



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:43 PM UTC

PDB ID : 4AKG / pdb_00004akg
Title : Dynein Motor Domain - ATP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

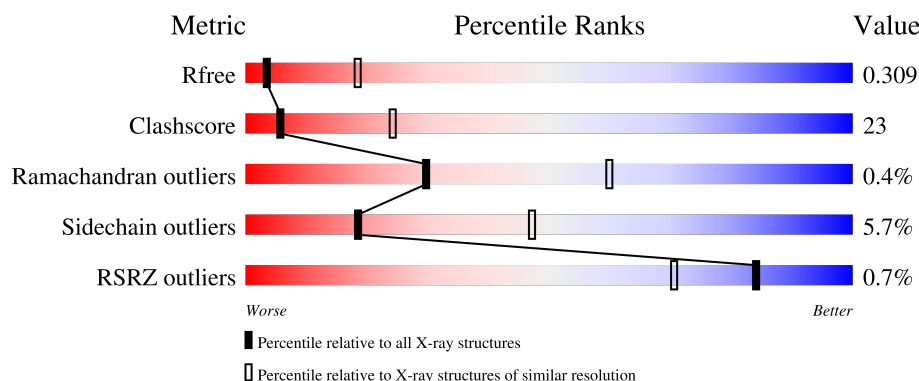
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	2695	
1	B	2695	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	5093	-	-	X	-
2	ATP	B	5093	-	-	X	-
5	SO4	A	5097	-	-	X	-
5	SO4	B	5096	-	-	X	-
5	SO4	B	5097	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41634 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 GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 8 discrepancies between the modelled and reference sequences:

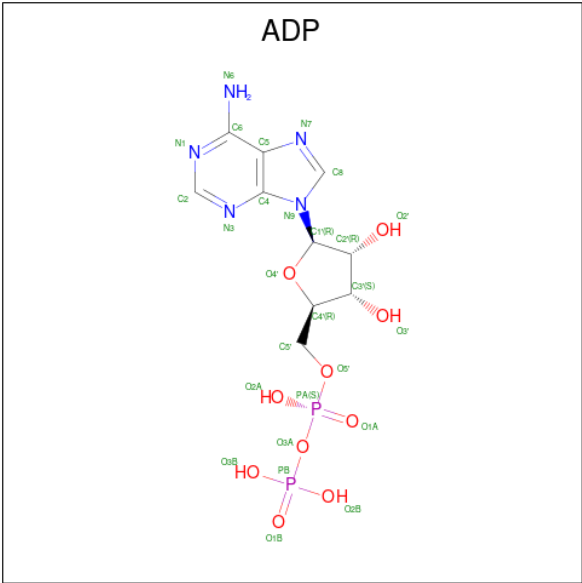
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

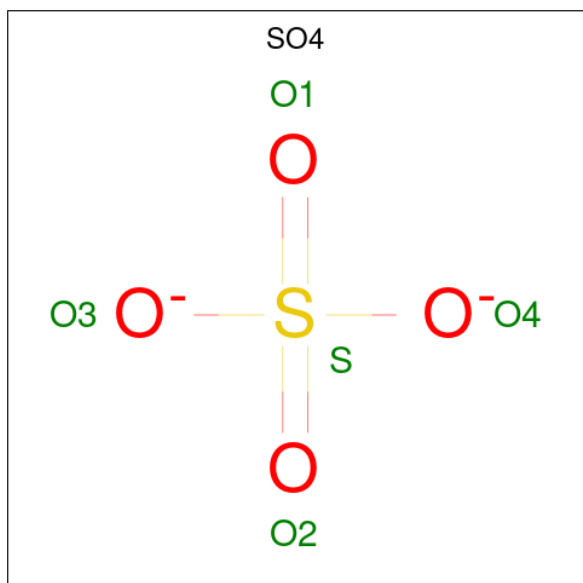


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- 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	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

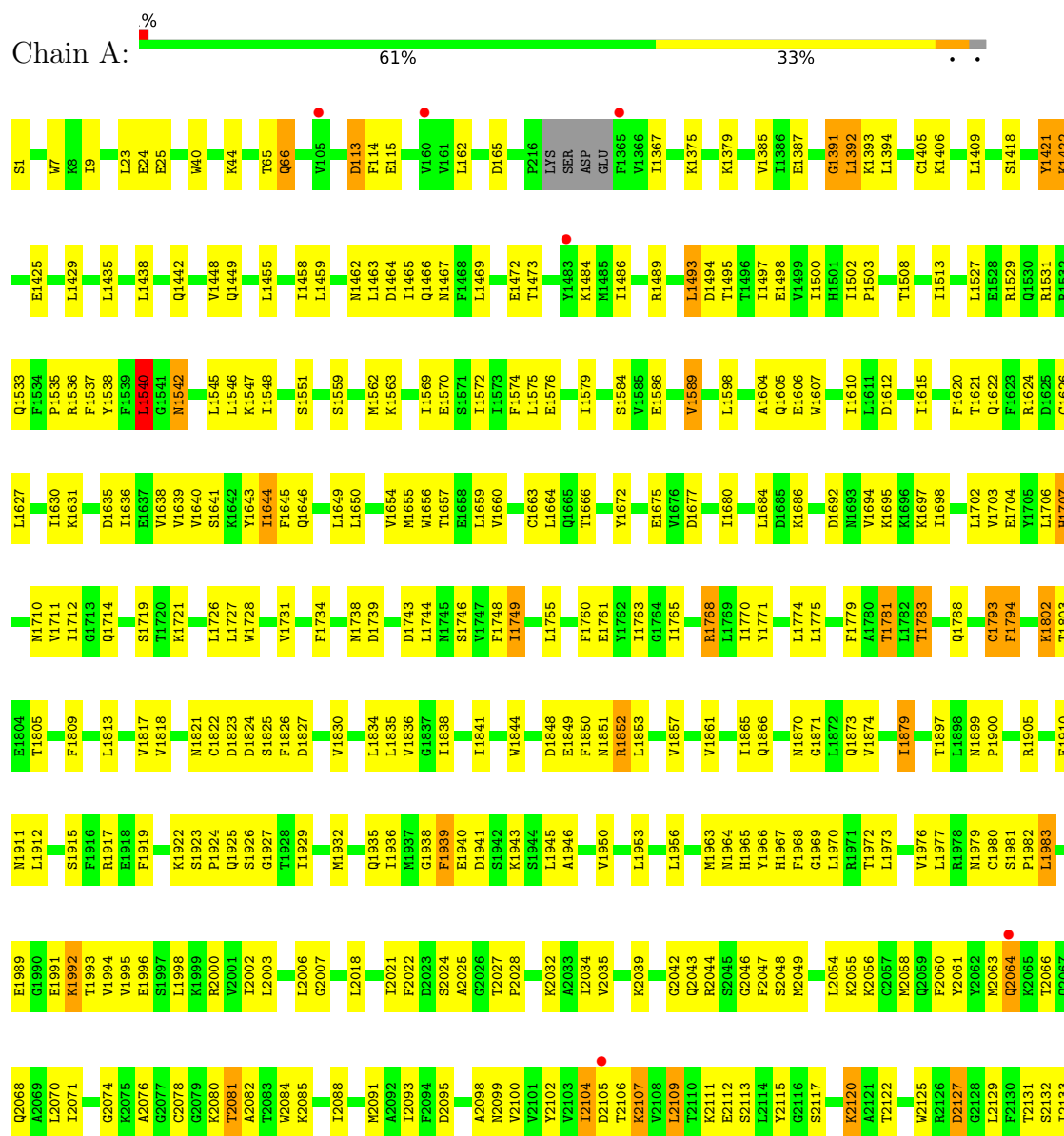


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

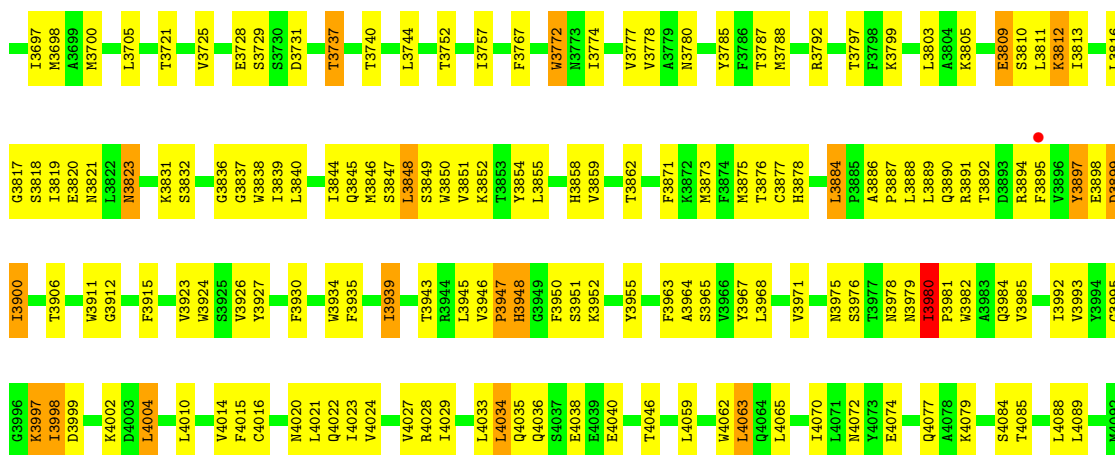
3 Residue-property plots

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.

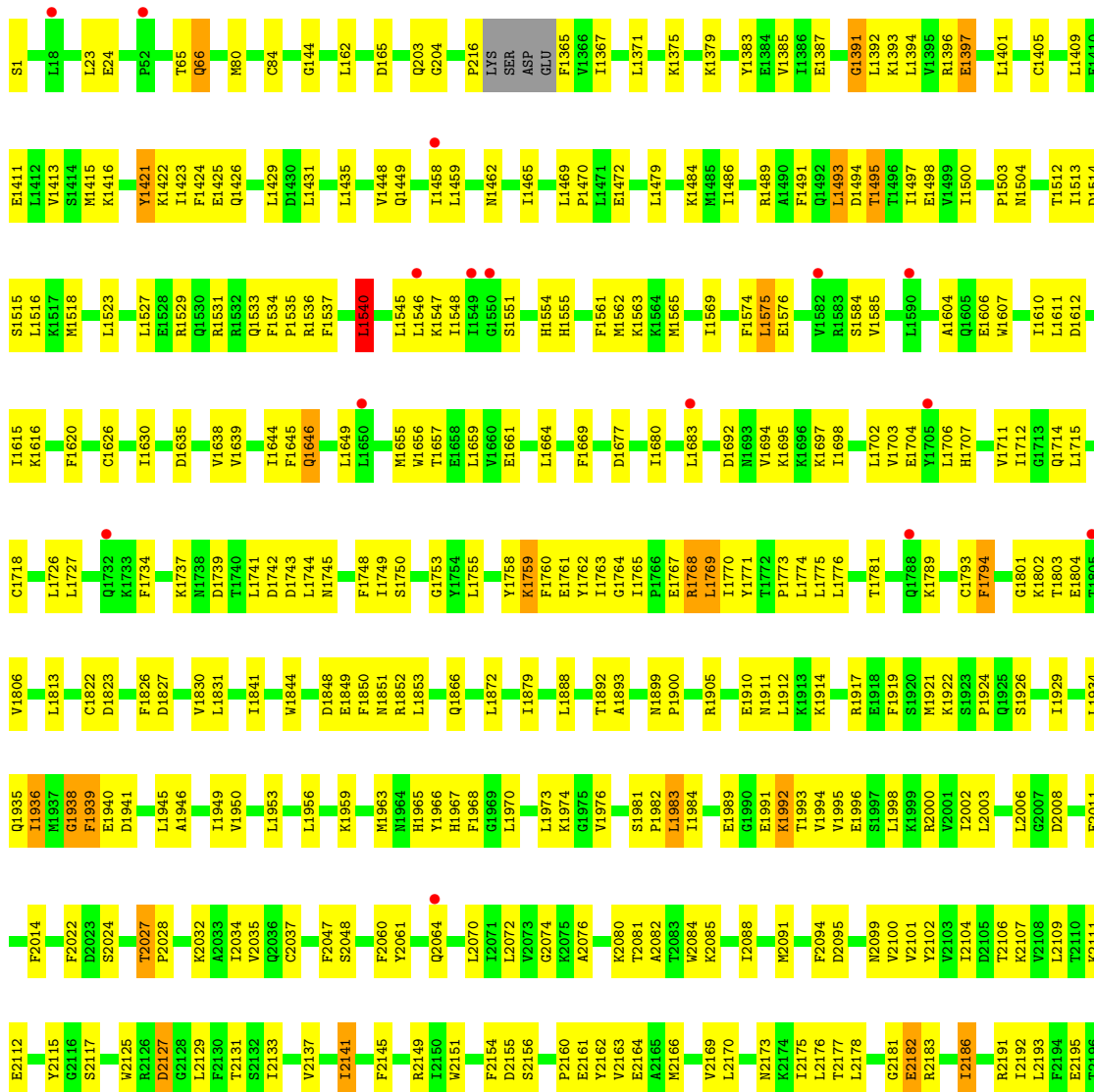
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



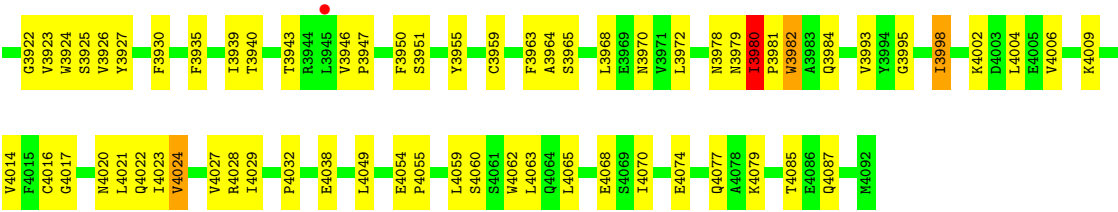
E3616	F3530	F3436	N3323	K2979	Q2783	V2677	L2569	E2488	I2403	Y2324	S2221	L2134
E3617	L3534	R3439	I3325	V2984	P2784	L2686	P2562	N2489	D2406	A2325	I2222	V2137
Y3618	T3535	L3440	T2985	N2985	I2786	P2686	S2563	N2490	L2407	L2326	S2223	N2138
G3622	T3536		P2986	P2987	R2787	I2689	S2564	L2491	G2332	G2326	K2225	G2137
V3626	E3536	A3443	I3329	R2987	H2788	S2680	G2563	N2492	N2408	E2333	K2226	I2141
K3627	E3537	Y3330	Y3330	S2988	R2789	S2691	K2565	K2493	K2410	S2334	H2228	F2145
F3628	N3538	E3331	E2907	P2989	F2795	S2691	S2566	L2494	S2411	Q2335	L2229	
F3629	F3334	F3334	L2908	G2990	D2796	L2694	L2567	D2496	K2412	R2336		
S3630			F2909	F2990	M2797		S2568	K2496	G2413		L2241	R2149
M3631	I2993	V3449	N2910	N2910	I2798	V2707	G2569	K2497	G2414	I2339	L2252	W2151
L3632		V3450	R2911	R2911	L2799	K2709	I2570	G2498	I2415	V2152		V2153
E3633	L3002		C2912	C2912	L2808	T2710	Y2571	S2499	I2416	V2153	F2257	F2154
F3634	K3350	E3456	I2913	I2913					G2417	Q2351		D2155
K3635	R3351	F3457	I2914	I2914	S2811	D2711	Y2574	V2502	G2418	L2353		S2156
G3636	L3352	F3458	N2915	N2915	R2812	L2712	Y2575	F2503	F2419	S2354	L2262	
	L3353	E3012	Y2916	Y2916	T2813	V2713	K2576	L2504	P2420	D2355		
	M2917		M2917	M2917			A2577	F2505	G2421	Y2356	I2265	M2166
F3641	F3356	I3461	V3017	V3017	I2816	E2727	I2578	L2506	K2424	S2357	F2266	E2161
Y3642	A3357	I3462	N3018	N3018	I2817	L2728		R2507	T2425	T2358		E2162
G3643	V3358		V3019	V3019			L2581	Q2508	N2425	I2359	V2273	V2163
I3644	K3359	R3464	E3012	E3012		K2732	V2582	L2509	N2426	V2367	H2274	
S3645	Y3360	L3465	Y3360	Y3360	N2821	R2747	K2517	M2510	I2427	F2368	I2275	M2166
I3646	D3361	I3466	L3024	L3024	I2822	S2737	T2609	E2511	N2428	A2362		
		S3467	V3028	V3028	L2823			K2512	N2429	G2277	G2277	V2169
F3649	R3365		LEU	LEU		H2741	Q2612	Q2513	N2430	K2365	V2278	
V3656	LYS	N3471	VAL	VAL	E2829	R2744	S2613	G2514	A2431	L2366	R2279	N2173
F3657	D3368	A3473	ASN	ASN	T2833	I2745	R2620	F2515	L2432	K2174	R2280	K2174
I3658	V3371		GLU	GLU	T2835	I2746	E2621	W2516	R2433	L2175	F2281	L2175
L3658	T3372		LEU	LEU	I2835	R2747	E2621	K2517		L2176	N2282	L2176
E3569	R3476		ASN	ASN	I2836	K2748	T2623	T2518	L2437	K2283	L2284	L2177
L3570	V3477		LYS	LYS	N2837	L2749		P2519		P2179	L2178	
	I3478		THR	THR	A2838	L2749		E2520	V2440	E2374	E2285	
S3573	W3379		LEU	LEU	D2839	Q2751	V2626	N2521	V2441	P2376	Q2289	N2190
L3578	L3391		SER	SER	I2840	K2752	W2523	K2522	F2445	E2377	Q2181	E2182
F3579			ILE	ILE	P2841	R2755	Y2630	W2524	S2446	V2378	A2291	R2183
ARG			THR	THR	D2842	K2756	T2631	T2525	K2447	S2379	V2292	L2184
ALA	M3394		SER	SER	L2843	K2757	A2632	L2526	D2448	E2381	H2293	
ALA	S3395		LEU	LEU	F2844	L2758	N2634	E2527	T2449	L2380	L2294	T2185
	I3396		VAL	VAL	Q2845	I2759	G2635		T2450	E2382	I2295	T2186
L3583		K3493	K3297	K3297	G2846	G2760	T2635	H2530	T2451	H2383		
M3584	S3298		S3298	S3298		K2761	G2636			E2384	R2299	L2193
T3669	F3301		F3301	F3301	Y2849	K2762	P2637	A2534	L2455	V2385		F2194
R3670	E3302		E3302	E3302		S2762	R2638	G2535		V2385	F2302	E2195
V3671	K3303		K3303	K3303	L2853	R2763	Q2639	N2536	N2463	M2386		T2196
D3672	E3304		E3304	E3304		T2764	T2640	P2537		R2387	D2197	
E3673	V3404		THR	THR	L2856	K2765			T2472	P2388	L2310	N2198
I3674	F3406		GLU	GLU		K2766	S2643	R2543	L2473	D2389	K2311	L2199
L3677	F3406		PR0	PR0	T2860	K2767		I2544	L2474	D2200	D2312	D2200
L3678			ILE	ILE		L2768	L2647	M2546	F2475	H2201	V2813	H2201
Y3679	N3308		N3308	N3308		I2769		P2545	K2476	I2392	T2315	T2202
					L2863			M2547		P2393	T2315	T2203
Y3683	K3311		K3311	K3311		T2770	W2653	S2547	S2477	T2394	L2316	P2204
	S3411		S3411	S3411	L2866	R2771	R2654	E2548	D2478	I2395	L2317	A2205
S3687	F3313		F3313	F3313	L2867	V2772	I2655	R2549	I2479	D2397	I2318	
						V2773		F2550	K2480	T2397	K2819	L2212
L3690	S3317		S3317	S3317	L2873		D2658	T2551	N2481	I2398	R2320	
D3691	I3318		I3318	I3318		L2779		R2552	L2482		S2321	F2215
K3692	E3319		E3319	E3319	F2889	K2780	L2673		F2485	E2401	L2322	
K3693	L3320		L3320	L3320	T2890			I2556		K2402	L2323	C2220



• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.33Å 117.92Å 202.76Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.30) 96.0 (50.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	REFMAC NULL	Depositor
R, R_{free}	0.239 , 0.305 0.239 , 0.309	Depositor DCC
R_{free} test set	5981 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 111.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41634	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: MG, ADP, ATP, SO4

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	0.85	15/21146 (0.1%)	1.22	96/28618 (0.3%)
1	B	0.70	5/21146 (0.0%)	1.10	53/28618 (0.2%)
All	All	0.77	20/42292 (0.0%)	1.16	149/57236 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2064	GLN	CA-C	-15.98	1.31	1.52
1	A	2495	ASP	C-N	-12.19	1.17	1.34
1	A	2412	ARG	CA-C	-10.96	1.39	1.52
1	B	1759	LYS	C-O	9.26	1.35	1.23
1	A	2412	ARG	C-N	-9.18	1.25	1.33
1	A	2392	ILE	CA-C	-8.31	1.46	1.53
1	B	2841	PRO	N-CD	-7.88	1.36	1.47
1	A	1983	LEU	CA-CB	-6.84	1.42	1.53
1	A	2494	LEU	C-N	6.55	1.42	1.33
1	A	2064	GLN	C-N	-6.51	1.25	1.33
1	A	3980	ILE	CA-C	5.58	1.58	1.52
1	A	2412	ARG	CZ-NH2	-5.51	1.26	1.33
1	B	1983	LEU	N-CA	5.41	1.52	1.46
1	A	3947	PRO	C-N	5.38	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2500	GLN	N-CA	5.34	1.52	1.46
1	B	2496	LYS	C-N	5.28	1.40	1.33
1	A	1983	LEU	C-N	5.22	1.40	1.34
1	A	1783	THR	CA-CB	5.21	1.61	1.53
1	A	1783	THR	CB-CG2	-5.16	1.35	1.52
1	A	1712	ILE	N-CA	5.12	1.52	1.46

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2138	ASN	N-CA-C	12.22	124.34	111.14
1	A	2127	ASP	N-CA-C	12.04	123.95	111.07
1	B	2127	ASP	N-CA-C	10.03	122.21	111.28
1	B	1424	PHE	N-CA-C	-9.14	101.23	112.38
1	A	2064	GLN	O-C-N	9.04	133.39	122.27
1	B	1426	GLN	N-CA-C	9.00	121.91	111.11
1	B	1	SER	CA-C-N	8.94	131.01	119.84
1	B	1	SER	C-N-CA	8.94	131.01	119.84
1	A	1794	PHE	N-CA-C	8.49	122.35	108.52
1	A	1464	ASP	N-CA-C	-8.25	101.55	111.69
1	A	1818	VAL	N-CA-CB	8.14	119.40	110.53
1	A	2392	ILE	N-CA-C	-8.03	99.60	107.55
1	A	2182	GLU	N-CA-C	8.01	120.31	108.14
1	B	1794	PHE	N-CA-C	7.93	121.45	108.52
1	B	3982	TRP	N-CA-C	7.90	121.86	111.75
1	B	2481	ASN	N-CA-C	7.80	120.95	110.35
1	A	3900	ILE	CB-CA-C	-7.73	101.97	110.85
1	A	2418	GLY	CA-C-N	7.68	128.29	120.38
1	A	2418	GLY	C-N-CA	7.68	128.29	120.38
1	B	3298	SER	N-CA-C	7.58	119.17	111.07
1	A	2333	GLU	N-CA-C	-7.51	103.11	111.82
1	A	3402	ASP	N-CA-C	-7.51	103.85	113.16
1	A	3948	HIS	N-CA-C	-7.47	98.83	109.96
1	A	1422	LYS	N-CA-C	7.39	118.98	111.07
1	B	1540	LEU	N-CA-C	7.37	119.10	111.14
1	A	2412	ARG	O-C-N	7.31	131.53	123.27
1	A	1542	ASN	N-CA-C	7.30	119.02	111.14
1	B	2182	GLU	N-CA-C	7.01	119.52	108.79
1	B	3771	GLU	N-CA-C	-6.92	99.78	110.10
1	A	1540	LEU	N-CA-C	6.86	118.41	111.07
1	A	2521	ASN	N-CA-C	6.73	120.37	111.28
1	A	1783	THR	N-CA-C	-6.71	103.77	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2429	ASN	N-CA-C	6.66	118.19	111.07
1	B	3870	LYS	N-CA-C	-6.64	100.06	109.96
1	B	2257	PHE	N-CA-C	6.59	119.15	108.41
1	A	2412	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	A	2220	CYS	N-CA-C	6.56	120.21	109.72
1	B	2430	ASN	N-CA-C	6.56	118.43	111.28
1	A	1666	THR	N-CA-C	6.50	118.36	111.28
1	A	1939	PHE	N-CA-C	6.47	117.99	111.07
1	B	2333	GLU	N-CA-C	-6.44	104.34	111.36
1	B	144	GLY	N-CA-C	6.41	121.31	112.52
1	A	3461	ILE	N-CA-C	6.40	116.56	110.42
1	B	2564	GLY	N-CA-C	-6.38	107.32	115.42
1	B	3459	ASP	CA-C-N	6.37	126.86	119.47
1	B	3459	ASP	C-N-CA	6.37	126.86	119.47
1	A	1803	THR	N-CA-CB	6.34	119.55	110.16
1	A	3459	ASP	CA-C-N	6.34	126.83	119.47
1	A	3459	ASP	C-N-CA	6.34	126.83	119.47
1	A	1865	ILE	N-CA-C	-6.33	104.33	110.72
1	B	84	CYS	N-CA-C	6.33	113.70	108.07
1	A	3521	ASN	N-CA-C	6.26	117.95	110.19
1	A	2942	ASP	N-CA-C	6.22	118.06	111.28
1	A	1793	CYS	CA-C-N	-6.21	114.35	123.05
1	A	1793	CYS	C-N-CA	-6.21	114.35	123.05
1	B	2916	TRP	N-CA-C	6.20	118.62	108.52
1	B	2220	CYS	N-CA-C	6.15	119.22	109.50
1	A	2537	PRO	CA-C-N	-6.15	113.87	121.00
1	A	2537	PRO	C-N-CA	-6.15	113.87	121.00
1	B	2373	SER	N-CA-C	6.14	120.34	111.56
1	B	80	MET	N-CA-C	6.12	120.36	112.41
1	A	3772	TRP	N-CA-C	6.08	119.17	110.10
1	A	3980	ILE	N-CA-C	6.08	122.02	108.88
1	B	1575	LEU	N-CA-C	-6.04	104.56	112.41
1	A	1802	LYS	CA-C-N	-6.03	111.73	120.29
1	A	1802	LYS	C-N-CA	-6.03	111.73	120.29
1	A	1783	THR	CB-CA-C	6.02	122.65	110.38
1	A	2564	GLY	N-CA-C	-6.01	107.47	115.40
1	B	1939	PHE	N-CA-C	5.93	117.42	111.07
1	A	3616	GLU	N-CA-C	5.93	117.82	111.36
1	A	2120	LYS	N-CA-C	5.89	117.70	111.28
1	A	2988	SER	CA-C-N	5.88	127.19	119.84
1	A	2988	SER	C-N-CA	5.88	127.19	119.84
1	A	3413	HIS	N-CA-C	-5.88	106.27	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2481	ASN	N-CA-C	5.87	117.87	110.24
1	A	2811	SER	N-CA-C	5.86	118.89	111.69
1	B	2418	GLY	CA-C-N	5.85	126.41	120.38
1	B	2418	GLY	C-N-CA	5.85	126.41	120.38
1	B	1759	LYS	O-C-N	-5.82	114.99	122.20
1	B	3922	GLY	N-CA-C	5.82	118.62	111.93
1	B	2618	SER	N-CA-C	5.79	113.22	108.07
1	A	3809	GLU	CB-CA-C	-5.78	109.89	116.54
1	B	2479	ILE	N-CA-C	5.77	118.30	111.09
1	A	2479	ILE	N-CA-C	5.70	118.17	111.05
1	A	3626	VAL	N-CA-CB	5.69	117.21	110.55
1	A	1707	HIS	N-CA-C	-5.67	104.71	111.69
1	A	3900	ILE	N-CA-C	5.67	114.19	107.73
1	A	1458	ILE	N-CA-C	5.66	116.43	110.72
1	A	3897	TYR	N-CA-C	-5.64	101.69	110.10
1	B	1458	ILE	N-CA-C	5.64	117.15	111.00
1	A	3975	ASN	N-CA-C	5.61	118.76	110.46
1	A	2257	PHE	N-CA-C	5.61	117.91	107.99
1	A	2156	SER	N-CA-C	5.59	117.74	110.53
1	A	2938	MET	N-CA-C	5.59	117.91	110.53
1	B	3809	GLU	CB-CA-C	-5.58	110.13	116.54
1	A	3848	LEU	N-CA-C	5.58	118.08	111.33
1	B	2471	LEU	CA-CB-CG	5.56	135.76	116.30
1	A	1821	ASN	N-CA-CB	5.54	118.80	109.94
1	A	1	SER	CA-C-N	5.53	126.75	119.84
1	A	1	SER	C-N-CA	5.53	126.75	119.84
1	B	2101	VAL	N-CA-C	5.53	116.27	108.36
1	B	1759	LYS	N-CA-C	-5.52	101.80	110.36
1	A	2761	ALA	CB-CA-C	-5.50	110.24	116.63
1	A	1464	ASP	N-CA-CB	5.47	118.34	110.20
1	A	4063	LEU	N-CA-C	-5.44	100.31	108.96
1	B	3980	ILE	N-CA-C	5.43	120.62	108.88
1	A	1879	ILE	CA-C-N	-5.43	115.23	122.72
1	A	1879	ILE	C-N-CA	-5.43	115.23	122.72
1	A	1781	THR	N-CA-C	-5.42	105.45	111.36
1	A	2502	VAL	CA-C-N	5.40	127.36	120.56
1	A	2502	VAL	C-N-CA	5.40	127.36	120.56
1	B	1938	GLY	N-CA-C	-5.38	100.42	113.18
1	A	4015	PHE	N-CA-C	5.37	119.77	111.56
1	A	2068	GLN	N-CA-C	-5.36	106.87	113.41
1	A	2837	ASN	N-CA-C	-5.36	102.53	110.46
1	B	3402	ASP	N-CA-C	-5.35	106.43	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2025	ALA	N-CA-C	5.34	117.19	109.07
1	A	2752	VAL	CB-CA-C	-5.32	105.17	111.81
1	A	2284	LEU	N-CA-C	5.31	117.48	111.11
1	A	2412	ARG	NH1-CZ-NH2	-5.25	112.48	119.30
1	A	2916	TRP	N-CA-C	5.24	116.95	108.41
1	B	2938	MET	N-CA-C	5.23	117.27	110.53
1	A	1976	VAL	N-CA-C	-5.22	105.30	110.62
1	A	2759	ILE	N-CA-C	5.21	114.80	106.88
1	B	1793	CYS	CA-C-N	-5.16	115.83	123.05
1	B	1793	CYS	C-N-CA	-5.16	115.83	123.05
1	B	2202	THR	N-CA-C	5.16	117.77	110.50
1	B	4032	PRO	CA-C-N	5.13	128.36	120.82
1	B	4032	PRO	C-N-CA	5.13	128.36	120.82
1	A	1836	VAL	N-CA-C	-5.12	105.54	110.72
1	B	1739	ASP	N-CA-C	5.11	116.85	111.28
1	A	3298	SER	N-CA-C	5.10	116.53	111.07
1	B	1397	GLU	N-CA-C	5.10	118.17	111.28
1	A	2522	LYS	N-CA-C	5.09	115.76	108.74
1	A	3404	VAL	CB-CA-C	-5.08	105.40	110.89
1	A	2357	SER	N-CA-C	5.06	118.13	110.64
1	B	2375	ILE	N-CA-C	5.06	113.63	107.61
1	A	2027	THR	CA-C-N	5.05	126.16	119.84
1	A	2027	THR	C-N-CA	5.05	126.16	119.84
1	A	1897	THR	N-CA-CB	5.05	118.67	110.43
1	A	2392	ILE	O-C-N	5.05	124.55	121.37
1	A	2373	SER	N-CA-C	5.05	118.78	111.56
1	B	1718	CYS	N-CA-C	5.05	117.36	110.24
1	B	1504	ASN	N-CA-C	5.03	118.33	111.39
1	A	2186	ILE	N-CA-C	5.03	113.37	107.89
1	A	2941	THR	CA-C-N	5.01	126.99	120.28
1	A	2941	THR	C-N-CA	5.01	126.99	120.28
1	A	2179	PRO	N-CA-C	-5.01	106.69	113.40
1	A	1589	VAL	N-CA-C	5.00	115.30	107.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASP	Peptide
1	A	2007	GLY	Peptide
1	A	2521	ASN	Peptide
1	B	2727	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	988	0
1	B	20748	0	20206	923	0
2	A	31	0	12	10	0
2	B	31	0	12	23	0
3	A	27	0	12	2	0
3	B	27	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	2	0
5	B	10	0	0	4	0
All	All	41634	0	40460	1913	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 23.

