



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:52 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

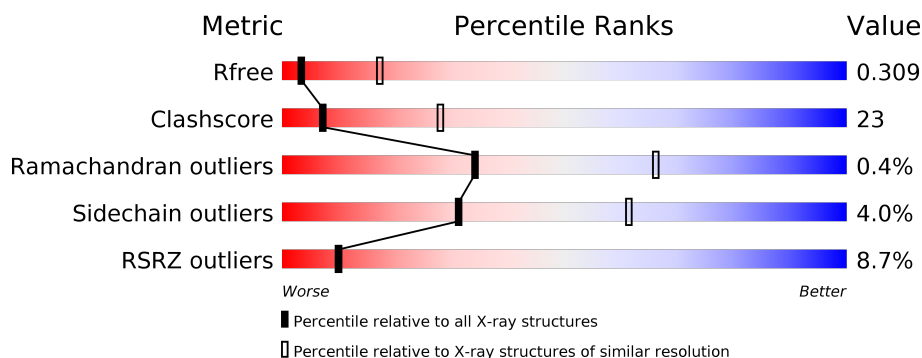
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 ≥ 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	<div> <div>5%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>
1	B	2695	<div> <div>12%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>

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

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

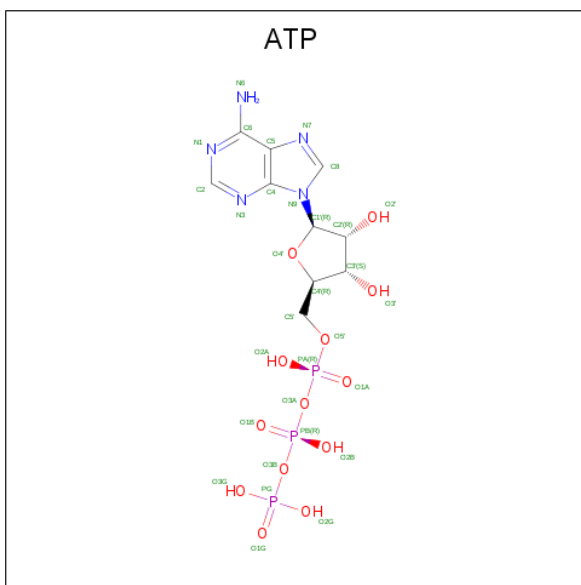
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 8 discrepancies between the modelled and reference sequences:

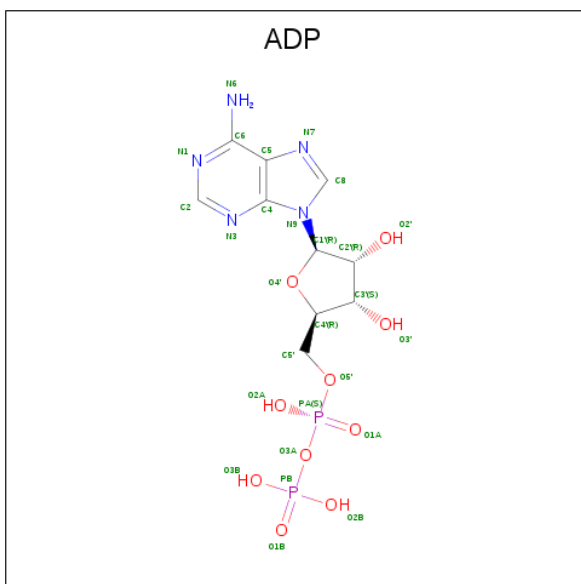
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

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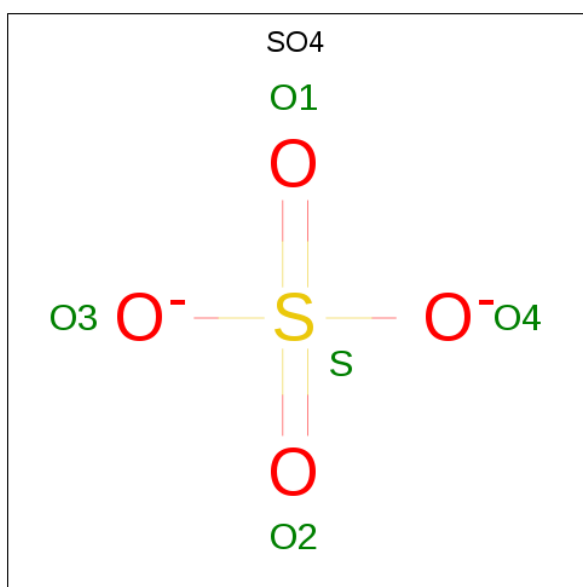
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

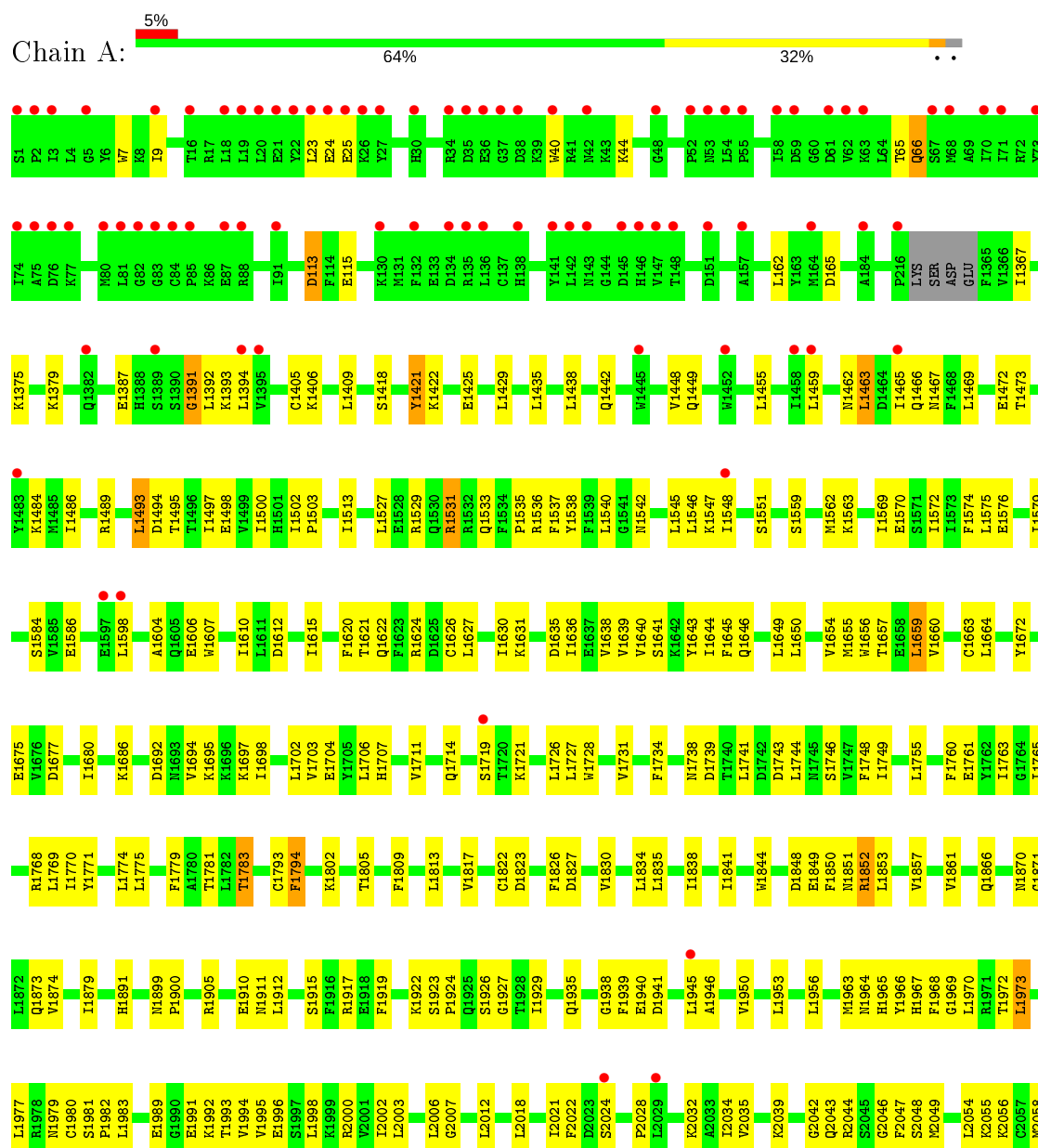


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

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

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





L2843	F2844	S2613	D2495	K2411	E2195	L2109	Z2023	M1937	L1831	T1740	L1649
Q2751	V2752	L2616	K2496	I2415	T2196	T2110	S2024	G1938	L1835	L1741	L1650
H2755	M2756	R2620	G2497	C2417	D2197	E2112	A2025	F1939	I1841	D1742	M1655
M2757	S2499	T2623	T2319	P2420	H2201	S2117	T2027	D1941	M1844	M1745	M1656
L2759	V2503	T2623	R2321	G2421	T2203	A2121	T2202	L1945	G1846	M1745	L1657
L2506	R2507	R2627	L2322	T2425	A2205	A2121	L2029	A1946	F1748	F1748	L1664
R2510	M2510	Y2630	L2326	T2425	T2207	W2125	K2032	I1949	I1749	S1750	F1669
T2510	T2631	T2632	G2332	I2427	T2206	W2125	K2032	V1950	G1753	G1753	Y1672
T2511	T2632	A2632	G2332	M2428	T2208	D2127	L2034	F1850	Y1754	Y1754	Y1673
T2512	M2429	T2633	Q2335	N2429	R2209	G2128	V2035	M1851	L1755	L1755	K1674
Q2513	N2430	T2635	Q2336	N2430	I2212	L2129	K2036	R1852	L1755	L1755	E1675
K2517	L2437	T2636	R2336	T2437	I2212	T2131	C2037	L1853	Y1758	Y1758	Y1676
T2518	T2437	T2637	L2339	T2437	F2215	T2131	Q2047	M1864	F1759	F1759	D1677
P2519	F2445	T2638	Q2351	F2445	C2220	L2133	S2048	N1865	F1760	F1760	M1678
E2520	S2446	T2639	E2352	S2446	S2224	V2137	Q2058	H1865	E1761	E1761	K1679
V2524	K2447	T2640	L2353	K2447	K2225	V2137	Q2059	H1866	Y1762	Y1762	I1680
T2525	D2448	S2643	S2354	D2448	S2225	I2141	F2061	F1967	I1763	I1763	K1681
T2526	T2449	T2647	D2355	T2449	E2228	F2145	Y2061	F1968	G1764	G1764	G1682
F2527	E2452	L2647	Y2356	E2452	E2228	F2145	Q2064	L1970	I1879	I1879	L1683
R2528	F2452	L2647	S2357	F2452	E2228	F2145	Q2064	L1970	T1880	T1880	L1684
C2535	L2455	K2653	T2361	L2455	L2241	R2149	Q2068	L1973	L1881	L1881	D1685
N2536	L2458	L2654	A2362	L2458	L2241	R2149	Q2068	L1973	L1882	L1882	K1686
R2543	H2459	T2655	N2363	H2459	L2252	L2150	K2069	K1974	L1888	L1888	D1692
R2544	R2460	L2655	D2364	R2460	L2262	W2151	G1975	V1976	Y1771	Y1771	M1693
R2549	N2463	L2656	K2365	N2463	L2262	F2154	L2071	S1981	A1893	A1893	V1694
F2550	Y2464	L2657	L2366	Y2464	L2266	D2155	L2072	P1982	V1894	V1894	K1695
T2551	T2467	Q2684	S2367	T2467	F2266	S2156	L2073	P1982	M1899	M1899	K1696
R2552	S2468	L2681	S2367	S2468	F2266	S2156	L2073	P1982	P1900	P1900	K1697
T2556	G2470	L2681	S2367	G2470	F2266	S2156	L2073	P1982	P1900	P1900	L1698
P2562	T2471	S2691	S2379	T2471	H2274	P2160	A2076	I1984	R1905	R1905	L1702
S2563	T2472	S2691	L2380	T2472	H2274	P2160	A2076	I1984	R1905	R1905	V1703
K2565	L2473	D2703	L2380	L2473	H2274	P2160	A2076	I1984	R1905	R1905	E1704
S2566	L2474	D2703	L2380	L2474	H2274	P2160	A2076	I1984	R1905	R1905	Y1705
Y2571	P2475	K2709	L2380	P2475	H2274	P2160	A2076	I1984	R1905	R1905	H1707
E2572	K2476	K2709	L2380	K2476	H2274	P2160	A2076	I1984	R1905	R1905	V1711
L2573	S2477	L2712	L2380	S2477	H2274	P2160	A2076	I1984	R1905	R1905	L1712
Y2574	K2480	L2728	L2380	K2480	H2274	P2160	A2076	I1984	R1905	R1905	G1713
L2578	N2481	L2728	L2380	N2481	H2274	P2160	A2076	I1984	R1905	R1905	G1713
F2579	L2484	S2737	T2394	L2484	L2289	G2181	N2099	L2006	Q1925	Q1925	K1730
K2580	L2488	S2737	L2395	L2488	L2289	G2181	N2099	L2006	Q1925	Q1925	V1731
T2581	E2488	H2741	L2395	E2488	F2302	R2183	Y2102	G2007	S1926	S1926	Q1732
V2582	I2489	R2744	T2397	I2489	F2302	R2183	Y2102	G2007	S1926	S1926	Q1732
R2586	Y2490	L2745	D2406	Y2490	L2305	L2186	V2103	E2011	I1929	I1929	K1733
P2590	L2491	L2745	D2406	L2491	D2307	R2191	V2103	E2011	I1929	I1929	F1734
E2590	P2492	D2746	D2406	P2492	D2307	R2191	V2103	E2011	I1929	I1929	D1827
	K2493	R2747	N2409	K2493	D2307	R2191	V2103	E2011	I1929	I1929	Y1828
	L2494	A2748	S2410	L2494	D2307	R2191	V2103	E2011	I1929	I1929	Q1829
											V1830
Q2751	V2752	L2616	K2496	I2415	T2196	T2110	S2024	F1938	L1831	T1740	L1649
H2755	M2756	R2620	G2497	C2417	D2197	E2112	A2025	F1939	I1841	D1742	M1655
M2757	S2499	T2623	T2319	P2420	H2201	S2117	T2027	D1941	M1844	M1745	M1656
L2759	V2503	T2623	R2321	G2421	T2203	A2121	T2202	L1945	G1846	F1748	L1664
L2506	R2507	R2627	L2322	T2425	A2205	A2121	L2029	A1946	F1748	S1750	F1669
R2510	M2510	Y2630	L2326	T2425	T2207	W2125	K2032	I1949	G1753	G1753	Y1672
T2510	T2631	T2632	G2332	I2427	T2208	D2127	L2034	F1850	Y1754	Y1754	Y1673
T2511	T2632	A2632	G2332	M2428	T2209	G2128	V2035	M1851	L1755	L1755	K1674
T2512	M2429	T2633	Q2335	N2429	R2209	L2129	K2036	R1852	L1755	L1755	E1675
Q2513	N2430	T2635	Q2336	N2430	I2212	T2131	C2037	L1853	Y1758	Y1758	Y1676
K2517	L2437	T2636	R2336	T2437	I2212	T2131	Q2047	M1864	F1759	F1759	D1677
T2518	T2437	T2637	L2339	T2437	F2215	L2133	S2048	N1865	F1760	F1760	M1678
P2519	F2445	T2638	Q2351	F2445	C2220	L2133	S2048	N1865	E1761	E1761	K1679
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V2524	K2447	T2640	L2353	K2447	K2225	I2141	F2061	F1967	I1763	I1763	K1681
T2525	D2448	S2643	S2354	D2448	S2225	I2141	F2061	F1968	G1764	G1764	G1682
T2526	T2449	T2647	D2355	T2449	E2228	F2145	Y2061	F1969	I1765	I1765	L1683
F2527	E2452	L2647	Y2356	E2452	E2228	F2145	Q2064	L1970	T1880	T1880	L1684
R2528	F2452	L2647	S2357	F2452	E2228	F2145	Q2064	L1970	L1881	L1881	D1685
C2535	L2455	K2653	T2361	L2455	L2241	R2149	Q2068	L1973	L1882	L1882	K1686
N2536	L2458	L2654	A2362	L2458	L2252	L2150	K2069	K1974	L1888	L1888	D1692
R2543	H2459	T2655	N2363	H2459	L2262	W2151	G1975	V1976	Y1771	Y1771	M1693
R2544	R2460	L2655	D2364	R2460	L2262	F2154	L2071	S1981	A1893	A1893	V1694
R2549	N2463	L2656	K2365	N2463	L2266	D2155	L2072	P1982	V1894	V1894	K1695
F2550	Y2464	L2657	L2366	Y2464	F2266	S2156	L2073	P1982	M1899	M1899	K1696
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T2556	G2470	L2681	S2379	T2470	H2274	P2160	A2076	I1984	R1905	R1905	L1702
P2562	T2471	S2691	L2380	T2471	H2274	P2160	A2076	I1984	R1905	R1905	V1703
S2563	T2472	S2691	L2380	T2472	H2274	P2160	A2076	I1984	R1905	R1905	E1704
K2565	L2473	D2703	L2380	L2473	H2274	P2160	A2076	I1984	R1905	R1905	Y1705
S2566	L2474	D2703	L2380	L2474	H2274	P2160	A2076	I1984	R1905	R1905	H1707
Y2571	P2475	K2709	L2380	P2475	H2274	P2160	A2076	I1984	R1905	R1905	V1711
E2572	K2476	K2709	L2380	K2476	H2274	P2160	A2076	I1984	R1905	R1905	L1712
L2573	S2477	L2712	L2380	S2477	H2274	P2160	A2076	I1984	R1905	R1905	G1713
Y2574	K2480	L2728	L2380	K2480	H2274	P2160	A2076	I1984	R1905	R1905	G1713
L2578	N2481	L2728	L2380	N2481	H2274	P2160	A2076	I1984	R1905	R1905	L1715
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T2581	E2488	H2741	L2395	E2488	F2302	R2183	Y2102	G2007	S1926	S1926	Q1732
V2582	I2489	R2744	T2397	I2489	F2302	R2183	Y2102	G2007	S1926	S1926	Q1732
R2586	Y2490	L2745	D2406	Y2490	L2305	L2186	V2103	E2011	I1929	I1929	K1733
P2590	L2491	L2745	D2406	L2491	D2307	R2191	V2103	E2011	I1929	I1929	F1734
E2590	P2492	D2746	D2406	P2492	D2307	R2191	V2103	E2011	I1929	I1929	D1827
	K2493	R2747	N2409	K2493	D2307	R2191	V2103	E2011	I1929	I1929	Y1828
	L2494	A2748	S2410	L2494	D2307	R2191	V2103	E2011	I1929	I1929	Q1829
											V1830
L2843	F2844	S2613	D2495	K2411	E2195	L2109	Z2023	M1937	L1831	T1740	L1649
Q2751	V2752	L2616	K2496	I2415	T2196	T2110	S2024	G1938	L1835	L1741	L1650
H2755	M2756	R2620	G2497	C2417	D2197	E2112	A2025	F1939	I1841	D1742	M1655
M2757	S2499	T2623	T2319	P2420	H2201	S2117	T2027	D1941	M1844	M1745	M1656
L2759	V2503	T2623	R2321	G2421	T2203	A2121	T2202	L1945	G1846	F1748	L1664
L2506	R2507	R2627	L2322	T2425	A2205	A2121	L2029	A1946	F1748	S1750	F1669
R2510	M2510	Y2630	L2326	T2425	T2207	W2125	K2032	I1949	G1753	G1753	Y1672
T2510	T2631	T2632	G2332	I2427	T2208	D2127	L2034	F1850	Y1754	Y1754	Y1673
T2511	T2632	A2632	G2332	M2428	T2209	G2128	V2035	M1851	L1755	L1755	K1674
T2512	M2429	T2633	Q2335	N2429	R2209	L2129	K2036	R1852	L1755	L1755	E1675
Q2513	N2430	T2635	Q2336	N2430	I2212	T2131	C2037	L1853	Y1758	Y1758	Y1676
K2517	L2437	T2636	R2336	T2437	I2212	T2131	Q2047	M1864	F1759	F1759	D1677
T2518	T2437	T2637	L2339	T2437	F2215	L2133	S2048	N1865	F1760	F1760	M1678
P2519	F2445	T2638	Q2351	F2445	C2220	L2133	S2048				

