



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:07 AM BST

PDB ID : 4AI6  
Title : Dynein Motor Domain - ADP complex  
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.  
Deposited on : 2012-02-08  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

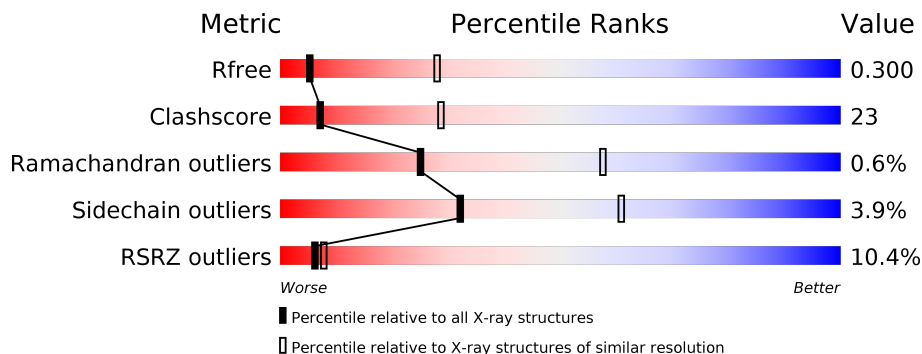
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	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	B	5400	-	-	X	-
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	A	5403	-	-	X	-
4	SO4	B	5403	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41678 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.

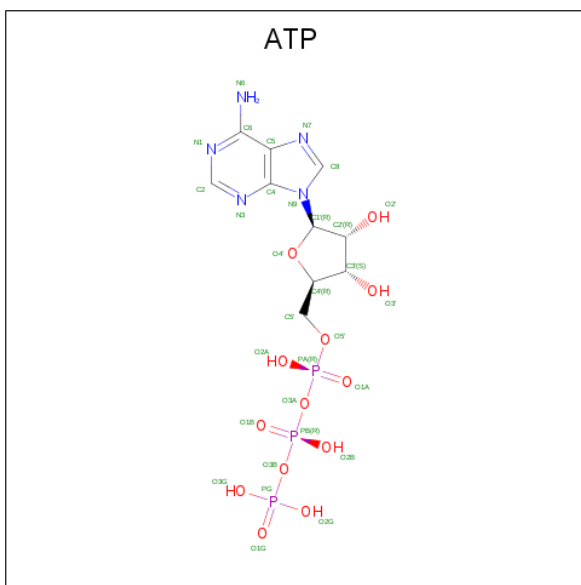
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 10 discrepancies between the modelled and reference sequences:

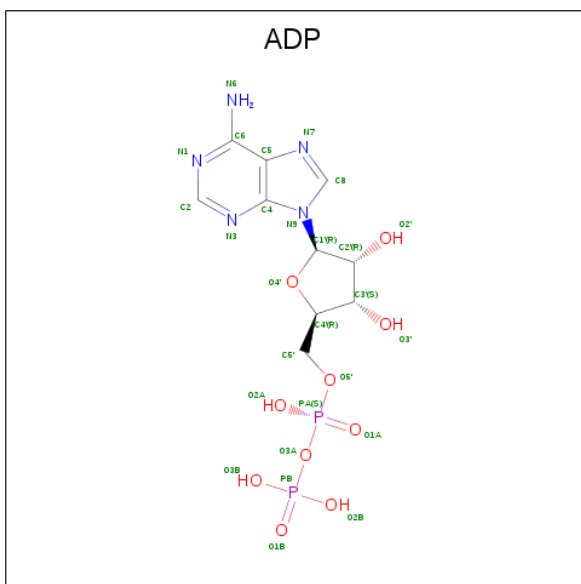
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	linker	UNP P36022
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	217	LYS	-	linker	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP P36022

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



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

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



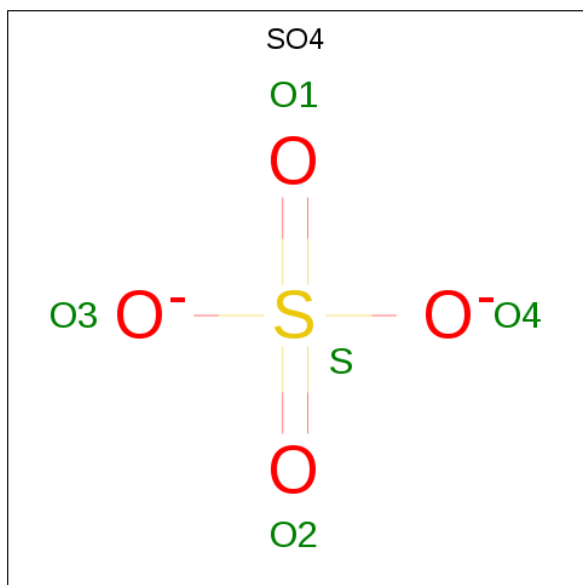
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

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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		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

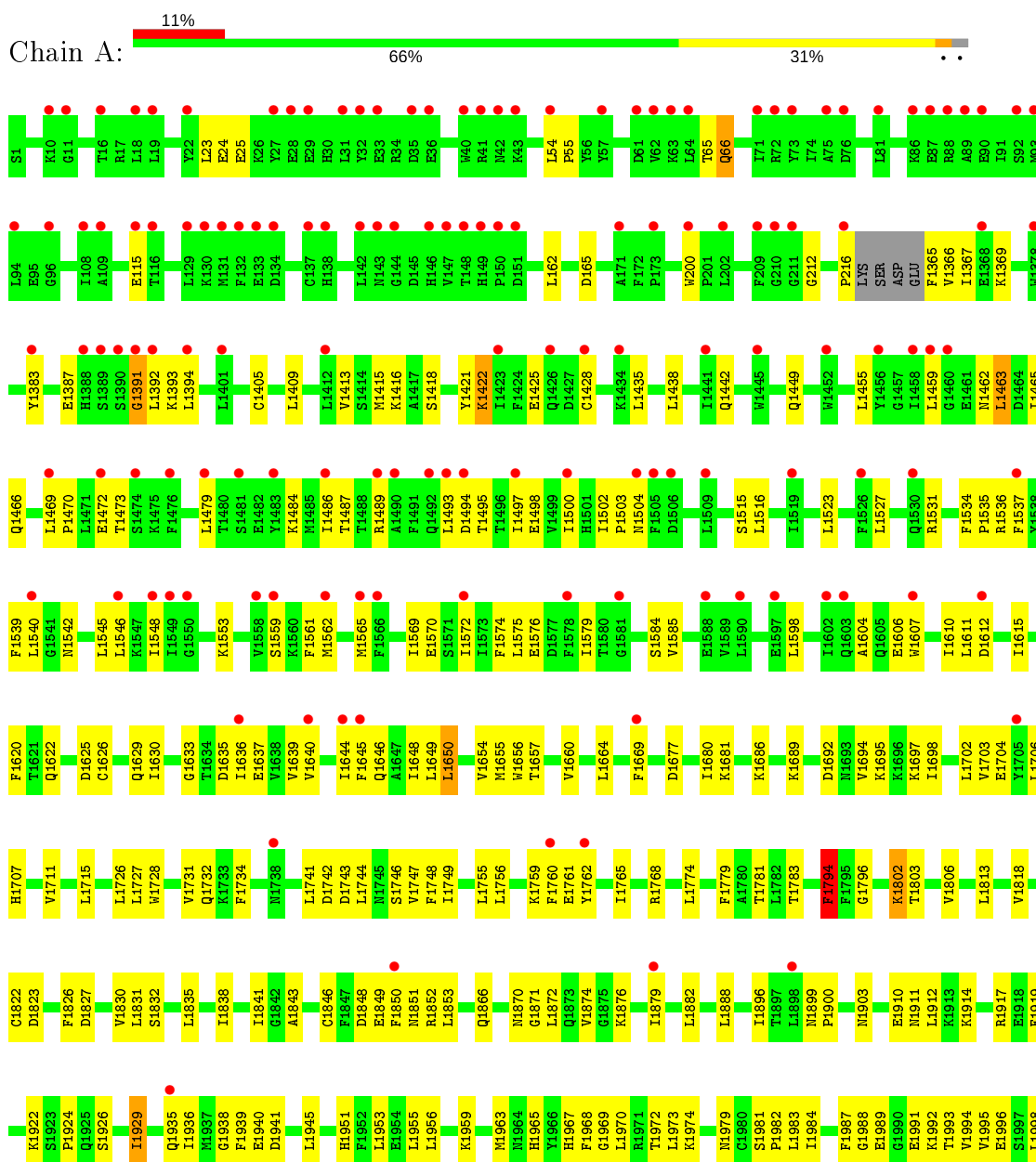
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

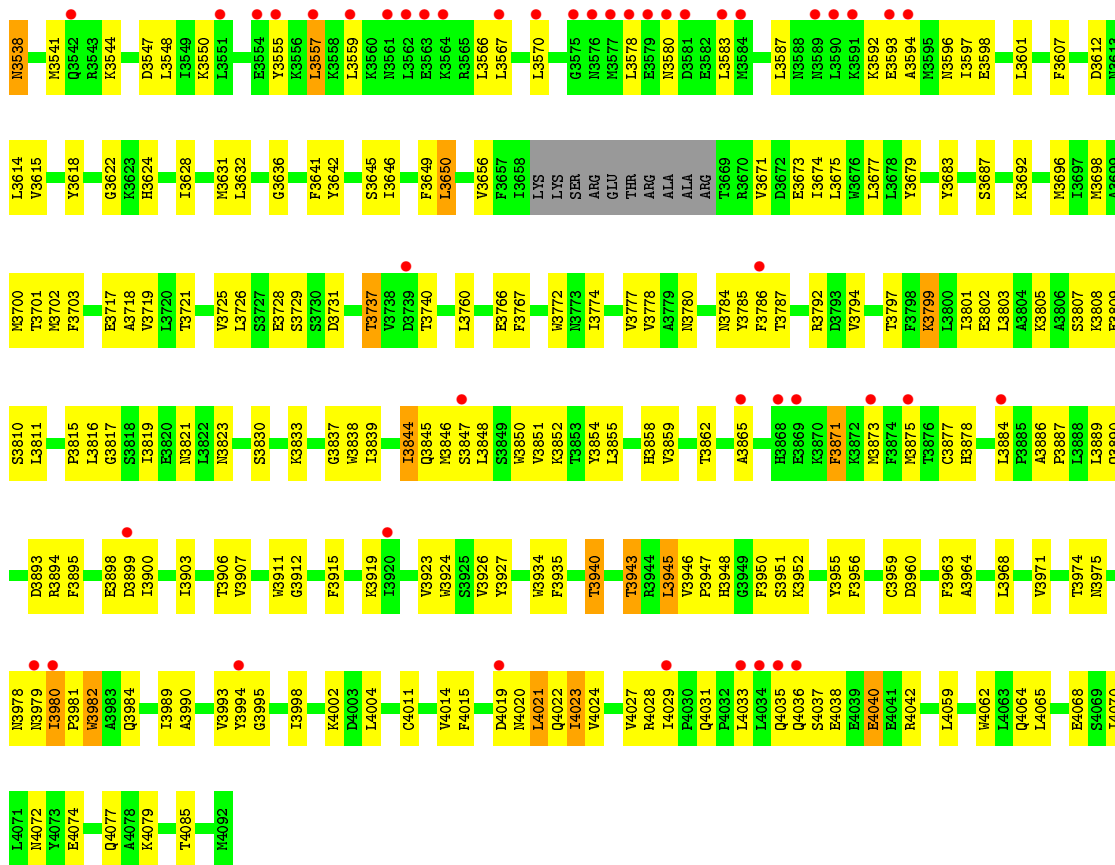
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

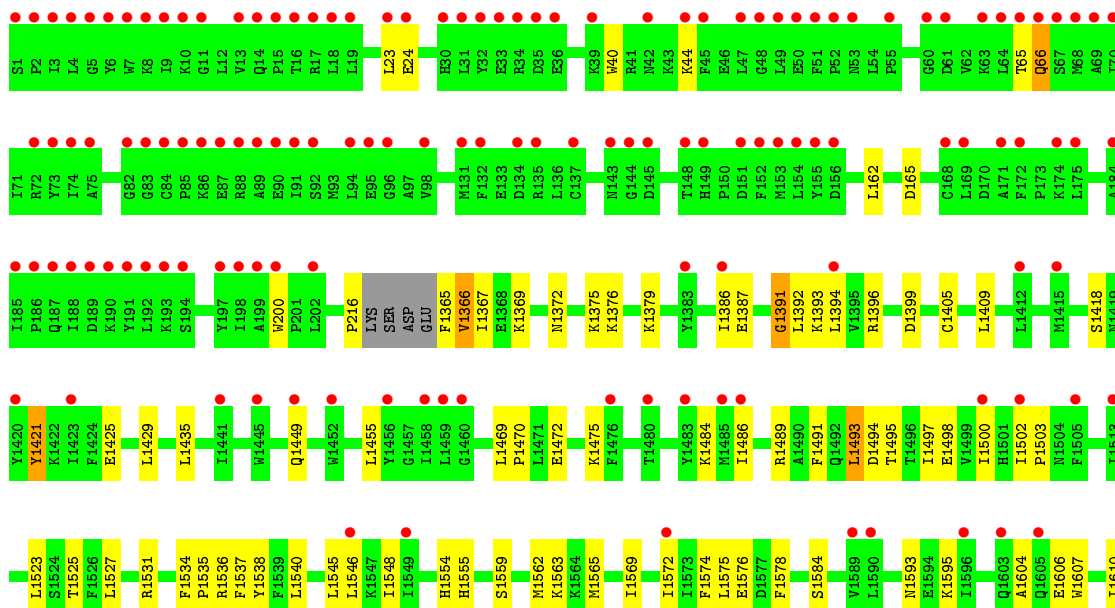


K1989	V2087	G2181	K2283	S2369	L2474	Q2569	L2681	H2787	F2889	K3311	I3416	K1989	V2087	G2181	K2283	S2369	L2474	Q2569	L2681	H2787	F2889	K3311	I3416
R2000	L2088	E2182	L2284	S2370	P2475	I2570	F2682	R2788	T2890	Q3312	K3425	R2000	L2088	E2182	L2284	S2370	P2475	I2570	F2682	R2788	T2890	Q3312	K3425
V2001	M2091	L2183	E2285	C2371	K2476	Y2571	L2686	F2795	I2891	F3313	T3426	V2001	M2091	L2183	E2285	C2371	K2476	Y2571	L2686	F2795	I2891	F3313	T3426
L2003	L2184	L2184	T2286	C2372	D2478	Y2574	G2687	L2799	D2892	T3316	F3436	L2003	L2184	L2184	T2286	C2372	K2476	Y2574	G2687	L2799	D2892	T3316	F3436
L2006	D2095	P2188	A2287	V2378	L2482	Y2575	I2688	L2808	S2992	S3317	R3438	L2006	D2095	P2188	A2287	V2378	L2482	Y2575	G2688	L2808	S2992	S3317	R3438
F2014	M2099	W2188	Q2289	S2379	L2485	R2576	S2689	L2809	M2902	E3319	R3440	F2014	M2099	W2188	Q2289	S2379	L2485	R2576	S2689	L2809	M2902	E3319	R3440
I2021	I2104	F2022	H2293	E2381	E2488	I2578	L2694	R2812	L2908	L3320	R3446	I2021	I2104	F2022	H2293	E2381	E2488	I2578	L2694	R2812	L2908	L3320	R3446
D2023	D2105	K2107	L2294	A2382	M2490	V2582	S2701	I2816	M2910	L3321	R3448	D2023	D2105	K2107	L2294	A2382	M2490	V2582	S2701	I2816	M2910	L3321	R3448
S2024	W2108	H2201	I2295	W2386	L2491	F2592	L2702	L2819	R2911	C3322	F3450	S2024	W2108	H2201	I2295	W2386	L2491	F2592	S2702	L2819	R2911	C3322	F3450
T2027	L2109	T2202	R2299	V2391	K2492	L2581	D2703	E2819	L2909	L3323	R3452	T2027	L2109	T2202	R2299	V2391	K2492	L2581	D2703	E2819	L2909	L3323	R3452
P2028	T2110	T2203	K2493	F2393	L2494	L2599	F2704	S2820	M2917	Y3007	R3454	P2028	T2110	T2203	K2493	F2393	L2494	L2599	F2704	S2820	M2917	Y3007	R3454
L2029	K2111	P2204	Q2302	P2394	L2495	L2598	V2707	I2822	R2917	L3010	F3456	L2029	K2111	P2204	Q2302	P2394	L2495	L2598	V2707	I2822	R2917	L3010	F3456
K2032	E2112	A2205	F2303	L2395	K2496	C2603	I2708	L2823	G2918	Q3014	R3458	K2032	E2112	A2205	F2303	L2395	K2496	C2603	I2708	L2823	G2918	Q3014	R3458
A2033	S2117	R2209	L2310	D2396	Y2497	Y2607	L2712	L2828	W2919	V3017	R3464	A2033	S2117	R2209	L2310	D2396	Y2497	Y2607	L2712	L2828	W2919	V3017	R3464
V2035	A2121	L2212	I2314	H2400	G2498	L2611	L2728	E2829	T2924	I3018	R3466	V2035	A2121	L2212	I2314	H2400	G2498	L2611	L2728	E2829	T2924	I3018	R3466
L2038	L2123	F2215	T2315	E2401	S2499	L2616	I2732	M2832	A2929	G3020	R3472	L2038	L2123	F2215	T2315	E2401	S2499	L2616	I2732	M2832	A2929	G3020	R3472
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G2042	R2126	C2220	S2321	L2408	K2517	Y2630	I2745	A2838	I2936	K3023	R3478	G2042	R2126	C2220	S2321	L2408	K2517	Y2630	I2745	A2838	I2936	K3023	R3478
Q2043	D2127	S2221	I2322	M2409	P2518	T2631	D2746	I2839	T2937	L3019	R3479	Q2043	D2127	S2221	I2322	M2409	P2518	T2631	D2746	I2839	T2937	L3019	R3479
S2048	G2128	I2222	L2323	R2411	K2512	A2632	R2747	D2840	G2937	G3021	R3481	S2048	G2128	I2222	L2323	R2411	K2512	A2632	R2747	D2840	G2937	G3021	R3481
H2049	L2129	S2223	L2323	K2411	G2514	M2634	E2741	D2841	M2938	L3021	R3482	H2049	L2129	S2223	L2323	K2411	G2514	M2634	E2741	D2841	M2938	L3021	R3482
F2060	F2130	S2224	L2326	R2412	R2517	I2633	R2744	L2843	E2939	V3028	R3484	F2060	F2130	S2224	L2326	R2412	R2517	I2633	R2744	L2843	E2939	V3028	R3484
Y2061	V2137	L2227	G2332	P2420	T2518	A2632	I2745	Q2845	F2940	L3028	R3486	Y2061	V2137	L2227	G2332	P2420	T2518	A2632	R2746	L2843	F2940	L3028	R3486
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Q2064	F2145	W2239	R2336	K2424	G2524	A2633	R2747	E2846	V2943	L3030	R3489	Q2064	F2145	W2239	R2336	K2424	G2524	A2633	R2747	E2846	V2943	L3030	R3489
R2065	K2241	K2240	I2339	T2426	L2525	M2634	G2754	E2848	P2940	L3031	R3490	R2065	K2241	K2240	I2339	T2426	L2525	M2634	G2754	E2848	P2940	L3031	R3490
T2066	R2149	L2246	F2346	M2428	L2526	I2635	R2756	I2849	I2941	L3032	R3492	T2066	R2149	L2246	F2346	M2428	L2526	I2635	R2756	I2849	I2941	L3032	R3492
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L2070	L2153	L2249	L2353	L2437	M2536	S2643	I2764	L2856	L2856	L3036	R3499	L2070	L2153	L2249	L2353	L2437	M2536	S2643	I2764	L2856	L2856	L3036	R3499
I2071	F2154	L2252	L2354	L2444	R2543	L2644	G2766	L2857	T2860	L3037	R3500	I2071	F2154	L2252	L2354	L2444	R2543	L2644	G2766	L2857	T2860	L3037	R3500
L2072	D2155	D2155	Y2355	F2445	R2549	V2653	I2768	G2765	L2865	L3038	R3502	L2072	D2155	D2155	Y2355	F2445	R2549	V2653	I2768	G2765	L2865	L3038	R3502
V2073	S2156	F2257	S2357	S2446	F2550	R2654	K2766	L2865	L2865	L3039	R3504	V2073	S2156	F2257	S2357	S2446	F2550	R2654	K2766	L2865	L2865	L3039	R3504
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A2076	L2170	L2262	T2358	D2448	F2552	R2657	L2768	L2871	L2871	L3041	R3508	A2076	L2170	L2262	T2358	D2448	F2552	R2657	L2768	L2871	L2871	L3041	R3508
G2077	C2078	F2266	F2360	T2448	R2552	F2657	L2768	E2871	L2871	L3042	R3510	G2077	C2078	F2266	F2360	T2448	R2552	F2657	L2768	E2871	L2871	L3042	R3510
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K2080	L2175	I2275	N2363	N2463	A2555	D2658	L2781	L2873	L2873	L3045	R3516	K2080	L2175	I2275	N2363	N2463	A2555	D2658	L2781	L2873	L2873	L3045	R3516
T2083	L2176	L2276	D2364	I2463	P2562	L2673	Q2783	W2872	W2872	L3046	R3518	T2083	L2176	L2276	D2364	I2463	P2562	L2673	Q2783	W2872	W2872	L3046	R3518
W2084	L2177	L2280	K2365	G2470	S2563	L2676	Q2783	F2877	F2877	L3047	R3520	W2084	L2177	L2280	K2365	G2470	S2563	L2676	Q2783	F2877	F2877	L3047	R3520
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T2086	N2180	N2282	F2368	L2473	S2566	V2677	I2786	H2886	H2886	L3049	R3524	T2086	N2180	N2282	F2368	L2473	S2566	V2677	I2786	H2886	H2886	L3049	R3524





