



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:53 pm BST

PDB ID : 4RH7  
Title : Crystal structure of human cytoplasmic dynein 2 motor domain in complex with ADP.Vi  
Authors : Schmidt, H.; Zalyte, R.; Urnavicius, L.; Carter, A.P.  
Deposited on : 2014-10-01  
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

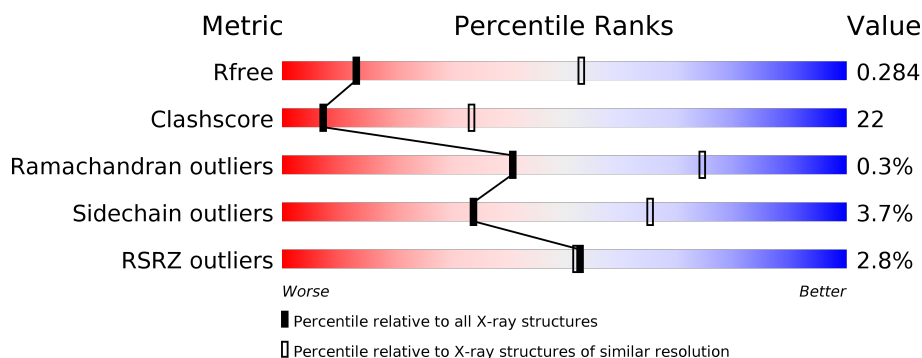
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	3450	<div> <div>2%</div> <div>59%</div> <div>27%</div> <div>• 13%</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	AOV	A	4401	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22816 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.

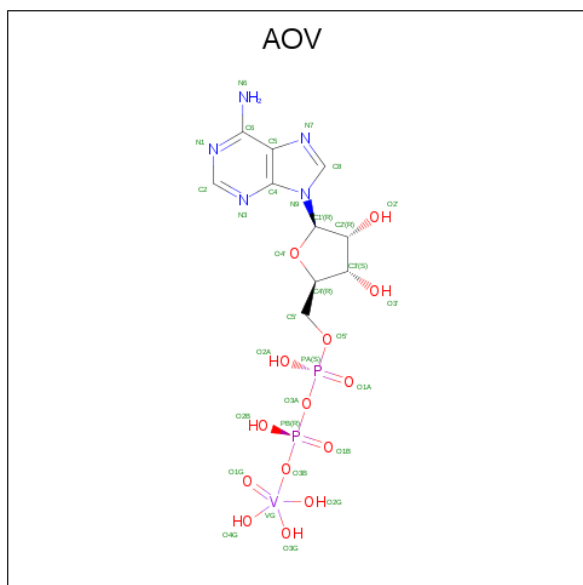
- Molecule 1 is a protein called Green fluorescent protein/Cytoplasmic dynein 2 heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	3005	22697	14414	3922	4263	98	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	GLY	-	LINKER	UNP Q8NCM8
A	1090	SER	-	LINKER	UNP Q8NCM8
A	1413	ARG	LYS	VARIANT	UNP Q8NCM8
A	2871	GLN	ARG	VARIANT	UNP Q8NCM8
A	3680	VAL	ALA	VARIANT	UNP Q8NCM8
A	4308	VAL	-	EXPRESSION TAG	UNP Q8NCM8

- Molecule 2 is ADP ORTHOVANADATE (three-letter code: AOV) (formula:  $C_{10}H_{17}N_5O_{14}P_2V$ ).

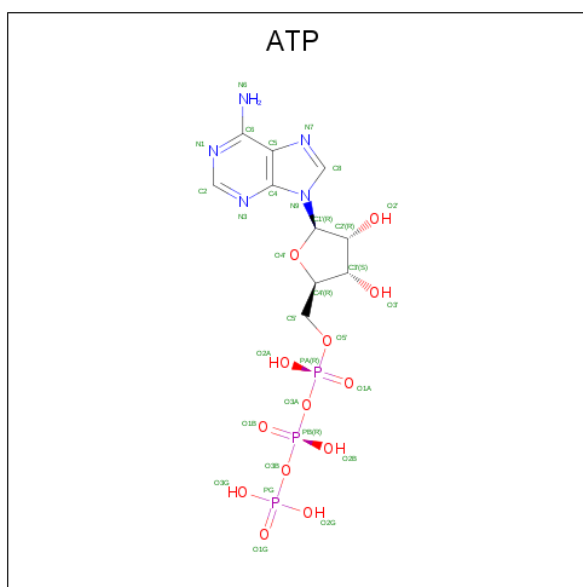


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	
			32	10	5	14	2	1	
									0
									0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg		
			2	2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

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



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



S3136	V2943	LYS	L2723	A2531	S2429	V2346	D2243	V2163	S2049	L1939	H1819	S1723
V3137	Q2944	GLU	L2723	R2532	I2430	R2347	L2249	V2164	S2050	L1939	H1820	S1723
G3138	D2945	GLU	L2626	R2533	I2431	P2348	L2249	E2165	W2051	L1943	D1821	F1728
Q3139	A2946	LYS	L2730	L2534	Y2432	P2348	D2253	T2166	I2052	K1944	N1822	V1729
S2947	S2947	LYS	L2739	R2535	R2435	C2351	E2255	S2167	D2055	I1955	E1823	G1730
E2948	Q2948	ASN	L2744	R2536	I2441	R2352	S2255	L2168	E2064	I1956	L1824	L1731
Q2949	Q2949	SER	E2745	E2544	Y2442	R2353	N2256	V2169	E2065	P1956	L1825	V1732
K2950	T2951	LYS	E2746	L2545	G2443	L2354	G2257	G2170	S2065	A1962	V1828	W1737
L2951	L2952	D2848	P2746	F2548	G2444	L2356	L2258	V2172	L2066	L1963	I1829	G1738
L2953	L2953	P2849	P2750	D2549	L2445	L2357	Q2264	N2174	N2067	L1964	F1740	F1739
L2956	L2956	D2850	L2749	L2550	L2446	L2358	Q2264	G2175	L2070	L1965	S1832	D1741
L2957	L2957	R2851	P2764	Q2557	Y2448	L2359	P2261	E2178	D2071	H1973	F1835	E1742
L2958	L2958	L2852	E2746	L2552	P2449	L2360	P2266	D2173	D2072	I1977	F1849	F1743
L2959	L2959	L2853	F2765	L2553	L2450	L2361	P2266	E2185	R2074	P1980	L1855	R1745
L2960	L2960	L2854	N2766	Q2557	L2451	L2362	Q2269	E2187	L2075	S1981	L1746	L1746
L2961	L2961	L2855	Y2767	W2560	N2453	L2363	Q2269	E2187	L2076	G1982	Q1859	E1747
L2962	L2962	L2856	T2768	W2560	I2459	L2366	R2270	E2188	T2077	G1983	Q1860	E1748
L2963	L2963	L2857	Y2770	L2564	W2460	L2367	Y2274	I2189	P2079	S1986	S1749	S1749
L2964	L2964	L2858	R2771	L2565	G2461	L2368	K2276	N2191	E2082	T1987	H1861	V1750
L2965	L2965	L2859	Q2773	D2566	S2462	L2378	P2277	L2192	R2083	L1988	Y1862	L1751
L2966	L2966	L2860	Q2774	D2570	W2465	L2382	K2284	L2196	F2092	H1989	W1864	S1752
L2967	L2967	L2861	M2782	Y2573	L2468	L2383	P2284	L2199	E2095	R1993	L1866	I1758
L2968	L2968	L2862	D2783	L2574	L2469	Y2384	P2287	L2200	A1995	A1994	R1867	V1781
L2969	L2969	L2863	K2802	T2575	L2575	L2384	P2288	N2201	A2105	A1996	L1869	N1784
L2970	L2970	L2864	C2803	W2576	M2473	D2389	P2292	R2205	R2109	C1997	L1879	I1787
L2971	L2971	L2865	Q2804	G2577	V2486	E2390	E2293	R2208	M2112	T1999	Q1882	F1788
L2972	L2972	L2866	V2805	A2578	P2496	L2391	C2294	T2209	I2113	G2000	E1894	I1789
L2973	L2973	L2867	L2806	H2580	T2495	E2392	G2296	T2209	F2114	V2002	S1895	H1791
L2974	L2974	L2868	G2810	G2583	C2497	G2396	K2297	V2212	L2115	K2004	H1896	N1792
L2975	L2975	L2869	W2811	ALA	I2498	L2397	L2301	E2214	S2116	Q2005	I1897	G1795
L2976	L2976	L2870	S2812	ALA	W2502	E2398	Q2307	W2215	L2130	Y2006	Q1900	K1796
L2977	L2977	L2871	M2816	A2587	L2504	N2399	Q2307	A2216	R2131	T2007	A1901	G1797
L2978	L2978	L2872	L2819	Q2590	D2510	L2402	S2310	S2219	R2132	K2011	L1902	G1799
L2979	L2979	L2873	E2821	P2591	L2511	W2406	T2311	E2219	Q2133	K2011	G1800	G1800
L2980	L2980	L2874	W2822	L2592	E2512	R2406	Q2312	E2223	P2134	L2019	A1801	A1801
L2981	L2981	L2875	L2823	P2593	E2512	R2411	E2223	E2224	A2135	L2019	M1907	Q1802
L2982	L2982	L2876	E2826	H2595	H2517	R2414	C2318	E2224	E2136	W2029	S1908	L1803
L2983	L2983	L2877	GLY	G2596	H2518	R2415	S2319	E2224	Y2137	S2030	K1909	L1804
L2984	L2984	L2878	GLY	K2597	P2519	H2415	A2320	E2224	R2138	S2030	F1910	P1805
L2985	L2985	L2879	GLY	L2601	L2521	K2416	Q2321	E2224	E2142	D2031	G1915	D1806
L2986	L2986	L2880	GLY	L2602	L2522	R2420	T2322	E2224	E2142	T2035	Q1810	Q1810
L2987	L2987	L2881	GLY	L2603	Y2522	R2421	L2327	E2224	A2152	T2035	L1811	L1811
L2988	L2988	L2882	GLY	L2604	Y2523	R2422	L2328	E2224	Q2154	A2038	F1812	F1812
L2989	L2989	L2883	GLY	L2605	L2524	R2423	L2329	E2224	Q2154	A2038	V1925	V1925
L2990	L2990	L2884	GLY	L2606	L2525	R2424	L2330	E2224	Q2154	A2038	V1926	V1926
L2991	L2991	L2885	GLY	L2607	L2526	R2425	L2331	E2224	Q2154	A2038	V1927	V1927
L2992	L2992	L2886	GLY	L2608	L2527	R2426	L2332	E2224	Q2154	A2038	V1928	V1928
L2993	L2993	L2887	GLY	L2609	L2528	R2427	L2333	E2224	Q2154	A2038	V1929	V1929
L2994	L2994	L2888	GLY	L2610	L2529	R2428	L2334	E2224	Q2154	A2038	V1930	V1930
L2995	L2995	L2889	GLY	L2611	L2530	R2429	L2335	E2224	Q2154	A2038	V1931	V1931
L2996	L2996	L2890	GLY	L2612	L2531	R2430	L2336	E2224	Q2154	A2038	V1932	V1932
L2997	L2997	L2891	GLY	L2613	L2532	R2431	L2337	E2224	Q2154	A2038	V1933	V1933
L2998	L2998	L2892	GLY	L2614	L2533	R2432	L2338	E2224	Q2154	A2038	V1934	V1934
L2999	L2999	L2893	GLY	L2615	L2534	R2433	L2339	E2224	Q2154	A2038	V1935	V1935
L3000	L3000	L2894	GLY	L2616	L2535	R2434	L2340	E2224	Q2154	A2038	V1936	V1936
L3001	L3001	L2895	GLY	L2617	L2536	R2435	L2341	E2224	Q2154	A2038	V1937	V1937
L3002	L3002	L2896	GLY	L2618	L2537	R2436	L2342	E2224	Q2154	A2038	V1938	V1938
L3003	L3003	L2897	GLY	L2619	L2538	R2437	L2343	E2224	Q2154	A2038	V1939	V1939
L3004	L3004	L2898	GLY	L2620	L2539	R2438	L2344	E2224	Q2154	A2038	V1940	V1940
L3005	L3005	L2899	GLY	L2621	L2540	R2439	L2345	E2224	Q2154	A2038	V1941	V1941
L3006	L3006	L2900	GLY	L2622	L2541	R2440	L2346	E2224	Q2154	A2038	V1942	V1942
L3007	L3007	L2901	GLY	L2623	L2542	R2441	L2347	E2224	Q2154	A2038	V1943	V1943
L3008	L3008	L2902	GLY	L2624	L2543	R2442	L2348	E2224	Q2154	A2038	V1944	V1944
L3009	L3009	L2903	GLY	L2625	L2544	R2443	L2349	E2224	Q2154	A2038	V1945	V1945
L3010	L3010	L2904	GLY	L2626	L2545	R2444	L2350	E2224	Q2154	A2038	V1946	V1946
L3011	L3011	L2905	GLY	L2627	L2546	R2445	L2351	E2224	Q2154	A2038	V1947	V1947
L3012	L3012	L2906	GLY	L2628	L2547	R2446	L2352	E2224	Q2154	A2038	V1948	V1948
L3013	L3013	L2907	GLY	L2629	L2548	R2447	L2353	E2224	Q2154	A2038	V1949	V1949
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L3015	L3015	L2909	GLY	L2631	L2550	R2449	L2355	E2224	Q2154	A2038	V1951	V1951
L3016	L3016	L2910	GLY	L2632	L2551	R2450	L2356	E2224	Q2154	A2038	V1952	V1952
L3017	L3017	L2911	GLY	L2633	L2552	R2451	L2357	E2224	Q2154	A2038	V1953	V1953
L3018	L3018	L2912	GLY	L2634	L2553	R2452	L2358	E2224	Q2154	A2038	V1954	V1954
L3019	L3019	L2913	GLY	L2635	L2554	R2453	L2359	E2224	Q2154	A2038	V1955	V1955
L3020	L3020	L2914	GLY	L2636	L2555	R2454	L2360	E2224	Q2154	A2038	V1956	V1956
L3021	L3021	L2915	GLY	L2637	L2556	R2455	L2361	E2224	Q2154	A2038	V1957	V1957
L3022	L3022	L2916	GLY	L2638	L2557	R2456	L2362	E2224	Q2154	A2038	V1958	V1958
L3023	L3023	L2917	GLY	L2639	L2558	R2457	L2363	E2224	Q2154	A2038	V1959	V1959
L3024	L3024	L2918	GLY	L2640	L2559	R2458	L2364	E2224	Q2154	A2038	V1960	V1960
L3025	L3025	L2919	GLY	L2641	L2560	R2459	L2365	E2224	Q2154	A2038	V1961	V1961
L3026	L3026	L2920	GLY	L2642	L2561	R2460	L2366	E2224	Q2154	A2038	V1962	V1962
L3027	L3027	L2921	GLY	L2643	L2562	R2461	L2367	E2224	Q2154	A2038	V1963	V1963
L3028	L3028	L2922	GLY	L2644	L2563	R2462	L2368	E2224	Q2154	A2038	V1964	V1964
L3029	L3029	L2923	GLY	L2645	L2564	R2463	L2369	E2224	Q2154	A2038	V1965	V1965
L3030	L3030	L2924	GLY	L2646	L2565	R2464	L2370	E2224	Q2154	A2038	V1966	V1966
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L3032	L3032	L2926	GLY	L2648	L2567	R2466	L2372	E2224	Q2154	A2038	V1968	V1968
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L3034	L3034	L2928	GLY	L2650	L2569	R2468	L2374	E2224	Q2154	A2038	V1970	V1970
L3035	L3035	L2929	GLY	L2651	L2570	R2469	L2375	E2224	Q2154	A2038	V1971	V1971
L3036	L3036	L2930	GLY	L2652	L2571	R2470	L2376	E2224	Q2154	A2038	V1972	V1972
L3037	L3037	L2931	GLY	L2653	L2572	R2471	L2377	E2224	Q2154	A2038	V1973	V1973
L3038	L3038	L2932	GLY	L2654	L2573	R2472	L2378	E2224	Q2154	A2038	V1974	V1974
L3039	L3039	L2933	GLY	L2655	L2574	R2473	L2379	E2224	Q2154	A2038	V1975	V1975
L3040	L3040	L2934	GLY	L2656	L2575	R2474	L2380	E2224	Q2154	A2038	V1976	V1976
L3041	L3041	L2935	GLY	L2657	L2576	R2475	L2381	E2224	Q2154	A2038	V1977	V1977
L3042	L3042	L2936	GLY	L2658	L2577	R2476	L2382	E2224	Q2154	A2038	V1978	V1978
L3043	L3043	L2937	GLY	L2659	L2578	R2477	L2383	E2224	Q2154	A2038	V1979	V1979
L3044	L3044	L2938	GLY	L2660	L2579	R2478	L2384	E2224	Q2154	A2038	V1980	V1980
L3045	L3045	L2939	GLY	L2661	L2580	R2479	L2385	E2224	Q2154	A2038	V1981	V