V4014	K3924	K3850	T3740	K3631	K3544	H3413	E3304	LYS
F4015	S3925	V3851	R3745	F3641	D3547	V3417	R3305	GLU
G4017	V3926	Y3854	R3745	F3641	L3543	V3417	W3306	LEU
		L3855	F3767	S3645	I3549	L3429	L3307	VAL
M4020	F3930	H3856	F3768	S3645	K3550	S3430	N3308	PHE
L4021	V3934	K3857	V3769	I3646	Y3555	F3431	T3310	THR
Q4022	V3935	H3858	W3772	K3854	K3556	R3439	K3311	GLU
I4023	F3935	V3859	N3773	V3656	L3557	L3440	Q3312	PRO
V4024	E3860	E3860	I3774	F3657	K3558	R3439	F3313	ILE
	A3865	E3866	V3777	L3658	L3559	I3453	T2960	GLN
V4027	T3943	K3869	V3778	LYS	R3565	F3458	S3317	T2961
R4028	K3944	K3870	V3778	LYS	L3566	D3459	I3318	R2962
I4029	L3945	SER	N3780	SER	L3567	P3460	E3319	D2963
E4038	P3947	F3871	N3780	ARG	L3570	I3461	L3320	A2964
L4049	F3950	K3872	Y3785	GLU	I3571	I3462	N3322	V2965
	S3951	F3874	F3786	THR	N3572	S3463	N3323	N2966
E4054	Y3955	T3875	T3787	ARG	S3573	I3462	I3324	N2967
P4055		T3876	ALA	ALA		S3463	I3325	L2968
L4059		C3877	R3792	ARG	E3579	L3465		L2969
S4060	D3958	H3878	K3799	T3669	N3580	A3473	V3329	V2982
S4061	C3959	D3882	L3803	R3670	D3581	R3476	Y3330	G2983
W4062	F3883	L3884	L3803	V3671	E3582	F3334	F3334	S2988
L4063	P3885	P3885	S3807	T3674	L3583	N3338	P2989	P2989
L4065	A3964	P3886	K3808	L3677	M3584	E3341	G2990	G2990
	S3965	P3887	F3809	L3678	V3585	I3481	L2999	L2999
		L3888	S3810	V3679	T3586	G3482	L3010	L3010
L3968	L3889	L3889	L3811		L3587	L3494	L3346	L3346
E3969	Q3890	Q3890	I3812	Y3683	N3588	D3500	K3350	V3017
N3970	Q3890	Q3890	I3813	Y3683	N3589	P3501	L3353	G3020
L3972	F3895	V3896	I3814	S3687	K3591	S3502	F3356	L3024
N3978	V3897	V3897	P3815	L3690	K3592	I3505	A3857	L3024
N3979	E3898	E3898	L3816	D3691	E3593	L3505	V3358	V3028
I3980	D3899	D3899	G3817	K3692	A3594	L3509	K3359	LEU
P3981	I3900	I3900	I3819	K3693	M3595	R3510	V3360	LYS
N3982	P3901	P3901	E3820	F3694	N3596	V3513	D3361	VAL
A3983	D3905	D3905	N3821	K3698	I3597	F3513		ASN
Q3984	T3906	T3906	L3822	A3699	E3598	F3518	I3367	GLU
V3985	V3907	V3907	N3823	P3700	K3600	V3519	D3368	LEU
V3993	K3908	K3908	I3834	T3701	E3603	T3520	V3369	ASN
G3995	V3911	V3911	G3837	K3702	E3604	N3521	L3370	LYS
	G3912	G3912	W3838	V3706	E3605	I3525	V3371	THR
	S3913	S3913	L3839	L3726	D3612	F3530	T3372	LEU
	Q3914	Q3914	L3840	S3727	N3613	F3530	L3373	SER
	F3915	F3915	L3841	E3728	V3615	T3533	D3374	ILE
	T3917	T3917	I3844	S3729	Y3618	L3534	L3391	SER
	F3916	F3916	Q3845		G3622	E3537	S3400	LEU
	T3917	T3917	N3846	F3734		N3538	F3406	VAL
	G3918	G3918	S3847	L3736				K3297
	K3919	K3919	L3848	T3737				T3300
	I3920	I3920	S3849					F3301
	V3923	V3923						E3302
								K3303