All (1913) 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:2380:LEU:CD2	1:A:2390:ILE:HD11	1.55	1.33
1:B:1826:PHE:CE2	1:B:1831:LEU:HB2	1.66	1.29
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.55	1.24
1:B:216:PRO:O	1:B:1365:PHE:HD1	1.21	1.22
1:B:216:PRO:O	1:B:1365:PHE:CD1	1.94	1.20
1:B:3458:PHE:CE1	1:B:3459:ASP:O	1.96	1.19
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.42	1.18
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.24	1.18
1:B:1416:LYS:HA	1:B:1421:TYR:CZ	1.77	1.18
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:1826:PHE:CZ	1:B:1831:LEU:HB2	1.78	1.16
1:B:2354:SER:OG	1:B:2357:SER:HB2	1.43	1.16
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.82	1.15
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.77	1.14
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.97	1.13
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.30	1.13
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.17	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2289:GLN:OE1	1:A:2412:ARG:HG2	1.49	1.13
1:A:1926:SER:HB2	1:A:1970:LEU:HD13	1.28	1.12
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.12
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.12
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.83	1.12
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.62	1.12
1:A:2757:MET:HG2	1:A:2889:PHE:HB2	1.29	1.12
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.32	1.12
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.16	1.12
1:B:2822:ILE:HG13	1:B:2822:ILE:O	1.51	1.11
1:B:2380:LEU:HD13	1:B:2390:ILE:HD11	1.33	1.10
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.23	1.10
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.33	1.09
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.17	1.09
1:B:2380:LEU:HD22	1:B:2384:GLU:OE1	1.49	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.99	1.08
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.84	1.08
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.84	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.24	1.08
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.33	1.07
1:B:3303:LYS:O	1:B:3306:TRP:HD1	1.37	1.07
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.67	1.06
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.34	1.06
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.32	1.06
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	1.11	1.06
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	1.90	1.06
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.32	1.05
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.05
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.08	1.05
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.92	1.05
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.57	1.04
1:B:1416:LYS:HG2	1:B:1421:TYR:OH	1.57	1.04
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.45	1.04
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.05	1.04
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.58	1.03
1:A:2380:LEU:HD21	1:A:2390:ILE:CD1	1.86	1.03
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.04	1.03
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	1.92	1.03
1:A:2476:LYS:N	1:A:2476:LYS:HD2	1.69	1.03
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.89	1.02
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2060:PHE:CZ	1:A:2064:GLN:NE2	2.27	1.02
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.59	1.02
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.40	1.01
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.90	1.01
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.04	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.90	1.01
1:B:1616:LYS:HZ1	1:B:1759:LYS:HE3	1.25	1.01
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	1.76	1.01
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.43	1.01
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.91	1.01
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.42	1.00
1:B:1983:LEU:CG	1:B:1993:THR:HG23	1.90	1.00
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.76	1.00
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.39	1.00
1:A:1620:PHE:HD2	1:A:1760:PHE:CZ	1.80	1.00
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.01	0.99
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.92	0.99
1:B:1422:LYS:O	1:B:1425:GLU:HB3	1.63	0.99
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.39	0.99
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.92	0.99
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.60	0.99
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.45	0.99
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.45	0.98
1:A:2378:VAL:HG22	1:A:2380:LEU:HD13	1.43	0.98
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.92	0.98
1:B:2471:LEU:O	1:B:2473:LEU:HD13	1.63	0.98
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.93	0.98
1:A:1970:LEU:HD12	1:A:1973:LEU:HG	1.46	0.97
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.45	0.97
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.76	0.97
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.82	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	0.97	0.97
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	1.94	0.97
1:B:2470:GLY:CA	1:B:2473:LEU:HD11	1.96	0.96
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.47	0.96
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.66	0.96
1:B:2470:GLY:HA3	1:B:2473:LEU:HD11	1.47	0.96
1:B:1616:LYS:NZ	1:B:1759:LYS:HE3	1.78	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2472:THR:C	1:B:2473:LEU:HD12	1.89	0.96
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.98	0.96
1:B:3460:PRO:O	1:B:3463:SER:HB2	1.65	0.96
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.45	0.95
1:A:2064:GLN:NE2	1:A:2151:TRP:CZ3	2.35	0.95
1:A:2378:VAL:CG2	1:A:2380:LEU:HD13	1.96	0.95
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.66	0.95
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.50	0.94
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.97	0.94
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.51	0.94
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.32	0.94
1:B:2064:GLN:NE2	1:B:2070:LEU:HG	1.82	0.94
1:B:2080:LYS:HD2	1:B:2195:GLU:HB2	1.48	0.94
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.49	0.94
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.97	0.93
1:A:2378:VAL:CG2	1:A:2380:LEU:CD1	2.46	0.93
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.69	0.93
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.96	0.93
1:B:1826:PHE:HE2	1:B:1831:LEU:HB2	1.27	0.93
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.48	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.50	0.93
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.98	0.93
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.92
1:A:2060:PHE:CE2	1:A:2064:GLN:NE2	2.37	0.92
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.82	0.92
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.68	0.92
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.22	0.92
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.52	0.92
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.94	0.92
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.51	0.91
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.36	0.91
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	2.00	0.91
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.98	0.91
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	2.06	0.91
1:B:1992:LYS:CG	1:B:2024:SER:HB2	2.01	0.91
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.51	0.91
1:B:2380:LEU:CD1	1:B:2390:ILE:HD11	2.00	0.91
1:B:2386:MET:CB	1:B:2627:ARG:HD3	2.01	0.91
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.88	0.91
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.91
1:A:1983:LEU:HG	1:A:1993:THR:HG23	1.49	0.90
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.23	0.90
1:A:2757:MET:HG2	1:A:2889:PHE:CB	2.01	0.90
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.01	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.01	0.90
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.70	0.90
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.90
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.37	0.90
1:A:2380:LEU:HD21	1:A:2390:ILE:HD11	0.92	0.89
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.20	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.25	0.89
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.72	0.89
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.13	0.89
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	2.02	0.89
1:A:3458:PHE:CE1	1:A:3459:ASP:O	2.26	0.88
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.74	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.54	0.88
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.09	0.88
1:B:2563:SER:HB3	1:B:2566:SER:H	1.39	0.88
1:B:2080:LYS:HE2	1:B:2195:GLU:OE1	1.73	0.88
1:A:1425:GLU:OE2	1:A:1429:LEU:CG	2.21	0.88
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.56	0.88
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.74	0.88
1:A:2378:VAL:HG22	1:A:2380:LEU:CD1	2.03	0.88
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.74	0.88
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.09	0.87
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.87
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.89	0.87
1:A:2380:LEU:CD2	1:A:2390:ILE:CD1	2.47	0.87
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.28	0.87
1:A:1425:GLU:OE2	1:A:1429:LEU:HG	1.74	0.87
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.55	0.87
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.08	0.87
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.75	0.87
1:A:1983:LEU:CG	1:A:1993:THR:HG23	2.04	0.87
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.09	0.87
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.57	0.86
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.58	0.86
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.64	0.86
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.75	0.86
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.57	0.86
1:B:1616:LYS:HZ1	1:B:1759:LYS:CE	1.87	0.86
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.11	0.86
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.11	0.86
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.06	0.86
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.58	0.86
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.58	0.85
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.76	0.85
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.37	0.85
1:B:2472:THR:O	1:B:2473:LEU:HD12	1.76	0.85
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.59	0.85
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.58	0.85
1:A:1970:LEU:HD12	1:A:1973:LEU:CG	2.07	0.84
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.59	0.84
1:A:2631:THR:O	1:A:2635:THR:HG22	1.76	0.84
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.77	0.84
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.07	0.84
1:B:3303:LYS:HA	1:B:3306:TRP:NE1	1.91	0.84
1:A:1621:THR:HA	1:A:1624:ARG:NH1	1.92	0.84
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.07	0.84
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.59	0.84
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.07	0.83
1:B:3303:LYS:C	1:B:3306:TRP:HD1	1.86	0.83
1:B:216:PRO:C	1:B:1365:PHE:CD1	2.56	0.83
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.78	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.07	0.83
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.61	0.83
1:A:2563:SER:HB3	1:A:2566:SER:H	1.42	0.83
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.42	0.83
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.82
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.28	0.82
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.13	0.82
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.61	0.82
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.77	0.82
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.07	0.82
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.62	0.82
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.09	0.82
1:A:2757:MET:HG2	1:A:2889:PHE:CD2	2.14	0.82
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.44	0.82
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.61	0.81
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.60	0.81
1:A:1783:THR:HG22	1:A:1809:PHE:HZ	1.44	0.81
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.81
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.09	0.81
1:A:1535:PRO:C	1:A:1841:ILE:HD11	2.05	0.81
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.81
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.60	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.62	0.81
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.62	0.81
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.11	0.81
1:A:2476:LYS:N	1:A:2476:LYS:CD	2.40	0.80
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.80
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.08	0.80
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.10	0.80
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.07	0.80
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.61	0.80
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.97	0.80
1:B:2048:SER:H	2:B:5093:ATP:HN62	1.29	0.80
1:A:2745:ILE:CG2	1:A:2756:MET:HE1	2.11	0.80
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.62	0.80
1:B:1983:LEU:HG	1:B:1993:THR:CG2	2.03	0.80
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.10	0.80
1:B:216:PRO:C	1:B:1365:PHE:HA	2.06	0.79
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.30	0.79
1:B:2471:LEU:O	1:B:2473:LEU:CD1	2.31	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.97	0.79
1:B:2728:LEU:HD12	1:B:2771:ARG:HH22	1.44	0.79
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.63	0.79
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.81	0.79
1:B:2354:SER:OG	1:B:2357:SER:CB	2.28	0.79
1:A:1620:PHE:CE1	1:A:1624:ARG:HD3	2.18	0.79
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	2.13	0.79
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.82	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.78
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.62	0.78
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.31	0.78
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.64	0.78
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.78
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.23	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.71	0.78
1:B:1416:LYS:CG	1:B:1421:TYR:OH	2.31	0.78
1:B:2224:SER:O	2:B:5093:ATP:H2	1.66	0.78
1:A:1783:THR:HG22	1:A:1809:PHE:CZ	2.19	0.78
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.99	0.78
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.78
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.90	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.62	0.78
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.99	0.77
1:A:2380:LEU:HG	1:A:2384:GLU:OE1	1.84	0.77
1:B:1826:PHE:CZ	1:B:1831:LEU:CB	2.66	0.77
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.32	0.77
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.84	0.77
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.49	0.77
1:A:2289:GLN:OE1	1:A:2412:ARG:CG	2.32	0.77
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.57	0.77
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.51	0.77
1:B:3303:LYS:CA	1:B:3306:TRP:CD1	2.66	0.77
1:A:2446:SER:H	1:A:2449:THR:CG2	1.97	0.77
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.28	0.77
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.65	0.77
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.24	0.77
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.67	0.77
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.99	0.77
1:B:1826:PHE:CE2	1:B:1831:LEU:CB	2.60	0.77
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.13	0.77
1:A:3458:PHE:HE1	1:A:3462:ILE:HB	1.50	0.77
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.09	0.77
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.67	0.77
1:A:1463:LEU:HA	1:A:1466:GLN:HG2	1.66	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.58	0.76
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.67	0.76
1:B:1759:LYS:CE	1:B:1761:GLU:OE2	2.33	0.76
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	2.01	0.76
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.84	0.76
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.62	0.76
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.16	0.76
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	2.01	0.76
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.15	0.76
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.16	0.76
1:B:2745:ILE:CG2	1:B:2756:MET:HE1	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.67	0.76
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.50	0.76
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.85	0.75
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.75
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.21	0.75
1:A:2757:MET:CG	1:A:2889:PHE:HB2	2.14	0.75
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.16	0.75
1:A:1620:PHE:HE1	1:A:1624:ARG:HD3	1.50	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.86	0.75
1:B:1421:TYR:O	1:B:1421:TYR:CG	2.37	0.75
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.69	0.75
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.22	0.75
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.74	0.75
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.86	0.75
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.51	0.74
1:B:2137:VAL:O	1:B:2141:ILE:HG23	1.86	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.52	0.74
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.13	0.74
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.74
1:B:2080:LYS:NZ	2:B:5093:ATP:O3G	2.21	0.74
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.74
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.65	0.74
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.14	0.74
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.03	0.74
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.18	0.74
1:B:2425:THR:HB	3:B:5094:ADP:O1A	1.85	0.74
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.18	0.74
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.22	0.74
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.18	0.74
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.53	0.74
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.69	0.74
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.51	0.74
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.66	0.73
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.18	0.73
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.68	0.73
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.69	0.73
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.88	0.73
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.51	0.73
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.70	0.73
1:B:3458:PHE:CD1	1:B:3459:ASP:O	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.04	0.73
1:B:1616:LYS:NZ	1:B:1759:LYS:CE	2.48	0.73
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.71	0.73
1:A:2048:SER:N	2:A:5093:ATP:HN62	1.86	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.71	0.73
1:B:2413:GLY:HA3	1:B:2510:MET:HE3	1.71	0.73
1:A:2064:GLN:NE2	1:A:2151:TRP:HZ3	1.86	0.73
1:B:2080:LYS:HG2	2:B:5093:ATP:O1B	1.89	0.73
1:B:2155:ASP:OD1	1:B:2549:ARG:NH2	2.22	0.73
1:A:1983:LEU:CD2	1:A:1993:THR:HG23	2.19	0.72
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.71	0.72
1:A:1620:PHE:CD2	1:A:1760:PHE:CZ	2.72	0.72
1:A:2757:MET:HG2	1:A:2889:PHE:CG	2.24	0.72
1:A:2932:MET:HE1	1:A:2993:ILE:HG23	1.70	0.72
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.14	0.72
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.68	0.72
1:B:2631:THR:O	1:B:2635:THR:HG22	1.88	0.72
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.72	0.72
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.77	0.72
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.20	0.72
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.00	0.72
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.53	0.72
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.34	0.72
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.72
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.70	0.72
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.19	0.72
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.48	0.72
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.90	0.72
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.19	0.72
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.25	0.72
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.77	0.71
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.18	0.71
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.20	0.71
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.84	0.71
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.21	0.71
1:B:3458:PHE:CZ	1:B:3459:ASP:O	2.43	0.71
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.53	0.71
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.71	0.71
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.31	0.71
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.91	0.71
1:B:3618:TYR:N	1:B:3618:TYR:CD1	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.23	0.71
1:B:2446:SER:H	1:B:2449:THR:HG23	1.56	0.71
1:B:3919:LYS:HZ2	1:B:4038:GLU:CD	1.98	0.71
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.19	0.71
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.09	0.71
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.26	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.14	0.71
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.90	0.71
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.73	0.71
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.97	0.71
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.72	0.71
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.21	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71
1:A:3618:TYR:N	1:A:3618:TYR:HD1	1.89	0.71
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	1.90	0.71
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.05	0.71
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.91	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.72	0.71
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.72	0.70
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.55	0.70
1:B:2476:LYS:H	1:B:2476:LYS:HD2	1.56	0.70
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.53	0.70
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.20	0.70
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.73	0.70
1:B:2446:SER:H	1:B:2449:THR:CG2	2.03	0.70
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.22	0.70
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.21	0.70
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.16	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.27	0.70
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.26	0.70
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.91	0.70
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.07	0.70
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.91	0.70
1:A:1744:LEU:HA	1:A:1760:PHE:CE1	2.25	0.70
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.21	0.70
1:B:3303:LYS:CA	1:B:3306:TRP:HD1	2.05	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.21	0.70
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.72	0.70
1:B:2476:LYS:H	1:B:2476:LYS:CD	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2048:SER:H	2:A:5093:ATP:N6	1.88	0.70
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.22	0.69
1:A:7:TRP:O	1:A:9:ILE:N	2.25	0.69
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.21	0.69
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.74	0.69
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.74	0.69
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.50	0.69
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.69
1:A:2490:ASN:HB3	1:A:2546:MET:HE2	1.74	0.69
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.73	0.69
1:A:1983:LEU:CD2	1:A:1993:THR:O	2.40	0.69
1:A:2064:GLN:NE2	1:A:2151:TRP:CH2	2.61	0.69
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.92	0.69
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.28	0.69
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.92	0.69
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.20	0.69
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.75	0.69
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.74	0.69
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.41	0.69
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.93	0.69
1:A:2475:PRO:C	1:A:2476:LYS:HD2	2.18	0.68
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.93	0.68
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.09	0.68
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.93	0.68
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.73	0.68
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.76	0.68
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.93	0.68
1:B:3618:TYR:N	1:B:3618:TYR:HD1	1.91	0.68
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.73	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:B:1759:LYS:HE2	1:B:1761:GLU:OE2	1.92	0.68
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	2.08	0.68
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.28	0.68
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.29	0.68