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



V2920	E2824	I2784	P2591	Y2497	D2406	S2309	D2197	L2109	F2014	I1929	F1826	V1703	L1611
T2924	T2825	S2737	T2609	G2498	N2409	L2310	N2198	Z2110	I1929	I1929	D1827	E1704	D1612
M2938	A2826	M2738	Q2612	S2499	S2410	R2311	L2199	K2111	Q1935	Q1935	I1828	Y1705	I1615
T2841	E2829	E2741	S2613	L2507	K2411	V2313	D2200	E2112	I1936	I1936	Q1829	H1707	K1616
D2944	L2832	L2742	R2620	R2508	R2412	L2314	T2202	S2117	M1937	M1937	L1830	V1711	E1620
F2943	L2833	L2743	R2625	Q2508	R2412	T2315	T2203	S2121	G1938	G1938	L1831	F1714	T1621
ILE	L2835	R2744	L2415	K2512	L2415	L2316	A2205	L2122	F1939	F1939	R1833	Q1714	C1626
VAL	L2838	I2745	C2417	Q2513	C2417	L2317	P2208	L2123	P2028	P2028	L1834	L1715	C1626
PRO	A2838	Q2751	P2420	K2517	R2320	R2319	L2212	D2127	K2032	K2032	I1835	S1719	I1630
GLU	D2842	G2754	R2321	R2518	S2321	R2321	C2220	T2131	L2033	L1945	I1838	T1720	I1630
VAL	L2843	H2755	L2322	E2520	S2222	L2322	S2220	V2137	L2034	I1949	I1841	K1721	G1683
ASN	F2844	M2756	L2326	T2425	S2223	L2326	I2222	V2137	V2035	I1949	G1842	L1726	I1636
GLU	Q2845	M2757	G2332	M2428	K2224	G2332	S2224	I2141	G2043	F1952	A1843	L1727	V1639
LEU	C2846	L2758	Q2336	L2437	S2225	Q2336	K2225	I2141	R2044	L1953	W1844	W1728	V1640
VAL	Y2849	I2759	P2337	L2437	L2229	Q2335	L2229	F2145	L1956	L1956	G1845	F1734	L1649
PHE	Y2849	G2760	R2638	L2437	L2230	R2336	L2230	R2149	H1967	H1967	E1849	Y1735	Y1643
THR	L2852	A2761	Q2639	V2440	L2230	R2336	L2230	I2150	F1968	F1968	F1850	L1741	I1644
GLU	L2853	R2762	Q2639	V2440	N2239	L2339	N2239	W2151	F1968	F1968	N1851	L1741	F1645
PRO	L2853	R2763	T2640	F2445	L2249	L2339	L2249	W2152	G1969	G1969	R1852	D1742	Q1646
ILE	L2856	T2764	L2641	S2446	L2249	F2346	L2249	V2152	L1970	L1970	L1853	D1743	L1649
GLN	L2856	G2765	R2642	K2447	F2346	F2346	L2249	V2155	R1971	R1971	G1857	L1744	L1649
T2960	L2860	K2766	S2643	D2448	S2350	S2350	L2252	D2154	T1972	T1972	V1857	F1748	M1655
I2961	T2860	T2767	R2646	T2448	Q2351	Q2351	L2252	K2065	C1980	C1980	M1870	Y1758	L1664
R2962	L2866	L2768	R2646	T2448	Q2351	Q2351	L2252	L2154	G1871	G1871	G1871	Y1758	Q1665
D2963	L2866	L2768	L2673	T2464	T2358	T2358	L2265	D2155	L1973	L1973	L1850	F1760	T1666
A2964	L2867	T2770	L2673	T2464	L2359	L2359	L2265	D2156	K1974	K1974	N1864	F1760	T1666
V2965	L2867	Q2783	V2677	S2468	L2361	L2361	E2274	D2157	L1974	L1974	I1865	I1749	W1657
V2966	E2870	P2784	V2677	S2468	A2362	A2362	E2274	D2158	L1974	L1974	L1865	S1750	T1657
N2967	L2873	K2785	L2886	L2468	L2362	L2362	E2275	D2159	L1978	L1978	Q1866	L1755	V1680
F2972	L2873	L2786	L2886	Y2464	S2367	S2367	L2276	D2160	R1979	R1979	M1870	L1755	V1680
V2982	F2877	V2782	L2886	Y2464	T2368	T2368	L2276	E2161	C1980	C1980	G1871	Y1758	L1664
G2983	V2878	Q2783	L2886	T2467	L2368	L2368	L2276	E2161	S1981	S1981	L1872	Y1758	Q1665
S2988	H2886	K2785	L2886	S2468	A2362	A2362	L2276	E2161	P1982	P1982	L1882	F1760	T1666
P2989	F2889	L2786	L2886	L2472	L2363	L2363	L2276	D2172	L1989	L1989	L1898	E1761	N1667
G2990	T2890	E2787	L2886	L2473	L2365	L2365	L2276	N2173	G1990	G1990	M1899	Y1762	Q1668
K3001	L2891	R2788	L2886	L2474	L2366	L2366	L2276	K2174	E1991	E1991	P1900	Y1762	Q1668
I3010	C2892	L2792	L2886	P2475	S2367	S2367	L2282	L2175	K1992	K1992	R1905	E1762	F1689
E3012	D2893	F2795	L2886	K2476	F2368	F2368	N2282	L2176	T1993	T1993	R1768	L1774	D1677
F3017	P2894	L2799	L2886	S2477	L2368	L2368	E2285	T2177	V1994	V1994	L1908	E1768	I1680
I3018	M2902	L2799	L2886	D2478	L2380	L2380	E2285	L2178	E1996	E1996	P1909	I1770	K1681
V3019	L2903	R2812	L2886	K2480	L2380	L2380	E2285	G2181	S1997	S1997	L1912	L1774	L1683
G3020	A2907	T2813	L2886	L2484	E2384	E2384	E2285	E2182	K1999	K1999	L1912	T1781	K1689
L2912	N2910	C2814	L2886	E2488	V2385	V2385	L2293	R2183	R2000	R2000	R1917	T1781	K1689
C2913	L2815	R2814	L2886	L2489	N2386	N2386	L2293	E2186	I2003	I2003	E1918	F1794	D1692
T2914	L2816	L2816	L2886	L2489	R2387	R2387	L2293	I2186	V2001	V2001	E1918	F1794	D1692
I2915	L2817	V2713	L2886	L2491	L2390	L2390	L2293	F2190	L2003	L2003	F1919	F1795	K1695
N2916	L2818	V2713	L2886	L2491	L2390	L2390	L2293	R2191	L2003	L2003	S1920	K1802	K1696
M3025	D2819	E2819	L2886	L2491	L2390	L2390	L2293	R2191	L2003	L2003	M1921	K1802	K1696
E3026	L2822	E2819	L2886	L2491	L2390	L2390	L2293	L2193	L2006	L2006	K1922	K1802	K1696
S3027	W2822	E2819	L2886	L2491	L2390	L2390	L2293	L2105	G2007	G2007	S1923	K1802	K1696
V3028	W2822	E2819	L2886	L2491	L2390	L2390	L2293	L2106	D2008	D2008	S1923	L1813	I1688
	L2823	L2823	L2886	L2496	L2397	L2397	L2293	L2106	E2011	E2011	Q1924	L1813	I1688
				K2496	T2397	T2397	L2293	L2106			Q1924	C1822	L1701
				K2496	T2397	T2397	L2293	L2106			Q1924	D1823	L1702