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.33Å 117.92Å 202.76Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 48.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.30) 96.1 (48.81-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	REFMAC NULL	Depositor
R, R_{free}	0.239 , 0.305 0.239 , 0.309	Depositor DCC
R_{free} test set	5980 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 102.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41634	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.62	7/21146 (0.0%)	0.85	21/28618 (0.1%)
1	B	0.51	2/21146 (0.0%)	0.72	4/28618 (0.0%)
All	All	0.57	9/42292 (0.0%)	0.79	25/57236 (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	3
1	B	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2064	GLN	CA-C	-8.38	1.31	1.52
1	B	2841	PRO	N-CD	-7.95	1.36	1.47
1	A	2495	ASP	C-N	-7.35	1.17	1.34
1	B	1759	LYS	C-O	6.47	1.35	1.23
1	A	2488	GLU	CD-OE1	5.63	1.31	1.25
1	A	3459	ASP	CB-CG	-5.33	1.40	1.51
1	A	2412	ARG	CA-C	-5.27	1.39	1.52
1	A	2412	ARG	CZ-NH2	-5.20	1.26	1.33
1	A	1783	THR	CB-CG2	-5.10	1.35	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2412	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	B	2471	LEU	CA-CB-CG	8.90	135.76	115.30
1	A	3459	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	2012	LEU	CA-CB-CG	7.53	132.62	115.30
1	A	2212	LEU	CB-CG-CD1	-7.18	98.80	111.00
1	A	1769	LEU	CA-CB-CG	6.83	131.00	115.30
1	A	2064	GLN	O-C-N	6.68	133.39	122.70
1	A	2487	ASP	CB-CG-OD1	6.48	124.14	118.30
1	A	2412	ARG	NH1-CZ-NH2	-6.29	112.48	119.40
1	A	1741	LEU	CB-CG-CD1	6.08	121.34	111.00
1	A	1973	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	2220	CYS	CA-CB-SG	-5.99	103.22	114.00
1	A	2336	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	1463	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	1659	LEU	CB-CG-CD2	-5.73	101.27	111.00
1	A	2078	CYS	CA-CB-SG	-5.69	103.76	114.00
1	B	2999	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	2176	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	4065	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	1973	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	2866	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	2012	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	1531	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	1938	GLY	N-CA-C	-5.07	100.42	113.10
1	B	2460	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20205	957	0
1	B	20748	0	20206	896	0
2	A	31	0	12	10	0
2	B	31	0	12	24	0
3	A	27	0	12	2	0
3	B	27	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	2	0
5	B	10	0	0	4	0
All	All	41634	0	40459	1855	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 (1855) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2380:LEU:CD2	1:A:2390:ILE:HD11	1.55	1.33
1:B:1826:PHE:CE2	1:B:1831:LEU:HB2	1.66	1.29
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.55	1.24
1:B:216:PRO:O	1:B:1365:PHE:HD1	1.21	1.22
1:B:216:PRO:O	1:B:1365:PHE:CD1	1.94	1.20
1:B:3458:PHE:CE1	1:B:3459:ASP:O	1.96	1.19
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.42	1.18
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.24	1.18
1:B:1416:LYS:HA	1:B:1421:TYR:CZ	1.77	1.18
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:1826:PHE:CZ	1:B:1831:LEU:HB2	1.78	1.16
1:B:2354:SER:OG	1:B:2357:SER:HB2	1.43	1.16
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.82	1.15
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.77	1.14
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.97	1.13
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.30	1.13
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.17	1.13
1:A:2289:GLN:OE1	1:A:2412:ARG:HG2	1.49	1.13
1:A:1926:SER:HB2	1:A:1970:LEU:HD13	1.28	1.12
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.12
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.62	1.12
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.12
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.83	1.12
1:A:2757:MET:HG2	1:A:2889:PHE:HB2	1.29	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.16	1.12
1:B:2822:ILE:O	1:B:2822:ILE:HG13	1.51	1.11
1:B:2380:LEU:HD13	1:B:2390:ILE:HD11	1.33	1.10
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.23	1.10
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.33	1.09
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.17	1.09
1:B:2380:LEU:HD22	1:B:2384:GLU:OE1	1.49	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.99	1.08
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.84	1.08
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.84	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.24	1.08
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.33	1.07
1:B:3303:LYS:O	1:B:3306:TRP:HD1	1.37	1.07
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.67	1.06
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	1.90	1.06
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.32	1.06
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	1.11	1.06
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.32	1.05
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.05
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.08	1.05
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.92	1.05
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.57	1.04
1:B:1416:LYS:HG2	1:B:1421:TYR:OH	1.57	1.04
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.45	1.04
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.05	1.04
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.58	1.03
1:A:2380:LEU:HD21	1:A:2390:ILE:CD1	1.86	1.03
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.04	1.03
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	1.92	1.03
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.37	1.03
1:A:2476:LYS:N	1:A:2476:LYS:HD2	1.69	1.03
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.89	1.02
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.88	1.02
1:A:2060:PHE:CZ	1:A:2064:GLN:NE2	2.27	1.02
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.59	1.02
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.40	1.01
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.90	1.01
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.04	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.90	1.01
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	1.76	1.01
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.91	1.01
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.42	1.00
1:B:1983:LEU:CG	1:B:1993:THR:HG23	1.90	1.00
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.76	1.00
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.39	1.00
1:A:1620:PHE:HD2	1:A:1760:PHE:CZ	1.80	1.00
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.01	0.99
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.92	0.99
1:B:1422:LYS:O	1:B:1425:GLU:HB3	1.63	0.99
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.39	0.99
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.92	0.99
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.60	0.99
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.45	0.99
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.45	0.98
1:A:2378:VAL:HG22	1:A:2380:LEU:HD13	1.43	0.98
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.92	0.98
1:B:2471:LEU:O	1:B:2473:LEU:HD13	1.63	0.98
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.93	0.98
1:A:1970:LEU:HD12	1:A:1973:LEU:HG	1.46	0.97
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.45	0.97
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.76	0.97
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.82	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	0.97	0.97
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	1.94	0.97
1:B:2470:GLY:CA	1:B:2473:LEU:HD11	1.96	0.96
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.47	0.96
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.66	0.96
1:B:2470:GLY:HA3	1:B:2473:LEU:HD11	1.47	0.96
1:B:1616:LYS:NZ	1:B:1759:LYS:HE3	1.78	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.30	0.96
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.98	0.96
1:B:3460:PRO:O	1:B:3463:SER:HB2	1.65	0.96
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.45	0.95
1:A:2064:GLN:NE2	1:A:2151:TRP:CZ3	2.35	0.95
1:A:2378:VAL:CG2	1:A:2380:LEU:HD13	1.96	0.95
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.66	0.95
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.97	0.94
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.50	0.94
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.51	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.32	0.94
1:B:2064:GLN:NE2	1:B:2070:LEU:HG	1.82	0.94
1:B:2080:LYS:HD2	1:B:2195:GLU:HB2	1.48	0.94
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.97	0.93
1:A:2378:VAL:CG2	1:A:2380:LEU:CD1	2.46	0.93
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.69	0.93
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.96	0.93
1:B:1826:PHE:HE2	1:B:1831:LEU:HB2	1.27	0.93
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.48	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.50	0.93
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.98	0.93
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.92
1:A:2060:PHE:CE2	1:A:2064:GLN:NE2	2.37	0.92
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.82	0.92
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.68	0.92
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.22	0.92
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.52	0.92
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.51	0.91
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.36	0.91
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	2.00	0.91
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.98	0.91
1:B:2472:THR:C	1:B:2473:LEU:HD12	1.89	0.91
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	2.06	0.91
1:B:1992:LYS:CG	1:B:2024:SER:HB2	2.01	0.91
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.51	0.91
1:B:2386:MET:CB	1:B:2627:ARG:HD3	2.01	0.91
1:B:2380:LEU:CD1	1:B:2390:ILE:HD11	2.00	0.91
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.88	0.91
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.53	0.91
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.91
1:A:1983:LEU:HG	1:A:1993:THR:HG23	1.49	0.90
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.23	0.90
1:A:2757:MET:HG2	1:A:2889:PHE:CB	2.01	0.90
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.01	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.01	0.90
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.70	0.90
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.90
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.37	0.90
1:A:2380:LEU:HD21	1:A:2390:ILE:HD11	0.92	0.89
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.25	0.89
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.72	0.89
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.13	0.89
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	2.02	0.89
1:A:3458:PHE:CE1	1:A:3459:ASP:O	2.26	0.88
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.74	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.54	0.88
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.09	0.88
1:B:2563:SER:HB3	1:B:2566:SER:H	1.39	0.88
1:B:2080:LYS:HE2	1:B:2195:GLU:OE1	1.73	0.88
1:A:1425:GLU:OE2	1:A:1429:LEU:CG	2.21	0.88
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.56	0.88
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.74	0.88
1:A:2378:VAL:HG22	1:A:2380:LEU:CD1	2.03	0.88
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.74	0.88
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.09	0.87
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.87
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.89	0.87
1:A:2380:LEU:CD2	1:A:2390:ILE:CD1	2.47	0.87
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.28	0.87
1:A:1425:GLU:OE2	1:A:1429:LEU:HG	1.74	0.87
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.55	0.87
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.08	0.87
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.75	0.87
1:A:1983:LEU:CG	1:A:1993:THR:HG23	2.04	0.87
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.94	0.87
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.09	0.87
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.57	0.86
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.58	0.86
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.05	0.86
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.64	0.86
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.75	0.86
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.57	0.86
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.11	0.86
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.11	0.86
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.06	0.86
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.58	0.86
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.58	0.85
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.76	0.85
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.37	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2472:THR:O	1:B:2473:LEU:HD12	1.76	0.85
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.59	0.85
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.58	0.85
1:A:1970:LEU:HD12	1:A:1973:LEU:CG	2.07	0.84
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.59	0.84
1:A:2631:THR:O	1:A:2635:THR:HG22	1.76	0.84
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.77	0.84
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.07	0.84
1:B:3303:LYS:HA	1:B:3306:TRP:NE1	1.91	0.84
1:A:1621:THR:HA	1:A:1624:ARG:NH1	1.92	0.84
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.07	0.84
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.59	0.84
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.07	0.83
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.78	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.07	0.83
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.61	0.83
1:A:2563:SER:HB3	1:A:2566:SER:H	1.42	0.83
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.42	0.83
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.82
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.28	0.82
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.13	0.82
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.61	0.82
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.77	0.82
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.07	0.82
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.62	0.82
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.09	0.82
1:A:2757:MET:HG2	1:A:2889:PHE:CD2	2.14	0.82
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.78	0.82
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.44	0.82
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.61	0.81
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.60	0.81
1:A:1783:THR:HG22	1:A:1809:PHE:HZ	1.44	0.81
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.81
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.09	0.81
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.81
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.60	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.62	0.81
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.62	0.81
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.11	0.81
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.40	0.80
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.08	0.80
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.10	0.80
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.07	0.80
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.61	0.80
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.97	0.80
1:B:2048:SER:H	2:B:5093:ATP:HN62	1.29	0.80
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.62	0.80
1:B:1983:LEU:HG	1:B:1993:THR:CG2	2.03	0.80
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.10	0.80
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.30	0.79
1:B:2471:LEU:O	1:B:2473:LEU:CD1	2.31	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.97	0.79
1:B:2728:LEU:HD12	1:B:2771:ARG:HH22	1.44	0.79
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.63	0.79
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.81	0.79
1:B:2354:SER:OG	1:B:2357:SER:CB	2.28	0.79
1:A:1620:PHE:CE1	1:A:1624:ARG:HD3	2.18	0.79
1:B:3303:LYS:C	1:B:3306:TRP:HD1	1.86	0.79
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	2.13	0.79
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.65	0.79
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.82	0.79
1:B:216:PRO:C	1:B:1365:PHE:CD1	2.56	0.79
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.78
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.62	0.78
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.31	0.78
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.64	0.78
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.78
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.23	0.78
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.71	0.78
1:B:1616:LYS:HZ1	1:B:1759:LYS:HE3	1.47	0.78
1:B:1416:LYS:CG	1:B:1421:TYR:OH	2.31	0.78
1:B:2224:SER:O	2:B:5093:ATP:H2	1.66	0.78
1:A:1783:THR:HG22	1:A:1809:PHE:CZ	2.19	0.78
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.99	0.78
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.62	0.78
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.99	0.77
1:A:2380:LEU:HG	1:A:2384:GLU:OE1	1.84	0.77
1:B:1826:PHE:CZ	1:B:1831:LEU:CB	2.66	0.77
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.32	0.77
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.49	0.77
1:A:2289:GLN:OE1	1:A:2412:ARG:CG	2.32	0.77
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.57	0.77
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.51	0.77
1:B:3303:LYS:CA	1:B:3306:TRP:CD1	2.66	0.77
1:A:2446:SER:H	1:A:2449:THR:CG2	1.97	0.77
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.28	0.77
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.65	0.77
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.24	0.77
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.67	0.77
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.99	0.77
1:B:1826:PHE:CE2	1:B:1831:LEU:CB	2.60	0.77
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.13	0.77
1:A:3458:PHE:HE1	1:A:3462:ILE:HB	1.50	0.77
1:B:1616:LYS:NZ	1:B:1759:LYS:CE	2.48	0.77
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.67	0.77
1:A:1463:LEU:HA	1:A:1466:GLN:HG2	1.66	0.76
1:A:1535:PRO:C	1:A:1841:ILE:HD11	2.05	0.76
1:B:1616:LYS:HZ2	1:B:1759:LYS:HE3	1.47	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.58	0.76
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.67	0.76
1:B:1759:LYS:CE	1:B:1761:GLU:OE2	2.33	0.76
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	2.01	0.76
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.84	0.76
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.62	0.76
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.16	0.76
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	2.01	0.76
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.15	0.76
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.16	0.76
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.67	0.76
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.50	0.76
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.85	0.75
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.75
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.21	0.75
1:A:2757:MET:CG	1:A:2889:PHE:HB2	2.14	0.75
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.16	0.75
1:A:1620:PHE:HE1	1:A:1624:ARG:HD3	1.50	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.86	0.75
1:B:216:PRO:C	1:B:1365:PHE:HA	2.06	0.75
1:B:1421:TYR:O	1:B:1421:TYR:CG	2.37	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.69	0.75
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.22	0.75
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.74	0.75
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.86	0.75
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.51	0.74
1:B:2137:VAL:O	1:B:2141:ILE:HG23	1.86	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.52	0.74
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.74
1:B:2080:LYS:NZ	2:B:5093:ATP:O3G	2.21	0.74
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.74
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.65	0.74
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.14	0.74
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.03	0.74
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.18	0.74
1:B:2425:THR:HB	3:B:5094:ADP:O1A	1.85	0.74
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.18	0.74
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.22	0.74
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.18	0.74
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.53	0.74
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.69	0.74
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.51	0.74
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.66	0.73
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.18	0.73
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.68	0.73
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.88	0.73
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.51	0.73
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.69	0.73
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.70	0.73
1:B:3458:PHE:CD1	1:B:3459:ASP:O	2.41	0.73
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.04	0.73
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.71	0.73
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.90	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.71	0.73
1:A:2048:SER:N	2:A:5093:ATP:HN62	1.86	0.73
1:A:2064:GLN:NE2	1:A:2151:TRP:HZ3	1.86	0.73
1:B:1616:LYS:HZ1	1:B:1759:LYS:CE	2.02	0.73
1:B:2080:LYS:HG2	2:B:5093:ATP:O1B	1.89	0.73
1:B:2155:ASP:OD1	1:B:2549:ARG:NH2	2.22	0.73
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.18	0.73
1:A:1983:LEU:CD2	1:A:1993:THR:HG23	2.19	0.72
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:PHE:CD2	1:A:1760:PHE:CZ	2.72	0.72
1:A:2757:MET:HG2	1:A:2889:PHE:CG	2.24	0.72
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.14	0.72
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.68	0.72
1:B:2631:THR:O	1:B:2635:THR:HG22	1.88	0.72
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.72	0.72
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.77	0.72
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.20	0.72
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.00	0.72
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.53	0.72
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.34	0.72
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.72
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.70	0.72
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.09	0.72
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.19	0.72
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.90	0.72
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.19	0.72
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.25	0.72
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.72	0.71
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.77	0.71
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.20	0.71
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.84	0.71
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.21	0.71
1:B:3458:PHE:CZ	1:B:3459:ASP:O	2.43	0.71
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.53	0.71
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.71	0.71
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.31	0.71
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.91	0.71
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.53	0.71
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.23	0.71
1:B:2446:SER:H	1:B:2449:THR:HG23	1.56	0.71
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.19	0.71
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.09	0.71
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.26	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.14	0.71
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.90	0.71
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.73	0.71
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.72	0.71
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.21	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	1.90	0.71
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.05	0.71
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.91	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.72	0.71
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.72	0.70
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.55	0.70
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.56	0.70
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.53	0.70
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.20	0.70
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.73	0.70
1:B:2446:SER:H	1:B:2449:THR:CG2	2.03	0.70
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.22	0.70
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.21	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.27	0.70
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.26	0.70
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.91	0.70
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.07	0.70
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.91	0.70
1:A:1744:LEU:HA	1:A:1760:PHE:CE1	2.25	0.70
1:B:3303:LYS:CA	1:B:3306:TRP:HD1	2.05	0.70
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.21	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.21	0.70
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.72	0.70
1:B:2476:LYS:CD	1:B:2476:LYS:H	2.04	0.70
1:A:2048:SER:H	2:A:5093:ATP:N6	1.88	0.70
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.13	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.22	0.69
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.21	0.69
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.74	0.69
1:A:7:TRP:O	1:A:9:ILE:N	2.25	0.69
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.74	0.69
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.50	0.69
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.69
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.73	0.69
1:A:2064:GLN:NE2	1:A:2151:TRP:CH2	2.61	0.69
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.28	0.69
1:A:1983:LEU:CD2	1:A:1993:THR:O	2.40	0.69
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.92	0.69
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.20	0.69
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.75	0.69
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.74	0.69
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.41	0.69
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.93	0.69
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.93	0.68
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.09	0.68
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.93	0.68
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.73	0.68
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.76	0.68
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.93	0.68
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.91	0.68
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.73	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:B:1759:LYS:HE2	1:B:1761:GLU:OE2	1.92	0.68
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	2.08	0.68
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.28	0.68
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.29	0.68
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.74	0.68
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.76	0.68
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.24	0.68
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.09	0.68
1:B:1826:PHE:HE2	1:B:1831:LEU:CB	2.04	0.68
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.57	0.68
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.12	0.68
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.59	0.68
1:A:2276:LEU:HD23	1:A:2556:ILE:HD13	1.76	0.68
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.59	0.68
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.75	0.67
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.24	0.67
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.57	0.67
1:B:3683:TYR:O	1:B:3687:SER:HB2	1.95	0.67
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.08	0.67
1:A:2391:VAL:HG22	1:A:2430:ASN:OD1	1.95	0.67
1:A:2762:SER:O	1:A:2763:ARG:HB2	1.95	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.24	0.67
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.76	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:A:1620:PHE:HD1	1:A:1624:ARG:NH1	1.93	0.67
1:B:2467:THR:HB	1:B:2473:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2463:ASN:HB2	1:A:2477:SER:HA	1.77	0.67
1:B:2081:THR:HB	2:B:5093:ATP:O1A	1.93	0.67
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	1.77	0.67
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.30	0.67
1:B:2224:SER:O	2:B:5093:ATP:C2	2.47	0.67
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.25	0.67
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.94	0.67
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.77	0.67
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.76	0.67
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.48	0.67
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.95	0.66
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.29	0.66
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.77	0.66
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.66
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.97	0.66
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.66
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.28	0.66
1:B:2517:LYS:HE3	1:B:2519:PRO:HD2	1.76	0.66
1:B:2552:ARG:NH2	2:B:5093:ATP:O2G	2.28	0.66
1:B:3919:LYS:HZ2	1:B:4038:GLU:CD	1.98	0.66
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.83	0.66
1:A:3460:PRO:O	1:A:3463:SER:CB	2.40	0.66
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.43	0.66
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.73	0.66
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.95	0.66
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.78	0.66
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.96	0.66
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.78	0.66
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.59	0.66
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.77	0.66
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.77	0.66
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.77	0.66
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.95	0.66
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.25	0.66
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.66
1:A:1983:LEU:HD23	1:A:1993:THR:O	1.96	0.66
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.16	0.65
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.61	0.65
1:A:1823:ASP:HB3	1:A:1852:ARG:O	1.95	0.65
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.60	0.65
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.79	0.65
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.96	0.65
1:B:2076:ALA:HA	2:B:5093:ATP:O1G	1.96	0.65
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.44	0.65
1:A:1983:LEU:HD23	1:A:1993:THR:CG2	2.26	0.65
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.30	0.65
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.25	0.65
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.77	0.65
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.96	0.65
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.77	0.65
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.37	0.65
1:A:2394:THR:H	1:A:2397:THR:HB	1.62	0.65
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.79	0.65
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.97	0.65
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.97	0.65
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.68	0.65
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.61	0.65
1:B:1983:LEU:HD21	1:B:1993:THR:O	1.94	0.65
1:A:1783:THR:CG2	1:A:1809:PHE:CZ	2.80	0.64
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.27	0.64
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.97	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.97	0.64
1:A:113:ASP:O	1:A:115:GLU:N	2.31	0.64
1:B:1826:PHE:HZ	1:B:1831:LEU:HB2	1.53	0.64
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.62	0.64
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.27	0.64
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.31	0.64
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.62	0.64
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.97	0.64
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.80	0.64
1:A:1425:GLU:OE2	1:A:1429:LEU:CD1	2.45	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.33	0.64
1:A:2134:LEU:CD1	1:A:2138:ASN:ND2	2.60	0.64
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.79	0.64
1:B:2574:TYR:HE2	3:B:5094:ADP:C2	2.16	0.64
1:A:2336:ARG:HD2	1:A:2355:ASP:OD2	1.97	0.64
1:A:2475:PRO:C	1:A:2476:LYS:HD2	2.18	0.64
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.13	0.64
1:B:2765:GLY:HA2	5:B:5096:SO4:O2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.28	0.64
1:B:2080:LYS:CD	1:B:2195:GLU:HB2	2.25	0.64
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.97	0.64
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.13	0.64
1:B:1493:LEU:O	1:B:1494:ASP:HB2	1.96	0.64
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.80	0.64
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.79	0.64
1:B:1852:ARG:HG3	1:B:1852:ARG:O	1.98	0.63
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.79	0.63
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.80	0.63
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.13	0.63
1:B:1991:GLU:O	1:B:1995:VAL:HG23	1.98	0.63
1:B:2064:GLN:OE1	1:B:2191:ARG:HD2	1.98	0.63
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.26	0.63
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.97	0.63
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.80	0.63
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.14	0.63
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.98	0.63
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.51	0.63
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.33	0.63
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.63	0.63
1:B:3460:PRO:O	1:B:3463:SER:CB	2.44	0.63
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.13	0.63
1:A:2426:MET:HG3	1:A:2427:ILE:N	2.11	0.63
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.64	0.63
1:A:2757:MET:CG	1:A:2889:PHE:CD2	2.80	0.63
1:A:3810:SER:O	1:A:3838:TRP:HB2	1.97	0.63
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.14	0.63
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.13	0.63
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.81	0.63
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.32	0.63
1:A:2054:LEU:O	1:A:2058:MET:HG2	1.99	0.62
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.99	0.62
1:B:3810:SER:O	1:B:3838:TRP:HB2	1.97	0.62
1:A:2620:ARG:NH1	1:A:2910:ASN:ND2	2.47	0.62
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.29	0.62
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.14	0.62
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.80	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.82	0.62
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.00	0.62
1:B:2426:MET:HG3	1:B:2427:ILE:H	1.64	0.62
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.79	0.62
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.81	0.62
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.98	0.62
1:A:2840:ILE:HB	1:A:2843:LEU:HD22	1.81	0.62
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.81	0.62
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.99	0.62
1:A:2163:VAL:HA	1:A:2166:MET:HG2	1.82	0.62
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.81	0.62
1:B:162:LEU:HA	1:B:165:ASP:O	1.98	0.62
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.82	0.62
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.00	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.53	0.62
1:B:2080:LYS:HZ3	2:B:5093:ATP:PG	2.22	0.62
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.15	0.62
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.30	0.62
1:A:2940:PHE:HZ	1:A:2943:PHE:HE2	1.48	0.62
1:A:1646:GLN:NE2	1:A:1761:GLU:O	2.24	0.61
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.81	0.61
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.65	0.61
1:B:3819:ILE:O	1:B:3823:ASN:HB2	2.01	0.61
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.64	0.61
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.81	0.61
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.20	0.61
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.35	0.61
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.35	0.61
1:B:2276:LEU:HD23	1:B:2556:ILE:HG21	1.83	0.61
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.00	0.61
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.78	0.61
1:A:2640:THR:HG23	1:A:2643:SER:H	1.66	0.61
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.29	0.61
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.40	0.61
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.83	0.61
1:B:2426:MET:HG3	1:B:2427:ILE:N	2.15	0.61
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.15	0.61
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.61
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.61
1:A:1802:LYS:NZ	5:A:5097:SO4:O2	2.34	0.61
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	1.81	0.61
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2048:SER:H	2:B:5093:ATP:N6	1.97	0.61
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.64	0.61
1:A:1563:LYS:HD2	1:A:1570:GLU:HG3	1.82	0.61
1:A:1783:THR:CG2	1:A:1809:PHE:CE1	2.83	0.61
1:A:2032:LYS:O	1:A:2035:VAL:HG12	2.00	0.61
1:A:2421:GLY:HA2	3:A:5094:ADP:O5'	2.00	0.61
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.31	0.61
1:A:3737:THR:HB	1:A:3740:THR:CB	2.31	0.61
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.30	0.61
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.34	0.61
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.82	0.61
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.36	0.61
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.82	0.61
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.61
1:B:3303:LYS:HA	1:B:3306:TRP:HE1	1.62	0.61
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.82	0.61
1:A:2064:GLN:CD	1:A:2151:TRP:CH2	2.74	0.61
1:B:2380:LEU:CD2	1:B:2384:GLU:OE1	2.37	0.61
1:B:2481:ASN:HD21	1:B:2528:ARG:HD3	1.64	0.61
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.82	0.60
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.83	0.60
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.60
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.84	0.60
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.01	0.60
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.20	0.60
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.82	0.60
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.01	0.60
1:A:2563:SER:CB	1:A:2566:SER:OG	2.49	0.60
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.83	0.60
1:B:2064:GLN:HE22	1:B:2070:LEU:HG	1.61	0.60
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.66	0.60
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.37	0.60
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.16	0.60
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.83	0.60
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.84	0.60
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.01	0.60
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.84	0.60
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.02	0.60
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.00	0.60
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.84	0.60
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.83	0.60
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.83	0.60
1:B:1416:LYS:CB	1:B:1421:TYR:OH	2.50	0.60
1:B:3737:THR:OG1	1:B:3740:THR:HB	2.01	0.60
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.01	0.59
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.37	0.59
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.59
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.17	0.59
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.67	0.59
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.83	0.59
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.84	0.59
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.32	0.59
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.32	0.59
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.90	0.59
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.83	0.59
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.59
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.38	0.59
1:B:2394:THR:H	1:B:2397:THR:HB	1.66	0.59
1:A:1620:PHE:CD1	1:A:1624:ARG:NH1	2.70	0.59
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.68	0.59
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.67	0.59
1:A:3818:SER:O	1:A:3821:ASN:N	2.35	0.59
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.21	0.59
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.67	0.59
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.59
1:B:1616:LYS:NZ	1:B:1759:LYS:NZ	2.49	0.59
1:B:2072:LEU:HD23	1:B:2215:PHE:CE1	2.37	0.59
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.67	0.59
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.59
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	2.90	0.59
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.85	0.59
1:A:2620:ARG:HH12	1:A:2910:ASN:ND2	1.99	0.59
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.32	0.59
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.37	0.59
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.59
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.68	0.59
1:B:1422:LYS:HA	1:B:1425:GLU:HB2	1.85	0.59
1:B:2386:MET:HB3	1:B:2627:ARG:NE	2.18	0.59
1:B:1416:LYS:HA	1:B:1421:TYR:OH	2.01	0.59
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.03	0.58
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.68	0.58
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.38	0.58
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.84	0.58
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.03	0.58
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.37	0.58
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.83	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.58
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.03	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.86	0.58
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.52	0.58
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.04	0.58
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.38	0.58
1:A:1983:LEU:HD23	1:A:1993:THR:HG23	1.84	0.58
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.86	0.58
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.51	0.58
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.39	0.58
1:A:3458:PHE:CZ	1:A:3459:ASP:O	2.57	0.58
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.34	0.58
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.85	0.58
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.84	0.58
1:A:162:LEU:HA	1:A:165:ASP:O	2.03	0.58
1:A:1929:ILE:HD12	1:A:1929:ILE:H	1.69	0.58
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.85	0.58
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.83	0.58
1:B:23:LEU:O	1:B:24:GLU:CB	2.52	0.58
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.84	0.58
1:A:3636:GLY:HA2	1:A:3642:TYR:O	2.04	0.58
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.32	0.58
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.69	0.58
1:B:2160:PRO:O	1:B:2164:GLU:HG3	2.04	0.58
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.85	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.44	0.57
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.33	0.57
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.85	0.57
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.84	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.84	0.57
1:B:2080:LYS:CG	2:B:5093:ATP:O1B	2.51	0.57
1:A:2047:PHE:HB3	2:A:5093:ATP:N6	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.82	0.57
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.86	0.57
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.86	0.57
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.69	0.57
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.86	0.57
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.87	0.57
1:B:2391:VAL:CG2	1:B:2426:MET:HE3	2.34	0.57
1:B:2745:ILE:HG23	1:B:2756:MET:HE3	1.85	0.57
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.86	0.57
1:A:2737:SER:HB2	1:A:2924:THR:HG21	1.87	0.57
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.58	0.57
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.86	0.57
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.92	0.57
1:A:3945:LEU:O	1:A:3948:HIS:O	2.23	0.57
1:B:1421:TYR:O	1:B:1421:TYR:CD1	2.58	0.57
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.39	0.57
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.85	0.57
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.04	0.57
1:A:1779:PHE:O	1:A:1783:THR:HG23	2.04	0.57
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.17	0.57
1:A:2064:GLN:CD	1:A:2151:TRP:HH2	2.08	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.35	0.57
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.86	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.25	0.57
1:A:2368:PHE:O	1:A:2369:SER:OG	2.16	0.57
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.23	0.57
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.16	0.57
1:A:1794:PHE:CZ	1:A:1805:THR:HG21	2.39	0.57
1:B:1416:LYS:HA	1:B:1421:TYR:CE1	2.34	0.57
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.85	0.57
1:B:2072:LEU:HD23	1:B:2215:PHE:HE1	1.68	0.57
1:B:3737:THR:HB	1:B:3740:THR:CB	2.34	0.57
1:A:1621:THR:CA	1:A:1624:ARG:NH1	2.66	0.57
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.88	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.86	0.57
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.38	0.57
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.85	0.57
1:A:2060:PHE:HZ	1:A:2064:GLN:NE2	1.99	0.56
1:A:65:THR:O	1:A:66:GLN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.86	0.56
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.06	0.56
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.39	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.86	0.56
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.86	0.56
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.14	0.56
1:A:3559:LEU:O	1:A:3563:GLU:HG3	2.06	0.56
1:B:2060:PHE:CZ	1:B:2064:GLN:NE2	2.73	0.56
1:B:2320:ARG:NH1	1:B:2406:ASP:OD2	2.33	0.56
1:B:3631:MET:HE3	1:B:3698:MET:HG3	1.86	0.56
1:A:1459:LEU:HD22	1:A:1473:THR:CG2	2.35	0.56
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.35	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.26	0.56
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.34	0.56
1:B:3690:LEU:HD23	1:B:3694:PHE:HB3	1.88	0.56
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.86	0.56
1:A:1463:LEU:HA	1:A:1466:GLN:CG	2.36	0.56
1:A:1794:PHE:HZ	1:A:1805:THR:HG21	1.71	0.56
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.19	0.56
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.45	0.56
1:A:3636:GLY:CA	1:A:3642:TYR:O	2.53	0.56
1:B:1416:LYS:CA	1:B:1421:TYR:CZ	2.71	0.56
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.05	0.56
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.05	0.56
1:B:2452:GLU:HA	1:B:2455:LEU:HD12	1.86	0.56
1:A:2389:ASP:HB3	1:A:2433:ARG:NH1	2.20	0.56
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.87	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.88	0.56
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.87	0.56
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.36	0.56
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.86	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.48	0.56
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.06	0.56
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.56
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.71	0.56
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.77	0.56
1:B:1802:LYS:NZ	5:B:5097:SO4:O3	2.39	0.56
1:A:3481:ILE:O	1:A:3483:ASP:N	2.38	0.56
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.87	0.56
1:A:1744:LEU:HA	1:A:1760:PHE:CD1	2.41	0.55
1:A:3303:LYS:CD	1:A:3306:TRP:CD1	2.80	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.86	0.55
1:B:1416:LYS:HG2	1:B:1421:TYR:CZ	2.40	0.55
1:B:3322:GLY:HA2	1:B:3325:ILE:HD12	1.88	0.55
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.42	0.55
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.88	0.55
1:B:2391:VAL:HG23	1:B:2426:MET:HE1	1.88	0.55
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.55
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.88	0.55
1:A:1646:GLN:CD	1:A:1763:ILE:HG12	2.27	0.55
1:A:3569:GLU:O	1:A:3573:SER:OG	2.20	0.55
1:B:2391:VAL:CG2	1:B:2426:MET:CE	2.84	0.55
1:A:1559:SER:HB2	1:A:1572:ILE:H	1.71	0.55
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.41	0.55
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.07	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.88	0.55
1:A:2757:MET:CE	1:A:2908:LEU:HB3	2.37	0.55
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.72	0.55
1:B:1983:LEU:CG	1:B:1993:THR:CG2	2.75	0.55
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.42	0.55
1:B:2391:VAL:HG23	1:B:2426:MET:CE	2.36	0.55
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.06	0.55
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.36	0.55
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	1.88	0.55
1:B:1396:ARG:HG3	1:B:1397:GLU:H	1.71	0.55
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.41	0.55
1:A:1851:ASN:ND2	1:A:1899:ASN:O	2.39	0.55
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.35	0.55
1:A:2163:VAL:HA	1:A:2166:MET:CG	2.36	0.55
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.27	0.55
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.21	0.55
1:B:2481:ASN:ND2	1:B:2528:ARG:HD3	2.22	0.55
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.60	0.55
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.10	0.55
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.55
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.72	0.55
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.69	0.55
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.54	0.55
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.71	0.55
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.55
1:B:1826:PHE:HZ	1:B:1831:LEU:CB	2.15	0.55
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.06	0.55
1:B:2380:LEU:HD13	1:B:2390:ILE:CD1	2.21	0.55
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.90	0.55
