Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:59 PM GMT

PDB ID	:	3VKH
Title	:	X-ray structure of a functional full-length dynein motor domain
Authors	:	Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on	:	2011-11-16
Resolution	:	3.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

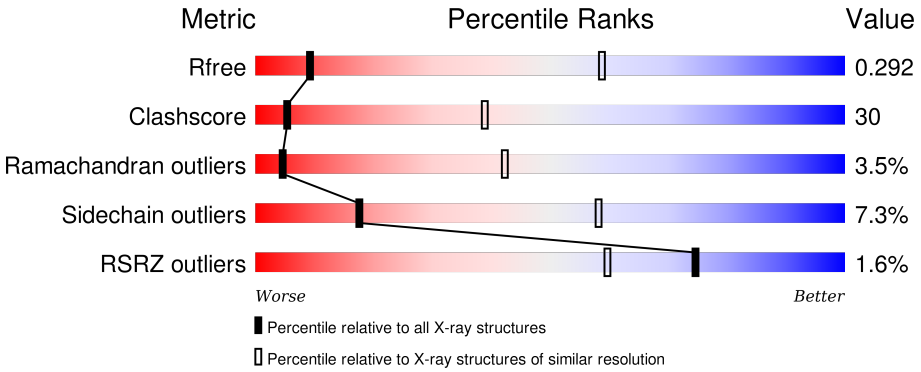
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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. 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 <=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	3367	2% 42% 42% 6% 10%
1	B	3367	% 46% 37% • 14%

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	ADP	A	9001	-	-	-	X
2	ADP	B	9007	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 45974 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	3042	Total	C	N	O	S	0	0	0
			23374	14951	3955	4368	100			
1	B	2908	Total	C	N	O	S	0	0	0
			22384	14307	3792	4190	95			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION TAG	UNP P34036
A	1371	HIS	-	EXPRESSION TAG	UNP P34036
A	1372	HIS	-	EXPRESSION TAG	UNP P34036
A	1373	GLY	-	EXPRESSION TAG	UNP P34036
A	1374	GLY	-	EXPRESSION TAG	UNP P34036
A	1375	GLY	-	EXPRESSION TAG	UNP P34036
A	1376	ASP	-	EXPRESSION TAG	UNP P34036
A	1377	TYR	-	EXPRESSION TAG	UNP P34036
A	1378	LYS	-	EXPRESSION TAG	UNP P34036
A	1379	ASP	-	EXPRESSION TAG	UNP P34036
A	1380	ASP	-	EXPRESSION TAG	UNP P34036
A	1381	ASP	-	EXPRESSION TAG	UNP P34036
A	1382	ASP	-	EXPRESSION TAG	UNP P34036
A	1383	LYS	-	EXPRESSION TAG	UNP P34036
A	1384	GLY	-	EXPRESSION TAG	UNP P34036
A	1385	GLY	-	EXPRESSION TAG	UNP P34036
A	1386	GLY	-	EXPRESSION TAG	UNP P34036
A	1387	LYS	-	EXPRESSION TAG	UNP P34036
B	1364	MET	-	EXPRESSION TAG	UNP P34036

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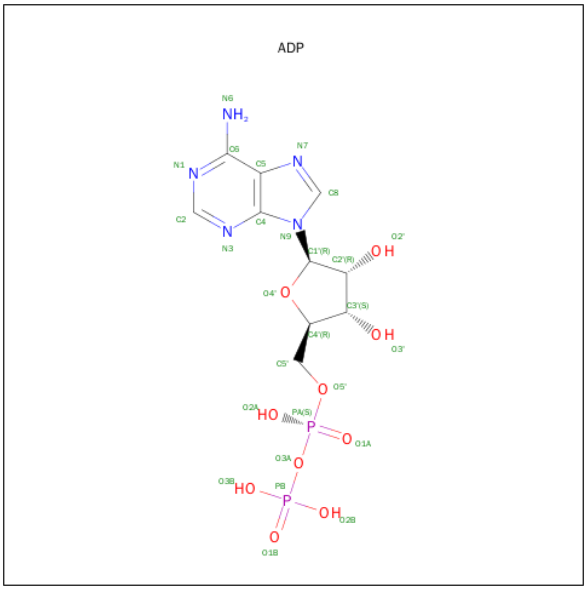
Chain	Residue	Modelled	Actual	Comment	Reference
B	1365	THR	-	EXPRESSION TAG	UNP P34036
B	1366	ARG	-	EXPRESSION TAG	UNP P34036
B	1367	HIS	-	EXPRESSION TAG	UNP P34036
B	1368	HIS	-	EXPRESSION TAG	UNP P34036
B	1369	HIS	-	EXPRESSION TAG	UNP P34036
B	1370	HIS	-	EXPRESSION TAG	UNP P34036
B	1371	HIS	-	EXPRESSION TAG	UNP P34036
B	1372	HIS	-	EXPRESSION TAG	UNP P34036
B	1373	GLY	-	EXPRESSION TAG	UNP P34036
B	1374	GLY	-	EXPRESSION TAG	UNP P34036
B	1375	GLY	-	EXPRESSION TAG	UNP P34036
B	1376	ASP	-	EXPRESSION TAG	UNP P34036
B	1377	TYR	-	EXPRESSION TAG	UNP P34036
B	1378	LYS	-	EXPRESSION TAG	UNP P34036
B	1379	ASP	-	EXPRESSION TAG	UNP P34036
B	1380	ASP	-	EXPRESSION TAG	UNP P34036
B	1381	ASP	-	EXPRESSION TAG	UNP P34036
B	1382	ASP	-	EXPRESSION TAG	UNP P34036
B	1383	LYS	-	EXPRESSION TAG	UNP P34036
B	1384	GLY	-	EXPRESSION TAG	UNP P34036
B	1385	GLY	-	EXPRESSION TAG	UNP P34036
B	1386	GLY	-	EXPRESSION TAG	UNP P34036
B	1387	LYS	-	EXPRESSION TAG	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