S4037	E4038	E4039	E4040	L4045	F4052	S4060	S4061	W4062	L4065	D3958	C3959	D3960	F3963	A3964	S3965	L3968	N3978	N3979	F3980	F3981	N3982	A3983	Q3984	Y3994	I3998	K4002	P4003	L4004	V4006	V4014	G4017	S4018	D4019	N4020	L4021	Q4022	L4023	V4024	V4027	R4028	L4029	P4030	Q4035	Q4036							
K3852	I3853	L3854	L3855	H3858	V3859	T3862	A3865	E3866	E3867	F3871	M3872	F3873	K3874	N3875	T3876	C3877	H3878	L3884	F3885	A3886	P3887	L3888	L3889	Q3890	R3894	F3895	V3896	Y3897	E3898	D3899	L3904	D3905	T3906	V3911	G3912	F3915	F3916	T3917	G3918	K3919	V3923	W3924	S3925	V3926	Y3927	W3934	F3935	F3936	V3851		
I3870	V3871	I3874	L3877	Y3883	F3886	N3887	T3888	L3889	L3890	D3891	K3892	F3893	F3894	N3898	N3700	T3701	N3702	F3703	F3708	Y3715	L3720	V3725	L3726	S3729	S3730	D3731	F3734	K3735	L3736	T3737	T3740	N3741	L3744	L3747	L3757	L3760	N3763	F3768	F3769	N3571	N3572	S3573	Q3574								
G3575	N3576	N3577	L3578	E3579	N3580	D3581	E3582	L3583	M3584	V3585	S3586	T3588	L3587	N3588	N3589	K3592	E3593	A3594	N3595	N3596	E3605	D3612	H3613	L3614	E3615	E3616	Y3617	Y3618	G3622	F3629	S3630	M3631	L3632	E3633	F3641	I3644	S3645	I3646	V3656	F3657	I3658	L35	SER	ARG	GLU	THR	ARG	ALA	ALA	ARG	T3669
G3482	D3483	V3488	S3502	I3505	L3509	R3510	E3592	N3593	S3400	Q3401	D3402	A3403	F3406	L3407	L3408	D3409	H3413	K3414	I3415	T3416	V3417	L3429	R3439	L3440	A3443	F3446	V3450	D3459	P3460	I3461	I3462	S3463	R3464	L3465	I3466	S3467	F3470	N3471	H3472	A3473	E3568	E3569	L3570	N3571	N3572	S3573	Q3574				
LEU	LYS	VAL	ASN	GLU	LEU	ASN	LYS	THR	SER	LEU	LEU	ILE	SER	LEU	VAL	T3300	K3303	E3304	R3305	W3306	L3307	N3308	K3311	Q3312	F3313	S3314	K3315	F3316	S3317	Q3318	E3319	N3323	I3326	I3329	Y3330	I3341	F3334	N3338	E3341	R3342	L3346	V3347	I3348	L3349	K3350	R3351	L3352	L3353	K3359		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.89Å 119.17Å 193.97Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	49.29 – 3.40 49.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.24-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.7.0019	Depositor
R, $R_{free}$	0.241 , 0.303 0.236 , 0.300	Depositor DCC
$R_{free}$ test set	5512 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	133.4	Xtrriage
Anisotropy	0.397	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 132.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	41678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	190.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, SO4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/21146	0.77	12/28618 (0.0%)
1	B	0.52	0/21146	0.76	9/28618 (0.0%)
All	All	0.53	0/42292	0.77	21/57236 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	2455	LEU	CB-CG-CD1	-8.01	97.38	111.00
1	A	3650	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	A	1882	LEU	CA-CB-CG	6.87	131.09	115.30
1	A	1463	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	3945	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	A	4021	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	A	4059	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	B	1872	LEU	CB-CG-CD2	5.95	121.11	111.00
1	B	1882	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	200	TRP	C-N-CA	5.77	146.22	122.00
1	B	200	TRP	C-N-CA	5.45	144.89	122.00
1	B	2158	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	4042	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	2471	LEU	CA-CB-CG	5.34	127.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3726	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	A	4023	ILE	CG1-CB-CG2	-5.29	99.77	111.40
1	A	1794	PHE	N-CA-CB	5.27	120.09	110.60
1	B	2158	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	2279	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	1938	GLY	N-CA-C	-5.23	100.03	113.10
1	A	1650	LEU	CB-CG-CD1	5.21	119.85	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3308	ASN	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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	934	0
1	B	20748	0	20207	930	0
2	A	31	0	12	6	0
2	B	31	0	12	22	0
3	A	54	0	24	28	0
3	B	54	0	24	29	0
4	A	5	0	0	2	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41678	0	40485	1867	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 (1867) 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:B:2732:MET:HB2	3:B:5402:ADP:C6	1.40	1.57
1:B:1365:PHE:CD1	1:B:1366:VAL:HG23	1.34	1.57
1:A:1365:PHE:CE2	1:A:1366:VAL:HG23	1.55	1.39
1:A:1365:PHE:CD2	1:A:1366:VAL:HG23	1.68	1.27
1:B:1365:PHE:CE1	1:B:1366:VAL:HG23	1.70	1.27
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.70	1.26
1:B:2386:MET:CG	1:B:2627:ARG:HD2	1.69	1.23
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.60	1.19
1:B:2380:LEU:CD2	1:B:2390:ILE:HD11	1.71	1.19
1:B:2473:LEU:CD2	1:B:2475:PRO:HD3	1.72	1.18
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.22	1.18
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.22	1.18
1:A:1365:PHE:CE2	1:A:1366:VAL:CG2	2.26	1.17
1:B:2732:MET:HB2	3:B:5402:ADP:C5	1.79	1.17
1:B:2732:MET:HE3	1:B:2768:ILE:HG23	1.25	1.17
1:A:2517:LYS:HE3	1:A:2524:VAL:CG2	1.73	1.17
1:A:1983:LEU:HG	1:A:1993:THR:HG23	1.26	1.17
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.62	1.15
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.23	1.15
1:B:2473:LEU:HD23	1:B:2475:PRO:HD3	1.17	1.15
1:B:1365:PHE:CD1	1:B:1366:VAL:CG2	2.30	1.15
1:A:1826:PHE:HE2	1:A:1831:LEU:HB2	1.13	1.14
1:B:2732:MET:CE	1:B:2768:ILE:HG21	1.78	1.14
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.17	1.13
1:B:2386:MET:HG2	1:B:2627:ARG:HD2	1.16	1.13
1:B:2732:MET:CE	1:B:2768:ILE:CG2	2.26	1.13
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.61	1.13
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.48	1.13
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.13	1.12
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.22	1.12
1:B:2380:LEU:HD21	1:B:2390:ILE:CD1	1.78	1.11
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.15	1.11
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.61	1.11
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	1.81	1.11
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.32	1.11
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	1.09	1.11
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.33	1.11
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.80	1.11
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.30	1.10
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.14	1.10
1:B:2732:MET:HE1	1:B:2768:ILE:HG21	1.17	1.10
1:A:1826:PHE:CE2	1:A:1831:LEU:HB2	1.86	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2732:MET:CB	3:B:5402:ADP:C6	2.34	1.10
1:B:2732:MET:HE3	1:B:2768:ILE:CG2	1.80	1.10
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.64	1.10
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.15	1.09
1:A:3306:TRP:CH2	1:A:3594:ALA:HB3	1.86	1.09
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.20	1.09
1:B:216:PRO:O	1:B:1365:PHE:HB2	1.50	1.08
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.53	1.08
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.14	1.08
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.28	1.07
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.34	1.07
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.52	1.06
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.33	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.37	1.06
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.53	1.06
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.11	1.05
1:B:2473:LEU:HD23	1:B:2475:PRO:CD	1.86	1.05
1:B:2785:LYS:HD3	1:B:3482:GLY:O	1.56	1.05
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.57	1.05
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.33	1.05
1:B:2473:LEU:CD2	1:B:2475:PRO:CD	2.33	1.05
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.09	1.04
1:B:2378:VAL:HG22	1:B:2380:LEU:CD1	1.86	1.04
1:B:2386:MET:CB	1:B:2627:ARG:HD2	1.87	1.04
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.88	1.03
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.04	1.03
1:A:1421:TYR:HD1	1:A:1425:GLU:HB2	1.18	1.03
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.56	1.03
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.36	1.03
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.38	1.02
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.19	1.02
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.39	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.02	1.02
1:A:1999:LYS:HG2	1:A:2014:PHE:CE1	1.95	1.01
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.88	1.01
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.90	1.01
1:B:2732:MET:HB2	3:B:5402:ADP:N1	1.76	1.01
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.61	1.00
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.91	1.00
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.41	1.00
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	1.00	1.00
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	1.97	1.00
1:B:2386:MET:HG2	1:B:2627:ARG:CD	1.92	0.99
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.44	0.99
1:B:1365:PHE:CE1	1:B:1366:VAL:CG2	2.45	0.99
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.51	0.99
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.93	0.99
1:B:1365:PHE:HD1	1:B:1366:VAL:CG2	1.71	0.99
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.93	0.99
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.93	0.99
1:B:1421:TYR:CE1	1:B:1425:GLU:CG	2.46	0.98
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.39	0.98
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	0.98	0.98
1:A:2732:MET:CE	1:A:2768:ILE:HG21	1.94	0.98
1:A:3307:LEU:HD12	1:A:3307:LEU:C	1.82	0.97
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.93	0.97
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.95	0.97
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.93	0.97
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.64	0.97
1:B:2137:VAL:O	1:B:2141:ILE:HG23	1.65	0.97
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	1.02	0.97
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.00	0.97
1:B:1535:PRO:CB	1:B:1841:ILE:HG13	1.95	0.97
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.05	0.97
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.43	0.96
1:A:2768:ILE:HG22	3:A:5402:ADP:O2A	1.65	0.96
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.49	0.96
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.94	0.96
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	2.00	0.96
1:A:1421:TYR:O	1:A:1421:TYR:CD1	2.19	0.95
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.45	0.95
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.53	0.95
1:B:1421:TYR:CE1	1:B:1425:GLU:HG3	2.02	0.95
1:A:2407:LEU:HD22	1:A:2412:ARG:HH12	1.32	0.95
1:A:2765:GLY:HA2	3:A:5402:ADP:PA	2.07	0.95
1:B:2412:ARG:NH1	1:B:2553:HIS:HA	1.82	0.94
1:A:3307:LEU:HD12	1:A:3307:LEU:O	1.67	0.94
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.02	0.94
1:A:3306:TRP:CZ2	1:A:3594:ALA:HB3	2.03	0.94
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.96	0.94
1:B:2080:LYS:HD2	1:B:2195:GLU:HB2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2732:MET:HE3	1:A:2768:ILE:HG21	1.47	0.94
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.66	0.94
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.49	0.94
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.03	0.94
1:A:2109:LEU:HD11	1:A:2129:LEU:HD22	1.48	0.94
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.86	0.94
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.96	0.94
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	1.98	0.94
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.47	0.93
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	1.98	0.93
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.68	0.93
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	1.99	0.93
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.47	0.93
1:B:2920:TRP:HB2	1:B:2989:PRO:CG	1.97	0.93
1:A:3303:LYS:HD2	1:A:3306:TRP:HB2	1.51	0.93
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.67	0.93
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.69	0.93
1:B:2761:ALA:O	1:B:2892:CYS:HB3	1.69	0.93
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.48	0.92
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.82	0.92
1:B:1421:TYR:CZ	1:B:1425:GLU:HG3	2.05	0.92
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.99	0.91
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.01	0.91
1:B:1535:PRO:HB2	1:B:1841:ILE:CD1	2.00	0.91
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.51	0.91
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.71	0.91
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.77	0.91
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	2.05	0.91
1:A:3304:GLU:O	1:A:3307:LEU:HG	1.68	0.90
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	2.01	0.90
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.50	0.90
1:A:3304:GLU:HG3	1:A:3307:LEU:HD23	1.51	0.90
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.36	0.90
1:A:1939:PHE:CD1	1:A:1940:GLU:O	2.24	0.90
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.53	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.51	0.90
1:A:2762:SER:O	1:A:2763:ARG:HB2	1.70	0.90
1:A:1421:TYR:CD1	1:A:1425:GLU:HB2	2.07	0.90
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.52	0.89
1:B:1365:PHE:CD1	1:B:1366:VAL:N	2.40	0.89
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.98	0.89
1:A:3306:TRP:CH2	1:A:3594:ALA:CB	2.54	0.89
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.73	0.89
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.08	0.89
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.70	0.89
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.03	0.89
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.03	0.88
1:B:2732:MET:CB	3:B:5402:ADP:C5	2.56	0.88
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.53	0.88
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.53	0.88
1:A:2517:LYS:HE3	1:A:2524:VAL:HG22	1.54	0.88
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.03	0.88
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.91	0.88
1:B:1939:PHE:CD1	1:B:1940:GLU:O	2.26	0.88
1:A:1929:ILE:HD13	1:A:1970:LEU:HD11	1.56	0.88
1:B:3792:ARG:HB2	1:B:3955:TYR:CD1	2.09	0.88
1:A:1416:LYS:HA	1:A:1421:TYR:CZ	2.09	0.88
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	2.03	0.88
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.04	0.88
1:A:2517:LYS:CE	1:A:2524:VAL:CG2	2.51	0.88
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.86	0.87
1:A:2988:SER:CB	1:A:2989:PRO:HD2	2.03	0.87
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.05	0.87
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	1.89	0.87
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.04	0.87
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.57	0.87
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.57	0.87
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.74	0.87
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.04	0.86
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.56	0.86
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.59	0.86
1:B:2080:LYS:NZ	1:B:2549:ARG:NH2	2.21	0.86
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.01	0.86
1:A:2763:ARG:O	3:A:5402:ADP:C8	2.27	0.86
1:B:1992:LYS:CG	1:B:2024:SER:HB2	2.04	0.86
1:B:2988:SER:CB	1:B:2989:PRO:HD2	2.00	0.86
1:B:2563:SER:HB3	1:B:2566:SER:H	1.39	0.86
1:B:2733:VAL:N	3:B:5402:ADP:N1	2.22	0.86
1:B:2378:VAL:CG2	1:B:2380:LEU:CD1	2.54	0.86
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.56	0.86
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2080:LYS:HZ2	1:B:2549:ARG:NH2	1.73	0.86
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.06	0.85
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	2.11	0.85
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.23	0.85
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.75	0.85
1:A:3792:ARG:HB2	1:A:3955:TYR:CD1	2.12	0.85
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.06	0.85
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.23	0.85
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.12	0.85
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.59	0.84
1:A:1926:SER:CB	1:A:1970:LEU:HD12	2.08	0.84
1:B:1983:LEU:CG	1:B:1993:THR:HG23	2.04	0.84
1:B:2412:ARG:HH11	1:B:2553:HIS:HA	1.35	0.84
1:A:2765:GLY:HA2	3:A:5402:ADP:O2A	1.76	0.84
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.92	0.84
1:B:2225:LYS:HA	2:B:5400:ATP:C2	2.12	0.84
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.58	0.84
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.08	0.84
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.78	0.84
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.60	0.83
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.08	0.83
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.78	0.83
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.61	0.83
1:A:2785:LYS:HD2	1:A:3482:GLY:O	1.78	0.83
1:B:1421:TYR:CE1	1:B:1425:GLU:HG2	2.10	0.83
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.43	0.83
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	2.04	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.08	0.83
1:A:2763:ARG:O	3:A:5402:ADP:H8	1.62	0.83
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.43	0.83
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.94	0.83
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.61	0.83
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.60	0.83
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.59	0.82
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.61	0.82
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.08	0.82
1:A:1640:VAL:HB	1:A:1686:LYS:HZ1	1.42	0.82
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.61	0.82
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.79	0.82
1:A:2563:SER:HB3	1:A:2566:SER:H	1.44	0.82
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.83	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.62	0.81
1:A:2517:LYS:CE	1:A:2524:VAL:HG21	2.11	0.81
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.78	0.81
1:A:1996:GLU:O	1:A:2000:ARG:HG3	1.78	0.81
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.46	0.81
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.59	0.81
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.28	0.81
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.96	0.81
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.62	0.80
1:A:1421:TYR:HE1	1:A:1425:GLU:CD	1.83	0.80
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.81	0.80
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.16	0.80
1:A:1535:PRO:C	1:A:1841:ILE:HD11	2.02	0.80
1:A:1983:LEU:CG	1:A:1993:THR:HG23	2.10	0.80
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.64	0.80
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.81	0.80
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.61	0.80
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.30	0.80
1:A:1983:LEU:HD23	1:A:1993:THR:O	1.81	0.79
1:A:2109:LEU:CD1	1:A:2129:LEU:HD22	2.12	0.79
1:B:2732:MET:HE1	1:B:2768:ILE:CG2	1.96	0.79
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.17	0.79
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.12	0.79
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.65	0.79
1:A:1999:LYS:HG2	1:A:2014:PHE:HE1	1.43	0.79
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.65	0.79
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.12	0.79
1:A:216:PRO:C	1:A:1365:PHE:HA	2.04	0.78
1:A:2424:LYS:HZ1	3:A:5401:ADP:PB	2.06	0.78
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.71	0.78
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.65	0.78
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.98	0.78
1:B:2080:LYS:HE2	2:B:5400:ATP:O1B	1.84	0.78
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.10	0.78
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.50	0.78
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.84	0.78
1:A:3792:ARG:HB2	1:A:3955:TYR:CE1	2.19	0.78
1:B:3690:LEU:HD23	1:B:3694:PHE:HB3	1.66	0.78
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.84	0.77
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.67	0.77
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.65	0.77
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.31	0.77
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.84	0.77
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.64	0.77
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.72	0.77
1:B:1425:GLU:OE2	1:B:1429:LEU:CG	2.32	0.77
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.85	0.77
1:B:2446:SER:H	1:B:2449:THR:HG23	1.49	0.77
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.15	0.77
1:A:2446:SER:H	1:A:2449:THR:CG2	1.97	0.77
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.49	0.77
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.14	0.76
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.67	0.76
1:A:3306:TRP:CZ2	1:A:3594:ALA:CB	2.69	0.76
1:B:2476:LYS:CD	1:B:2476:LYS:H	1.98	0.76
1:B:3303:LYS:O	1:B:3306:TRP:HD1	1.68	0.76
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.85	0.76
1:A:1983:LEU:CD2	1:A:1993:THR:O	2.34	0.76
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	2.00	0.76
1:A:1802:LYS:HG3	4:A:5403:SO4:O2	1.86	0.76
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.34	0.76
1:B:2517:LYS:HD2	1:B:2524:VAL:CG2	2.15	0.76
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.85	0.76
1:B:1983:LEU:HG	1:B:1993:THR:CG2	2.07	0.76
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.68	0.76
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.64	0.76
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.68	0.76
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.00	0.76
1:A:3737:THR:HB	1:A:3740:THR:CB	2.15	0.75
1:A:1939:PHE:HD1	1:A:1940:GLU:O	1.69	0.75
1:B:2378:VAL:HG22	1:B:2380:LEU:HD12	1.66	0.75
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.68	0.75
1:B:2473:LEU:HD11	1:B:2527:GLU:CG	2.16	0.75
1:A:2513:GLN:O	1:A:2526:ILE:HG13	1.86	0.75
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.87	0.75
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.68	0.75
1:B:2732:MET:HA	3:B:5402:ADP:C2	2.22	0.75
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.68	0.74
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	2.02	0.74
1:A:3785:TYR:HE1	1:A:3859:VAL:HG22	1.52	0.74
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.69	0.74
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.87	0.74
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.17	0.74
1:A:1421:TYR:CE1	1:A:1425:GLU:CD	2.61	0.74
1:B:2473:LEU:CD2	1:B:2475:PRO:CG	2.66	0.74
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.87	0.74
1:A:2424:LYS:NZ	3:A:5401:ADP:PB	2.61	0.74
1:B:1535:PRO:HB2	1:B:1841:ILE:HD11	1.68	0.74
1:B:2380:LEU:HD21	1:B:2390:ILE:HD11	0.82	0.74
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.51	0.74
1:B:2473:LEU:HD22	1:B:2475:PRO:HD3	1.69	0.74
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.03	0.73
1:B:1425:GLU:OE2	1:B:1429:LEU:HG	1.87	0.73
1:B:2080:LYS:HG2	2:B:5400:ATP:PB	2.27	0.73
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.88	0.73
1:A:2763:ARG:HE	3:A:5402:ADP:H4'	1.53	0.73
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.86	0.73
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.69	0.73
1:B:2517:LYS:HD2	1:B:2524:VAL:HG21	1.69	0.73
1:A:3304:GLU:O	1:A:3307:LEU:CG	2.37	0.73
1:B:1365:PHE:HD1	1:B:1366:VAL:H	1.11	0.73
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.18	0.73
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.53	0.73
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.69	0.73
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.89	0.73
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.54	0.73
1:B:1826:PHE:CE2	1:B:1853:LEU:HD22	2.23	0.73
1:A:1929:ILE:HD13	1:A:1970:LEU:CD1	2.18	0.72
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.53	0.72
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.18	0.72
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.71	0.72
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.72	0.72
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.70	0.72
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.18	0.72
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.89	0.72
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.19	0.72
1:B:1983:LEU:HD21	1:B:1993:THR:O	1.90	0.72
1:B:2446:SER:H	1:B:2449:THR:CG2	2.03	0.72
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.71	0.72
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.18	0.72
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.90	0.72
1:B:2762:SER:C	1:B:2764:THR:H	1.94	0.72
1:B:2080:LYS:NZ	2:B:5400:ATP:O3G	2.23	0.72
1:B:2425:THR:HB	3:B:5401:ADP:O2A	1.90	0.72
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.89	0.71
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.20	0.71
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.89	0.71
1:B:2424:LYS:NZ	3:B:5401:ADP:O2B	2.23	0.71
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.18	0.71
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.50	0.71
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.70	0.71
1:A:3302:GLU:O	1:A:3305:ARG:HB2	1.90	0.71
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.36	0.71
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.90	0.71
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.72	0.71
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.72	0.71
1:A:2448:ASP:HB2	1:A:2829:GLU:OE1	1.90	0.71
1:B:3303:LYS:HA	1:B:3306:TRP:HD1	1.49	0.71
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.72	0.71
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.05	0.71
1:A:2446:SER:H	1:A:2449:THR:HG23	1.56	0.71
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.11	0.71
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.37	0.71
1:A:2226:ILE:HG23	1:A:2288:VAL:HG21	1.71	0.71
1:A:4020:ASN:HB3	1:A:4028:ARG:HH21	1.56	0.71
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.20	0.71
1:A:2765:GLY:HA2	3:A:5402:ADP:O3A	1.89	0.71
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.54	0.71
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.57	0.71
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.72	0.71
1:B:2473:LEU:HD11	1:B:2527:GLU:HG2	1.72	0.71
1:A:1409:LEU:HD21	1:A:1435:LEU:HB2	1.72	0.71
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.31	0.71
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.72	0.71
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.72	0.71
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.05	0.70
1:B:2473:LEU:HD22	1:B:2475:PRO:HG3	1.73	0.70
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.90	0.70
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.90	0.70
1:A:2620:ARG:NH2	3:A:5401:ADP:PA	2.64	0.70
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.21	0.70
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.74	0.70
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.72	0.70
1:B:2631:THR:O	1:B:2635:THR:HG22	1.92	0.70
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.32	0.70
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	2.27	0.70
1:A:2763:ARG:HE	3:A:5402:ADP:C4'	2.04	0.70
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.65	0.70
1:A:1455:LEU:HD12	1:A:1516:LEU:HD23	1.74	0.70
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.19	0.70
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.21	0.70
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.22	0.70
1:A:3304:GLU:O	1:A:3307:LEU:CB	2.40	0.70
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.78	0.70
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.55	0.70
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.73	0.70
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	2.07	0.70
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	1.91	0.70
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.74	0.70
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.92	0.70
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.90	0.69
1:A:3307:LEU:CD1	1:A:3307:LEU:C	2.57	0.69
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.74	0.69
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.69	0.69
1:B:2080:LYS:HE2	2:B:5400:ATP:PB	2.32	0.69
1:B:2378:VAL:CG2	1:B:2380:LEU:HD11	2.23	0.69
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.19	0.69
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.51	0.69
1:B:2728:LEU:HD12	1:B:2771:ARG:HH22	1.57	0.69
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.27	0.69
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.22	0.69
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.74	0.69
1:A:1415:MET:O	1:A:1421:TYR:CD2	2.46	0.69
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.73	0.69
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.91	0.69
1:B:2732:MET:CE	1:B:2768:ILE:HG23	1.99	0.69
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.75	0.69
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.58	0.69
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.68	0.69
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	2.07	0.69
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1365:PHE:HE1	1:B:1366:VAL:CG2	2.04	0.68
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.57	0.68
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.76	0.68
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.71	0.68
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.14	0.68
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.28	0.68
1:A:2282:ASN:CB	1:A:2552:ARG:HG3	2.20	0.68
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.93	0.68
1:B:1366:VAL:HG13	1:B:1369:LYS:HE3	1.75	0.68
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.23	0.68
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.93	0.68
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.74	0.68
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.46	0.68
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.24	0.68
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.93	0.68
1:B:3460:PRO:O	1:B:3463:SER:HB2	1.94	0.68
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.93	0.68
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.14	0.68
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.76	0.68
3:B:5401:ADP:N3	3:B:5401:ADP:H2'	2.09	0.68
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.58	0.68
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.76	0.68
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.76	0.68
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.75	0.67
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.14	0.67
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.94	0.67
1:A:1926:SER:HA	1:A:1970:LEU:HD12	1.76	0.67
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.24	0.67
1:B:2080:LYS:NZ	1:B:2549:ARG:CZ	2.57	0.67
1:B:2386:MET:HB2	1:B:2627:ARG:HD2	1.75	0.67
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.23	0.67
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.22	0.67
1:A:2763:ARG:NE	3:A:5402:ADP:H4'	2.10	0.67
1:A:1910:GLU:HB2	1:A:3846:MET:CB	2.23	0.67
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.82	0.67
1:B:1365:PHE:HD1	1:B:1366:VAL:HG23	0.91	0.67
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.48	0.67
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.76	0.67
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.09	0.67
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	1.76	0.67
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.75	0.67
1:B:2768:ILE:HG22	3:B:5402:ADP:O2A	1.94	0.67
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.60	0.67
1:B:2080:LYS:HG3	1:B:2081:THR:N	2.10	0.67
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.24	0.67
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.59	0.67
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.76	0.67
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.30	0.67
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.77	0.67
1:B:2728:LEU:CD1	1:B:2771:ARG:HH22	2.08	0.67
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.25	0.67
1:B:3792:ARG:HB2	1:B:3955:TYR:CE1	2.29	0.67
1:B:2762:SER:O	1:B:2764:THR:N	2.28	0.66
1:A:3322:GLY:HA2	1:A:3325:ILE:HD12	1.77	0.66
1:B:1802:LYS:N	4:B:5403:SO4:O1	2.28	0.66
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.25	0.66
1:B:2080:LYS:CG	2:B:5400:ATP:O1B	2.44	0.66
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.76	0.66
1:A:2407:LEU:HD22	1:A:2412:ARG:NH1	2.09	0.66
1:A:2620:ARG:NH2	3:A:5401:ADP:O3A	2.29	0.66
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.78	0.66
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.78	0.66
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.31	0.66
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.35	0.66
1:A:3303:LYS:HD2	1:A:3306:TRP:CB	2.25	0.66
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.61	0.65
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.61	0.65
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.71	0.65
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.19	0.65
1:B:3010:LEU:HD21	1:B:3317:SER:HB3	1.77	0.65
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.77	0.65
1:A:2476:LYS:NZ	1:A:2528:ARG:HD2	2.11	0.65
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.62	0.65
1:A:1421:TYR:CE1	1:A:1425:GLU:OE1	2.48	0.65
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.00	0.65
1:A:3306:TRP:CE3	1:A:3306:TRP:HA	2.31	0.65
1:B:2386:MET:HB3	1:B:2627:ARG:HE	1.60	0.65
1:A:2517:LYS:HE2	1:A:2524:VAL:HG21	1.78	0.65
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.96	0.65
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.62	0.65
1:B:1939:PHE:HD1	1:B:1940:GLU:O	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.78	0.65
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.36	0.65
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.27	0.65
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.55	0.65
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.79	0.65
1:B:3737:THR:HB	1:B:3740:THR:CB	2.27	0.65
1:A:1999:LYS:CG	1:A:2014:PHE:HE1	2.10	0.65
1:A:2109:LEU:CD1	1:A:2129:LEU:CD2	2.74	0.65
1:A:3810:SER:O	1:A:3838:TRP:HB2	1.97	0.64
1:B:1991:GLU:O	1:B:1995:VAL:HG23	1.97	0.64
1:B:2412:ARG:HH11	1:B:2553:HIS:CA	2.09	0.64
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	2.12	0.64
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.80	0.64
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.26	0.64
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.32	0.64
1:A:3306:TRP:HE3	1:A:3306:TRP:HA	1.63	0.64
1:B:2080:LYS:HG3	1:B:2081:THR:H	1.60	0.64
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.79	0.64
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.61	0.64
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.27	0.64
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.78	0.64
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.98	0.64
1:B:2411:LYS:HG2	1:B:2530:HIS:HE1	1.62	0.64
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.26	0.64
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.94	0.64
1:A:2421:GLY:N	3:A:5401:ADP:O2B	2.29	0.64
1:A:2765:GLY:CA	3:A:5402:ADP:O3A	2.46	0.64
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.97	0.64
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.61	0.64
1:A:1917:ARG:HD2	1:A:3963:PHE:CZ	2.33	0.64
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.61	0.64
1:B:2386:MET:HB3	1:B:2627:ARG:NE	2.13	0.64
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.28	0.64
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.63	0.64
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.79	0.64
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.62	0.64
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.63	0.64
1:B:2437:LEU:HA	1:B:2480:LYS:HD3	1.80	0.64
1:A:2224:SER:O	2:A:5400:ATP:H2	1.80	0.64
1:B:1681:LYS:HE2	1:B:1939:PHE:HZ	1.62	0.64
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.28	0.64
1:B:3688:THR:HG21	1:B:3777:VAL:HG21	1.80	0.64
1:A:2380:LEU:HD12	1:A:2577:ALA:HB1	1.80	0.64
1:A:3737:THR:CB	1:A:3740:THR:HB	2.27	0.64
1:B:2080:LYS:HZ2	1:B:2549:ARG:CZ	2.11	0.64
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.13	0.64
1:B:1493:LEU:HD23	1:B:1498:GLU:HB3	1.79	0.64
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.78	0.64
1:A:1527:LEU:HD22	1:A:1545:LEU:HD22	1.80	0.63
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.33	0.63
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.63	0.63
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.24	0.63
1:A:3307:LEU:CD1	1:A:3307:LEU:O	2.44	0.63
1:A:2424:LYS:NZ	3:A:5401:ADP:O1B	2.30	0.63
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.79	0.63
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.12	0.63
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.27	0.63
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.80	0.63
1:A:3302:GLU:O	1:A:3305:ARG:N	2.31	0.63
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.81	0.63
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.31	0.63
1:B:2732:MET:HB2	3:B:5402:ADP:C2	2.32	0.63
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.27	0.63
1:A:1741:LEU:O	1:A:1742:ASP:HB2	1.98	0.63
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.63	0.63
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.99	0.63
1:A:1611:LEU:O	1:A:1615:ILE:HG23	1.98	0.63
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.29	0.63
1:B:1421:TYR:O	1:B:1425:GLU:N	2.32	0.63
1:A:1926:SER:HB2	1:A:1970:LEU:HD12	1.79	0.63
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.80	0.63
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.13	0.63
1:A:1365:PHE:CE2	1:A:1366:VAL:HG21	2.29	0.62
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.33	0.62
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.81	0.62
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.98	0.62
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.32	0.62
1:A:3698:MET:O	1:A:3702:MET:HG3	1.98	0.62
1:B:2315:THR:HG21	1:B:2350:SER:HB3	1.81	0.62
1:B:3401:GLN:C	1:B:3403:ALA:H	2.00	0.62
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.57	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1926:SER:CA	1:A:1970:LEU:HD12	2.29	0.62
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.14	0.62
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.64	0.62
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.34	0.62
1:B:3303:LYS:CA	1:B:3306:TRP:HD1	2.11	0.62
1:B:2225:LYS:HA	2:B:5400:ATP:H2	1.64	0.62
1:A:1416:LYS:HA	1:A:1421:TYR:OH	1.99	0.62
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.81	0.62
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.81	0.62
1:B:2764:THR:O	3:B:5402:ADP:C8	2.52	0.62
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.64	0.62
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.66	0.62
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.14	0.62
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.32	0.62
1:A:1999:LYS:CG	1:A:2014:PHE:CE1	2.79	0.62
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.34	0.62
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.64	0.62
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.11	0.62
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.12	0.62
1:B:2080:LYS:NZ	1:B:2549:ARG:HH21	1.95	0.62
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.82	0.62
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.28	0.62
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.29	0.62
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.63	0.62
1:A:1979:ASN:OD1	1:A:2066:THR:HG21	2.00	0.62
1:A:2624:ARG:NH2	1:A:2910:ASN:O	2.32	0.62
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.81	0.62
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.29	0.62
1:A:1421:TYR:HD1	1:A:1425:GLU:CB	2.05	0.62
1:B:162:LEU:HA	1:B:165:ASP:O	1.99	0.62
1:B:2709:LYS:O	1:B:2713:VAL:HG23	1.99	0.62
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.18	0.62
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.09	0.62
1:B:1802:LYS:NZ	4:B:5403:SO4:S	2.71	0.62
1:A:1938:GLY:O	1:A:1989:GLU:HB3	2.00	0.62
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.64	0.62
1:B:1698:ILE:O	1:B:1702:LEU:HG	2.00	0.62
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.64	0.62
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.77	0.61
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.82	0.61
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.34	0.61
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.29	0.61
1:B:2081:THR:O	1:B:2085:LYS:HB2	1.99	0.61
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.15	0.61
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.35	0.61
1:B:2760:GLY:O	1:B:2761:ALA:C	2.38	0.61
1:B:3816:LEU:HD23	1:B:3847:SER:OG	2.00	0.61
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.81	0.61
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.35	0.61
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.35	0.61
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.00	0.61
1:B:1967:HIS:C	1:B:1968:PHE:HD1	2.04	0.61
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.99	0.61
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.36	0.61
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.82	0.61
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.76	0.61
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.00	0.61
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.14	0.61
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.30	0.61
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.64	0.61
1:B:216:PRO:O	1:B:1365:PHE:CB	2.36	0.61
1:B:1983:LEU:HD23	1:B:1993:THR:O	2.00	0.61
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.01	0.61
1:A:1756:LEU:HD13	1:A:1813:LEU:HD11	1.82	0.61
1:A:1646:GLN:OE1	1:A:1762:TYR:HA	1.99	0.61
1:A:4022:GLN:HA	1:A:4027:VAL:O	2.01	0.61
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.54	0.61
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.41	0.61
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.00	0.61
1:A:1744:LEU:HA	1:A:1760:PHE:HE2	1.60	0.61
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	2.00	0.61
1:A:3737:THR:CB	1:A:3740:THR:CB	2.79	0.61
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.16	0.61
1:A:3308:ASN:C	1:A:3310:THR:N	2.54	0.61
1:B:3785:TYR:CE1	1:B:3859:VAL:HG22	2.36	0.61
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.82	0.60
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.30	0.60
1:A:2391:VAL:HG23	1:A:2426:MET:SD	2.41	0.60
1:A:2512:LYS:O	1:A:2513:GLN:HB2	2.00	0.60
1:A:3303:LYS:CD	1:A:3306:TRP:HB2	2.28	0.60
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.99	0.60
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.36	0.60
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.31	0.60
1:A:2380:LEU:HD12	1:A:2577:ALA:CB	2.31	0.60
1:A:2563:SER:HB2	1:A:2566:SER:OG	2.01	0.60
1:A:3982:TRP:CD1	1:A:4015:PHE:O	2.55	0.60
1:A:2620:ARG:NH2	3:A:5401:ADP:O1A	2.34	0.60
1:A:1425:GLU:HG3	1:A:1428:CYS:SG	2.41	0.60
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.35	0.60
1:B:1425:GLU:OE2	1:B:1429:LEU:HD21	2.02	0.60
1:B:2473:LEU:HD23	1:B:2474:LEU:N	2.17	0.60
1:A:2631:THR:O	1:A:2635:THR:HG22	2.00	0.60
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.83	0.60
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.82	0.60
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.36	0.60
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.67	0.60
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.01	0.60
1:B:1534:PHE:HD2	1:B:1537:PHE:CE2	2.20	0.60
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.31	0.60
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.14	0.60
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.16	0.60
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.83	0.60
1:A:2080:LYS:O	1:A:2084:TRP:CD1	2.54	0.60
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.37	0.60
1:A:3774:ILE:O	1:A:3778:VAL:HG23	2.02	0.60
1:A:2109:LEU:CD2	1:A:2518:THR:HG22	2.32	0.59
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.84	0.59
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.21	0.59
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.83	0.59
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.32	0.59
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.02	0.59
1:B:1849:GLU:CG	1:B:1899:ASN:HD22	2.15	0.59
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.83	0.59
1:A:1779:PHE:O	1:A:1783:THR:HG22	2.02	0.59
1:A:2002:ILE:HB	1:A:2014:PHE:HE2	1.66	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.02	0.59
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.32	0.59
1:B:2764:THR:O	3:B:5402:ADP:H8	1.85	0.59
1:B:3512:ARG:NH2	3:B:5402:ADP:O3B	2.35	0.59
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.02	0.59
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2378:VAL:HG22	1:B:2380:LEU:HD13	1.80	0.59
1:A:1409:LEU:CD2	1:A:1435:LEU:HB2	2.32	0.59
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.35	0.59
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.37	0.59
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.37	0.59
1:B:2473:LEU:CD2	1:B:2475:PRO:HG3	2.30	0.59
1:B:2732:MET:CB	3:B:5402:ADP:N1	2.54	0.59
1:B:3017:VAL:HG21	1:B:3313:PHE:HE2	1.68	0.59
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.63	0.59
1:B:2428:MET:HE1	1:B:2440:VAL:HG21	1.84	0.59
1:A:1415:MET:O	1:A:1421:TYR:CE2	2.55	0.59
1:A:1640:VAL:HB	1:A:1686:LYS:NZ	2.16	0.59
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.67	0.59
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.84	0.59
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.91	0.59
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.84	0.59
1:B:2677:VAL:HG11	1:B:2686:LEU:HD21	1.85	0.59
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.38	0.58
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.20	0.58
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.17	0.58
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.56	0.58
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.33	0.58
1:B:3819:ILE:O	1:B:3823:ASN:HB2	2.02	0.58
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.16	0.58
1:A:3308:ASN:O	1:A:3310:THR:N	2.36	0.58
1:B:3737:THR:CB	1:B:3740:THR:HB	2.34	0.58
1:B:2080:LYS:HG2	2:B:5400:ATP:O2B	2.03	0.58
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.04	0.58
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.39	0.58
1:A:2286:THR:HA	1:A:2412:ARG:NE	2.18	0.58
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.85	0.58
1:B:1418:SER:HB2	1:B:3446:PHE:HB3	1.83	0.58
1:B:2513:GLN:O	1:B:2526:ILE:CG1	2.52	0.58
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.84	0.58
1:B:1852:ARG:HG3	1:B:1852:ARG:O	2.03	0.58
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.31	0.58
1:A:1999:LYS:HG2	1:A:2014:PHE:CZ	2.38	0.58
1:A:2032:LYS:O	1:A:2035:VAL:HG12	2.04	0.58
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.87	0.58
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.33	0.58
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.03	0.58
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.57	0.58
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.38	0.58
1:A:4065:LEU:O	1:A:4065:LEU:HD12	2.03	0.58
1:B:1493:LEU:CD2	1:B:1498:GLU:HB3	2.33	0.58
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.83	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.69	0.58
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	2.03	0.58
1:A:2080:LYS:NZ	2:A:5400:ATP:O3G	2.37	0.58
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.68	0.58
1:B:1372:ASN:O	1:B:1376:LYS:HG3	2.03	0.58
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.21	0.58
1:B:3461:ILE:C	1:B:3463:SER:H	2.07	0.58
1:A:1991:GLU:O	1:A:1995:VAL:HG23	2.04	0.58
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.67	0.58
1:B:1826:PHE:HE2	1:B:1853:LEU:HD22	1.66	0.58
1:B:2276:LEU:HD23	1:B:2556:ILE:HD13	1.86	0.58
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.16	0.58
1:A:1637:GLU:O	1:A:1686:LYS:NZ	2.31	0.58
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.69	0.58
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.39	0.58
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.85	0.58
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.34	0.58
1:B:1425:GLU:OE2	1:B:1429:LEU:CD2	2.52	0.58
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.24	0.58
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.85	0.58
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.86	0.58
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.39	0.57
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	1.86	0.57
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.84	0.57
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.35	0.57
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.37	0.57
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.86	0.57
1:A:1421:TYR:CG	1:A:1421:TYR:O	2.58	0.57
1:B:2042:GLY:HA3	1:B:2049:MET:CE	2.33	0.57
1:B:2763:ARG:O	3:B:5402:ADP:O4'	2.22	0.57
1:A:2109:LEU:HD23	1:A:2518:THR:HG22	1.86	0.57
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.33	0.57
1:A:2768:ILE:CG2	3:A:5402:ADP:O2A	2.47	0.57
1:A:4020:ASN:HB3	1:A:4028:ARG:NH2	2.18	0.57
1:B:2745:ILE:HG23	1:B:2756:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.39	0.57
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.04	0.57
1:A:2386:MET:HB2	1:A:2627:ARG:CD	2.22	0.57
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.70	0.57
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.35	0.57
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.04	0.57
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.40	0.57
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.86	0.57
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.58	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.53	0.57
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.51	0.57
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.05	0.56
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	1.86	0.56
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.87	0.56
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.04	0.56
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.68	0.56
1:A:2513:GLN:O	1:A:2526:ILE:CG1	2.52	0.56
1:A:2737:SER:HB2	1:A:2924:THR:HG21	1.88	0.56
1:A:2314:ILE:HG22	1:A:2318:ILE:HD12	1.87	0.56
1:B:2517:LYS:CE	1:B:2520:GLU:OE1	2.53	0.56
1:A:1826:PHE:CZ	1:A:1831:LEU:HB2	2.37	0.56
1:A:2495:ASP:O	1:A:2498:GLY:N	2.38	0.56
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	2.05	0.56
1:B:2225:LYS:HA	2:B:5400:ATP:N3	2.20	0.56
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.36	0.56
1:A:1796:GLY:O	1:A:1900:PRO:HD3	2.05	0.56
1:A:2420:PRO:HG2	1:A:2616:LEU:HD21	1.88	0.56
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.26	0.56
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.88	0.56
1:B:2081:THR:HB	2:B:5400:ATP:PA	2.45	0.56
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.70	0.56
1:B:2387:ARG:O	1:B:2390:ILE:HG22	2.05	0.56
1:A:1850:PHE:HB2	1:A:1896:ILE:HG23	1.88	0.56
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.88	0.56
1:A:1366:VAL:HG13	1:A:1369:LYS:HE3	1.88	0.56
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.38	0.56
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.88	0.56
1:A:2732:MET:HA	3:A:5402:ADP:C2	2.40	0.56
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.21	0.56
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	2.36	0.56
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HA	1:A:165:ASP:O	2.06	0.56
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.06	0.56
1:A:3785:TYR:CE1	1:A:3859:VAL:HG22	2.37	0.56
1:B:1984:ILE:CG2	1:B:1989:GLU:HG3	2.36	0.56
1:B:2517:LYS:HE2	1:B:2520:GLU:OE1	2.04	0.56
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.31	0.56
1:A:2107:LYS:CE	1:A:2499:SER:HB3	2.34	0.56
1:A:3302:GLU:O	1:A:3305:ARG:CB	2.53	0.56