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.72	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:B:2391:VAL:HG21	1:B:2426:MET:HE3	1.88	0.55
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.07	0.54
1:B:2470:GLY:C	1:B:2473:LEU:HD11	2.27	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.96	0.54
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.36	0.54
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.87	0.54
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.89	0.54
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.89	0.54
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.37	0.54
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.89	0.54
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.71	0.54
1:A:2081:THR:OG1	1:A:2195:GLU:OE2	2.26	0.54
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.40	0.54
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.89	0.54
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.06	0.54
1:B:3010:LEU:HD21	1:B:3317:SER:HB3	1.90	0.54
1:A:2475:PRO:O	1:A:2476:LYS:C	2.46	0.54
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.08	0.54
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.05	0.54
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.91	0.54
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.85	0.54
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.07	0.54
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.87	0.54
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.42	0.54
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.61	0.54
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.88	0.54
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.38	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.87	0.54
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.90	0.54
1:B:1416:LYS:HA	1:B:1421:TYR:CE2	2.36	0.54
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.73	0.54
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.54
1:A:1425:GLU:OE2	1:A:1429:LEU:CD2	2.56	0.54
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.72	0.54
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.89	0.54
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.73	0.54
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.08	0.54
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.90	0.54
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.08	0.54
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.08	0.54
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.90	0.54
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.25	0.54
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.90	0.54
1:A:2513:GLN:O	1:A:2526:ILE:HG13	2.09	0.53
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.37	0.53
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.90	0.53
1:A:1743:ASP:HA	1:A:1746:SER:HB3	1.90	0.53
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.73	0.53
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.43	0.53
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.89	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.41	0.53
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.56	0.53
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.73	0.53
1:A:2451:THR:O	1:A:2455:LEU:HD12	2.08	0.53
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.91	0.53
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.38	0.53
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.08	0.53
1:B:1421:TYR:CD1	1:B:1421:TYR:C	2.82	0.53
1:A:1783:THR:HG23	1:A:1809:PHE:CE1	2.44	0.53
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.08	0.53
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.71	0.53
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.89	0.53
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.90	0.53
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.57	0.53
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.22	0.53
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.44	0.53
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.53
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.23	0.53
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.91	0.53
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.49	0.53
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.74	0.53
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3303:LYS:C	1:B:3306:TRP:CD1	2.74	0.53
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.44	0.53
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.26	0.53
1:A:1367:ILE:H	1:A:1367:ILE:HD12	1.73	0.53
1:A:1620:PHE:CE2	1:A:1743:ASP:HB3	2.43	0.53
1:A:1970:LEU:HD12	1:A:1973:LEU:CD1	2.38	0.53
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.74	0.53
1:B:1396:ARG:HG3	1:B:1397:GLU:N	2.24	0.53
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.91	0.53
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.39	0.53
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.90	0.53
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.43	0.53
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.91	0.52
1:A:2060:PHE:HZ	1:A:2064:GLN:HE21	1.51	0.52
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.55	0.52
1:A:2967:ASN:HB3	1:A:3356:PHE:CE2	2.44	0.52
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.13	0.52
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.74	0.52
1:A:2463:ASN:CB	1:A:2477:SER:HA	2.39	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.75	0.52
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.56	0.52
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.90	0.52
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.08	0.52
1:A:2421:GLY:N	3:A:5094:ADP:O2B	2.35	0.52
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.45	0.52
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.09	0.52
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.37	0.52
1:B:2276:LEU:HD21	1:B:2415:ILE:HG21	1.91	0.52
1:A:2441:VAL:HG21	1:A:2482:LEU:HD21	1.91	0.52
1:B:1422:LYS:O	1:B:1425:GLU:CB	2.48	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.90	0.52
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.75	0.52
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.35	0.52
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.98	0.52
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.73	0.52
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.25	0.52
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.90	0.52
1:B:1635:ASP:HB2	1:B:1638:VAL:HG23	1.91	0.52
1:B:1616:LYS:HZ1	1:B:1759:LYS:NZ	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.52
1:B:3736:LEU:HD11	1:B:3745:ARG:HG3	1.92	0.52
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.33	0.52
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.64	0.52
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.91	0.52
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.40	0.52
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.92	0.52
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.10	0.52
1:A:2448:ASP:O	1:A:2829:GLU:OE2	2.27	0.52
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	1.92	0.52
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.57	0.52
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.39	0.52
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.92	0.52
1:B:2476:LYS:HZ2	1:B:2528:ARG:HD2	1.72	0.52
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.10	0.52
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.32	0.52
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.68	0.52
1:B:1448:VAL:HG22	1:B:1513:ILE:HB	1.92	0.52
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.92	0.52
1:B:2640:THR:HG23	1:B:2643:SER:H	1.75	0.52
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.10	0.52
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.24	0.52
1:B:1970:LEU:HD23	1:B:1974:LYS:HE3	1.92	0.52
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.92	0.52
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.91	0.51
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.39	0.51
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.58	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.87	0.51
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.91	0.51
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.91	0.51
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.10	0.51
1:A:1995:VAL:CG1	1:A:2018:LEU:HD21	2.40	0.51
1:B:1771:TYR:HA	1:B:1775:LEU:HD13	1.92	0.51
1:B:2228:HIS:HB3	2:B:5093:ATP:C2	2.44	0.51
1:A:1983:LEU:HD23	1:A:1993:THR:HG22	1.92	0.51
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.41	0.51
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.45	0.51
1:A:3737:THR:CB	1:A:3740:THR:HB	2.40	0.51
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.76	0.51
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.92	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2792:LEU:HD13	1:B:2826:ALA:HB3	1.92	0.51
1:A:1771:TYR:HA	1:A:1775:LEU:HD13	1.92	0.51
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.40	0.51
1:A:3458:PHE:CD1	1:A:3459:ASP:O	2.63	0.51
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.51
1:B:2225:LYS:HA	2:B:5093:ATP:H2	1.71	0.51
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.40	0.51
1:A:2494:LEU:O	1:A:2495:ASP:O	2.29	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.39	0.51
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.74	0.51
1:B:2276:LEU:HD23	1:B:2556:ILE:CG2	2.41	0.51
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.39	0.51
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.75	0.51
1:A:2055:LYS:HE3	1:A:2056:LYS:HE2	1.93	0.51
1:A:2965:VAL:HG13	1:A:3325:ILE:HD11	1.92	0.51
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.22	0.51
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.11	0.51
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.14	0.51
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.40	0.51
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.92	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:B:2064:GLN:NE2	1:B:2070:LEU:CG	2.67	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:A:1744:LEU:HD22	1:A:1760:PHE:CD1	2.45	0.51
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.63	0.51
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.76	0.51
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.51
1:A:2378:VAL:HG21	1:A:2380:LEU:HD13	1.89	0.51
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.11	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.58	0.51
1:B:1826:PHE:HZ	1:B:1831:LEU:CA	2.24	0.51
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.91	0.50
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.93	0.50
1:A:2446:SER:H	1:A:2449:THR:HG21	1.76	0.50
1:A:2425:THR:HG22	1:A:2485:PHE:HE2	1.77	0.50
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.24	0.50
1:B:3530:PHE:CE1	1:B:3618:TYR:HD2	2.26	0.50
1:A:2762:SER:O	1:A:2763:ARG:CB	2.60	0.50
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.11	0.50
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.11	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2378:VAL:HG22	1:B:2380:LEU:HG	1.92	0.50
1:B:2517:LYS:HG2	1:B:2520:GLU:HB2	1.93	0.50
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.41	0.50
1:A:1425:GLU:OE2	1:A:1429:LEU:HD21	2.12	0.50
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.94	0.50
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.41	0.50
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.32	0.50
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.15	0.50
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.76	0.50
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.11	0.50
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.77	0.50
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.42	0.50
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.94	0.50
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.93	0.50
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	1.93	0.50
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.50
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.76	0.50
1:A:1645:PHE:HB3	1:A:1765:ILE:HG21	1.90	0.50
1:A:2380:LEU:HD23	1:A:2384:GLU:HB3	1.94	0.50
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.76	0.50
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.42	0.50
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.76	0.50
1:B:3461:ILE:C	1:B:3463:SER:H	2.14	0.50
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.60	0.50
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.94	0.50
1:A:2755:HIS:CE1	1:A:2835:LEU:HG	2.47	0.50
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.68	0.50
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.45	0.50
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.76	0.50
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.93	0.50
1:A:1969:GLY:O	1:A:1972:THR:HB	2.11	0.50
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.47	0.50
1:A:4023:ILE:HD11	1:A:4029:ILE:HD12	1.93	0.50
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.32	0.50
1:A:2228:HIS:HB3	2:A:5093:ATP:C2	2.47	0.50
1:B:2428:MET:SD	1:B:2428:MET:C	2.90	0.50
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.32	0.50
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.60	0.50
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.45	0.50
1:A:3628:ILE:HG22	1:A:3649:PHE:CE2	2.47	0.50
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.99	0.50
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.44	0.50
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.94	0.50
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.70	0.50
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.93	0.50
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.94	0.49
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.94	0.49
1:B:2786:ILE:HG12	1:B:2821:ASN:HA	1.94	0.49
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.94	0.49
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.75	0.49
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	1.94	0.49
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.94	0.49
1:A:3818:SER:O	1:A:3820:GLU:N	2.45	0.49
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.60	0.49
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.52	0.49
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.94	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:1929:ILE:H	1:B:1929:ILE:HD12	1.77	0.49
1:B:2467:THR:CB	1:B:2473:LEU:HD22	2.40	0.49
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.11	0.49
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.76	0.49
1:B:1616:LYS:HZ2	1:B:1759:LYS:CE	2.19	0.49
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.74	0.49
1:B:2822:ILE:O	1:B:2822:ILE:CG1	2.38	0.49
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.53	0.49
1:A:23:LEU:O	1:A:25:GLU:N	2.45	0.49
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.26	0.49
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.95	0.49
1:B:2181:GLY:O	1:B:2182:GLU:HG3	2.12	0.49
1:B:2574:TYR:CE2	3:B:5094:ADP:C2	2.98	0.49
1:B:3737:THR:CB	1:B:3740:THR:CB	2.90	0.49
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.78	0.49
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.93	0.49
1:A:1448:VAL:HG22	1:A:1513:ILE:HB	1.95	0.49
1:A:2476:LYS:O	1:A:2476:LYS:HD3	2.11	0.49
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.13	0.49
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.12	0.49
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.46	0.49
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.48	0.49
1:B:2080:LYS:CE	2:B:5093:ATP:O3G	2.60	0.49
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3579:GLU:O	1:B:3582:GLU:N	2.44	0.49
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.77	0.49
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.48	0.49
3:B:5094:ADP:N3	3:B:5094:ADP:H2'	2.27	0.49
1:A:1459:LEU:HD22	1:A:1473:THR:HG22	1.95	0.49
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	1.94	0.49
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.94	0.49
2:B:5093:ATP:O3G	2:B:5093:ATP:O1B	2.30	0.49
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.48	0.49
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.13	0.49
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.49
1:B:1422:LYS:CA	1:B:1425:GLU:HB2	2.43	0.49
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.94	0.49
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.91	0.49
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.48	0.49
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.42	0.49
1:B:2495:ASP:O	1:B:2498:GLY:N	2.46	0.49
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.42	0.49
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.39	0.49
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.95	0.48
1:A:1823:ASP:CG	1:A:1823:ASP:O	2.51	0.48
1:A:2134:LEU:HD12	1:A:2138:ASN:ND2	2.28	0.48
1:A:2920:TRP:CG	1:A:2989:PRO:HG3	2.47	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.94	0.48
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.48	0.48
1:A:4022:GLN:HA	1:A:4027:VAL:O	2.12	0.48
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.36	0.48
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.13	0.48
1:A:1466:GLN:HB2	1:A:1473:THR:HG21	1.95	0.48
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.94	0.48
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.60	0.48
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.78	0.48
1:B:2476:LYS:HE3	1:B:2528:ARG:HB3	1.95	0.48
1:B:2763:ARG:HA	5:B:5096:SO4:O3	2.13	0.48
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.29	0.48
1:B:2080:LYS:HE2	2:B:5093:ATP:O3G	2.13	0.48
1:A:2154:PHE:HD1	1:A:2154:PHE:N	2.10	0.48
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.48
1:A:2475:PRO:O	1:A:2476:LYS:O	2.30	0.48
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.81	0.48
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.92	0.48
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.96	0.48
1:B:2467:THR:HG22	1:B:2468:SER:N	2.29	0.48
1:B:3618:TYR:O	1:B:3622:GLY:N	2.42	0.48
1:B:3737:THR:CB	1:B:3740:THR:HB	2.44	0.48
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.95	0.48
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.14	0.48
1:A:3618:TYR:O	1:A:3622:GLY:N	2.38	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.42	0.48
1:A:2942:ASP:HB3	1:A:3357:ALA:HB1	1.95	0.48
1:A:3462:ILE:N	1:A:3462:ILE:HD13	2.28	0.48
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.79	0.48
1:B:2467:THR:HB	1:B:2473:LEU:CD2	2.42	0.48
1:B:65:THR:O	1:B:66:GLN:CB	2.61	0.48
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.13	0.48
1:A:2154:PHE:CD1	1:A:2154:PHE:N	2.79	0.48
1:A:2494:LEU:O	1:A:2494:LEU:HD12	2.14	0.48
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.48	0.48
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.44	0.48
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.43	0.48
1:B:4074:GLU:HA	1:B:4077:GLN:HE21	1.79	0.48
1:A:1620:PHE:HD2	1:A:1760:PHE:HZ	1.49	0.48
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.14	0.48
1:B:1423:ILE:C	1:B:1425:GLU:N	2.66	0.48
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	1.96	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.40	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.13	0.48
1:A:3934:TRP:CG	1:A:4023:ILE:HD12	2.49	0.48
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.96	0.48
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.48	0.48
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	1.96	0.48
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.14	0.48
1:A:2426:MET:HG3	1:A:2427:ILE:H	1.79	0.48
1:A:3307:LEU:O	1:A:3311:LYS:HB3	2.14	0.48
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.95	0.48
1:B:3628:ILE:HD11	1:B:3679:TYR:CZ	2.49	0.48
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.79	0.48
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2473:LEU:HD23	1:A:2525:THR:HB	1.96	0.47
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.14	0.47
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.49	0.47
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.79	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.96	0.47
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.16	0.47
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.96	0.47
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.44	0.47
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.29	0.47
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.47
1:A:2134:LEU:HD11	1:A:2138:ASN:HD21	1.79	0.47
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.83	0.47
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.14	0.47
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.71	0.47
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.30	0.47
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.14	0.47
1:A:2441:VAL:CG2	1:A:2482:LEU:HD21	2.43	0.47
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.62	0.47
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	1.95	0.47
1:B:2060:PHE:CE1	1:B:2064:GLN:NE2	2.81	0.47
1:B:3461:ILE:C	1:B:3463:SER:N	2.67	0.47
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.47
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	1.96	0.47
1:A:2378:VAL:CG1	1:A:2392:ILE:HD12	2.44	0.47
1:A:2563:SER:C	1:A:2565:LYS:H	2.17	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.29	0.47
1:A:1646:GLN:OE1	1:A:1763:ILE:N	2.42	0.47
1:A:2354:SER:H	1:A:2357:SER:HB2	1.80	0.47
1:A:2760:GLY:HA2	1:A:2917:MET:HB2	1.96	0.47
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	1.97	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.96	0.47
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.98	0.47
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.47
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.55	0.47
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.14	0.47
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.83	0.47
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.96	0.47
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.95	0.47
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	1.97	0.47
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2967:ASN:HB3	1:A:3356:PHE:CZ	2.49	0.47
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.45	0.47
1:B:2470:GLY:O	1:B:2471:LEU:HB2	2.15	0.47
1:B:2473:LEU:N	1:B:2473:LEU:HD12	2.28	0.47
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.96	0.47
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.66	0.47
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.44	0.47
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.78	0.47
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.50	0.47
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	1.96	0.47
1:B:3367:ILE:O	1:B:3371:VAL:HG22	2.15	0.47
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.97	0.47
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.50	0.47
1:A:1802:LYS:NZ	5:A:5097:SO4:S	2.88	0.47
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.39	0.47
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.47
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	1.97	0.47
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.51	0.47
1:B:2446:SER:H	1:B:2449:THR:HG21	1.79	0.47
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.63	0.47
1:B:2920:TRP:CG	1:B:2989:PRO:HG3	2.50	0.46
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.44	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.97	0.46
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.97	0.46
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.17	0.46
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.46	0.46
1:A:3927:TYR:HE1	1:A:4029:ILE:HG22	1.80	0.46
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	1.96	0.46
1:B:2709:LYS:O	1:B:2713:VAL:HG23	2.15	0.46
1:B:2421:GLY:N	3:B:5094:ADP:O2B	2.39	0.46
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.15	0.46
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.50	0.46
1:A:2507:ARG:HG3	1:A:2550:PHE:HA	1.97	0.46
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.46
1:B:1714:GLN:HB3	1:B:1727:LEU:HD11	1.98	0.46
1:B:1826:PHE:CE1	1:B:1830:VAL:HG13	2.51	0.46
1:B:1938:GLY:O	1:B:1989:GLU:HB3	2.15	0.46
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.97	0.46
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.15	0.46
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.15	0.46
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	1.98	0.46
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.42	0.46
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.97	0.46
1:A:3818:SER:O	1:A:3819:ILE:C	2.54	0.46
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.46
1:B:2620:ARG:HH11	1:B:2910:ASN:ND2	2.13	0.46
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.96	0.46
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.44	0.46
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.97	0.46
1:A:3431:PHE:CZ	1:A:3458:PHE:HD1	2.33	0.46
1:B:1422:LYS:C	1:B:1425:GLU:HB3	2.33	0.46
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.16	0.46
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.78	0.46
1:B:203:GLN:O	1:B:204:GLY:C	2.54	0.46
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.62	0.46
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.51	0.46
1:A:2905:SER:HA	1:A:2906:PRO:HD2	1.70	0.46
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.16	0.46
1:B:2305:LEU:HB3	1:B:2310:LEU:CD1	2.45	0.46
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.51	0.46
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.97	0.46
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.80	0.46
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.97	0.46
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.46
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.98	0.46
1:B:1939:PHE:HD1	1:B:1939:PHE:H	1.61	0.46
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.46	0.46
1:B:3462:ILE:O	1:B:3465:LEU:N	2.49	0.46
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.80	0.46
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.49	0.46
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.15	0.46
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.15	0.46
1:A:1977:LEU:O	1:A:1980:CYS:HB3	2.16	0.46
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	1.97	0.46
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.51	0.46
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.85	0.46
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.16	0.46
1:B:2170:LEU:HB3	1:B:2209:ARG:HD3	1.98	0.46
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.62	0.46
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.81	0.46
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.96	0.46
1:A:2228:HIS:HD2	2:A:5093:ATP:O2'	1.99	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.15	0.46
1:B:2204:PRO:HA	1:B:2207:ILE:HD12	1.97	0.46
1:B:2563:SER:C	1:B:2565:LYS:H	2.19	0.46
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.16	0.46
1:A:1848:ASP:O	1:A:1849:GLU:HB2	2.16	0.46
1:A:23:LEU:O	1:A:24:GLU:C	2.50	0.46
1:A:2475:PRO:HB3	1:A:2527:GLU:HB2	1.98	0.46
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.16	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.97	0.46
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.16	0.46
1:B:3687:SER:HA	1:B:3698:MET:HE1	1.98	0.46
1:A:1621:THR:HA	1:A:1624:ARG:CZ	2.44	0.45
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.17	0.45
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.97	0.45
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.31	0.45
1:A:2129:LEU:O	1:A:2133:ILE:HG12	2.16	0.45
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:3816:LEU:HD21	1:A:3850:TRP:HZ3	1.81	0.45
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.66	0.45
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.97	0.45
1:A:1694:VAL:HG23	1:A:1697:LYS:HE2	1.98	0.45
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.81	0.45
1:A:1927:GLY:HA2	1:A:1950:VAL:HG21	1.97	0.45
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.99	0.45
1:B:3017:VAL:HG21	1:B:3313:PHE:HE2	1.81	0.45
1:B:3500:ASP:HA	1:B:3501:PRO:HD3	1.88	0.45
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.17	0.45
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.84	0.45
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.51	0.45
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.51	0.45
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.46	0.45
1:A:2567:LEU:HD22	1:A:2622:LEU:HD13	1.98	0.45
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.51	0.45
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.51	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.51	0.45
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.51	0.45
1:A:1575:LEU:HA	1:A:1575:LEU:HD12	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1852:ARG:HG3	1:A:1852:ARG:O	2.17	0.45
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.90	0.45
1:A:2163:VAL:O	1:A:2166:MET:HG3	2.16	0.45
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	1.98	0.45
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.81	0.45
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.98	0.45
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.15	0.45
1:A:2425:THR:HG22	1:A:2485:PHE:CE2	2.51	0.45
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.64	0.45
1:A:3799:LYS:HG3	1:A:3803:LEU:HD11	1.98	0.45
1:A:3891:ARG:HA	1:A:3891:ARG:HD2	1.79	0.45
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.16	0.45
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.37	0.45
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.17	0.45
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.52	0.45
1:A:2727:GLU:O	1:A:2728:LEU:C	2.55	0.45
1:B:2037:CYS:SG	1:B:2094:PHE:HB2	2.56	0.45
1:B:2276:LEU:CD2	1:B:2556:ILE:HG21	2.45	0.45
1:B:2491:LEU:HD21	1:B:2543:ARG:CZ	2.47	0.45
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.39	0.45
1:A:1946:ALA:O	1:A:1950:VAL:HG23	2.17	0.45
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.28	0.45
1:A:2115:TYR:O	1:A:2131:THR:CG2	2.65	0.45
1:A:2134:LEU:CD1	1:A:2138:ASN:HD21	2.28	0.45
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.16	0.45
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.16	0.45
1:A:1640:VAL:CG1	1:A:1686:LYS:NZ	2.79	0.45
1:A:2891:ILE:CD1	1:A:2903:ILE:HD11	2.43	0.45
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ3	1.81	0.45
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	1.99	0.45
1:B:1941:ASP:O	1:B:1945:LEU:HG	2.17	0.45
1:B:2563:SER:CB	1:B:2566:SER:H	2.20	0.45
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.80	0.45
1:A:2474:LEU:N	1:A:2475:PRO:HD3	2.32	0.45
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.99	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.98	0.45
1:A:3304:GLU:C	1:A:3306:TRP:H	2.21	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:B:1753:GLY:HA3	1:B:3970:ASN:HD21	1.81	0.45
1:B:2467:THR:O	1:B:2471:LEU:N	2.50	0.45
1:A:2100:VAL:N	1:A:2149:ARG:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2412:ARG:HH11	1:A:2412:ARG:HG3	1.82	0.44
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.99	0.44
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.78	0.44
1:B:2580:LYS:HG2	1:B:2586:ARG:HH22	1.82	0.44
1:B:2752:VAL:HG13	1:B:2883:LYS:HB3	1.98	0.44
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.98	0.44
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.32	0.44
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.98	0.44
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.20	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:A:2220:CYS:SG	1:A:2221:SER:N	2.91	0.44
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.53	0.44
1:A:2755:HIS:CB	1:A:2912:CYS:HA	2.47	0.44
1:B:1367:ILE:HD12	1:B:1367:ILE:H	1.83	0.44
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.44
1:B:3600:LYS:HA	1:B:3603:GLU:HG2	1.99	0.44
1:A:2386:MET:HB2	1:A:2627:ARG:CD	2.39	0.44
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.98	0.44
1:B:2091:MET:CE	1:B:2149:ARG:NH1	2.80	0.44
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.32	0.44
1:B:2988:SER:CB	1:B:2989:PRO:CD	2.62	0.44
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.16	0.44
1:B:3810:SER:HB3	1:B:3838:TRP:H	1.83	0.44
1:A:3440:LEU:HD22	1:A:3462:ILE:HD12	1.98	0.44
1:A:3459:ASP:HB2	1:A:3460:PRO:HD2	1.98	0.44
1:A:3464:ARG:O	1:A:3467:SER:O	2.35	0.44
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.53	0.44
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.18	0.44
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.99	0.44
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.53	0.44
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.99	0.44
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.81	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:B:1851:ASN:HD21	1:B:1899:ASN:HB2	1.81	0.44
1:B:2178:LEU:HD12	1:B:2182:GLU:HB2	1.99	0.44
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.95	0.44
1:B:3509:LEU:O	1:B:3513:VAL:HG23	2.17	0.44
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.28	0.44
1:A:1646:GLN:CG	1:A:1763:ILE:HG12	2.47	0.44
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.85	0.44
1:A:2424:LYS:HZ3	1:A:2424:LYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.17	0.44
1:A:2755:HIS:CB	1:A:2911:ARG:O	2.58	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.06	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.98	0.44
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.17	0.44
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.78	0.44
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	2.00	0.44
1:A:1664:LEU:O	1:A:1721:LYS:HE3	2.18	0.44
1:A:1983:LEU:HD21	1:A:1993:THR:O	2.16	0.44
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.48	0.44
1:A:2428:MET:SD	1:A:2428:MET:C	2.96	0.44
1:A:3788:MET:HG3	1:A:3788:MET:O	2.18	0.44
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.82	0.44
1:B:1970:LEU:CD2	1:B:1974:LYS:HE3	2.47	0.44
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.53	0.44
1:B:2387:ARG:O	1:B:2390:ILE:HG22	2.18	0.44
1:B:2276:LEU:HD13	1:B:2417:CYS:SG	2.58	0.44
1:B:2967:ASN:HB3	1:B:3356:PHE:HE2	1.80	0.44
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.50	0.44
1:A:2446:SER:N	1:A:2449:THR:CG2	2.75	0.44
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.00	0.44
1:A:2940:PHE:CE1	1:A:2941:THR:O	2.71	0.44
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	2.00	0.44
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.53	0.44
1:B:3373:LEU:HD13	1:B:3557:LEU:CD1	2.48	0.44
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.18	0.44
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.17	0.44
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.48	0.44
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.53	0.44
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.44
1:B:1540:LEU:HA	1:B:1540:LEU:HD23	1.70	0.44
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.18	0.44
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.99	0.44
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.18	0.43
1:A:1968:PHE:N	1:A:1968:PHE:CD1	2.85	0.43
1:A:2120:LYS:H	1:A:2120:LYS:HG3	1.64	0.43
1:A:2361:ILE:HG22	1:A:2367:SER:O	2.18	0.43
1:B:1512:THR:HG22	1:B:1516:LEU:HD12	1.98	0.43
1:B:1849:GLU:CG	1:B:1899:ASN:ND2	2.81	0.43
1:B:2137:VAL:O	1:B:2141:ILE:CG2	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.99	0.43
1:B:2578:ILE:HG21	1:B:2630:TYR:HB2	1.99	0.43
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.17	0.43
1:B:2420:PRO:HA	3:B:5094:ADP:O2B	2.17	0.43
1:A:2042:GLY:HA3	1:A:2049:MET:CE	2.48	0.43
1:A:2228:HIS:CD2	2:A:5093:ATP:O2'	2.71	0.43
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.18	0.43
1:A:2904:SER:O	1:A:2905:SER:C	2.56	0.43
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.79	0.43
1:B:3024:LEU:HD13	1:B:3303:LYS:HG3	1.96	0.43
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.31	0.43
1:A:1622:GLN:NE2	1:A:1644:ILE:H	2.15	0.43
1:A:1983:LEU:CD2	1:A:1993:THR:CG2	2.88	0.43
1:A:2755:HIS:O	1:A:2913:ILE:N	2.49	0.43
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.48	0.43
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.52	0.43
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.16	0.43
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.17	0.43
1:A:2418:GLY:CA	1:A:2424:LYS:HE3	2.47	0.43
1:A:2391:VAL:CG2	1:A:2430:ASN:OD1	2.65	0.43
1:A:2708:ASN:ND2	1:A:2710:THR:OG1	2.52	0.43
1:B:1849:GLU:CG	1:B:1899:ASN:HD22	2.31	0.43
1:B:2833:THR:HG21	1:B:2841:PRO:CD	2.49	0.43
1:B:2935:VAL:C	1:B:2937:PRO:HD3	2.39	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.99	0.43
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.64	0.43
1:A:1392:LEU:CD1	1:A:1393:LYS:O	2.67	0.43
1:A:1970:LEU:CD1	1:A:1973:LEU:HD11	2.48	0.43
1:A:2064:GLN:OE1	1:A:2091:MET:SD	2.77	0.43
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.52	0.43
1:B:1422:LYS:C	1:B:1425:GLU:CB	2.87	0.43
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.33	0.43
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.53	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.52	0.43
1:A:1620:PHE:HA	1:A:1760:PHE:CE2	2.53	0.43
1:A:2526:ILE:O	1:A:2526:ILE:HG13	2.18	0.43
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.71	0.43
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	2.01	0.43
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.43
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2109:LEU:HD11	1:A:2129:LEU:HD23	1.99	0.43
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.18	0.43
1:A:3436:PHE:HE2	1:A:3462:ILE:HD11	1.82	0.43
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	2.00	0.43
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	2.00	0.43
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.18	0.43
1:B:2745:ILE:HA	1:B:2756:MET:SD	2.58	0.43
1:B:2785:LYS:HE2	1:B:3480:GLU:OE1	2.18	0.43
1:B:3307:LEU:HA	1:B:3310:THR:HB	2.00	0.43
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.38	0.43
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.93	0.43
1:A:1794:PHE:HZ	1:A:1805:THR:CG2	2.31	0.43
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.18	0.43
1:A:2266:PHE:CD1	1:A:2326:LEU:HD21	2.48	0.43
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.33	0.43
1:B:1527:LEU:HD21	1:B:1546:LEU:CD2	2.48	0.43
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.43
1:B:2361:ILE:HG22	1:B:2367:SER:O	2.19	0.43
1:A:2197:ASP:CB	1:A:2549:ARG:HD2	2.45	0.43
1:A:3352:LEU:O	1:A:3356:PHE:HD1	2.02	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.84	0.43
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.48	0.43
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.28	0.43
1:A:1463:LEU:O	1:A:1467:ASN:HB2	2.19	0.43
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.19	0.43
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.18	0.43
1:A:3500:ASP:HA	1:A:3501:PRO:HD3	1.82	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.48	0.43
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.43
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.19	0.42
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	2.00	0.42
1:A:3592:LYS:O	1:A:3596:ASN:N	2.52	0.42
1:B:1416:LYS:CA	1:B:1421:TYR:OH	2.65	0.42
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.19	0.42
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.29	0.42
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.19	0.42
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.49	0.42
1:A:2418:GLY:N	1:A:2424:LYS:HE3	2.34	0.42
1:A:4084:SER:O	1:A:4088:LEU:HG	2.19	0.42
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1976:VAL:HG11	1:B:1998:LEU:HD23	2.01	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:B:3979:ASN:OD1	1:B:3979:ASN:N	2.52	0.42
1:B:4054:GLU:HA	1:B:4055:PRO:HD3	1.90	0.42
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	2.01	0.42
1:A:2395:ILE:H	1:A:2395:ILE:HD12	1.83	0.42
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	2.01	0.42
1:B:1910:GLU:CB	1:B:3846:MET:HB3	2.49	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.99	0.42
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	2.01	0.42
1:A:1660:VAL:HG11	1:A:1728:TRP:CH2	2.54	0.42
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	2.02	0.42
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	2.01	0.42
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.49	0.42
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	2.00	0.42
1:B:2383:HIS:CE1	1:B:2384:GLU:HG3	2.53	0.42
1:B:2788:ARG:H	1:B:3459:ASP:CB	2.32	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.52	0.42
1:A:1540:LEU:CD1	1:A:1548:ILE:HD12	2.50	0.42
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.54	0.42
1:A:3436:PHE:CE2	1:A:3462:ILE:HD11	2.54	0.42
1:A:3832:SER:O	1:A:3836:GLY:N	2.46	0.42
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.85	0.42
1:B:1759:LYS:CD	1:B:1761:GLU:OE2	2.67	0.42
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.53	0.42
1:B:2080:LYS:HG2	2:B:5093:ATP:PB	2.60	0.42
1:B:2380:LEU:HD11	1:B:2390:ILE:HD11	1.97	0.42
1:B:2428:MET:SD	1:B:2429:ASN:N	2.93	0.42
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.48	0.42
1:A:2354:SER:OG	1:A:2357:SER:CA	2.68	0.42
1:A:2385:VAL:HG13	1:A:2386:MET:N	2.33	0.42
1:A:2416:LEU:HB3	1:A:2424:LYS:CD	2.50	0.42
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.39	0.42
1:A:3945:LEU:HD21	1:A:4059:LEU:HD22	2.02	0.42
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	2.02	0.42
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.85	0.42
1:B:2866:LEU:HD12	1:B:2867:LEU:H	1.85	0.42
1:B:3846:MET:HG3	1:B:3847:SER:N	2.34	0.42
1:B:2048:SER:N	2:B:5093:ATP:HN62	2.08	0.42
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.50	0.42
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.55	0.42
1:A:1873:GLN:HE22	1:A:1915:SER:HA	1.84	0.42
1:A:2312:ASP:HB3	1:A:2351:GLN:HG3	2.01	0.42
1:A:3997:LYS:H	1:A:3997:LYS:HG3	1.53	0.42
1:A:4023:ILE:HD11	1:A:4029:ILE:CD1	2.50	0.42
1:B:1742:ASP:HB3	1:B:1745:ASN:HD22	1.85	0.42
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.19	0.42
1:B:2368:PHE:O	1:B:2368:PHE:CD1	2.72	0.42
1:B:2437:LEU:HA	1:B:2480:LYS:HD3	2.02	0.42
1:B:3631:MET:HE1	1:B:3698:MET:HG3	2.00	0.42
1:B:2549:ARG:HG2	2:B:5093:ATP:O1G	2.19	0.42
1:A:1406:LYS:HB3	1:A:1406:LYS:HE2	1.84	0.42
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.20	0.42
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	2.02	0.42
1:A:2324:TYR:CD1	1:A:2403:ILE:HG12	2.55	0.42
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.40	0.42
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.41	0.42
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	2.01	0.42
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.00	0.42
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.42
1:A:2224:SER:O	2:A:5093:ATP:H2	2.03	0.42
1:A:2389:ASP:OD1	1:A:2389:ASP:O	2.37	0.42
1:B:1946:ALA:O	1:B:1950:VAL:HG23	2.20	0.42
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.20	0.42
1:B:2756:MET:O	1:B:2888:VAL:HA	2.20	0.42
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.42
1:A:1635:ASP:HB2	1:A:1638:VAL:HG23	2.02	0.42
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	2.02	0.42
1:A:2134:LEU:HD11	1:A:2138:ASN:ND2	2.34	0.42
1:A:2153:VAL:C	1:A:2154:PHE:HD1	2.24	0.42
1:A:2278:VAL:O	1:A:2283:LYS:HE2	2.19	0.42
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.98	0.42
1:A:3669:THR:HA	1:A:3672:ASP:HB2	2.00	0.42
1:A:3888:LEU:O	1:A:3892:THR:HG22	2.19	0.42
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.50	0.42
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.50	0.42
1:B:1801:GLY:N	5:B:5097:SO4:O3	2.52	0.42
1:B:2081:THR:OG1	2:B:5093:ATP:O2A	2.37	0.42
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.20	0.42
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	2.19	0.42
1:B:2278:VAL:O	1:B:2283:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.55	0.42
1:B:3965:SER:HA	1:B:3968:LEU:HD12	2.02	0.42
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ3	1.84	0.41
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.84	0.41
1:A:1910:GLU:HB2	1:A:3846:MET:HA	2.01	0.41
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.41
1:A:3411:SER:O	1:A:3413:HIS:N	2.50	0.41
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.54	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.41
1:B:1758:TYR:CD1	1:B:1759:LYS:O	2.73	0.41
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.53	0.41
1:B:2627:ARG:NH1	1:B:2630:TYR:CE2	2.87	0.41
1:B:3702:MET:CB	1:B:3767:PHE:HZ	2.32	0.41
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.02	0.41
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	2.02	0.41
1:A:2571:TYR:HD1	1:A:2626:VAL:HG21	1.85	0.41
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.41
1:B:1645:PHE:CZ	1:B:1649:LEU:HD22	2.55	0.41
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.20	0.41
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.54	0.41
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.85	0.41
1:A:1659:LEU:O	1:A:1663:CYS:HB2	2.20	0.41
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.20	0.41
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.02	0.41
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.85	0.41
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.03	0.41
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.55	0.41
1:A:1422:LYS:O	1:A:1425:GLU:HB3	2.21	0.41
1:A:1495:THR:HB	1:A:1498:GLU:CG	2.51	0.41
1:A:1926:SER:HA	1:A:1929:ILE:HD13	2.02	0.41
1:A:2412:ARG:NH1	1:A:2412:ARG:HG3	2.34	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.33	0.41
1:B:1802:LYS:O	1:B:1806:VAL:HG23	2.20	0.41
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.02	0.41
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.85	0.41
1:A:1979:ASN:OD1	1:A:2066:THR:HG21	2.20	0.41
1:A:2098:ALA:O	1:A:2149:ARG:N	2.50	0.41
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.41
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.20	0.41
1:A:2397:THR:HG22	1:A:2398:ILE:HD13	2.03	0.41
1:A:2757:MET:HG2	1:A:2889:PHE:HD2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.21	0.41
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.34	0.41
1:B:2491:LEU:HD21	1:B:2543:ARG:NH1	2.35	0.41
1:B:2786:ILE:H	1:B:2786:ILE:HG13	1.68	0.41
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.50	0.41
1:A:2428:MET:SD	1:A:2429:ASN:N	2.94	0.41
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.41
1:A:3642:TYR:CD1	1:A:3642:TYR:N	2.87	0.41
1:A:4085:THR:O	1:A:4089:LEU:HG	2.21	0.41
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.46	0.41
1:B:2632:ALA:HB3	1:B:2647:LEU:HD21	2.01	0.41
1:B:2757:MET:HB2	1:B:2889:PHE:HB2	2.01	0.41
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	1.76	0.41
1:B:3431:PHE:CE1	1:B:3458:PHE:HD1	2.37	0.41
1:A:1765:ILE:HD13	1:A:1765:ILE:HG21	1.72	0.41
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	2.02	0.41
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41
1:B:2464:TYR:CE1	1:B:2474:LEU:HD12	2.56	0.41
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	2.01	0.41
1:B:2824:GLU:HG2	1:B:2825:THR:H	1.86	0.41
1:B:3901:PRO:HB2	1:B:3906:THR:HG23	2.02	0.41
1:A:2039:LYS:O	1:A:2043:GLN:HG2	2.21	0.41
1:A:2046:GLY:O	1:A:2228:HIS:HB2	2.20	0.41
1:A:2475:PRO:HB3	1:A:2527:GLU:CB	2.50	0.41
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.41
1:A:2765:GLY:HA2	1:A:2768:ILE:HG22	2.02	0.41
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.69	0.41
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.55	0.41
1:B:3850:TRP:NE1	1:B:3854:TYR:CB	2.82	0.41
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	3.04	0.41
1:A:2780:LYS:HB3	1:A:2813:THR:HG22	2.02	0.41
1:A:3331:GLU:HA	1:A:3396:ILE:HG12	2.03	0.41
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.03	0.41
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.82	0.41
1:B:1945:LEU:HD21	1:B:1991:GLU:HB3	2.03	0.41
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.21	0.41
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.21	0.41
1:A:1462:ASN:HB3	1:A:1465:ILE:HG22	2.00	0.41
1:A:2455:LEU:HD21	1:A:2515:PHE:CE2	2.56	0.41
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.02	0.41
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	2.02	0.41
1:B:216:PRO:C	1:B:1365:PHE:CA	2.82	0.41
1:B:2391:VAL:CG2	1:B:2426:MET:HE1	2.49	0.41
1:B:2481:ASN:ND2	1:B:2528:ARG:HB3	2.36	0.41
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.84	0.41
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.21	0.41
1:B:2788:ARG:H	1:B:3459:ASP:HB2	1.86	0.41
1:A:1838:ILE:HG21	1:A:1838:ILE:HD13	1.81	0.41
1:A:2412:ARG:HD2	1:A:2412:ARG:HA	1.86	0.41
1:A:2426:MET:CG	1:A:2427:ILE:N	2.81	0.41
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.50	0.41
1:A:2502:VAL:O	1:A:2505:PHE:HB3	2.20	0.41
1:A:4034:LEU:C	1:A:4034:LEU:HD23	2.41	0.41
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.86	0.41
1:B:2354:SER:OG	1:B:2357:SER:CA	2.68	0.41
1:B:2494:LEU:HD12	1:B:2494:LEU:C	2.41	0.41
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	2.03	0.41
1:A:1817:VAL:HG22	1:A:1844:TRP:CB	2.51	0.40
1:A:2290:LEU:HD23	1:A:2321:SER:HA	2.02	0.40
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	2.03	0.40
1:A:2416:LEU:O	1:A:2534:ALA:HA	2.22	0.40
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.49	0.40
1:B:1547:LYS:O	1:B:1551:SER:HB3	2.21	0.40
1:B:2368:PHE:O	1:B:2369:SER:OG	2.28	0.40
1:B:2637:PRO:HD3	1:B:2703:ASP:HB3	2.03	0.40
1:A:2060:PHE:CZ	1:A:2193:LEU:HD21	2.57	0.40
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.55	0.40
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.35	0.40
1:A:3848:LEU:O	1:A:3849:SER:C	2.59	0.40
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.61	0.40
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	2.02	0.40
1:B:2507:ARG:HG3	1:B:2550:PHE:HA	2.03	0.40
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.61	0.40
1:A:1375:LYS:O	1:A:1379:LYS:HG2	2.21	0.40
1:A:1531:ARG:HD3	1:A:1538:TYR:HA	2.03	0.40
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.22	0.40
1:A:2488:GLU:O	1:A:2491:LEU:HB2	2.21	0.40
1:A:2514:GLY:HA3	1:A:2525:THR:HA	2.03	0.40
1:A:3379:TRP:CD2	1:A:3394:MET:HG3	2.56	0.40
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.21	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.03	0.40
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.02	0.40
1:B:1534:PHE:CD2	1:B:1537:PHE:CE1	3.05	0.40
1:B:2745:ILE:CG1	1:B:2756:MET:HE3	2.43	0.40
1:B:3848:LEU:O	1:B:3849:SER:C	2.59	0.40
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.69	0.40
1:A:1857:VAL:O	1:A:1861:VAL:HG23	2.21	0.40
1:A:23:LEU:C	1:A:25:GLU:N	2.74	0.40
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.56	0.40
1:B:1409:LEU:O	1:B:1413:VAL:HG23	2.22	0.40
1:B:1529:ARG:O	1:B:1533:GLN:HG2	2.21	0.40
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.20	0.40
1:B:1826:PHE:CZ	1:B:1831:LEU:CA	3.04	0.40
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.03	0.40
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	2.03	0.40
1:B:2160:PRO:HA	1:B:2163:VAL:HG22	2.04	0.40
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	2.02	0.40
1:B:3908:LYS:HG2	1:B:4049:LEU:HD13	2.03	0.40
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.86	0.40
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.51	0.40
1:A:1421:TYR:CD2	1:A:1425:GLU:HG2	2.55	0.40
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.22	0.40
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.49	0.40
1:B:2582:VAL:O	1:B:2582:VAL:HG23	2.21	0.40
1:B:3924:TRP:CD1	1:B:3924:TRP:O	2.75	0.40
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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%)	2511 (95%)	118 (4%)	11 (0%)	34	66
1	B	2640/2695 (98%)	2525 (96%)	107 (4%)	8 (0%)	41	71
All	All	5280/5390 (98%)	5036 (95%)	225 (4%)	19 (0%)	34	66