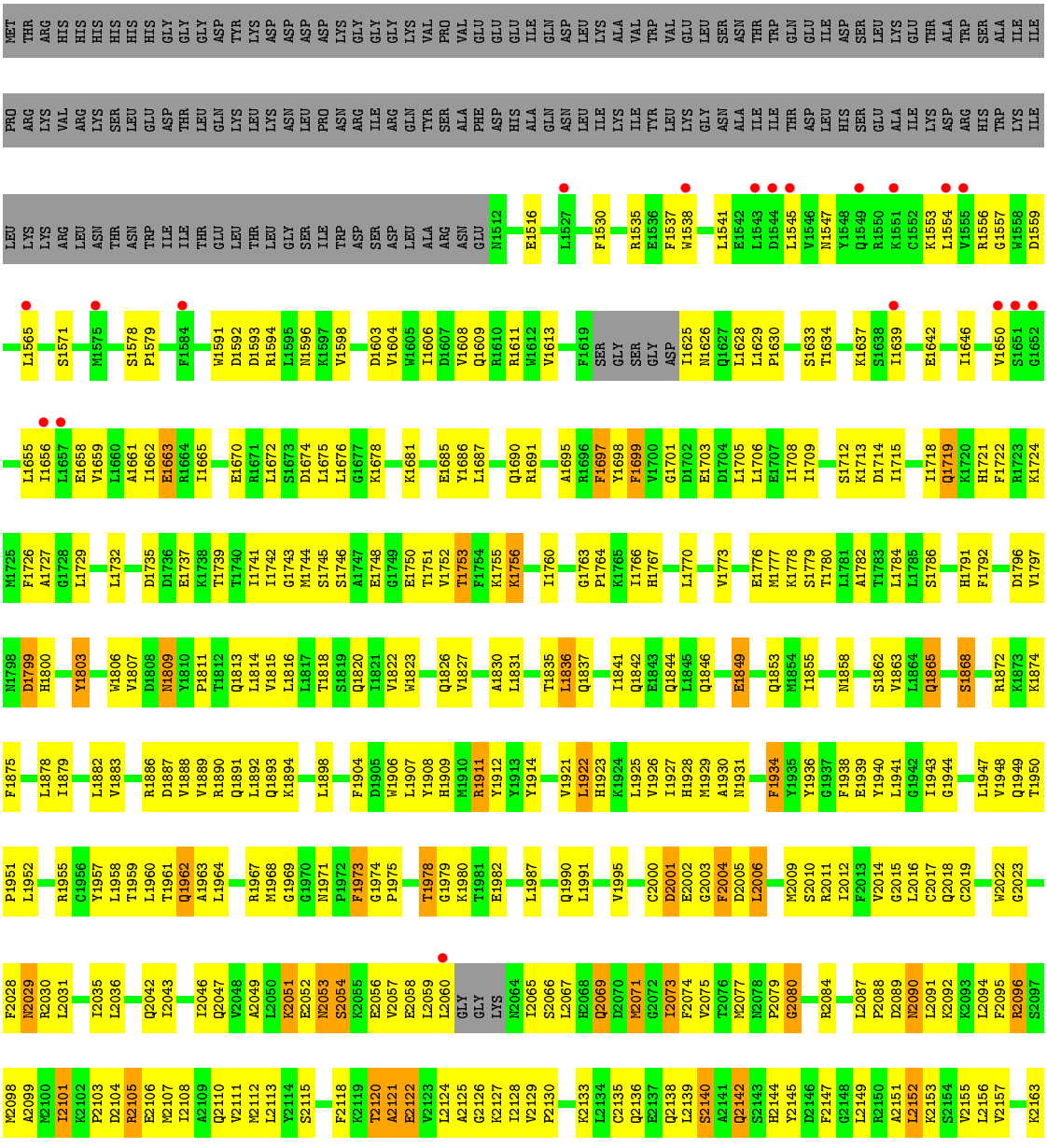
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