S4239	I4150	R4033	D3932	Y3830	K3711	ILE	R3525	D3357	S3248
P4240	I4151	E4034	R3953	E3831	L3718	ARG	R3533	D3361	E3249
S4241	Q4152		Y3934	L3836	E3719		D3536	N3363	I3252
V4245	N4153	S4037	Y3939	K3837	I3720		R3543	F3366	E3256
L4246	N4154	N4038	Y3943	L3840	E3721		I3544	R3367	D3261
P4247	K4157	E4039	L3944	M3841	Q3730		Q3545	L3368	D3262
C4248	L4164	S4041	L3944	R3842	A3731		R3555	F3369	D3370
P4249	S4165	P4042	Y3952	T3843	D3732		V3555	S3371	
W4252	E4166	V4043	V3953	Y3844	P3733		C3560	T3372	V3270
I4253	T4167	L4046	ASP	W3847	E3736		I3548	F3373	I3271
P4254	S4171		VAL	K3854	L3740		L3551	N3374	L3272
Q4255	E4172	N4051	PHE	K3854	L3740		Q3552	P3375	Q3273
E4265	E4172	Q4052	ASN	N3857	Y3750		V3555	N3376	V3276
C4266	D4177	N4053	GLN	T3858	Y3750		V3555	P3377	C3277
I4267	S4054	S4054	ARG	T3858	M3755		C3560	I3379	P3278
S4268	N4055	L4056	ASN	H3859	Q3756		I3563	P3380	F3279
L4269	L4180	I4057	LYS	R3860			D3567	F3381	L3280
P4270	R4184	I4072	SER	L3864	Q3759		D3567	A3383	I3281
V4271	Q4185	L4073	F3965	H3871	A3760		D3567	S3385	S3285
V4281	T4187	S4074	P3966	Q3875	D3761		M3570	V3387	T3288
T4282	A4188	F4075		E3876	L3762		F3575	T3388	E3289
N4283	G4192	I4076	V3869	R3877	A3771		V3575	N3391	W3290
I4284	R4193	L4077	S3970	T3881	W3776		V3576	F3397	K3291
D4285	T4197	E4079	C3975	P3882	K3780		G3578	D3448	K3292
V4286	K4199	Q4080	S3976	W3885	N3781		R3579	D3486	H3294
P4287	F4200	V4090	I3984	Y3900	V3785		H3580	D3490	L3295
C4288	W4201	L4094	E3989	D3900	W3788		P3581	A3491	D3296
Q4289	A4202	L4097	D3991	I3903	W3788		E3582	Y3492	S3298
Q4290	W4203	V4100	F3996	D3904	P3790		L3583	L3493	R3299
N4291	W4204	T4105	P3999	R3905	V3791		F3584	P3494	L3300
Q4292	W4204	L4106	A4000	L3906	L3792		Q3585	D3495	Q3305
D4293	L4208	L4107	N4001	F3907	E3793		E3586	N3309	
Q4294	L4208	V4111	I4002	D3908	K3794		N3588	F3320	
W4295	Q4214	L4118	L4002	G3909	K3802		W3589	G3321	
I4296	T4215	L4118	Q4007	A3910			D3590	K3322	
Q4297	I4216	P4124	Q4017	K3911	F3805		T3591	T3323	
C4298	I4217	W4127	Q4017	Q3914	T3810		V3595	L3324	
L4302	L4220	W4127	L4021	W3915	T3810		VAL	I3325	
F4303	L4221	P4134	L4022	E3916	H3814		VAL	I3326	
L4304	E4222	P4134	R4023	F3917	P3815		GLY	I3326	
K4305	E4223	P4137	S4024	V3918	P3815		ASP	I3326	
N4306	G4224	L4137	L4025	H3919	P3819		MET	S3510	
Q4307	C4225	L4138	T4026	G3920	L3921		LEU	K3511	
V4308	S4226	Y4139	A4027	L3921	L3821		ARG	Y3337	
	F4227	Y4140	Q4028	L3922	L3822		LYS	P3338	
	D4228	Q4029	S4029	A3925	K3701		ALA	N3513	
	G4229	F4031	R4030	G3929	P3705		ASP	N3514	
	N4230	A4148	D4032		L3826		SER	N3515	
	Q4231	L4149			T3829		GLN	R3517	
	L4232						LYS	F3518	
	Q4236								
	L4237								
	D4238								



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.03Å 487.15Å 276.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.60 – 3.41 56.54 – 3.41	Depositor EDS
% Data completeness (in resolution range)	62.2 (56.60-3.41) 62.2 (56.54-3.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.237 , 0.285 0.239 , 0.284	Depositor DCC
$R_{free}$ test set	3915 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 110.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: AOV, MG, ATP, 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	0.61	2/23147 (0.0%)	0.78	5/31474 (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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2275	PHE	CB-CG	-5.18	1.42	1.51
1	A	2826	GLU	CD-OE2	5.06	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2426	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	2275	PHE	CB-CA-C	-5.82	98.76	110.40
1	A	1915	CYS	CA-CB-SG	5.68	124.22	114.00
1	A	4253	ILE	CB-CA-C	-5.50	100.59	111.60
1	A	2426	ARG	NE-CZ-NH2	5.42	123.01	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	LEU	Peptide
1	A	2247	GLU	Peptide
1	A	2275	PHE	Peptide
1	A	2310	SER	Peptide
1	A	2416	LYS	Peptide
1	A	2659	VAL	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	22697	0	21503	995	0
2	A	32	0	12	12	0
3	A	2	0	0	0	0
4	A	31	0	12	4	0
5	A	54	0	24	10	0
All	All	22816	0	21551	996	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 22.