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	A	2495	ASP
1	B	1391	GLY
1	A	2476	LYS
1	A	2728	LEU
1	B	66	GLN
1	A	2519	PRO
1	B	2519	PRO
1	B	2990	GLY
1	B	3914	GLN
1	A	66	GLN
1	A	2990	GLY
1	A	3980	ILE
1	A	2562	PRO
1	B	2562	PRO
1	B	3980	ILE
1	A	3462	ILE
1	B	1470	PRO
1	A	2028	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2218/2453 (90%)	2115 (95%)	103 (5%)	27	58
1	B	2218/2453 (90%)	2145 (97%)	73 (3%)	38	66
All	All	4436/4906 (90%)	4260 (96%)	176 (4%)	31	61

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1421	TYR
1	A	1455	LEU
1	A	1486	ILE
1	A	1493	LEU
1	A	1641	SER
1	A	1719	SER
1	A	1793	CYS
1	A	1794	PHE
1	A	1852	ARG
1	A	1891	HIS
1	A	1923	SER
1	A	1964	ASN
1	A	2081	THR
1	A	2109	LEU
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2202	THR
1	A	2228	HIS
1	A	2229	LEU
1	A	2273	VAL
1	A	2320	ARG
1	A	2351	GLN
1	A	2357	SER
1	A	2387	ARG
1	A	2390	ILE
1	A	2397	THR
1	A	2425	THR
1	A	2428	MET
1	A	2430	ASN
1	A	2472	THR
1	A	2476	LYS
1	A	2482	LEU
1	A	2510	MET
1	A	2522	LYS
1	A	2526	ILE
1	A	2535	CYS
1	A	2547	SER
1	A	2548	GLU
1	A	2563	SER
1	A	2566	SER
1	A	2574	TYR