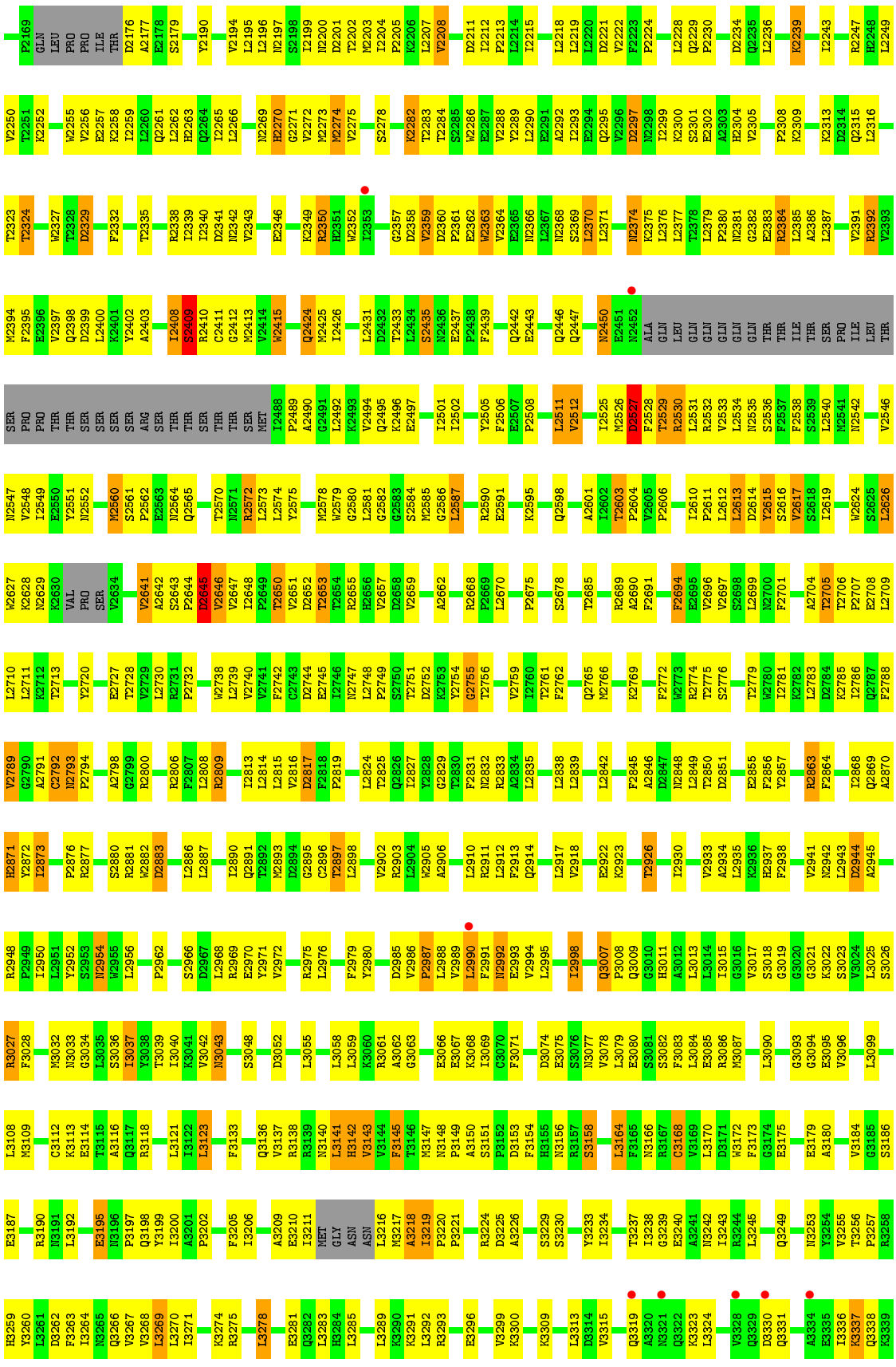
3 Residue-property plots (i)

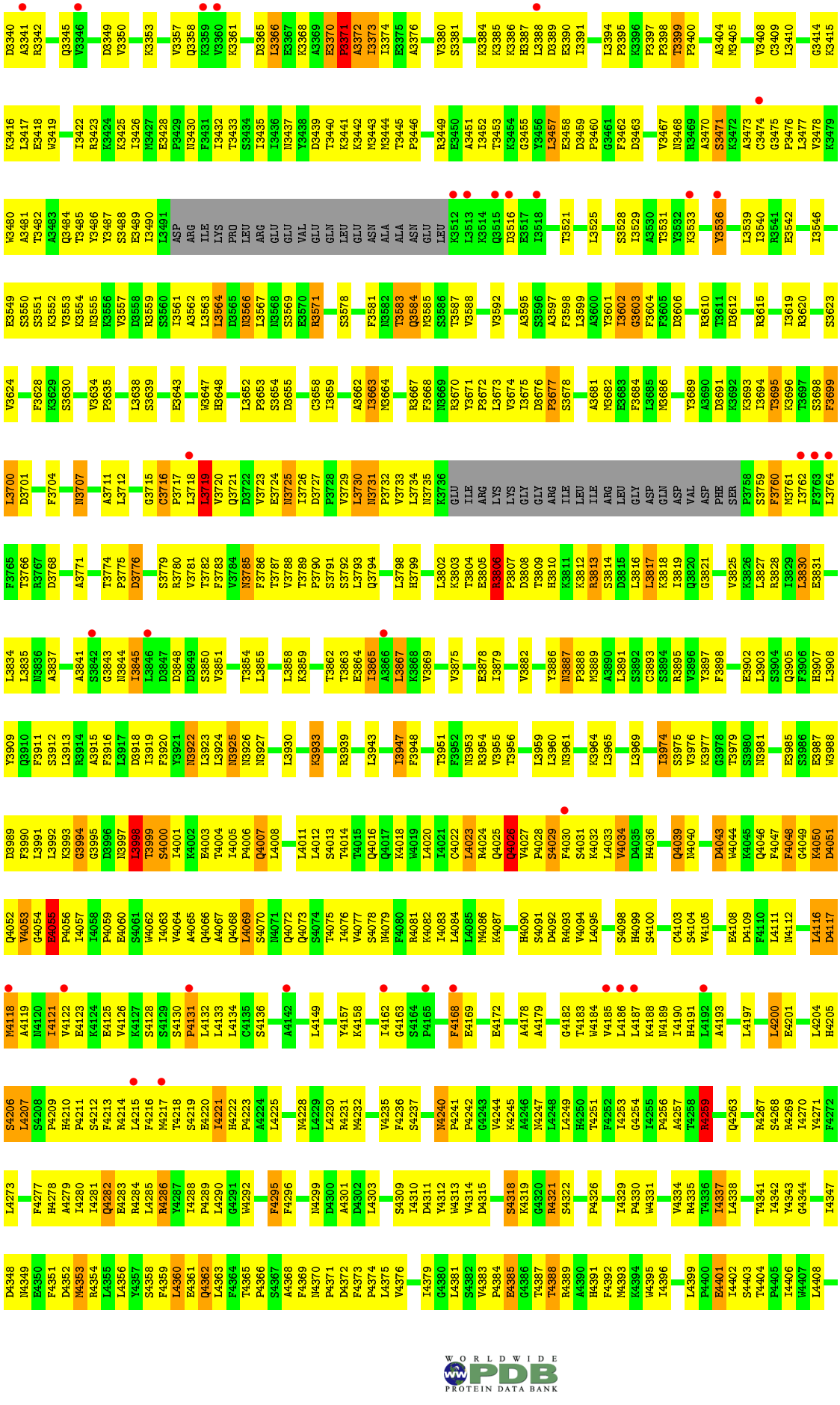
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