All (996) 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:3581:PRO:HA	1:A:3584:PHE:CE1	1.16	1.63
1:A:2284:LYS:CE	1:A:2401:GLN:HG3	1.33	1.55
1:A:2284:LYS:HE3	1:A:2401:GLN:CG	1.49	1.40
1:A:3291:LEU:O	1:A:3294:HIS:CE1	1.75	1.39
1:A:3581:PRO:CA	1:A:3584:PHE:CE1	2.04	1.38
1:A:2284:LYS:CD	1:A:2353:ARG:HH22	1.37	1.37
1:A:2659:VAL:CG2	1:A:2811:TRP:HE1	1.45	1.30
1:A:2847:VAL:CG1	1:A:2849:PRO:HD2	1.61	1.30
1:A:3291:LEU:O	1:A:3294:HIS:ND1	1.63	1.29
1:A:2284:LYS:HD2	1:A:2353:ARG:NH2	1.47	1.27
1:A:2473:MET:HE2	1:A:2502:TRP:CD2	1.70	1.26
1:A:3238:PHE:HZ	1:A:3243:PHE:CD1	1.51	1.25
1:A:4030:LYS:HG3	1:A:4034:GLU:OE1	1.34	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2660:GLY:HA3	5:A:4406:ADP:O1A	1.34	1.21
1:A:4054:SER:HB3	1:A:4057:ILE:CD1	1.71	1.19
1:A:2592:LEU:HD21	1:A:2707:GLN:OE1	1.37	1.19
1:A:3238:PHE:CZ	1:A:3243:PHE:CD1	2.32	1.18
1:A:2284:LYS:HG3	1:A:2401:GLN:OE1	1.38	1.18
1:A:4054:SER:CB	1:A:4057:ILE:HD12	1.73	1.17
1:A:1690:PRO:HA	1:A:1798:TYR:OH	1.47	1.15
1:A:2004:LYS:HG3	1:A:2006:TYR:CE1	1.82	1.14
1:A:2659:VAL:CB	1:A:2811:TRP:HE1	1.61	1.13
1:A:2131:ARG:HA	1:A:2138:ARG:NH2	1.66	1.11
1:A:4100:VAL:HG12	1:A:4105:THR:HG21	1.31	1.10
1:A:4100:VAL:HG12	1:A:4105:THR:CG2	1.83	1.08
1:A:2473:MET:CE	1:A:2502:TRP:CE2	2.14	1.08
1:A:2847:VAL:HG12	1:A:2849:PRO:CD	1.83	1.08
1:A:4171:SER:HB2	1:A:4308:VAL:O	1.54	1.08
1:A:2661:ARG:O	1:A:2665:THR:HG23	1.55	1.06
1:A:3581:PRO:HA	1:A:3584:PHE:CZ	1.89	1.06
1:A:4100:VAL:HA	1:A:4105:THR:HG22	1.36	1.06
1:A:1867:ARG:NH1	2:A:4401:AOV:O3B	1.89	1.05
1:A:3580:HIS:O	1:A:3584:PHE:CZ	2.08	1.05
1:A:1716:ASP:CG	1:A:1745:ARG:NH2	2.10	1.05
1:A:2659:VAL:CG2	1:A:2811:TRP:NE1	2.20	1.03
1:A:2607:LEU:HD23	1:A:2634:LEU:CD1	1.86	1.03
1:A:3291:LEU:HD12	1:A:3294:HIS:CE1	1.95	1.02
1:A:4100:VAL:HA	1:A:4105:THR:CG2	1.90	1.02
1:A:2607:LEU:CD2	1:A:2634:LEU:HD12	1.89	1.01
1:A:2607:LEU:HD23	1:A:2634:LEU:HD12	1.01	1.01
1:A:2653:LEU:HB3	1:A:2661:ARG:HG2	1.44	1.00
1:A:2473:MET:HE2	1:A:2502:TRP:CE2	1.47	0.98
1:A:2284:LYS:HE3	1:A:2401:GLN:CB	1.93	0.98
1:A:3581:PRO:CA	1:A:3584:PHE:HE1	1.56	0.97
1:A:2284:LYS:CE	1:A:2353:ARG:HH22	1.76	0.96
1:A:2811:TRP:HB2	1:A:2816:MET:CE	1.96	0.96
1:A:2359:LYS:O	1:A:2360:ASP:OD1	1.83	0.96
1:A:2284:LYS:CE	1:A:2401:GLN:CG	2.23	0.96
1:A:2847:VAL:HG12	1:A:2849:PRO:HD2	0.97	0.95
1:A:3511:LYS:NZ	1:A:4021:LEU:O	1.98	0.94
1:A:2284:LYS:HD2	1:A:2353:ARG:HH22	0.79	0.93
1:A:2659:VAL:HG23	1:A:2811:TRP:HE1	1.33	0.93
1:A:4054:SER:HB3	1:A:4057:ILE:HD12	0.94	0.92
1:A:1584:PRO:HB2	1:A:1587:THR:CG2	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4100:VAL:CG1	1:A:4105:THR:HG21	1.98	0.92
1:A:4171:SER:CB	1:A:4308:VAL:O	2.16	0.92
1:A:3581:PRO:CB	1:A:3584:PHE:HE1	1.82	0.92
1:A:1896:HIS:CD2	1:A:1929:ILE:HG23	2.05	0.92
1:A:3238:PHE:HZ	1:A:3243:PHE:HD1	0.98	0.91
1:A:1716:ASP:OD2	1:A:1745:ARG:NH2	2.03	0.91
1:A:2847:VAL:CG1	1:A:2849:PRO:CD	2.42	0.91
1:A:2659:VAL:HB	1:A:2811:TRP:HE1	1.33	0.91
1:A:2284:LYS:CD	1:A:2401:GLN:HG3	2.01	0.90
1:A:1662:LEU:HD11	1:A:1697:GLU:HB3	1.54	0.90
1:A:2284:LYS:HE2	1:A:2401:GLN:HG3	1.51	0.90
1:A:1584:PRO:HB2	1:A:1587:THR:HG22	1.55	0.89
1:A:4057:ILE:HD13	1:A:4149:LEU:HD23	1.54	0.89
1:A:3581:PRO:HA	1:A:3584:PHE:HE1	1.08	0.88
1:A:3291:LEU:C	1:A:3294:HIS:CE1	2.46	0.88
1:A:1674:THR:HG22	1:A:3925:ALA:HA	1.54	0.88
1:A:1716:ASP:OD1	1:A:1745:ARG:NH2	2.06	0.88
1:A:2004:LYS:CG	1:A:2006:TYR:CE1	2.56	0.88
1:A:2659:VAL:HB	1:A:2811:TRP:NE1	1.88	0.88
1:A:1796:LYS:HD3	1:A:1797:GLY:N	1.88	0.87
1:A:1690:PRO:CA	1:A:1798:TYR:OH	2.22	0.87
1:A:2284:LYS:CD	1:A:2353:ARG:NH2	2.19	0.87
1:A:2284:LYS:HE3	1:A:2401:GLN:HG3	0.88	0.87
1:A:2660:GLY:CA	5:A:4406:ADP:O1A	2.22	0.87
1:A:3377:PRO:CB	1:A:3378:PHE:HB2	2.05	0.86
1:A:4100:VAL:CA	1:A:4105:THR:CG2	2.53	0.86
1:A:4030:LYS:HB2	1:A:4034:GLU:HG3	1.57	0.85
1:A:2284:LYS:CE	1:A:2353:ARG:NH2	2.36	0.85
1:A:2660:GLY:O	1:A:2664:ILE:HD13	1.76	0.85
1:A:2284:LYS:HG3	1:A:2401:GLN:CD	1.97	0.84
1:A:2592:LEU:CD2	1:A:2707:GLN:OE1	2.24	0.84
1:A:2510:ASP:O	1:A:2522:TYR:OH	1.96	0.83
1:A:4171:SER:C	1:A:4308:VAL:O	2.16	0.83
1:A:2659:VAL:HG23	1:A:2811:TRP:NE1	1.87	0.83
1:A:2284:LYS:HD2	1:A:2353:ARG:CZ	2.07	0.83
1:A:1716:ASP:OD1	1:A:1745:ARG:CZ	2.27	0.82
1:A:2004:LYS:HG3	1:A:2006:TYR:HE1	1.41	0.82
1:A:2811:TRP:HB2	1:A:2816:MET:HE2	1.61	0.82
1:A:4057:ILE:HD13	1:A:4149:LEU:CD2	2.09	0.82
1:A:2658:GLY:HA3	1:A:2870:SER:HB3	1.62	0.81
1:A:3291:LEU:HA	1:A:3294:HIS:CE1	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2055:ASP:OD1	1:A:2420:ARG:NH2	2.14	0.81
1:A:1716:ASP:OD2	1:A:2065:SER:HA	1.80	0.81
1:A:4171:SER:CB	1:A:4305:LYS:CB	2.59	0.80
1:A:1554:ALA:HA	1:A:1560:LEU:HD12	1.63	0.80
1:A:2288:ILE:HD11	1:A:2425:VAL:HG21	1.63	0.80
1:A:3238:PHE:CZ	1:A:3243:PHE:HD1	1.85	0.80
1:A:4171:SER:HB3	1:A:4305:LYS:CB	2.12	0.80
1:A:4057:ILE:CD1	1:A:4149:LEU:CD2	2.60	0.80
1:A:3291:LEU:HD12	1:A:3294:HIS:HE1	1.46	0.79
1:A:2575:THR:HG21	1:A:2645:SER:OG	1.80	0.79
1:A:3857:ASN:HB2	1:A:3975:CYS:SG	2.21	0.79
1:A:1715:CYS:SG	1:A:1743:PHE:HA	2.22	0.79
1:A:4100:VAL:CG1	1:A:4105:THR:CG2	2.57	0.79
1:A:3377:PRO:HB2	1:A:3378:PHE:HB2	1.65	0.78
1:A:3640:LEU:HG	1:A:3642:PHE:CE2	2.18	0.78
1:A:2263:ILE:HD13	1:A:2441:ILE:HA	1.65	0.78
1:A:3640:LEU:HG	1:A:3642:PHE:CZ	2.20	0.77
1:A:3581:PRO:HA	1:A:3584:PHE:CD1	2.11	0.77
1:A:1513:GLN:HG3	1:A:1514:LEU:N	2.00	0.76
1:A:2847:VAL:HG13	1:A:2849:PRO:HD2	1.66	0.76
1:A:2658:GLY:HA3	1:A:2870:SER:CB	2.16	0.76
1:A:3291:LEU:C	1:A:3294:HIS:ND1	2.40	0.76
1:A:3512:ILE:HG23	1:A:4021:LEU:CD2	2.16	0.76
1:A:4171:SER:CA	1:A:4308:VAL:O	2.33	0.76
1:A:4304:LEU:HD12	1:A:4305:LYS:N	2.00	0.76
1:A:4030:LYS:CG	1:A:4034:GLU:OE1	2.28	0.75
1:A:2811:TRP:HB2	1:A:2816:MET:HE3	1.66	0.75
1:A:2821:GLU:HB2	1:A:2852:LEU:HD13	1.68	0.75
1:A:3291:LEU:CA	1:A:3294:HIS:CE1	2.70	0.75
1:A:2473:MET:HE2	1:A:2502:TRP:CE3	1.91	0.74
1:A:3760:ALA:HA	1:A:3788:TRP:CH2	2.22	0.74
1:A:2810:GLY:O	1:A:2811:TRP:HD1	1.70	0.74
1:A:4208:LEU:O	1:A:4214:GLN:NE2	2.20	0.74
1:A:2685:TYR:HB2	1:A:2718:VAL:HG21	1.68	0.73
1:A:2135:ALA:HA	1:A:2138:ARG:CB	1.71	0.73
1:A:4057:ILE:CD1	1:A:4152:GLN:HE22	2.01	0.73
1:A:1583:ASP:N	1:A:1584:PRO:HD2	2.02	0.73
1:A:1696:THR:OG1	2:A:4401:AOV:O2B	2.05	0.73
1:A:2659:VAL:CB	1:A:2811:TRP:NE1	2.41	0.73
1:A:1896:HIS:HA	1:A:1929:ILE:HD13	1.69	0.73
1:A:2205:ARG:NH2	1:A:2429:SER:OG	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2653:LEU:CB	1:A:2661:ARG:HG2	2.17	0.72
1:A:3587:ASN:OD1	1:A:3590:ASP:OD2	2.07	0.72
1:A:1752:SER:OG	1:A:3755:MET:O	2.06	0.72
1:A:1283:ASP:HB3	1:A:1353:GLU:OE2	1.89	0.72
1:A:1693:THR:HG23	1:A:1817:MET:O	1.89	0.72
1:A:1460:GLY:HA3	1:A:1655:TYR:HD2	1.54	0.72
1:A:2135:ALA:N	1:A:2138:ARG:HG3	1.73	0.71
1:A:1801:ARG:NH1	1:A:2064:GLU:OE1	2.23	0.71
1:A:1279:ILE:HD12	1:A:1293:LYS:HG3	1.71	0.71
1:A:1514:LEU:CD1	1:A:1534:PHE:CE1	2.74	0.71
1:A:1690:PRO:HD2	1:A:1818:SER:HA	1.72	0.71
1:A:2661:ARG:O	1:A:2665:THR:CG2	2.37	0.71
1:A:3642:PHE:HA	1:A:3648:TRP:NE1	2.06	0.70
1:A:3881:ILE:HG23	1:A:3882:PRO:HA	1.72	0.70
1:A:3512:ILE:HD12	1:A:3513:ASN:HB2	1.72	0.70
1:A:4100:VAL:HG12	1:A:4105:THR:HG23	1.72	0.70
1:A:2607:LEU:CD2	1:A:2634:LEU:CD1	2.61	0.70
1:A:3966:PRO:HB2	1:A:3969:VAL:HG12	1.73	0.70
1:A:2004:LYS:CG	1:A:2006:TYR:HE1	2.00	0.70
1:A:2658:GLY:CA	1:A:2870:SER:HB3	2.21	0.70
1:A:4100:VAL:CB	1:A:4105:THR:CG2	2.70	0.70
1:A:2135:ALA:HA	1:A:2138:ARG:HB2	1.72	0.69
1:A:1587:THR:OG1	1:A:1590:GLY:HA3	1.93	0.69
1:A:3847:TRP:HH2	1:A:3900:TYR:HB2	1.56	0.69
1:A:4097:LEU:HD13	1:A:4111:VAL:CG1	2.23	0.69
1:A:2867:ALA:HA	1:A:2871:GLN:OE1	1.93	0.69
1:A:1900:GLN:N	1:A:1900:GLN:OE1	2.22	0.68
1:A:4236:GLN:O	1:A:4239:SER:OG	2.10	0.68
1:A:3291:LEU:C	1:A:3294:HIS:HD1	1.95	0.68
1:A:2284:LYS:CG	1:A:2401:GLN:HG3	2.22	0.68
1:A:2274:TYR:CE2	1:A:2428:CYS:HB3	2.28	0.68
1:A:4057:ILE:HD11	1:A:4152:GLN:HE22	1.57	0.68
1:A:1397:ILE:HD12	1:A:1398:ARG:N	2.09	0.67
1:A:1665:THR:OG1	1:A:1666:PRO:HD2	1.94	0.67
1:A:2719:HIS:ND1	1:A:2720:PRO:HD2	2.09	0.67
1:A:1752:SER:CB	1:A:3755:MET:O	2.43	0.67
1:A:4046:LEU:HD11	1:A:4138:LEU:HD13	1.77	0.67
1:A:4222:LEU:HD23	1:A:4223:GLU:N	2.09	0.67
1:A:1540:CYS:SG	1:A:1599:LEU:HD12	2.35	0.67
1:A:3837:LYS:HB2	1:A:3984:ILE:HG23	1.75	0.67
1:A:3877:ARG:CZ	1:A:3943:TYR:OH	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2131:ARG:HA	1:A:2138:ARG:CZ	2.24	0.67
1:A:1514:LEU:HD12	1:A:1534:PHE:HE1	1.58	0.67
1:A:2390:GLU:O	1:A:2391:ASN:CB	2.43	0.67
1:A:1514:LEU:HD12	1:A:1534:PHE:CE1	2.30	0.66
1:A:2473:MET:HE1	1:A:2502:TRP:CE2	2.12	0.66
1:A:3099:TYR:O	1:A:3103:LEU:N	2.29	0.66
1:A:4154:TRP:NE1	1:A:4172:GLU:OE2	2.28	0.66
1:A:3814:HIS:ND1	1:A:3815:PRO:O	2.21	0.66
1:A:2450:LEU:HD11	1:A:2460:TRP:HB3	1.78	0.66
1:A:2242:VAL:O	1:A:2269:GLN:NE2	2.28	0.66
1:A:2284:LYS:HG3	1:A:2401:GLN:CG	2.25	0.66
1:A:2265:THR:HB	1:A:2266:PRO:CD	2.26	0.66
1:A:2518:HIS:N	1:A:2519:PRO:HA	2.10	0.66
1:A:4171:SER:O	1:A:4308:VAL:O	2.13	0.66
1:A:2109:ARG:NH2	2:A:4401:AOV:O3G	2.28	0.66
1:A:2295:CYS:SG	1:A:2430:ILE:HG13	2.35	0.66
1:A:1624:TRP:CD2	1:A:3917:PHE:HB3	2.31	0.66
1:A:3847:TRP:HH2	1:A:3900:TYR:CB	2.09	0.66
1:A:4051:ASN:N	1:A:4051:ASN:OD1	2.29	0.66
1:A:1662:LEU:HD11	1:A:1697:GLU:CB	2.25	0.65
1:A:2135:ALA:H	1:A:2138:ARG:HG3	1.56	0.65
1:A:3374:ASN:ND2	1:A:3377:PRO:HD2	2.10	0.65
1:A:2212:VAL:HA	1:A:2215:TRP:HE3	1.62	0.65
1:A:4030:LYS:HB2	1:A:4034:GLU:CG	2.25	0.65
1:A:4215:ILE:HB	1:A:4217:ILE:HD11	1.77	0.65
1:A:2816:MET:HB2	1:A:2856:LEU:HD21	1.78	0.65
1:A:2292:PRO:O	1:A:2295:CYS:HB2	1.96	0.65
1:A:4307:GLN:HG3	1:A:4307:GLN:O	1.97	0.65
1:A:2131:ARG:CA	1:A:2138:ARG:NH2	2.52	0.65
1:A:1693:THR:CG2	1:A:1817:MET:O	2.44	0.65
1:A:2004:LYS:HE3	1:A:2006:TYR:CZ	2.32	0.65
1:A:4057:ILE:CD1	1:A:4149:LEU:HD22	2.27	0.65
1:A:2168:LEU:O	1:A:2169:VAL:C	2.34	0.65
1:A:2354:LEU:HD23	1:A:2355:VAL:N	2.12	0.65
1:A:1696:THR:OG1	1:A:1741:ASP:OD1	2.15	0.64
1:A:2362:ASN:HD21	1:A:2406:MET:HB2	1.62	0.64
1:A:1584:PRO:HB2	1:A:1587:THR:HG21	1.77	0.64
1:A:2651:LEU:HD23	1:A:2653:LEU:HD21	1.78	0.64
1:A:2135:ALA:N	1:A:2138:ARG:CG	2.38	0.64
1:A:2442:TYR:O	1:A:2446:LEU:HB2	1.97	0.64
1:A:2473:MET:CE	1:A:2502:TRP:CD2	2.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2656:ARG:NH1	1:A:2783:ASP:OD1	2.31	0.64
1:A:1938:GLU:OE2	1:A:1938:GLU:N	2.31	0.64
1:A:2653:LEU:HB3	1:A:2661:ARG:CG	2.25	0.63
1:A:3273:GLN:OE1	1:A:3276:VAL:N	2.31	0.63
1:A:4025:ILE:N	1:A:4025:ILE:HD12	2.14	0.63
1:A:1482:GLU:OE1	1:A:1658:ASN:ND2	2.32	0.63
1:A:3871:HIS:NE2	1:A:3875:GLN:OE1	2.32	0.63
1:A:1752:SER:HB3	1:A:3755:MET:O	1.99	0.63
1:A:3762:LEU:C	1:A:3762:LEU:HD12	2.18	0.63
1:A:2261:PRO:O	1:A:2445:TYR:OH	2.08	0.62
1:A:1279:ILE:HD12	1:A:1293:LYS:CG	2.28	0.62
1:A:1499:TRP:CZ3	1:A:1503:LEU:HD11	2.34	0.62
1:A:2264:GLN:HA	1:A:2268:MET:HG3	1.80	0.62
1:A:4220:LEU:HB2	1:A:4245:VAL:HG13	1.80	0.62
1:A:3080:LYS:CB	1:A:3087:ALA:HB2	2.30	0.62
1:A:3374:ASN:HB2	1:A:3820:ILE:HD11	1.82	0.62
1:A:1715:CYS:O	1:A:1716:ASP:OD1	2.18	0.62
1:A:3836:LEU:HD23	1:A:3991:ASP:CB	2.30	0.62
1:A:4052:GLN:HA	1:A:4055:ASN:OD1	1.98	0.62
1:A:2660:GLY:HA3	5:A:4406:ADP:PA	2.38	0.62
1:A:2664:ILE:N	1:A:2664:ILE:HD12	2.14	0.62
1:A:2699:GLN:NE2	1:A:2704:GLU:OE1	2.33	0.62
1:A:3511:LYS:CE	1:A:4021:LEU:O	2.48	0.61
1:A:2375:VAL:HA	1:A:2378:LEU:HD12	1.82	0.61
1:A:1472:HIS:ND1	1:A:1490:VAL:O	2.33	0.61
1:A:2239:ALA:O	1:A:2240:THR:HG23	2.00	0.61
1:A:1645:VAL:HG12	1:A:1646:ASP:H	1.66	0.61
1:A:2597:LYS:HB2	1:A:2645:SER:HB3	1.82	0.61
1:A:4057:ILE:HG23	1:A:4152:GLN:OE1	2.01	0.61
1:A:4281:VAL:HG21	1:A:4304:LEU:HD23	1.81	0.61
1:A:2335:CYS:HG	1:A:2347:ARG:C	2.04	0.61
1:A:3238:PHE:CZ	1:A:3243:PHE:CG	2.86	0.61
1:A:3755:MET:HG3	1:A:3785:VAL:HG21	1.83	0.61
1:A:1509:LYS:NZ	1:A:1512:GLU:OE1	2.34	0.61
1:A:3238:PHE:CZ	1:A:3243:PHE:HB2	2.36	0.61
1:A:3377:PRO:HB2	1:A:3378:PHE:CB	2.29	0.61
1:A:4030:LYS:HG3	1:A:4034:GLU:CD	2.16	0.61
1:A:2517:ASN:CB	1:A:2519:PRO:HB3	2.31	0.60
1:A:4265:GLU:O	1:A:4288:CYS:CB	2.49	0.60
1:A:2265:THR:HB	1:A:2266:PRO:HD2	1.83	0.60
1:A:2517:ASN:HB3	1:A:2519:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3374:ASN:HD22	1:A:3377:PRO:HD2	1.66	0.60
1:A:3904:ASP:O	1:A:3908:ASP:N	2.34	0.60
1:A:2284:LYS:CG	1:A:2401:GLN:CG	2.79	0.60
1:A:2288:ILE:HD11	1:A:2425:VAL:CG2	2.32	0.60
1:A:3292:LYS:O	1:A:3295:LEU:HB2	2.01	0.60
1:A:2284:LYS:NZ	1:A:2353:ARG:NH2	2.49	0.60
1:A:1795:GLY:HA3	1:A:1798:TYR:HD1	1.66	0.60
1:A:4217:ILE:HD12	1:A:4217:ILE:N	2.17	0.60
1:A:1583:ASP:N	1:A:1584:PRO:CD	2.64	0.60
1:A:2816:MET:CB	1:A:2856:LEU:HD21	2.32	0.59
1:A:3837:LYS:O	1:A:3841:MET:N	2.30	0.59
1:A:1662:LEU:HB3	2:A:4401:AOV:C6	2.31	0.59
1:A:2363:LEU:N	1:A:2364:PRO:HD2	2.17	0.59
1:A:2659:VAL:O	1:A:2659:VAL:HG22	2.01	0.59
1:A:3372:THR:HG22	1:A:3374:ASN:H	1.67	0.59
1:A:2548:PHE:HA	1:A:2551:ILE:HD12	1.84	0.59
1:A:3245:CYS:SG	1:A:3249:GLU:HB2	2.43	0.59
1:A:4100:VAL:CA	1:A:4105:THR:HG21	2.30	0.59
1:A:1943:LEU:HA	1:A:1995:ALA:HB2	1.85	0.59
1:A:2011:LYS:NZ	1:A:2367:ASP:OD2	2.33	0.59
1:A:2284:LYS:HD2	1:A:2353:ARG:NH1	2.17	0.59
1:A:4281:VAL:HG21	1:A:4304:LEU:CD2	2.32	0.59
1:A:2135:ALA:CA	1:A:2138:ARG:HB2	2.30	0.59
1:A:2353:ARG:HG2	1:A:2354:LEU:N	2.16	0.59
1:A:2847:VAL:CG1	1:A:2849:PRO:CG	2.80	0.59
1:A:1747:GLU:HB3	1:A:1750:VAL:HG23	1.84	0.59
1:A:3512:ILE:CG2	1:A:4021:LEU:CD2	2.80	0.59
1:A:3844:TYR:HA	1:A:3847:TRP:HB2	1.85	0.58
1:A:3585:GLN:NE2	1:A:3585:GLN:O	2.36	0.58
1:A:4306:ASN:O	1:A:4307:GLN:HB3	2.03	0.58
1:A:2335:CYS:SG	1:A:2347:ARG:O	2.58	0.58
1:A:1554:ALA:CA	1:A:1560:LEU:HD12	2.32	0.58
1:A:2357:TYR:C	1:A:2358:LEU:HD23	2.24	0.58
1:A:3711:LYS:HG2	1:A:3740:LEU:HD13	1.85	0.58
1:A:1973:MET:SD	1:A:2074:ARG:NH1	2.77	0.58
1:A:2162:TYR:HB2	1:A:2199:ASN:O	2.03	0.58
1:A:2185:HIS:CE1	1:A:2189:ILE:HD11	2.39	0.58
1:A:3591:THR:HG21	1:A:3632:ALA:HB1	1.85	0.58
1:A:1584:PRO:CB	1:A:1587:THR:HG22	2.31	0.58
1:A:3781:ASN:H	1:A:3810:THR:HB	1.67	0.58
1:A:1796:LYS:HD3	1:A:1797:GLY:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2544:GLU:N	1:A:2544:GLU:OE1	2.37	0.58
1:A:2676:LEU:O	1:A:2676:LEU:HD23	2.04	0.58
1:A:3877:ARG:NH1	1:A:3943:TYR:OH	2.37	0.58
1:A:1986:SER:OG	4:A:4403:ATP:O2B	2.16	0.57
1:A:1496:VAL:HA	1:A:1499:TRP:NE1	2.18	0.57
1:A:2625:LEU:HB3	1:A:2627:ILE:HD13	1.85	0.57
1:A:2858:ILE:O	1:A:2861:SER:OG	2.16	0.57
1:A:2366:LEU:HD11	1:A:2415:HIS:HB3	1.85	0.57
1:A:1437:LEU:CD2	1:A:1441:LEU:HD12	2.34	0.57
1:A:2462:SER:O	1:A:2465:LYS:N	2.37	0.57
1:A:3621:GLU:HG3	1:A:3622:ARG:N	2.19	0.57
1:A:3492:TYR:O	1:A:3495:LEU:HB3	2.05	0.57
1:A:2095:GLU:OE2	4:A:4403:ATP:O3G	2.23	0.57
1:A:3067:LEU:O	1:A:3071:LYS:N	2.38	0.57
1:A:1397:ILE:HD12	1:A:1398:ARG:H	1.69	0.57
1:A:1514:LEU:CD1	1:A:1534:PHE:HE1	2.16	0.57
1:A:2739:TYR:HB3	1:A:2744:LEU:HD21	1.87	0.57
1:A:3525:ARG:NH2	1:A:3721:GLU:OE1	2.38	0.57
1:A:1440:ILE:HD11	1:A:1453:HIS:CG	2.40	0.56
1:A:4220:LEU:HB3	1:A:4302:LEU:HD21	1.84	0.56
1:A:3921:LEU:HD23	1:A:3922:LEU:N	2.19	0.56
1:A:4054:SER:HB3	1:A:4057:ILE:CG1	2.34	0.56
1:A:1534:PHE:HB2	1:A:1539:LEU:HD11	1.86	0.56
1:A:2643:VAL:HG11	1:A:2651:LEU:CD1	2.36	0.56
1:A:3640:LEU:HD12	1:A:3642:PHE:CE1	2.40	0.56
1:A:2130:LEU:O	1:A:2138:ARG:NE	2.38	0.56
1:A:3245:CYS:SG	1:A:3249:GLU:CB	2.93	0.56
1:A:3642:PHE:HA	1:A:3648:TRP:CD1	2.40	0.56
1:A:1908:SER:N	1:A:1964:GLU:OE2	2.39	0.56
1:A:3291:LEU:O	1:A:3294:HIS:HE1	1.74	0.56
1:A:3864:LEU:HD23	1:A:3903:ILE:HD12	1.87	0.56