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Mol	Chain	Res	Type
1	A	2576	LYS
1	A	2613	SER
1	A	2623	THR
1	A	2689	ILE
1	A	2738	MET
1	A	2769	LEU
1	A	2785	LYS
1	A	2822	ILE
1	A	2823	LEU
1	A	2833	THR
1	A	2843	LEU
1	A	2856	LEU
1	A	2863	LEU
1	A	2911	ARG
1	A	2967	ASN
1	A	2979	LYS
1	A	3012	GLU
1	A	3019	VAL
1	A	3301	PHE
1	A	3329	ILE
1	A	3372	THR
1	A	3391	LEU
1	A	3400	SER
1	A	3401	GLN
1	A	3512	ARG
1	A	3543	ARG
1	A	3548	LEU
1	A	3560	LYS
1	A	3567	LEU
1	A	3578	LEU
1	A	3595	MET
1	A	3598	GLU
1	A	3601	LEU
1	A	3618	TYR
1	A	3634	LYS
1	A	3673	GLU
1	A	3677	LEU
1	A	3729	SER
1	A	3737	THR
1	A	3788	MET
1	A	3812	LYS
1	A	3823	ASN

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Mol	Chain	Res	Type
1	A	3831	LYS
1	A	3862	THR
1	A	3871	PHE
1	A	3876	THR
1	A	3884	LEU
1	A	3899	ASP
1	A	3905	ASP
1	A	3906	THR
1	A	3943	THR
1	A	3952	LYS
1	A	3958	ASP
1	A	3960	ASP
1	A	3982	TRP
1	A	3992	ILE
1	A	3997	LYS
1	A	4016	CYS
1	A	4040	GLU
1	A	4042	ARG
1	A	4046	THR
1	B	1383	TYR
1	B	1421	TYR
1	B	1422	LYS
1	B	1426	GLN
1	B	1486	ILE
1	B	1504	ASN
1	B	1646	GLN
1	B	1694	VAL
1	B	1767	GLU
1	B	1794	PHE
1	B	1936	ILE
1	B	2027	THR
1	B	2068	GLN
1	B	2141	ILE
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2351	GLN
1	B	2381	GLU
1	B	2386	MET
1	B	2390	ILE
1	B	2395	ILE
1	B	2428	MET

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Mol	Chain	Res	Type
1	B	2430	ASN
1	B	2474	LEU
1	B	2476	LYS
1	B	2510	MET
1	B	2566	SER
1	B	2574	TYR
1	B	2613	SER
1	B	2616	LEU
1	B	2623	THR
1	B	2681	LEU
1	B	2689	ILE
1	B	2747	ARG
1	B	2829	GLU
1	B	2835	LEU
1	B	2853	LEU
1	B	2856	LEU
1	B	2920	TRP
1	B	2967	ASN
1	B	2969	LEU
1	B	3329	ILE
1	B	3360	TYR
1	B	3372	THR
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3538	ASN
1	B	3548	LEU
1	B	3559	LEU
1	B	3565	ARG
1	B	3567	LEU
1	B	3581	ASP
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3677	LEU
1	B	3729	SER
1	B	3737	THR
1	B	3844	ILE
1	B	3860	GLU
1	B	3871	PHE
1	B	3899	ASP
1	B	3905	ASP

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Mol	Chain	Res	Type
1	B	3906	THR
1	B	3917	THR
1	B	3943	THR
1	B	3960	ASP
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL
1	B	4087	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1605	GLN
1	A	1622	GLN
1	A	1745	ASN
1	A	1864	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1965	HIS
1	A	2064	GLN
1	A	2068	GLN
1	A	2099	ASN
1	A	2138	ASN
1	A	2228	HIS
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2481	ASN
1	A	2530	HIS
1	A	2536	ASN
1	A	2634	ASN
1	A	2688	ASN
1	A	2896	ASN
1	A	2910	ASN
1	A	2927	GLN
1	A	3323	ASN
1	A	3497	HIS
1	A	3521	ASN
1	A	3624	HIS

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Mol	Chain	Res	Type
1	A	3780	ASN
1	A	3842	GLN
1	A	3890	GLN
1	A	4020	ASN
1	A	4077	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1707	HIS
1	B	1736	GLN
1	B	1745	ASN
1	B	1851	ASN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN
1	B	1951	HIS
1	B	2068	GLN
1	B	2228	HIS
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2335	GLN
1	B	2351	GLN
1	B	2383	HIS
1	B	2409	ASN
1	B	2481	ASN
1	B	2536	ASN
1	B	2753	GLN
1	B	2910	ASN
1	B	3308	ASN
1	B	3338	ASN
1	B	3471	ASN
1	B	3497	HIS
1	B	3521	ASN
1	B	3542	GLN
1	B	3624	HIS
1	B	3685	GLN
1	B	3780	ASN
1	B	3783	ASN
1	B	3890	GLN
1	B	3962	GLN
1	B	3970	ASN

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Mol	Chain	Res	Type
1	B	4020	ASN
1	B	4031	GLN
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 carbohydrates 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	$\# Z > 2$
5	SO4	B	5096	-	4,4,4	0.93	0	6,6,6	1.19	0
5	SO4	A	5096	-	4,4,4	1.03	1 (25%)	6,6,6	1.46	1 (16%)
2	ATP	B	5093	4	26,33,33	1.05	2 (7%)	31,52,52	1.64	5 (16%)
5	SO4	B	5097	-	4,4,4	0.38	0	6,6,6	0.43	0
5	SO4	A	5097	-	4,4,4	0.37	0	6,6,6	0.59	0
2	ATP	A	5093	4	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
3	ADP	B	5094	-	24,29,29	1.26	2 (8%)	29,45,45	1.67	5 (17%)
3	ADP	A	5094	-	24,29,29	1.15	1 (4%)	29,45,45	1.62	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5093	4	-	6/18/38/38	0/3/3/3
2	ATP	B	5093	4	-	4/18/38/38	0/3/3/3
3	ADP	B	5094	-	-	5/12/32/32	0/3/3/3
3	ADP	A	5094	-	-	7/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ADP	C5-C4	2.96	1.48	1.40
3	A	5094	ADP	C5-C4	2.95	1.48	1.40
2	B	5093	ATP	C5-C4	2.75	1.48	1.40
3	B	5094	ADP	C4-N3	2.70	1.39	1.35
2	A	5093	ATP	C5-C4	2.50	1.47	1.40
2	B	5093	ATP	C2-N3	2.13	1.35	1.32
5	A	5096	SO4	O1-S	2.04	1.57	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ADP	N3-C2-N1	-4.82	121.14	128.68
3	B	5094	ADP	N3-C2-N1	-4.44	121.73	128.68
3	B	5094	ADP	C3'-C2'-C1'	4.05	107.07	100.98
2	B	5093	ATP	C3'-C2'-C1'	3.77	106.65	100.98
2	B	5093	ATP	PA-O3A-PB	-3.61	120.43	132.83
2	B	5093	ATP	PB-O3B-PG	-3.60	120.47	132.83
2	A	5093	ATP	PA-O3A-PB	-3.59	120.51	132.83
2	A	5093	ATP	PB-O3B-PG	-3.58	120.53	132.83
2	A	5093	ATP	C3'-C2'-C1'	3.53	106.29	100.98
2	B	5093	ATP	C4-C5-N7	-3.16	106.11	109.40
2	A	5093	ATP	N3-C2-N1	-3.14	123.77	128.68
3	A	5094	ADP	PA-O3A-PB	-3.08	122.24	132.83
3	A	5094	ADP	C2-N1-C6	3.01	123.91	118.75
3	B	5094	ADP	PA-O3A-PB	-2.94	122.74	132.83
2	A	5093	ATP	C4-C5-N7	-2.68	106.60	109.40
3	B	5094	ADP	C5'-C4'-C3'	-2.65	105.26	115.18
2	B	5093	ATP	N3-C2-N1	-2.61	124.60	128.68
3	A	5094	ADP	C2'-C3'-C4'	2.60	107.69	102.64
5	A	5096	SO4	O4-S-O1	2.41	121.86	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5094	ADP	C2-N1-C6	2.36	122.80	118.75
3	A	5094	ADP	C3'-C2'-C1'	2.28	104.41	100.98

There are no chirality outliers.