1:A:3308:ASN:O	1:A:3311:LYS:N	2.38	0.56
1:B:2728:LEU:HD12	1:B:2771:ARG:HH12	1.71	0.56
1:B:2763:ARG:HG3	1:B:2990:GLY:HA3	1.87	0.56
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.70	0.55
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.36	0.55
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.39	0.55
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.26	0.55
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.82	0.55
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.41	0.55
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.36	0.55
1:B:1939:PHE:H	1:B:1939:PHE:HD2	1.55	0.55
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.87	0.55
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.07	0.55
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.06	0.55
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.49	0.55
1:A:1459:LEU:HD22	1:A:1473:THR:CG2	2.36	0.55
1:A:1637:GLU:HA	1:A:1686:LYS:HZ3	1.72	0.55
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.07	0.55
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.95	0.55
1:A:2763:ARG:HA	3:A:5402:ADP:C5'	2.37	0.55
1:B:2380:LEU:CD2	1:B:2390:ILE:CD1	2.57	0.55
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.06	0.55
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.88	0.55
1:B:2473:LEU:HD23	1:B:2475:PRO:N	2.20	0.55
1:B:3305:ARG:O	1:B:3307:LEU:N	2.36	0.55
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.88	0.55
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.88	0.55
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.40	0.55
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.71	0.55
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.88	0.55
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.87	0.55
1:B:2620:ARG:HH21	3:B:5401:ADP:PB	2.29	0.55
1:B:2732:MET:CB	3:B:5402:ADP:C2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:PHE:HB2	1:A:1760:PHE:CE1	2.42	0.55
1:A:1939:PHE:HD2	1:A:1939:PHE:H	1.55	0.55
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.07	0.55
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.37	0.55
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.89	0.55
1:B:2728:LEU:HD12	1:B:2771:ARG:NH1	2.22	0.55
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.20	0.54
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.07	0.54
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.89	0.54
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.22	0.54
1:B:3303:LYS:C	1:B:3306:TRP:HD1	2.09	0.54
1:A:1910:GLU:HB2	1:A:3846:MET:HB2	1.89	0.54
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.21	0.54
1:B:3401:GLN:C	1:B:3403:ALA:N	2.61	0.54
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.90	0.54
3:B:5401:ADP:N3	3:B:5401:ADP:C2'	2.70	0.54
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.89	0.54
1:A:1852:ARG:HG3	1:A:1852:ARG:O	2.08	0.54
1:A:2763:ARG:HD2	3:A:5402:ADP:H4'	1.90	0.54
1:A:1983:LEU:HD21	1:A:1996:GLU:HB2	1.88	0.54
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.72	0.54
1:A:4037:SER:HB3	1:A:4040:GLU:HB2	1.90	0.54
1:B:1835:LEU:O	1:B:1838:ILE:HG22	2.08	0.54
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.95	0.54
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.37	0.54
1:A:2446:SER:H	1:A:2449:THR:HG21	1.72	0.54
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	1.89	0.54
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.55	0.54
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.36	0.54
1:B:3460:PRO:O	1:B:3463:SER:CB	2.55	0.54
1:B:4023:ILE:HD12	1:B:4029:ILE:HD11	1.90	0.54
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.96	0.54
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.73	0.54
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.07	0.54
1:B:2860:THR:HG21	1:B:2867:LEU:HD12	1.89	0.54
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.96	0.54
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.08	0.54
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	1.89	0.54
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	2.08	0.54
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.90	0.54
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.08	0.54
1:A:2517:LYS:HE3	1:A:2524:VAL:HG23	1.81	0.54
1:A:3855:LEU:HD12	1:A:3859:VAL:HG23	1.88	0.54
1:B:1795:PHE:HE2	1:B:1918:GLU:HB3	1.73	0.54
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.89	0.54
1:A:3304:GLU:CG	1:A:3307:LEU:HD23	2.33	0.53
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.41	0.53
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.76	0.53
1:B:1898:LEU:HD11	1:B:1908:LEU:HD23	1.90	0.53
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.07	0.53
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	2.96	0.53
1:B:1365:PHE:C	1:B:1367:ILE:N	2.59	0.53
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.37	0.53
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.91	0.53
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.90	0.53
1:B:3618:TYR:O	1:B:3622:GLY:N	2.40	0.53
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.39	0.53
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.89	0.53
1:A:1983:LEU:HD21	1:A:1993:THR:O	2.09	0.53
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.90	0.53
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.55	0.53
1:A:3989:ILE:HD13	1:A:4015:PHE:CZ	2.43	0.53
1:A:2763:ARG:CD	3:A:5402:ADP:H4'	2.38	0.53
1:B:1645:PHE:CZ	1:B:1649:LEU:HD22	2.42	0.53
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.08	0.53
1:B:2428:MET:HE1	1:B:2440:VAL:CG2	2.38	0.53
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	1.91	0.53
1:B:2732:MET:CA	3:B:5402:ADP:N1	2.72	0.53
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.88	0.53
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.08	0.53
1:A:1872:LEU:HG	1:A:1888:LEU:HD21	1.90	0.53
1:A:2786:ILE:HD12	1:A:3460:PRO:HG2	1.91	0.53
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.73	0.53
1:B:2582:VAL:HG23	1:B:2582:VAL:O	2.08	0.53
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.87	0.53
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.90	0.53
1:A:2563:SER:CB	1:A:2566:SER:OG	2.57	0.53
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.29	0.53
1:A:3367:ILE:O	1:A:3371:VAL:HG22	2.09	0.53
1:A:3819:ILE:O	1:A:3823:ASN:HB2	2.09	0.53
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:SER:O	1:A:1421:TYR:CE2	2.62	0.53
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.08	0.53
1:A:1826:PHE:CZ	1:A:1830:VAL:HG13	2.44	0.53
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.43	0.53
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.09	0.53
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.96	0.53
1:B:3342:ARG:NH1	1:B:3393:ASN:OD1	2.38	0.53
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.09	0.53
1:B:3760:LEU:HD21	1:B:4078:ALA:HA	1.91	0.53
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.39	0.53
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.73	0.53
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.41	0.53
1:A:2220:CYS:SG	1:A:2221:SER:N	2.82	0.53
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.29	0.53
1:B:1770:ILE:HD11	1:B:1936:ILE:HD11	1.90	0.53
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.32	0.53
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.91	0.53
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.90	0.53
1:A:2380:LEU:CD1	1:A:2577:ALA:CB	2.86	0.53
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.74	0.53
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.38	0.53
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.08	0.53
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.57	0.53
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.43	0.52
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.44	0.52
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.39	0.52
1:B:2080:LYS:HZ1	1:B:2549:ARG:NE	2.07	0.52
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.09	0.52
1:B:3737:THR:CB	1:B:3740:THR:CB	2.87	0.52
1:B:3862:THR:HB	1:B:3865:ALA:HB2	1.91	0.52
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.24	0.52
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.74	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	1.90	0.52
1:A:2941:THR:HG22	1:A:2942:ASP:N	2.22	0.52
1:A:4024:VAL:CG2	1:A:4027:VAL:HB	2.40	0.52
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.10	0.52
1:B:1866:GLN:O	1:B:1870:ASN:HB2	2.08	0.52
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.73	0.52
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.10	0.52
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	1.91	0.52
1:B:2891:ILE:HD11	1:B:2903:ILE:HD11	1.90	0.52
1:B:2081:THR:HB	2:B:5400:ATP:O1A	2.09	0.52
1:A:1416:LYS:O	1:A:1421:TYR:OH	2.25	0.52
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.91	0.52
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.54	0.52
1:A:3701:THR:OG1	1:A:4085:THR:HG22	2.08	0.52
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.45	0.52
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.74	0.52
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.92	0.52
1:A:2473:LEU:HD22	1:A:2527:GLU:HG2	1.91	0.52
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.44	0.52
1:A:1416:LYS:O	1:A:1421:TYR:CE2	2.63	0.52
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.44	0.52
1:A:3304:GLU:O	1:A:3307:LEU:HB3	2.10	0.52
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.91	0.52
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.50	0.52
1:B:2624:ARG:NH2	1:B:2910:ASN:O	2.43	0.52
1:B:3934:TRP:CB	1:B:4023:ILE:HD13	2.40	0.52
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.91	0.52
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.10	0.52
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.30	0.52
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.44	0.52
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.90	0.52
1:A:1970:LEU:CD2	1:A:1974:LYS:HE2	2.40	0.52
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.50	0.52
1:B:2073:VAL:HG21	1:B:2199:LEU:HD11	1.92	0.52
1:B:23:LEU:O	1:B:24:GLU:CB	2.57	0.52
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.91	0.52
1:A:1956:LEU:CB	1:A:1968:PHE:CE2	2.87	0.52
1:B:2044:ARG:NH2	1:B:2093:ILE:HD11	2.24	0.52
1:A:1527:LEU:HD21	1:A:1546:LEU:HD21	1.91	0.52
1:A:1706:LEU:HD22	1:A:1935:GLN:CG	2.38	0.52
1:A:2076:ALA:CB	1:A:2549:ARG:HG2	2.40	0.52
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.57	0.52
1:A:3304:GLU:HG3	1:A:3307:LEU:CD2	2.32	0.52
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.50	0.52
1:B:2728:LEU:CG	1:B:2771:ARG:HH22	2.22	0.52
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.09	0.51
1:B:2080:LYS:HG2	2:B:5400:ATP:O1B	2.07	0.51
1:A:2421:GLY:H	3:A:5401:ADP:PB	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.86	0.51
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.46	0.51
1:B:2080:LYS:HG3	1:B:2195:GLU:OE1	2.10	0.51
1:B:2386:MET:HB2	1:B:2627:ARG:CD	2.37	0.51
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.29	0.51
1:B:3934:TRP:HB3	1:B:4023:ILE:HD13	1.93	0.51
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.11	0.51
1:B:2080:LYS:HG3	2:B:5400:ATP:O1B	2.11	0.51
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.92	0.51
1:A:2633:ILE:HD11	1:A:2644:LEU:CD2	2.41	0.51
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.89	0.51
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.92	0.51
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	1.92	0.51
1:A:2517:LYS:HG3	1:A:2524:VAL:HG23	1.93	0.51
1:A:3303:LYS:HA	1:A:3306:TRP:HB2	1.92	0.51
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.40	0.51
1:B:2257:PHE:HD1	1:B:2262:LEU:HD11	1.75	0.51
1:B:3911:TRP:HH2	1:B:3926:VAL:HG13	1.76	0.51
1:A:3460:PRO:O	1:A:3463:SER:CB	2.59	0.51
1:B:1910:GLU:CB	1:B:3846:MET:HB3	2.41	0.51
1:B:2506:LEU:HD22	1:B:2531:ILE:HD12	1.91	0.51
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.92	0.51
1:B:2786:ILE:HD12	1:B:3460:PRO:HG2	1.92	0.51
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.91	0.51
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.30	0.51
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.11	0.51
1:A:2154:PHE:CD1	1:A:2154:PHE:N	2.79	0.51
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.93	0.51
1:B:2105:ASP:OD2	1:B:2508:GLN:HB2	2.11	0.51
1:B:3978:ASN:O	1:B:3981:PRO:HD3	2.11	0.51
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.92	0.51
1:A:2494:LEU:HB2	1:A:2499:SER:N	2.26	0.51
1:A:2563:SER:CB	1:A:2566:SER:H	2.22	0.51
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.92	0.51
1:A:3342:ARG:NH1	1:A:3393:ASN:OD1	2.40	0.51
1:A:3989:ILE:HD13	1:A:4015:PHE:CE2	2.46	0.51
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.51	0.51
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.11	0.51
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	1.93	0.51
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.92	0.51
1:B:3566:LEU:HD23	1:B:3587:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.44	0.51
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.11	0.51
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.46	0.51
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	1.93	0.51
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.46	0.51
1:B:2410:SER:O	1:B:2411:LYS:HB2	2.11	0.51
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.71	0.51
1:A:3785:TYR:CE1	1:A:3859:VAL:HG13	2.46	0.50
1:B:1365:PHE:CG	1:B:1366:VAL:N	2.76	0.50
1:B:2473:LEU:HD22	1:B:2475:PRO:CG	2.32	0.50
1:B:2224:SER:O	2:B:5400:ATP:H2	1.93	0.50
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.74	0.50
1:A:2048:SER:H	2:A:5400:ATP:N6	2.08	0.50
1:A:3308:ASN:C	1:A:3310:THR:H	2.12	0.50
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.91	0.50
1:B:2380:LEU:HG	1:B:2384:GLU:OE1	2.11	0.50
1:B:2571:TYR:HD1	1:B:2626:VAL:HG21	1.75	0.50
1:B:2081:THR:OG1	2:B:5400:ATP:O1B	2.26	0.50
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.93	0.50
1:A:2282:ASN:ND2	1:A:2552:ARG:HD2	2.26	0.50
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.92	0.50
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.92	0.50
1:B:2080:LYS:CG	1:B:2081:THR:H	2.25	0.50
1:B:2473:LEU:HD21	1:B:2527:GLU:HB2	1.94	0.50
1:A:1493:LEU:HD22	1:A:1502:ILE:HD11	1.93	0.50
1:A:1926:SER:HA	1:A:1970:LEU:CD1	2.40	0.50
1:A:2083:THR:O	1:A:2087:VAL:HG23	2.12	0.50
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.11	0.50
1:B:2137:VAL:O	1:B:2141:ILE:CG2	2.49	0.50
1:B:3401:GLN:O	1:B:3403:ALA:N	2.44	0.50
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.93	0.50
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.32	0.50
1:B:3461:ILE:C	1:B:3463:SER:N	2.65	0.50
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.26	0.50
1:A:2081:THR:HA	1:A:2084:TRP:NE1	2.27	0.50
1:A:2364:ASP:O	1:A:2365:LYS:HG3	2.11	0.50
1:A:2762:SER:O	1:A:2763:ARG:CB	2.47	0.50
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.47	0.50
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.58	0.50
1:B:3965:SER:HA	1:B:3968:LEU:HD12	1.92	0.50
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2780:LYS:HB3	1:A:2813:THR:HG22	1.94	0.50
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.50
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.60	0.50
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.74	0.50
1:B:2080:LYS:HE2	2:B:5400:ATP:PG	2.52	0.50
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.82	0.50
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.11	0.50
1:A:3461:ILE:C	1:A:3463:SER:H	2.16	0.50
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.77	0.50
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.12	0.50
1:A:2424:LYS:NZ	3:A:5401:ADP:O2B	2.32	0.50
1:A:1802:LYS:NZ	4:A:5403:SO4:O2	2.32	0.50
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.12	0.50
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.93	0.50
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	1.94	0.50
1:A:2394:THR:H	1:A:2397:THR:HB	1.76	0.49
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.25	0.49
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.42	0.49
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.11	0.49
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.47	0.49
1:B:1681:LYS:CE	1:B:1939:PHE:HZ	2.24	0.49
1:B:1973:LEU:O	1:B:1977:LEU:HG	2.12	0.49
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.11	0.49
1:B:2732:MET:HB2	3:B:5402:ADP:C4	2.41	0.49
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.94	0.49
1:A:2170:LEU:HB3	1:A:2209:ARG:HD3	1.92	0.49
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.96	0.49
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.42	0.49
1:A:1495:THR:CG2	1:A:1497:ILE:HG22	2.40	0.49
1:A:1802:LYS:O	1:A:1806:VAL:HG23	2.12	0.49
1:A:1926:SER:HB2	1:A:1973:LEU:HD21	1.93	0.49
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.12	0.49
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	1.95	0.49
1:B:3481:ILE:O	1:B:3483:ASP:N	2.45	0.49
1:A:1850:PHE:CB	1:A:1896:ILE:HG23	2.42	0.49
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.27	0.49
1:A:1970:LEU:CD2	1:A:1974:LYS:CE	2.90	0.49
1:A:2829:GLU:HA	1:A:2832:ASN:HD22	1.76	0.49
1:A:3631:MET:HE3	1:A:3698:MET:HG3	1.93	0.49
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.95	0.49
1:B:2354:SER:H	1:B:2357:SER:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.13	0.49
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.31	0.49
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.93	0.49
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.26	0.49
1:B:3306:TRP:CH2	1:B:3594:ALA:HB1	2.48	0.49
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.13	0.49
1:A:1637:GLU:HA	1:A:1686:LYS:NZ	2.27	0.49
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.26	0.49
1:A:1910:GLU:HB2	1:A:3846:MET:CA	2.42	0.49
1:B:2580:LYS:HG2	1:B:2586:ARG:HH22	1.77	0.49
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.77	0.49
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.11	0.49
1:A:1838:ILE:HG13	1:A:1843:ALA:HB3	1.93	0.49
1:B:1795:PHE:CE2	1:B:1918:GLU:HB3	2.48	0.49
1:B:2229:LEU:HB3	1:B:2288:VAL:HG11	1.94	0.49
1:B:2732:MET:CA	3:B:5402:ADP:C2	2.93	0.49
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.95	0.49
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.46	0.49
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.77	0.49
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.33	0.49
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.51	0.49
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	1.94	0.49
1:B:1838:ILE:CD1	1:B:1845:GLY:HA3	2.43	0.49
1:B:1929:ILE:HD12	1:B:1929:ILE:H	1.78	0.49
1:B:2080:LYS:CG	1:B:2081:THR:N	2.76	0.49
1:B:2305:LEU:HD11	1:B:2368:PHE:HB3	1.94	0.49
1:B:2792:LEU:HD13	1:B:2826:ALA:HB3	1.95	0.49
1:A:3010:LEU:CD2	1:A:3317:SER:HB3	2.41	0.49
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.13	0.49
1:A:3989:ILE:HA	1:A:3993:VAL:HB	1.95	0.49
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	3.01	0.49
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.12	0.49
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.48	0.49
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.32	0.49
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.78	0.48
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.95	0.48
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.13	0.48
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.27	0.48
1:A:2027:THR:HA	1:A:2028:PRO:HD3	1.62	0.48
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	1.94	0.48
1:A:3737:THR:HB	1:A:3740:THR:HB	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3971:VAL:O	1:A:3975:ASN:HB2	2.13	0.48
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.94	0.48
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.13	0.48
1:B:2257:PHE:CD1	1:B:2262:LEU:HD11	2.48	0.48
1:B:2316:LEU:HD13	1:B:2351:GLN:HB3	1.95	0.48
1:B:2473:LEU:CD2	1:B:2475:PRO:N	2.76	0.48
1:B:3688:THR:HG21	1:B:3777:VAL:CG2	2.42	0.48
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.27	0.48
1:B:3785:TYR:HE1	1:B:3859:VAL:HG22	1.74	0.48
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.94	0.48
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.94	0.48
1:A:2985:ASN:N	1:A:2986:PRO:HD3	2.28	0.48
1:A:3440:LEU:HD22	1:A:3462:ILE:HD12	1.95	0.48
1:B:3592:LYS:O	1:B:3596:ASN:N	2.46	0.48
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.14	0.48
1:B:1917:ARG:HD2	1:B:3963:PHE:CZ	2.48	0.48
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.94	0.48
1:A:65:THR:O	1:A:66:GLN:CB	2.60	0.48
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.48	0.48
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.95	0.48
1:A:2394:THR:HG22	1:A:2395:ILE:H	1.78	0.48
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	1.95	0.48
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.02	0.48
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.27	0.48
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.78	0.48
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.80	0.48
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.14	0.48
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.79	0.48
1:B:4020:ASN:HB3	1:B:4028:ARG:HH21	1.77	0.48
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.96	0.48
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.14	0.48
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.95	0.48
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.96	0.48
1:B:1535:PRO:C	1:B:1841:ILE:HD11	2.33	0.48
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.14	0.48
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.13	0.48
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.14	0.48
1:A:2079:GLY:HA2	2:A:5400:ATP:H5'2	1.96	0.48
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.78	0.48
1:A:2728:LEU:HD12	1:A:2771:ARG:NH1	2.27	0.48
1:A:2982:VAL:CG1	1:A:2983:GLY:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3797:THR:O	1:A:3801:ILE:HG12	2.13	0.48
1:B:1386:ILE:HG22	1:B:1396:ARG:HG2	1.95	0.48
1:B:1714:GLN:HB3	1:B:1727:LEU:HD11	1.96	0.48
1:B:2642:ARG:O	1:B:2646:ARG:HG3	2.14	0.48
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.77	0.48
1:A:1455:LEU:HD12	1:A:1516:LEU:CD2	2.41	0.48
1:A:2463:ASN:O	1:A:2475:PRO:HD2	2.13	0.48
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.96	0.48
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.85	0.48
1:A:1969:GLY:O	1:A:1972:THR:HB	2.14	0.48
1:A:2771:ARG:HG2	1:A:2781:ILE:HG21	1.96	0.48
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	1.96	0.48
1:B:2295:ILE:HG12	1:B:2314:ILE:HD12	1.96	0.48
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.43	0.48
1:A:1941:ASP:O	1:A:1945:LEU:HG	2.13	0.47
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	1.91	0.47
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.39	0.47
1:B:2754:GLY:HA3	1:B:2886:HIS:CE1	2.49	0.47
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	2.97	0.47
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	1.94	0.47
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.29	0.47
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.49	0.47
1:B:2467:THR:HG22	1:B:2468:SER:N	2.28	0.47
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.44	0.47
1:A:2201:HIS:CE1	1:A:2497:TYR:HB3	2.48	0.47
1:A:3628:ILE:HG22	1:A:3649:PHE:CE2	2.49	0.47
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.96	0.47
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.14	0.47
1:B:2122:THR:O	1:B:2123:LEU:C	2.53	0.47
1:B:2220:CYS:SG	2:B:5400:ATP:C6	3.07	0.47
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.63	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.97	0.47
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.14	0.47
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.80	0.47
1:B:2732:MET:CB	3:B:5402:ADP:C4	2.97	0.47
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.62	0.47
1:A:2889:PHE:CD1	1:A:2902:MET:HE1	2.50	0.47
1:A:3940:THR:O	1:A:3943:THR:HB	2.14	0.47
1:B:1979:ASN:OD1	1:B:2066:THR:HG21	2.15	0.47
1:B:2106:THR:H	1:B:2156:SER:HB2	1.79	0.47
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2757:MET:HG2	1:B:2914:ILE:HG13	1.96	0.47
1:A:1938:GLY:HA3	1:A:1989:GLU:HG2	1.96	0.47
1:A:3979:ASN:O	1:A:3981:PRO:CD	2.57	0.47
1:B:2473:LEU:HD23	1:B:2473:LEU:C	2.34	0.47
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	1.97	0.47
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.49	0.47
1:B:2891:ILE:CD1	1:B:2903:ILE:HD11	2.44	0.47
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.50	0.47
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.45	0.47
1:A:1422:LYS:HA	1:A:1422:LYS:HD3	1.63	0.47
1:A:1992:LYS:HG2	1:A:2024:SER:CB	2.43	0.47
1:A:2368:PHE:O	1:A:2369:SER:CB	2.62	0.47
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.97	0.47
1:B:1534:PHE:CD2	1:B:1537:PHE:CE2	3.02	0.47
1:B:2361:ILE:HG22	1:B:2367:SER:O	2.15	0.47
1:B:2734:ILE:HD12	1:B:2734:ILE:H	1.80	0.47
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.30	0.47
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.79	0.47
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.25	0.47
1:B:3326:ILE:HA	1:B:3349:LEU:HD21	1.96	0.47
1:B:3994:TYR:O	1:B:3998:ILE:HD12	2.15	0.47
1:B:2424:LYS:N	3:B:5401:ADP:O1B	2.48	0.47
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.80	0.47
1:A:3302:GLU:O	1:A:3305:ARG:CA	2.63	0.47
1:A:3718:ALA:O	1:A:3721:THR:HG22	2.15	0.47
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.96	0.47
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.18	0.47
1:B:1910:GLU:HB2	1:B:3846:MET:HB2	1.97	0.47
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.79	0.47
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.96	0.47
1:B:2354:SER:OG	1:B:2357:SER:CB	2.63	0.47
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.97	0.47
1:B:4037:SER:HB3	1:B:4040:GLU:HB2	1.97	0.47
1:A:1970:LEU:HD23	1:A:1974:LYS:HE3	1.97	0.46
1:A:3956:PHE:CD1	1:A:3994:TYR:HD1	2.33	0.46
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.45	0.46
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.97	0.46
1:B:2819:GLU:O	1:B:2822:ILE:HG13	2.15	0.46
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.97	0.46
1:B:1828:TYR:HB2	1:B:1857:VAL:HG13	1.98	0.46
1:B:2152:VAL:HG12	1:B:2154:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4074:GLU:HA	1:B:4077:GLN:HE21	1.80	0.46
1:A:2856:LEU:HD21	1:A:2877:PHE:HB2	1.97	0.46
1:A:3304:GLU:O	1:A:3307:LEU:N	2.48	0.46
1:A:3509:LEU:O	1:A:3513:VAL:HG23	2.16	0.46
1:A:3624:HIS:ND1	1:A:3675:LEU:HD11	2.30	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.97	0.46
1:A:3945:LEU:HD21	1:A:4070:ILE:CD1	2.45	0.46
1:B:1563:LYS:HA	1:B:1569:ILE:O	2.15	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG23	2.15	0.46
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.15	0.46
1:B:2080:LYS:CE	1:B:2549:ARG:HH21	2.28	0.46
1:B:4023:ILE:CD1	1:B:4029:ILE:HD11	2.45	0.46
1:A:1970:LEU:HD21	1:A:1974:LYS:HE2	1.97	0.46
1:A:3990:ALA:HB2	1:A:4011:CYS:SG	2.56	0.46
1:B:1386:ILE:CG2	1:B:1396:ARG:HG2	2.46	0.46
1:B:2081:THR:HG22	1:B:2085:LYS:HD2	1.97	0.46
1:B:2732:MET:SD	3:B:5402:ADP:N7	2.89	0.46
1:B:2824:GLU:HG2	1:B:2825:THR:H	1.80	0.46
1:B:2961:ILE:O	1:B:2965:VAL:HG23	2.14	0.46
1:B:2786:ILE:HD12	1:B:3460:PRO:CG	2.46	0.46
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.28	0.46
1:A:2068:GLN:HE22	1:A:2188:PRO:HA	1.81	0.46
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.81	0.46
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.69	0.46
1:A:4019:ASP:H	1:A:4031:GLN:HE21	1.64	0.46
3:A:5401:ADP:H2'	3:A:5401:ADP:N3	2.31	0.46
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.68	0.46
1:B:2064:GLN:OE1	1:B:2065:LYS:HG3	2.15	0.46
1:B:2424:LYS:HE2	1:B:2424:LYS:HB2	1.55	0.46
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.97	0.46
1:A:2420:PRO:CG	1:A:2616:LEU:HD21	2.45	0.46
1:A:2938:MET:SD	1:A:3321:ILE:CG2	3.03	0.46
1:A:2999:LEU:HD11	1:A:3325:ILE:HG12	1.97	0.46
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.50	0.46
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.55	0.46
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.98	0.46
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.63	0.46
1:B:3911:TRP:CH2	1:B:3926:VAL:HG13	2.51	0.46
1:A:1418:SER:O	1:A:1421:TYR:CD2	2.68	0.46
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.96	0.46
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.97	0.46
1:A:2219:VAL:HG21	2:A:5400:ATP:N7	2.31	0.46
1:B:3701:THR:OG1	1:B:4085:THR:HG22	2.15	0.46
1:B:2081:THR:HB	2:B:5400:ATP:O2A	2.15	0.46
1:B:3725:VAL:HG22	1:B:3731:ASP:HA	1.96	0.46
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.46	0.46
1:B:2080:LYS:HZ1	1:B:2549:ARG:CZ	2.26	0.46
1:B:3367:ILE:O	1:B:3371:VAL:HG22	2.16	0.46
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.16	0.46
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.16	0.46
1:A:23:LEU:O	1:A:25:GLU:N	2.49	0.46
1:A:2754:GLY:HA3	1:A:2886:HIS:CE1	2.51	0.46
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	1.97	0.46
1:B:1838:ILE:HD11	1:B:1845:GLY:CA	2.46	0.46
1:B:2394:THR:H	1:B:2397:THR:HB	1.81	0.46
1:A:1644:ILE:O	1:A:1648:ILE:HG22	2.16	0.45
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.16	0.45
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.97	0.45
1:B:2358:THR:HG22	1:B:2359:ILE:N	2.31	0.45
1:A:2763:ARG:HA	3:A:5402:ADP:C4'	2.47	0.45
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.64	0.45
1:B:1366:VAL:CG1	1:B:1369:LYS:HE3	2.45	0.45
1:B:2856:LEU:HD21	1:B:2877:PHE:HB2	1.98	0.45
1:A:2072:LEU:HB3	1:A:2215:PHE:HE1	1.80	0.45
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.16	0.45
1:A:3373:LEU:HD13	1:A:3557:LEU:CD1	2.47	0.45
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.81	0.45
1:B:2088:ILE:HG12	1:B:2151:TRP:CZ2	2.51	0.45
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.63	0.45
1:B:2473:LEU:HD21	1:B:2475:PRO:CG	2.47	0.45
1:B:65:THR:O	1:B:66:GLN:CB	2.64	0.45
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.84	0.45
1:A:1968:PHE:N	1:A:1968:PHE:CD1	2.84	0.45
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.51	0.45
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.16	0.45
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.97	0.45
1:A:2853:LEU:HD21	1:A:2870:GLU:HG3	1.98	0.45
1:A:2893:ASP:HA	1:A:2894:PRO:HD2	1.89	0.45
1:A:3636:GLY:CA	1:A:3642:TYR:O	2.64	0.45
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.29	0.45
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2068:GLN:HA	1:B:2191:ARG:HG2	1.98	0.45
1:B:216:PRO:HA	1:B:1365:PHE:HA	1.98	0.45
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.38	0.45
1:B:40:TRP:O	1:B:44:LYS:N	2.50	0.45
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.98	0.45
1:A:2982:VAL:CG1	1:A:2983:GLY:H	2.29	0.45
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.99	0.45
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.47	0.45
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.94	0.45
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.00	0.45
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	1.98	0.45
1:B:2249:LEU:HA	1:B:2252:LEU:HD12	1.99	0.45
1:B:2467:THR:O	1:B:2471:LEU:N	2.48	0.45
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.16	0.45
1:B:4084:SER:O	1:B:4088:LEU:HG	2.17	0.45
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.73	0.45
1:A:1995:VAL:HG22	1:A:2022:PHE:HD2	1.80	0.45
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.99	0.45
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.36	0.45
1:B:2476:LYS:HE3	1:B:2528:ARG:CB	2.47	0.45
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.97	0.45
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.98	0.45
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.99	0.45
1:A:1956:LEU:HB3	1:A:1968:PHE:CD2	2.51	0.45
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.45
1:A:2241:LEU:HD21	1:A:2249:LEU:HD12	1.99	0.45
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.17	0.45
1:A:3306:TRP:CH2	1:A:3594:ALA:HB1	2.45	0.45
1:B:2609:THR:HA	1:B:2612:GLN:O	2.17	0.45
1:B:2695:LEU:HD23	1:B:2743:LEU:HD11	1.99	0.45
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.51	0.45
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.81	0.45
1:B:2941:THR:CG2	1:B:2942:ASP:H	2.29	0.45
1:B:3470:PHE:CE1	1:B:3488:VAL:HG21	2.52	0.45
1:A:1416:LYS:CA	1:A:1421:TYR:OH	2.65	0.45
1:A:1646:GLN:OE1	1:A:1762:TYR:HD1	2.00	0.45
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.51	0.45
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.31	0.45
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.50	0.45
1:A:3592:LYS:O	1:A:3596:ASN:N	2.50	0.45
1:B:1536:ARG:HD3	1:B:1841:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2285:GLU:HB2	1:B:2412:ARG:NH2	2.32	0.45
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.99	0.45
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.17	0.45
1:B:4018:SER:O	1:B:4019:ASP:HB2	2.17	0.45
1:A:3002:LEU:HD21	1:A:3370:LEU:HD11	1.99	0.45
1:B:2091:MET:CE	1:B:2149:ARG:NH1	2.80	0.45
1:B:2822:ILE:O	1:B:2822:ILE:HG13	2.17	0.45
1:B:2960:THR:CG2	1:B:2961:ILE:N	2.80	0.45
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.16	0.45
1:A:2764:THR:HG21	1:A:2917:MET:HB3	1.99	0.44
1:A:3338:ASN:HB2	1:A:3341:GLU:HG2	1.99	0.44
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.99	0.44
1:A:4033:LEU:HD12	1:A:4035:GLN:H	1.82	0.44
1:B:1421:TYR:O	1:B:1425:GLU:CA	2.65	0.44
1:B:1660:VAL:HG13	1:B:1728:TRP:CH2	2.51	0.44
1:B:1967:HIS:NE2	1:B:2204:PRO:HB3	2.31	0.44
1:B:1945:LEU:HD13	1:B:1994:VAL:HG21	1.99	0.44
1:A:2042:GLY:HA3	1:A:2049:MET:CE	2.46	0.44
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.16	0.44
1:A:2635:THR:O	1:A:2704:PHE:N	2.40	0.44
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.63	0.44
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.98	0.44
1:B:2757:MET:HB2	1:B:2889:PHE:HB2	1.98	0.44
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.99	0.44
1:B:3632:LEU:HD13	1:B:3644:ILE:HD13	1.98	0.44
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.52	0.44
1:A:2048:SER:O	2:A:5400:ATP:N6	2.45	0.44
1:B:1365:PHE:HE1	1:B:1366:VAL:HG21	1.81	0.44
1:B:1421:TYR:CD1	1:B:1425:GLU:CG	2.99	0.44
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.50	0.44
1:B:2517:LYS:NZ	1:B:2520:GLU:OE1	2.50	0.44
1:B:4020:ASN:HD22	1:B:4028:ARG:HB3	1.82	0.44
1:A:1416:LYS:O	1:A:1421:TYR:HE2	2.01	0.44
1:A:1995:VAL:HG21	1:A:2024:SER:CB	2.44	0.44
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.17	0.44
1:B:3946:VAL:HB	1:B:3947:PRO:HA	2.00	0.44
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.85	0.44
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.48	0.44
1:A:1575:LEU:O	1:A:1576:GLU:HB3	2.16	0.44
1:A:1620:PHE:CB	1:A:1760:PHE:CE1	3.00	0.44
1:A:2122:THR:O	1:A:2123:LEU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.17	0.44
1:A:2623:THR:HG21	3:A:5401:ADP:O2'	2.17	0.44
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.75	0.44
1:A:3919:LYS:HG3	1:A:3919:LYS:O	2.18	0.44
1:B:1735:TYR:HB2	1:B:1748:PHE:CZ	2.53	0.44
1:B:2385:VAL:HG23	1:B:2574:TYR:HD1	1.82	0.44
1:B:2640:THR:HG23	1:B:2643:SER:H	1.83	0.44
1:B:2728:LEU:HG	1:B:2771:ARG:HH22	1.81	0.44
1:B:3348:ILE:HA	1:B:3351:ARG:HG2	1.99	0.44
1:B:3631:MET:HE3	1:B:3698:MET:HG3	1.98	0.44
1:B:3708:PHE:HZ	1:B:3720:LEU:HD21	1.82	0.44
1:A:2745:ILE:HG12	1:A:2756:MET:CE	2.44	0.44
1:A:3305:ARG:HA	1:A:3305:ARG:HD3	1.42	0.44
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.66	0.44
1:A:4024:VAL:HG23	1:A:4027:VAL:HB	2.00	0.44
1:B:1969:GLY:O	1:B:1972:THR:HB	2.17	0.44
1:B:1980:CYS:O	1:B:1983:LEU:HB3	2.17	0.44
1:B:2733:VAL:H	3:B:5402:ADP:N6	2.16	0.44
1:B:3407:LEU:HD23	1:B:3518:PHE:CE2	2.52	0.44
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.53	0.44
1:A:1849:GLU:CD	1:A:1899:ASN:ND2	2.70	0.44
1:A:2111:LYS:CD	1:A:2161:GLU:CG	2.87	0.44
1:A:2936:ILE:HG22	1:A:2962:ARG:HD3	1.99	0.44
1:B:2786:ILE:HD13	1:B:2823:LEU:HD11	1.98	0.44
1:A:2099:ASN:HD22	1:A:2151:TRP:HE1	1.66	0.44
1:A:3703:PHE:CE1	1:A:3766:GLU:HG2	2.53	0.44
1:A:3785:TYR:CD2	1:A:3785:TYR:N	2.85	0.44
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.99	0.44
1:A:1650:LEU:HD11	1:A:1747:VAL:HG11	1.99	0.44
1:A:1806:VAL:HG11	1:A:1846:CYS:HB2	1.99	0.44
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.51	0.44
1:B:1365:PHE:O	1:B:1366:VAL:C	2.56	0.44
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.78	0.44
1:B:1926:SER:HA	1:B:1970:LEU:CD1	2.48	0.44
1:B:2080:LYS:HZ1	1:B:2549:ARG:HE	1.65	0.44
1:B:2673:LEU:HD23	1:B:2689:ILE:HG23	2.00	0.44
1:B:4022:GLN:HA	1:B:4028:ARG:HA	2.00	0.44
1:A:1983:LEU:HD13	1:A:2000:ARG:HE	1.82	0.43
1:A:2039:LYS:O	1:A:2043:GLN:HG2	2.17	0.43
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.53	0.43
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3461:ILE:C	1:A:3463:SER:N	2.71	0.43
1:B:1645:PHE:HZ	1:B:1768:ARG:HD2	1.82	0.43
1:B:2473:LEU:HD11	1:B:2527:GLU:HG3	1.98	0.43
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.46	0.43
1:B:2738:MET:HG2	1:B:2769:LEU:HD21	1.99	0.43
1:B:3443:ALA:HB1	1:B:3450:VAL:CG2	2.48	0.43
1:B:3407:LEU:HD23	1:B:3518:PHE:HE2	1.83	0.43
1:A:1459:LEU:HD23	1:A:1465:ILE:HG13	1.99	0.43
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	3.01	0.43
1:B:3024:LEU:HD13	1:B:3303:LYS:HG3	1.91	0.43
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.48	0.43
1:A:1963:MET:HG2	1:A:1965:HIS:CE1	2.53	0.43
1:A:3407:LEU:HD23	1:A:3518:PHE:CE2	2.53	0.43
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.81	0.43
1:B:2754:GLY:HA3	1:B:2886:HIS:ND1	2.32	0.43
1:B:3579:GLU:O	1:B:3582:GLU:N	2.44	0.43
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.18	0.43
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.54	0.43
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.19	0.43
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.76	0.43
1:B:2060:PHE:HD2	1:B:2087:VAL:HG11	1.83	0.43
1:B:2473:LEU:HD22	1:B:2475:PRO:CD	2.30	0.43
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.99	0.43
1:B:3303:LYS:CA	1:B:3306:TRP:CD1	2.86	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.17	0.43
1:A:1866:GLN:O	1:A:1870:ASN:HB2	2.18	0.43
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.66	0.43
1:A:3815:PRO:O	1:A:3821:ASN:HB3	2.17	0.43
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	2.01	0.43
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.53	0.43
1:B:2080:LYS:HZ1	1:B:2549:ARG:NH2	2.11	0.43
1:A:1469:LEU:HD13	1:A:1523:LEU:CD2	2.49	0.43
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.33	0.43
1:A:1987:PHE:HB3	1:A:1988:GLY:H	1.69	0.43
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.19	0.43
1:A:2581:LEU:HD11	1:A:2634:ASN:HD22	1.84	0.43
1:A:3544:LYS:HE3	1:A:3607:PHE:CD1	2.54	0.43
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.59	0.43
1:B:1924:PRO:CB	1:B:1929:ILE:HD11	2.37	0.43
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.54	0.43
1:A:3696:MET:SD	1:A:3760:LEU:HB3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.32	0.43
1:B:1898:LEU:HD11	1:B:1908:LEU:CD2	2.49	0.43
1:B:1926:SER:HB2	1:B:1973:LEU:HD21	2.00	0.43
1:B:2160:PRO:O	1:B:2164:GLU:HG3	2.18	0.43
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	2.00	0.43
1:B:2733:VAL:N	3:B:5402:ADP:C6	2.80	0.43
1:A:1689:LYS:HG3	1:A:1689:LYS:O	2.19	0.43
1:B:1945:LEU:HD21	1:B:1991:GLU:CB	2.49	0.43
1:B:2581:LEU:HD11	1:B:2634:ASN:HD22	1.82	0.43
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	2.01	0.43
1:A:1998:LEU:CD1	1:A:2022:PHE:CZ	3.02	0.43
1:A:2354:SER:OG	1:A:2357:SER:CB	2.67	0.43
1:A:2356:TYR:O	1:A:2372:CYS:HB2	2.19	0.43
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.49	0.43
1:A:3934:TRP:CB	1:A:4023:ILE:HD13	2.49	0.43
1:A:4033:LEU:CD1	1:A:4036:GLN:H	2.32	0.43
1:B:1365:PHE:O	1:B:1367:ILE:N	2.52	0.43
1:B:2154:PHE:CD1	1:B:2154:PHE:N	2.86	0.43
1:B:2464:TYR:CE2	1:B:2474:LEU:HD12	2.54	0.43
1:B:2759:ILE:HG21	1:B:2916:TRP:CZ2	2.54	0.43
1:B:3978:ASN:ND2	1:B:3980:ILE:HG22	2.34	0.43
1:A:2437:LEU:HD12	1:A:2437:LEU:H	1.84	0.43
1:A:2514:GLY:HA3	1:A:2525:THR:HA	2.01	0.43
1:A:3618:TYR:O	1:A:3622:GLY:N	2.51	0.43
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.18	0.43
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.52	0.43
1:B:1910:GLU:HB2	1:B:3846:MET:CA	2.48	0.43
1:B:3833:LYS:NZ	1:B:3862:THR:HG21	2.34	0.43
1:B:2080:LYS:CE	2:B:5400:ATP:O1B	2.60	0.43
1:A:1574:PHE:HB3	1:A:1576:GLU:N	2.24	0.42
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.54	0.42
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.54	0.42
1:A:2506:LEU:HA	1:A:2509:LEU:HD12	2.01	0.42
1:A:2763:ARG:HA	1:A:2763:ARG:HD2	1.55	0.42
1:B:3848:LEU:O	1:B:3849:SER:C	2.57	0.42
1:A:1365:PHE:CG	1:A:1366:VAL:N	2.86	0.42
1:B:1770:ILE:HD13	1:B:1770:ILE:HA	1.93	0.42
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.76	0.42
1:B:2764:THR:HG22	1:B:2765:GLY:N	2.34	0.42
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.01	0.42
1:A:1367:ILE:H	1:A:1367:ILE:HD12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:PHE:N	1:A:1539:PHE:CD1	2.87	0.42
1:A:1826:PHE:CE1	1:A:1830:VAL:HG13	2.55	0.42
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.67	0.42
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.33	0.42
1:A:1421:TYR:HE1	1:A:1425:GLU:OE2	2.02	0.42
1:A:1981:SER:CB	1:A:1982:PRO:HD3	2.45	0.42
1:A:2106:THR:H	1:A:2156:SER:HB2	1.84	0.42
1:A:2507:ARG:HB2	1:A:2550:PHE:HB2	2.01	0.42
1:B:1939:PHE:N	1:B:1939:PHE:CD2	2.87	0.42
1:B:2021:ILE:HG22	1:B:2022:PHE:HD1	1.83	0.42
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.85	0.42
1:B:2889:PHE:CD1	1:B:2902:MET:HE1	2.54	0.42
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.84	0.42
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	2.02	0.42
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.39	0.42
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.20	0.42
1:B:1977:LEU:O	1:B:1980:CYS:HB3	2.20	0.42
1:B:2158:LEU:HD13	1:B:2202:THR:HB	2.02	0.42
1:B:3584:MET:HA	1:B:3587:LEU:HB2	1.99	0.42
1:A:1421:TYR:O	1:A:1425:GLU:HB3	2.18	0.42
1:A:1743:ASP:HA	1:A:1746:SER:HB3	2.00	0.42
1:B:2080:LYS:CE	2:B:5400:ATP:O3G	2.67	0.42
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.20	0.42
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.39	0.42
1:B:3519:VAL:CG1	1:B:3521:ASN:ND2	2.82	0.42
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.67	0.42
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	2.01	0.42
1:B:3846:MET:HG3	1:B:3847:SER:N	2.34	0.42
1:A:2109:LEU:HD12	1:A:2129:LEU:HD23	2.01	0.42
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.68	0.42
1:A:3321:ILE:H	1:A:3321:ILE:HD12	1.84	0.42
1:A:3934:TRP:HB3	1:A:4023:ILE:HD13	2.01	0.42
1:B:2159:ASP:HB2	1:B:2160:PRO:HD2	2.01	0.42
1:B:2893:ASP:HA	1:B:2894:PRO:HD2	1.96	0.42
1:A:1681:LYS:HE2	1:A:1939:PHE:HZ	1.84	0.42
1:A:1914:LYS:HD3	1:A:3959:CYS:SG	2.60	0.42
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.39	0.42
1:A:2060:PHE:CZ	1:A:2193:LEU:HD21	2.54	0.42
1:A:2356:TYR:CE1	1:A:2399:LYS:HD2	2.54	0.42
1:A:2476:LYS:N	1:A:2476:LYS:HD3	2.31	0.42
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	2.02	0.42
1:A:3799:LYS:HG3	1:A:3803:LEU:HD11	2.02	0.42
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.02	0.42
1:B:3843:ASN:O	1:B:3846:MET:HG2	2.19	0.42
1:A:216:PRO:CB	1:A:1365:PHE:N	2.83	0.42
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.67	0.42
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.20	0.42
1:B:2034:ILE:HD12	1:B:2061:TYR:CE2	2.54	0.42
1:B:2071:ILE:HB	1:B:2212:LEU:HD12	2.01	0.42
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.01	0.42
1:A:1874:VAL:HG21	1:A:1876:LYS:NZ	2.34	0.42
1:A:2081:THR:HG22	1:A:2085:LYS:HD2	2.01	0.42
1:A:2412:ARG:HH11	1:A:2555:ALA:HB2	1.85	0.42
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.42
1:A:2847:GLU:HG3	1:A:2848:GLU:N	2.34	0.42
1:A:3302:GLU:O	1:A:3306:TRP:N	2.49	0.42
1:A:3327:SER:O	1:A:3331:GLU:HG3	2.20	0.42
1:A:3636:GLY:HA2	1:A:3642:TYR:O	2.20	0.42
1:A:3830:SER:HA	1:A:3833:LYS:HE3	2.02	0.42
1:A:3839:ILE:HG22	1:A:3873:MET:HA	2.02	0.42
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	2.01	0.42
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	2.02	0.42
1:B:2178:LEU:HD12	1:B:2182:GLU:HB2	2.02	0.42
1:B:2415:ILE:O	1:B:2556:ILE:HA	2.20	0.42
1:B:2082:ALA:N	2:B:5400:ATP:O2A	2.53	0.42
1:A:1625:ASP:O	1:A:1629:GLN:HG3	2.19	0.41
1:A:2701:SER:HB2	1:A:2703:ASP:O	2.20	0.41
1:A:3555:TYR:HB3	1:A:3597:ILE:HD11	2.02	0.41
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.99	0.41
1:A:3903:ILE:O	1:A:3907:VAL:HG23	2.20	0.41
1:B:1664:LEU:O	1:B:1721:LYS:HE3	2.19	0.41
1:B:2222:ILE:H	1:B:2222:ILE:HG13	1.67	0.41
1:B:2852:LEU:O	1:B:2856:LEU:HB2	2.20	0.41
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.20	0.41
1:B:4019:ASP:O	1:B:4030:PRO:HA	2.19	0.41
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.20	0.41
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	2.02	0.41
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.85	0.41
1:A:2828:LEU:HD11	1:A:2908:LEU:HD11	2.01	0.41
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.20	0.41
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.55	0.41
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.49	0.41
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.50	0.41
1:B:1534:PHE:HD2	1:B:1537:PHE:CD2	2.38	0.41
1:B:3466:ILE:HD13	1:B:3509:LEU:HD13	2.02	0.41
1:B:3471:ASN:HB2	1:B:3478:THR:HG23	2.01	0.41
1:A:1392:LEU:HD22	1:A:1393:LYS:H	1.86	0.41
1:A:1956:LEU:CB	1:A:1968:PHE:CD2	3.04	0.41
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.87	0.41
1:A:3330:TYR:CE1	1:A:3334:PHE:CE2	3.08	0.41
1:A:3631:MET:HE2	1:A:3632:LEU:HG	2.02	0.41
1:A:4023:ILE:HD13	1:A:4023:ILE:HG21	1.70	0.41
1:B:2091:MET:HE3	1:B:2149:ARG:NH1	2.35	0.41
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.80	0.41
1:A:1534:PHE:HD2	1:A:1537:PHE:CE2	2.38	0.41
1:A:2095:ASP:CG	1:A:2149:ARG:HH21	2.23	0.41
1:A:2339:ILE:HG23	1:A:2353:LEU:HD23	2.03	0.41
1:A:2929:ALA:O	1:A:2933:VAL:HG22	2.21	0.41
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.41
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	2.02	0.41
1:A:54:LEU:HA	1:A:55:PRO:HA	1.83	0.41
1:B:2493:LYS:HA	1:B:2493:LYS:HD2	1.81	0.41
1:B:3464:ARG:O	1:B:3467:SER:O	2.37	0.41
1:B:3519:VAL:CG1	1:B:3521:ASN:HD21	2.33	0.41
1:B:2220:CYS:SG	2:B:5400:ATP:N1	2.89	0.41
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.55	0.41
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.20	0.41
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.54	0.41
1:A:1826:PHE:HE2	1:A:1831:LEU:CB	2.05	0.41
1:A:1951:HIS:HD2	1:A:2021:ILE:HD12	1.84	0.41
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	2.02	0.41
1:A:2474:LEU:HB3	1:A:2526:ILE:HG22	2.01	0.41
1:A:2754:GLY:HA3	1:A:2886:HIS:ND1	2.36	0.41
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.50	0.41
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	2.01	0.41
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.31	0.41
1:B:1838:ILE:HD11	1:B:1845:GLY:N	2.35	0.41
1:B:2866:LEU:HD12	1:B:2867:LEU:H	1.84	0.41
1:B:3311:LYS:HG2	1:B:3315:LYS:NZ	2.35	0.41
1:B:3832:SER:O	1:B:3836:GLY:N	2.49	0.41
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:THR:HB	1:A:1498:GLU:HB2	2.01	0.41
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.02	0.41
1:A:2476:LYS:HB3	1:A:2482:LEU:HB2	2.02	0.41
1:A:2640:THR:HG23	1:A:2643:SER:H	1.85	0.41
1:A:2821:ASN:O	1:A:2823:LEU:HD13	2.21	0.41
1:A:3786:PHE:CD1	1:A:3893:ASP:HB2	2.56	0.41
1:A:3692:LYS:HG3	1:A:3898:GLU:HG3	2.02	0.41
1:A:1726:LEU:HD13	1:A:3984:GLN:HB3	2.01	0.41
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.21	0.41
1:B:1626:CYS:HB2	1:B:1643:TYR:CD2	2.56	0.41
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.35	0.41
1:B:3896:VAL:HG12	1:B:3898:GLU:HG2	2.02	0.41
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.81	0.41
1:A:2765:GLY:CA	3:A:5402:ADP:O2A	2.59	0.41
1:B:1578:PHE:HB3	1:B:1595:LYS:HB2	2.02	0.41
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.51	0.41
1:B:2285:GLU:CB	1:B:2412:ARG:NH2	2.83	0.41
1:B:2788:ARG:H	1:B:3459:ASP:HB2	1.85	0.41
1:B:3950:PHE:HE1	1:B:4006:VAL:HB	1.86	0.41
1:B:2732:MET:CG	3:B:5402:ADP:C6	3.02	0.41
1:A:1409:LEU:O	1:A:1413:VAL:HG23	2.20	0.41
1:A:1744:LEU:CD2	1:A:1760:PHE:CD2	3.03	0.41
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.50	0.41
1:A:2728:LEU:HB2	1:A:2771:ARG:HH12	1.86	0.41
1:A:2982:VAL:HG12	1:A:2983:GLY:H	1.85	0.41
1:A:3971:VAL:HA	1:A:3974:THR:HG22	2.03	0.41
1:B:1697:LYS:O	1:B:1701:LEU:HG	2.20	0.41
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.97	0.41
1:B:3304:GLU:O	1:B:3305:ARG:C	2.59	0.41
1:B:3409:ASP:HB3	1:B:3518:PHE:CB	2.47	0.41
1:B:3757:ILE:HD11	1:B:4074:GLU:HG2	2.02	0.41
1:B:3826:GLN:HB2	1:B:3854:TYR:CZ	2.56	0.41
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.99	0.41
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.61	0.41
1:A:2226:ILE:HG23	1:A:2288:VAL:CG2	2.46	0.41
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.83	0.41
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.41
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.21	0.41
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	2.02	0.41
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.86	0.41
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	2.02	0.41
1:B:1838:ILE:HD11	1:B:1845:GLY:HA3	2.03	0.41
1:B:2099:ASN:HD22	1:B:2151:TRP:HE1	1.68	0.41
1:B:2590:GLU:N	1:B:2591:PRO:HD2	2.36	0.41
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.45	0.41
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.42	0.41
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.56	0.41
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.48	0.41
1:A:2485:PHE:CZ	1:A:2534:ALA:HB2	2.56	0.41
1:A:3528:ARG:HH11	1:A:3650:LEU:HD11	1.86	0.41
1:A:3703:PHE:HE2	1:A:3719:VAL:HG21	1.86	0.41
1:B:1830:VAL:HG23	1:B:1833:ARG:NH2	2.36	0.41
1:B:2782:VAL:HB	1:B:2815:LEU:HD12	2.02	0.41
1:A:1664:LEU:HD21	1:A:1715:LEU:HD22	2.03	0.41
1:A:2266:PHE:CD1	1:A:2326:LEU:HD21	2.53	0.41
1:A:2408:LEU:HD13	1:A:2432:LEU:HD21	2.03	0.41
1:A:2985:ASN:N	1:A:2986:PRO:CD	2.84	0.41
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.34	0.41
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.56	0.40
1:A:2332:GLY:HA2	1:A:2335:GLN:CG	2.50	0.40
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.40
1:B:2225:LYS:HD2	1:B:2281:PHE:CZ	2.55	0.40
1:B:2299:ARG:HA	1:B:2302:PHE:CD2	2.56	0.40
1:B:2320:ARG:NH1	1:B:2406:ASP:OD2	2.40	0.40
1:B:2766:LYS:HD2	1:B:2890:THR:HG22	2.02	0.40
1:B:3629:PHE:O	1:B:3633:GLU:HB2	2.20	0.40
1:B:3833:LYS:HZ3	1:B:3862:THR:HG21	1.85	0.40
1:B:3839:ILE:HG22	1:B:3871:PHE:HE1	1.86	0.40
1:A:1392:LEU:HD21	1:A:1487:THR:HG21	2.02	0.40
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	2.02	0.40
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.91	0.40
1:A:2060:PHE:HZ	1:A:2193:LEU:HD21	1.86	0.40
1:A:2380:LEU:HD12	1:A:2380:LEU:C	2.42	0.40
1:A:3458:PHE:HD2	1:A:3506:PRO:HG2	1.86	0.40
1:A:3844:ILE:HD11	1:A:3855:LEU:HD22	2.03	0.40
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.03	0.40
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.21	0.40
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.40
1:A:1637:GLU:C	1:A:1686:LYS:HZ2	2.20	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.03	0.40
1:B:2306:ASP:HB2	1:B:2309:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.37	0.40
1:B:2575:TYR:HD1	1:B:2578:ILE:HD11	1.85	0.40
1:B:2757:MET:CB	1:B:2889:PHE:HB2	2.52	0.40
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	2.03	0.40
1:A:1703:VAL:HG21	1:A:1768:ARG:HB2	2.03	0.40
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.97	0.40
1:B:2572:GLU:CG	1:B:2590:GLU:HG3	2.51	0.40
1:B:2751:GLN:H	1:B:2751:GLN:HG2	1.74	0.40
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.62	0.40
1:B:2972:PHE:CE2	1:B:3329:ILE:HG12	2.57	0.40
1:B:3939:ILE:HG22	1:B:3956:PHE:CE2	2.57	0.40
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.35	0.40
1:A:3528:ARG:HD2	1:A:3650:LEU:HD11	2.03	0.40
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.42	0.40
1:A:3848:LEU:HD12	1:A:3884:LEU:HD12	2.04	0.40
1:B:1495:THR:HB	1:B:1498:GLU:CG	2.51	0.40
1:B:2276:LEU:HD13	1:B:2417:CYS:SG	2.62	0.40
1:B:2542:GLY:O	1:B:2544:ILE:HD12	2.21	0.40
1:B:2832:ASN:OD1	1:B:2907:ALA:HB3	2.21	0.40
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.57	0.40
1:B:3772:TRP:HZ3	1:B:3780:ASN:ND2	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	2503 (95%)	121 (5%)	16 (1%)	25	57
1	B	2640/2695 (98%)	2506 (95%)	116 (4%)	18 (1%)	22	55
All	All	5280/5390 (98%)	5009 (95%)	237 (4%)	34 (1%)	25	57