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.74	0.68
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.76	0.68
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.24	0.68
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.51	0.68
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1826:PHE:HE2	1:B:1831:LEU:CB	2.04	0.68
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.57	0.68
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.12	0.68
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.59	0.68
1:A:2276:LEU:HD23	1:A:2556:ILE:HD13	1.76	0.68
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.59	0.68
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.75	0.67
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.24	0.67
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.57	0.67
1:B:3683:TYR:O	1:B:3687:SER:HB2	1.95	0.67
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.08	0.67
1:A:2391:VAL:HG22	1:A:2430:ASN:OD1	1.95	0.67
1:A:2762:SER:O	1:A:2763:ARG:HB2	1.95	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.24	0.67
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.76	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:A:1620:PHE:HD1	1:A:1624:ARG:NH1	1.93	0.67
1:B:2467:THR:HB	1:B:2473:LEU:HD22	1.77	0.67
1:A:2463:ASN:HB2	1:A:2477:SER:HA	1.77	0.67
1:B:2081:THR:HB	2:B:5093:ATP:O1A	1.93	0.67
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	1.77	0.67
1:B:2428:MET:HE2	1:B:2432:LEU:HD12	1.77	0.67
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.30	0.67
1:B:2224:SER:O	2:B:5093:ATP:C2	2.47	0.67
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.25	0.67
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.94	0.67
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.77	0.67
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.76	0.67
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.95	0.66
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.29	0.66
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.77	0.66
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.66
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.66
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.28	0.66
1:B:2517:LYS:HE3	1:B:2519:PRO:HD2	1.76	0.66
1:B:2552:ARG:NH2	2:B:5093:ATP:O2G	2.28	0.66
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.83	0.66
1:A:3460:PRO:O	1:A:3463:SER:CB	2.40	0.66
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.43	0.66
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.73	0.66
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.78	0.66
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.96	0.66
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.78	0.66
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.77	0.66
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.20	0.66
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.77	0.66
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.95	0.66
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.25	0.66
1:A:1983:LEU:HD23	1:A:1993:THR:O	1.96	0.66
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.61	0.65
1:A:1823:ASP:HB3	1:A:1852:ARG:O	1.95	0.65
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.60	0.65
1:A:2064:GLN:CD	1:A:2151:TRP:CH2	2.74	0.65
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.31	0.65
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.79	0.65
1:B:2076:ALA:HA	2:B:5093:ATP:O1G	1.96	0.65
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.96	0.65
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.44	0.65
1:A:1983:LEU:HD23	1:A:1993:THR:CG2	2.26	0.65
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.30	0.65
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.25	0.65
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.77	0.65
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.96	0.65
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.77	0.65
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.37	0.65
1:A:2394:THR:H	1:A:2397:THR:HB	1.62	0.65
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.79	0.65
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.97	0.65
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.97	0.65
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.68	0.65
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.61	0.65
1:B:1983:LEU:HD21	1:B:1993:THR:O	1.94	0.65
1:A:1783:THR:CG2	1:A:1809:PHE:CZ	2.80	0.64
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.27	0.64
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.97	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.97	0.64
1:A:113:ASP:O	1:A:115:GLU:N	2.31	0.64
1:B:1826:PHE:HZ	1:B:1831:LEU:HB2	1.53	0.64
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.62	0.64
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.31	0.64
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.62	0.64
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.97	0.64
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.80	0.64
1:A:1425:GLU:OE2	1:A:1429:LEU:CD1	2.45	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.33	0.64
1:A:2428:MET:HE2	1:A:2432:LEU:HD12	1.79	0.64
1:A:2134:LEU:CD1	1:A:2138:ASN:ND2	2.60	0.64
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.79	0.64
1:B:2574:TYR:HE2	3:B:5094:ADP:C2	2.16	0.64
1:A:2336:ARG:HD2	1:A:2355:ASP:OD2	1.97	0.64
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.13	0.64
1:B:2765:GLY:HA2	5:B:5096:SO4:O2	1.98	0.64
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.28	0.64
1:B:2080:LYS:CD	1:B:2195:GLU:HB2	2.25	0.64
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.97	0.64
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.13	0.64
1:B:1493:LEU:O	1:B:1494:ASP:HB2	1.96	0.64
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.80	0.64
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.79	0.64
1:B:1852:ARG:O	1:B:1852:ARG:HG3	1.98	0.63
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.79	0.63
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.13	0.63
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.80	0.63
1:B:1991:GLU:O	1:B:1995:VAL:HG23	1.98	0.63
1:B:2064:GLN:OE1	1:B:2191:ARG:HD2	1.98	0.63
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.26	0.63
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.97	0.63
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.80	0.63
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.14	0.63
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.98	0.63
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.33	0.63
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.63	0.63
1:B:3460:PRO:O	1:B:3463:SER:CB	2.44	0.63
1:A:2426:MET:HG3	1:A:2427:ILE:N	2.11	0.63
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.63
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.64	0.63
1:A:2757:MET:CG	1:A:2889:PHE:CD2	2.80	0.63
1:A:3810:SER:O	1:A:3838:TRP:HB2	1.97	0.63
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.13	0.63
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.13	0.63
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.32	0.63
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.81	0.63
1:A:2054:LEU:O	1:A:2058:MET:HG2	1.99	0.62
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.99	0.62
1:B:3810:SER:O	1:B:3838:TRP:HB2	1.97	0.62
1:A:2620:ARG:NH1	1:A:2910:ASN:ND2	2.47	0.62
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.29	0.62
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.14	0.62
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.80	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.82	0.62
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.82	0.62
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.00	0.62
1:B:2426:MET:HG3	1:B:2427:ILE:H	1.64	0.62
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.79	0.62
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.81	0.62
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.98	0.62
1:A:2840:ILE:HB	1:A:2843:LEU:HD22	1.81	0.62
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.81	0.62
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.99	0.62
1:A:2163:VAL:HA	1:A:2166:MET:HG2	1.82	0.62
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.81	0.62
1:B:162:LEU:HA	1:B:165:ASP:O	1.98	0.62
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.58	0.62
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.82	0.62
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.00	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.53	0.62
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.25	0.62
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.15	0.62
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.30	0.62
1:A:2940:PHE:HZ	1:A:2943:PHE:HE2	1.48	0.62
1:A:1646:GLN:NE2	1:A:1761:GLU:O	2.24	0.61
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.81	0.61
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.65	0.61
1:B:3819:ILE:O	1:B:3823:ASN:HB2	2.01	0.61
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.64	0.61
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.81	0.61
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.35	0.61
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2276:LEU:HD23	1:B:2556:ILE:HG21	1.83	0.61
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.00	0.61
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.78	0.61
1:A:2640:THR:HG23	1:A:2643:SER:H	1.66	0.61
1:A:2745:ILE:HG12	1:A:2756:MET:HE1	1.82	0.61
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.29	0.61
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.83	0.61
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.40	0.61
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.15	0.61
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.61
1:B:2391:VAL:HG23	1:B:2426:MET:HE1	1.83	0.61
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.61
1:A:1802:LYS:NZ	5:A:5097:SO4:O2	2.34	0.61
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	1.81	0.61
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.31	0.61
1:B:2048:SER:H	2:B:5093:ATP:N6	1.97	0.61
1:B:2980:MET:HE3	1:B:3337:LEU:HD13	1.82	0.61
1:A:2064:GLN:CD	1:A:2151:TRP:HH2	2.08	0.61
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.64	0.61
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.26	0.61
1:A:1563:LYS:HD2	1:A:1570:GLU:HG3	1.82	0.61
1:A:1783:THR:CG2	1:A:1809:PHE:CE1	2.83	0.61
1:A:2032:LYS:O	1:A:2035:VAL:HG12	2.00	0.61
1:A:2421:GLY:HA2	3:A:5094:ADP:O5'	2.00	0.61
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.31	0.61
1:A:3737:THR:HB	1:A:3740:THR:CB	2.31	0.61
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.30	0.61
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.34	0.61
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.36	0.61
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.82	0.61
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.82	0.61
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.61
1:B:3303:LYS:HA	1:B:3306:TRP:HE1	1.62	0.61
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.82	0.61
1:B:2380:LEU:CD2	1:B:2384:GLU:OE1	2.37	0.61
1:B:2481:ASN:HD21	1:B:2528:ARG:HD3	1.64	0.61
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.82	0.60
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.83	0.60
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.60
1:B:2426:MET:HG3	1:B:2427:ILE:N	2.15	0.60
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.01	0.60
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.20	0.60
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.82	0.60
1:A:1646:GLN:CD	1:A:1763:ILE:HG12	2.27	0.60
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.01	0.60
1:A:2563:SER:CB	1:A:2566:SER:OG	2.49	0.60
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.83	0.60
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.27	0.60
1:B:2064:GLN:HE22	1:B:2070:LEU:HG	1.61	0.60
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.66	0.60
1:A:3631:MET:HE1	1:A:3698:MET:HG3	1.82	0.60
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.37	0.60
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.16	0.60
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.83	0.60
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.84	0.60
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.01	0.60
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.84	0.60
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.02	0.60
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.00	0.60
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.84	0.60
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.83	0.60
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.83	0.60
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.83	0.60
1:B:1416:LYS:CB	1:B:1421:TYR:OH	2.50	0.60
1:B:3737:THR:OG1	1:B:3740:THR:HB	2.01	0.60
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.01	0.59
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.10	0.59
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.37	0.59
1:A:3569:GLU:O	1:A:3573:SER:OG	2.20	0.59
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.59
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.17	0.59
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.67	0.59
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.83	0.59
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.84	0.59
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.32	0.59
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.32	0.59
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.90	0.59
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.83	0.59
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.59
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.38	0.59
1:B:2394:THR:H	1:B:2397:THR:HB	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:PHE:CD1	1:A:1624:ARG:NH1	2.70	0.59
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.68	0.59
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.67	0.59
1:A:3818:SER:O	1:A:3821:ASN:N	2.35	0.59
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.21	0.59
1:B:2470:GLY:C	1:B:2473:LEU:HD11	2.27	0.59
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.67	0.59
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.59
1:B:1616:LYS:NZ	1:B:1759:LYS:NZ	2.49	0.59
1:B:2072:LEU:HD23	1:B:2215:PHE:CE1	2.37	0.59
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.67	0.59
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.59
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	2.90	0.59
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.37	0.59
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.85	0.59
1:A:2620:ARG:HH12	1:A:2910:ASN:ND2	1.99	0.59
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.32	0.59
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.59
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.68	0.59
1:A:2475:PRO:O	1:A:2476:LYS:C	2.46	0.59
1:B:1422:LYS:HA	1:B:1425:GLU:HB2	1.85	0.59
1:B:2386:MET:HB3	1:B:2627:ARG:NE	2.18	0.59
1:B:1416:LYS:HA	1:B:1421:TYR:OH	2.01	0.59
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.03	0.58
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.68	0.58
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.38	0.58
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.84	0.58
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.03	0.58
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.37	0.58
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.83	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.03	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.86	0.58
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.52	0.58
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.04	0.58
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.38	0.58
1:A:1983:LEU:HD23	1:A:1993:THR:HG23	1.84	0.58
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.86	0.58
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.39	0.58
1:A:3458:PHE:CZ	1:A:3459:ASP:O	2.57	0.58
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.34	0.58
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.85	0.58
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.84	0.58
1:A:162:LEU:HA	1:A:165:ASP:O	2.03	0.58
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.69	0.58
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.85	0.58
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.83	0.58
1:B:23:LEU:O	1:B:24:GLU:CB	2.52	0.58
1:B:1421:TYR:CD1	1:B:1421:TYR:C	2.82	0.58
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.84	0.58
1:A:3636:GLY:HA2	1:A:3642:TYR:O	2.04	0.58
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.32	0.58
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.69	0.58
1:B:2160:PRO:O	1:B:2164:GLU:HG3	2.04	0.58
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.85	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.44	0.57
1:B:2932:MET:HE1	1:B:2993:ILE:HG23	1.85	0.57
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.33	0.57
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.85	0.57
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.84	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.84	0.57
1:B:2080:LYS:CG	2:B:5093:ATP:O1B	2.51	0.57
1:A:2047:PHE:HB3	2:A:5093:ATP:N6	2.19	0.57
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.82	0.57
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.86	0.57
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.86	0.57
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.69	0.57
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.86	0.57
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.87	0.57
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.86	0.57
1:A:2737:SER:HB2	1:A:2924:THR:HG21	1.87	0.57
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.86	0.57
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.92	0.57
1:A:3945:LEU:O	1:A:3948:HIS:O	2.23	0.57
1:B:1421:TYR:O	1:B:1421:TYR:CD1	2.58	0.57
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.39	0.57
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.85	0.57
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1779:PHE:O	1:A:1783:THR:HG23	2.04	0.57
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.17	0.57
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.13	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.35	0.57
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.86	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57
1:A:2368:PHE:O	1:A:2369:SER:OG	2.16	0.57
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.23	0.57
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.16	0.57
1:B:3303:LYS:C	1:B:3306:TRP:CD1	2.74	0.57
1:A:1794:PHE:CZ	1:A:1805:THR:HG21	2.39	0.57
1:B:1416:LYS:HA	1:B:1421:TYR:CE1	2.34	0.57
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.85	0.57
1:B:2072:LEU:HD23	1:B:2215:PHE:HE1	1.68	0.57
1:B:3737:THR:HB	1:B:3740:THR:CB	2.34	0.57
1:A:1621:THR:CA	1:A:1624:ARG:NH1	2.66	0.57
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.88	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.86	0.57
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.38	0.57
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.85	0.57
1:B:1616:LYS:HZ2	1:B:1759:LYS:HE3	1.69	0.56
1:A:65:THR:O	1:A:66:GLN:CB	2.53	0.56
1:A:2060:PHE:HZ	1:A:2064:GLN:NE2	1.99	0.56
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.86	0.56
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.06	0.56
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.39	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.86	0.56
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.86	0.56
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.14	0.56
1:A:3559:LEU:O	1:A:3563:GLU:HG3	2.06	0.56
1:B:1655:MET:HE3	1:B:1659:LEU:HD12	1.86	0.56
1:B:2060:PHE:CZ	1:B:2064:GLN:NE2	2.73	0.56
1:B:2320:ARG:NH1	1:B:2406:ASP:OD2	2.33	0.56
1:A:1459:LEU:HD22	1:A:1473:THR:CG2	2.35	0.56
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.35	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.34	0.56
1:B:3690:LEU:HD23	1:B:3694:PHE:HB3	1.88	0.56
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.86	0.56
1:A:1463:LEU:HA	1:A:1466:GLN:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:PHE:HZ	1:A:1805:THR:HG21	1.71	0.56
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.19	0.56
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.45	0.56
1:A:3636:GLY:CA	1:A:3642:TYR:O	2.53	0.56
1:B:1416:LYS:CA	1:B:1421:TYR:CZ	2.71	0.56
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.05	0.56
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.05	0.56
1:B:2452:GLU:HA	1:B:2455:LEU:HD12	1.86	0.56
1:A:2389:ASP:HB3	1:A:2433:ARG:NH1	2.20	0.56
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.70	0.56
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.87	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.88	0.56
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.87	0.56
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.36	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.48	0.56
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.86	0.56
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.06	0.56
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.56
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.71	0.56
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.77	0.56
1:B:1802:LYS:NZ	5:B:5097:SO4:O3	2.39	0.56
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.14	0.56
1:A:3481:ILE:O	1:A:3483:ASP:N	2.38	0.56
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.36	0.56
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.87	0.56
1:A:1744:LEU:HA	1:A:1760:PHE:CD1	2.41	0.55
1:A:3303:LYS:CD	1:A:3306:TRP:CD1	2.80	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.86	0.55
1:B:1416:LYS:HG2	1:B:1421:TYR:CZ	2.40	0.55
1:B:3322:GLY:HA2	1:B:3325:ILE:HD12	1.88	0.55
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.42	0.55
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.88	0.55
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.55
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.88	0.55
1:B:2391:VAL:CG2	1:B:2426:MET:CE	2.84	0.55
1:A:1559:SER:HB2	1:A:1572:ILE:H	1.71	0.55
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.41	0.55
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.07	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.88	0.55
1:A:2757:MET:CE	1:A:2908:LEU:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.72	0.55
1:B:1983:LEU:CG	1:B:1993:THR:CG2	2.75	0.55
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.42	0.55
1:B:2391:VAL:HG23	1:B:2426:MET:CE	2.36	0.55
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.06	0.55
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.36	0.55
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	1.88	0.55
1:B:1396:ARG:HG3	1:B:1397:GLU:H	1.71	0.55
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.41	0.55
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.32	0.55
1:A:1851:ASN:ND2	1:A:1899:ASN:O	2.39	0.55
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.35	0.55
1:A:2163:VAL:HA	1:A:2166:MET:CG	2.36	0.55
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.21	0.55
1:B:2481:ASN:ND2	1:B:2528:ARG:HD3	2.22	0.55
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.55
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.72	0.55
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.69	0.55
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.54	0.55
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.71	0.55
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.37	0.55
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.55
1:B:1826:PHE:HZ	1:B:1831:LEU:CB	2.15	0.55
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.32	0.55
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.06	0.55
1:B:2380:LEU:HD13	1:B:2390:ILE:CD1	2.21	0.55
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.90	0.55
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.72	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:B:2428:MET:SD	1:B:2428:MET:C	2.90	0.55
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.32	0.55
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.07	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.96	0.54
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.36	0.54
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.87	0.54
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.89	0.54
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.89	0.54
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.37	0.54
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.89	0.54
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.71	0.54
1:B:3461:ILE:C	1:B:3463:SER:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2081:THR:OG1	1:A:2195:GLU:OE2	2.26	0.54
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.40	0.54
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.89	0.54
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.06	0.54
1:B:3010:LEU:HD21	1:B:3317:SER:HB3	1.90	0.54
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.08	0.54
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.05	0.54
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.91	0.54
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.85	0.54
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.07	0.54
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.87	0.54
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.42	0.54
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.61	0.54
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.88	0.54
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.38	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.87	0.54