All (22) torsion outliers are listed below:

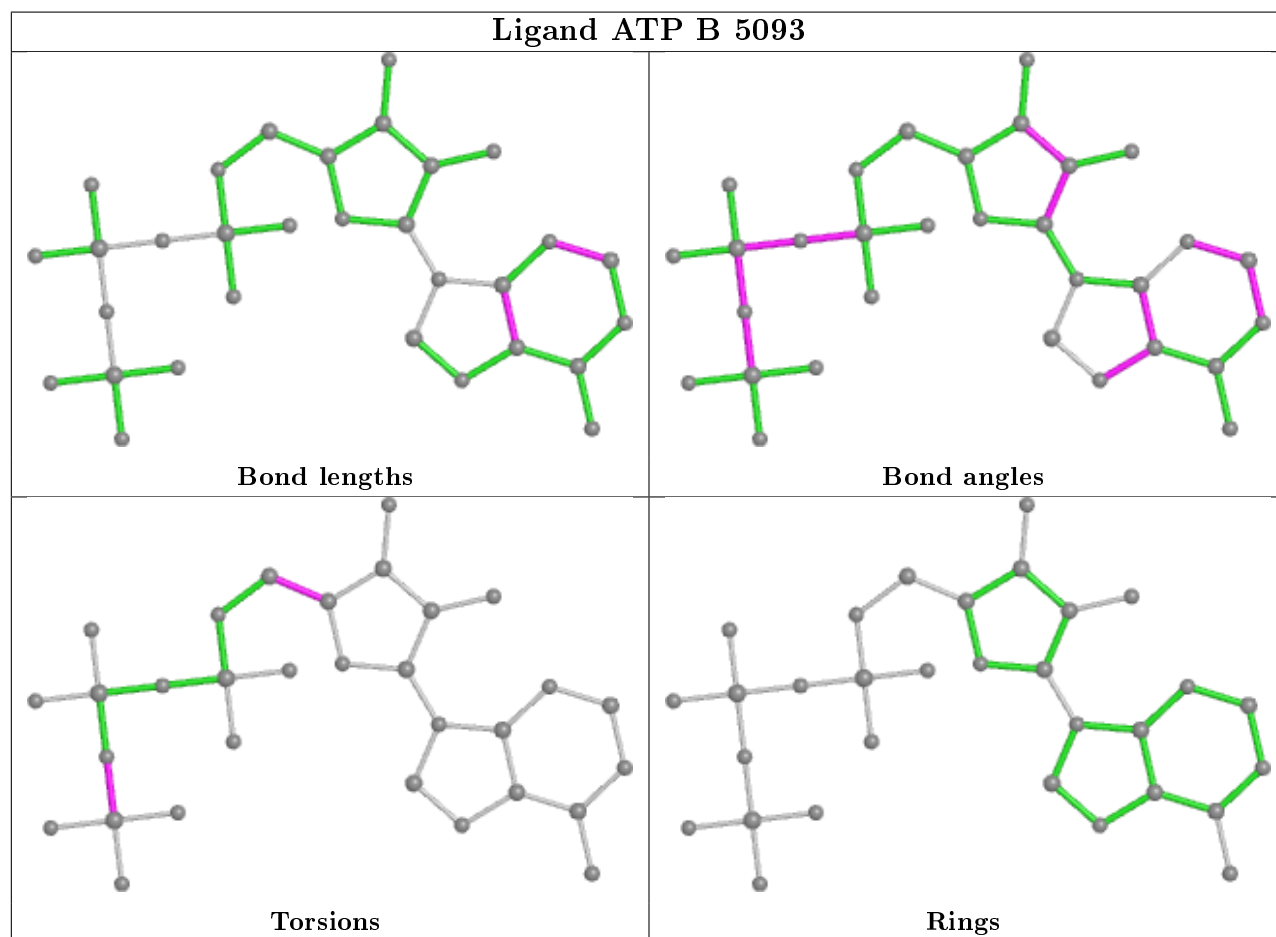
Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	PB-O3B-PG-O2G
2	B	5093	ATP	PB-O3B-PG-O3G
2	A	5093	ATP	C5'-O5'-PA-O1A
3	B	5094	ADP	C5'-O5'-PA-O1A
3	B	5094	ADP	C3'-C4'-C5'-O5'
3	A	5094	ADP	C5'-O5'-PA-O1A
2	B	5093	ATP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C3'-C4'-C5'-O5'
2	A	5093	ATP	O4'-C4'-C5'-O5'
2	A	5093	ATP	C3'-C4'-C5'-O5'
3	A	5094	ADP	O4'-C4'-C5'-O5'
3	A	5094	ADP	C3'-C4'-C5'-O5'
3	B	5094	ADP	O4'-C4'-C5'-O5'
3	B	5094	ADP	C4'-C5'-O5'-PA
2	A	5093	ATP	C5'-O5'-PA-O3A
3	A	5094	ADP	C5'-O5'-PA-O3A
2	A	5093	ATP	PA-O3A-PB-O1B
3	A	5094	ADP	PB-O3A-PA-O2A
3	A	5094	ADP	PB-O3A-PA-O1A
3	B	5094	ADP	C5'-O5'-PA-O3A
2	A	5093	ATP	PA-O3A-PB-O2B
3	A	5094	ADP	C5'-O5'-PA-O2A

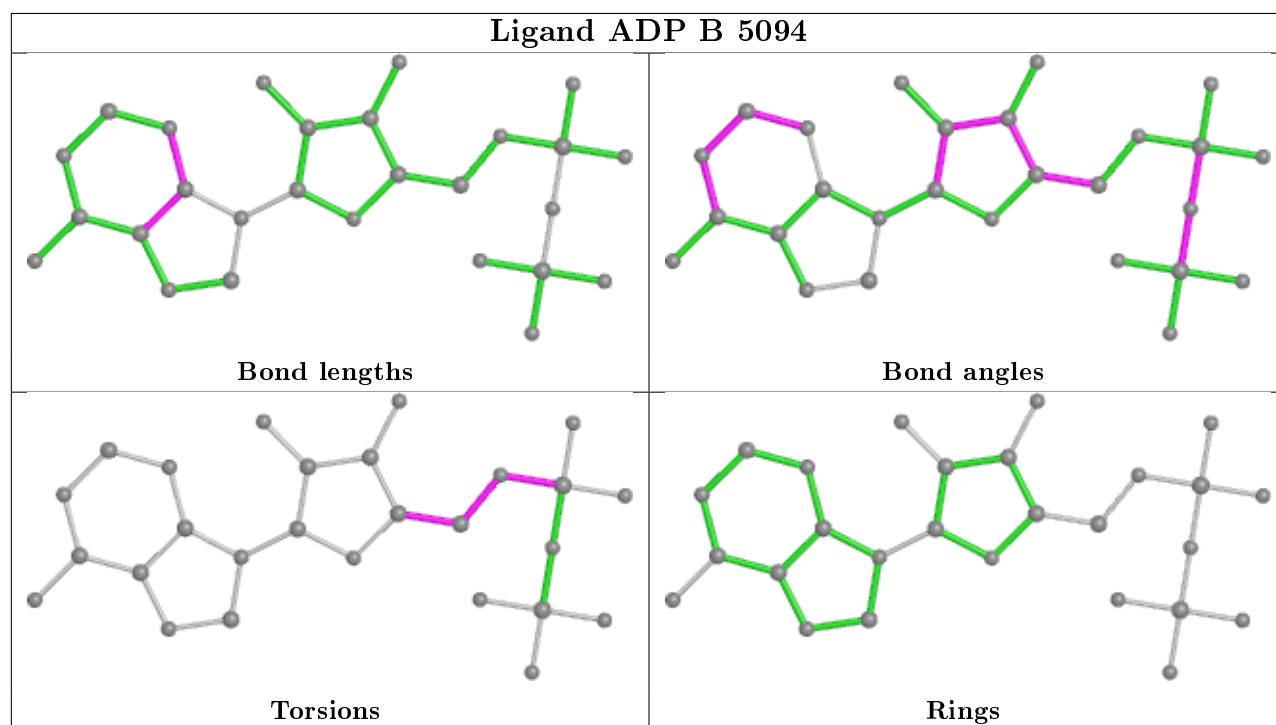
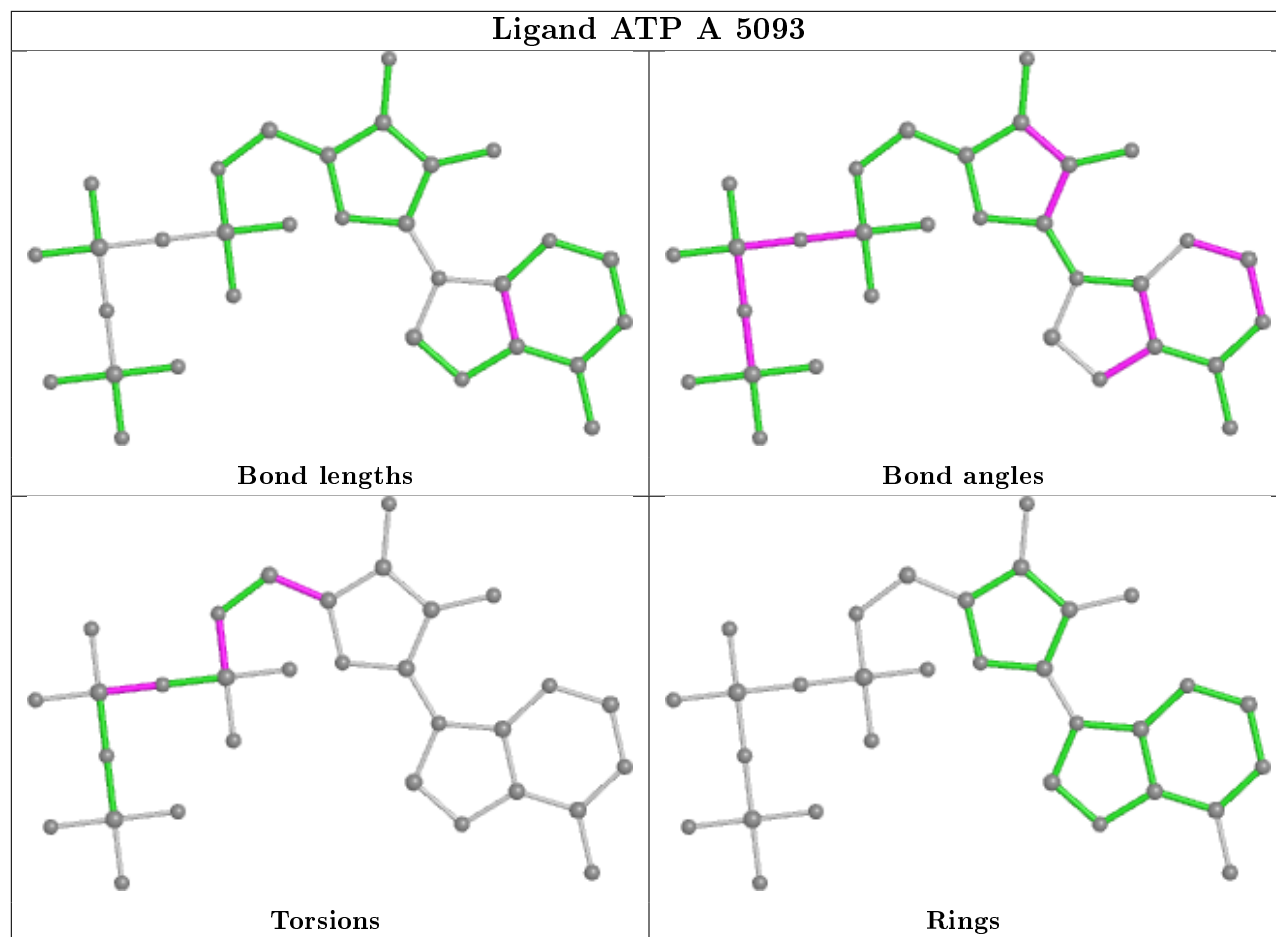
There are no ring outliers.

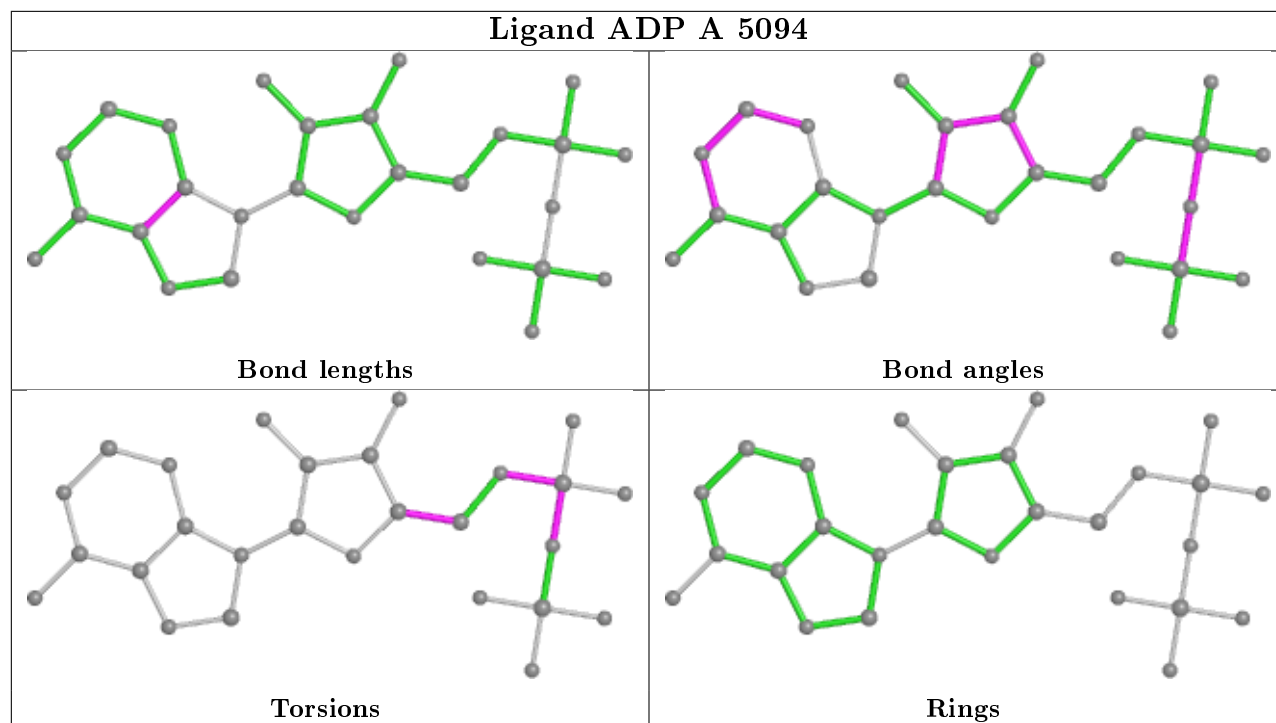
7 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5096	SO4	2	0
2	B	5093	ATP	24	0
5	B	5097	SO4	2	0
5	A	5097	SO4	2	0
2	A	5093	ATP	10	0
3	B	5094	ADP	6	0
3	A	5094	ADP	2	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

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

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.18	139 (5%) 27 25	62, 134, 265, 480	1 (0%)
1	B	2650/2695 (98%)	0.66	323 (12%) 4 3	83, 185, 334, 500	1 (0%)
All	All	5300/5390 (98%)	0.42	462 (8%) 10 10	62, 158, 303, 500	2 (0%)

