/3/3
3	SPM	A	9016	-	-	11/11/11/11	-
2	ADP	A	9003	-	-	5/16/32/32	0/3/3/3
2	ADP	A	9001	-	-	6/16/32/32	0/3/3/3
2	ADP	A	9002	4	-	5/16/32/32	0/3/3/3
3	SPM	A	9012	-	-	5/11/11/11	-
3	SPM	B	9022	-	-	7/11/11/11	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9009	ADP	C5-C4	5.65	1.49	1.39
2	B	9008	ADP	C5-C4	5.40	1.48	1.39
2	A	9004	ADP	C5-C4	5.30	1.48	1.39
2	A	9001	ADP	C5-C4	5.20	1.48	1.39
2	A	9003	ADP	C5-C4	5.18	1.48	1.39
2	A	9002	ADP	C5-C4	4.95	1.47	1.39
2	B	9007	ADP	C5-C4	4.70	1.47	1.39
2	B	9010	ADP	PA-O3A	4.66	1.64	1.59
2	B	9010	ADP	C5-C4	4.38	1.46	1.39
2	B	9008	ADP	PA-O3A	3.79	1.63	1.59
2	A	9004	ADP	PA-O3A	3.77	1.63	1.59
2	B	9007	ADP	C5-N7	-3.74	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9010	ADP	C5-N7	-3.22	1.33	1.39
2	A	9004	ADP	C5-N7	-3.18	1.33	1.39
2	B	9009	ADP	C5-C6	3.16	1.49	1.41
2	B	9009	ADP	PA-O3A	3.15	1.62	1.59
2	A	9001	ADP	C4-N9	-3.07	1.31	1.37
2	A	9003	ADP	PA-O3A	3.06	1.62	1.59
2	A	9002	ADP	C5-C6	3.06	1.49	1.41
2	A	9003	ADP	C5-C6	3.04	1.49	1.41
2	B	9007	ADP	C4-N9	-3.03	1.31	1.37
2	B	9008	ADP	C5-N7	-2.93	1.33	1.39
2	A	9002	ADP	C5-N7	-2.92	1.33	1.39
2	A	9001	ADP	C5-C6	2.88	1.49	1.41
2	B	9010	ADP	C4-N9	-2.78	1.31	1.37
2	B	9008	ADP	C5-C6	2.78	1.48	1.41
2	B	9009	ADP	C5-N7	-2.66	1.34	1.39
2	A	9003	ADP	C8-N7	2.65	1.36	1.31
2	B	9010	ADP	C5-C6	2.63	1.48	1.41
2	A	9003	ADP	C5-N7	-2.60	1.34	1.39
2	A	9004	ADP	C5-C6	2.56	1.48	1.41
2	B	9009	ADP	C8-N7	2.55	1.36	1.31
2	A	9004	ADP	C4-N9	-2.47	1.32	1.37
2	A	9001	ADP	C5-N7	-2.29	1.34	1.39
2	A	9003	ADP	C4-N3	2.22	1.38	1.34
2	B	9008	ADP	C4-N9	-2.19	1.33	1.37
2	A	9001	ADP	O4'-C4'	-2.15	1.40	1.45
2	B	9008	ADP	C8-N7	2.12	1.35	1.31
2	A	9004	ADP	C8-N7	2.10	1.35	1.31
2	A	9002	ADP	C4-N9	-2.01	1.33	1.37
2	A	9002	ADP	PA-O3A	2.01	1.61	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9002	ADP	C5-C4-N3	-5.96	118.52	126.72
2	A	9003	ADP	C5-C4-N3	-5.79	118.74	126.72
2	B	9009	ADP	C5-C4-N3	-5.55	119.07	126.72
2	B	9008	ADP	C5-C4-N3	-5.38	119.30	126.72
2	A	9004	ADP	C5-C4-N3	-5.26	119.47	126.72
2	A	9001	ADP	C5-C4-N3	-5.05	119.76	126.72
2	B	9010	ADP	C5-C4-N3	-5.04	119.77	126.72
2	B	9007	ADP	C5-C4-N3	-5.01	119.81	126.72
2	B	9007	ADP	N3-C2-N1	-4.92	121.13	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9002	ADP	N3-C4-N9	4.86	135.44	127.17
2	A	9003	ADP	N3-C4-N9	4.74	135.22	127.17
2	A	9003	ADP	N3-C2-N1	-4.57	121.67	128.58
2	B	9009	ADP	N3-C4-N9	4.54	134.88	127.17
2	A	9001	ADP	N3-C2-N1	-4.44	121.86	128.58
2	B	9010	ADP	N3-C4-N9	4.43	134.70	127.17
2	B	9008	ADP	N3-C4-N9	4.40	134.65	127.17
2	A	9004	ADP	N3-C4-N9	4.38	134.61	127.17
2	A	9002	ADP	N3-C2-N1	-4.33	122.03	128.58
2	B	9007	ADP	N3-C4-N9	4.25	134.40	127.17
2	B	9008	ADP	N3-C2-N1	-4.24	122.17	128.58
2	B	9010	ADP	N3-C2-N1	-4.21	122.21	128.58
2	A	9003	ADP	C2-N3-C4	4.21	122.11	111.83
2	B	9009	ADP	N3-C2-N1	-4.18	122.25	128.58
2	A	9002	ADP	C2-N3-C4	4.13	121.92	111.83
2	A	9004	ADP	N3-C2-N1	-4.03	122.48	128.58
2	A	9001	ADP	C2-N3-C4	4.02	121.65	111.83
2	A	9001	ADP	N3-C4-N9	3.99	133.95	127.17
2	B	9009	ADP	C2-N3-C4	3.96	121.50	111.83
2	B	9007	ADP	C2-N3-C4	3.90	121.35	111.83
2	A	9004	ADP	C2-N3-C4	3.80	121.11	111.83
2	B	9010	ADP	C2-N3-C4	3.76	121.03	111.83
2	B	9008	ADP	C2-N3-C4	3.74	120.96	111.83
2	A	9002	ADP	C4-C5-N7	-3.47	106.61	110.58
2	B	9009	ADP	C4-C5-N7	-3.26	106.86	110.58
2	A	9003	ADP	C4-C5-N7	-3.20	106.92	110.58
2	A	9001	ADP	C4-C5-N7	-3.16	106.96	110.58
2	B	9008	ADP	C4-C5-N7	-3.12	107.01	110.58
2	B	9010	ADP	C3'-C2'-C1'	3.00	107.13	101.46
2	A	9004	ADP	C4-C5-N7	-2.96	107.20	110.58
2	A	9004	ADP	C3'-C2'-C1'	2.95	107.05	101.46
2	B	9010	ADP	C2'-C1'-N9	-2.89	106.13	113.30
2	A	9001	ADP	C4-N9-C8	2.83	108.71	105.74
2	A	9003	ADP	O4'-C1'-N9	2.77	113.40	108.09
2	A	9003	ADP	C5-N7-C8	2.76	107.80	103.45
2	B	9007	ADP	C4-N9-C8	2.68	108.55	105.74
2	B	9010	ADP	C4-C5-N7	-2.65	107.55	110.58
2	A	9002	ADP	C5-N7-C8	2.64	107.60	103.45
2	A	9003	ADP	C2'-C3'-C4'	2.64	107.70	102.61
2	B	9007	ADP	C4-C5-N7	-2.63	107.58	110.58
2	B	9007	ADP	C2-N1-C6	2.60	123.00	118.73
2	B	9009	ADP	C5-N7-C8	2.60	107.53	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9008	ADP	C5-N7-C8	2.57	107.49	103.45
2	A	9001	ADP	C6-C5-N7	2.53	136.97	132.09
2	A	9004	ADP	C2-N1-C6	2.52	122.87	118.73
2	A	9004	ADP	C4-N9-C8	2.47	108.33	105.74
2	B	9010	ADP	C2-N1-C6	2.46	122.78	118.73
2	A	9001	ADP	C2-N1-C6	2.46	122.77	118.73
2	A	9003	ADP	C3'-C2'-C1'	2.41	106.03	101.46
2	A	9003	ADP	C2-N1-C6	2.41	122.69	118.73
2	B	9007	ADP	C3'-C2'-C1'	2.39	105.99	101.46
2	A	9004	ADP	C5-N7-C8	2.38	107.19	103.45
2	B	9008	ADP	C2'-C3'-C4'	2.37	107.19	102.61
2	A	9003	ADP	C6-C5-N7	2.37	136.65	132.09
2	A	9002	ADP	C3'-C2'-C1'	2.36	105.93	101.46
2	B	9008	ADP	C4-N9-C8	2.35	108.21	105.74
2	B	9010	ADP	C4-N9-C8	2.34	108.19	105.74
2	B	9009	ADP	C2-N1-C6	2.33	122.56	118.73
2	B	9008	ADP	C2-N1-C6	2.33	122.55	118.73
2	A	9003	ADP	C4-N9-C8	2.32	108.17	105.74
2	B	9009	ADP	C2'-C3'-C4'	2.31	107.08	102.61
2	B	9007	ADP	C5-N7-C8	2.30	107.06	103.45
2	B	9010	ADP	C5-N7-C8	2.29	107.05	103.45
2	A	9001	ADP	C5-N7-C8	2.22	106.94	103.45
2	A	9001	ADP	C2'-C3'-C4'	2.22	106.90	102.61
2	B	9008	ADP	C6-C5-N7	2.20	136.34	132.09
2	A	9002	ADP	C2-N1-C6	2.20	122.34	118.73
2	B	9008	ADP	C3'-C2'-C1'	2.18	105.59	101.46
2	A	9002	ADP	C4-N9-C8	2.16	108.01	105.74
2	A	9002	ADP	C6-C5-N7	2.14	136.22	132.09
2	B	9009	ADP	C6-C5-N7	2.14	136.22	132.09
2	B	9009	ADP	C4-N9-C8	2.12	107.97	105.74
2	B	9010	ADP	C6-C5-N7	2.10	136.13	132.09
2	B	9009	ADP	C3'-C2'-C1'	2.07	105.38	101.46
2	B	9007	ADP	N9-C8-N7	-2.05	111.02	113.94
2	A	9001	ADP	C3'-C2'-C1'	2.05	105.34	101.46
2	B	9007	ADP	O3B-PB-O2B	2.05	115.48	107.80
2	A	9003	ADP	N9-C8-N7	-2.02	111.08	113.94
2	A	9001	ADP	N9-C8-N7	-2.00	111.09	113.94
2	A	9004	ADP	C2'-C1'-N9	-2.00	108.33	113.30