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	1391	GLY
1	A	2369	SER
1	A	3309	THR
1	B	1391	GLY
1	B	2761	ALA
1	B	3306	TRP
1	A	212	GLY
1	A	1633	GLY
1	B	2763	ARG
1	B	2764	THR
1	B	2990	GLY
1	B	3482	GLY
1	A	2562	PRO
1	A	2990	GLY
1	A	3980	ILE
1	A	115	GLU
1	A	2513	GLN
1	A	2519	PRO
1	A	3809	GLU
1	B	66	GLN
1	B	2519	PRO
1	B	3402	ASP
1	A	66	GLN
1	B	2562	PRO
1	A	3482	GLY
1	B	1366	VAL
1	B	3462	ILE
1	B	3980	ILE
1	B	1633	GLY
1	B	2028	PRO
1	B	1470	PRO
1	B	2141	ILE
1	A	1470	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%)	2128 (96%)	90 (4%)	30	59
1	B	2218/2453 (90%)	2133 (96%)	85 (4%)	33	61
All	All	4436/4906 (90%)	4261 (96%)	175 (4%)	32	61

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1383	TYR
1	A	1422	LYS
1	A	1463	LEU
1	A	1486	ILE
1	A	1504	ASN
1	A	1553	LYS
1	A	1635	ASP
1	A	1694	VAL
1	A	1794	PHE
1	A	1802	LYS
1	A	1818	VAL
1	A	1832	SER
1	A	1903	ASN
1	A	1929	ILE
1	A	1936	ILE
1	A	1959	LYS
1	A	2064	GLN
1	A	2075	LYS
1	A	2078	CYS
1	A	2080	LYS
1	A	2122	THR
1	A	2154	PHE
1	A	2155	ASP
1	A	2202	THR
1	A	2239	ASN
1	A	2246	LEU
1	A	2276	LEU
1	A	2285	GLU
1	A	2323	LEU
1	A	2346	PHE
1	A	2428	MET
1	A	2472	THR
1	A	2474	LEU
1	A	2476	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2566	SER
1	A	2681	LEU
1	A	2694	LEU
1	A	2785	LYS
1	A	2829	GLU
1	A	2843	LEU
1	A	2856	LEU
1	A	2865	LEU
1	A	2873	LEU
1	A	2961	ILE
1	A	3023	LYS
1	A	3304	GLU
1	A	3305	ARG
1	A	3306	TRP
1	A	3307	LEU
1	A	3312	GLN
1	A	3316	THR
1	A	3355	LYS
1	A	3372	THR
1	A	3386	LYS
1	A	3391	LEU
1	A	3400	SER
1	A	3439	ARG
1	A	3483	ASP
1	A	3534	LEU
1	A	3536	GLU
1	A	3538	ASN
1	A	3557	LEU
1	A	3559	LEU
1	A	3567	LEU
1	A	3578	LEU
1	A	3598	GLU
1	A	3601	LEU
1	A	3673	GLU
1	A	3717	GLU
1	A	3729	SER
1	A	3737	THR
1	A	3794	VAL
1	A	3799	LYS
1	A	3802	GLU
1	A	3805	LYS
1	A	3811	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	3844	ILE
1	A	3871	PHE
1	A	3899	ASP
1	A	3900	ILE
1	A	3906	THR
1	A	3940	THR
1	A	3943	THR
1	A	3952	LYS
1	A	3960	ASP
1	A	3980	ILE
1	A	3982	TRP
1	A	4040	GLU
1	A	4064	GLN
1	A	4068	GLU
1	B	1399	ASP
1	B	1421	TYR
1	B	1455	LEU
1	B	1475	LYS
1	B	1486	ILE
1	B	1491	PHE
1	B	1493	LEU
1	B	1525	THR
1	B	1689	LYS
1	B	1794	PHE
1	B	1832	SER
1	B	1936	ILE
1	B	1939	PHE
1	B	1971	ARG
1	B	2003	LEU
1	B	2035	VAL
1	B	2064	GLN
1	B	2109	LEU
1	B	2155	ASP
1	B	2202	THR
1	B	2222	ILE
1	B	2239	ASN
1	B	2255	ASP
1	B	2295	ILE
1	B	2310	LEU
1	B	2346	PHE
1	B	2351	GLN
1	B	2357	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	2387	ARG
1	B	2395	ILE
1	B	2428	MET
1	B	2476	LYS
1	B	2563	SER
1	B	2566	SER
1	B	2574	TYR
1	B	2587	SER
1	B	2613	SER
1	B	2664	LYS
1	B	2689	ILE
1	B	2694	LEU
1	B	2702	LEU
1	B	2757	MET
1	B	2829	GLU
1	B	2833	THR
1	B	2843	LEU
1	B	2853	LEU
1	B	2873	LEU
1	B	2967	ASN
1	B	3001	LYS
1	B	3012	GLU
1	B	3329	ILE
1	B	3360	TYR
1	B	3372	THR
1	B	3391	LEU
1	B	3400	SER
1	B	3401	GLN
1	B	3502	SER
1	B	3510	ARG
1	B	3531	ASP
1	B	3534	LEU
1	B	3536	GLU
1	B	3538	ASN
1	B	3565	ARG
1	B	3567	LEU
1	B	3605	GLU
1	B	3618	TYR
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3811	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	3813	ILE
1	B	3831	LYS
1	B	3871	PHE
1	B	3876	THR
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3943	THR
1	B	3958	ASP
1	B	3960	ASP
1	B	3980	ILE
1	B	3982	TRP
1	B	4004	LEU
1	B	4021	LEU
1	B	4040	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1533	GLN
1	A	1605	GLN
1	A	1622	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1864	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	2068	GLN
1	A	2099	ASN
1	A	2228	HIS
1	A	2274	HIS
1	A	2282	ASN
1	A	2335	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2536	ASN
1	A	2598	HIS
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2753	GLN
1	A	3323	ASN
1	A	3338	ASN
1	A	3420	ASN
1	A	3521	ASN
1	A	3588	ASN
1	A	3685	GLN
1	A	3780	ASN
1	A	3890	GLN
1	A	4020	ASN
1	A	4031	GLN
1	A	4077	GLN
1	B	1449	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1736	GLN
1	B	1899	ASN
1	B	1951	HIS
1	B	2068	GLN
1	B	2099	ASN
1	B	2228	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2383	HIS
1	B	2409	ASN
1	B	2536	ASN
1	B	2601	ASN
1	B	2634	ASN
1	B	2688	ASN
1	B	2753	GLN
1	B	3323	ASN
1	B	3338	ASN
1	B	3497	HIS
1	B	3521	ASN
1	B	3624	HIS
1	B	3780	ASN
1	B	3783	ASN
1	B	3868	HIS
1	B	3890	GLN
1	B	4020	ASN
1	B	4077	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	B	5401	-	24,29,29	1.22	2 (8%)	29,45,45	1.56	6 (20%)
2	ATP	B	5400	-	26,33,33	1.02	1 (3%)	31,52,52	1.61	6 (19%)
2	ATP	A	5400	-	26,33,33	1.02	1 (3%)	31,52,52	1.62	6 (19%)
4	SO4	B	5403	-	4,4,4	0.34	0	6,6,6	0.45	0
3	ADP	A	5402	-	24,29,29	1.02	1 (4%)	29,45,45	1.58	5 (17%)
3	ADP	B	5402	-	24,29,29	0.98	1 (4%)	29,45,45	1.53	5 (17%)
4	SO4	A	5403	-	4,4,4	0.36	0	6,6,6	0.74	0
3	ADP	A	5401	-	24,29,29	1.20	2 (8%)	29,45,45	1.46	7 (24%)