All (462) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	20.3
1	B	69	ALA	17.4
1	B	59	ASP	17.2
1	B	31	LEU	16.8
1	B	60	GLY	15.0
1	B	70	ILE	14.7
1	B	52	PRO	14.7
1	B	46	GLU	14.7
1	B	1572	ILE	13.8
1	B	94	LEU	13.8
1	B	18	LEU	13.4
1	B	1549	ILE	13.4
1	B	61	ASP	13.0
1	B	58	ILE	12.2
1	B	47	LEU	11.9
1	B	1550	GLY	11.4
1	B	87	GLU	10.9
1	B	71	ILE	10.6
1	B	95	GLU	10.5
1	A	147	VAL	10.3
1	A	2	PRO	10.1
1	A	20	LEU	9.8
1	B	30	HIS	9.6
1	B	1581	GLY	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	63	LYS	9.1
1	B	1592	LEU	9.0
1	B	2	PRO	8.8
1	B	1582	VAL	8.8
1	B	8	LYS	8.7
1	B	1459	LEU	8.4
1	B	1596	ILE	8.3
1	B	1680	ILE	8.1
1	B	1546	LEU	8.1
1	B	27	TYR	8.1
1	A	148	THR	8.0
1	B	17	ARG	8.0
1	B	1669	PHE	8.0
1	A	216	PRO	7.9
1	B	19	LEU	7.9
1	B	149	HIS	7.8
1	B	184	ALA	7.8
1	B	1452	TRP	7.7
1	B	1683	LEU	7.7
1	B	199	ALA	7.6
1	B	155	TYR	7.4
1	B	186	PRO	7.4
1	B	3915	PHE	7.4
1	B	1845	GLY	7.2
1	B	63	LYS	7.2
1	B	79	ASN	7.2
1	B	1602	ILE	7.2
1	B	151	ASP	7.1
1	B	148	THR	7.1
1	B	55	PRO	6.8
1	A	74	ILE	6.7
1	B	16	THR	6.7
1	B	1394	LEU	6.7
1	B	49	LEU	6.7
1	A	76	ASP	6.6
1	B	45	PHE	6.6
1	B	1483	TYR	6.6
1	B	86	LYS	6.6
1	A	71	ILE	6.4
1	A	1	SER	6.3
1	A	1483	TYR	6.3
1	A	84	CYS	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	1601	SER	6.3
1	B	1684	LEU	6.3
1	B	1574	PHE	6.3
1	B	73	TYR	6.2
1	B	193	LYS	6.2
1	B	88	ARG	6.1
1	B	96	GLY	6.1
1	B	1647	ALA	6.1
1	A	27	TYR	6.0
1	A	54	LEU	6.0
1	B	1603	GLN	6.0
1	B	3919	LYS	6.0
1	B	44	LYS	5.9
1	B	78	HIS	5.8
1	B	72	ARG	5.8
1	B	1579	ILE	5.8
1	B	91	ILE	5.8
1	B	62	VAL	5.8
1	B	202	LEU	5.8
1	A	59	ASP	5.8
1	A	135	ARG	5.7
1	B	93	MET	5.7
1	B	1460	GLY	5.7
1	B	187	GLN	5.6
1	B	1456	TYR	5.6
1	B	67	SER	5.6
1	B	3580	ASN	5.5
1	B	92	SER	5.5
1	A	73	TYR	5.5
1	B	84	CYS	5.3
1	B	1545	LEU	5.2
1	B	134	ASP	5.2
1	B	7	TRP	5.1
1	B	1573	ILE	5.1
1	B	85	PRO	5.0
1	B	161	VAL	5.0
1	B	43	LYS	5.0
1	B	1644	ILE	5.0
1	B	28	GLU	5.0
1	B	54	LEU	5.0
1	B	143	ASN	5.0
1	B	42	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	1730	LYS	5.0
1	B	1894	VAL	4.9
1	A	23	LEU	4.9
1	B	80	MET	4.9
1	B	1760	PHE	4.9
1	B	1551	SER	4.9
1	B	26	LYS	4.8
1	B	1606	GLU	4.8
1	A	3575	GLY	4.8
1	B	1476	PHE	4.7
1	B	1458	ILE	4.7
1	B	3916	PHE	4.7
1	B	1590	LEU	4.7
1	B	1679	LYS	4.7
1	B	1937	MET	4.7
1	B	1767	GLU	4.7
1	B	1497	ILE	4.6
1	A	48	GLY	4.6
1	B	1580	THR	4.6
1	B	3304	GLU	4.6
1	B	3566	LEU	4.6
1	B	3555	TYR	4.6
1	B	210	GLY	4.5
1	B	2353	LEU	4.5
1	B	89	ALA	4.5
1	B	1492	GLN	4.5
1	B	3588	ASN	4.5
1	B	216	PRO	4.4
1	A	61	ASP	4.4
1	B	1605	GLN	4.4
1	A	62	VAL	4.4
1	A	83	GLY	4.4
1	B	64	LEU	4.3
1	A	3567	LEU	4.3
1	B	183	GLU	4.3
1	A	77	LYS	4.3
1	B	25	GLU	4.3
1	B	1505	PHE	4.2
1	B	1506	ASP	4.2
1	A	3566	LEU	4.2
1	B	3572	ASN	4.2
1	B	32	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	20	LEU	4.1
1	B	74	ILE	4.1
1	B	150	PRO	4.1
1	A	3568	GLU	4.1
1	B	1682	GLY	4.0
1	A	81	LEU	4.0
1	A	143	ASN	4.0
1	A	151	ASP	4.0
1	A	25	GLU	4.0
1	B	66	GLN	3.9
1	B	1445	TRP	3.9
1	B	1675	GLU	3.9
1	B	1792	GLY	3.9
1	B	2938	MET	3.9
1	B	75	ALA	3.9
1	B	1465	ILE	3.9
1	A	142	LEU	3.9
1	B	3585	VAL	3.9
1	A	19	LEU	3.8
1	A	88	ARG	3.8
1	B	2363	ASN	3.8
1	B	198	ILE	3.8
1	B	48	GLY	3.8
1	B	1486	ILE	3.8
1	B	192	LEU	3.8
1	B	3571	ASN	3.8
1	B	152	PHE	3.8
1	B	3734	PRO	3.8
1	A	75	ALA	3.7
1	A	184	ALA	3.7
1	B	215	PRO	3.7
1	B	3934	TRP	3.6
1	A	2364	ASP	3.6
1	B	138	HIS	3.6
1	A	3580	ASN	3.6
1	B	1893	ALA	3.6
1	B	24	GLU	3.6
1	A	91	ILE	3.6
1	B	1395	VAL	3.6
1	A	85	PRO	3.6
1	B	1594	GLU	3.6
1	B	50	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	68	MET	3.5
1	B	5	GLY	3.5
1	A	3555	TYR	3.5
1	B	1595	LYS	3.5
1	B	2121	ALA	3.5
1	A	132	PHE	3.5
1	B	1604	ALA	3.5
1	A	80	MET	3.5
1	B	1676	VAL	3.5
1	B	51	PHE	3.5
1	A	3564	LYS	3.4
1	B	53	ASN	3.4
1	B	1566	PHE	3.4
1	B	201	PRO	3.4
1	B	1835	LEU	3.4
1	B	1994	VAL	3.4
1	B	209	PHE	3.3
1	B	1562	MET	3.3
1	A	67	SER	3.3
1	B	133	GLU	3.3
1	B	1472	GLU	3.3
1	B	1532	ARG	3.3
1	B	1711	VAL	3.3
1	B	1732	GLN	3.3
1	B	3020	GLY	3.3
1	A	2029	LEU	3.3
1	B	1489	ARG	3.2
1	A	35	ASP	3.2
1	A	18	LEU	3.2
1	B	1423	ILE	3.2
1	B	200	TRP	3.2
1	B	6	TYR	3.2
1	A	22	TYR	3.1
1	A	82	GLY	3.1
1	B	3920	ILE	3.1
1	B	3811	LEU	3.1
1	B	1608	LEU	3.1
1	A	2676	THR	3.1
1	A	55	PRO	3.1
1	A	1458	ILE	3.1
1	B	1737	LYS	3.1
1	B	1828	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	3583	LEU	3.1
1	B	162	LEU	3.1
1	B	3024	LEU	3.0
1	B	1591	ASN	3.0
1	A	68	MET	3.0
1	A	2470	GLY	3.0
1	B	2863	LEU	3.0
1	A	3418	ILE	3.0
1	B	170	ASP	3.0
1	B	1552	GLY	3.0
1	B	189	ASP	3.0
1	B	1487	THR	3.0
1	A	145	ASP	3.0
1	A	1445	TRP	3.0
1	B	3301	PHE	3.0
1	B	194	SER	2.9
1	A	3	ILE	2.9
1	A	52	PRO	2.9
1	B	3694	PHE	2.9
1	B	3300	THR	2.9
1	B	83	GLY	2.9
1	B	2058	MET	2.9
1	A	146	HIS	2.9
1	A	2361	ILE	2.9
1	B	1705	TYR	2.9
1	A	3865	ALA	2.9
1	B	1490	ALA	2.9
1	B	2364	ASP	2.9
1	B	1479	LEU	2.9
1	B	2370	SER	2.8
1	B	3866	GLU	2.8
1	B	2856	LEU	2.8
1	A	2302	PHE	2.8
1	B	135	ARG	2.8
1	A	26	LYS	2.8
1	B	2064	GLN	2.8
1	A	138	HIS	2.8
1	A	130	LYS	2.8
1	A	3301	PHE	2.8
1	B	159	ASP	2.8
1	A	34	ARG	2.8
1	B	76	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	40	TRP	2.8
1	B	3590	LEU	2.8
1	B	1424	PHE	2.8
1	B	1583	ARG	2.8
1	B	56	TYR	2.8
1	A	2940	PHE	2.8
1	B	1768	ARG	2.8
1	B	1762	TYR	2.8
1	B	2025	ALA	2.8
1	B	2179	PRO	2.8
1	B	1734	PHE	2.8
1	A	2757	MET	2.8
1	B	164	MET	2.8
1	A	3300	THR	2.8
1	B	211	GLY	2.8
1	B	3846	MET	2.8
1	B	3726	LEU	2.7
1	A	3923	VAL	2.7
1	B	1593	ASN	2.7
1	A	58	ILE	2.7
1	B	15	PRO	2.7
1	B	1401	LEU	2.7
1	A	1597	GLU	2.7
1	A	2064	GLN	2.7
1	B	1672	TYR	2.7
1	A	1719	SER	2.7
1	B	2844	PHE	2.7
1	A	9	ILE	2.7
1	A	1382	GLN	2.7
1	B	35	ASP	2.7
1	B	1739	ASP	2.7
1	A	3021	LEU	2.7
1	B	190	LYS	2.7
1	B	3735	LYS	2.7
1	B	3768	PHE	2.7
1	B	4023	ILE	2.7
1	A	3617	GLU	2.7
1	B	206	GLN	2.7
1	A	87	GLU	2.7
1	B	2241	LEU	2.6
1	B	1421	TYR	2.6
1	A	21	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	3561	ASN	2.6
1	A	3589	ASN	2.6
1	B	207	ALA	2.6
1	A	30	HIS	2.6
1	A	37	GLY	2.6
1	B	1881	LEU	2.6
1	B	145	ASP	2.6
1	B	3618	TYR	2.6
1	B	1715	LEU	2.6
1	B	4088	LEU	2.6
1	B	81	LEU	2.6
1	B	3654	LYS	2.6
1	B	3656	VAL	2.6
1	A	3025	ASN	2.6
1	A	16	THR	2.6
1	B	9	ILE	2.6
1	B	3451	ILE	2.6
1	A	2310	LEU	2.5
1	B	1991	GLU	2.5
1	B	41	ARG	2.5
1	A	3582	GLU	2.5
1	A	141	TYR	2.5
1	B	1493	LEU	2.5
1	A	38	ASP	2.5
1	B	1383	TYR	2.5
1	B	3586	THR	2.5
1	B	3591	LYS	2.5
1	B	3845	GLN	2.5
1	B	1740	THR	2.5
1	B	1547	LYS	2.5
1	B	204	GLY	2.5
1	B	3573	SER	2.5
1	B	3356	PHE	2.5
1	B	3533	THR	2.5
1	B	3589	ASN	2.5
1	A	4034	LEU	2.5
1	B	1650	LEU	2.5
1	A	134	ASP	2.5
1	A	3020	GLY	2.4
1	A	3586	THR	2.4
1	A	3581	ASP	2.4
1	A	3563	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	2.4
1	A	2363	ASN	2.4
1	B	2022	PHE	2.4
1	A	2942	ASP	2.4
1	B	160	VAL	2.4
1	B	2684	GLN	2.4
1	B	3865	ALA	2.4
1	B	23	LEU	2.4
1	A	3305	ARG	2.4
1	B	203	GLN	2.4
1	B	1513	ILE	2.4
1	B	1548	ILE	2.4
1	B	1482	GLU	2.3
1	A	1465	ILE	2.3
1	B	1771	TYR	2.3
1	B	3856	HIS	2.3
1	A	3584	MET	2.3
1	B	57	TYR	2.3
1	A	2941	THR	2.3
1	A	70	ILE	2.3
1	B	2669	PHE	2.3
1	B	1905	ARG	2.3
1	B	4092	MET	2.3
1	B	185	ILE	2.3
1	B	3945	LEU	2.3
1	B	90	GLU	2.3
1	A	3870	LYS	2.3
1	B	3994	TYR	2.3
1	B	1509	LEU	2.3
1	A	42	ASN	2.3
1	B	1420	TYR	2.3
1	B	3980	ILE	2.3
1	A	1459	LEU	2.3
1	A	1389	SER	2.3
1	A	1452	TRP	2.2
1	B	1933	ILE	2.2
1	A	36	GLU	2.2
1	A	1598	LEU	2.2
1	A	1945	LEU	2.2
1	B	1415	MET	2.2
1	B	2125	TRP	2.2
1	A	136	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1394	LEU	2.2
1	B	1673	TRP	2.2
1	B	1882	LEU	2.2
1	B	2808	LEU	2.2
1	B	1558	VAL	2.2
1	B	1426	GLN	2.2
1	B	1649	LEU	2.2
1	B	3706	TYR	2.2
1	A	3299	LEU	2.2
1	B	3841	LEU	2.2
1	A	1548	ILE	2.2
1	B	10	LYS	2.2
1	B	137	CYS	2.2
1	A	3593	GLU	2.2
1	A	3019	VAL	2.2
1	B	1588	GLU	2.2
1	A	5	GLY	2.2
1	B	1686	LYS	2.2
1	B	2024	SER	2.2
1	A	3915	PHE	2.2
1	B	3985	VAL	2.2
1	A	40	TRP	2.1
1	A	3026	GLU	2.1
1	B	98	VAL	2.1
1	B	3923	VAL	2.1
1	B	4029	ILE	2.1
1	A	1395	VAL	2.1
1	B	1503	PRO	2.1
1	A	3576	ASN	2.1
1	B	3565	ARG	2.1
1	B	33	GLU	2.1
1	A	2024	SER	2.1
1	A	3419	SER	2.1
1	B	4	LEU	2.1
1	B	1455	LEU	2.1
1	B	3597	ILE	2.1
1	B	29	GLU	2.1
1	A	3588	ASN	2.1
1	B	65	THR	2.1
1	B	3834	ILE	2.1
1	B	3494	LEU	2.1
1	B	2030	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLU	2.1
1	A	2852	LEU	2.1
1	B	1827	ASP	2.1
1	A	164	MET	2.1
1	A	3027	SER	2.1
1	B	3369	TYR	2.1
1	A	2916	TRP	2.0
1	B	3958	ASP	2.0
1	B	1504	ASN	2.0
1	B	1698	ILE	2.0
1	B	3874	PHE	2.0
1	A	3579	GLU	2.0
1	B	1569	ILE	2.0
1	A	2732	MET	2.0
1	A	53	ASN	2.0
1	B	1864	ASN	2.0
1	B	14	GLN	2.0
1	B	2000	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

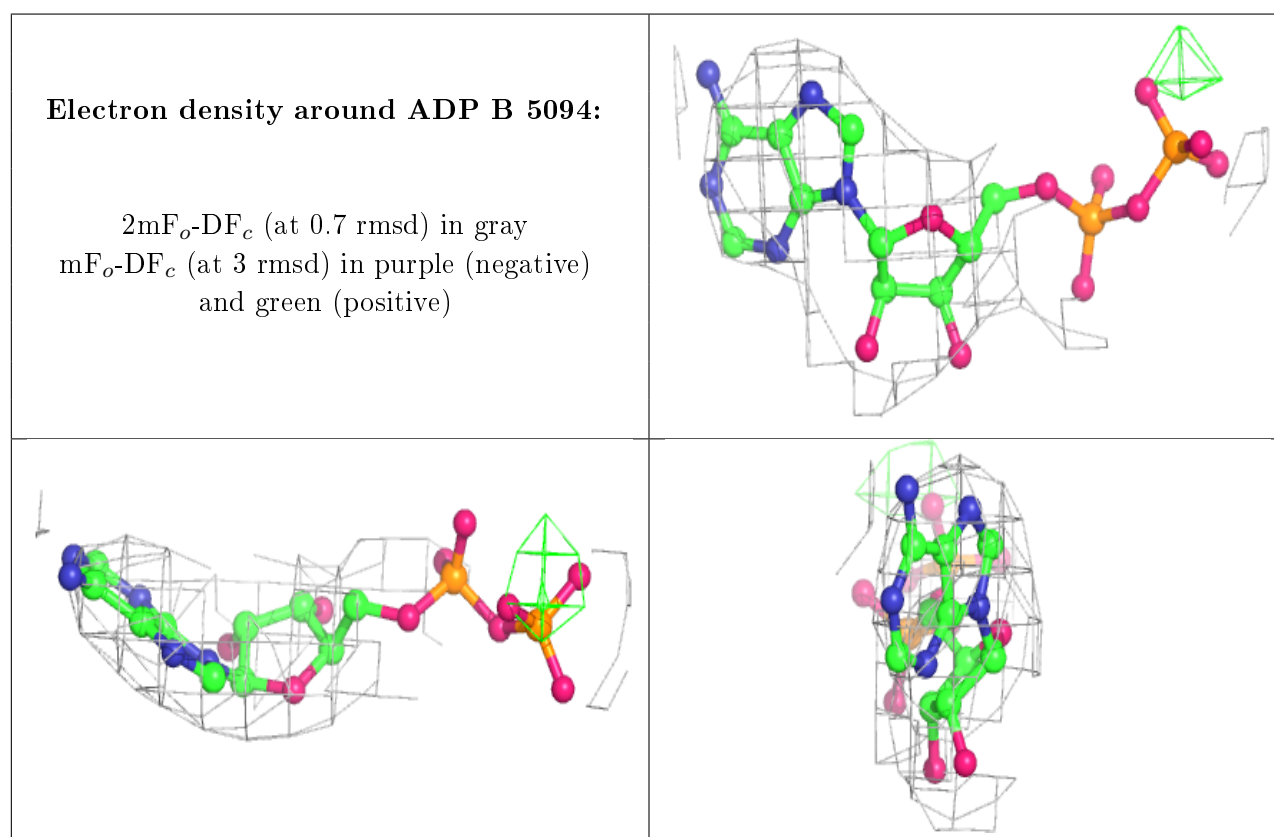
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	B	5096	5/5	0.87	0.53	86,103,146,179	0
4	MG	A	5095	1/1	0.89	0.40	76,76,76,76	0
3	ADP	B	5094	27/27	0.90	0.27	81,114,155,168	0
2	ATP	B	5093	31/31	0.92	0.26	93,138,174,217	0
5	SO4	A	5096	5/5	0.92	0.45	77,106,130,132	0

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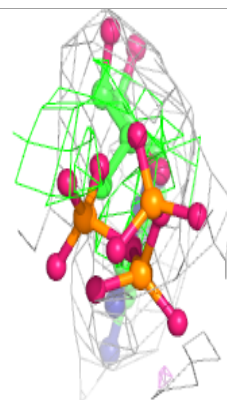
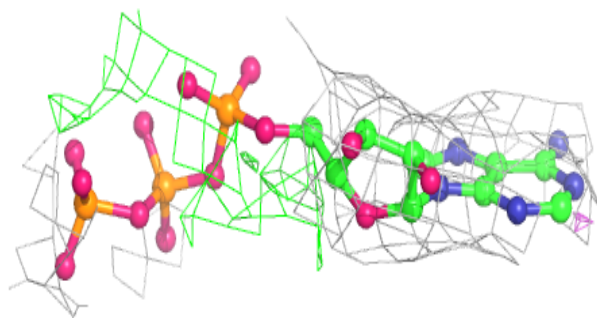
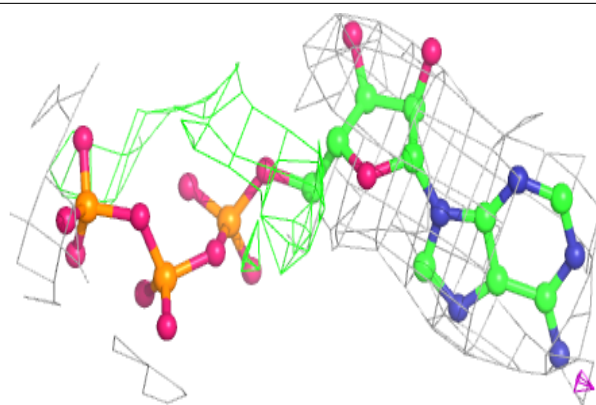
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	A	5093	31/31	0.93	0.29	78,92,129,144	0
3	ADP	A	5094	27/27	0.94	0.25	91,101,113,131	0
4	MG	B	5095	1/1	0.97	0.34	86,86,86,86	0
5	SO4	B	5097	5/5	0.97	0.17	157,162,176,183	0
5	SO4	A	5097	5/5	0.97	0.22	82,93,104,115	0

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

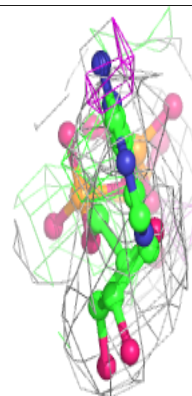
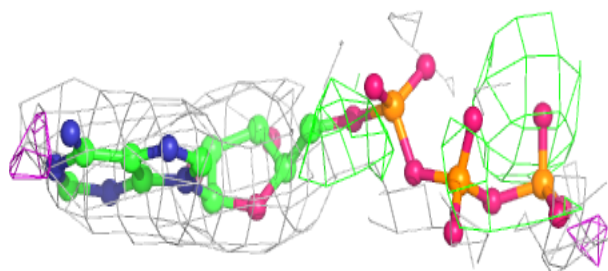
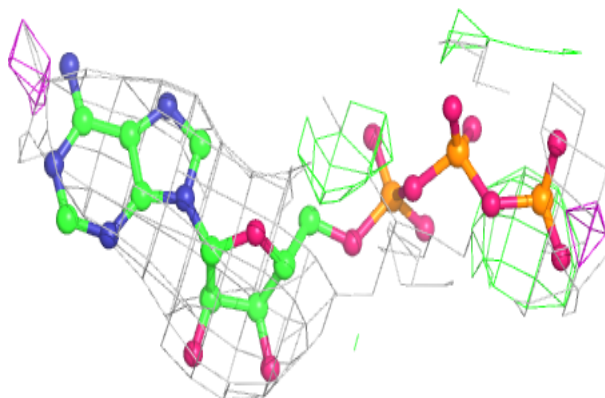


Electron density around ATP B 5093:

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

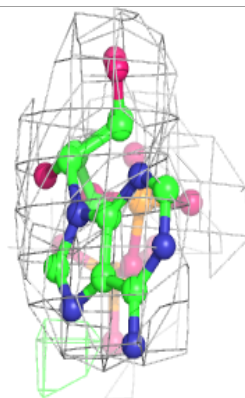
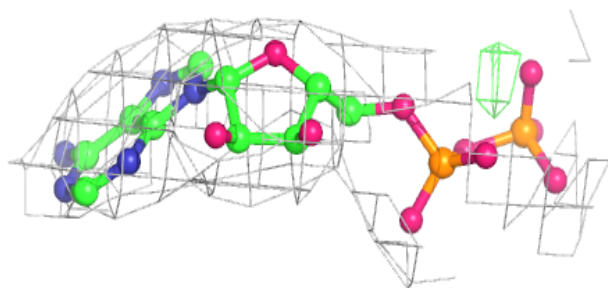
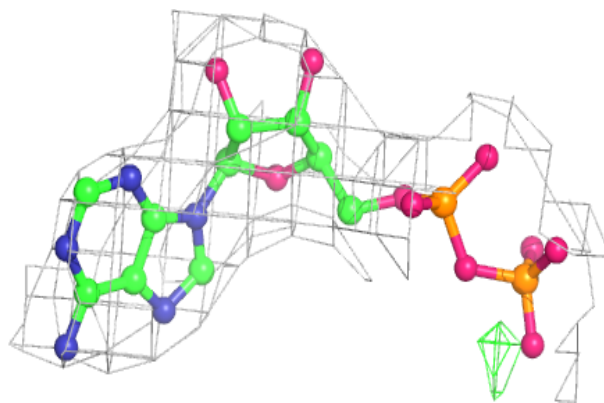
**Electron density around ATP A 5093:**

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



Electron density around ADP A 5094:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.