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	A	9001	ADP	C5'-O5'-PA-O3A
2	A	9002	ADP	C5'-O5'-PA-O3A
2	A	9003	ADP	C5'-O5'-PA-O1A
2	A	9003	ADP	C5'-O5'-PA-O2A
2	A	9003	ADP	C5'-O5'-PA-O3A
2	B	9007	ADP	C5'-O5'-PA-O1A
2	B	9007	ADP	C5'-O5'-PA-O2A
2	B	9007	ADP	C5'-O5'-PA-O3A
2	B	9008	ADP	C5'-O5'-PA-O3A
2	B	9009	ADP	C5'-O5'-PA-O1A
2	B	9009	ADP	C5'-O5'-PA-O2A
2	B	9009	ADP	C5'-O5'-PA-O3A
2	B	9010	ADP	C5'-O5'-PA-O2A
2	B	9010	ADP	C5'-O5'-PA-O3A
3	A	9012	SPM	C2-C3-C4-N5
3	A	9016	SPM	C7-C8-C9-N10
3	B	9018	SPM	C2-C3-C4-N5
3	B	9022	SPM	C2-C3-C4-N5
3	A	9016	SPM	C3-C4-N5-C6
3	B	9018	SPM	N10-C11-C12-C13
3	A	9012	SPM	C12-C11-N10-C9
3	A	9016	SPM	C7-C6-N5-C4
3	A	9012	SPM	N1-C2-C3-C4
3	A	9016	SPM	N10-C11-C12-C13
3	A	9016	SPM	C6-C7-C8-C9
3	B	9022	SPM	C3-C4-N5-C6
3	A	9016	SPM	C2-C3-C4-N5
3	A	9012	SPM	C7-C8-C9-N10
3	B	9018	SPM	C11-C12-C13-N14
3	A	9012	SPM	N10-C11-C12-C13
3	A	9016	SPM	C12-C11-N10-C9
2	A	9001	ADP	PB-O3A-PA-O2A
2	A	9002	ADP	PB-O3A-PA-O2A
2	A	9003	ADP	PB-O3A-PA-O2A
2	A	9004	ADP	PB-O3A-PA-O2A
2	B	9007	ADP	PB-O3A-PA-O2A
2	B	9008	ADP	PB-O3A-PA-O2A
2	B	9009	ADP	PB-O3A-PA-O2A
2	B	9010	ADP	PB-O3A-PA-O2A
3	A	9016	SPM	C8-C9-N10-C11
3	B	9022	SPM	N10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	B	9018	SPM	C6-C7-C8-C9
2	A	9002	ADP	C5'-O5'-PA-O1A
2	B	9008	ADP	C5'-O5'-PA-O1A
2	B	9010	ADP	C5'-O5'-PA-O1A
3	A	9016	SPM	N5-C6-C7-C8
3	A	9016	SPM	N1-C2-C3-C4
3	B	9022	SPM	N1-C2-C3-C4
3	B	9018	SPM	C7-C6-N5-C4
3	B	9022	SPM	C12-C11-N10-C9
3	B	9018	SPM	C12-C11-N10-C9
3	B	9022	SPM	C7-C6-N5-C4
2	B	9007	ADP	O4'-C4'-C5'-O5'
2	A	9002	ADP	PB-O3A-PA-O1A
2	A	9003	ADP	PB-O3A-PA-O1A
2	A	9004	ADP	PB-O3A-PA-O1A
2	B	9009	ADP	PB-O3A-PA-O1A
2	B	9010	ADP	PB-O3A-PA-O1A
2	A	9001	ADP	O4'-C4'-C5'-O5'
2	A	9004	ADP	O4'-C4'-C5'-O5'
2	B	9008	ADP	O4'-C4'-C5'-O5'
2	B	9010	ADP	O4'-C4'-C5'-O5'
3	A	9016	SPM	C11-C12-C13-N14
3	B	9018	SPM	N1-C2-C3-C4
3	B	9022	SPM	C11-C12-C13-N14
2	A	9002	ADP	O4'-C4'-C5'-O5'
2	B	9009	ADP	O4'-C4'-C5'-O5'
2	A	9001	ADP	PB-O3A-PA-O1A
2	B	9007	ADP	PB-O3A-PA-O1A
2	B	9008	ADP	PB-O3A-PA-O1A

There are no ring outliers.

12 monomers are involved in 30 short contacts:

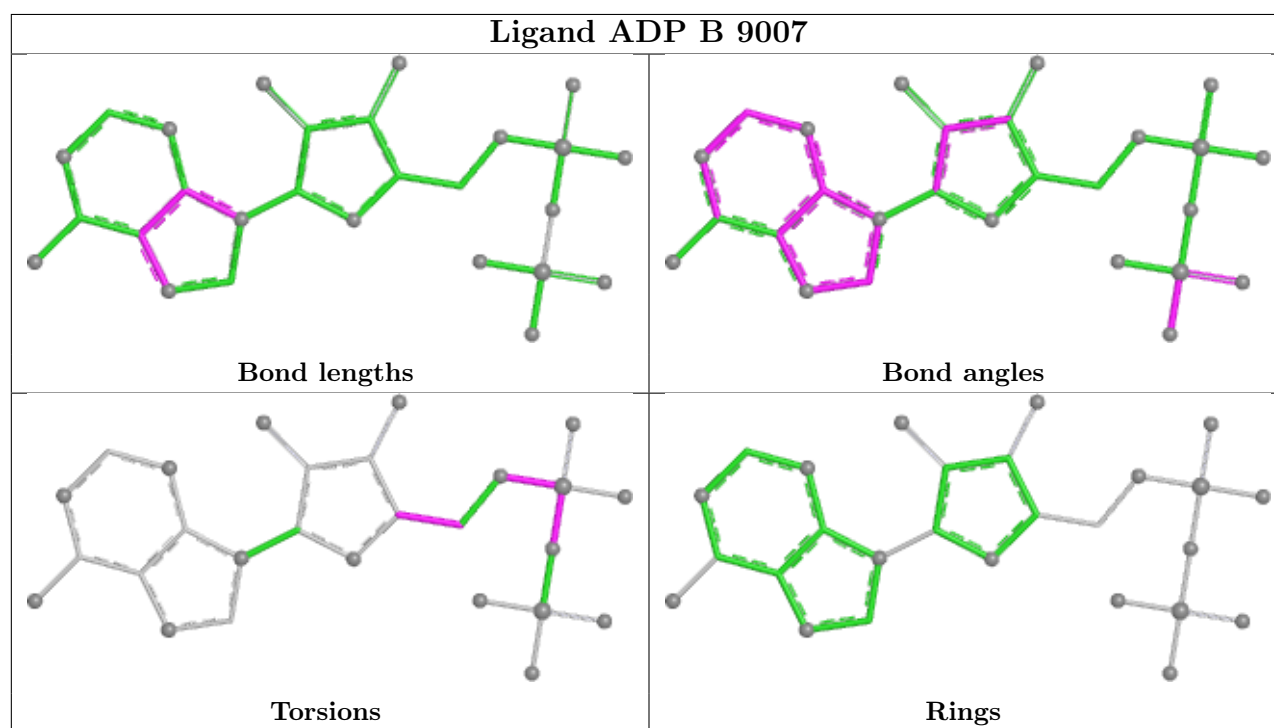
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9007	ADP	2	0
2	A	9004	ADP	6	0
2	B	9008	ADP	2	0
3	B	9018	SPM	2	0
2	B	9010	ADP	3	0
2	B	9009	ADP	2	0
3	A	9016	SPM	1	0
2	A	9003	ADP	4	0

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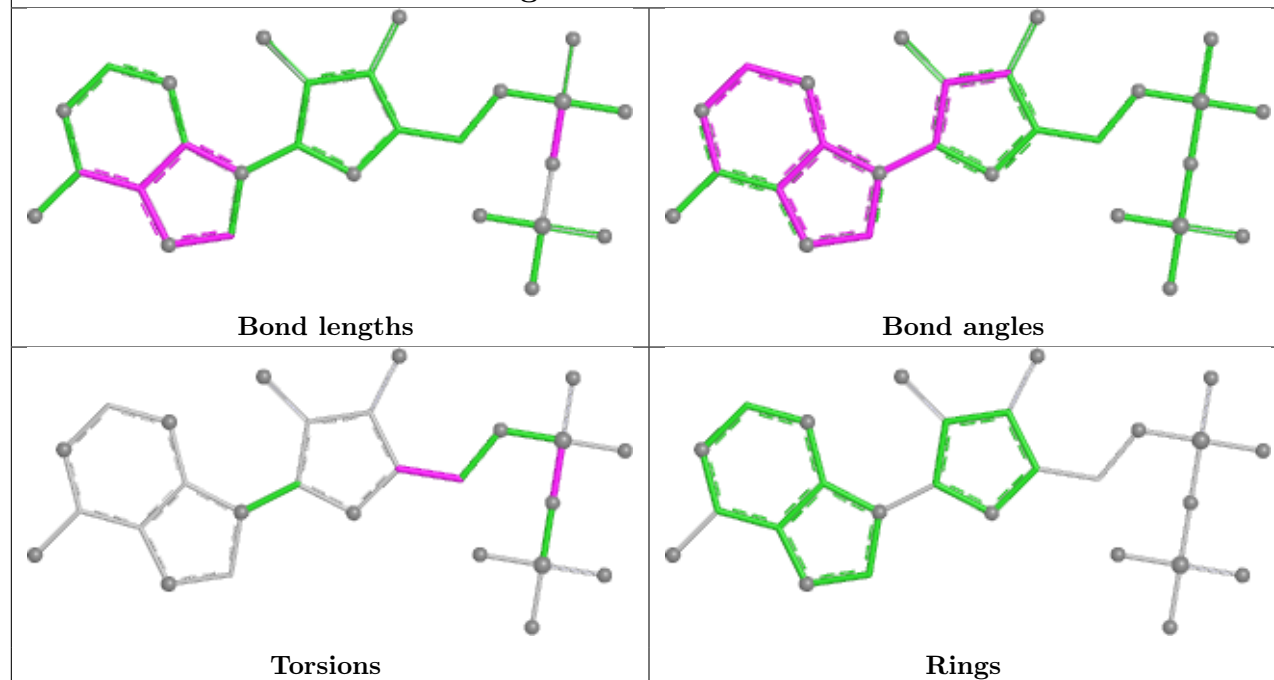
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	A	9002	ADP	3	0
3	A	9012	SPM	1	0
3	B	9022	SPM	3	0

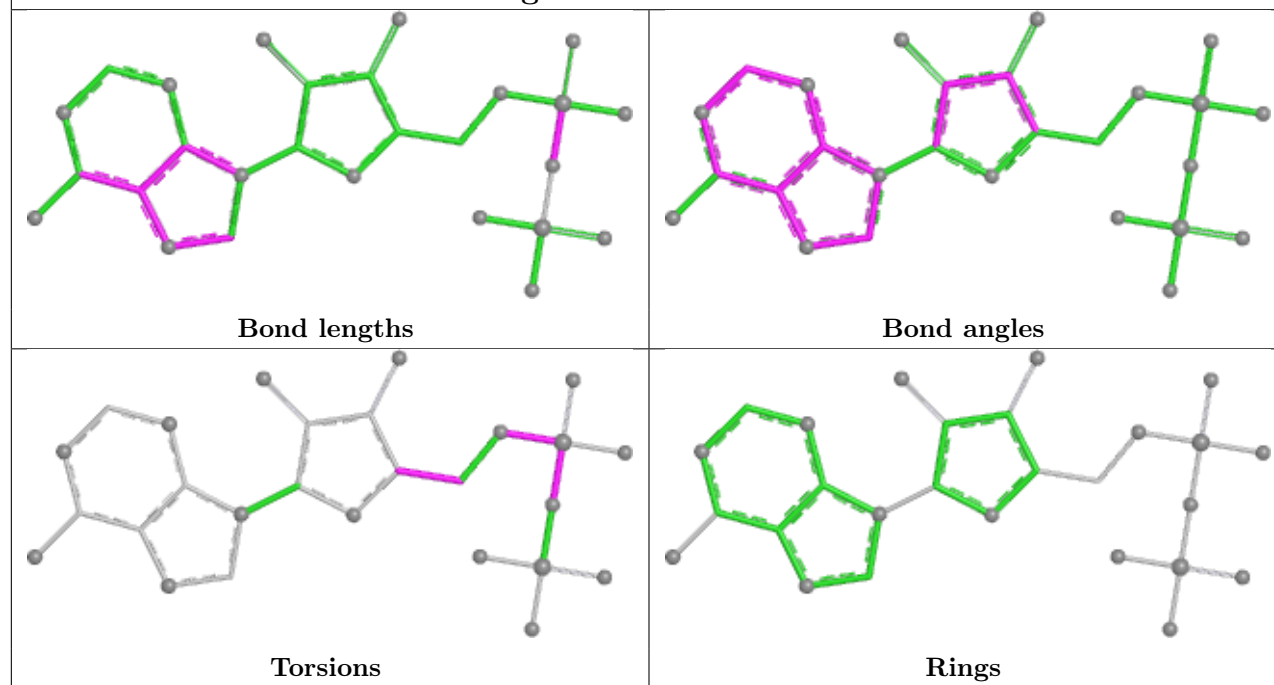
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