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.90	0.54
1:B:1416:LYS:HA	1:B:1421:TYR:CE2	2.36	0.54
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.73	0.54
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.15	0.54
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	1.90	0.54
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.54
1:A:1425:GLU:OE2	1:A:1429:LEU:CD2	2.56	0.54
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.72	0.54
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.89	0.54
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.73	0.54
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.08	0.54
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.90	0.54
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.72	0.54
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.08	0.54
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.08	0.54
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.90	0.54
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.25	0.54
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.90	0.54
1:A:2513:GLN:O	1:A:2526:ILE:HG13	2.09	0.53
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.37	0.53
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.90	0.53
1:A:1743:ASP:HA	1:A:1746:SER:HB3	1.90	0.53
1:A:1823:ASP:CG	1:A:1823:ASP:O	2.51	0.53
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.73	0.53
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.43	0.53
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.89	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.41	0.53
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.56	0.53
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.73	0.53
1:A:2451:THR:O	1:A:2455:LEU:HD12	2.08	0.53
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.91	0.53
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.91	0.53
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.38	0.53
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.08	0.53
1:B:2428:MET:HE1	1:B:2440:VAL:HG13	1.91	0.53
1:A:1783:THR:HG23	1:A:1809:PHE:CE1	2.44	0.53
1:A:2563:SER:C	1:A:2565:LYS:H	2.17	0.53
1:B:1616:LYS:HZ1	1:B:1759:LYS:NZ	2.07	0.53
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.53
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.08	0.53
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.71	0.53
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.89	0.53
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.90	0.53
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.57	0.53
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.22	0.53
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.44	0.53
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.53
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.23	0.53
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.60	0.53
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.91	0.53
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.49	0.53
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.74	0.53
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.90	0.53
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.44	0.53
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.26	0.53
1:A:1367:ILE:H	1:A:1367:ILE:HD12	1.73	0.53
1:A:1620:PHE:CE2	1:A:1743:ASP:HB3	2.43	0.53
1:A:1970:LEU:HD12	1:A:1973:LEU:CD1	2.38	0.53
1:A:2413:GLY:HA3	1:A:2510:MET:HE3	1.90	0.53
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.74	0.53
1:B:1396:ARG:HG3	1:B:1397:GLU:N	2.24	0.53
1:B:1423:ILE:C	1:B:1425:GLU:N	2.66	0.53
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.91	0.53
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.90	0.53
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.43	0.53
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.91	0.52
1:A:2060:PHE:HZ	1:A:2064:GLN:HE21	1.51	0.52
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.55	0.52
1:A:2967:ASN:HB3	1:A:3356:PHE:CE2	2.44	0.52
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.74	0.52
1:A:2463:ASN:CB	1:A:2477:SER:HA	2.39	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.75	0.52
1:B:2391:VAL:CG2	1:B:2426:MET:HE3	2.39	0.52
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.56	0.52
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.90	0.52
1:A:2421:GLY:N	3:A:5094:ADP:O2B	2.35	0.52
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.08	0.52
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.45	0.52
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.09	0.52
1:B:2276:LEU:HD21	1:B:2415:ILE:HG21	1.91	0.52
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.37	0.52
1:A:2441:VAL:HG21	1:A:2482:LEU:HD21	1.91	0.52
1:B:1422:LYS:O	1:B:1425:GLU:CB	2.48	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.90	0.52
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.75	0.52
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.35	0.52
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.73	0.52
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.98	0.52
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.52
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.25	0.52
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.90	0.52
1:B:1635:ASP:HB2	1:B:1638:VAL:HG23	1.91	0.52
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.52
1:B:2428:MET:HE1	1:B:2440:VAL:CG1	2.39	0.52
1:B:3736:LEU:HD11	1:B:3745:ARG:HG3	1.92	0.52
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.33	0.52
1:A:2476:LYS:HD2	1:A:2476:LYS:H	1.64	0.52
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.91	0.52
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.40	0.52
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.92	0.52
1:B:3461:ILE:C	1:B:3463:SER:N	2.67	0.52
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2448:ASP:O	1:A:2829:GLU:OE2	2.27	0.52
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	1.92	0.52
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.57	0.52
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.39	0.52
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.92	0.52
1:B:2476:LYS:HZ2	1:B:2528:ARG:HD2	1.72	0.52
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.10	0.52
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.32	0.52
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.68	0.52
1:B:1448:VAL:HG22	1:B:1513:ILE:HB	1.92	0.52
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.92	0.52
1:B:2640:THR:HG23	1:B:2643:SER:H	1.75	0.52
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.10	0.52
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.24	0.52
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.83	0.52
1:B:1970:LEU:HD23	1:B:1974:LYS:HE3	1.92	0.52
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.92	0.52
1:B:2745:ILE:HG12	1:B:2756:MET:HE1	1.92	0.52
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.91	0.51
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.39	0.51
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.58	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.87	0.51
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.91	0.51
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.91	0.51
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.10	0.51
1:A:1995:VAL:CG1	1:A:2018:LEU:HD21	2.40	0.51
1:B:216:PRO:C	1:B:1365:PHE:CA	2.82	0.51
1:B:1771:TYR:HA	1:B:1775:LEU:HD13	1.92	0.51
1:B:2228:HIS:HB3	2:B:5093:ATP:C2	2.44	0.51
1:A:1983:LEU:HD23	1:A:1993:THR:HG22	1.92	0.51
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.41	0.51
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.45	0.51
1:A:3737:THR:CB	1:A:3740:THR:HB	2.40	0.51
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.76	0.51
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.92	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51
1:B:2792:LEU:HD13	1:B:2826:ALA:HB3	1.92	0.51
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.40	0.51
1:A:1771:TYR:HA	1:A:1775:LEU:HD13	1.92	0.51
1:A:3458:PHE:CD1	1:A:3459:ASP:O	2.63	0.51
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2225:LYS:HA	2:B:5093:ATP:H2	1.71	0.51
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.40	0.51
1:A:2494:LEU:O	1:A:2495:ASP:O	2.29	0.51
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.74	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.39	0.51
1:B:2276:LEU:HD23	1:B:2556:ILE:CG2	2.41	0.51
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.39	0.51
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.75	0.51
1:A:2055:LYS:HE3	1:A:2056:LYS:HE2	1.93	0.51
1:A:2965:VAL:HG13	1:A:3325:ILE:HD11	1.92	0.51
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.22	0.51
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.11	0.51
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.40	0.51
1:A:3818:SER:O	1:A:3819:ILE:C	2.54	0.51
1:B:203:GLN:O	1:B:204:GLY:C	2.54	0.51
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.51
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.92	0.51
1:B:1422:LYS:C	1:B:1425:GLU:HB3	2.33	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:B:2064:GLN:NE2	1:B:2070:LEU:CG	2.67	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:A:1744:LEU:HD22	1:A:1760:PHE:CD1	2.45	0.51
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.63	0.51
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.76	0.51
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.51
1:A:2378:VAL:HG21	1:A:2380:LEU:HD13	1.89	0.51
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.11	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.58	0.51
1:B:1826:PHE:HZ	1:B:1831:LEU:CA	2.24	0.51
1:B:2391:VAL:HG21	1:B:2426:MET:HE3	1.91	0.51
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.91	0.50
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.93	0.50
1:A:2425:THR:HG22	1:A:2485:PHE:HE2	1.77	0.50
1:A:2446:SER:H	1:A:2449:THR:HG21	1.76	0.50
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.24	0.50
1:B:3530:PHE:CE1	1:B:3618:TYR:HD2	2.26	0.50
1:A:2762:SER:O	1:A:2763:ARG:CB	2.60	0.50
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.11	0.50
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.11	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50
1:B:2378:VAL:HG22	1:B:2380:LEU:HG	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2517:LYS:HG2	1:B:2520:GLU:HB2	1.93	0.50
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.41	0.50
1:A:23:LEU:O	1:A:24:GLU:C	2.50	0.50
1:A:1425:GLU:OE2	1:A:1429:LEU:HD21	2.12	0.50
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.94	0.50
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.84	0.50
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.41	0.50
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.76	0.50
1:B:2563:SER:C	1:B:2565:LYS:H	2.19	0.50
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.11	0.50
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.77	0.50
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.42	0.50
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.94	0.50
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.93	0.50
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	1.93	0.50
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.85	0.50
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.50
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.76	0.50
1:A:1645:PHE:HB3	1:A:1765:ILE:HG21	1.90	0.50
1:A:2380:LEU:HD23	1:A:2384:GLU:HB3	1.94	0.50
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.76	0.50
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.42	0.50
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.76	0.50
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.60	0.50
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.94	0.50
1:A:2755:HIS:CE1	1:A:2835:LEU:HG	2.47	0.50
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.45	0.50
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.68	0.50
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.76	0.50
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.93	0.50
1:A:1969:GLY:O	1:A:1972:THR:HB	2.11	0.50
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.47	0.50
1:A:2228:HIS:HB3	2:A:5093:ATP:C2	2.47	0.50
1:A:4023:ILE:HD11	1:A:4029:ILE:HD12	1.93	0.50
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.60	0.50
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.90	0.50
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.45	0.50
1:A:3628:ILE:HG22	1:A:3649:PHE:CE2	2.47	0.50
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.93	0.50
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.99	0.50
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.94	0.50
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.70	0.50
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.93	0.50
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.37	0.50
1:A:2727:GLU:O	1:A:2728:LEU:C	2.55	0.49
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.94	0.49
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.94	0.49
1:B:2786:ILE:HG12	1:B:2821:ASN:HA	1.94	0.49
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.94	0.49
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.75	0.49
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	1.94	0.49
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.94	0.49
1:A:3818:SER:O	1:A:3820:GLU:N	2.45	0.49
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.60	0.49
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.52	0.49
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.94	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:1929:ILE:H	1:B:1929:ILE:HD12	1.77	0.49
1:B:2467:THR:CB	1:B:2473:LEU:HD22	2.40	0.49
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.11	0.49
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.76	0.49
1:B:2476:LYS:CD	1:B:2476:LYS:N	2.74	0.49
1:B:2822:ILE:O	1:B:2822:ILE:CG1	2.38	0.49
1:A:23:LEU:O	1:A:25:GLU:N	2.45	0.49
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.53	0.49
1:A:2428:MET:HE1	1:A:2440:VAL:CG1	2.42	0.49
1:A:3304:GLU:C	1:A:3306:TRP:H	2.21	0.49
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.26	0.49
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.95	0.49
1:B:2181:GLY:O	1:B:2182:GLU:HG3	2.12	0.49
1:B:2574:TYR:CE2	3:B:5094:ADP:C2	2.98	0.49
1:B:3737:THR:CB	1:B:3740:THR:CB	2.90	0.49
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.78	0.49
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.93	0.49
1:A:1448:VAL:HG22	1:A:1513:ILE:HB	1.95	0.49
1:A:2476:LYS:O	1:A:2476:LYS:HD3	2.11	0.49
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.13	0.49
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.12	0.49
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.46	0.49
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.48	0.49
1:B:2080:LYS:CE	2:B:5093:ATP:O3G	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.93	0.49
1:B:3579:GLU:O	1:B:3582:GLU:N	2.44	0.49
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.77	0.49
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.48	0.49
3:B:5094:ADP:H2'	3:B:5094:ADP:N3	2.27	0.49
1:A:1459:LEU:HD22	1:A:1473:THR:HG22	1.95	0.49
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	1.94	0.49
1:A:2428:MET:HE1	1:A:2440:VAL:HG11	1.95	0.49
1:A:2757:MET:HE1	1:A:2908:LEU:HB3	1.95	0.49
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.94	0.49
2:B:5093:ATP:O3G	2:B:5093:ATP:O1B	2.30	0.49
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.48	0.49
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.13	0.49
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.49
1:B:1422:LYS:CA	1:B:1425:GLU:HB2	2.43	0.49
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.94	0.49
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.48	0.49
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.42	0.49
1:B:2495:ASP:O	1:B:2498:GLY:N	2.46	0.49
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.42	0.49
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.39	0.49
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.95	0.48
1:A:2134:LEU:HD12	1:A:2138:ASN:ND2	2.28	0.48
1:A:2920:TRP:CG	1:A:2989:PRO:HG3	2.47	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.94	0.48
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.48	0.48
1:A:4022:GLN:HA	1:A:4027:VAL:O	2.12	0.48
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.36	0.48
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.13	0.48
1:A:1466:GLN:HB2	1:A:1473:THR:HG21	1.95	0.48
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.94	0.48
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.78	0.48
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.60	0.48
1:B:2080:LYS:HE2	2:B:5093:ATP:O3G	2.13	0.48
1:B:2476:LYS:HE3	1:B:2528:ARG:HB3	1.95	0.48
1:B:2763:ARG:HA	5:B:5096:SO4:O3	2.13	0.48
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.29	0.48
1:A:2154:PHE:N	1:A:2154:PHE:HD1	2.10	0.48
1:A:2475:PRO:O	1:A:2476:LYS:O	2.30	0.48
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.81	0.48
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.96	0.48
1:B:2467:THR:HG22	1:B:2468:SER:N	2.29	0.48
1:B:3618:TYR:O	1:B:3622:GLY:N	2.42	0.48
1:B:3737:THR:CB	1:B:3740:THR:HB	2.44	0.48
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.95	0.48
1:A:2428:MET:SD	1:A:2428:MET:C	2.96	0.48
1:A:2904:SER:O	1:A:2905:SER:C	2.56	0.48
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.14	0.48
1:A:3618:TYR:O	1:A:3622:GLY:N	2.38	0.48
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.71	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.42	0.48
1:A:2942:ASP:HB3	1:A:3357:ALA:HB1	1.95	0.48
1:A:3462:ILE:HD13	1:A:3462:ILE:N	2.28	0.48
1:B:65:THR:O	1:B:66:GLN:CB	2.61	0.48
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.79	0.48
1:B:2467:THR:HB	1:B:2473:LEU:CD2	2.42	0.48
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.13	0.48
1:A:2154:PHE:N	1:A:2154:PHE:CD1	2.79	0.48
1:A:2494:LEU:HD12	1:A:2494:LEU:O	2.14	0.48
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.48	0.48
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.44	0.48
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.43	0.48
1:B:2935:VAL:C	1:B:2937:PRO:HD3	2.39	0.48
1:B:4074:GLU:HA	1:B:4077:GLN:HE21	1.79	0.48
1:A:1620:PHE:HD2	1:A:1760:PHE:HZ	1.49	0.48
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.14	0.48
1:B:1422:LYS:C	1:B:1425:GLU:CB	2.87	0.48
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	1.96	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.48
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.40	0.48
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.13	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:3934:TRP:CG	1:A:4023:ILE:HD12	2.49	0.48
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.96	0.48
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.48	0.48
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	1.96	0.48
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.14	0.48
1:A:2426:MET:HG3	1:A:2427:ILE:H	1.79	0.48
1:A:3307:LEU:O	1:A:3311:LYS:HB3	2.14	0.48
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3628:ILE:HD11	1:B:3679:TYR:CZ	2.49	0.48
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.79	0.48
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.38	0.48
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.94	0.47
1:A:2473:LEU:HD23	1:A:2525:THR:HB	1.96	0.47
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.14	0.47
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.49	0.47
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.79	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.96	0.47
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.96	0.47
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.16	0.47
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.44	0.47
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.79	0.47
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.29	0.47
1:A:2134:LEU:HD11	1:A:2138:ASN:HD21	1.79	0.47
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.14	0.47
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.71	0.47
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.30	0.47
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.14	0.47
1:A:2441:VAL:CG2	1:A:2482:LEU:HD21	2.43	0.47
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.62	0.47
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	1.95	0.47
1:B:2060:PHE:CE1	1:B:2064:GLN:NE2	2.81	0.47
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.47
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	1.96	0.47
1:A:2378:VAL:CG1	1:A:2392:ILE:HD12	2.44	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.29	0.47
1:A:1646:GLN:OE1	1:A:1763:ILE:N	2.42	0.47
1:A:2354:SER:H	1:A:2357:SER:HB2	1.80	0.47
1:A:2745:ILE:CG1	1:A:2756:MET:HE1	2.45	0.47
1:A:2760:GLY:HA2	1:A:2917:MET:HB2	1.96	0.47
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	1.97	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.96	0.47
1:B:1421:TYR:C	1:B:1425:GLU:HB2	2.31	0.47
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.98	0.47
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.14	0.47
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.83	0.47
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.47
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.96	0.47
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.95	0.47
1:B:3687:SER:HA	1:B:3698:MET:HE1	1.96	0.47
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	1.97	0.47
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	1.96	0.47
1:A:2967:ASN:HB3	1:A:3356:PHE:CZ	2.49	0.47
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.39	0.47
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.45	0.47
1:B:2470:GLY:O	1:B:2471:LEU:HB2	2.15	0.47
1:B:2473:LEU:HD12	1:B:2473:LEU:N	2.28	0.47
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.96	0.47
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.66	0.47
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.44	0.47
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.78	0.47
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.50	0.47
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	1.96	0.47
1:B:3367:ILE:O	1:B:3371:VAL:HG22	2.15	0.47
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.97	0.47
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.50	0.47
1:A:1802:LYS:NZ	5:A:5097:SO4:S	2.88	0.47
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.39	0.47
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.47
1:A:2797:MET:HE2	1:A:2797:MET:HB3	1.82	0.47
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	1.97	0.47
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.51	0.47
1:B:2446:SER:H	1:B:2449:THR:HG21	1.79	0.47
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.63	0.47
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.44	0.46
1:B:2920:TRP:CG	1:B:2989:PRO:HG3	2.50	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.97	0.46
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.97	0.46
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.17	0.46
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.46	0.46
1:A:3927:TYR:HE1	1:A:4029:ILE:HG22	1.80	0.46
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	1.96	0.46
1:B:2421:GLY:N	3:B:5094:ADP:O2B	2.39	0.46
1:B:2709:LYS:O	1:B:2713:VAL:HG23	2.15	0.46
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.15	0.46
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.50	0.46
1:A:2153:VAL:C	1:A:2154:PHE:HD1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2507:ARG:HG3	1:A:2550:PHE:HA	1.97	0.46
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.46
1:B:1714:GLN:HB3	1:B:1727:LEU:HD11	1.98	0.46
1:B:1826:PHE:CE1	1:B:1830:VAL:HG13	2.51	0.46
1:B:1938:GLY:O	1:B:1989:GLU:HB3	2.15	0.46
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.96	0.46
1:B:2391:VAL:CG2	1:B:2426:MET:HE1	2.44	0.46
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.97	0.46
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.15	0.46
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.15	0.46
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	1.98	0.46
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.42	0.46
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.46
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.97	0.46
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.46
1:B:2620:ARG:HH11	1:B:2910:ASN:ND2	2.13	0.46
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.96	0.46
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.44	0.46
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.97	0.46
1:A:3431:PHE:CZ	1:A:3458:PHE:HD1	2.33	0.46
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.16	0.46
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.78	0.46
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.62	0.46
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.51	0.46
1:A:2905:SER:HA	1:A:2906:PRO:HD2	1.70	0.46
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.16	0.46
1:B:2305:LEU:HB3	1:B:2310:LEU:CD1	2.45	0.46
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.51	0.46
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.97	0.46
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.80	0.46
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.97	0.46
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.98	0.46
1:B:1939:PHE:H	1:B:1939:PHE:HD1	1.61	0.46
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.46	0.46
1:B:3462:ILE:O	1:B:3465:LEU:N	2.49	0.46
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.80	0.46
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.49	0.46
1:B:4022:GLN:O	1:B:4022:GLN:HG2	2.15	0.46
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.15	0.46
1:A:1977:LEU:O	1:A:1980:CYS:HB3	2.16	0.46
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.51	0.46
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.16	0.46