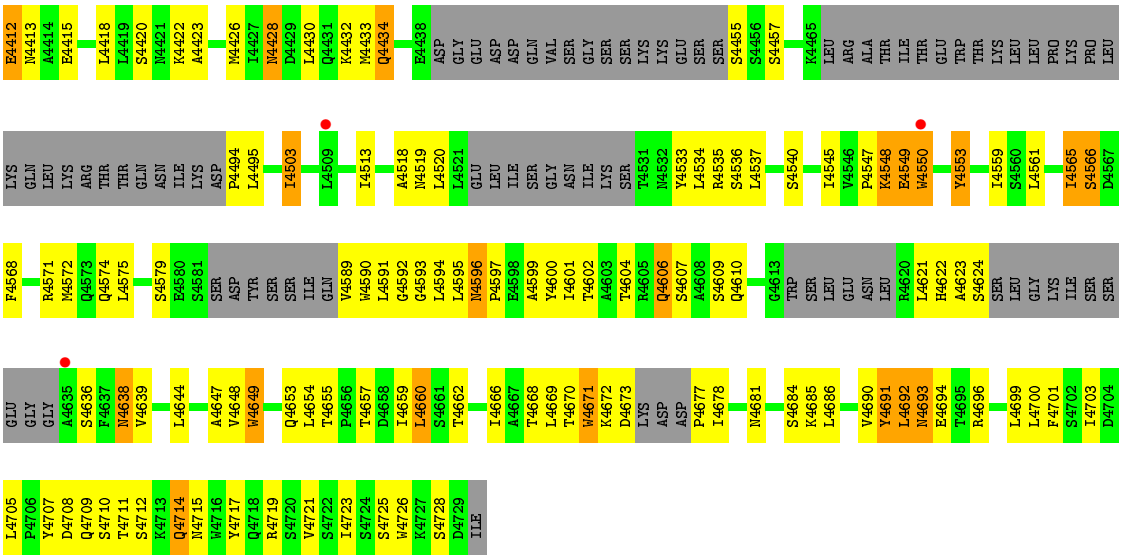
- Molecule 1: Dynein heavy chain, cytoplasmic

Chain A:

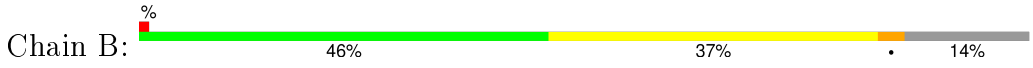


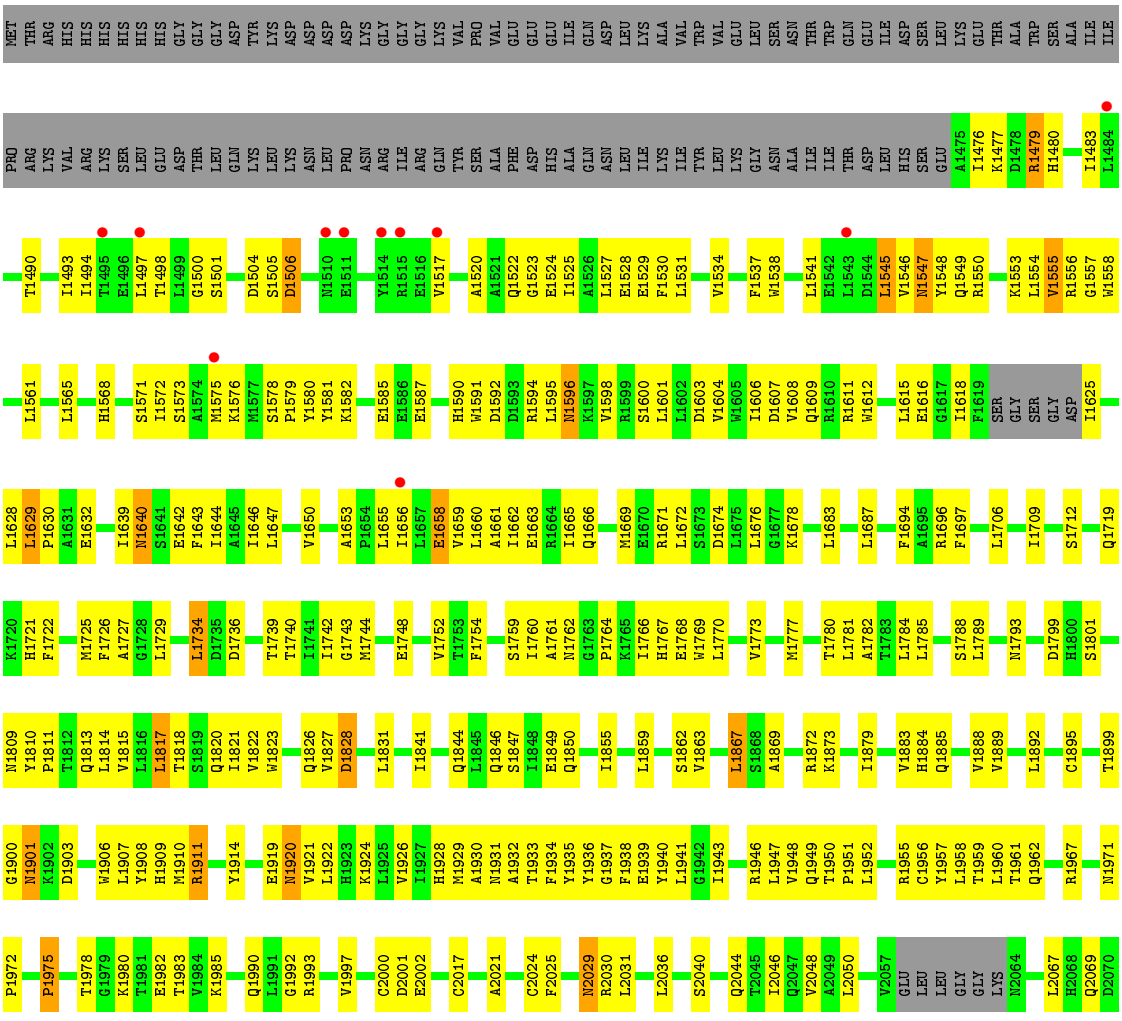

P2169 GLN LEU PRO PRO ILE THR D2176 A2177 E2178 S2179 V2190 V2194 L2195 L2196 N2197 S2198 I2199 N2200 D2201 T2202 M2203 I2204 P2205 K2206 L2207 V2208 D2211 I2212 P2213 L2214 I2215 L2218 L2219 L2220 D2221 V2222 F2223 P2224 L2228 Q2229 P2230 D2234 Q2235 L2236 K2239 I2243 R2247 H2248 L2249
V2250 T2251 K2252 W2255 V2256 E2257 K2258 I2259 L2260 Q2261 L2262 H2263 Q2264 I2265 L2266 N2269 H2270 G2271 V2272 M2273 M2274 V2275 S2278 K2282 T2283 T2284 S2285 W2286 E2287 V2288 Y2289 L2290 E2291 A2292 I2293 E2294 Q2295 V2296 D2297 N2298 I2299 K2300 S2301 E2302 A2303 H2304 V2305 P2308 K2309 K2313 D2314 Q2315 L2316
T2323 T2324 W2327 T2328 D2329 F2332 T2335 R2338 I2339 I2340 D2341 N2342 V2343 E2346 K2349 R2350 H2351 W2352 I2353 G2357 D2358 V2359 D2360 P2361 E2362 W2363 V2364 E2365 N2366 L2367 N2368 S2369 L2370 L2371 N2374 K2375 L2376 L2377 T2378 L2379 P2380 N2381 G2382 E2383 R2384 L2385 A2386 L2387 V2391 R2392 V2393
M2394 F2395 E2396 V2397 Q2398 D2399 L2400 K2401 Y2402 A2403 I2408 S2409 R2410 C2411 G2412 M2413 V2414 W2415 Q2424 M2425 I2426 L2431 D2432 T2433 L2434 S2435 N2436 E2437 P2438 F2439 Q2442 E2443 Q2446 Q2447 N2450 E2451 N2452 ALA GLN LEU GLN GLN GLN GLN GLN THR THR ILE THR SER PRO ILE LEU THR
SER PRO PRO THR THR SER SER SER SER ARG SER THR THR SER THR THR THR SER MET I2488 P2489 A2490 G2491 L2492 K2493 V2494 Q2495 K2496 E2497 I2501 I2502 Y2505 F2506 E2507 P2508 L2511 V2512 I2525 M2526 D2527 F2528 T2529 R2530 L2531 R2532 V2533 L2534 N2535 S2536 F2537 F2538 S2539 L2540 M2541 N2542 V2546
N2547 V2548 I2549 E2550 V2551 N2552 M2560 S2561 P2562 E2563 N2564 Q2565 T2570 N2571 R2572 L2573 L2574 Y2575 M2578 W2579 G2580 L2581 G2582 G2583 S2584 M2585 G2586 L2587 R2590 E2591 K2595 Q2598 A2601 I2602 T2603 P2604 V2605 P2606 I2610 P2611 L2612 L2613 D2614 Y2615 S2616 V2617 S2618 I2619 W2624 S2625 L2626
W2627 K2628 N2629 K2630 VAL PRO SER V2634 V2641 A2642 S2643 P2644 D2645 V2646 V2647 I2648 P2649 T2650 V2651 D2652 T2653 T2654 R2655 H2656 V2657 D2658 V2659 A2662 R2668 P2669 L2670 P2675 S2678 T2685 R2689 A2690 F2691 F2694 E2695 V2696 V2697 S2698 L2699 N2700 F2701 A2704 T2705 T2706 P2707 E2708 L2709