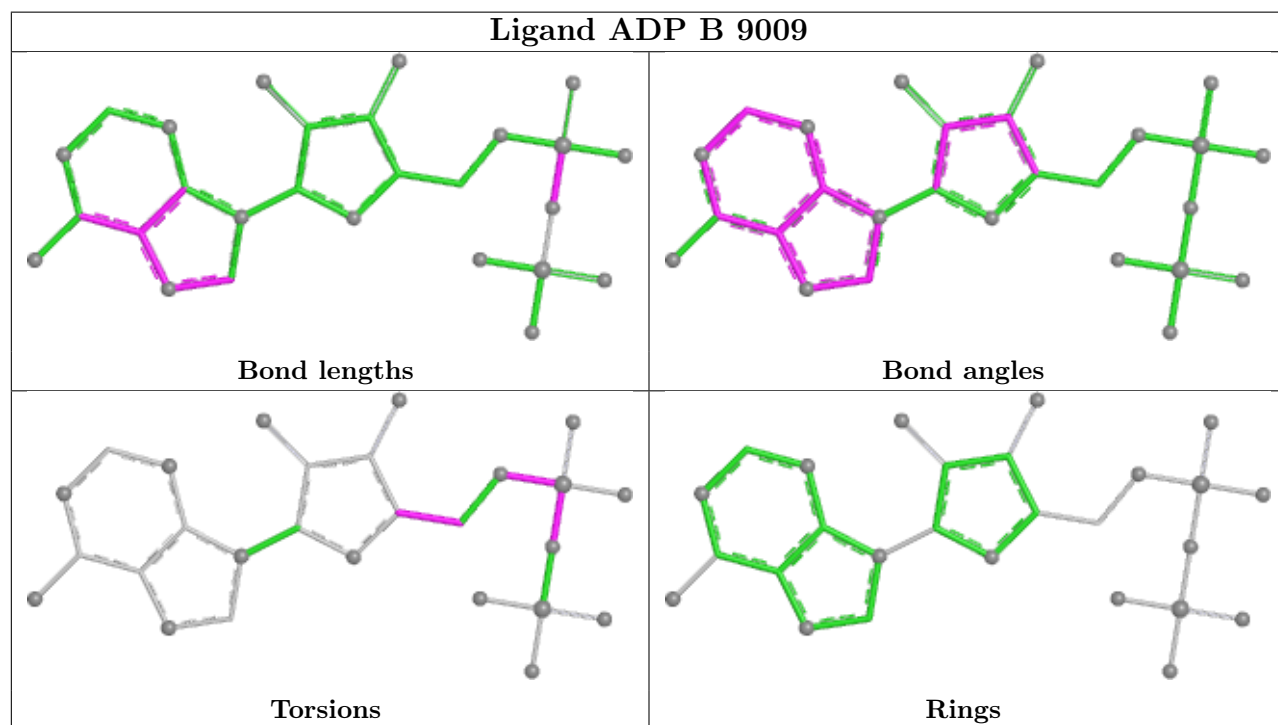
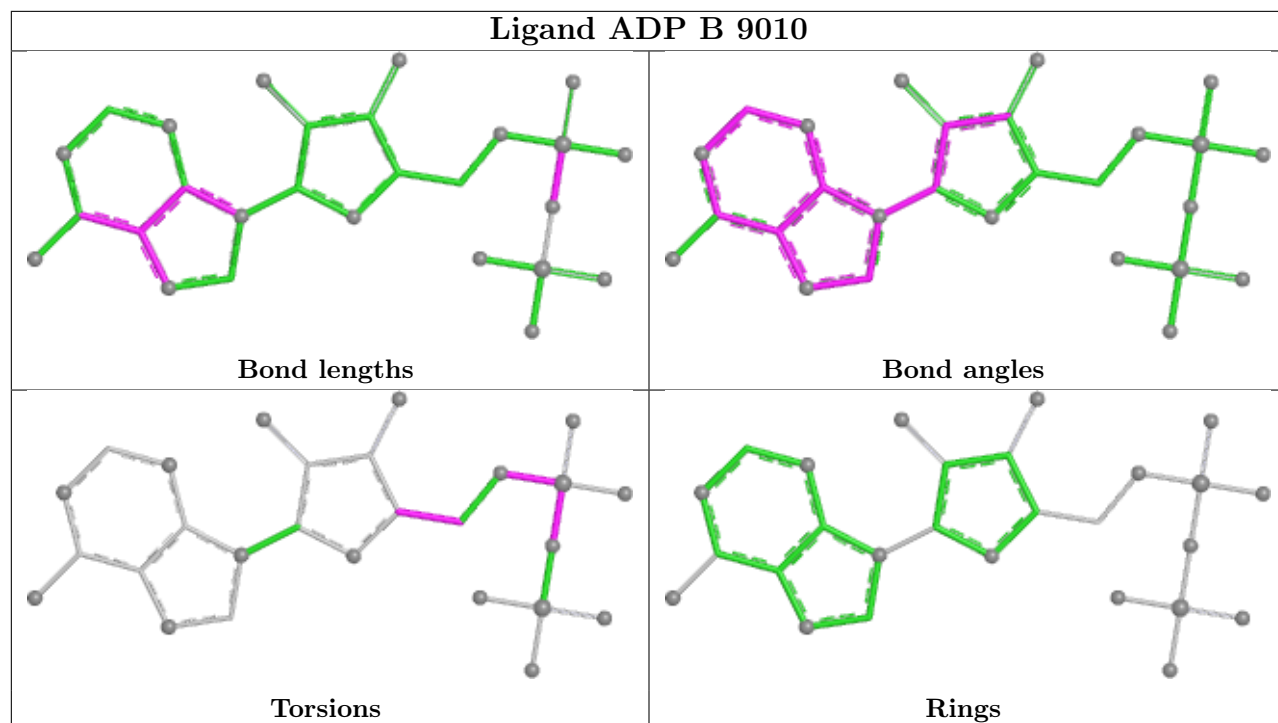