1:B:2170:LEU:HB3	1:B:2209:ARG:HD3	1.98	0.46
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.62	0.46
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.15	0.46
1:A:2228:HIS:HD2	2:A:5093:ATP:O2'	1.99	0.46
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.81	0.46
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.96	0.46
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.40	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.15	0.46
1:B:2204:PRO:HA	1:B:2207:ILE:HD12	1.97	0.46
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.16	0.46
1:A:2475:PRO:HB3	1:A:2527:GLU:HB2	1.98	0.46
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.16	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.97	0.46
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.16	0.46
1:A:1621:THR:HA	1:A:1624:ARG:CZ	2.44	0.45
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.97	0.45
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.17	0.45
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.31	0.45
1:A:2129:LEU:O	1:A:2133:ILE:HG12	2.16	0.45
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:3816:LEU:HD21	1:A:3850:TRP:HZ3	1.81	0.45
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.66	0.45
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.97	0.45
1:A:1694:VAL:HG23	1:A:1697:LYS:HE2	1.98	0.45
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.81	0.45
1:A:1927:GLY:HA2	1:A:1950:VAL:HG21	1.97	0.45
1:B:1411:GLU:HG2	1:B:1415:MET:HE3	1.98	0.45
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.99	0.45
1:B:3017:VAL:HG21	1:B:3313:PHE:HE2	1.81	0.45
1:B:3500:ASP:HA	1:B:3501:PRO:HD3	1.88	0.45
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.17	0.45
1:A:4034:LEU:HD23	1:A:4034:LEU:C	2.41	0.45
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.51	0.45
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.51	0.45
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.46	0.45
1:A:2567:LEU:HD22	1:A:2622:LEU:HD13	1.98	0.45
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.45
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.51	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.51	0.45
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.51	0.45
1:B:3919:LYS:HZ1	1:B:4038:GLU:CD	2.25	0.45
1:A:1575:LEU:HD12	1:A:1575:LEU:HA	1.87	0.45
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.17	0.45
1:A:2163:VAL:O	1:A:2166:MET:HG3	2.16	0.45
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	1.98	0.45
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.81	0.45
1:B:2494:LEU:C	1:B:2494:LEU:HD12	2.41	0.45
1:A:1848:ASP:O	1:A:1849:GLU:HB2	2.16	0.45
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.98	0.45
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.15	0.45
1:A:2425:THR:HG22	1:A:2485:PHE:CE2	2.51	0.45
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.64	0.45
1:A:3799:LYS:HG3	1:A:3803:LEU:HD11	1.98	0.45
1:A:3891:ARG:HA	1:A:3891:ARG:HD2	1.79	0.45
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.16	0.45
1:B:3848:LEU:O	1:B:3849:SER:C	2.59	0.45
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.17	0.45
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.52	0.45
1:B:2037:CYS:SG	1:B:2094:PHE:HB2	2.56	0.45
1:B:2276:LEU:CD2	1:B:2556:ILE:HG21	2.45	0.45
1:B:2491:LEU:HD21	1:B:2543:ARG:CZ	2.47	0.45
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.39	0.45
1:A:1946:ALA:O	1:A:1950:VAL:HG23	2.17	0.45
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.28	0.45
1:A:2115:TYR:O	1:A:2131:THR:CG2	2.65	0.45
1:A:2134:LEU:CD1	1:A:2138:ASN:HD21	2.28	0.45
1:A:3848:LEU:O	1:A:3849:SER:C	2.59	0.45
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.16	0.45
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.16	0.45
1:A:1640:VAL:CG1	1:A:1686:LYS:NZ	2.79	0.45
1:A:2891:ILE:CD1	1:A:2903:ILE:HD11	2.43	0.45
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	1.99	0.45
1:B:1941:ASP:O	1:B:1945:LEU:HG	2.17	0.45
1:B:2391:VAL:HG21	1:B:2426:MET:CE	2.47	0.45
1:B:2563:SER:CB	1:B:2566:SER:H	2.20	0.45
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.80	0.45
1:A:2474:LEU:N	1:A:2475:PRO:HD3	2.32	0.45
1:A:2546:MET:HE3	1:A:2546:MET:HB2	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.99	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.98	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:B:1753:GLY:HA3	1:B:3970:ASN:HD21	1.81	0.45
1:B:2467:THR:O	1:B:2471:LEU:N	2.50	0.45
1:A:1392:LEU:C	1:A:1392:LEU:CD1	2.86	0.44
1:A:2100:VAL:N	1:A:2149:ARG:O	2.48	0.44
1:A:2412:ARG:HG3	1:A:2412:ARG:HH11	1.82	0.44
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.78	0.44
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.99	0.44
1:B:2580:LYS:HG2	1:B:2586:ARG:HH22	1.82	0.44
1:B:2752:VAL:HG13	1:B:2883:LYS:HB3	1.98	0.44
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.98	0.44
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.32	0.44
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.98	0.44
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.20	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:A:2220:CYS:SG	1:A:2221:SER:N	2.91	0.44
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.53	0.44
1:A:2755:HIS:CB	1:A:2912:CYS:HA	2.47	0.44
1:B:1367:ILE:H	1:B:1367:ILE:HD12	1.83	0.44
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.44
1:B:2470:GLY:C	1:B:2473:LEU:CD1	2.90	0.44
1:B:3600:LYS:HA	1:B:3603:GLU:HG2	1.99	0.44
1:B:4065:LEU:C	1:B:4065:LEU:HD12	2.43	0.44
1:A:2386:MET:HB2	1:A:2627:ARG:CD	2.39	0.44
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.98	0.44
1:B:2091:MET:CE	1:B:2149:ARG:NH1	2.80	0.44
1:B:2095:ASP:CG	1:B:2149:ARG:HH21	2.26	0.44
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.32	0.44
1:B:2988:SER:CB	1:B:2989:PRO:CD	2.62	0.44
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.16	0.44
1:B:3810:SER:HB3	1:B:3838:TRP:H	1.83	0.44
1:B:3924:TRP:CD1	1:B:3924:TRP:C	2.94	0.44
1:A:3440:LEU:HD22	1:A:3462:ILE:HD12	1.98	0.44
1:A:3459:ASP:HB2	1:A:3460:PRO:HD2	1.98	0.44
1:A:3464:ARG:O	1:A:3467:SER:O	2.35	0.44
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.53	0.44
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.18	0.44
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.99	0.44
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.99	0.44
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.81	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:B:1851:ASN:HD21	1:B:1899:ASN:HB2	1.81	0.44
1:B:2178:LEU:HD12	1:B:2182:GLU:HB2	1.99	0.44
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.95	0.44
1:B:3509:LEU:O	1:B:3513:VAL:HG23	2.17	0.44
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.28	0.44
1:A:1646:GLN:CG	1:A:1763:ILE:HG12	2.47	0.44
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.85	0.44
1:A:2064:GLN:CD	1:A:2151:TRP:CZ3	2.95	0.44
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.17	0.44
1:A:2755:HIS:CB	1:A:2911:ARG:O	2.58	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.06	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44
1:A:3737:THR:HB	1:A:3740:THR:HG1	1.79	0.44
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.98	0.44
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.17	0.44
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.78	0.44
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	2.00	0.44
1:A:1664:LEU:O	1:A:1721:LYS:HE3	2.18	0.44
1:A:1983:LEU:HD21	1:A:1993:THR:O	2.16	0.44
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.48	0.44
1:A:3788:MET:O	1:A:3788:MET:HG3	2.18	0.44
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.82	0.44
1:B:1970:LEU:CD2	1:B:1974:LYS:HE3	2.47	0.44
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.53	0.44
1:B:2276:LEU:HD13	1:B:2417:CYS:SG	2.58	0.44
1:B:2387:ARG:O	1:B:2390:ILE:HG22	2.18	0.44
1:B:2967:ASN:HB3	1:B:3356:PHE:HE2	1.80	0.44
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.50	0.44
1:A:2446:SER:N	1:A:2449:THR:CG2	2.75	0.44
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.00	0.44
1:A:2940:PHE:CE1	1:A:2941:THR:O	2.71	0.44
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	2.00	0.44
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.53	0.44
1:B:3373:LEU:HD13	1:B:3557:LEU:CD1	2.48	0.44
1:A:23:LEU:C	1:A:25:GLU:N	2.74	0.44
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.18	0.44
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.17	0.44
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.48	0.44
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.44
1:B:1540:LEU:HD23	1:B:1540:LEU:HA	1.70	0.44
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.18	0.44
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.99	0.44
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.18	0.43
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.85	0.43
1:A:2120:LYS:H	1:A:2120:LYS:HG3	1.64	0.43
1:A:2361:ILE:HG22	1:A:2367:SER:O	2.18	0.43
1:B:1512:THR:HG22	1:B:1516:LEU:HD12	1.98	0.43
1:B:1849:GLU:CG	1:B:1899:ASN:ND2	2.81	0.43
1:B:2137:VAL:O	1:B:2141:ILE:CG2	2.62	0.43
1:B:2420:PRO:HA	3:B:5094:ADP:O2B	2.17	0.43
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.99	0.43
1:B:2578:ILE:HG21	1:B:2630:TYR:HB2	1.99	0.43
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.17	0.43
1:A:2042:GLY:HA3	1:A:2049:MET:CE	2.48	0.43
1:A:2228:HIS:CD2	2:A:5093:ATP:O2'	2.71	0.43
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.18	0.43
1:A:2494:LEU:HD12	1:A:2494:LEU:C	2.43	0.43
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.79	0.43
1:B:3024:LEU:HD13	1:B:3303:LYS:HG3	1.96	0.43
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.31	0.43
1:A:1622:GLN:NE2	1:A:1644:ILE:H	2.15	0.43
1:A:1983:LEU:CD2	1:A:1993:THR:CG2	2.88	0.43
1:A:2755:HIS:O	1:A:2913:ILE:N	2.49	0.43
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.48	0.43
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.52	0.43
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.16	0.43
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.17	0.43
1:A:1655:MET:HE3	1:A:1659:LEU:HD12	2.00	0.43
1:A:2391:VAL:CG2	1:A:2430:ASN:OD1	2.65	0.43
1:A:2418:GLY:CA	1:A:2424:LYS:HE3	2.47	0.43
1:A:2708:ASN:ND2	1:A:2710:THR:OG1	2.52	0.43
1:B:1849:GLU:CG	1:B:1899:ASN:HD22	2.31	0.43
1:B:2833:THR:HG21	1:B:2841:PRO:CD	2.49	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.99	0.43
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.64	0.43
1:A:1392:LEU:CD1	1:A:1393:LYS:O	2.67	0.43
1:A:1970:LEU:CD1	1:A:1973:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.52	0.43
1:A:2064:GLN:OE1	1:A:2091:MET:SD	2.77	0.43
1:A:2199:LEU:O	1:A:2200:ASP:C	2.61	0.43
1:A:3946:VAL:HG12	1:A:3950:PHE:C	2.37	0.43
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.33	0.43
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.53	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.52	0.43
1:A:1620:PHE:HA	1:A:1760:PHE:CE2	2.53	0.43
1:A:2526:ILE:HG13	1:A:2526:ILE:O	2.18	0.43
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	2.01	0.43
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.43
1:A:2109:LEU:HD11	1:A:2129:LEU:HD23	1.99	0.43
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.18	0.43
1:A:3436:PHE:HE2	1:A:3462:ILE:HD11	1.82	0.43
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	2.00	0.43
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	2.00	0.43
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.18	0.43
1:B:2745:ILE:HA	1:B:2756:MET:SD	2.58	0.43
1:B:2779:LEU:HD23	1:B:2812:ARG:C	2.44	0.43
1:B:2785:LYS:HE2	1:B:3480:GLU:OE1	2.18	0.43
1:B:3307:LEU:HA	1:B:3310:THR:HB	2.00	0.43
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.93	0.43
1:A:1794:PHE:HZ	1:A:1805:THR:CG2	2.31	0.43
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.18	0.43
1:A:2266:PHE:CD1	1:A:2326:LEU:HD21	2.48	0.43
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.33	0.43
1:B:1527:LEU:HD21	1:B:1546:LEU:CD2	2.48	0.43
1:B:2064:GLN:CD	1:B:2151:TRP:HZ3	2.26	0.43
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.43
1:B:2361:ILE:HG22	1:B:2367:SER:O	2.19	0.43
1:A:2197:ASP:CB	1:A:2549:ARG:HD2	2.45	0.43
1:A:3352:LEU:O	1:A:3356:PHE:HD1	2.02	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.84	0.43
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.48	0.43
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.28	0.43
1:A:1463:LEU:O	1:A:1467:ASN:HB2	2.19	0.43
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.19	0.43
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.18	0.43
1:A:3500:ASP:HA	1:A:3501:PRO:HD3	1.82	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.43
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.19	0.42
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	2.00	0.42
1:A:3592:LYS:O	1:A:3596:ASN:N	2.52	0.42
1:B:1416:LYS:CA	1:B:1421:TYR:OH	2.65	0.42
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.19	0.42
1:B:2620:ARG:NH1	1:B:2910:ASN:CG	2.77	0.42
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.29	0.42
1:B:4022:GLN:O	1:B:4023:ILE:C	2.61	0.42
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.19	0.42
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.49	0.42
1:A:2418:GLY:N	1:A:2424:LYS:HE3	2.34	0.42
1:A:3428:LEU:HD23	1:A:3428:LEU:C	2.43	0.42
1:A:4084:SER:O	1:A:4088:LEU:HG	2.19	0.42
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.54	0.42
1:B:1976:VAL:HG11	1:B:1998:LEU:HD23	2.01	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:B:3979:ASN:OD1	1:B:3979:ASN:N	2.52	0.42
1:B:4054:GLU:HA	1:B:4055:PRO:HD3	1.90	0.42
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	2.01	0.42
1:A:2395:ILE:H	1:A:2395:ILE:HD12	1.83	0.42
1:A:2745:ILE:HG12	1:A:2756:MET:CE	2.49	0.42
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	2.01	0.42
1:B:1910:GLU:CB	1:B:3846:MET:HB3	2.49	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.99	0.42
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	2.01	0.42
1:A:1660:VAL:HG11	1:A:1728:TRP:CH2	2.54	0.42
1:A:1710:ASN:HB2	1:A:1932:MET:HE1	2.02	0.42
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	2.02	0.42
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	2.01	0.42
1:A:3855:LEU:HD11	1:A:3873:MET:HE1	2.00	0.42
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.49	0.42
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	2.00	0.42
1:B:2166:MET:HE1	1:B:2192:ILE:HD13	2.00	0.42
1:B:2383:HIS:CE1	1:B:2384:GLU:HG3	2.53	0.42
1:B:2788:ARG:H	1:B:3459:ASP:CB	2.32	0.42
1:B:3738:VAL:C	1:B:3740:THR:H	2.27	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.52	0.42
1:A:1540:LEU:CD1	1:A:1548:ILE:HD12	2.50	0.42
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.54	0.42
1:A:3436:PHE:CE2	1:A:3462:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3832:SER:O	1:A:3836:GLY:N	2.46	0.42
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.85	0.42
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.53	0.42
1:B:1759:LYS:CD	1:B:1761:GLU:OE2	2.67	0.42
1:B:2080:LYS:HG2	2:B:5093:ATP:PB	2.60	0.42
1:B:2380:LEU:HD11	1:B:2390:ILE:HD11	1.97	0.42
1:B:2428:MET:SD	1:B:2429:ASN:N	2.93	0.42
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.48	0.42
1:A:2354:SER:OG	1:A:2357:SER:CA	2.68	0.42
1:A:2385:VAL:HG13	1:A:2386:MET:N	2.33	0.42
1:A:2416:LEU:HB3	1:A:2424:LYS:CD	2.50	0.42
1:A:3945:LEU:HD21	1:A:4059:LEU:HD22	2.02	0.42
1:A:3980:ILE:C	1:A:3982:TRP:H	2.26	0.42
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	2.02	0.42
1:B:2048:SER:N	2:B:5093:ATP:HN62	2.08	0.42
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.28	0.42
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.85	0.42
1:B:2866:LEU:HD12	1:B:2867:LEU:H	1.85	0.42
1:B:3846:MET:HG3	1:B:3847:SER:N	2.34	0.42
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.50	0.42
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.55	0.42
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	2.01	0.42
1:A:1873:GLN:HE22	1:A:1915:SER:HA	1.84	0.42
1:A:2312:ASP:HB3	1:A:2351:GLN:HG3	2.01	0.42
1:A:3997:LYS:H	1:A:3997:LYS:HG3	1.53	0.42
1:A:4023:ILE:HD11	1:A:4029:ILE:CD1	2.50	0.42
1:B:1742:ASP:HB3	1:B:1745:ASN:HD22	1.85	0.42
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.19	0.42
1:B:2368:PHE:CD1	1:B:2368:PHE:O	2.72	0.42
1:B:2437:LEU:HA	1:B:2480:LYS:HD3	2.02	0.42
1:B:2549:ARG:HG2	2:B:5093:ATP:O1G	2.19	0.42
1:A:113:ASP:O	1:A:114:PHE:C	2.62	0.42
1:A:1406:LYS:HE2	1:A:1406:LYS:HB3	1.84	0.42
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.20	0.42
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	2.02	0.42
1:A:2324:TYR:CD1	1:A:2403:ILE:HG12	2.55	0.42
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.41	0.42
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	2.01	0.42
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.00	0.42
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.42
1:A:2224:SER:O	2:A:5093:ATP:H2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2389:ASP:O	1:A:2389:ASP:OD1	2.37	0.42
1:B:1946:ALA:O	1:B:1950:VAL:HG23	2.20	0.42
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.20	0.42
1:B:2756:MET:O	1:B:2888:VAL:HA	2.20	0.42
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.42
1:A:1635:ASP:HB2	1:A:1638:VAL:HG23	2.02	0.42
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	2.02	0.42
1:A:2134:LEU:HD11	1:A:2138:ASN:ND2	2.34	0.42
1:A:2278:VAL:O	1:A:2283:LYS:HE2	2.19	0.42
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.98	0.42
1:A:3669:THR:HA	1:A:3672:ASP:HB2	2.00	0.42
1:A:3888:LEU:O	1:A:3892:THR:HG22	2.19	0.42
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.50	0.42
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.50	0.42
1:B:1801:GLY:N	5:B:5097:SO4:O3	2.52	0.42
1:B:2081:THR:OG1	2:B:5093:ATP:O2A	2.37	0.42
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.20	0.42
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	2.19	0.42
1:B:2278:VAL:O	1:B:2283:LYS:HE2	2.19	0.42
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.55	0.42
1:B:3965:SER:HA	1:B:3968:LEU:HD12	2.02	0.42
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.84	0.41
1:A:1910:GLU:HB2	1:A:3846:MET:HA	2.01	0.41
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.41
1:A:3411:SER:O	1:A:3413:HIS:N	2.50	0.41
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.54	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.41
1:B:1758:TYR:CD1	1:B:1759:LYS:O	2.73	0.41
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.53	0.41
1:B:2627:ARG:NH1	1:B:2630:TYR:CE2	2.87	0.41
1:B:3702:MET:CB	1:B:3767:PHE:HZ	2.32	0.41
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.02	0.41
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	2.02	0.41
1:A:2571:TYR:HD1	1:A:2626:VAL:HG21	1.85	0.41
1:A:4022:GLN:O	1:A:4023:ILE:C	2.64	0.41
1:B:1645:PHE:CZ	1:B:1649:LEU:HD22	2.55	0.41
1:B:1849:GLU:CD	1:B:1899:ASN:ND2	2.77	0.41
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.20	0.41
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.54	0.41
1:A:1659:LEU:O	1:A:1663:CYS:HB2	2.20	0.41
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.02	0.41
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.85	0.41
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.03	0.41
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.55	0.41
1:A:1422:LYS:O	1:A:1425:GLU:HB3	2.21	0.41
1:A:1495:THR:HB	1:A:1498:GLU:CG	2.51	0.41
1:A:1926:SER:HA	1:A:1929:ILE:HD13	2.02	0.41
1:A:2412:ARG:HG3	1:A:2412:ARG:NH1	2.34	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.33	0.41
1:B:1802:LYS:O	1:B:1806:VAL:HG23	2.20	0.41
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.02	0.41
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.45	0.41
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.85	0.41
1:A:1979:ASN:OD1	1:A:2066:THR:HG21	2.20	0.41
1:A:2098:ALA:O	1:A:2149:ARG:N	2.50	0.41
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.41
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.20	0.41
1:A:2397:THR:HG22	1:A:2398:ILE:HD13	2.03	0.41
1:A:2757:MET:HG2	1:A:2889:PHE:HD2	1.78	0.41
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.21	0.41
1:B:1612:ASP:C	1:B:1615:ILE:HG12	2.45	0.41
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.34	0.41
1:B:2491:LEU:HD21	1:B:2543:ARG:NH1	2.35	0.41
1:B:2762:SER:C	1:B:2764:THR:H	2.29	0.41
1:B:2786:ILE:H	1:B:2786:ILE:HG13	1.68	0.41
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.50	0.41
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.41
1:A:2428:MET:SD	1:A:2429:ASN:N	2.94	0.41
1:A:2779:LEU:HD23	1:A:2812:ARG:C	2.44	0.41
1:A:2940:PHE:CD1	1:A:2940:PHE:C	2.99	0.41
1:A:3642:TYR:N	1:A:3642:TYR:CD1	2.87	0.41
1:A:4085:THR:O	1:A:4089:LEU:HG	2.21	0.41
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.46	0.41
1:B:2632:ALA:HB3	1:B:2647:LEU:HD21	2.01	0.41
1:B:2757:MET:HB2	1:B:2889:PHE:HB2	2.01	0.41
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	1.76	0.41
1:B:3431:PHE:CE1	1:B:3458:PHE:HD1	2.37	0.41
1:B:3671:VAL:C	1:B:3674:ILE:HG22	2.46	0.41
1:A:1765:ILE:HG21	1:A:1765:ILE:HD13	1.72	0.41
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41
1:B:2464:TYR:CE1	1:B:2474:LEU:HD12	2.56	0.41
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	2.01	0.41
1:B:2824:GLU:HG2	1:B:2825:THR:H	1.86	0.41
1:B:3901:PRO:HB2	1:B:3906:THR:HG23	2.02	0.41
1:A:2039:LYS:O	1:A:2043:GLN:HG2	2.21	0.41
1:A:2046:GLY:O	1:A:2228:HIS:HB2	2.20	0.41
1:A:2475:PRO:HB3	1:A:2527:GLU:CB	2.50	0.41
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.41
1:A:2765:GLY:HA2	1:A:2768:ILE:HG22	2.02	0.41
1:A:3854:TYR:CD1	1:A:3854:TYR:C	2.99	0.41
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.69	0.41
1:B:2620:ARG:HH12	1:B:2910:ASN:CG	2.28	0.41
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.55	0.41
1:B:3850:TRP:NE1	1:B:3854:TYR:CB	2.82	0.41
1:A:1462:ASN:HB3	1:A:1465:ILE:HG22	2.00	0.41
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	3.04	0.41
1:A:2455:LEU:HD21	1:A:2515:PHE:CE2	2.56	0.41
1:A:2780:LYS:HB3	1:A:2813:THR:HG22	2.02	0.41
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	2.03	0.41
1:A:3331:GLU:HA	1:A:3396:ILE:HG12	2.03	0.41
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.02	0.41
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	2.02	0.41
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.03	0.41
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.82	0.41
1:B:1945:LEU:HD21	1:B:1991:GLU:HB3	2.03	0.41
1:B:2155:ASP:CG	1:B:2507:ARG:HH22	2.28	0.41
1:B:2481:ASN:ND2	1:B:2528:ARG:HB3	2.36	0.41
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.84	0.41
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.21	0.41
1:B:2788:ARG:H	1:B:3459:ASP:HB2	1.86	0.41
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.21	0.41
1:B:3773:ASN:O	1:B:3774:ILE:C	2.62	0.41
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.21	0.41
1:A:1626:CYS:O	1:A:1627:LEU:C	2.63	0.41
1:A:1838:ILE:HD13	1:A:1838:ILE:HG21	1.81	0.41
1:A:2412:ARG:HA	1:A:2412:ARG:HD2	1.86	0.41
1:A:2426:MET:CG	1:A:2427:ILE:N	2.81	0.41
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.50	0.41
1:A:2502:VAL:O	1:A:2505:PHE:HB3	2.20	0.41
1:A:3924:TRP:CD1	1:A:3924:TRP:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2354:SER:OG	1:B:2357:SER:CA	2.68	0.41
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.46	0.41
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	2.03	0.41
1:A:1817:VAL:HG22	1:A:1844:TRP:CB	2.51	0.40
1:A:2290:LEU:HD23	1:A:2321:SER:HA	2.02	0.40
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	2.03	0.40
1:A:2416:LEU:O	1:A:2534:ALA:HA	2.22	0.40
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.49	0.40
1:B:1547:LYS:O	1:B:1551:SER:HB3	2.21	0.40
1:B:2368:PHE:O	1:B:2369:SER:OG	2.28	0.40
1:B:2637:PRO:HD3	1:B:2703:ASP:HB3	2.03	0.40
1:A:2060:PHE:CZ	1:A:2193:LEU:HD21	2.57	0.40
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.55	0.40
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.35	0.40
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.61	0.40
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	2.02	0.40
1:B:2507:ARG:HG3	1:B:2550:PHE:HA	2.03	0.40
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.61	0.40
1:A:1375:LYS:O	1:A:1379:LYS:HG2	2.21	0.40
1:A:1531:ARG:HD3	1:A:1538:TYR:HA	2.03	0.40
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.22	0.40
1:A:2488:GLU:O	1:A:2491:LEU:HB2	2.21	0.40
1:A:2514:GLY:HA3	1:A:2525:THR:HA	2.03	0.40
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.40	0.40
1:A:3379:TRP:CD2	1:A:3394:MET:HG3	2.56	0.40
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.21	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.03	0.40
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.02	0.40
1:B:1534:PHE:CD2	1:B:1537:PHE:CE1	3.05	0.40
1:B:3570:LEU:HD23	1:B:3580:ASN:CG	2.47	0.40
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.69	0.40
1:A:1857:VAL:O	1:A:1861:VAL:HG23	2.21	0.40
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.56	0.40
1:A:2906:PRO:O	1:A:2907:ALA:C	2.63	0.40
1:B:1409:LEU:O	1:B:1413:VAL:HG23	2.22	0.40
1:B:1529:ARG:O	1:B:1533:GLN:HG2	2.21	0.40
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.20	0.40
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.03	0.40
1:B:1826:PHE:CZ	1:B:1831:LEU:CA	3.04	0.40
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	2.03	0.40
1:B:2160:PRO:HA	1:B:2163:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	2.02	0.40
1:B:3908:LYS:HG2	1:B:4049:LEU:HD13	2.03	0.40
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.51	0.40
1:A:1421:TYR:CD2	1:A:1425:GLU:HG2	2.55	0.40
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.22	0.40
1:A:1824:ASP:O	1:A:1825:SER:C	2.65	0.40
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.49	0.40
1:B:2582:VAL:O	1:B:2582:VAL:HG23	2.21	0.40
1:B:3924:TRP:O	1:B:3924:TRP:CD1	2.75	0.40
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.33	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	2640/2695 (98%)	2511 (95%)	118 (4%)	11 (0%)	30	60
1	B	2640/2695 (98%)	2525 (96%)	107 (4%)	8 (0%)	36	65
All	All	5280/5390 (98%)	5036 (95%)	225 (4%)	19 (0%)	30	60