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	B	5401	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	5400	-	-	5/18/38/38	0/3/3/3
2	ATP	A	5400	-	-	5/18/38/38	0/3/3/3
3	ADP	A	5402	-	-	5/12/32/32	0/3/3/3
3	ADP	B	5402	-	-	1/12/32/32	0/3/3/3
3	ADP	A	5401	-	-	6/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5401	ADP	C5-C4	2.91	1.48	1.40
3	A	5401	ADP	C2-N3	2.69	1.36	1.32
3	B	5401	ADP	C5-C4	2.63	1.47	1.40
3	B	5402	ADP	C5-C4	2.60	1.47	1.40
2	B	5400	ATP	C5-C4	2.45	1.47	1.40
3	A	5402	ADP	C5-C4	2.42	1.47	1.40
2	A	5400	ATP	C5-C4	2.38	1.47	1.40
3	B	5401	ADP	C2'-C1'	-2.09	1.50	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5402	ADP	C3'-C2'-C1'	4.03	107.04	100.98
3	A	5402	ADP	N3-C2-N1	-3.88	122.61	128.68
3	B	5401	ADP	PA-O3A-PB	-3.74	119.99	132.83
3	B	5401	ADP	N3-C2-N1	-3.72	122.86	128.68
2	B	5400	ATP	C3'-C2'-C1'	3.64	106.46	100.98
2	A	5400	ATP	C3'-C2'-C1'	3.58	106.36	100.98
3	B	5402	ADP	PA-O3A-PB	-3.57	120.58	132.83
2	A	5400	ATP	PB-O3B-PG	-3.55	120.64	132.83
3	B	5402	ADP	C3'-C2'-C1'	3.52	106.28	100.98
2	A	5400	ATP	PA-O3A-PB	-3.52	120.76	132.83
2	B	5400	ATP	PB-O3B-PG	-3.51	120.80	132.83
3	B	5402	ADP	N3-C2-N1	-3.45	123.28	128.68
2	B	5400	ATP	PA-O3A-PB	-3.33	121.41	132.83
3	A	5402	ADP	PA-O3A-PB	-3.22	121.78	132.83
2	B	5400	ATP	N3-C2-N1	-3.14	123.77	128.68
2	A	5400	ATP	N3-C2-N1	-3.12	123.80	128.68
3	A	5401	ADP	O4'-C1'-C2'	2.89	111.14	106.93
3	A	5401	ADP	PA-O3A-PB	-2.88	122.95	132.83
3	A	5402	ADP	C4-C5-N7	-2.75	106.53	109.40
2	A	5400	ATP	C4-C5-N7	-2.71	106.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5400	ATP	C4-C5-N7	-2.69	106.59	109.40
3	B	5401	ADP	C3'-C2'-C1'	2.66	104.99	100.98
3	A	5401	ADP	N3-C2-N1	-2.64	124.55	128.68
3	A	5401	ADP	C2'-C3'-C4'	2.47	107.43	102.64
3	B	5402	ADP	C4-C5-N7	-2.33	106.97	109.40
3	B	5402	ADP	O3B-PB-O2B	2.27	116.31	107.64
2	B	5400	ATP	O3G-PG-O2G	2.25	116.24	107.64
3	A	5401	ADP	N6-C6-N1	2.21	123.16	118.57
3	B	5401	ADP	C4-C5-N7	-2.13	107.18	109.40
3	A	5401	ADP	O2A-PA-O1A	2.09	122.58	112.24
3	A	5401	ADP	C4-C5-N7	-2.08	107.23	109.40
3	A	5402	ADP	O3B-PB-O2B	2.04	115.44	107.64
3	B	5401	ADP	C2-N1-C6	2.04	122.24	118.75
2	A	5400	ATP	O3G-PG-O2G	2.02	115.34	107.64
3	B	5401	ADP	O2'-C2'-C3'	-2.00	105.35	111.82

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5401	ADP	C3'-C4'-C5'-O5'
2	B	5400	ATP	C5'-O5'-PA-O2A
2	A	5400	ATP	C5'-O5'-PA-O2A
3	A	5402	ADP	C5'-O5'-PA-O3A
3	A	5402	ADP	O4'-C4'-C5'-O5'
3	A	5401	ADP	PA-O3A-PB-O2B
3	A	5401	ADP	C5'-O5'-PA-O1A
3	A	5401	ADP	C5'-O5'-PA-O2A
3	A	5401	ADP	C5'-O5'-PA-O3A
3	A	5401	ADP	O4'-C4'-C5'-O5'
3	A	5401	ADP	C3'-C4'-C5'-O5'
2	B	5400	ATP	O4'-C4'-C5'-O5'
2	B	5400	ATP	C3'-C4'-C5'-O5'
2	A	5400	ATP	O4'-C4'-C5'-O5'
2	A	5400	ATP	C3'-C4'-C5'-O5'
3	A	5402	ADP	C3'-C4'-C5'-O5'
3	B	5401	ADP	O4'-C4'-C5'-O5'
2	B	5400	ATP	C5'-O5'-PA-O3A
2	A	5400	ATP	C5'-O5'-PA-O3A
3	A	5402	ADP	C5'-O5'-PA-O1A
3	A	5402	ADP	C5'-O5'-PA-O2A
3	B	5401	ADP	PB-O3A-PA-O2A