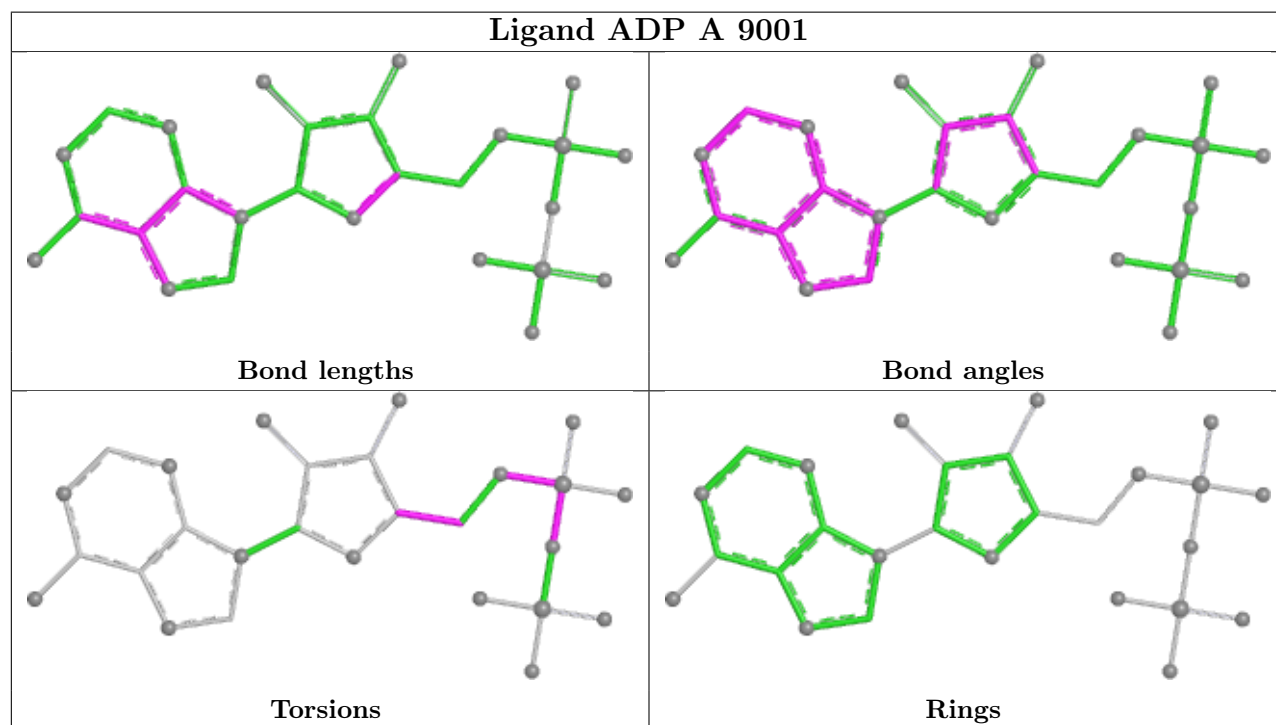
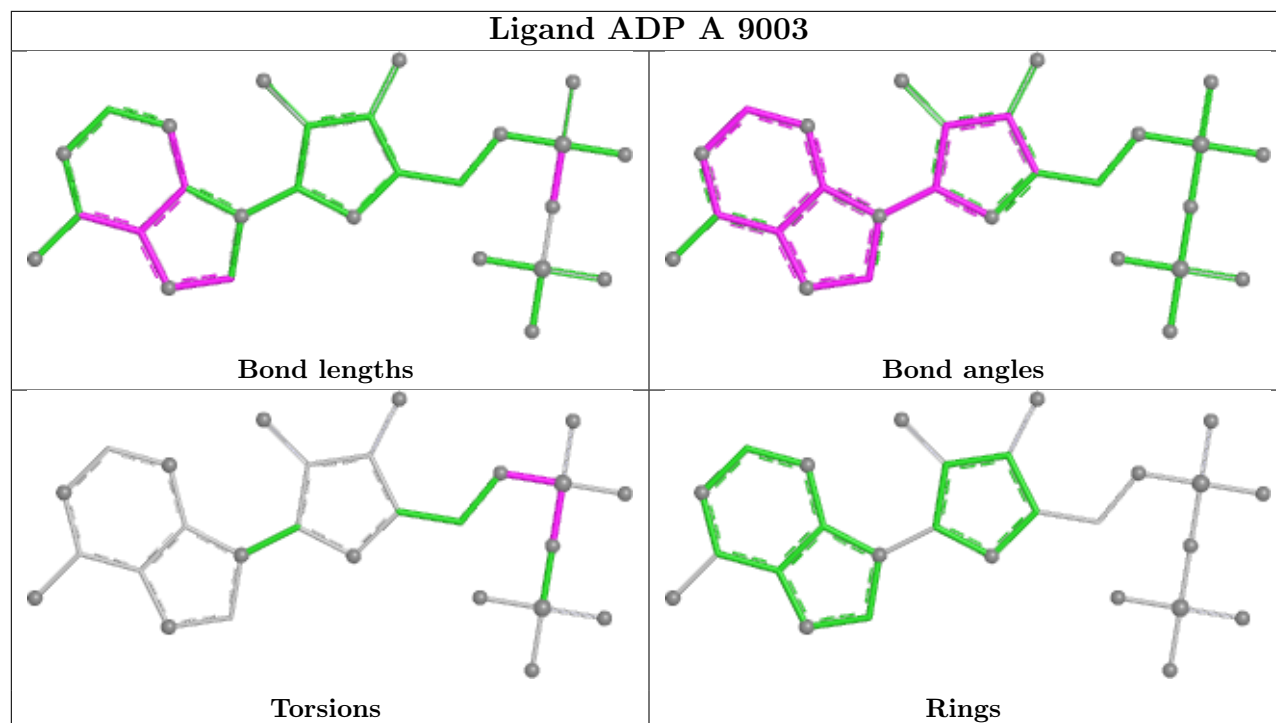
Ligand ADP A 9004