L2710 L2711 K2712 T2713 Y2720 E2727 T2728 V2729 L2730 R2731 P2732 W2738 L2739 V2740 V2741 F2742 C2743 D2744 E2745 I2746 N2747 L2748 P2749 S2750 T2751 D2752 K2753 Y2754 G2755 T2756 V2759 I2760 T2761 F2762 Q2765 M2766 K2769 F2772 W2773 R2774 T2775 S2776 T2779 W2780 I2781 K2782 L2783 D2784 K2785 I2786 Q2787 F2788
V2789 G2790 A2791 C2792 N2793 P2794 A2798 G2799 R2800 R2806 F2807 L2808 R2809 I2813 L2814 L2815 V2816 D2817 F2818 P2819 L2824 T2825 Q2826 I2827 Y2828 G2829 T2830 F2831 N2832 R2833 A2834 L2835 L2838 L2839 L2842 F2845 A2846 D2847 N2848 L2849 T2850 D2851 E2855 F2856 Y2857 R2863 F2864 I2868 Q2869 A2870
H2871 V2872 I2873 P2876 R2877 S2880 R2881 W2882 D2883 L2886 L2887 I2890 Q2891 T2892 M2893 D2894 G2895 C2896 T2897 L2898 V2902 R2903 L2904 W2905 A2906 L2910 R2911 L2912 F2913 Q2914 L2917 V2918 E2922 K2923 T2926 I2930 V2933 A2934 L2935 K2936 H2937 F2938 V2941 N2942 L2943 D2944 A2945
R2948 P2949 I2950 L2951 V2952 S2953 N2954 W2955 L2956 P2962 S2966 D2967 L2968 R2969 E2970 Y2971 V2972 R2975 L2976 F2979 Y2980 D2985 V2986 P2987 L2988 V2989 L2990 F2991 N2992 E2993 V2994 L2995 I2998 Q3007 P3008 Q3009 G3010 H3011 A3012 L3013 L3014 I3015 G3016 V3017 S3018 G3019 G3020 G3021 K3022 S3023 V3024 L3025 S3026
R3027 F3028 M3032 N3033 G3034 L3035 S3036 I3037 Y3038 T3039 I3040 K3041 V3042 N3043 S3048 D3052 L3055 L3058 L3059 K3060 R3061 A3062 G3063 E3066 E3067 K3068 I3069 C3070 F3071 D3074 E3075 S3076 N3077 V3078 L3079 E3080 S3081 S3082 F3083 L3084 E3085 R3086 M3087 L3090 G3093 G3094 E3095 V3096 L3099
L3108 M3109 C3112 K3113 E3114 T3115 A3116 Q3117 R3118 L3121 I3122 L3123 F3133 Q3136 V3137 R3138 R3139 N3140 L3141 H3142 V3143 V3144 F3145 T3146 M3147 N3148 P3149 A3150 S3151 P3152 D3153 F3154 H3155 N3156 R3157 S3158 L3164 F3165 N3166 R3167 C3168 V3169 L3170 D3171 W3172 F3173 G3174 E3175 E3179 A3180 V3184 G3185 S3186
E3187 R3190 N3191 L3192 E3195 N3196 P3197 Q3198 Y3199 I3200 A3201 P3202 F3205 I3206 A3209 E3210 I3211 MET GLY ASN ASN L3216 M3217 A3218 I3219 P3220 P3221 R3224 D3225 A3226 S3229 S3230 Y3233 I3234 T3237 I3238 G3239 E3240 A3241 N3242 I3243 R3244 L3245 Q3249 N3253 Y3254 V3255 T3256 P3257 R3258
H3259 Y3260 L3261 D3262 F3263 I3264 N3265 Q3266 V3267 V3268 L3269 L3270 I3271 K3274 R3275 L3278 E3281 Q3282 L3283 H3284 L3285 L3289 K3290 K3291 L3292 R3293 E3296 V3299 K3300 K3309 L3313 D3314 V3315 Q3319 A3320 N3321 Q3322 K3323 L3324 V3328 Q3329 D3330 Q3331 A3334 E3335 I3336 K3337 Q3338 K3339