1:A:4164:LEU:HD13	1:A:4214:GLN:O	2.05	0.56
1:A:4204:TRP:CZ2	1:A:4248:CYS:SG	2.99	0.56
1:A:3249:GLU:N	1:A:3249:GLU:OE1	2.39	0.56
1:A:3580:HIS:O	1:A:3584:PHE:CE2	2.55	0.56
1:A:3577:ARG:O	1:A:3584:PHE:HZ	1.89	0.56
1:A:3591:THR:CG2	1:A:3632:ALA:HB1	2.36	0.56
1:A:1353:GLU:HB3	1:A:1354:PRO:HD3	1.87	0.56
1:A:2565:LEU:HG	1:A:2566:ASP:O	2.06	0.56
1:A:4100:VAL:CB	1:A:4105:THR:HG23	2.35	0.56
1:A:2382:LEU:HD21	1:A:2402:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2810:GLY:O	1:A:2811:TRP:CD1	2.58	0.55
1:A:1282:GLU:HA	1:A:1287:ARG:O	2.06	0.55
1:A:1813:ARG:HD3	1:A:1814:PRO:HD2	1.89	0.55
1:A:1824:LEU:O	1:A:1828:VAL:HG23	2.06	0.55
1:A:2402:ILE:N	1:A:2402:ILE:HD12	2.21	0.55
1:A:2664:ILE:O	1:A:2668:VAL:HG23	2.05	0.55
1:A:4220:LEU:O	1:A:4221:LEU:HD23	2.06	0.55
1:A:3581:PRO:HB3	1:A:3584:PHE:HE1	1.69	0.55
1:A:1260:ILE:HD12	1:A:1317:TYR:HB2	1.87	0.55
1:A:1667:LEU:HD22	1:A:1819:HIS:O	2.06	0.55
1:A:4137:PRO:O	1:A:4140:TYR:HB3	2.07	0.55
1:A:2536:ARG:HG2	1:A:2545:LEU:HD22	1.88	0.55
1:A:3239:ASP:O	1:A:3242:ARG:HG2	2.06	0.55
1:A:3570:MET:SD	1:A:4017:GLN:HB3	2.47	0.55
1:A:2767:TYR:CE2	1:A:2771:ARG:HD2	2.42	0.55
1:A:3294:HIS:CE1	1:A:3295:LEU:HG	2.42	0.55
1:A:1694:GLY:HA3	2:A:4401:AOV:H8	1.89	0.55
1:A:2592:LEU:HD22	1:A:2645:SER:O	2.05	0.55
1:A:1408:LEU:HA	1:A:1411:CYS:SG	2.46	0.55
1:A:1716:ASP:CG	1:A:1745:ARG:HH22	1.97	0.55
1:A:2348:PRO:HB3	1:A:2354:LEU:HB2	1.88	0.55
1:A:2390:GLU:O	1:A:2391:ASN:HB3	2.07	0.55
1:A:3718:LEU:HD13	1:A:3720:ILE:HB	1.89	0.55
1:A:1439:GLU:HB2	1:A:1440:ILE:HD12	1.87	0.55
1:A:1835:PHE:CE2	1:A:1894:GLU:HB3	2.42	0.55
1:A:2659:VAL:HG21	1:A:2811:TRP:NE1	2.20	0.55
1:A:3238:PHE:CE1	1:A:3243:PHE:HB2	2.41	0.55
1:A:1996:LEU:O	1:A:2000:GLY:N	2.36	0.54
1:A:2230:TYR:OH	1:A:2266:PRO:O	2.24	0.54
1:A:3991:ASP:OD1	1:A:3991:ASP:N	2.40	0.54
1:A:4051:ASN:O	1:A:4055:ASN:N	2.40	0.54
1:A:1925:VAL:HG23	1:A:1926:PHE:HD1	1.72	0.54
1:A:2167:SER:O	1:A:2168:LEU:C	2.43	0.54
1:A:1810:GLN:HG3	1:A:3732:ASP:HB2	1.90	0.54
1:A:3658:GLU:OE1	1:A:3658:GLU:N	2.41	0.54
1:A:3291:LEU:C	1:A:3294:HIS:HE1	2.08	0.54
1:A:1711:LEU:HD12	1:A:1731:LEU:HD21	1.89	0.54
1:A:3512:ILE:CG2	1:A:4021:LEU:HD21	2.38	0.54
1:A:2536:ARG:NH1	1:A:2549:ASP:OD2	2.41	0.54
1:A:4025:ILE:HG22	1:A:4027:ALA:N	2.24	0.54
1:A:1645:VAL:HG12	1:A:1646:ASP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2134:PRO:O	1:A:2135:ALA:HB3	2.08	0.53
1:A:3854:LYS:O	1:A:3857:ASN:HB3	2.07	0.53
1:A:1663:VAL:CG2	1:A:1829:ILE:HD11	2.38	0.53
1:A:3296:LYS:C	1:A:3298:SER:H	2.10	0.53
1:A:3750:TYR:HA	1:A:3776:TRP:O	2.08	0.53
1:A:4057:ILE:HD12	1:A:4149:LEU:CD2	2.35	0.53
1:A:2663:THR:OG1	5:A:4406:ADP:H5'1	2.09	0.53
1:A:4051:ASN:O	1:A:4055:ASN:OD1	2.27	0.53
1:A:4308:VAL:O	1:A:4308:VAL:HG12	2.08	0.53
1:A:1411:CYS:O	1:A:1414:SER:OG	2.19	0.53
1:A:1879:LEU:HD12	1:A:1897:ILE:HG23	1.90	0.53
1:A:2135:ALA:CA	1:A:2138:ARG:CB	2.56	0.53
1:A:2396:GLY:C	1:A:2397:LEU:HD22	2.28	0.53
1:A:2450:LEU:O	1:A:2453:ASN:O	2.27	0.53
1:A:3740:LEU:O	1:A:3740:LEU:HD12	2.07	0.53
1:A:4147:ARG:O	1:A:4151:ILE:HG12	2.08	0.53
1:A:4265:GLU:O	1:A:4288:CYS:N	2.35	0.53
1:A:1709:GLN:HG3	1:A:1709:GLN:O	2.09	0.53
1:A:2689:GLN:HG3	1:A:2690:PHE:N	2.24	0.53
1:A:4199:LYS:CD	1:A:4255:GLN:HG2	2.39	0.53
1:A:1376:ARG:O	1:A:1379:MET:HB3	2.08	0.53
1:A:2041:VAL:CG2	1:A:2050:SER:CB	2.87	0.53
1:A:2249:LEU:HB2	1:A:2448:PRO:HG3	1.91	0.53
1:A:1590:GLY:C	1:A:1591:ILE:HG13	2.29	0.53
1:A:3299:ARG:HH21	1:A:3322:LYS:HD3	1.73	0.53
1:A:3577:ARG:HA	1:A:3584:PHE:HE2	1.72	0.53
1:A:2660:GLY:HA2	5:A:4406:ADP:PB	2.49	0.53
1:A:2639:ARG:O	1:A:2642:ARG:HG2	2.09	0.52
1:A:3864:LEU:CD2	1:A:3903:ILE:HG21	2.39	0.52
1:A:1343:ASN:OD1	1:A:1344:HIS:N	2.42	0.52
1:A:1472:HIS:HA	1:A:1490:VAL:O	2.10	0.52
1:A:3212:THR:HG23	1:A:3213:TYR:CD2	2.44	0.52
1:A:3262:ASP:N	1:A:3262:ASP:OD1	2.42	0.52
1:A:1624:TRP:CZ2	1:A:3906:LEU:HD13	2.44	0.52
1:A:1993:ARG:HB2	1:A:2003:VAL:HG11	1.92	0.52
1:A:2004:LYS:HE2	1:A:2006:TYR:OH	2.09	0.52
1:A:2175:GLY:CA	1:A:2196:LEU:HD23	2.39	0.52
1:A:2389:ASP:N	1:A:2393:GLU:O	2.43	0.52
1:A:2848:ASP:N	1:A:2849:PRO:HD2	2.24	0.52
1:A:3296:LYS:HA	1:A:3300:LEU:HD21	1.92	0.52
1:A:4052:GLN:HA	1:A:4055:ASN:CG	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4188:ALA:O	1:A:4192:GLY:N	2.42	0.52
1:A:2650:SER:HB2	1:A:2803:CYS:HB3	1.91	0.52
1:A:3238:PHE:CA	1:A:3242:ARG:HH21	2.23	0.52
1:A:4199:LYS:CE	1:A:4255:GLN:HG2	2.39	0.52
1:A:1691:ALA:HB1	1:A:2105:ALA:HA	1.91	0.52
1:A:1908:SER:HB2	1:A:2113:ILE:HA	1.91	0.52
1:A:3324:LEU:HG	1:A:3325:ILE:N	2.25	0.52
1:A:3675:ILE:HD11	1:A:3693:PHE:HB2	1.92	0.52
1:A:4265:GLU:O	1:A:4288:CYS:HB3	2.09	0.52
1:A:1861:HIS:HB2	1:A:2112:MET:SD	2.50	0.52
1:A:2131:ARG:HA	1:A:2138:ARG:HH22	1.64	0.52
1:A:2254:PHE:O	1:A:2595:HIS:HE1	1.92	0.52
1:A:4046:LEU:CD1	1:A:4138:LEU:HD22	2.40	0.52
1:A:1631:ARG:O	1:A:1642:VAL:HG13	2.10	0.52
1:A:1811:LEU:N	1:A:1811:LEU:HD12	2.25	0.52
1:A:1896:HIS:CD2	1:A:1929:ILE:CG2	2.88	0.52
1:A:2486:VAL:HB	1:A:4106:LEU:HD21	1.91	0.52
1:A:2254:PHE:O	1:A:2595:HIS:CE1	2.63	0.52
1:A:2774:GLN:N	1:A:2774:GLN:OE1	2.42	0.52
1:A:3218:PRO:HD2	1:A:3221:LEU:HD12	1.92	0.52
1:A:3635:SER:O	1:A:3639:THR:HG23	2.09	0.52
1:A:4026:THR:O	1:A:4027:ALA:HB3	2.10	0.52
1:A:4204:TRP:CE2	1:A:4248:CYS:SG	3.03	0.52
1:A:1398:ARG:O	1:A:1402:LEU:HG	2.09	0.52
1:A:1408:LEU:O	1:A:1411:CYS:SG	2.67	0.52
1:A:2577:GLY:HA3	1:A:2602:LEU:HD11	1.92	0.52
1:A:2465:LYS:O	1:A:2468:LEU:HB3	2.10	0.51
1:A:2823:LEU:HD13	1:A:2826:GLU:OE1	2.09	0.51
1:A:3877:ARG:HB2	1:A:3885:TRP:CD1	2.46	0.51
1:A:3965:PHE:HB3	1:A:3966:PRO:CD	2.40	0.51
1:A:1285:GLN:O	1:A:1287:ARG:HG3	2.10	0.51
1:A:2133:GLN:O	1:A:2138:ARG:HD2	2.11	0.51
1:A:3380:PRO:HD2	1:A:3383:ALA:HB3	1.92	0.51
1:A:4100:VAL:CG1	1:A:4105:THR:HG23	2.35	0.51
1:A:2263:ILE:HD11	1:A:2444:ALA:HB3	1.93	0.51
1:A:3640:LEU:CD1	1:A:3648:TRP:CZ2	2.93	0.51
1:A:4052:GLN:HA	1:A:4055:ASN:ND2	2.26	0.51
1:A:1800:GLY:C	1:A:1801:ARG:HG3	2.29	0.51
1:A:1993:ARG:HG3	1:A:1994:ALA:N	2.25	0.51
1:A:3240:LEU:HA	1:A:3243:PHE:HB3	1.92	0.51
1:A:2592:LEU:HD11	1:A:2707:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3577:ARG:NH2	1:A:3577:ARG:HB3	2.26	0.51
1:A:1806:ASP:OD2	1:A:3730:GLY:N	2.43	0.51
1:A:1628:LYS:HB2	1:A:3917:PHE:CZ	2.46	0.51
1:A:2284:LYS:NZ	1:A:2401:GLN:N	2.59	0.51
1:A:2811:TRP:CE2	1:A:2869:PRO:HB3	2.46	0.51
1:A:3325:ILE:HA	1:A:3369:PHE:O	2.11	0.51
1:A:3515:MET:HA	1:A:3822:LEU:HD13	1.93	0.51
1:A:2847:VAL:HG13	1:A:2849:PRO:CD	2.30	0.50
1:A:3586:GLU:O	1:A:3587:ASN:HB3	2.11	0.50
1:A:3640:LEU:HD12	1:A:3648:TRP:CZ2	2.46	0.50
1:A:1472:HIS:C	1:A:1473:ILE:HD12	2.31	0.50
1:A:1804:LEU:HD12	1:A:1805:PRO:HD2	1.92	0.50
1:A:2187:GLU:HG2	1:A:2191:ASN:OD1	2.11	0.50
1:A:3577:ARG:CZ	1:A:3577:ARG:HB3	2.42	0.50
1:A:1697:GLU:OE2	1:A:2072:ASP:HB3	2.12	0.50
1:A:1973:MET:HG3	1:A:2070:LEU:HD23	1.94	0.50
1:A:1458:PHE:HB3	1:A:1461:ILE:CD1	2.42	0.50
1:A:1728:PHE:CZ	1:A:1758:ILE:HD11	2.47	0.50
1:A:1802:GLN:N	1:A:1802:GLN:OE1	2.45	0.50
1:A:2294:GLY:O	1:A:2496:PRO:HG2	2.11	0.50
1:A:3514:ASN:O	1:A:3515:MET:HB2	2.11	0.50
1:A:3881:ILE:CG2	1:A:3882:PRO:HA	2.41	0.50
1:A:3932:ASP:OD1	1:A:3932:ASP:N	2.45	0.50
1:A:3910:ALA:O	1:A:3911:LYS:HG3	2.12	0.50
1:A:1337:GLU:O	1:A:1341:ASN:ND2	2.45	0.50
1:A:2004:LYS:CE	1:A:2006:TYR:CZ	2.95	0.50
1:A:3291:LEU:HA	1:A:3294:HIS:ND1	2.27	0.50
1:A:4227:PHE:CD2	1:A:4232:LEU:CD2	2.94	0.50
1:A:1499:TRP:CE3	1:A:1503:LEU:HD11	2.47	0.49
1:A:2078:MET:HG3	1:A:2082:GLU:HB3	1.94	0.49
1:A:2284:LYS:CG	1:A:2401:GLN:OE1	2.33	0.49
1:A:2659:VAL:HG21	1:A:2811:TRP:CD1	2.47	0.49
1:A:4171:SER:HB2	1:A:4305:LYS:CB	2.39	0.49
1:A:1388:VAL:HG13	1:A:1389:THR:N	2.27	0.49
1:A:2318:CYS:HB2	1:A:2360:ASP:O	2.12	0.49
1:A:2363:LEU:HD22	1:A:2363:LEU:N	2.27	0.49
1:A:2769:THR:HA	1:A:2772:ILE:HD12	1.94	0.49
1:A:1582:GLU:C	1:A:1584:PRO:HD2	2.33	0.49
1:A:3291:LEU:CA	1:A:3294:HIS:ND1	2.75	0.49
1:A:2045:PRO:O	1:A:2048:VAL:HG22	2.13	0.49
1:A:2173:MET:HB3	1:A:2426:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3922:LEU:C	1:A:3922:LEU:HD13	2.32	0.49
1:A:4038:ASN:O	1:A:4042:PRO:HD3	2.13	0.49
1:A:1825:ILE:O	1:A:1829:ILE:HG12	2.12	0.49
1:A:2362:ASN:HB2	1:A:2363:LEU:HD22	1.94	0.49
1:A:1547:PHE:CE1	1:A:1606:ASN:HB3	2.48	0.49
1:A:1862:TYR:CD2	1:A:1864:TRP:CH2	3.01	0.49
1:A:2473:MET:CE	1:A:2502:TRP:CE3	2.79	0.49
1:A:2512:GLU:OE2	1:A:2579:ARG:HG3	2.12	0.49
1:A:1879:LEU:O	1:A:1882:GLN:N	2.43	0.49
1:A:1896:HIS:O	1:A:1900:GLN:OE1	2.30	0.49
1:A:2284:LYS:CE	1:A:2401:GLN:CA	2.91	0.49
1:A:2683:ARG:NH2	1:A:3305:GLN:O	2.46	0.49
1:A:3587:ASN:OD1	1:A:3590:ASP:CG	2.51	0.49
1:A:3674:GLN:O	1:A:3677:VAL:HB	2.13	0.49
1:A:2175:GLY:HA2	1:A:2196:LEU:HD23	1.93	0.49
1:A:2320:ALA:HA	1:A:2364:PRO:HA	1.95	0.49
1:A:3847:TRP:CH2	1:A:3900:TYR:HB2	2.41	0.49
1:A:2223:PHE:CE2	1:A:2224:HIS:HB2	2.47	0.49
1:A:2625:LEU:HD22	1:A:2627:ILE:HD13	1.94	0.49
1:A:3636:LEU:HA	1:A:3639:THR:OG1	2.12	0.49
1:A:4253:ILE:HG22	1:A:4254:PRO:HD2	1.95	0.49
1:A:1695:LYS:NZ	2:A:4401:AOV:O1G	2.44	0.49
1:A:2051:TRP:C	1:A:2052:ILE:HD13	2.34	0.49
1:A:2530:GLU:O	1:A:2531:ALA:C	2.51	0.49
1:A:2819:ILE:HB	1:A:2820:PRO:HD3	1.95	0.49
1:A:3300:LEU:HA	1:A:3323:THR:O	2.13	0.49
1:A:1514:LEU:HD11	1:A:1534:PHE:CE1	2.47	0.48
1:A:1696:THR:HA	1:A:1790:THR:HG21	1.95	0.48
1:A:2274:TYR:HE2	1:A:2428:CYS:HB3	1.76	0.48
1:A:3536:ASP:O	1:A:3543:ARG:NH1	2.46	0.48
1:A:3577:ARG:HA	1:A:3584:PHE:CE2	2.48	0.48
1:A:2579:ARG:C	1:A:2580:HIS:CD2	2.87	0.48
1:A:4171:SER:OG	1:A:4308:VAL:HG12	2.13	0.48
1:A:2041:VAL:HG21	1:A:2050:SER:CB	2.43	0.48
1:A:2284:LYS:HZ1	1:A:2401:GLN:N	2.11	0.48
1:A:2459:ILE:HD12	1:A:2519:PRO:HD2	1.95	0.48
1:A:2749:LEU:N	1:A:2750:PRO:CD	2.76	0.48
1:A:1516:LYS:HD3	1:A:1638:HIS:HB3	1.94	0.48
1:A:1939:LEU:HD23	1:A:1939:LEU:O	2.14	0.48
1:A:2396:GLY:O	1:A:2397:LEU:HD22	2.13	0.48
1:A:4030:LYS:HB2	1:A:4034:GLU:CD	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4222:LEU:HD22	1:A:4225:CYS:O	2.13	0.48
1:A:1280:ASP:HA	1:A:1289:MET:O	2.13	0.48
1:A:1276:PHE:HE1	1:A:1388:VAL:HA	1.79	0.48
1:A:2723:LEU:N	1:A:2723:LEU:HD22	2.29	0.48
1:A:1378:ILE:O	1:A:1382:ILE:HD12	2.13	0.48
1:A:2529:TYR:O	1:A:2533:ARG:HG2	2.13	0.48
1:A:3291:LEU:O	1:A:3295:LEU:HG	2.14	0.48
1:A:3829:THR:HG22	1:A:3831:GLU:HG3	1.96	0.48
1:A:4043:VAL:HG21	1:A:4118:LEU:CD2	2.44	0.48
1:A:1749:SER:O	1:A:3756:GLY:CA	2.61	0.48
1:A:3374:ASN:HB2	1:A:3820:ILE:CG1	2.44	0.48
1:A:4046:LEU:HD12	1:A:4138:LEU:HD22	1.96	0.48
1:A:1795:GLY:HA3	1:A:1798:TYR:CD1	2.48	0.48
1:A:1792:ASN:HB3	1:A:1798:TYR:CE2	2.49	0.48
1:A:1943:LEU:HA	1:A:1995:ALA:CB	2.44	0.48
1:A:2284:LYS:HD2	1:A:2353:ARG:HH12	1.79	0.48
1:A:3296:LYS:O	1:A:3296:LYS:HD2	2.14	0.48
1:A:3347:GLN:HG3	1:A:3352:VAL:CG2	2.44	0.48
1:A:3238:PHE:HA	1:A:3242:ARG:HH21	1.79	0.47
1:A:3245:CYS:SG	1:A:3249:GLU:HB3	2.53	0.47
1:A:4188:ALA:HB1	1:A:4193:ARG:O	2.14	0.47
1:A:1716:ASP:OD2	1:A:2065:SER:CA	2.57	0.47
1:A:1879:LEU:N	1:A:1879:LEU:HD23	2.29	0.47
1:A:2168:LEU:O	1:A:2171:THR:OG1	2.26	0.47
1:A:2345:VAL:HG21	1:A:2398:GLU:HB2	1.96	0.47
1:A:2625:LEU:HD22	1:A:2627:ILE:CD1	2.44	0.47
1:A:3219:GLU:OE1	1:A:3219:GLU:N	2.47	0.47
1:A:3238:PHE:N	1:A:3242:ARG:HH21	2.12	0.47
1:A:3256:GLU:OE1	1:A:3290:TRP:NE1	2.47	0.47
1:A:1987:THR:O	1:A:1988:LEU:C	2.49	0.47
1:A:2235:ARG:HB3	1:A:2237:ARG:CG	2.44	0.47
1:A:2848:ASP:N	1:A:2849:PRO:CD	2.77	0.47
1:A:3629:LEU:HD22	1:A:3680:VAL:HG21	1.95	0.47
1:A:3966:PRO:HB2	1:A:3969:VAL:CG1	2.43	0.47
1:A:4270:PRO:HA	1:A:4283:ASN:HB3	1.97	0.47
1:A:1902:LEU:HD21	1:A:1918:PHE:HZ	1.78	0.47
1:A:2208:PHE:O	1:A:2209:THR:C	2.51	0.47
1:A:2238:LEU:N	1:A:2238:LEU:HD22	2.28	0.47
1:A:2230:TYR:N	1:A:2239:ALA:HB1	2.28	0.47
1:A:2632:GLU:OE2	1:A:2812:SER:N	2.48	0.47
1:A:2643:VAL:HG11	1:A:2651:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2659:VAL:CG2	1:A:2811:TRP:CD1	2.95	0.47
1:A:2704:GLU:O	1:A:2705:ALA:HB3	2.14	0.47
1:A:3640:LEU:CD1	1:A:3642:PHE:CE1	2.96	0.47
1:A:3877:ARG:HH22	1:A:3996:PHE:HA	1.80	0.47
1:A:4072:ILE:HG23	1:A:4073:LEU:N	2.30	0.47
1:A:4077:ILE:O	1:A:4080:GLN:HB3	2.15	0.47
1:A:1643:GLN:HG3	1:A:1647:SER:O	2.14	0.47
1:A:1742:GLU:OE2	2:A:4401:AOV:O2G	2.32	0.47
1:A:2495:THR:H	1:A:2498:ILE:HG12	1.80	0.47
1:A:3321:GLY:HA3	1:A:3363:ASN:OD1	2.13	0.47
1:A:4033:ARG:O	1:A:4037:SER:N	2.46	0.47
1:A:1746:LEU:HB3	1:A:1751:LEU:HD21	1.96	0.47
1:A:1792:ASN:OD1	2:A:4401:AOV:O2G	2.32	0.47
1:A:1993:ARG:HB2	1:A:2003:VAL:HG21	1.95	0.47
1:A:3197:LEU:HD12	1:A:3197:LEU:C	2.35	0.47
1:A:1280:ASP:OD1	1:A:1290:LYS:HE3	2.14	0.47
1:A:2319:SER:N	1:A:2322:THR:OG1	2.42	0.47
1:A:2764:VAL:O	1:A:2767:TYR:HB3	2.14	0.47
1:A:3291:LEU:CD1	1:A:3294:HIS:HE1	2.23	0.47
1:A:1815:VAL:HA	1:A:3929:GLY:HA2	1.97	0.47
1:A:1732:VAL:HB	1:A:1781:VAL:HG23	1.96	0.47
1:A:1440:ILE:HD11	1:A:1453:HIS:CD2	2.49	0.47
1:A:2447:GLU:HB3	1:A:2448:PRO:HD3	1.97	0.47
1:A:2469:LEU:HD22	1:A:2560:TRP:HZ2	1.80	0.47
1:A:2639:ARG:O	1:A:2643:VAL:HG23	2.14	0.47
1:A:3357:ASP:OD1	1:A:3357:ASP:N	2.48	0.47
2:A:4401:AOV:O4G	2:A:4401:AOV:O2B	2.33	0.47
1:A:1508:LYS:O	1:A:1512:GLU:HB2	2.15	0.46
1:A:1529:VAL:C	1:A:1531:PRO:HD3	2.36	0.46
1:A:2004:LYS:CG	1:A:2006:TYR:CZ	2.98	0.46
1:A:2019:LEU:O	1:A:2035:THR:HG21	2.14	0.46
1:A:2076:LEU:HD12	1:A:2077:THR:N	2.31	0.46
1:A:2166:THR:OG1	1:A:2171:THR:HG23	2.15	0.46
1:A:2256:ASN:OD1	1:A:2257:GLY:N	2.48	0.46
1:A:3771:ALA:HA	1:A:3805:PHE:CD1	2.50	0.46
1:A:2297:LYS:HZ3	5:A:4405:ADP:PB	2.38	0.46
1:A:1444:SER:HB3	1:A:1496:VAL:HG22	1.96	0.46
1:A:2607:LEU:O	1:A:2610:VAL:N	2.48	0.46
1:A:3337:TYR:N	1:A:3338:PRO:HD2	2.31	0.46
1:A:3560:CYS:HA	1:A:3563:LEU:HG	1.98	0.46
1:A:1534:PHE:CB	1:A:1539:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:TRP:HE1	1:A:2531:ALA:HB2	1.81	0.46
1:A:3864:LEU:HD21	1:A:3903:ILE:HG21	1.97	0.46
1:A:1363:LYS:O	1:A:1366:THR:OG1	2.33	0.46
1:A:2287:PHE:HA	1:A:2426:ARG:O	2.15	0.46
1:A:3347:GLN:HG3	1:A:3352:VAL:HG22	1.96	0.46
1:A:3560:CYS:HB3	1:A:3705:PRO:HG3	1.97	0.46
1:A:1411:CYS:SG	1:A:1412:GLN:N	2.89	0.46
1:A:2284:LYS:HE3	1:A:2353:ARG:NH2	2.29	0.46
1:A:2664:ILE:N	1:A:2664:ILE:CD1	2.78	0.46
1:A:1518:CYS:HB2	1:A:1534:PHE:CZ	2.51	0.46
1:A:1747:GLU:O	1:A:1750:VAL:HB	2.15	0.46
1:A:3587:ASN:OD1	1:A:3590:ASP:HB2	2.16	0.46
1:A:3780:LYS:HA	1:A:3810:THR:HB	1.96	0.46
1:A:4229:GLY:O	1:A:4230:ASN:HB2	2.16	0.46
1:A:1446:ASN:HB3	1:A:1449:VAL:HB	1.98	0.46
1:A:1719:ILE:HG22	1:A:1723:SER:HB3	1.96	0.46
1:A:2004:LYS:HG2	1:A:2006:TYR:CE1	2.47	0.46
1:A:2077:THR:HA	1:A:2083:ARG:HG2	1.97	0.46
1:A:2155:TRP:CZ3	1:A:2208:PHE:HB2	2.51	0.46
1:A:2213:PHE:HB3	1:A:2219:SER:HA	1.98	0.46
1:A:3563:LEU:HD11	1:A:3571:PHE:CD2	2.50	0.46
1:A:1624:TRP:HB3	1:A:3917:PHE:CB	2.46	0.46
1:A:2041:VAL:HG23	1:A:2050:SER:CB	2.45	0.46
1:A:2360:ASP:HB3	1:A:2363:LEU:HD23	1.97	0.46
1:A:3216:ALA:O	1:A:3391:ASN:ND2	2.48	0.46
1:A:3621:GLU:HG3	1:A:3622:ARG:H	1.81	0.46
1:A:4057:ILE:CG2	1:A:4152:GLN:OE1	2.63	0.46
1:A:2307:GLN:OE1	1:A:2307:GLN:HA	2.16	0.46
1:A:3505:ILE:HG21	1:A:3575:PHE:HA	1.98	0.46
1:A:4177:ASP:O	1:A:4180:LEU:HB2	2.16	0.46
1:A:4199:LYS:HD2	1:A:4255:GLN:HG2	1.96	0.46
1:A:1401:LEU:HA	1:A:1404:ILE:HD12	1.96	0.46
1:A:1499:TRP:HZ3	1:A:1503:LEU:HD11	1.80	0.46
1:A:2134:PRO:HB2	1:A:2136:GLU:HG3	1.98	0.46
1:A:1982:GLY:HA3	1:A:2169:VAL:HG21	1.98	0.46
1:A:2223:PHE:CG	1:A:2224:HIS:N	2.84	0.46
1:A:3325:ILE:HG22	1:A:3326:ILE:N	2.30	0.46
1:A:4177:ASP:OD1	1:A:4177:ASP:N	2.49	0.46
1:A:2805:VAL:O	1:A:2806:LEU:HD23	2.17	0.45