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	A	2495	ASP
1	B	1391	GLY
1	A	2476	LYS
1	A	2728	LEU
1	B	66	GLN
1	A	2519	PRO
1	B	2519	PRO

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Mol	Chain	Res	Type
1	B	2990	GLY
1	B	3914	GLN
1	A	66	GLN
1	A	2990	GLY
1	A	3980	ILE
1	A	2562	PRO
1	B	2562	PRO
1	B	3980	ILE
1	A	3462	ILE
1	B	1470	PRO
1	A	2028	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2218/2453 (90%)	2071 (93%)	147 (7%)	15	43
1	B	2218/2453 (90%)	2110 (95%)	108 (5%)	22	51
All	All	4436/4906 (90%)	4181 (94%)	255 (6%)	18	47

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1385	VAL
1	A	1392	LEU
1	A	1421	TYR
1	A	1455	LEU
1	A	1486	ILE
1	A	1493	LEU
1	A	1508	THR
1	A	1540	LEU
1	A	1589	VAL
1	A	1605	GLN
1	A	1641	SER
1	A	1644	ILE

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Mol	Chain	Res	Type
1	A	1684	LEU
1	A	1719	SER
1	A	1749	ILE
1	A	1768	ARG
1	A	1788	GLN
1	A	1793	CYS
1	A	1852	ARG
1	A	1923	SER
1	A	1925	GLN
1	A	1936	ILE
1	A	1943	LYS
1	A	1964	ASN
1	A	1992	LYS
1	A	2081	THR
1	A	2104	ILE
1	A	2107	LYS
1	A	2109	LEU
1	A	2122	THR
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2166	MET
1	A	2169	VAL
1	A	2186	ILE
1	A	2202	THR
1	A	2228	HIS
1	A	2229	LEU
1	A	2273	VAL
1	A	2292	VAL
1	A	2295	ILE
1	A	2310	LEU
1	A	2318	ILE
1	A	2320	ARG
1	A	2323	LEU
1	A	2351	GLN
1	A	2361	ILE
1	A	2390	ILE
1	A	2397	THR
1	A	2424	LYS
1	A	2425	THR
1	A	2430	ASN
1	A	2437	LEU

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Mol	Chain	Res	Type
1	A	2472	THR
1	A	2476	LYS
1	A	2482	LEU
1	A	2510	MET
1	A	2517	LYS
1	A	2522	LYS
1	A	2526	ILE
1	A	2544	ILE
1	A	2547	SER
1	A	2548	GLU
1	A	2559	LEU
1	A	2566	SER
1	A	2576	LYS
1	A	2613	SER
1	A	2623	THR
1	A	2626	VAL
1	A	2689	ILE
1	A	2694	LEU
1	A	2751	GLN
1	A	2769	LEU
1	A	2785	LYS
1	A	2822	ILE
1	A	2823	LEU
1	A	2833	THR
1	A	2843	LEU
1	A	2856	LEU
1	A	2863	LEU
1	A	2866	LEU
1	A	2911	ARG
1	A	2936	ILE
1	A	2961	ILE
1	A	2967	ASN
1	A	2979	LYS
1	A	3002	LEU
1	A	3012	GLU
1	A	3019	VAL
1	A	3301	PHE
1	A	3329	ILE
1	A	3371	VAL
1	A	3372	THR
1	A	3391	LEU
1	A	3400	SER

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Mol	Chain	Res	Type
1	A	3456	GLU
1	A	3481	ILE
1	A	3485	GLU
1	A	3512	ARG
1	A	3534	LEU
1	A	3536	GLU
1	A	3538	ASN
1	A	3543	ARG
1	A	3548	LEU
1	A	3559	LEU
1	A	3565	ARG
1	A	3567	LEU
1	A	3578	LEU
1	A	3584	MET
1	A	3595	MET
1	A	3598	GLU
1	A	3601	LEU
1	A	3618	TYR
1	A	3634	LYS
1	A	3646	ILE
1	A	3677	LEU
1	A	3697	ILE
1	A	3729	SER
1	A	3737	THR
1	A	3744	LEU
1	A	3752	THR
1	A	3805	LYS
1	A	3809	GLU
1	A	3811	LEU
1	A	3812	LYS
1	A	3823	ASN
1	A	3831	LYS
1	A	3862	THR
1	A	3876	THR
1	A	3884	LEU
1	A	3899	ASP
1	A	3900	ILE
1	A	3906	THR
1	A	3939	ILE
1	A	3943	THR
1	A	3952	LYS
1	A	3976	SER

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Mol	Chain	Res	Type
1	A	3980	ILE
1	A	3992	ILE
1	A	3997	LYS
1	A	3998	ILE
1	A	4004	LEU
1	A	4016	CYS
1	A	4034	LEU
1	A	4040	GLU
1	A	4046	THR
1	B	1371	LEU
1	B	1421	TYR
1	B	1486	ILE
1	B	1493	LEU
1	B	1495	THR
1	B	1540	LEU
1	B	1644	ILE
1	B	1646	GLN
1	B	1661	GLU
1	B	1694	VAL
1	B	1737	LYS
1	B	1767	GLU
1	B	1768	ARG
1	B	1769	LEU
1	B	1892	THR
1	B	1936	ILE
1	B	1959	LYS
1	B	1992	LYS
1	B	2027	THR
1	B	2141	ILE
1	B	2186	ILE
1	B	2202	THR
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2310	LEU
1	B	2318	ILE
1	B	2323	LEU
1	B	2351	GLN
1	B	2352	GLU
1	B	2361	ILE
1	B	2381	GLU
1	B	2390	ILE

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Mol	Chain	Res	Type
1	B	2395	ILE
1	B	2397	THR
1	B	2430	ASN
1	B	2471	LEU
1	B	2474	LEU
1	B	2476	LYS
1	B	2510	MET
1	B	2526	ILE
1	B	2544	ILE
1	B	2566	SER
1	B	2576	LYS
1	B	2613	SER
1	B	2616	LEU
1	B	2623	THR
1	B	2681	LEU
1	B	2689	ILE
1	B	2694	LEU
1	B	2747	ARG
1	B	2751	GLN
1	B	2752	VAL
1	B	2829	GLU
1	B	2833	THR
1	B	2835	LEU
1	B	2843	LEU
1	B	2853	LEU
1	B	2856	LEU
1	B	2936	ILE
1	B	2961	ILE
1	B	2967	ASN
1	B	2969	LEU
1	B	3329	ILE
1	B	3348	ILE
1	B	3372	THR
1	B	3391	LEU
1	B	3400	SER
1	B	3415	ILE
1	B	3425	LYS
1	B	3456	GLU
1	B	3461	ILE
1	B	3502	SER
1	B	3507	ILE
1	B	3534	LEU

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Mol	Chain	Res	Type
1	B	3536	GLU
1	B	3538	ASN
1	B	3548	LEU
1	B	3559	LEU
1	B	3566	LEU
1	B	3567	LEU
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3646	ILE
1	B	3677	LEU
1	B	3717	GLU
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3771	GLU
1	B	3811	LEU
1	B	3813	ILE
1	B	3844	ILE
1	B	3860	GLU
1	B	3862	THR
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3940	THR
1	B	3943	THR
1	B	3980	ILE
1	B	3982	TRP
1	B	3998	ILE
1	B	4016	CYS
1	B	4024	VAL
1	B	4068	GLU
1	B	4087	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1442	GLN
1	A	1449	GLN
1	A	1533	GLN
1	A	1605	GLN
1	A	1622	GLN

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Mol	Chain	Res	Type
1	A	1629	GLN
1	A	1709	ASN
1	A	1717	ASN
1	A	1757	GLN
1	A	1873	GLN
1	A	1899	ASN
1	A	1965	HIS
1	A	2064	GLN
1	A	2068	GLN
1	A	2138	ASN
1	A	2228	HIS
1	A	2239	ASN
1	A	2264	ASN
1	A	2270	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2304	ASN
1	A	2335	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2481	ASN
1	A	2500	GLN
1	A	2508	GLN
1	A	2530	HIS
1	A	2536	ASN
1	A	2601	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	2708	ASN
1	A	2755	HIS
1	A	2783	GLN
1	A	2896	ASN
1	A	2910	ASN
1	A	2927	GLN
1	A	3008	GLN
1	A	3025	ASN
1	A	3323	ASN
1	A	3336	HIS
1	A	3363	ASN

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Mol	Chain	Res	Type
1	A	3413	HIS
1	A	3497	HIS
1	A	3521	ASN
1	A	3538	ASN
1	A	3576	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	3962	GLN
1	A	4020	ASN
1	A	4077	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1667	ASN
1	B	1714	GLN
1	B	1717	ASN
1	B	1736	GLN
1	B	1745	ASN
1	B	1787	HIS
1	B	1821	ASN
1	B	1851	ASN
1	B	1873	GLN
1	B	1899	ASN
1	B	1951	HIS
1	B	1965	HIS
1	B	2228	HIS
1	B	2264	ASN
1	B	2270	ASN
1	B	2282	ASN
1	B	2293	HIS
1	B	2335	GLN
1	B	2351	GLN
1	B	2383	HIS
1	B	2409	ASN
1	B	2461	HIS
1	B	2481	ASN
1	B	2513	GLN
1	B	2521	ASN
1	B	2530	HIS
1	B	2536	ASN
1	B	2598	HIS

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Mol	Chain	Res	Type
1	B	2601	ASN
1	B	2634	ASN
1	B	2667	ASN
1	B	2683	ASN
1	B	2753	GLN
1	B	2755	HIS
1	B	2777	ASN
1	B	2837	ASN
1	B	2896	ASN
1	B	2910	ASN
1	B	2927	GLN
1	B	3008	GLN
1	B	3323	ASN
1	B	3336	HIS
1	B	3338	ASN
1	B	3363	ASN
1	B	3413	HIS
1	B	3471	ASN
1	B	3497	HIS
1	B	3521	ASN
1	B	3542	GLN
1	B	3561	ASN
1	B	3624	HIS
1	B	3890	GLN
1	B	3948	HIS
1	B	3962	GLN
1	B	3970	ASN
1	B	4020	ASN
1	B	4031	GLN
1	B	4036	GLN
1	B	4077	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	5094	-	28,29,29	1.68	5 (17%)	43,45,45	1.75	6 (13%)
3	ADP	B	5094	-	28,29,29	1.64	6 (21%)	43,45,45	2.08	13 (30%)
5	SO4	B	5097	-	4,4,4	0.48	0	6,6,6	0.44	0
5	SO4	B	5096	-	4,4,4	0.99	0	6,6,6	1.17	1 (16%)
5	SO4	A	5096	-	4,4,4	1.05	1 (25%)	6,6,6	1.40	1 (16%)
2	ATP	A	5093	4	32,33,33	1.41	4 (12%)	48,52,52	1.78	9 (18%)
5	SO4	A	5097	-	4,4,4	0.46	0	6,6,6	0.57	0
2	ATP	B	5093	4	32,33,33	1.55	5 (15%)	48,52,52	1.75	7 (14%)

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
3	ADP	A	5094	-	-	6/16/32/32	0/3/3/3
3	ADP	B	5094	-	-	7/16/32/32	0/3/3/3
2	ATP	B	5093	4	-	4/22/38/38	0/3/3/3
2	ATP	A	5093	4	-	5/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ADP	C5-C4	5.42	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5094	ADP	C5-C4	5.40	1.48	1.39
2	B	5093	ATP	C5-C4	5.11	1.48	1.39
2	A	5093	ATP	C5-C4	4.74	1.47	1.39
3	A	5094	ADP	C5-N7	-3.52	1.32	1.39
3	A	5094	ADP	C8-N7	3.23	1.37	1.31
3	B	5094	ADP	C8-N7	2.95	1.37	1.31
2	B	5093	ATP	C5-C6	2.91	1.49	1.41
2	B	5093	ATP	C8-N7	2.87	1.37	1.31
3	B	5094	ADP	C5-C6	2.87	1.49	1.41
2	B	5093	ATP	C5-N7	-2.77	1.34	1.39
2	A	5093	ATP	C5-C6	2.75	1.48	1.41
3	B	5094	ADP	C4-N3	2.65	1.39	1.34
2	A	5093	ATP	C8-N7	2.35	1.36	1.31
2	A	5093	ATP	C5-N7	-2.24	1.35	1.39
3	B	5094	ADP	PA-O3A	2.22	1.61	1.59
3	A	5094	ADP	C4-N9	-2.21	1.33	1.37
2	B	5093	ATP	PB-O3B	2.12	1.61	1.59
3	A	5094	ADP	C5-C6	2.07	1.46	1.41
3	B	5094	ADP	PB-O3B	-2.06	1.47	1.54
5	A	5096	SO4	O1-S	2.05	1.57	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5093	ATP	C5-C4-N3	-6.10	118.32	126.72
2	A	5093	ATP	C5-C4-N3	-5.82	118.70	126.72
3	B	5094	ADP	C5-C4-N3	-5.39	119.29	126.72
3	A	5094	ADP	N3-C2-N1	-4.91	121.14	128.58
3	B	5094	ADP	N3-C4-N9	4.89	135.49	127.17
3	A	5094	ADP	C5-C4-N3	-4.70	120.24	126.72
2	A	5093	ATP	N3-C4-N9	4.61	135.01	127.17
3	B	5094	ADP	N3-C2-N1	-4.53	121.73	128.58
2	B	5093	ATP	N3-C4-N9	4.34	134.55	127.17
3	B	5094	ADP	C2-N3-C4	4.16	121.98	111.83
2	B	5093	ATP	C4-C5-N7	-3.91	106.11	110.58
3	A	5094	ADP	N3-C4-N9	3.85	133.72	127.17
3	A	5094	ADP	C2-N3-C4	3.78	121.06	111.83
2	A	5093	ATP	C2-N3-C4	3.68	120.83	111.83
2	A	5093	ATP	C4-C5-N7	-3.48	106.60	110.58
2	B	5093	ATP	C2-N3-C4	3.47	120.30	111.83
2	A	5093	ATP	N3-C2-N1	-3.18	123.77	128.58
3	A	5094	ADP	C2-N1-C6	3.15	123.91	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5094	ADP	C4-N9-C8	3.05	108.94	105.74
3	B	5094	ADP	C3'-C2'-C1'	2.96	107.07	101.46
3	B	5094	ADP	C5'-C4'-C3'	-2.77	105.26	115.21
2	B	5093	ATP	C3'-C2'-C1'	2.74	106.65	101.46
3	B	5094	ADP	C6-C5-N7	2.67	137.24	132.09
3	B	5094	ADP	C4-C5-N7	-2.64	107.57	110.58
2	A	5093	ATP	C4-N9-C8	2.63	108.50	105.74
2	B	5093	ATP	N3-C2-N1	-2.63	124.60	128.58
3	A	5094	ADP	C2'-C3'-C4'	2.63	107.69	102.61
2	B	5093	ATP	C5-N7-C8	2.56	107.48	103.45
2	A	5093	ATP	C5-N7-C8	2.56	107.48	103.45
2	A	5093	ATP	C3'-C2'-C1'	2.55	106.29	101.46
3	B	5094	ADP	C2-N1-C6	2.48	122.80	118.73
3	B	5094	ADP	C5-N7-C8	2.36	107.16	103.45
5	A	5096	SO4	O4-S-O1	2.35	121.86	109.56
3	B	5094	ADP	C2'-C1'-N9	-2.29	107.61	113.30
3	B	5094	ADP	O2A-PA-O3A	2.27	113.40	107.27
2	A	5093	ATP	C6-C5-N7	2.10	136.13	132.09
5	B	5096	SO4	O2-S-O1	2.05	123.48	109.06

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5093	ATP	C5'-O5'-PA-O1A
2	B	5093	ATP	PB-O3B-PG-O2G
2	B	5093	ATP	PB-O3B-PG-O3G
3	A	5094	ADP	C5'-O5'-PA-O1A
3	B	5094	ADP	C5'-O5'-PA-O1A
3	B	5094	ADP	C5'-O5'-PA-O3A
2	B	5093	ATP	O4'-C4'-C5'-O5'
3	B	5094	ADP	C3'-C4'-C5'-O5'
3	A	5094	ADP	O4'-C4'-C5'-O5'
3	B	5094	ADP	O4'-C4'-C5'-O5'
2	A	5093	ATP	O4'-C4'-C5'-O5'
2	A	5093	ATP	C3'-C4'-C5'-O5'
2	B	5093	ATP	C3'-C4'-C5'-O5'
3	A	5094	ADP	C3'-C4'-C5'-O5'
2	A	5093	ATP	PA-O3A-PB-O1B
3	A	5094	ADP	PB-O3A-PA-O2A
3	B	5094	ADP	C4'-C5'-O5'-PA
3	A	5094	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	A	5094	ADP	PB-O3A-PA-O1A
3	B	5094	ADP	C2'-C1'-N9-C4
3	B	5094	ADP	C2'-C1'-N9-C8
2	A	5093	ATP	PA-O3A-PB-O2B

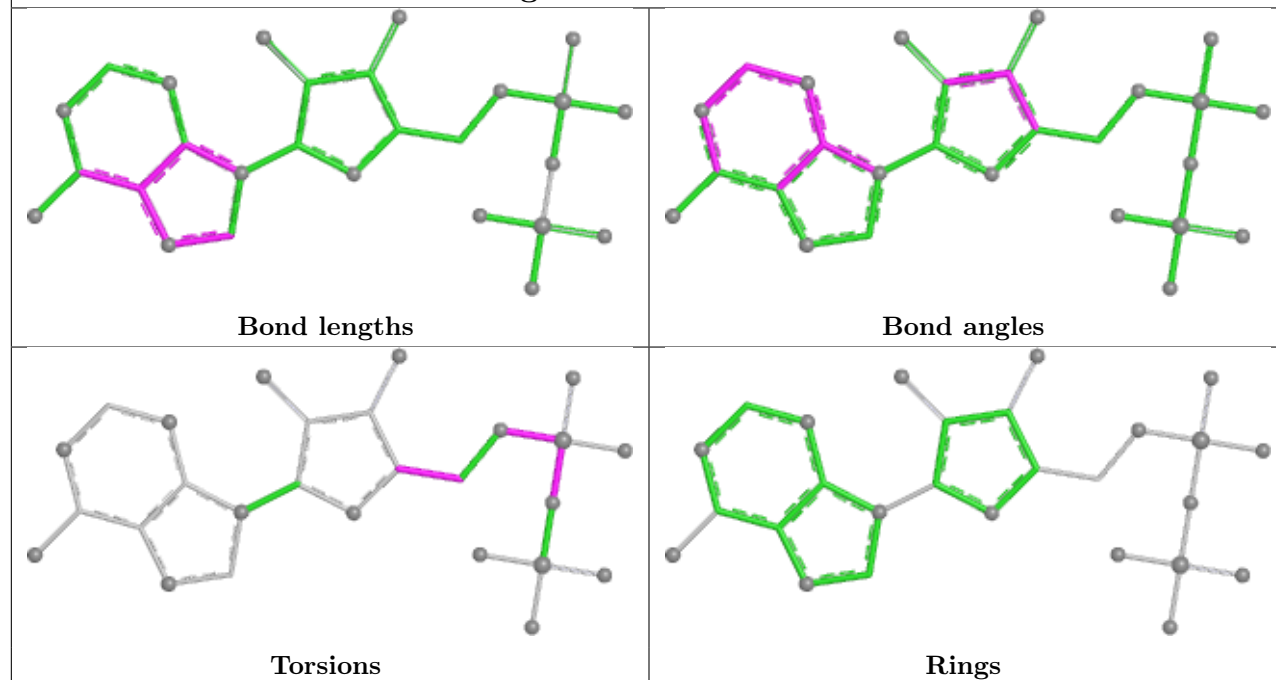
There are no ring outliers.