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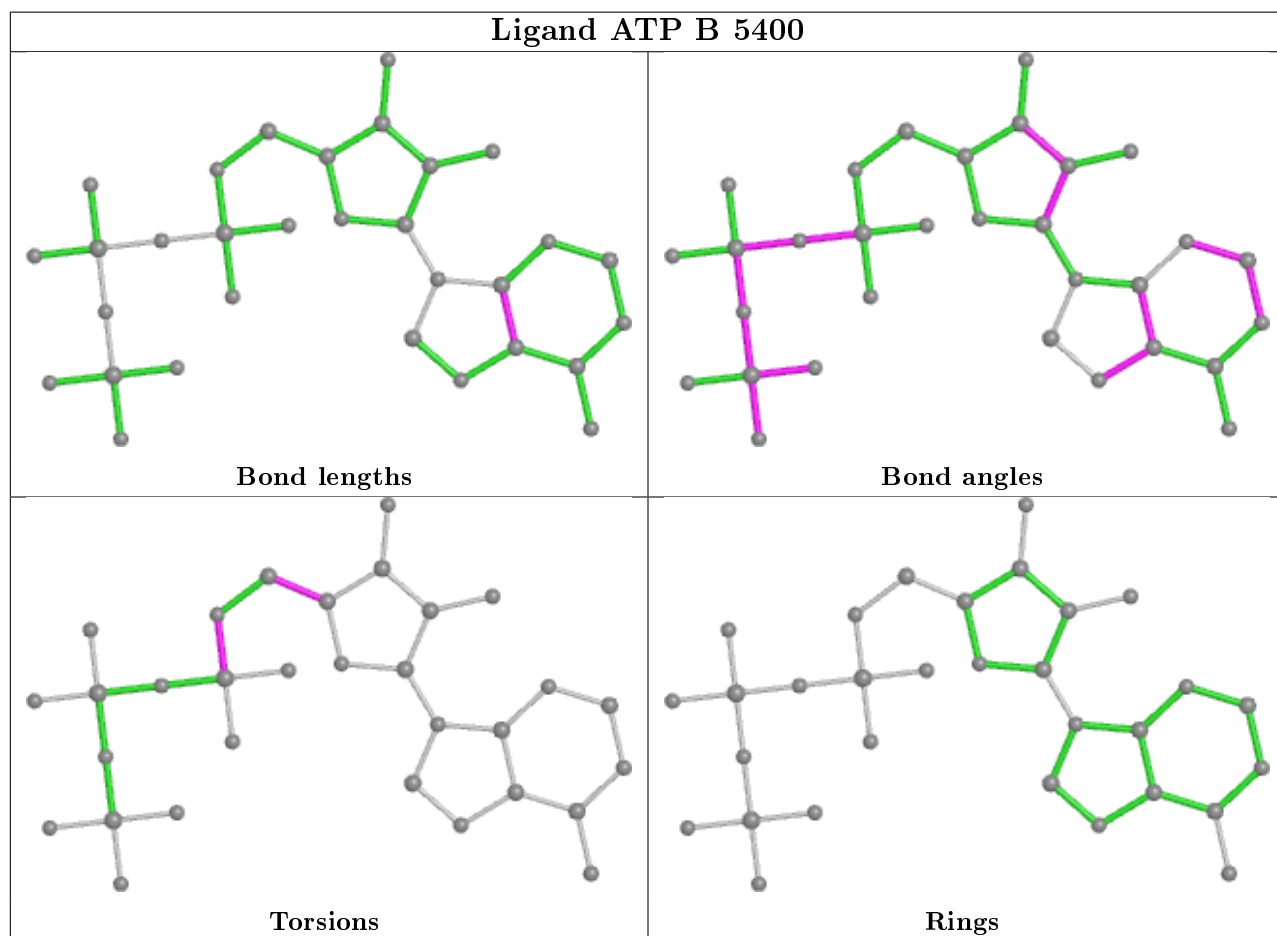
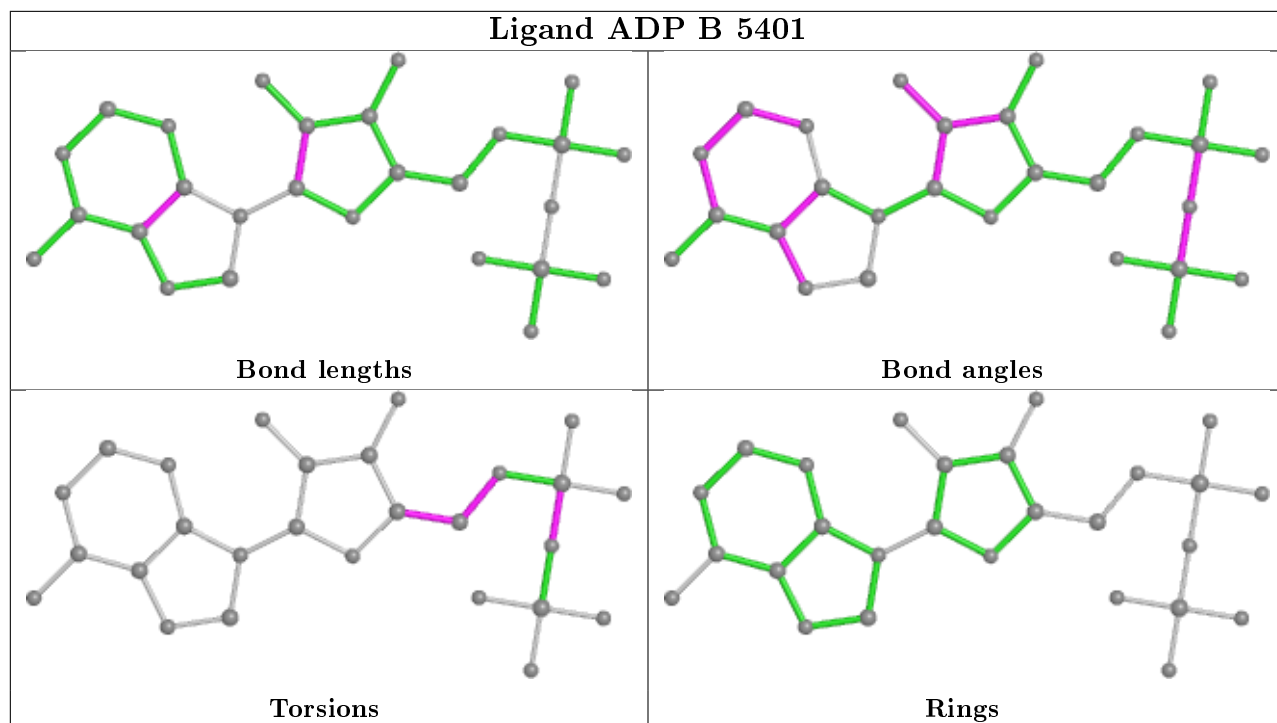
Mol	Chain	Res	Type	Atoms
3	B	5401	ADP	C4'-C5'-O5'-PA
3	B	5402	ADP	O4'-C4'-C5'-O5'
3	B	5401	ADP	PB-O3A-PA-O1A
2	B	5400	ATP	C5'-O5'-PA-O1A
2	A	5400	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

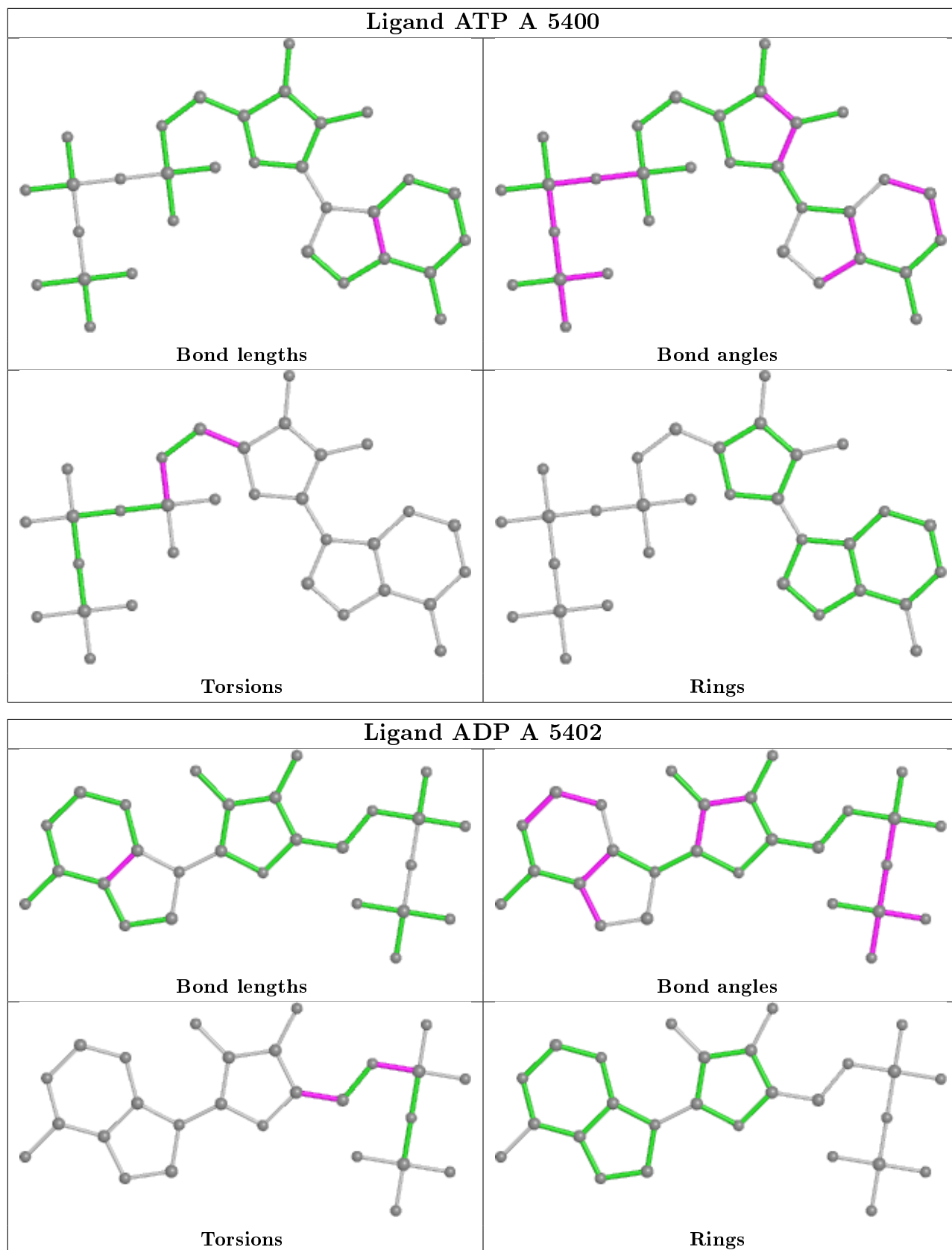
8 monomers are involved in 89 short contacts:

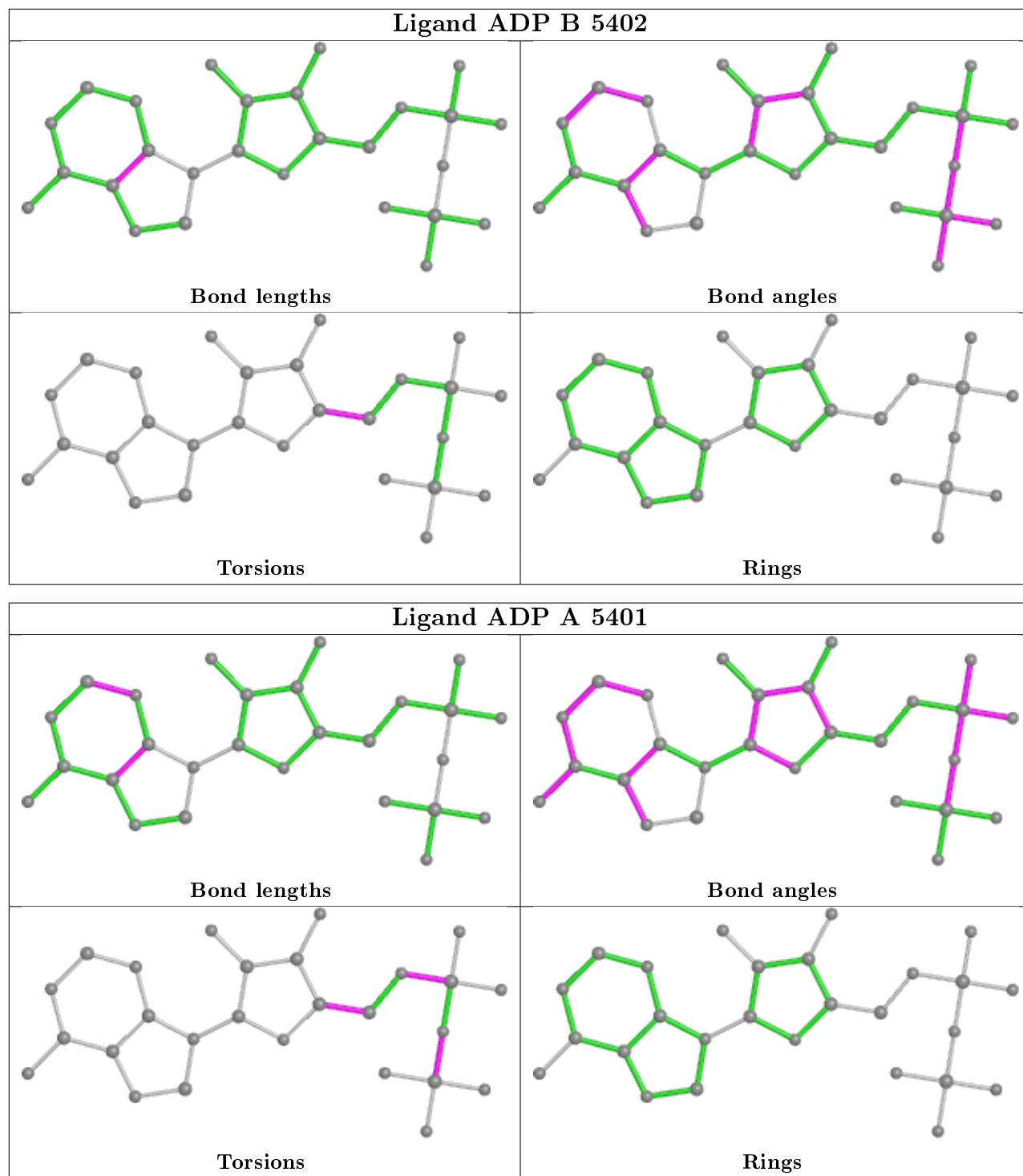
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5401	ADP	6	0
2	B	5400	ATP	22	0
2	A	5400	ATP	6	0
4	B	5403	SO4	2	0
3	A	5402	ADP	17	0
3	B	5402	ADP	23	0
4	A	5403	SO4	2	0
3	A	5401	ADP	11	0

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









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	2650/2695 (98%)	0.60	296 (11%) <b>5</b> <b>6</b>	88, 185, 310, 500	1 (0%)
1	B	2650/2695 (98%)	0.70	256 (9%) <b>7</b> <b>9</b>	96, 180, 317, 500	1 (0%)
All	All	5300/5390 (98%)	0.65	552 (10%) <b>6</b> <b>8</b>	88, 183, 311, 500	2 (0%)

All (552) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	35.4
1	B	33	GLU	29.6
1	B	83	GLY	28.0
1	B	69	ALA	26.8
1	A	131	MET	25.1
1	B	91	ILE	24.1
1	B	199	ALA	23.9
1	B	198	ILE	23.4
1	B	66	GLN	22.9
1	B	84	CYS	22.1
1	B	16	THR	21.6
1	B	92	SER	19.4
1	A	1460	GLY	18.9
1	B	52	PRO	18.7
1	B	15	PRO	18.6
1	B	35	ASP	17.5
1	B	4	LEU	15.5
1	B	155	TYR	15.3
1	A	132	PHE	15.2
1	B	189	ASP	15.1
1	B	34	ARG	14.9
1	B	200	TRP	14.9
1	B	152	PHE	14.2
1	B	50	GLU	13.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	95	GLU	13.5
1	B	14	GLN	13.1
1	B	68	MET	13.1
1	A	1459	LEU	13.0
1	B	17	ARG	12.4
1	B	32	TYR	12.3
1	B	186	PRO	11.9
1	B	88	ARG	11.8
1	B	89	ALA	11.7
1	B	87	GLU	11.6
1	B	18	LEU	11.1
1	B	48	GLY	10.4
1	A	143	ASN	10.3
1	A	27	TYR	10.2
1	B	149	HIS	10.0
1	B	5	GLY	9.8
1	B	65	THR	9.7
1	B	151	ASP	9.6
1	B	90	GLU	9.5
1	A	31	LEU	9.4
1	A	3580	ASN	9.0
1	B	171	ALA	8.8
1	A	1483	TYR	8.6
1	B	1483	TYR	8.4
1	B	194	SER	8.3
1	A	42	ASN	8.3
1	A	108	ILE	8.2
1	B	168	CYS	8.1
1	B	36	GLU	8.0
1	A	3575	GLY	7.9
1	B	193	LYS	7.7
1	A	3581	ASP	7.7
1	B	45	PHE	7.6
1	B	70	ILE	7.6
1	B	73	TYR	7.6
1	A	115	GLU	7.5
1	B	53	ASN	7.4
1	A	210	GLY	7.4
1	A	28	GLU	7.3
1	A	202	LEU	7.3
1	B	11	GLY	7.2
1	B	6	TYR	7.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	19	LEU	7.2
1	B	3580	ASN	7.2
1	A	40	TRP	7.1
1	B	96	GLY	7.1
1	B	8	LYS	7.1
1	A	35	ASP	7.0
1	A	148	THR	6.8
1	A	3578	LEU	6.8
1	B	3	ILE	6.7
1	A	3979	ASN	6.7
1	A	1549	ILE	6.7
1	A	2364	ASP	6.5
1	B	72	ARG	6.3
1	A	1500	ILE	6.3
1	A	134	ASP	6.2
1	B	143	ASN	6.2
1	A	2687	GLY	6.2
1	B	174	LYS	6.1
1	A	2362	ALA	6.0
1	A	173	PRO	6.0
1	A	2942	ASP	6.0
1	B	2941	THR	5.9
1	A	1504	ASN	5.9
1	A	29	GLU	5.9
1	B	3567	LEU	5.9
1	B	94	LEU	5.9
1	B	55	PRO	5.9
1	A	1458	ILE	5.9
1	B	190	LYS	5.9
1	A	1445	TRP	5.9
1	B	3300	THR	5.8
1	A	1490	ALA	5.7
1	B	172	PHE	5.7
1	A	150	PRO	5.7
1	A	130	LYS	5.7
1	A	1390	SER	5.7
1	B	169	LEU	5.7
1	A	3306	TRP	5.6
1	B	1669	PHE	5.6
1	A	1548	ILE	5.6
1	B	2938	MET	5.6
1	A	54	LEU	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	13	VAL	5.5
1	B	1459	LEU	5.5
1	B	3575	GLY	5.4
1	B	3735	LYS	5.3
1	B	2368	PHE	5.3
1	B	30	HIS	5.3
1	A	1392	LEU	5.3
1	B	61	ASP	5.2
1	A	3579	GLU	5.2
1	A	3577	MET	5.1
1	B	98	VAL	5.0
1	A	2302	PHE	5.0
1	B	7	TRP	5.0
1	A	41	ARG	5.0
1	A	1368	GLU	5.0
1	B	10	LYS	4.9
1	B	85	PRO	4.9
1	A	1389	SER	4.9
1	B	2	PRO	4.9
1	A	1558	VAL	4.9
1	A	3980	ILE	4.8
1	A	2363	ASN	4.8
1	A	1383	TYR	4.7
1	B	39	LYS	4.7
1	A	1434	LYS	4.7
1	B	184	ALA	4.7
1	A	64	LEU	4.6
1	A	2248	LYS	4.6
1	B	3741	ASN	4.6
1	B	137	CYS	4.6
1	A	2808	LEU	4.6
1	A	3562	LEU	4.5
1	B	134	ASP	4.5
1	A	89	ALA	4.5
1	A	116	THR	4.5
1	A	1879	ILE	4.5
1	A	63	LYS	4.5
1	B	2121	ALA	4.5
1	A	3576	ASN	4.5
1	A	90	GLU	4.4
1	B	187	GLN	4.4
1	A	3555	TYR	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	133	GLU	4.4
1	A	1388	HIS	4.4
1	B	3024	LEU	4.3
1	B	74	ILE	4.3
1	A	81	LEU	4.3
1	A	144	GLY	4.3
1	A	216	PRO	4.3
1	A	129	LEU	4.2
1	A	32	TYR	4.2
1	B	67	SER	4.2
1	B	192	LEU	4.1
1	B	1394	LEU	4.1
1	B	3542	GLN	4.1
1	B	1458	ILE	4.1
1	A	2854	ASN	4.1
1	B	24	GLU	4.1
1	B	86	LYS	4.1
1	A	3301	PHE	4.1
1	A	75	ALA	4.1
1	B	154	LEU	4.0
1	B	3734	PRO	4.0
1	B	3016	PHE	4.0
1	B	153	MET	4.0
1	A	1493	LEU	4.0
1	A	209	PHE	4.0
1	A	3583	LEU	4.0
1	B	3304	GLU	3.9
1	B	1727	LEU	3.9
1	A	3739	ASP	3.9
1	B	3573	SER	3.9
1	A	1492	GLN	3.9
1	B	3763	PHE	3.9
1	A	3017	VAL	3.9
1	B	1485	MET	3.9
1	B	3303	LYS	3.9
1	A	1452	TRP	3.9
1	B	145	ASP	3.9
1	B	3585	VAL	3.8
1	A	2941	THR	3.8
1	A	3564	LYS	3.8
1	B	202	LEU	3.8
1	B	4035	GLN	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1479	LEU	3.8
1	A	1546	LEU	3.8
1	B	31	LEU	3.8
1	B	1945	LEU	3.8
1	B	64	LEU	3.7
1	A	3591	LYS	3.7
1	B	9	ILE	3.7
1	A	86	LYS	3.7
1	B	1	SER	3.7
1	A	1644	ILE	3.7
1	A	1394	LEU	3.7
1	A	142	LEU	3.7
1	B	2172	ASP	3.7
1	B	42	ASN	3.7
1	A	1572	ILE	3.6
1	B	3703	PHE	3.6
1	A	4034	LEU	3.6
1	B	1502	ILE	3.6
1	A	2852	LEU	3.6
1	A	147	VAL	3.6
1	B	1383	TYR	3.6
1	A	19	LEU	3.6
1	A	1602	ILE	3.6
1	A	2676	THR	3.6
1	A	1378	TRP	3.6
1	B	2364	ASP	3.6
1	B	1705	TYR	3.6
1	B	3020	GLY	3.5
1	A	1530	GLN	3.5
1	A	2916	TRP	3.5
1	A	3920	ILE	3.5
1	A	211	GLY	3.5
1	B	1762	TYR	3.5
1	A	2965	VAL	3.5
1	B	3617	GLU	3.5
1	A	3024	LEU	3.5
1	A	1550	GLY	3.5
1	A	2937	PRO	3.5
1	A	3589	ASN	3.4
1	A	138	HIS	3.4
1	A	2574	TYR	3.4
1	B	63	LYS	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1456	TYR	3.4
1	A	1738	ASN	3.4
1	A	1401	LEU	3.4
1	A	151	ASP	3.4
1	B	135	ARG	3.4
1	A	3570	LEU	3.4
1	B	3569	GLU	3.4
1	A	72	ARG	3.4
1	B	3919	LYS	3.4
1	A	1472	GLU	3.4
1	A	1489	ARG	3.3
1	B	3571	ASN	3.3
1	A	1391	GLY	3.3
1	A	2371	PHE	3.3
1	A	171	ALA	3.3
1	B	3579	GLU	3.3
1	A	18	LEU	3.3
1	A	2870	GLU	3.2
1	B	44	LYS	3.2
1	A	87	GLU	3.2
1	A	1441	ILE	3.2
1	A	2029	LEU	3.2
1	A	2611	LEU	3.2
1	B	1445	TRP	3.2
1	B	148	THR	3.2
1	A	3561	ASN	3.2
1	A	16	THR	3.2
1	B	23	LEU	3.2
1	B	3566	LEU	3.2
1	B	3543	ARG	3.2
1	B	131	MET	3.2
1	A	1607	TRP	3.1
1	B	3984	GLN	3.1
1	B	3572	ASN	3.1
1	A	3551	LEU	3.1
1	A	1597	GLU	3.1
1	A	88	ARG	3.1
1	A	109	ALA	3.1
1	A	57	TYR	3.1
1	A	1636	ILE	3.1
1	A	1565	MET	3.1
1	A	2918	GLY	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1767	GLU	3.0
1	A	1581	GLY	3.0
1	B	3873	MET	3.0
1	B	1898	LEU	3.0
1	A	2368	PHE	3.0
1	B	3028	VAL	3.0
1	A	3584	MET	3.0
1	B	4052	THR	3.0
1	A	3019	VAL	3.0
1	B	82	GLY	3.0
1	A	2179	PRO	3.0
1	A	2303	GLN	3.0
1	B	3568	GLU	3.0
1	B	1549	ILE	3.0
1	A	137	CYS	3.0
1	B	132	PHE	2.9
1	A	4029	ILE	2.9
1	B	51	PHE	2.9
1	B	2173	ASN	2.9
1	A	3425	LYS	2.9
1	B	3927	TYR	2.9
1	A	1578	PHE	2.9
1	B	3715	TYR	2.9
1	A	33	GLU	2.9
1	B	1513	ILE	2.9
1	A	3436	PHE	2.9
1	A	1486	ILE	2.9
1	A	2582	VAL	2.9
1	B	1486	ILE	2.9
1	A	2130	PHE	2.9
1	B	2942	ASP	2.9
1	B	185	ILE	2.9
1	B	1590	LEU	2.9
1	B	1449	GLN	2.9
1	A	2359	ILE	2.8
1	B	1441	ILE	2.8
1	B	3577	MET	2.8
1	B	1460	GLY	2.8
1	A	2361	ILE	2.8
1	B	1452	TRP	2.8
1	B	2022	PHE	2.8
1	B	188	ILE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	3554	GLU	2.8
1	A	3484	HIS	2.8
1	A	2249	LEU	2.8
1	A	3868	HIS	2.8
1	A	2091	MET	2.8
1	B	1937	MET	2.8
1	A	3020	GLY	2.8
1	A	3309	THR	2.8
1	A	3594	ALA	2.8
1	A	1519	ILE	2.8
1	B	3564	LYS	2.8
1	A	1760	PHE	2.7
1	A	2938	MET	2.7
1	A	2943	PHE	2.7
1	A	4033	LEU	2.7
1	A	4036	GLN	2.7
1	B	3744	LEU	2.7
1	A	1526	PHE	2.7
1	A	3026	GLU	2.7
1	B	3581	ASP	2.7
1	B	3934	TRP	2.7
1	A	2689	ILE	2.7
1	A	1505	PHE	2.7
1	A	3313	PHE	2.7
1	A	92	SER	2.7
1	B	60	GLY	2.7
1	B	3025	ASN	2.7
1	B	3747	LEU	2.7
1	A	3446	PHE	2.7
1	B	1719	SER	2.7
1	A	1562	MET	2.7
1	B	3017	VAL	2.7
1	B	3853	THR	2.7
1	A	2190	PHE	2.6
1	B	75	ALA	2.6
1	B	1596	ILE	2.6
1	B	1683	LEU	2.6
1	B	144	GLY	2.6
1	A	94	LEU	2.6
1	A	1497	ILE	2.6
1	A	1456	TYR	2.6
1	A	76	ASP	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1476	PHE	2.6
1	B	1905	ARG	2.6
1	A	3025	ASN	2.6
1	A	3567	LEU	2.6
1	B	191	TYR	2.6
1	A	2739	VAL	2.6
1	B	1952	PHE	2.6
1	A	2838	ALA	2.6
1	B	2024	SER	2.6
1	B	3582	GLU	2.6
1	B	3576	ASN	2.6
1	A	3873	MET	2.5
1	B	3867	GLU	2.5
1	A	2853	LEU	2.5
1	A	1476	PHE	2.5
1	B	1505	PHE	2.5
1	B	3618	TYR	2.5
1	A	1469	LEU	2.5
1	A	2581	LEU	2.5
1	A	146	HIS	2.5
1	A	3865	ALA	2.5
1	B	3026	GLU	2.5
1	B	3726	LEU	2.5
1	B	1480	THR	2.5
1	B	1415	MET	2.5
1	A	2121	ALA	2.5
1	B	3019	VAL	2.5
1	B	3686	PHE	2.5
1	A	36	GLU	2.5
1	A	3847	SER	2.5
1	B	3904	LEU	2.5
1	A	3305	ARG	2.5
1	A	4035	GLN	2.5
1	A	11	GLY	2.5
1	B	1864	ASN	2.5
1	A	96	GLY	2.5
1	A	1898	LEU	2.5
1	A	2607	TYR	2.5
1	A	2682	PRO	2.5
1	A	3014	GLN	2.5
1	A	1590	LEU	2.4
1	A	2681	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	3587	LEU	2.4
1	B	156	ASP	2.4
1	B	1672	TYR	2.4
1	B	1760	PHE	2.4
1	A	1506	ASP	2.4
1	A	1559	SER	2.4
1	A	2656	PHE	2.4
1	A	200	TRP	2.4
1	A	1669	PHE	2.4
1	A	1705	TYR	2.4
1	A	1423	ILE	2.4
1	A	62	VAL	2.4
1	B	1850	PHE	2.4
1	B	3557	LEU	2.4
1	A	2844	PHE	2.4
1	A	2024	SER	2.4
1	A	3415	ILE	2.4
1	B	175	LEU	2.4
1	A	1494	ASP	2.4
1	A	3028	VAL	2.4
1	B	197	TYR	2.4
1	A	10	LYS	2.4
1	A	1640	VAL	2.4
1	B	3565	ARG	2.4
1	A	3326	ILE	2.4
1	B	1572	ILE	2.4
1	A	2129	LEU	2.4
1	B	2014	PHE	2.4
1	A	3357	ALA	2.4
1	B	3555	TYR	2.4
1	A	2038	LEU	2.4
1	A	3875	MET	2.3
1	A	3007	TYR	2.3
1	A	2782	VAL	2.3
1	A	2876	TRP	2.3
1	B	2943	PHE	2.3
1	A	1426	GLN	2.3
1	A	2385	VAL	2.3
1	A	22	TYR	2.3
1	B	1423	ILE	2.3
1	A	2444	ASN	2.3
1	B	4092	MET	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	71	ILE	2.3
1	B	1953	LEU	2.3
1	B	1589	VAL	2.3
1	B	2302	PHE	2.3
1	A	3593	GLU	2.3
1	B	3562	LEU	2.3
1	B	3839	ILE	2.3
1	A	93	MET	2.3
1	A	3559	LEU	2.3
1	A	2367	SER	2.3
1	A	3021	LEU	2.3
1	B	47	LEU	2.3
1	B	1664	LEU	2.3
1	A	73	TYR	2.3
1	A	2912	CYS	2.3
1	B	1666	THR	2.3
1	B	2122	THR	2.3
1	A	2366	LEU	2.3
1	A	2022	PHE	2.3
1	A	2977	TYR	2.3
1	B	3768	PHE	2.3
1	A	2856	LEU	2.2
1	B	2962	ARG	2.2
1	A	3542	GLN	2.2
1	A	2470	GLY	2.2
1	A	2314	ILE	2.2
1	A	3563	GLU	2.2
1	B	1942	SER	2.2
1	B	3415	ILE	2.2
1	B	3948	HIS	2.2
1	A	2150	ILE	2.2
1	A	2940	PHE	2.2
1	A	61	ASP	2.2
1	A	2874	TYR	2.2
1	B	3589	ASN	2.2
1	B	3847	SER	2.2
1	B	3725	VAL	2.2
1	A	2784	PRO	2.2
1	B	2990	GLY	2.2
1	A	3590	LEU	2.2
1	B	2795	PHE	2.2
1	A	2686	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1668	GLN	2.2
1	A	2962	ARG	2.2
1	A	1588	GLU	2.2
1	A	1762	TYR	2.2
1	B	3841	LEU	2.2
1	B	2021	ILE	2.2
1	A	1474	SER	2.2
1	B	1605	GLN	2.2
1	A	3899	ASP	2.2
1	A	43	LYS	2.2
1	A	1540	LEU	2.2
1	A	2310	LEU	2.2
1	B	2006	LEU	2.2
1	B	2190	PHE	2.2
1	B	1500	ILE	2.2
1	A	3884	LEU	2.1
1	B	1546	LEU	2.1
1	A	3869	GLU	2.1
1	B	3923	VAL	2.1
1	A	149	HIS	2.1
1	A	1509	LEU	2.1
1	A	1935	GLN	2.1
1	A	2603	CYS	2.1
1	A	3994	TYR	2.1
1	A	1603	GLN	2.1
1	B	4045	LEU	2.1
1	A	1537	PHE	2.1
1	A	1428	CYS	2.1
1	B	1603	GLN	2.1
1	A	2999	LEU	2.1
1	B	3390	PHE	2.1
1	A	4019	ASP	2.1
1	A	2106	THR	2.1
1	A	2252	LEU	2.1
1	A	3426	THR	2.1
1	A	3557	LEU	2.1
1	B	1420	TYR	2.1
1	A	3480	GLU	2.1
1	B	3027	SER	2.1
1	B	2295	ILE	2.1
1	B	3958	ASP	2.1
1	A	2673	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3895	PHE	2.1
1	B	1386	ILE	2.1
1	A	2292	VAL	2.1
1	A	2170	LEU	2.1
1	A	2474	LEU	2.1
1	A	2237	LEU	2.1
1	B	1828	TYR	2.0
1	A	2304	ASN	2.0
1	B	2989	PRO	2.0
1	A	1566	PHE	2.0
1	A	2257	PHE	2.0
1	B	3657	PHE	2.0
1	A	1612	ASP	2.0
1	A	1412	LEU	2.0
1	A	2592	PHE	2.0
1	A	2599	LEU	2.0
1	A	1850	PHE	2.0
1	A	1481	SER	2.0
1	B	3816	LEU	2.0
1	A	3786	PHE	2.0
1	A	3325	ILE	2.0
1	B	1412	LEU	2.0
1	A	1645	PHE	2.0
1	B	3406	PHE	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](#)