1:A:3701:LYS:HE2	1:A:3989:GLU:OE1	2.16	0.45
1:A:2130:LEU:HD13	1:A:2142:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2392:LEU:HD12	1:A:2392:LEU:N	2.31	0.45
1:A:2292:PRO:HG2	1:A:2432:TYR:HE1	1.82	0.45
1:A:3292:LYS:O	1:A:3296:LYS:N	2.49	0.45
1:A:3499:ALA:HA	1:A:3502:MET:HE2	1.98	0.45
1:A:3512:ILE:HG23	1:A:4021:LEU:HD23	1.97	0.45
1:A:3685:ARG:O	1:A:3686:LEU:C	2.53	0.45
1:A:3819:PRO:HA	1:A:3822:LEU:HD12	1.98	0.45
1:A:2311:THR:OG1	1:A:2312:GLN:N	2.50	0.45
1:A:2447:GLU:N	1:A:2448:PRO:CD	2.78	0.45
1:A:2650:SER:O	1:A:2803:CYS:HB2	2.16	0.45
1:A:3299:ARG:NH2	1:A:3320:PHE:O	2.48	0.45
1:A:3970:SER:OG	1:A:3970:SER:O	2.34	0.45
1:A:4090:VAL:HG12	1:A:4094:LEU:HD12	1.97	0.45
1:A:1654:GLU:HB3	1:A:1707:GLY:O	2.17	0.45
1:A:1955:ILE:CG2	1:A:1956:PRO:HD2	2.46	0.45
1:A:2164:VAL:O	1:A:2166:THR:HG23	2.16	0.45
1:A:3261:ASP:OD1	1:A:3262:ASP:N	2.50	0.45
1:A:3272:LEU:HD23	1:A:3272:LEU:C	2.37	0.45
1:A:3721:GLU:HG3	1:A:3826:LEU:HD11	1.98	0.45
1:A:2235:ARG:HB3	1:A:2237:ARG:HG2	1.98	0.45
1:A:2327:LEU:O	1:A:2328:LEU:C	2.53	0.45
1:A:2460:TRP:HE1	1:A:2519:PRO:HB2	1.80	0.45
1:A:2593:PRO:HG2	1:A:2597:LYS:HA	1.99	0.45
1:A:2749:LEU:HB3	1:A:2750:PRO:HD3	1.98	0.45
1:A:3279:PHE:HA	1:A:3370:LEU:HD12	1.99	0.45
1:A:4184:ARG:HG3	1:A:4252:TRP:CD2	2.52	0.45
1:A:4227:PHE:HD2	1:A:4232:LEU:CD2	2.28	0.45
1:A:1601:LEU:HD21	1:A:1832:SER:HB3	1.99	0.45
1:A:3577:ARG:O	1:A:3584:PHE:CZ	2.69	0.45
1:A:4025:ILE:CD1	1:A:4025:ILE:N	2.79	0.45
1:A:4097:LEU:HD13	1:A:4111:VAL:HG12	1.98	0.45
1:A:1741:ASP:O	1:A:1742:GLU:CB	2.64	0.45
1:A:2495:THR:HB	1:A:2496:PRO:HD2	1.99	0.45
1:A:2870:SER:OG	1:A:3385:SER:HB2	2.17	0.45
1:A:4025:ILE:HG22	1:A:4027:ALA:H	1.81	0.45
1:A:1274:ALA:HB1	1:A:1388:VAL:CG1	2.47	0.45
1:A:1663:VAL:N	2:A:4401:AOV:N1	2.64	0.45
1:A:1708:ARG:NH1	1:A:1784:ASN:O	2.49	0.45
1:A:2651:LEU:HD12	1:A:2651:LEU:N	2.32	0.45
1:A:1624:TRP:CE3	1:A:3917:PHE:HB3	2.51	0.45
1:A:4134:PRO:HG2	1:A:4140:TYR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:ASP:O	1:A:1385:ASP:HB3	2.17	0.45
1:A:1906:THR:HG21	1:A:1918:PHE:CZ	2.52	0.45
1:A:2007:THR:HG21	1:A:2384:TYR:CE2	2.52	0.45
1:A:4201:VAL:HG12	1:A:4202:ALA:H	1.81	0.45
1:A:1560:LEU:HD23	1:A:1560:LEU:HA	1.80	0.45
1:A:1787:ILE:O	1:A:1788:PHE:CD1	2.70	0.45
1:A:1820:PRO:O	1:A:1822:ASN:OD1	2.35	0.45
1:A:3368:LEU:HD23	1:A:3369:PHE:N	2.32	0.45
1:A:3580:HIS:C	1:A:3584:PHE:CZ	2.86	0.45
1:A:4057:ILE:CD1	1:A:4152:GLN:NE2	2.77	0.45
1:A:1315:SER:O	1:A:1318:TYR:HB3	2.17	0.44
1:A:1372:ASP:OD1	1:A:1376:ARG:NH1	2.49	0.44
1:A:1749:SER:O	1:A:3756:GLY:HA3	2.17	0.44
1:A:2004:LYS:HG2	1:A:2006:TYR:OH	2.17	0.44
1:A:2041:VAL:HG23	1:A:2050:SER:OG	2.17	0.44
1:A:2382:LEU:CD2	1:A:2402:ILE:HD13	2.47	0.44
1:A:2411:ARG:CB	1:A:2414:ARG:CZ	2.94	0.44
1:A:3200:LEU:N	1:A:3201:PRO:CD	2.80	0.44
1:A:3640:LEU:CG	1:A:3642:PHE:CZ	2.98	0.44
1:A:3732:ASP:HA	1:A:3733:PRO:HD3	1.81	0.44
1:A:3847:TRP:HH2	1:A:3900:TYR:CG	2.35	0.44
1:A:1550:ASP:O	1:A:1554:ALA:N	2.49	0.44
1:A:1547:PHE:O	1:A:1551:VAL:HG23	2.17	0.44
1:A:2004:LYS:CE	1:A:2006:TYR:OH	2.64	0.44
1:A:2517:ASN:HB3	1:A:2519:PRO:CB	2.47	0.44
1:A:3864:LEU:HD21	1:A:3903:ILE:CG2	2.47	0.44
1:A:4134:PRO:CG	1:A:4140:TYR:HA	2.48	0.44
1:A:4057:ILE:HG12	1:A:4152:GLN:OE1	2.17	0.44
1:A:4001:ASN:ND2	1:A:4241:SER:HA	2.33	0.44
1:A:1278:LEU:HD12	1:A:1278:LEU:N	2.32	0.44
1:A:1444:SER:CB	1:A:1496:VAL:HG22	2.47	0.44
1:A:1591:ILE:HB	1:A:1592:LEU:HD12	1.98	0.44
1:A:1671:CYS:O	1:A:1675:LEU:HG	2.16	0.44
1:A:1699:VAL:HG11	1:A:1788:PHE:CD2	2.52	0.44
1:A:1719:ILE:HG13	1:A:2079:PRO:HB3	2.00	0.44
1:A:2213:PHE:HA	1:A:2216:ALA:HB3	1.99	0.44
1:A:2503:VAL:HG13	1:A:2504:LEU:CD1	2.48	0.44
1:A:2711:LEU:O	1:A:2712:LEU:HD23	2.17	0.44
1:A:1862:TYR:CD2	1:A:1864:TRP:HH2	2.36	0.44
1:A:2002:VAL:HG12	1:A:2003:VAL:N	2.30	0.44
1:A:1401:LEU:HB2	1:A:1402:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:THR:HG22	1:A:1474:THR:O	2.16	0.44
1:A:2168:LEU:O	1:A:2171:THR:N	2.50	0.44
1:A:2821:GLU:HB2	1:A:2852:LEU:CD1	2.44	0.44
1:A:3193:ILE:HG22	1:A:3197:LEU:HD23	1.99	0.44
1:A:3291:LEU:CA	1:A:3294:HIS:HE1	2.25	0.44
1:A:3577:ARG:HD2	1:A:3589:TRP:CH2	2.53	0.44
1:A:3755:MET:N	1:A:3755:MET:CE	2.81	0.44
1:A:4286:VAL:HG13	1:A:4287:PRO:HD2	2.00	0.44
1:A:4288:CYS:SG	1:A:4290:GLY:CA	3.06	0.44
1:A:2629:LEU:HD12	1:A:2629:LEU:N	2.32	0.44
1:A:2643:VAL:CG1	1:A:2651:LEU:HD11	2.48	0.44
1:A:3755:MET:CG	1:A:3785:VAL:HG21	2.47	0.44
1:A:4040:LEU:HD22	1:A:4118:LEU:HD23	1.99	0.44
1:A:4266:CYS:HB3	1:A:4285:ASP:HB3	1.98	0.44
1:A:2730:LEU:HB3	1:A:2802:LYS:HG3	2.00	0.44
1:A:3587:ASN:OD1	1:A:3590:ASP:CB	2.66	0.44
1:A:3654:ASN:O	1:A:3682:ARG:NH1	2.50	0.44
1:A:1810:GLN:HG3	1:A:3732:ASP:CB	2.48	0.44
1:A:1624:TRP:CG	1:A:3917:PHE:HB3	2.52	0.44
1:A:3965:PHE:CB	1:A:3966:PRO:CD	2.94	0.44
1:A:1276:PHE:CD2	1:A:1292:ILE:HD12	2.53	0.44
1:A:1713:PHE:HB2	1:A:1740:PHE:CD1	2.52	0.44
1:A:2000:GLY:O	1:A:2001:LYS:C	2.54	0.44
1:A:2284:LYS:HE3	1:A:2401:GLN:CA	2.46	0.44
1:A:2717:PHE:CD1	1:A:2723:LEU:HD21	2.53	0.44
1:A:3837:LYS:HB2	1:A:3984:ILE:CG2	2.45	0.44
1:A:4307:GLN:O	1:A:4308:VAL:HG23	2.18	0.44
1:A:2038:ALA:HA	1:A:2041:VAL:HG12	2.00	0.43
1:A:3217:ALA:O	1:A:3222:ARG:NE	2.51	0.43
1:A:3244:LEU:HA	1:A:3244:LEU:HD22	1.85	0.43
1:A:3285:SER:O	1:A:3288:THR:OG1	2.26	0.43
1:A:3999:PRO:HG2	1:A:4002:ILE:HG12	2.00	0.43
1:A:4227:PHE:HD2	1:A:4232:LEU:HD21	1.84	0.43
1:A:1506:GLU:OE2	1:A:1510:THR:OG1	2.36	0.43
1:A:2579:ARG:O	1:A:2580:HIS:CD2	2.71	0.43
1:A:1274:ALA:HB1	1:A:1388:VAL:HG11	2.00	0.43
1:A:1397:ILE:O	1:A:1398:ARG:C	2.56	0.43
1:A:1500:LEU:HA	1:A:1503:LEU:HG	2.00	0.43
1:A:1699:VAL:CG1	1:A:1788:PHE:CD2	3.01	0.43
1:A:2765:PHE:O	1:A:2768:PHE:HB3	2.18	0.43
1:A:3273:GLN:OE1	1:A:3276:VAL:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3581:PRO:CA	1:A:3584:PHE:CZ	2.73	0.43
1:A:3802:LYS:O	1:A:3805:PHE:HB3	2.18	0.43
1:A:4202:ALA:HA	1:A:4249:PHE:O	2.19	0.43
1:A:1458:PHE:HB3	1:A:1461:ILE:HD12	1.98	0.43
1:A:1859:GLN:HB2	1:A:1862:TYR:CD2	2.53	0.43
1:A:1973:MET:HG3	1:A:2070:LEU:CD2	2.49	0.43
1:A:2052:ILE:HB	1:A:2092:PHE:CE1	2.53	0.43
1:A:3185:ARG:O	1:A:3189:GLN:NE2	2.51	0.43
1:A:3673:GLN:HA	1:A:3676:LEU:HD12	2.01	0.43
1:A:4030:LYS:O	1:A:4034:GLU:HB2	2.18	0.43
1:A:4100:VAL:HB	1:A:4105:THR:HG23	1.99	0.43
1:A:4124:PRO:HD2	1:A:4127:TRP:CE3	2.53	0.43
1:A:4147:ARG:HG2	1:A:4172:GLU:O	2.19	0.43
1:A:1558:HIS:HB3	1:A:1560:LEU:HG	1.99	0.43
1:A:1603:ILE:O	1:A:1606:ASN:HB2	2.19	0.43
1:A:2004:LYS:HB3	1:A:2050:SER:HA	2.00	0.43
1:A:2114:PHE:C	1:A:2115:LEU:HD12	2.39	0.43
1:A:2284:LYS:CE	1:A:2401:GLN:CB	2.77	0.43
1:A:3654:ASN:O	1:A:3657:CYS:HB3	2.19	0.43
1:A:4201:VAL:HG23	1:A:4253:ILE:CD1	2.48	0.43
1:A:1294:ASP:O	1:A:1297:ASP:HB3	2.19	0.43
1:A:1518:CYS:HB2	1:A:1534:PHE:CE1	2.53	0.43
1:A:1855:LEU:HD12	1:A:1855:LEU:C	2.39	0.43
1:A:2805:VAL:C	1:A:2806:LEU:HD23	2.39	0.43
1:A:3374:ASN:ND2	1:A:3377:PRO:CD	2.78	0.43
1:A:3281:ILE:HD12	1:A:3391:ASN:HB3	1.99	0.43
1:A:3686:LEU:HD22	1:A:3690:MET:SD	2.59	0.43
1:A:4100:VAL:N	1:A:4105:THR:HG21	2.34	0.43
1:A:1281:TYR:O	1:A:1288:THR:HA	2.19	0.43
1:A:2201:ASN:OD1	1:A:2201:ASN:N	2.51	0.43
1:A:1475:ALA:HB1	1:A:1484:VAL:O	2.19	0.43
1:A:2590:GLN:HG3	1:A:2591:PRO:HD3	2.01	0.43
1:A:4227:PHE:CD1	1:A:4227:PHE:C	2.92	0.43
1:A:2288:ILE:HD12	1:A:2426:ARG:O	2.19	0.43
1:A:2312:GLN:HB2	1:A:2351:CYS:SG	2.59	0.43
1:A:2357:TYR:O	1:A:2358:LEU:HD23	2.19	0.43
1:A:2745:GLU:N	1:A:2746:PRO:HD2	2.34	0.43
1:A:3510:SER:HA	1:A:3516:TYR:HB2	2.00	0.43
1:A:2296:GLY:CA	5:A:4405:ADP:O1A	2.67	0.43
1:A:3230:THR:HG23	1:A:3235:LEU:O	2.19	0.42
1:A:3239:ASP:OD1	1:A:3239:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3493:LEU:N	1:A:3494:PRO:CD	2.82	0.42
1:A:3577:ARG:HD2	1:A:3589:TRP:CZ3	2.54	0.42
1:A:2652:LEU:HD22	1:A:2805:VAL:HG13	2.01	0.42
1:A:2851:PHE:CE2	1:A:3201:PRO:HB2	2.54	0.42
1:A:3238:PHE:CZ	1:A:3243:PHE:CB	3.01	0.42
1:A:3336:LEU:N	1:A:3336:LEU:CD2	2.82	0.42
1:A:3512:ILE:HG23	1:A:4021:LEU:HD21	1.95	0.42
1:A:4057:ILE:HD12	1:A:4149:LEU:HD22	1.98	0.42
1:A:4288:CYS:SG	1:A:4290:GLY:C	2.97	0.42
1:A:2167:SER:O	1:A:2170:GLY:N	2.52	0.42
1:A:2200:LEU:HD12	1:A:2205:ARG:HA	2.01	0.42
1:A:2301:LEU:HD13	1:A:2357:TYR:CE1	2.55	0.42
1:A:2503:VAL:HG13	1:A:2504:LEU:HD13	2.01	0.42
1:A:2606:ASP:O	1:A:2610:VAL:HG23	2.19	0.42
1:A:2664:ILE:HD12	1:A:2664:ILE:H	1.83	0.42
1:A:1515:LEU:HD13	1:A:1538:ILE:HG23	2.01	0.42
1:A:2029:TRP:HE1	1:A:2031:ASP:HA	1.84	0.42
1:A:2163:VAL:HG23	1:A:2164:VAL:HG23	1.99	0.42
1:A:2212:VAL:HA	1:A:2215:TRP:CE3	2.48	0.42
1:A:4072:ILE:HB	1:A:4186:GLU:HG3	2.00	0.42
1:A:4075:PHE:O	1:A:4078:LEU:HB2	2.20	0.42
1:A:4227:PHE:CD2	1:A:4232:LEU:HD21	2.54	0.42
1:A:1593:GLU:N	1:A:1593:GLU:OE1	2.47	0.42
1:A:3321:GLY:HA2	1:A:3366:PHE:HB2	2.02	0.42
1:A:3374:ASN:HB2	1:A:3820:ILE:CD1	2.47	0.42
1:A:3545:GLN:HA	1:A:3548:ILE:HG22	2.01	0.42
1:A:1684:GLY:O	1:A:1812:PHE:HA	2.19	0.42
1:A:1731:LEU:HA	1:A:1731:LEU:HD23	1.91	0.42
1:A:1862:TYR:HB3	1:A:1864:TRP:CH2	2.54	0.42
1:A:2193:ILE:HG21	1:A:2209:THR:HG22	2.02	0.42
1:A:1514:LEU:HD11	1:A:1534:PHE:CD1	2.54	0.42
1:A:2041:VAL:HG21	1:A:2050:SER:HB2	2.01	0.42
1:A:2135:ALA:C	1:A:2138:ARG:H	2.23	0.42
1:A:2276:LYS:N	1:A:2277:PRO:HD2	2.35	0.42
1:A:3277:CYS:SG	1:A:3368:LEU:CD2	3.07	0.42
1:A:4134:PRO:HG2	1:A:4140:TYR:CA	2.50	0.42
1:A:2652:LEU:HD23	1:A:2652:LEU:C	2.40	0.42
1:A:2662:ARG:NH1	1:A:2662:ARG:HG2	2.35	0.42
1:A:3248:SER:O	1:A:3252:ILE:HG13	2.20	0.42
1:A:3299:ARG:HE	1:A:3322:LYS:HD2	1.84	0.42
1:A:3518:PHE:N	1:A:3518:PHE:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3583:LEU:HG	1:A:3583:LEU:H	1.68	0.42
1:A:3788:TRP:HD1	1:A:3788:TRP:O	2.03	0.42
1:A:3860:ARG:HB3	1:A:3907:PHE:CD2	2.55	0.42
1:A:4271:VAL:HA	1:A:4302:LEU:O	2.19	0.42
1:A:1866:LEU:HD12	2:A:4401:AOV:O4'	2.20	0.42
1:A:2296:GLY:HA2	5:A:4405:ADP:O1A	2.20	0.42
1:A:2517:ASN:HB2	1:A:2519:PRO:HB3	1.99	0.42
1:A:4281:VAL:CG2	1:A:4304:LEU:HD23	2.48	0.42
1:A:1481:GLY:O	1:A:1591:ILE:HD13	2.20	0.42
1:A:1693:THR:HG21	1:A:1817:MET:HB2	2.01	0.42
1:A:2076:LEU:HD12	1:A:2077:THR:H	1.85	0.42
1:A:3512:ILE:HD12	1:A:3513:ASN:CB	2.46	0.42
1:A:1688:TYR:CD1	1:A:1688:TYR:C	2.93	0.41
1:A:1906:THR:HG22	1:A:1910:PHE:CE1	2.55	0.41
1:A:3847:TRP:CH2	1:A:3900:TYR:CG	3.08	0.41
1:A:3919:HIS:HB2	1:A:3944:LEU:HB3	2.03	0.41
1:A:3965:PHE:HB3	1:A:3966:PRO:HD3	2.02	0.41
1:A:4030:LYS:O	1:A:4034:GLU:N	2.44	0.41
1:A:1962:ALA:O	1:A:1965:LEU:HB3	2.19	0.41
1:A:1986:SER:HB3	1:A:2095:GLU:OE2	2.19	0.41
1:A:3309:ASN:OD1	1:A:3309:ASN:N	2.53	0.41
1:A:3567:ASP:O	1:A:3570:MET:HB2	2.19	0.41
1:A:3836:LEU:O	1:A:3840:LEU:HD13	2.19	0.41
1:A:1624:TRP:HZ2	1:A:3906:LEU:HD13	1.85	0.41
1:A:2153:LEU:HD22	1:A:2157:LEU:HD11	2.03	0.41
1:A:2230:TYR:O	1:A:2239:ALA:HA	2.20	0.41
1:A:2276:LYS:N	1:A:2277:PRO:CD	2.83	0.41
1:A:2460:TRP:CH2	1:A:2523:VAL:HG11	2.55	0.41
1:A:3836:LEU:HD23	1:A:3991:ASP:HB3	2.00	0.41
1:A:3915:TRP:O	1:A:3918:VAL:HB	2.20	0.41
1:A:3934:TYR:C	1:A:3934:TYR:CD1	2.93	0.41
1:A:1496:VAL:HA	1:A:1499:TRP:HE1	1.84	0.41
1:A:1982:GLY:HA2	4:A:4403:ATP:C5'	2.50	0.41
1:A:2186:ASP:HB3	1:A:2238:LEU:HD21	2.01	0.41
1:A:3214:LEU:HD12	1:A:3214:LEU:N	2.35	0.41
1:A:1691:ALA:HA	2:A:4401:AOV:O1G	2.20	0.41
1:A:1289:MET:CE	1:A:1379:MET:HG2	2.51	0.41
1:A:1514:LEU:HD23	1:A:1538:ILE:CD1	2.50	0.41
1:A:3551:LEU:HD13	1:A:3555:VAL:HG23	2.02	0.41
1:A:3790:PRO:O	1:A:3794:LYS:HB2	2.20	0.41
1:A:2296:GLY:HA2	5:A:4405:ADP:H5'1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1440:ILE:HD11	1:A:1453:HIS:CB	2.51	0.41
1:A:1563:ILE:O	1:A:1566:GLN:HB3	2.20	0.41
1:A:3270:VAL:O	1:A:3273:GLN:HB3	2.19	0.41
1:A:1849:PHE:CE2	1:A:1869:LEU:HB2	2.56	0.41
1:A:3238:PHE:CG	1:A:3238:PHE:O	2.72	0.41
1:A:3249:GLU:HA	1:A:3252:ILE:HD12	2.03	0.41
1:A:3648:TRP:CZ3	1:A:3662:PRO:HG3	2.56	0.41
1:A:1690:PRO:CD	1:A:1818:SER:HA	2.48	0.41
1:A:2223:PHE:CD2	1:A:2224:HIS:HB2	2.55	0.41
1:A:2335:CYS:SG	1:A:2348:PRO:HA	2.60	0.41
1:A:2534:LEU:HD12	1:A:2534:LEU:N	2.36	0.41
1:A:4153:ASN:O	1:A:4157:LYS:HG2	2.21	0.41
1:A:4166:GLU:HG2	1:A:4167:THR:N	2.36	0.41
1:A:1352:LEU:O	1:A:1356:PHE:N	2.47	0.41
1:A:1486:PHE:CD1	1:A:1506:GLU:OE1	2.74	0.41
1:A:1591:ILE:O	1:A:1592:LEU:HB2	2.21	0.41
1:A:1729:VAL:O	1:A:1732:VAL:HG22	2.21	0.41
1:A:1718:GLY:HA2	1:A:1746:LEU:HD12	2.03	0.41
1:A:1925:VAL:HG23	1:A:1926:PHE:CD1	2.53	0.41
1:A:2067:ASN:O	1:A:2071:ASP:HB2	2.20	0.41
1:A:2421:PHE:HA	1:A:2424:ILE:HD12	2.02	0.41
1:A:2524:LEU:HD12	1:A:2564:ILE:HG21	2.03	0.41
1:A:3502:MET:HE1	1:A:3551:LEU:HD12	2.03	0.41
1:A:3505:ILE:HD11	1:A:3578:GLY:HA3	2.03	0.41
1:A:4238:ASP:OD1	1:A:4239:SER:N	2.54	0.41
1:A:1388:VAL:CG1	1:A:1389:THR:N	2.84	0.41
1:A:1480:GLU:CD	1:A:1480:GLU:H	2.25	0.41
1:A:1640:CYS:SG	1:A:1641:CYS:N	2.94	0.41
1:A:2152:ALA:O	1:A:2156:VAL:HG23	2.21	0.41
1:A:2573:TYR:CZ	1:A:2601:LYS:HG3	2.56	0.41
1:A:3759:GLN:O	1:A:3762:LEU:HG	2.21	0.41
1:A:4072:ILE:O	1:A:4075:PHE:HB3	2.21	0.41
1:A:4291:ASN:OD1	1:A:4294:GLN:HB2	2.21	0.41
1:A:1906:THR:CG2	1:A:1910:PHE:CE1	3.04	0.41
1:A:2230:TYR:OH	1:A:2270:ARG:N	2.53	0.41
1:A:2338:ILE:HD11	1:A:2345:VAL:HG13	2.03	0.41
1:A:2689:GLN:CG	1:A:2690:PHE:N	2.83	0.41
1:A:3552:GLN:O	1:A:3555:VAL:HB	2.21	0.41
1:A:1591:ILE:HG22	1:A:1592:LEU:N	2.36	0.40
1:A:1693:THR:HG21	1:A:1817:MET:CB	2.51	0.40
1:A:1710:VAL:HA	1:A:1737:TRP:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1789:ILE:HG13	1:A:1789:ILE:O	2.21	0.40
1:A:1980:PRO:O	1:A:1983:ALA:HB2	2.21	0.40
1:A:2156:VAL:HG13	1:A:2200:LEU:HD21	2.04	0.40
1:A:2523:VAL:O	1:A:2527:VAL:HG23	2.21	0.40
1:A:2739:TYR:CB	1:A:2744:LEU:HD21	2.51	0.40
1:A:3202:LYS:O	1:A:3206:LEU:HG	2.21	0.40
1:A:3230:THR:CG2	1:A:3235:LEU:O	2.70	0.40
1:A:3387:VAL:HG12	1:A:3388:THR:N	2.36	0.40
1:A:3512:ILE:CG2	1:A:4021:LEU:HD23	2.52	0.40
1:A:3640:LEU:CD1	1:A:3642:PHE:CZ	3.04	0.40
1:A:3686:LEU:O	1:A:3689:ALA:HB3	2.21	0.40
1:A:1624:TRP:CD1	1:A:3914:GLN:HB2	2.56	0.40
1:A:1539:LEU:O	1:A:1543:GLU:HG2	2.21	0.40
1:A:2399:ASN:C	1:A:2400:ILE:HD12	2.41	0.40
1:A:2553:THR:HG22	1:A:2557:GLN:NE2	2.36	0.40
1:A:3670:SER:OG	1:A:3673:GLN:HG3	2.22	0.40
1:A:3675:ILE:HD11	1:A:3693:PHE:CB	2.49	0.40
1:A:3687:GLN:HB3	1:A:4007:GLN:OE1	2.22	0.40
1:A:4075:PHE:C	1:A:4075:PHE:CD1	2.94	0.40
1:A:2296:GLY:C	5:A:4405:ADP:O1A	2.60	0.40
1:A:1741:ASP:O	1:A:1742:GLU:HB2	2.21	0.40
1:A:2174:ASN:HA	1:A:2426:ARG:HD2	2.03	0.40
1:A:2766:ASN:O	1:A:2769:THR:HB	2.21	0.40
1:A:3710:LEU:CD1	1:A:3736:GLU:CD	2.89	0.40
1:A:4288:CYS:HG	1:A:4290:GLY:C	2.24	0.40
1:A:1982:GLY:HA2	4:A:4403:ATP:H5'1	2.04	0.40
1:A:1986:SER:HA	1:A:1989:TRP:NE1	2.37	0.40
1:A:2453:ASN:ND2	1:A:2512:GLU:HA	2.36	0.40
1:A:2664:ILE:CD1	1:A:2664:ILE:H	2.34	0.40
1:A:3858:THR:HG23	1:A:3859:HIS:N	2.36	0.40
1:A:4200:PHE:HB2	1:A:4252:TRP:CZ3	2.57	0.40
1:A:1567:LEU:HB3	1:A:1607:ILE:HD11	2.04	0.40
1:A:2175:GLY:HA3	1:A:2196:LEU:CD2	2.51	0.40
1:A:2659:VAL:HG13	1:A:2659:VAL:O	2.21	0.40
1:A:3277:CYS:SG	1:A:3368:LEU:HD23	2.61	0.40
1:A:3486:ASP:O	1:A:3490:ASP:N	2.42	0.40
1:A:3588:GLU:HA	1:A:3633:LEU:HD11	2.03	0.40
1:A:3755:MET:HB2	1:A:3780:LYS:O	2.21	0.40
1:A:3939:VAL:HG22	1:A:4296:ILE:HG22	2.04	0.40
1:A:4073:LEU:O	1:A:4077:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2995/3450 (87%)	2834 (95%)	153 (5%)	8 (0%)	41 74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1820	PRO
1	A	3965	PHE
1	A	1589	SER
1	A	1645	VAL
1	A	3375	PRO
1	A	4027	ALA
1	A	1529	VAL
1	A	3952	VAL