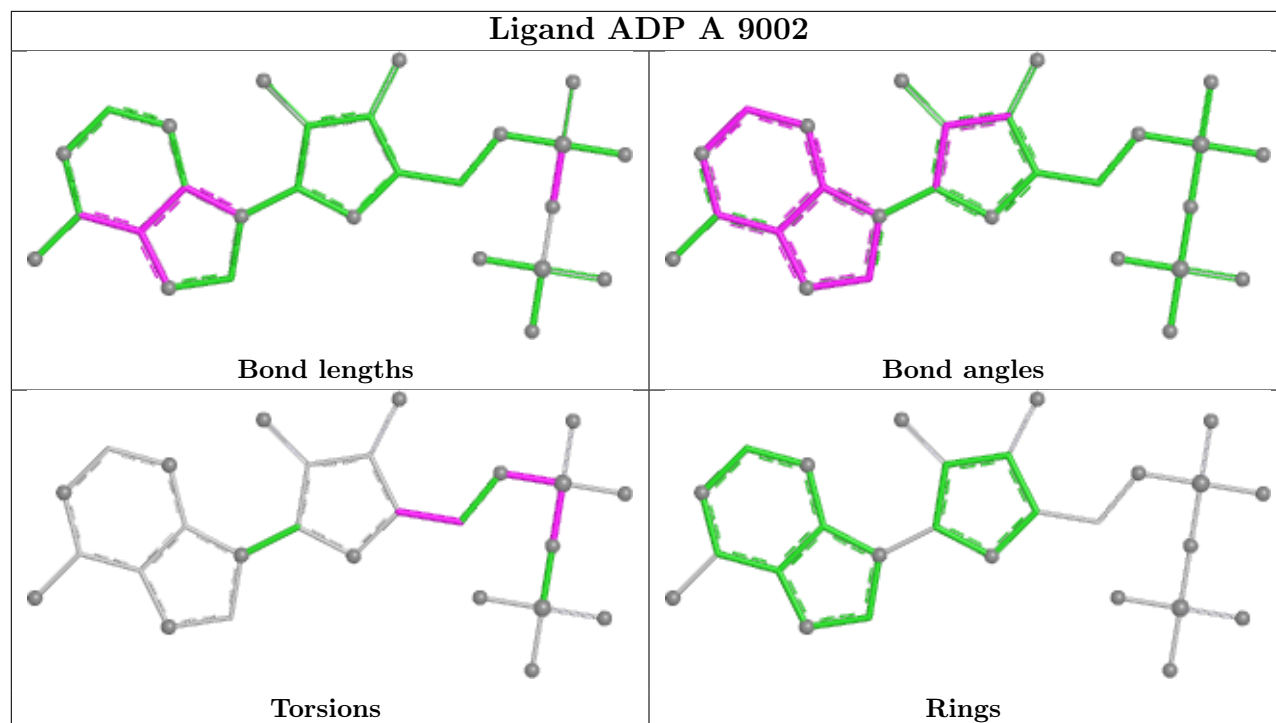


Ligand ADP B 9008









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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	2954/3245 (91%)	0.50	187 (6%)	26	19	17, 53, 78, 102	0
1	B	2853/3245 (87%)	0.39	121 (4%)	40	32	24, 52, 75, 100	0
All	All	5807/6490 (89%)	0.44	308 (5%)	32	24	17, 52, 77, 102	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4677	PRO	5.9
1	B	3108	LEU	4.8
1	B	4456	SER	4.8
1	A	4613	GLY	4.7
1	B	2323	THR	4.6
1	A	2001	ASP	4.6
1	B	2631	VAL	4.5
1	B	1591	TRP	4.4
1	A	4581	SER	4.3
1	A	4455	SER	4.3
1	A	2630	LYS	4.2
1	A	4494	PRO	4.2
1	A	2169	PRO	4.2
1	A	1625	ILE	4.2
1	A	4191	HIS	4.2
1	A	4678	ILE	4.1
1	B	4614	TRP	3.8
1	A	4521	LEU	3.8
1	B	1545	LEU	3.8
1	B	1561	LEU	3.8
1	B	3101	GLU	3.7
1	B	4051	ASP	3.7
1	B	4491	ILE	3.7
1	A	4166	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	2887	LEU	3.6
1	A	3084	LEU	3.6
1	A	4462	GLY	3.5
1	A	3502	GLU	3.5
1	A	4116	LEU	3.5
1	B	4529	LYS	3.5
1	A	4624	SER	3.5
1	B	4073	GLN	3.4
1	B	2001	ASP	3.4
1	B	3153	ASP	3.4
1	B	3044	ASN	3.4
1	A	3931	VAL	3.4
1	A	1450	ALA	3.4
1	B	1565	LEU	3.3
1	B	4523	LEU	3.3
1	A	2407	THR	3.3
1	A	3817	LEU	3.3
1	A	3098	GLY	3.3
1	B	2491	GLY	3.3
1	A	3826	LYS	3.3
1	A	3777	LEU	3.3
1	B	4049	GLY	3.3
1	A	3932	ASP	3.2
1	B	1564	LYS	3.2
1	A	2262	LEU	3.2
1	A	4608	ALA	3.2
1	A	1714	ASP	3.2
1	A	4673	ASP	3.2
1	B	1605	TRP	3.2
1	B	1861	ASP	3.2
1	A	3079	LEU	3.2
1	A	2987	PRO	3.2
1	B	1595	LEU	3.1
1	B	3161	SER	3.1
1	B	2324	THR	3.1
1	A	4564	TRP	3.1
1	A	4168	PHE	3.1
1	B	4515	ASN	3.1
1	B	2635	GLU	3.1
1	B	2736	GLY	3.0
1	B	2166	CYS	3.0
1	B	1643	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	4150	ALA	3.0
1	B	1604	VAL	3.0
1	B	3095	GLU	3.0
1	A	1559	ASP	2.9
1	A	2267	ASN	2.9
1	A	1836	LEU	2.9
1	A	4152	GLN	2.9
1	A	1413	SER	2.9
1	B	1593	ASP	2.9
1	A	4165	PRO	2.9
1	B	1555	VAL	2.9
1	B	4166	GLU	2.9
1	A	1506	ASP	2.9
1	A	4053	VAL	2.9
1	B	3165	PHE	2.9
1	B	1562	PHE	2.8
1	B	1559	ASP	2.8
1	A	3220	PRO	2.8
1	A	4519	ASN	2.8
1	B	3509	ASN	2.8
1	A	1420	SER	2.8
1	A	2889	ALA	2.8
1	A	2374	ASN	2.8
1	A	2573	LEU	2.8
1	A	2629	ASN	2.8
1	A	1412	ASP	2.8
1	B	4624	SER	2.8
1	B	2737	LYS	2.8
1	B	2225	GLY	2.8
1	A	4223	PRO	2.8
1	A	4195	GLN	2.8
1	A	3870	GLU	2.8
1	A	3869	VAL	2.8
1	B	3145	PHE	2.8
1	A	3825	VAL	2.7
1	A	1494	ILE	2.7
1	A	4611	LEU	2.7
1	B	3782	THR	2.7
1	B	4072	GLN	2.7
1	A	1414	LEU	2.7
1	A	4518	ALA	2.7
1	B	3712	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1568	HIS	2.7
1	A	3506	ASN	2.7
1	B	2565	GLN	2.7
1	B	2064	ASN	2.7
1	B	3758	PRO	2.7
1	A	4217	MET	2.6
1	B	1570	ASN	2.6
1	A	1488	LEU	2.6
1	A	1837	GLN	2.6
1	A	2740	VAL	2.6
1	A	3867	LEU	2.6
1	B	4588	GLN	2.6
1	A	4183	THR	2.6
1	A	3122	ILE	2.6
1	A	3820	GLN	2.6
1	A	1461	TYR	2.6
1	A	3822	GLU	2.6
1	B	3727	ASP	2.6
1	B	2716	HIS	2.6
1	A	1492	TRP	2.6
1	A	3040	ILE	2.6
1	A	3161	SER	2.5
1	B	1558	TRP	2.5
1	A	3830	LEU	2.5
1	B	1569	LEU	2.5
1	A	2891	GLN	2.5
1	B	4522	GLU	2.5
1	A	3321	ASN	2.5
1	A	4154	HIS	2.5
1	A	2576	SER	2.5
1	A	3868	LYS	2.5
1	A	1424	PRO	2.5
1	A	3816	LEU	2.5
1	B	3058	LEU	2.5
1	B	2746	ILE	2.5
1	B	1567	GLU	2.5
1	A	1626	ASN	2.5
1	A	3821	GLY	2.5
1	A	2838	LEU	2.5
1	B	1650	VAL	2.5
1	A	3773	PHE	2.5
1	B	3128	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	3863	THR	2.5
1	A	4218	THR	2.5
1	A	2405	LEU	2.4
1	B	2322	LEU	2.4
1	B	1566	ALA	2.4
1	B	4109	ASP	2.4
1	A	2634	VAL	2.4
1	A	3501	VAL	2.4
1	B	1863	VAL	2.4
1	A	2338	ARG	2.4
1	A	3520	ALA	2.4
1	A	1453	HIS	2.4
1	B	3708	LEU	2.4
1	A	1762	ASN	2.4
1	A	1458	ILE	2.4
1	A	2962	PRO	2.4
1	B	2268	ILE	2.4
1	B	1896	LYS	2.4
1	A	3823	PHE	2.4
1	A	4580	GLU	2.4
1	A	2177	ALA	2.4
1	B	4464	ALA	2.4
1	A	4151	LEU	2.4
1	A	3328	VAL	2.4
1	B	3133	PHE	2.4
1	B	3356	ALA	2.4
1	A	1901	ASN	2.3
1	A	3498	ARG	2.3
1	B	2057	VAL	2.3
1	B	4319	LYS	2.3
1	A	2453	ALA	2.3
1	B	3502	GLU	2.3
1	A	2060	LEU	2.3
1	A	4132	LEU	2.3
1	B	4462	GLY	2.3
1	A	3124	ASP	2.3
1	B	3709	GLU	2.3
1	A	2673	CYS	2.3
1	B	4156	GLN	2.3
1	A	2725	SER	2.3
1	A	4560	SER	2.3
1	B	1573	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	4636	SER	2.3
1	B	3220	PRO	2.3
1	B	3669	ASN	2.3
1	A	3704	PHE	2.3
1	A	2658	ASP	2.3
1	A	1627	GLN	2.3
1	B	4484	LEU	2.3
1	A	4164	SER	2.3
1	B	4533	TYR	2.3
1	B	2604	PRO	2.3
1	A	2291	GLU	2.3
1	A	4142	ALA	2.3
1	B	2490	ALA	2.3
1	A	1870	GLN	2.3
1	B	3064	CYS	2.3
1	A	4113	THR	2.3
1	B	1852	THR	2.3
1	B	3125	SER	2.3
1	A	4216	PHE	2.2
1	B	3212	MET	2.2
1	A	4577	GLU	2.2
1	A	1629	LEU	2.2
1	A	1896	LYS	2.2
1	A	2600	ILE	2.2
1	A	3845	ILE	2.2
1	A	1797	VAL	2.2
1	A	1489	ASN	2.2
1	B	1731	ASN	2.2
1	B	3736	LYS	2.2
1	A	2408	ILE	2.2
1	A	4578	ILE	2.2
1	A	3936	PRO	2.2
1	B	2256	VAL	2.2
1	A	2409	SER	2.2
1	A	2940	SER	2.2
1	A	1507	LEU	2.2
1	A	2602	ILE	2.2
1	A	4497	ARG	2.2
1	A	2918	VAL	2.2
1	A	4517	LEU	2.2
1	A	1945	GLU	2.2
1	A	2690	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	3027	ARG	2.2
1	A	4666	ILE	2.2
1	B	1671	ARG	2.2
1	A	3707	ASN	2.2
1	A	4428	ASN	2.2
1	A	3907	HIS	2.2
1	A	2168	PRO	2.2
1	A	3496	PRO	2.2
1	B	3349	ASP	2.2
1	A	3041	LYS	2.2
1	A	3714	PHE	2.2
1	A	4135	CYS	2.2
1	A	1602	LEU	2.2
1	A	4144	SER	2.2
1	A	4170	LEU	2.2
1	B	1864	LEU	2.2
1	B	4536	SER	2.2
1	A	1502	ILE	2.1
1	A	1716	ILE	2.1
1	A	2263	HIS	2.1
1	B	2407	THR	2.1
1	A	3504	LEU	2.1
1	B	1647	LEU	2.1
1	A	3683	GLU	2.1
1	B	1663	GLU	2.1
1	A	3865	ILE	2.1
1	A	4190	ILE	2.1
1	A	2628	LYS	2.1
1	A	2059	LEU	2.1
1	A	2714	PHE	2.1
1	B	4069	LEU	2.1
1	A	2882	TRP	2.1
1	A	4435	SER	2.1
1	A	4146	VAL	2.1
1	B	3825	VAL	2.1
1	A	4509	LEU	2.1
1	A	3857	THR	2.1
1	B	2959	ASP	2.1
1	A	3813	ARG	2.1
1	A	2235	GLN	2.1
1	B	4165	PRO	2.1
1	A	4515	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3164	LEU	2.1
1	A	1421	ALA	2.1
1	B	2960	TYR	2.1
1	B	4317	TYR	2.1
1	A	2840	PRO	2.0
1	A	4495	LEU	2.0
1	A	4568	PHE	2.0
1	B	3063	GLY	2.0
1	A	2892	THR	2.0
1	B	2065	ILE	2.0
1	A	2642	ALA	2.0
1	B	1661	ALA	2.0
1	A	4465	LYS	2.0
1	B	4543	LYS	2.0
1	A	3772	HIS	2.0
1	A	3875	VAL	2.0
1	A	4579	SER	2.0
1	A	1864	LEU	2.0
1	B	3129	LEU	2.0
1	A	2913	PHE	2.0
1	B	3051	PHE	2.0
1	A	1493	ILE	2.0
1	A	3518	ILE	2.0
1	B	4057	ILE	2.0
1	B	3334	ALA	2.0
1	A	2365	GLU	2.0
1	B	2784	ASP	2.0
1	B	4658	ASP	2.0
1	B	3353	LYS	2.0
1	B	3109	MET	2.0
1	A	2980	TYR	2.0
1	B	1598	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