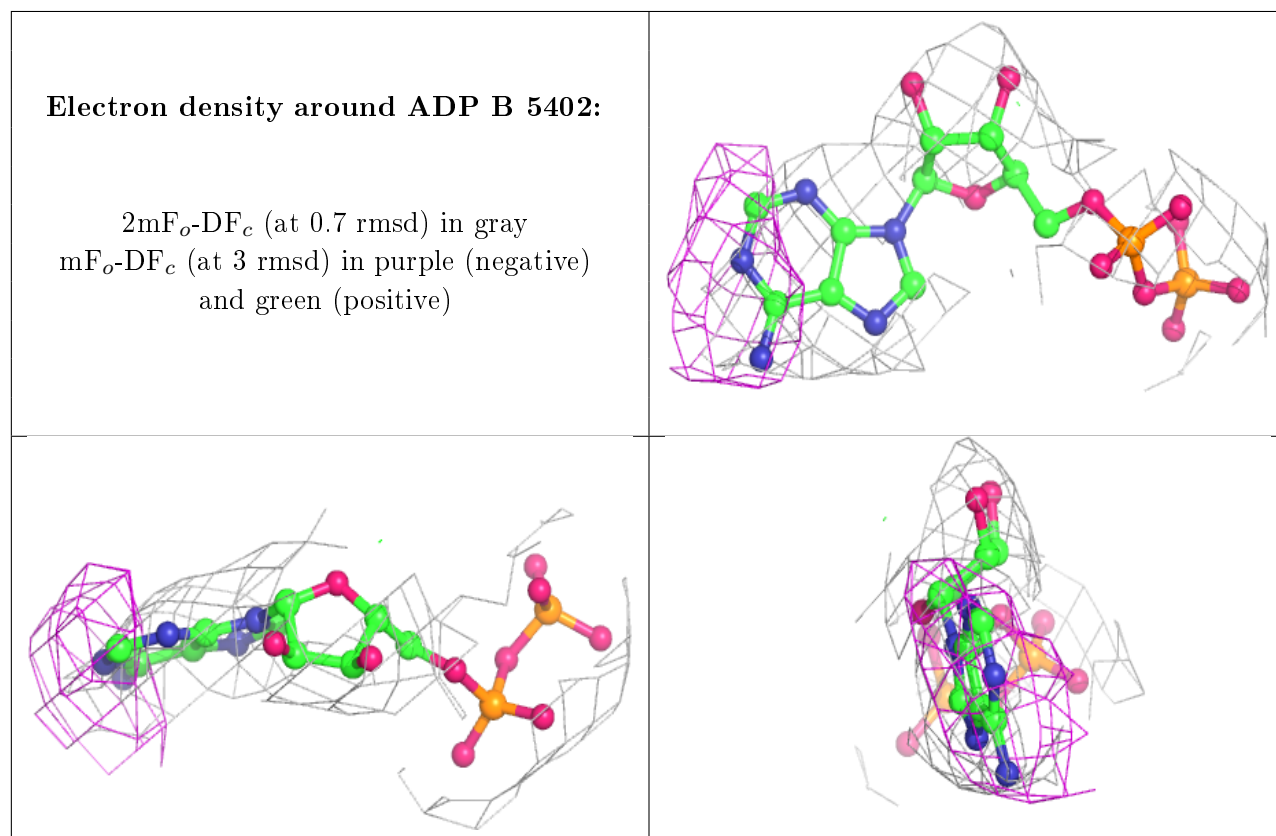
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

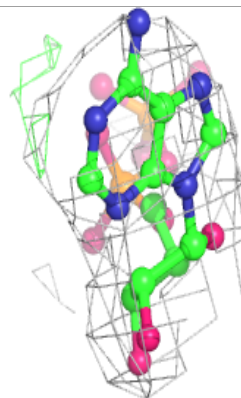
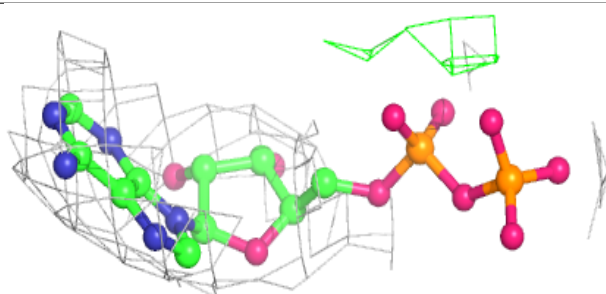
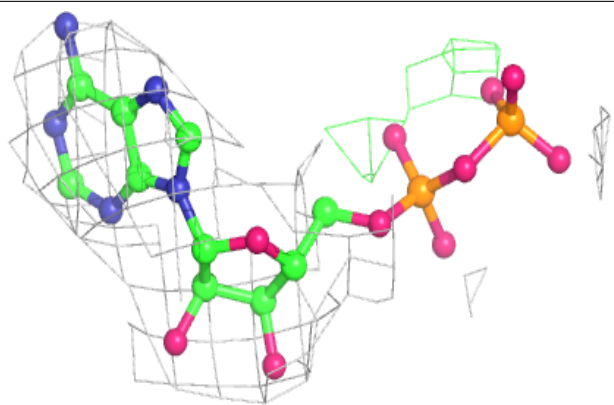
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	5404	1/1	0.77	0.17	97,97,97,97	0
3	ADP	B	5402	27/27	0.87	0.33	108,145,183,194	0
3	ADP	A	5401	27/27	0.89	0.28	126,146,191,198	0
5	MG	B	5404	1/1	0.90	0.30	107,107,107,107	0
2	ATP	B	5400	31/31	0.91	0.27	124,160,195,221	0
4	SO4	B	5403	5/5	0.91	0.16	139,143,171,171	0
4	SO4	A	5403	5/5	0.92	0.23	101,136,142,145	0
3	ADP	A	5402	27/27	0.93	0.25	134,176,208,218	0
2	ATP	A	5400	31/31	0.94	0.31	122,147,224,246	0
3	ADP	B	5401	27/27	0.94	0.27	98,121,138,153	0

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

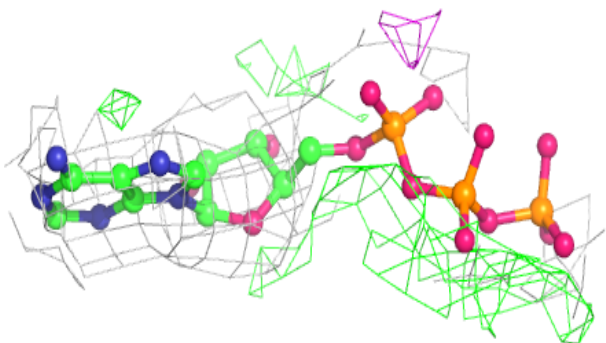
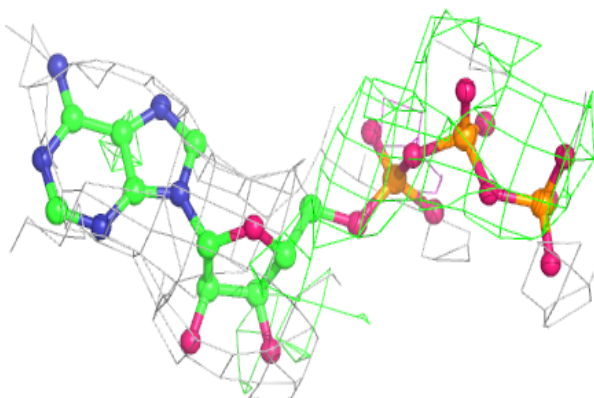


**Electron density around ADP A 5401:**

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

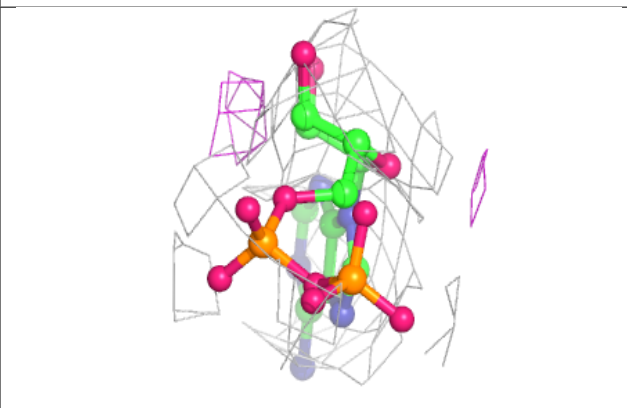
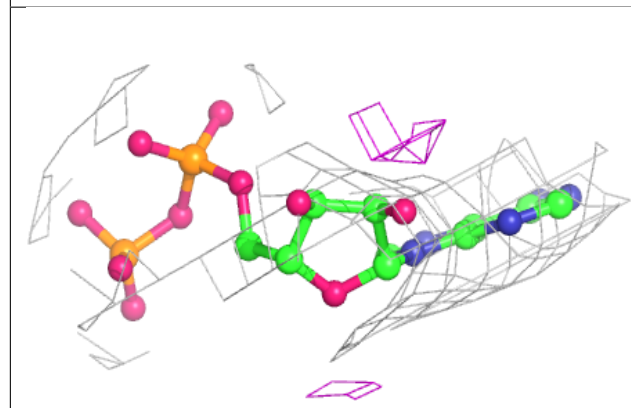
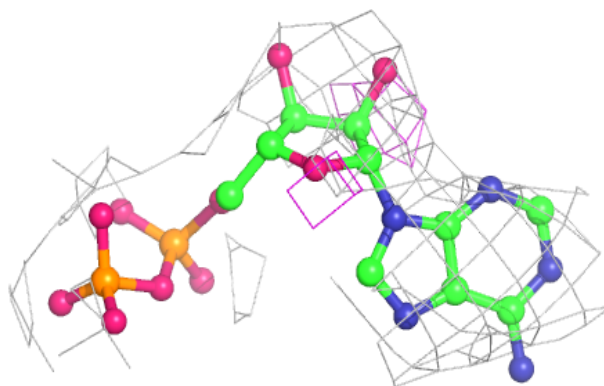
**Electron density around ATP B 5400:**

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

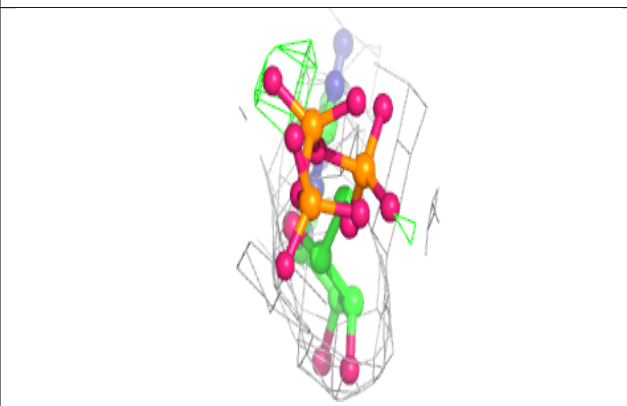
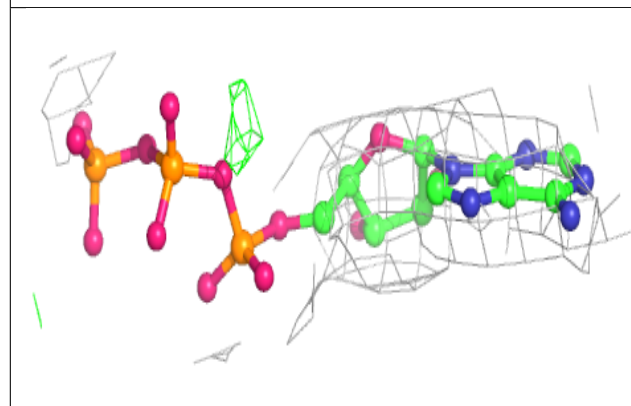
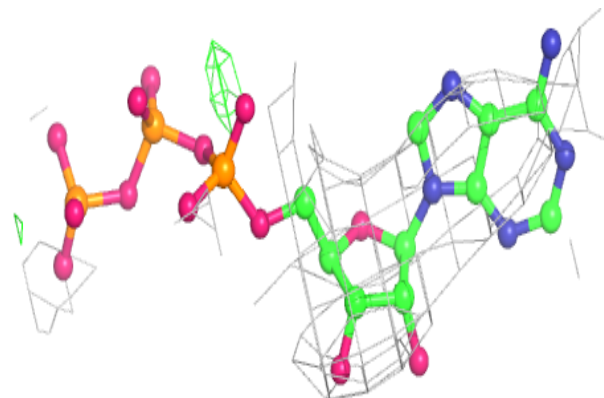


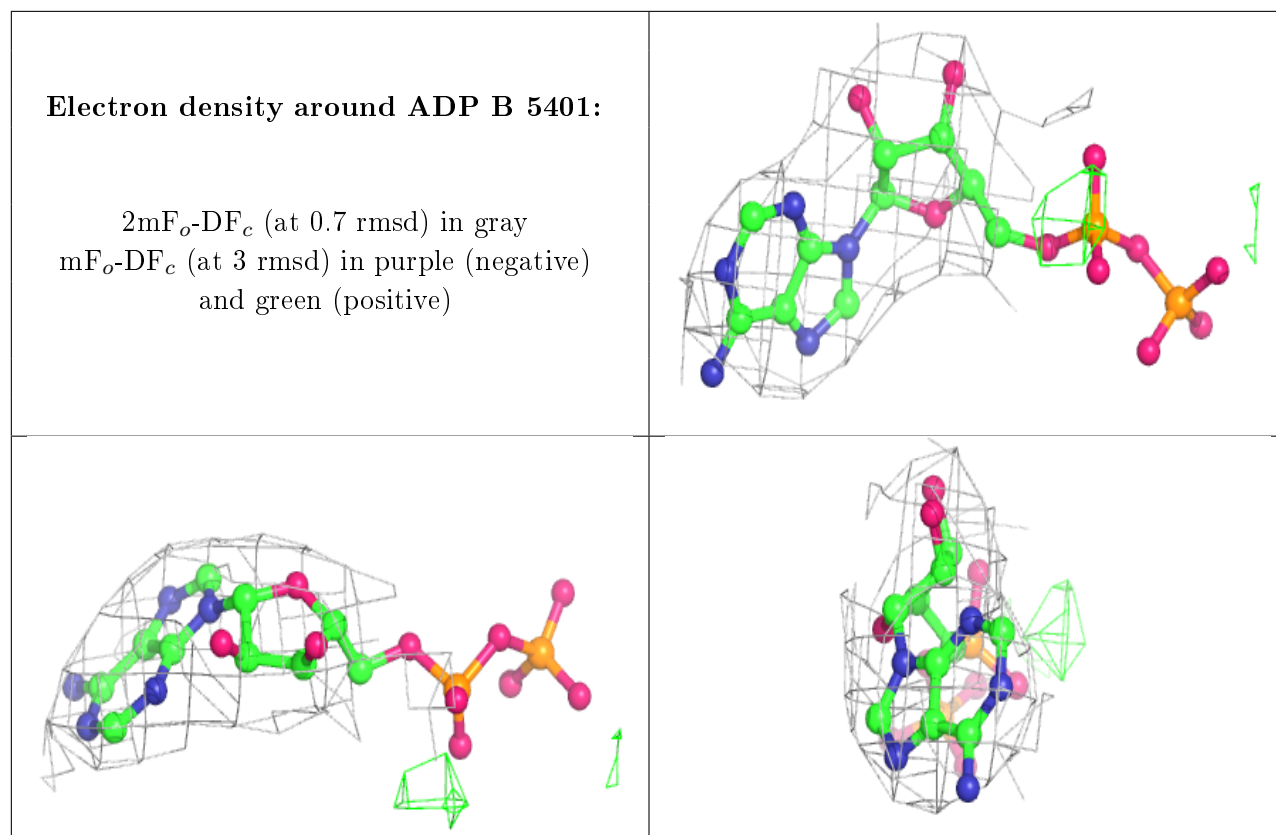
**Electron density around ADP A 5402:**

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

**Electron density around ATP A 5400:**

$2mF_o-DF_c$  (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.