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2286/3065 (75%)	2201 (96%)	85 (4%)	34 65

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1307	CYS
1	A	1392	THR
1	A	1465	CYS

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Mol	Chain	Res	Type
1	A	1513	GLN
1	A	1536	SER
1	A	1570	LYS
1	A	1705	LEU
1	A	1737	TRP
1	A	1739	CYS
1	A	1744	ASN
1	A	1787	ILE
1	A	1796	LYS
1	A	1944	LYS
1	A	1977	ILE
1	A	1997	CYS
1	A	1999	THR
1	A	2050	SER
1	A	2064	GLU
1	A	2116	SER
1	A	2178	HIS
1	A	2248	ASP
1	A	2253	ASP
1	A	2258	LEU
1	A	2322	THR
1	A	2435	ARG
1	A	2521	ASP
1	A	2570	ASP
1	A	2615	LEU
1	A	2627	ILE
1	A	2635	GLU
1	A	2661	ARG
1	A	2782	MET
1	A	2821	GLU
1	A	2875	PHE
1	A	3239	ASP
1	A	3262	ASP
1	A	3279	PHE
1	A	3309	ASN
1	A	3336	LEU
1	A	3343	ASP
1	A	3357	ASP
1	A	3391	ASN
1	A	3397	SER
1	A	3495	LEU
1	A	3518	PHE