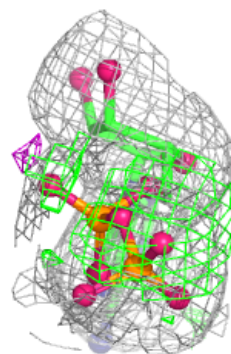
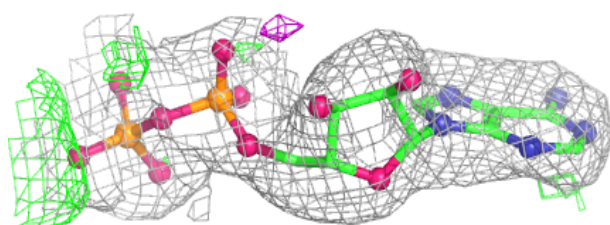
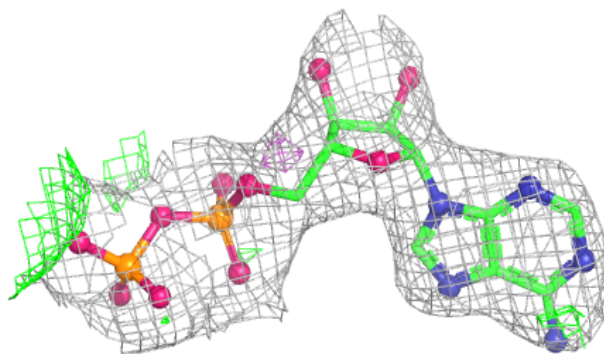
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	2	1/1	0.85	0.13	50,50,50,50	0
3	SPM	A	9016	14/14	0.86	0.17	43,50,54,55	0
3	SPM	B	9018	14/14	0.88	0.15	57,57,59,59	0
2	ADP	B	9008	27/27	0.89	0.13	41,51,53,54	0
3	SPM	A	9012	14/14	0.90	0.14	37,41,45,47	0
2	ADP	A	9002	27/27	0.90	0.12	47,49,52,54	0
3	SPM	B	9022	14/14	0.91	0.13	37,43,49,49	0
2	ADP	A	9003	27/27	0.91	0.11	41,45,50,52	0
2	ADP	A	9004	27/27	0.92	0.09	44,49,54,56	0
4	MG	B	3	1/1	0.92	0.15	28,28,28,28	0
2	ADP	B	9007	27/27	0.94	0.11	38,47,50,52	0
2	ADP	A	9001	27/27	0.94	0.11	32,38,42,44	0
2	ADP	B	9009	27/27	0.95	0.09	39,45,48,51	0
2	ADP	B	9010	27/27	0.95	0.09	31,37,46,48	0
4	MG	A	1	1/1	0.98	0.11	44,44,44,44	0

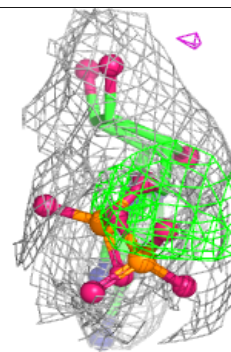
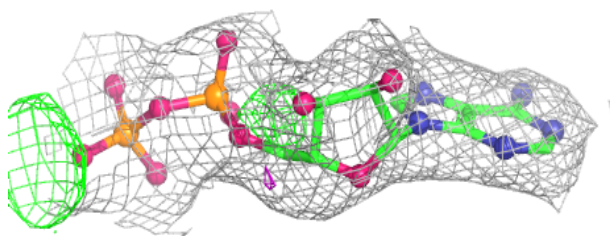
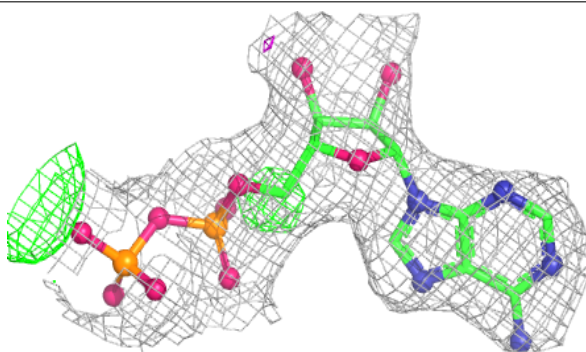
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 9008:

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

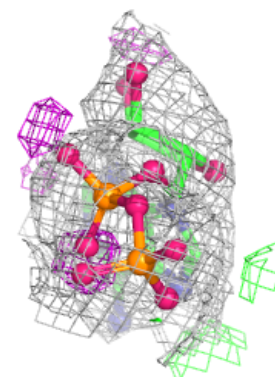
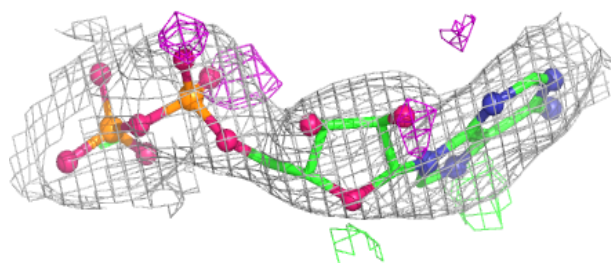
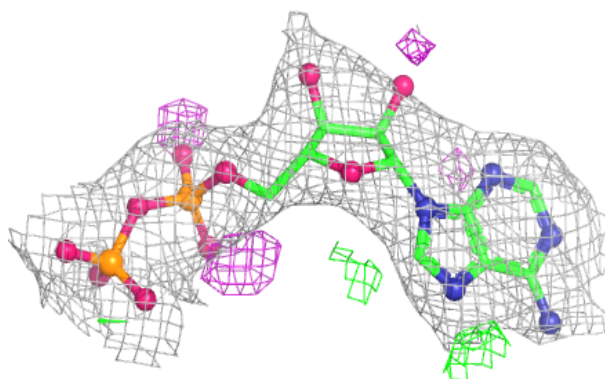
**Electron density around ADP A 9002:**