7 monomers are involved in 47 short contacts:

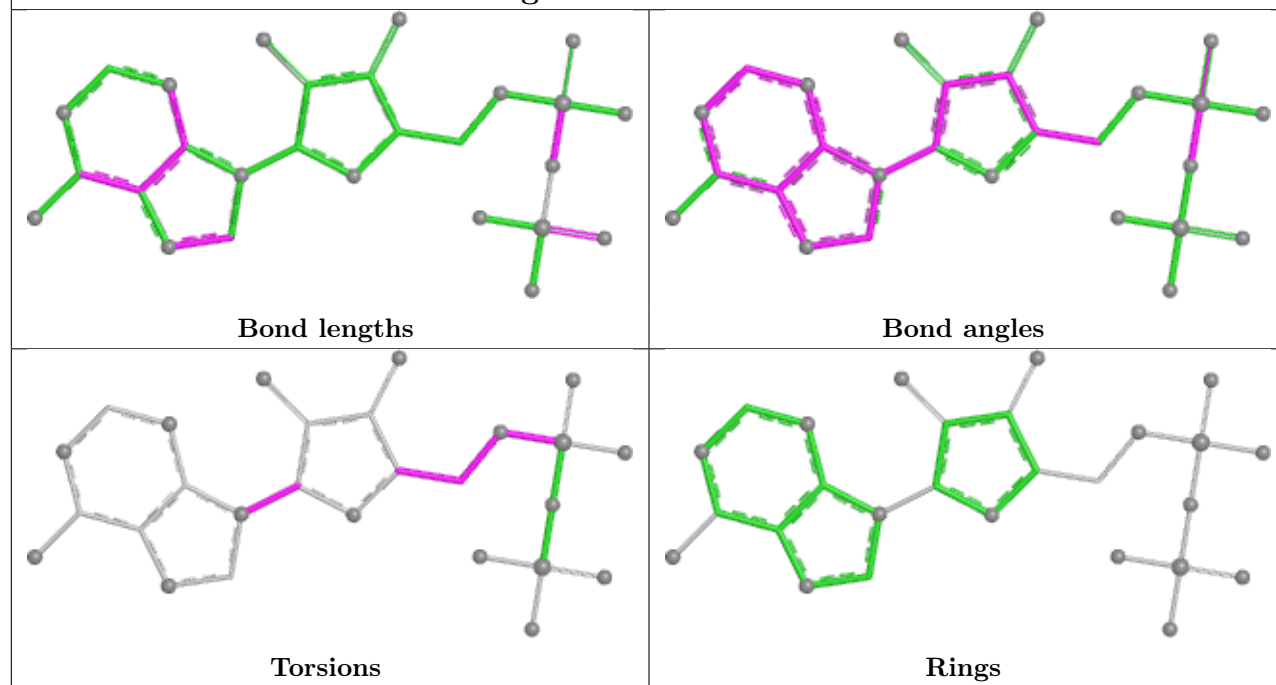
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5094	ADP	2	0
3	B	5094	ADP	6	0
5	B	5097	SO4	2	0
5	B	5096	SO4	2	0
2	A	5093	ATP	10	0
5	A	5097	SO4	2	0
2	B	5093	ATP	23	0

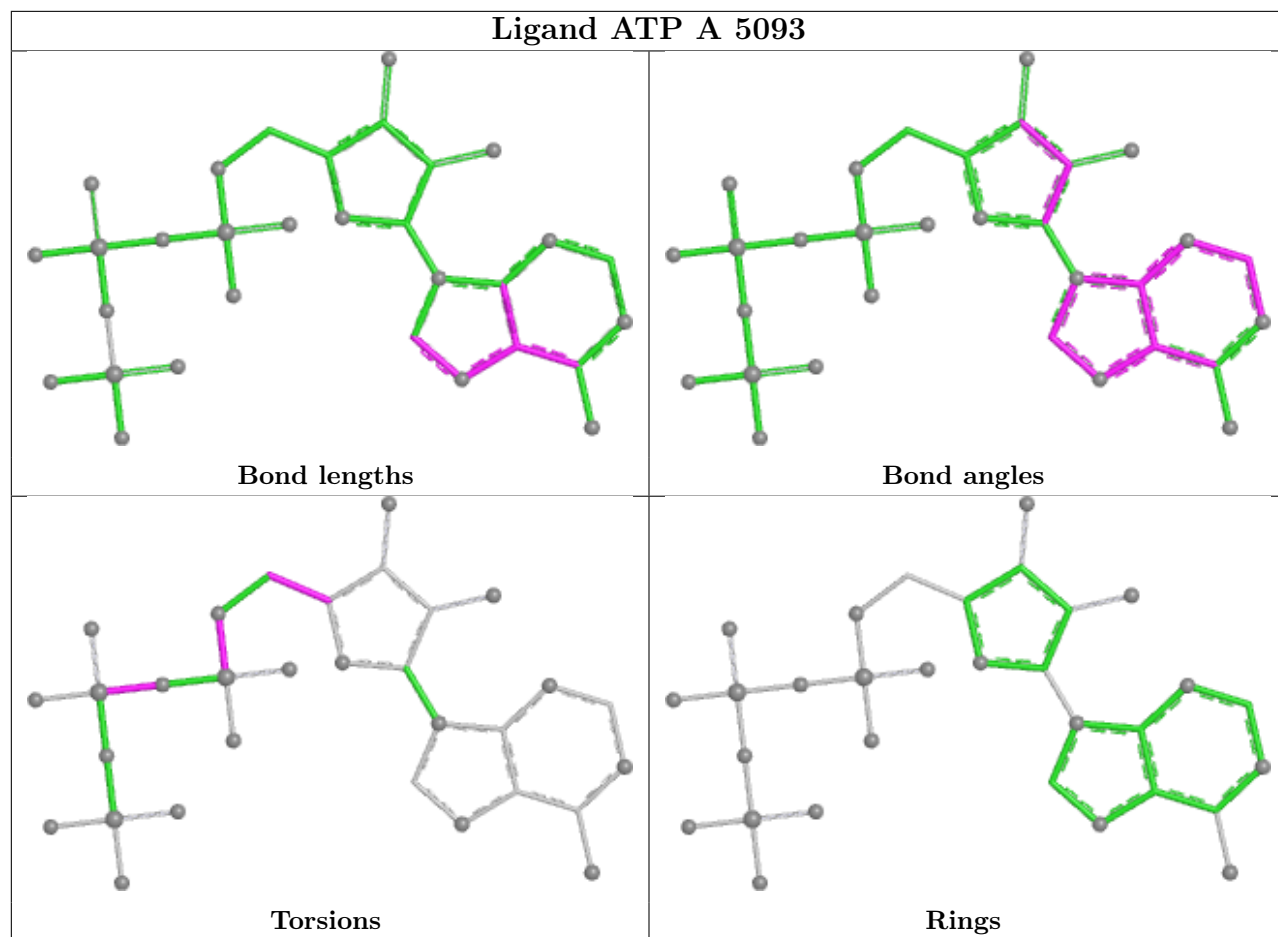
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

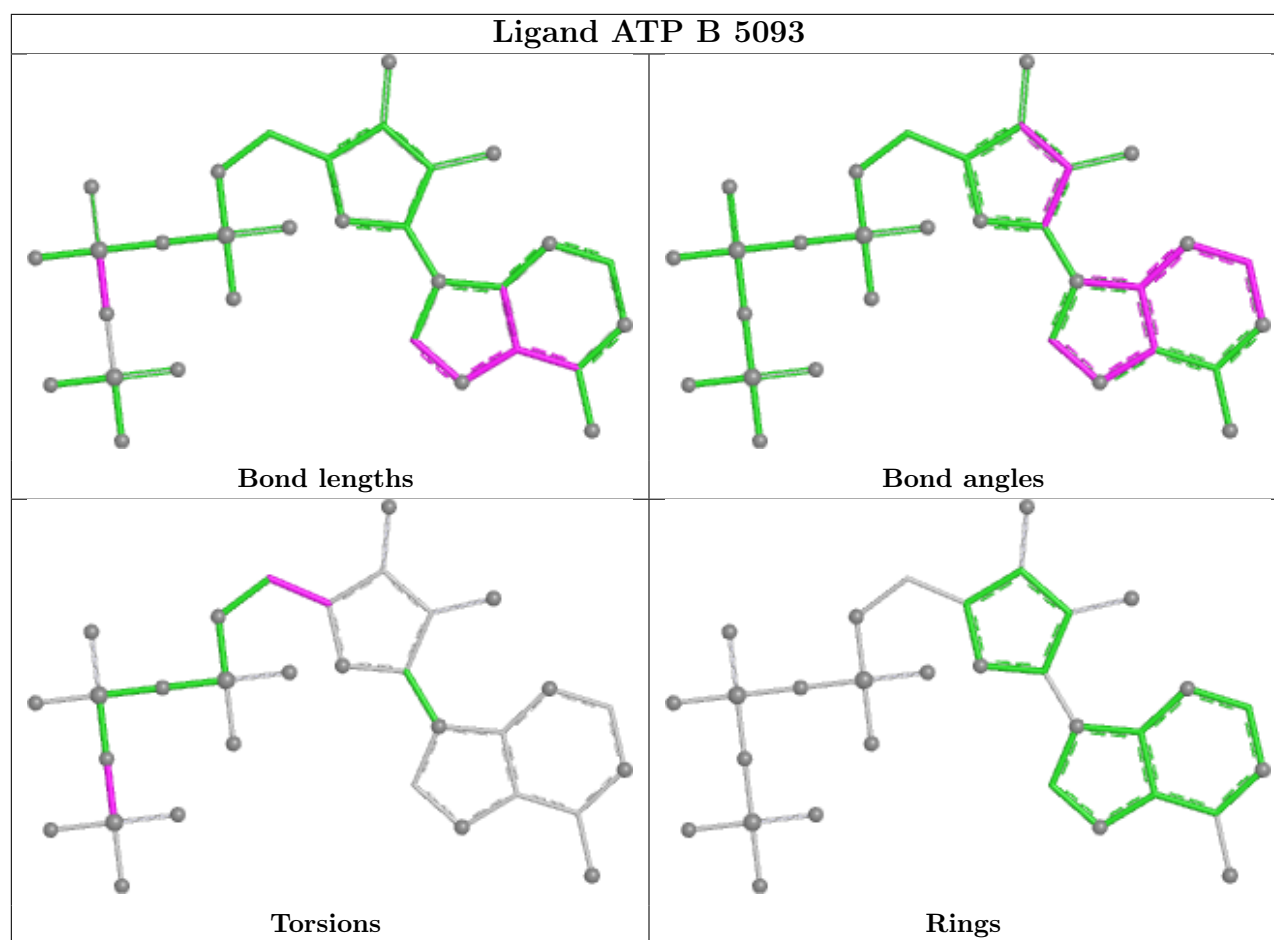
Ligand ADP A 5094



Ligand ADP B 5094







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2495:ASP	C	2496:LYS	N	1.17

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	2650/2695 (98%)	-0.34	18 (0%) 84 70	62, 134, 265, 480	1 (0%)
1	B	2650/2695 (98%)	-0.18	20 (0%) 82 68	83, 185, 334, 500	1 (0%)
All	All	5300/5390 (98%)	-0.26	38 (0%) 84 70	62, 158, 302, 500	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1546	LEU	5.3
1	A	1483	TYR	5.0
1	B	18	LEU	4.4
1	A	2757	MET	4.2
1	A	3895	PHE	4.0
1	B	2064	GLN	3.9
1	A	2064	GLN	3.7
1	A	2105	ASP	3.6
1	B	1732	GLN	3.4
1	B	1582	VAL	3.3
1	B	3393	ASN	3.1
1	A	2928	VAL	3.0
1	B	1705	TYR	3.0
1	B	1788	GLN	3.0
1	B	3330	TYR	2.9
1	B	1805	THR	2.9
1	A	2512	LYS	2.8
1	B	1458	ILE	2.8
1	B	2937	PRO	2.7
1	B	52	PRO	2.7
1	A	2732	MET	2.6
1	A	160	VAL	2.6
1	B	1590	LEU	2.6
1	A	1365	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1683	LEU	2.5
1	A	3562	LEU	2.4
1	B	3945	LEU	2.4
1	A	2574	TYR	2.4
1	B	1549	ILE	2.4
1	A	2302	PHE	2.4
1	A	2986	PRO	2.3
1	A	2518	THR	2.3
1	B	1650	LEU	2.3
1	B	3656	VAL	2.2
1	A	105	VAL	2.1
1	A	3617	GLU	2.1
1	B	1550	GLY	2.0
1	A	2184	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	5096	5/5	0.82	0.13	86,103,146,179	0
5	SO4	A	5096	5/5	0.87	0.11	77,106,130,132	0
4	MG	A	5095	1/1	0.87	0.14	76,76,76,76	0
5	SO4	B	5097	5/5	0.90	0.05	157,162,176,183	0
4	MG	B	5095	1/1	0.94	0.10	86,86,86,86	0
2	ATP	A	5093	31/31	0.94	0.10	78,92,129,144	0
3	ADP	B	5094	27/27	0.95	0.08	81,114,155,168	0
2	ATP	B	5093	31/31	0.95	0.08	93,138,174,217	0
5	SO4	A	5097	5/5	0.96	0.05	82,93,104,115	0

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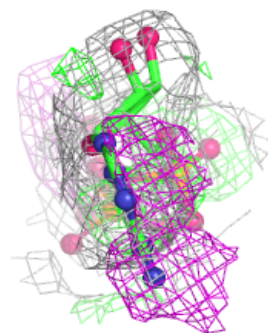
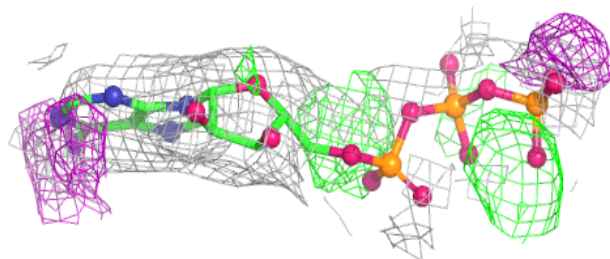
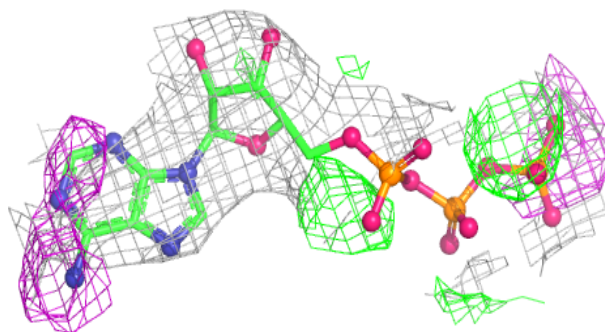
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	A	5094	27/27	0.97	0.06	91,101,113,131	0

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.

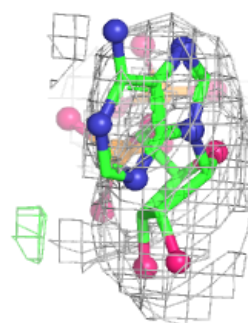
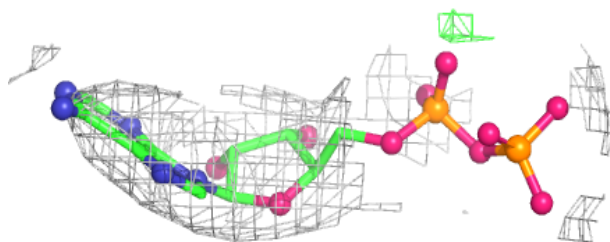
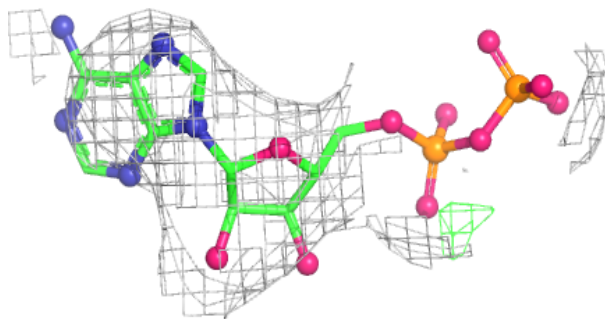
Electron density around ATP A 5093:

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

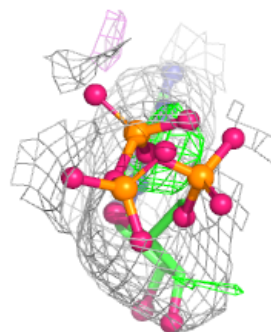
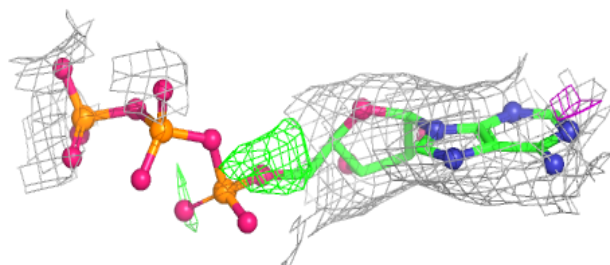
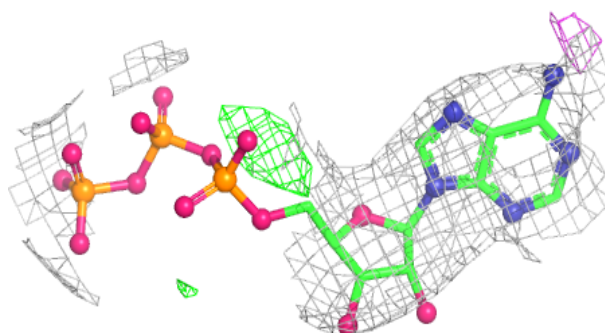


Electron density around ADP B 5094:

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

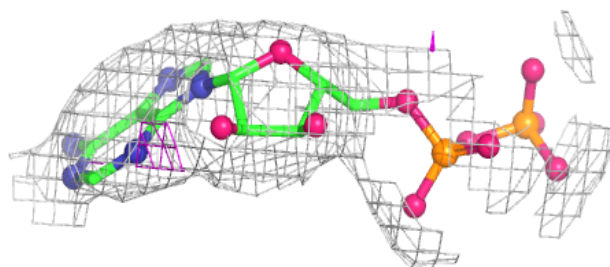
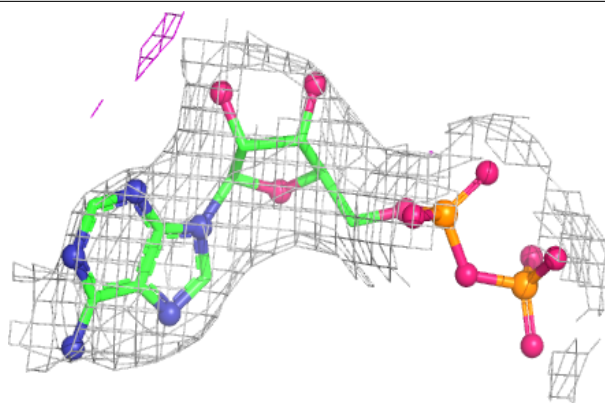
**Electron density around ATP B 5093:**

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



Electron density around ADP A 5094:

$2mF_o-DF_c$ (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.