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Mol	Chain	Res	Type
1	A	3582	GLU
1	A	3583	LEU
1	A	3584	PHE
1	A	3590	ASP
1	A	3640	LEU
1	A	3641	CYS
1	A	3652	TYR
1	A	3667	LYS
1	A	3671	LEU
1	A	3688	SER
1	A	3690	MET
1	A	3718	LEU
1	A	3755	MET
1	A	3761	ASP
1	A	3762	LEU
1	A	3792	LEU
1	A	3821	LEU
1	A	3842	ARG
1	A	3847	TRP
1	A	3877	ARG
1	A	3904	ASP
1	A	3921	LEU
1	A	3976	SER
1	A	4023	ARG
1	A	4026	THR
1	A	4030	LYS
1	A	4031	PHE
1	A	4032	ASP
1	A	4051	ASN
1	A	4100	VAL
1	A	4164	LEU
1	A	4180	LEU
1	A	4201	VAL
1	A	4215	ILE
1	A	4228	ASP
1	A	4246	LEU
1	A	4268	SER
1	A	4293	ASP
1	A	4298	CYS
1	A	4302	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1792	ASN
1	A	1810	GLN
1	A	2140	ASN
1	A	2178	HIS
1	A	2269	GLN
1	A	2362	ASN
1	A	2391	ASN
1	A	2580	HIS
1	A	2595	HIS
1	A	2777	HIS
1	A	3738	GLN
1	A	3742	ASN
1	A	4214	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ADP	A	4405	-	24,29,29	1.07	1 (4%)	29,45,45	1.67	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ADP	A	4406	-	24,29,29	1.12	1 (4%)	29,45,45	1.65	7 (24%)
4	ATP	A	4403	3	26,33,33	0.88	1 (3%)	31,52,52	1.99	5 (16%)
2	AOV	A	4401	3	27,34,34	5.35	3 (11%)	26,56,56	1.55	3 (11%)

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
5	ADP	A	4405	-	-	3/12/32/32	0/3/3/3
5	ADP	A	4406	-	-	0/12/32/32	0/3/3/3
4	ATP	A	4403	3	-	0/18/38/38	0/3/3/3
2	AOV	A	4401	3	-	0/12/39/39	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4401	AOV	O1G-VG	27.32	2.10	1.61
5	A	4406	ADP	PB-O1B	3.16	1.60	1.50
2	A	4401	AOV	C5-C4	2.50	1.47	1.40
2	A	4401	AOV	C2-N3	2.37	1.35	1.32
5	A	4405	ADP	C4-N3	-2.31	1.32	1.35
4	A	4403	ATP	C2-N3	2.07	1.35	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4403	ATP	PA-O3A-PB	-6.39	110.88	132.83
4	A	4403	ATP	PB-O3B-PG	-6.11	111.86	132.83
2	A	4401	AOV	PA-O3A-PB	-4.77	116.47	132.83
5	A	4405	ADP	C4-C5-N7	-4.16	105.06	109.40
2	A	4401	AOV	C4-C5-N7	-3.87	105.36	109.40
5	A	4406	ADP	N3-C2-N1	-3.77	122.78	128.68
4	A	4403	ATP	N3-C2-N1	-3.74	122.83	128.68
5	A	4405	ADP	C3'-C2'-C1'	3.60	106.40	100.98
5	A	4405	ADP	PA-O3A-PB	-3.59	120.50	132.83
2	A	4401	AOV	N3-C2-N1	-3.45	123.28	128.68
5	A	4406	ADP	PA-O3A-PB	-3.17	121.94	132.83
5	A	4406	ADP	O3B-PB-O2B	2.85	118.52	107.64
5	A	4406	ADP	C3'-C2'-C1'	2.67	105.00	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4403	ATP	C4-C5-N7	-2.58	106.71	109.40
5	A	4406	ADP	C4-C5-N7	-2.54	106.75	109.40
5	A	4406	ADP	O2A-PA-O1A	2.46	124.41	112.24
5	A	4406	ADP	O4'-C4'-C3'	2.27	109.60	105.11
5	A	4405	ADP	N3-C2-N1	-2.23	125.19	128.68
5	A	4405	ADP	O2A-PA-O1A	2.20	123.10	112.24
5	A	4405	ADP	O2B-PB-O3A	2.13	111.76	104.64
4	A	4403	ATP	O4'-C4'-C3'	2.05	109.17	105.11
5	A	4405	ADP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4405	ADP	C5'-O5'-PA-O2A
5	A	4405	ADP	C5'-O5'-PA-O3A
5	A	4405	ADP	O4'-C4'-C5'-O5'

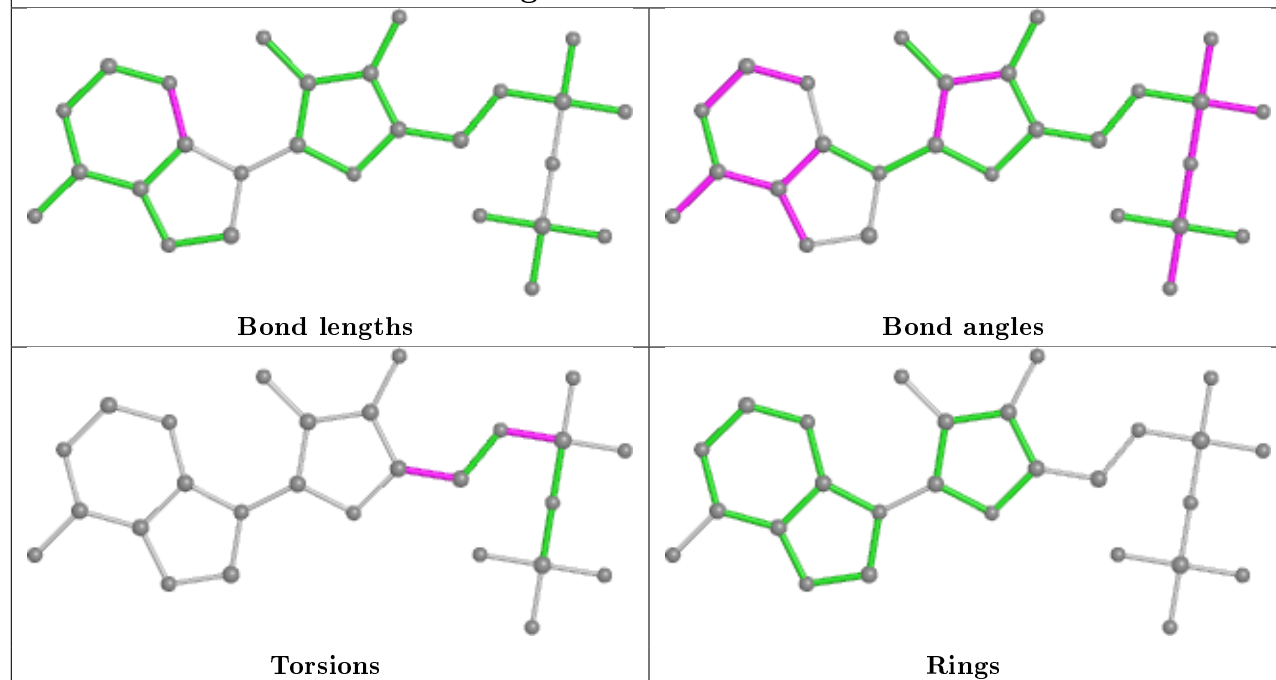
There are no ring outliers.