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

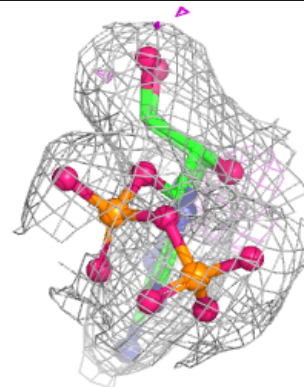
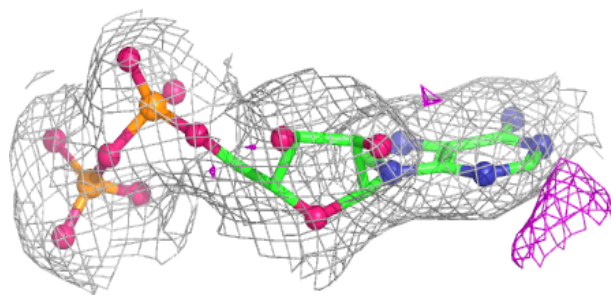
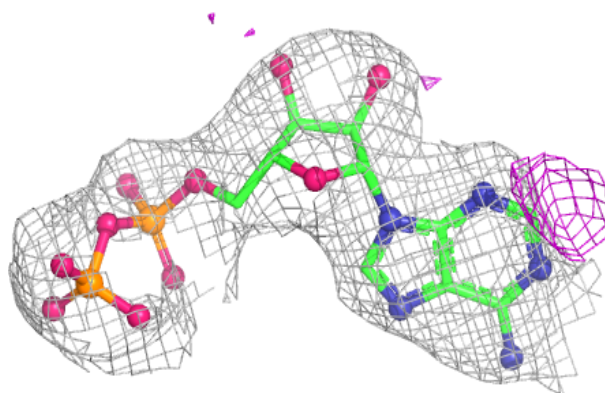


Electron density around ADP A 9003:

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

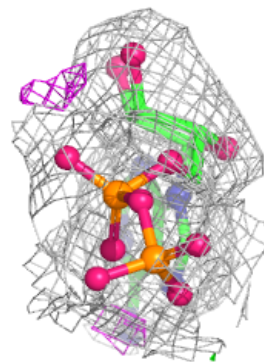
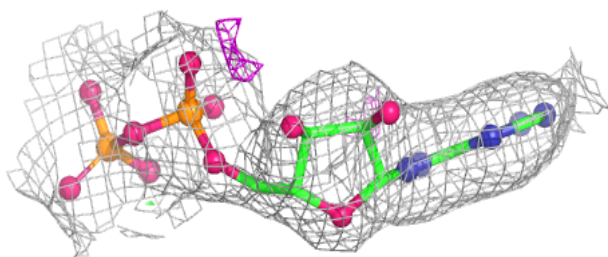
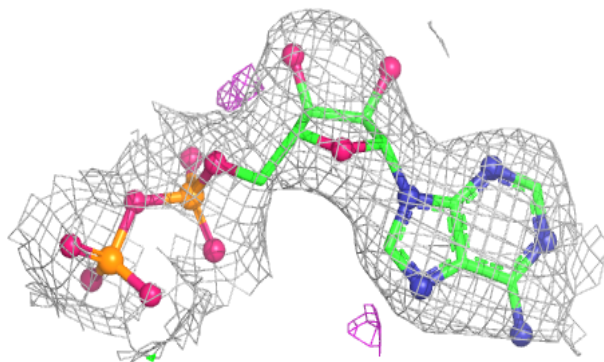
**Electron density around ADP A 9004:**

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

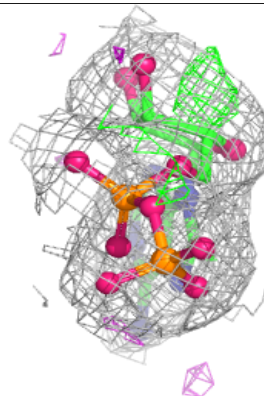
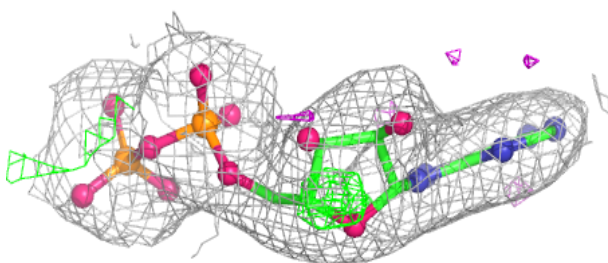
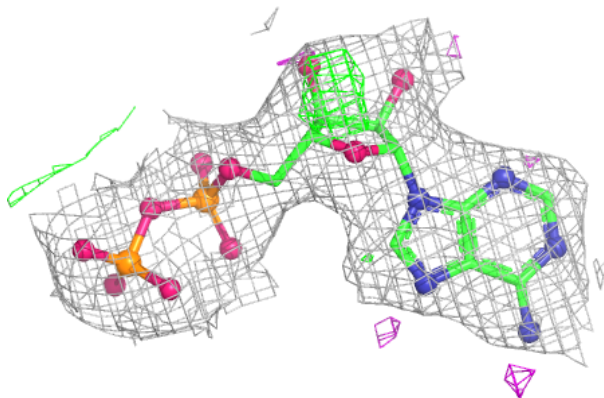


Electron density around ADP B 9007:

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

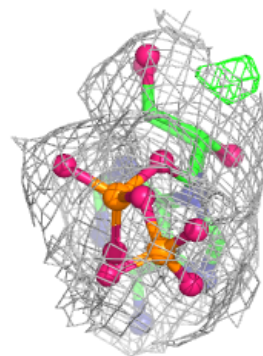
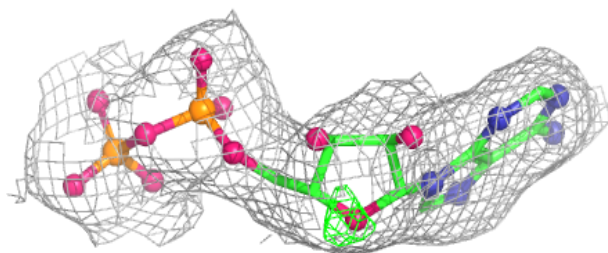
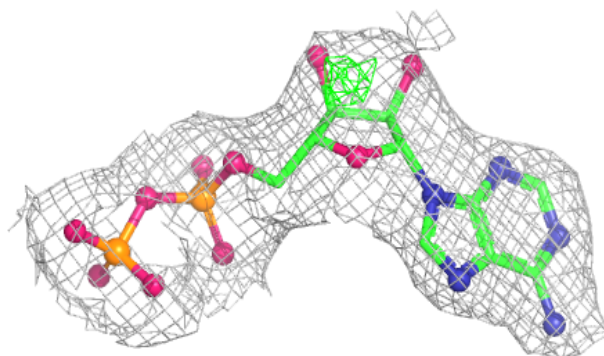
**Electron density around ADP A 9001:**

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

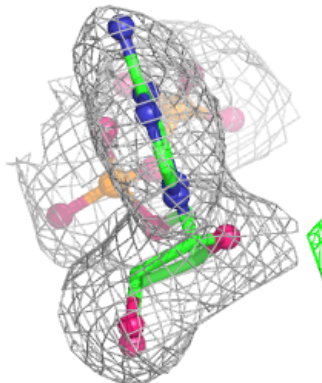
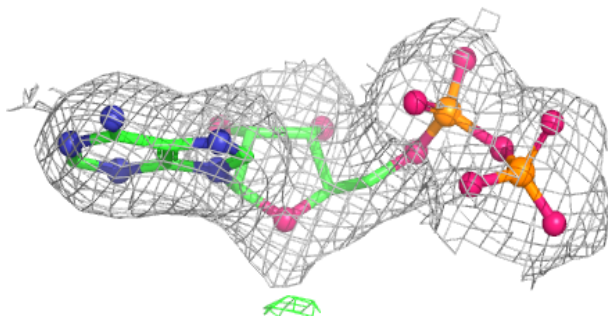
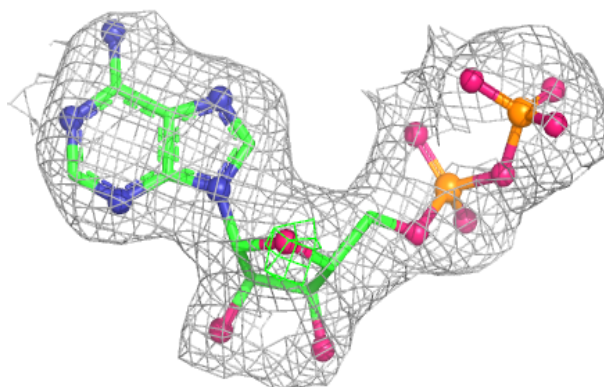


Electron density around ADP B 9009:

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

**Electron density around ADP B 9010:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.