4 monomers are involved in 26 short contacts:

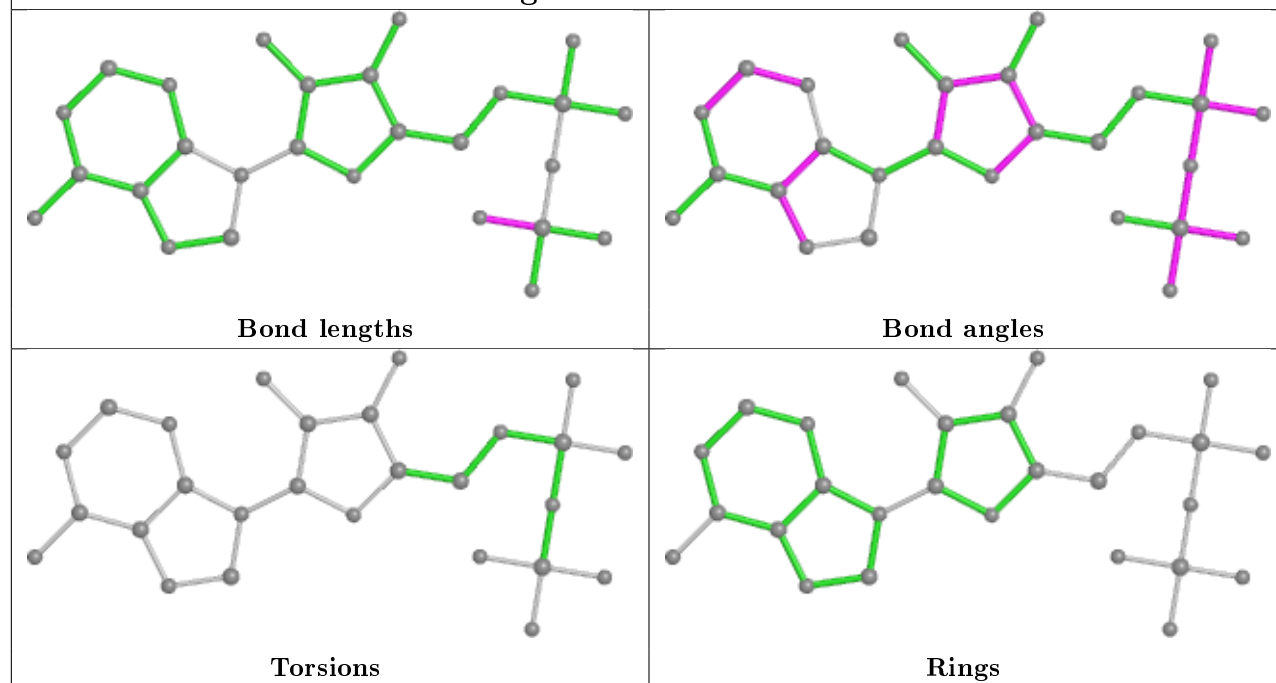
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4405	ADP	5	0
5	A	4406	ADP	5	0
4	A	4403	ATP	4	0
2	A	4401	AOV	12	0

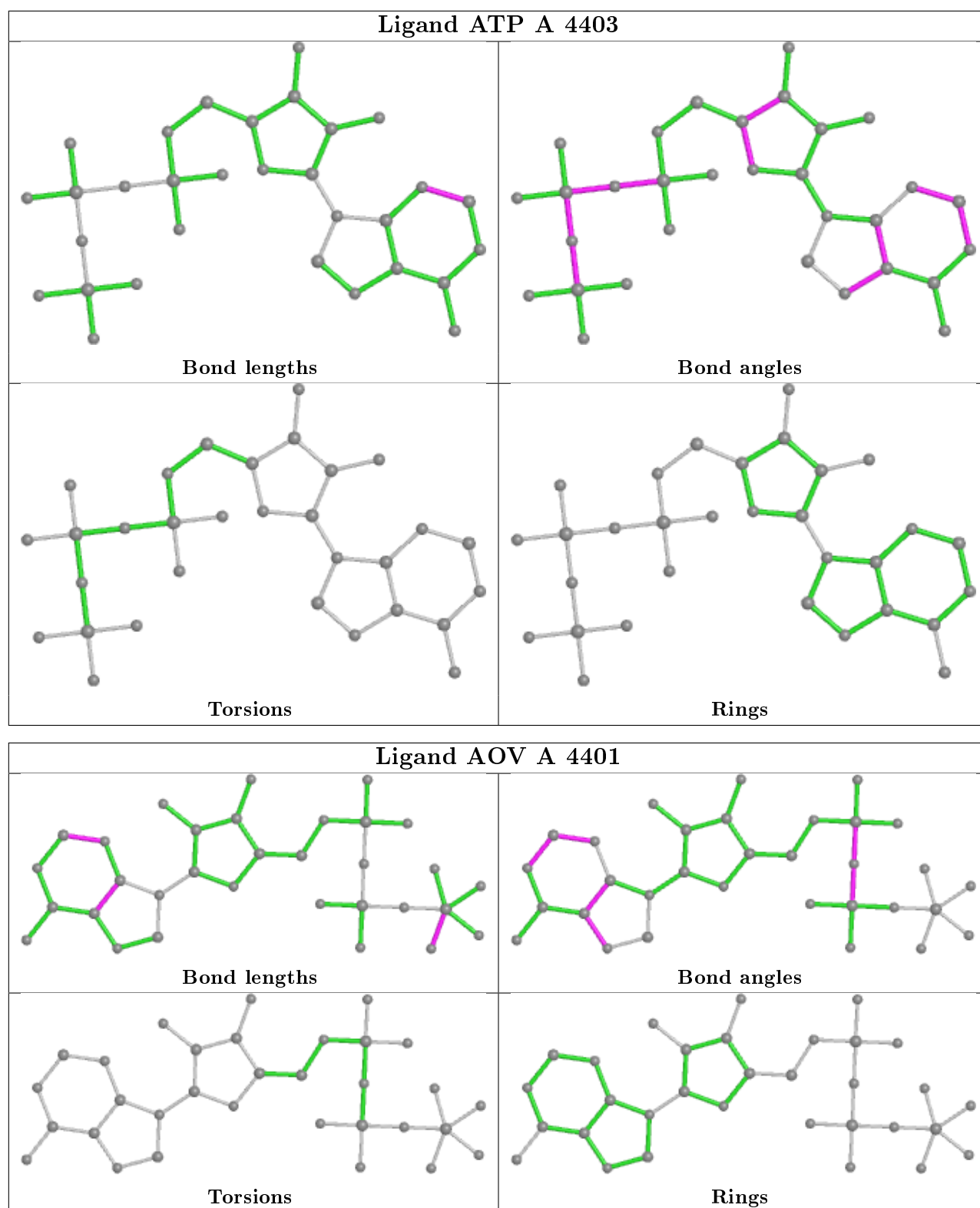
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand ADP A 4405



## Ligand ADP A 4406





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	3005/3450 (87%)	-0.31	85 (2%) 53 52	39, 110, 274, 477	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3130	LEU	8.1
1	A	2975	ASP	5.9
1	A	3136	SER	5.5
1	A	2942	SER	4.7
1	A	2946	ALA	4.5
1	A	3134	LEU	4.4
1	A	2949	GLN	4.1
1	A	2945	ASP	4.0
1	A	3138	GLY	3.9
1	A	3133	LEU	3.9
1	A	2915	ASN	3.8
1	A	2953	LEU	3.7
1	A	3139	GLN	3.7
1	A	3123	THR	3.7
1	A	3135	ASN	3.7
1	A	2918	ALA	3.6
1	A	3131	GLU	3.6
1	A	2909	ALA	3.5
1	A	2964	VAL	3.5
1	A	2947	SER	3.5
1	A	2911	VAL	3.4
1	A	2907	ALA	3.3
1	A	2937	GLN	3.2
1	A	3238	PHE	3.2
1	A	3142	SER	3.2
1	A	2956	LEU	3.2
1	A	3137	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1579	THR	3.1
1	A	3019	GLY	3.1
1	A	2938	MET	3.1
1	A	2951	THR	3.0
1	A	4030	LYS	3.0
1	A	3156	ALA	2.9
1	A	3533	ASN	2.8
1	A	4056	LEU	2.8
1	A	3128	ARG	2.8
1	A	3144	LEU	2.8
1	A	1318	TYR	2.7
1	A	3642	PHE	2.7
1	A	2935	ALA	2.7
1	A	3451	ILE	2.7
1	A	3910	ALA	2.7
1	A	4029	SER	2.6
1	A	2902	SER	2.6
1	A	2912	ASP	2.6
1	A	4031	PHE	2.6
1	A	2906	GLU	2.6
1	A	3187	ASN	2.6
1	A	3132	GLU	2.6
1	A	4026	THR	2.6
1	A	3143	GLU	2.5
1	A	3154	GLU	2.5
1	A	1321	PHE	2.5
1	A	3125	ASP	2.5
1	A	3025	GLY	2.5
1	A	1653	TYR	2.5
1	A	2944	GLN	2.5
1	A	3159	GLU	2.4
1	A	3129	LYS	2.4
1	A	3121	LYS	2.4
1	A	3153	SER	2.4
1	A	3127	LYS	2.4
1	A	3155	ALA	2.3
1	A	3448	GLN	2.3
1	A	3141	VAL	2.3
1	A	2962	GLU	2.3
1	A	3037	PHE	2.3
1	A	3168	THR	2.2
1	A	2900	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	3126	ARG	2.2
1	A	3119	ASN	2.2
1	A	2943	MET	2.2
1	A	2939	ILE	2.2
1	A	2950	LYS	2.2
1	A	2941	VAL	2.2
1	A	2952	GLU	2.1
1	A	2979	LYS	2.1
1	A	2919	GLY	2.1
1	A	2933	ASP	2.1
1	A	3076	PRO	2.1
1	A	2965	VAL	2.0
1	A	2893	ARG	2.0
1	A	4057	ILE	2.0
1	A	2922	SER	2.0
1	A	3145	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

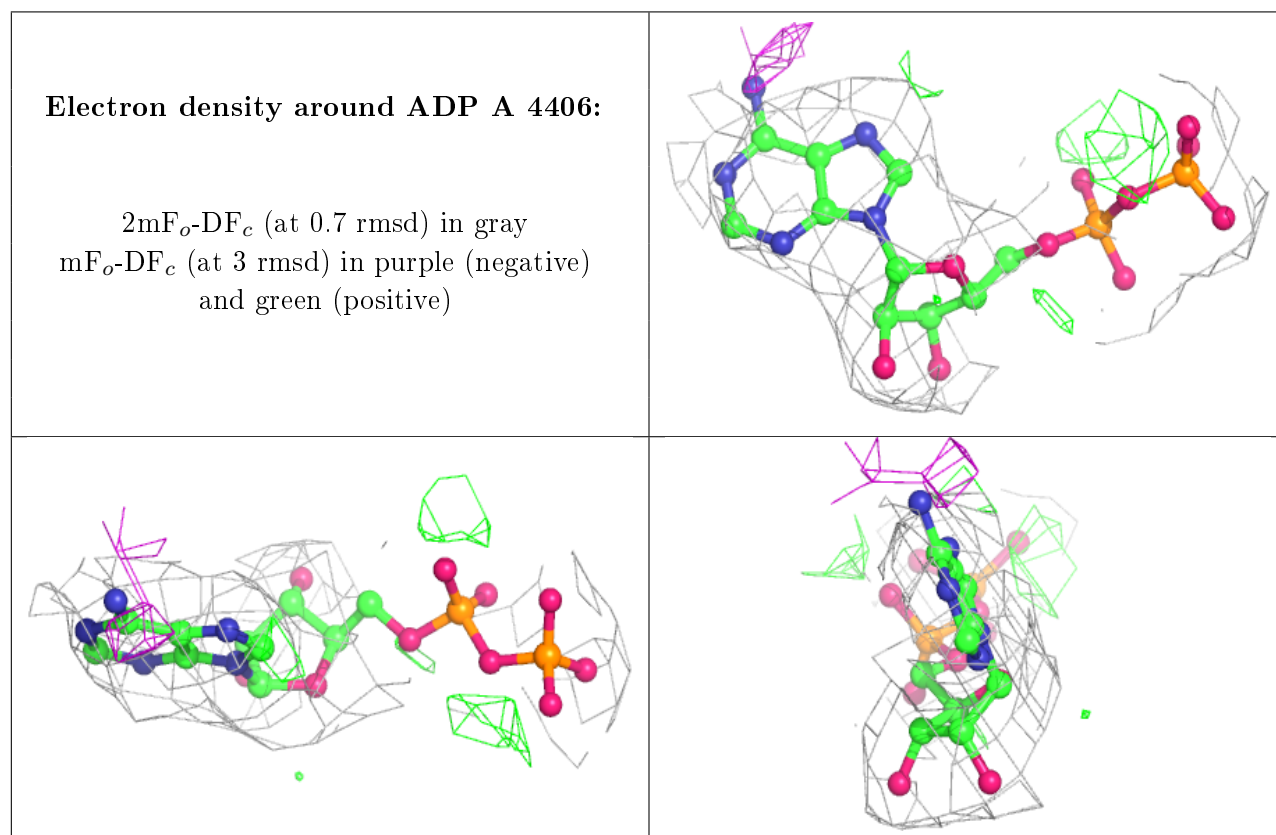
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ADP	A	4406	27/27	0.95	0.20	66,85,103,111	0
5	ADP	A	4405	27/27	0.97	0.18	42,46,57,61	0
4	ATP	A	4403	31/31	0.97	0.18	49,80,97,108	0
2	AOV	A	4401	32/32	0.98	0.20	41,69,88,93	0
3	MG	A	4402	1/1	0.99	0.21	31,31,31,31	0
3	MG	A	4404	1/1	1.00	0.22	22,22,22,22	0

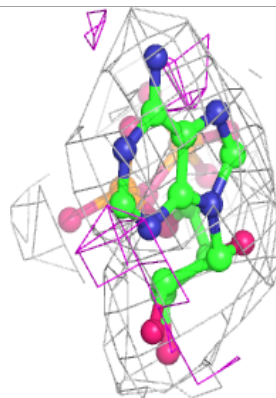
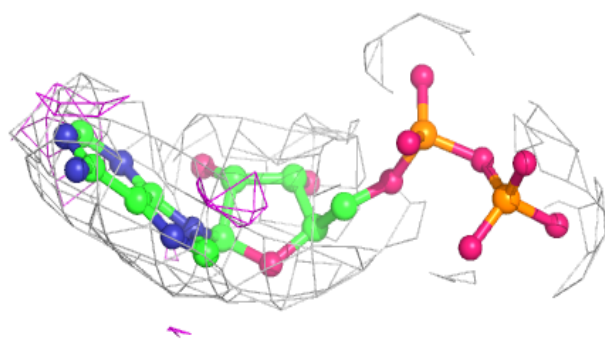
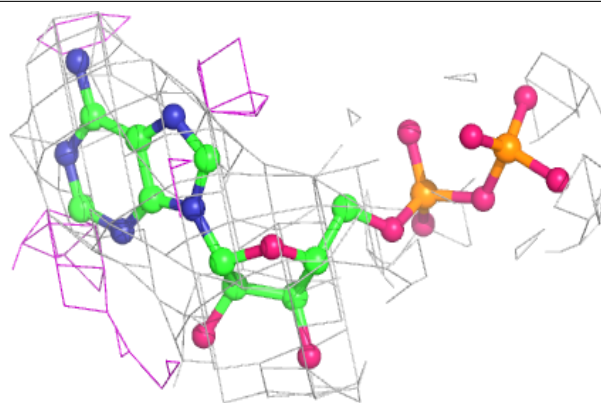
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



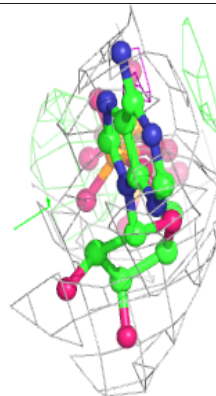
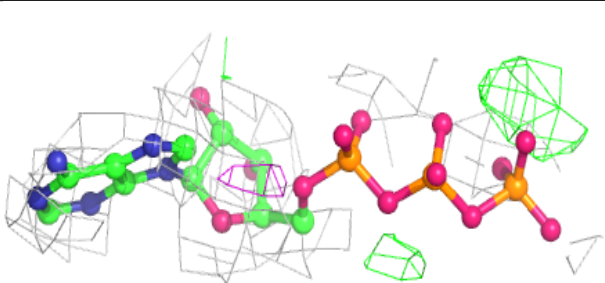
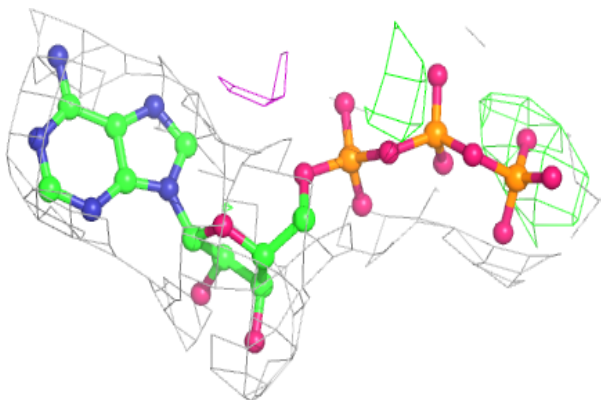


**Electron density around ADP A 4405:**

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

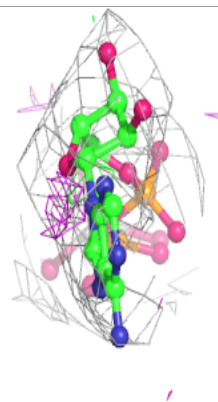
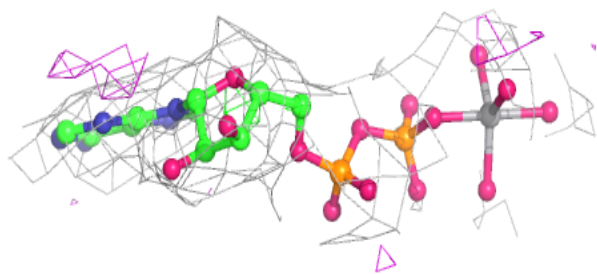
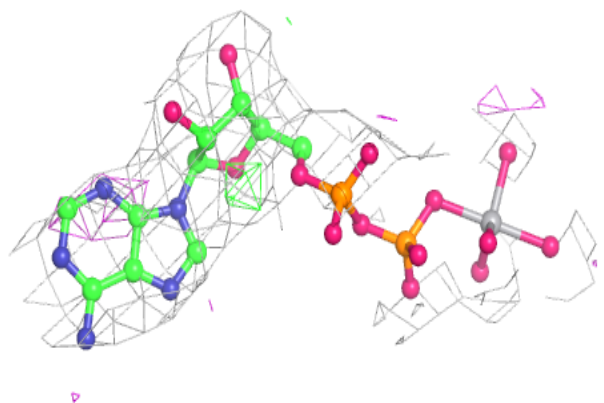
**Electron density around ATP A 4403:**

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



**Electron density around AOV A 4401:**

$2mF_o-DF_c$  (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.