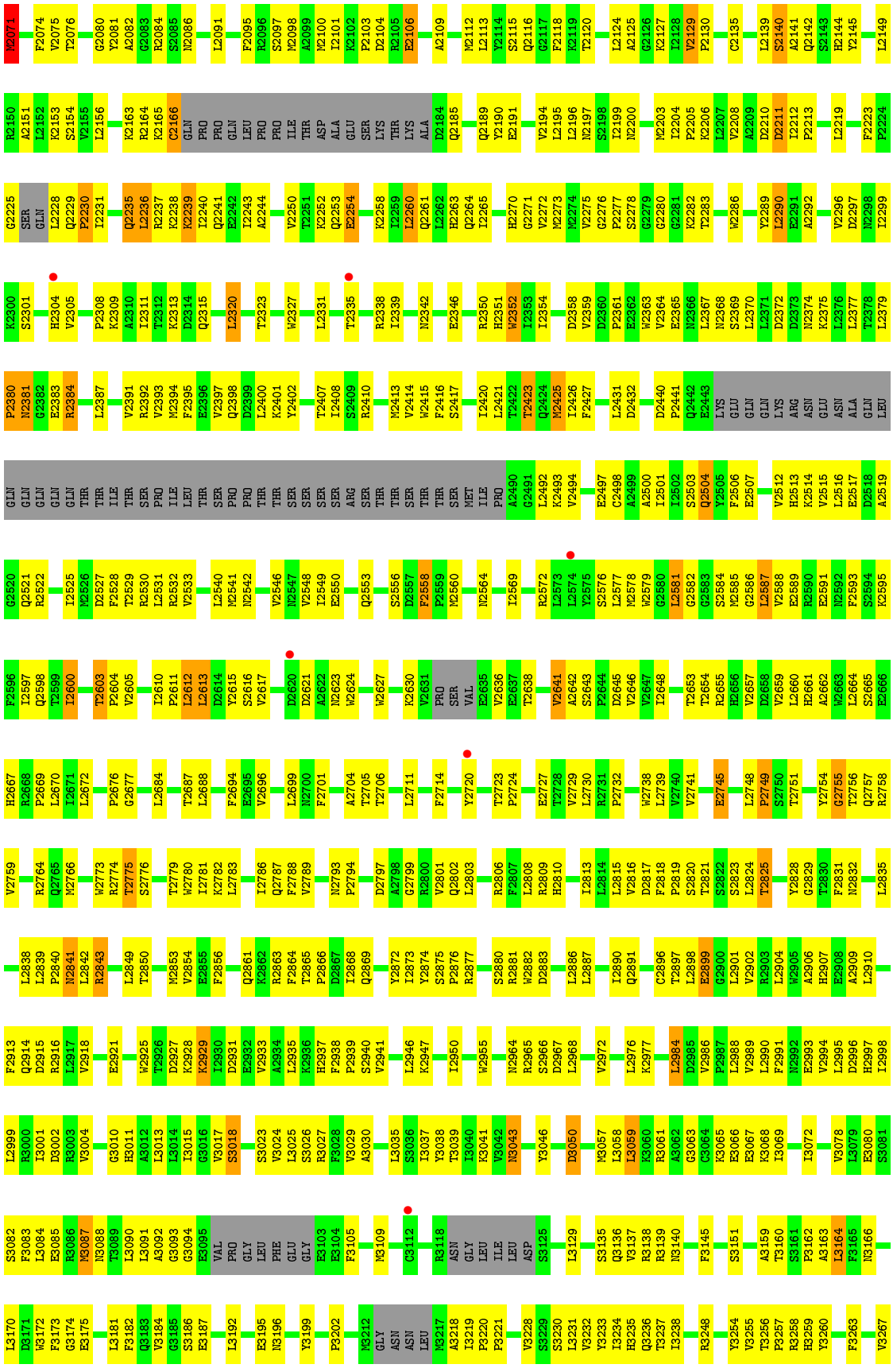


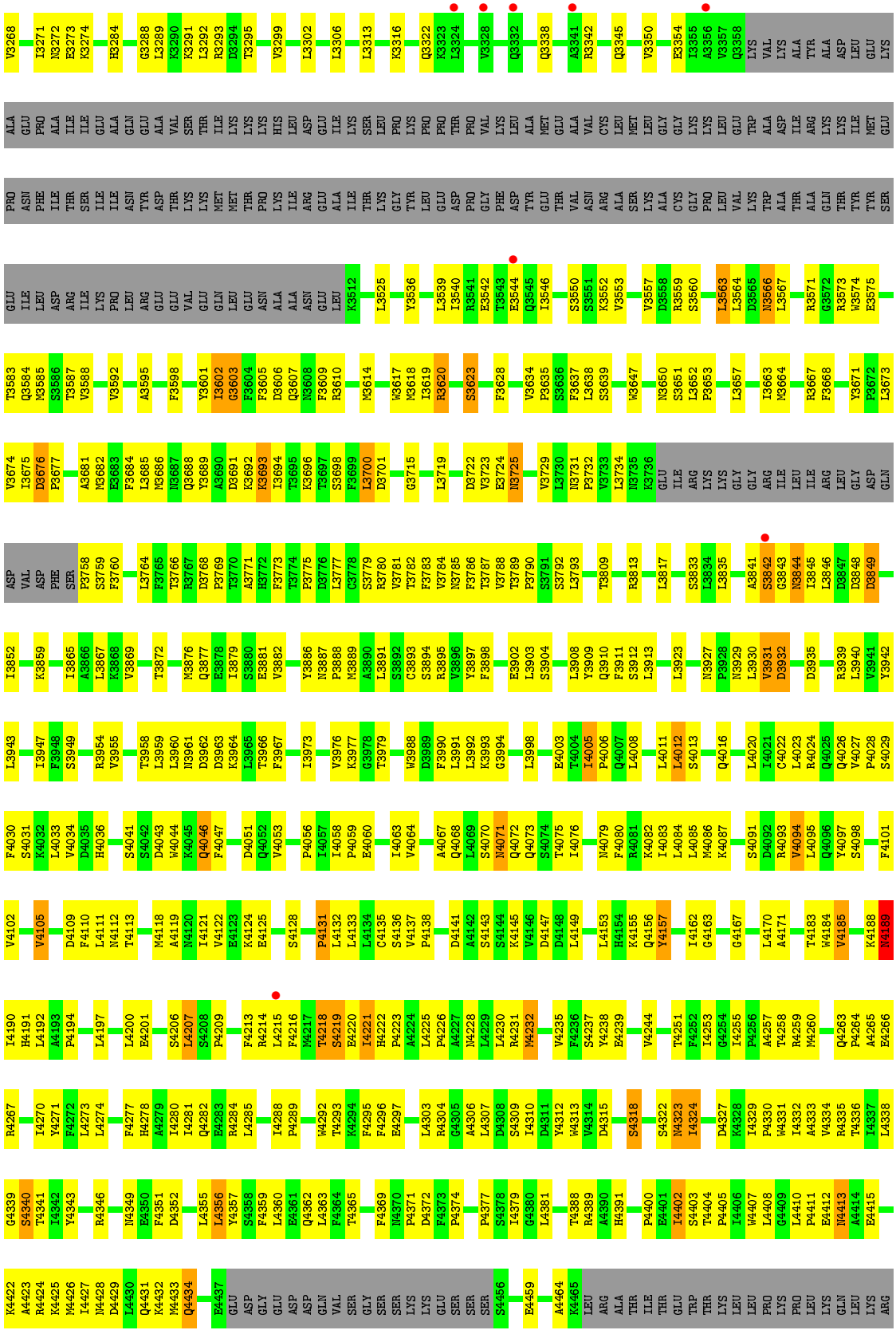


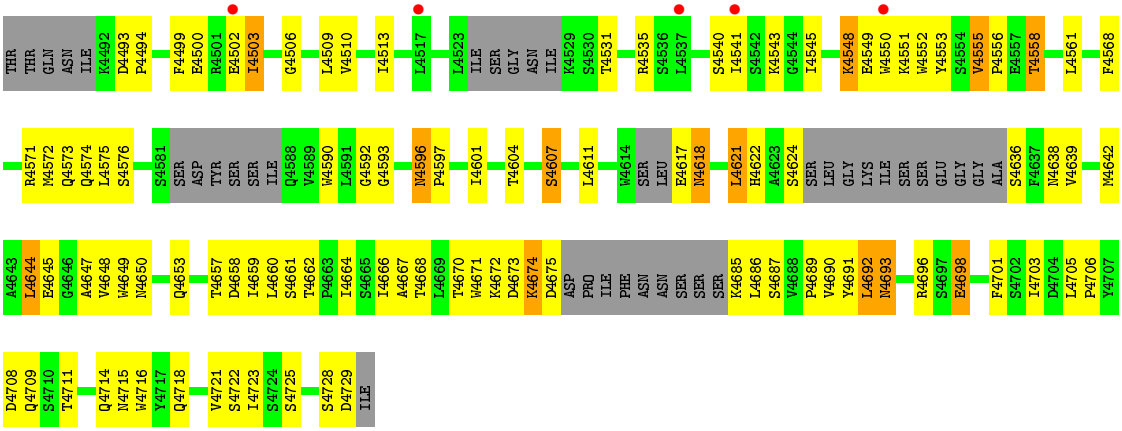
• Molecule 1: Dynein heavy chain, cytoplasmic










THR THR GLN ASN ILE K4492 D4493 P4494 F4499 E4500 R4501 E4502 I4503 G4506 L4509 V4510 I4513 L4517 L4523 ILE SER GLY ASN ILE K4529 S4530 T4531 R4535 S4536 L4537 S4540 I4541 S4542 K4543 G4544 I4545 K4548 E4549 W4550 K4551 W4552 Y4553 S4554 V4555 P4556 E4557 T4558 L4561 F4568
R4571 M4572 Q4573 Q4574 L4575 S4576 S4581 SER ASP TYR SER SER ILE Q4588 V4589 W4590 L4591 G4592 G4593 M4596 P4597 I4601 T4604 S4607 L4611 W4614 SER LEU E4617 M4618 L4621 H4622 A4623 S4624 SER LEU GLY LYS ILE SER SER GLU GLY GLY ALA S4636 F4637 N4638 V4639 M4642
A4643 L4644 E4645 G4646 A4647 V4648 W4649 N4650 Q4653 T4657 D4658 I4659 L4660 S4661 T4662 P4663 I4664 S4665 I4666 A4667 T4668 L4669 T4670 W4671 K4672 D4673 K4674 D4675 ASP PRO ILE PHE ASN ASN SER SER SER K4685 L4686 S4687 V4688 P4689 V4690 Y4691 L4692 N4693 R4696 S4697 E4698 F4701 S4702 I4703 D4704 L4705 P4706 V4707
D4708 Q4709 S4710 T4711 Q4714 N4715 W4716 Y4717 Q4718 V4721 S4722 I4723 S4724 S4725 S4728 D4729 ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.78 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.0 (48.78-3.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.219 , 0.292 0.220 , 0.292	Depositor DCC
R_{free} test set	4442 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 112.1	EDS
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 89309 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.24	0/23866	0.44	1/32482 (0.0%)
1	B	0.24	0/22846	0.43	0/31076
All	All	0.24	0/46712	0.44	1/63558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3371	PRO	N-CA-CB	5.32	109.68	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23374	0	22545	1559	0
1	B	22384	0	21550	1149	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2704	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 30.

All (2704) 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:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00
1:A:3373:ILE:HD13	1:A:3373:ILE:H	1.29	0.98
1:A:3673:LEU:HB2	1:A:3781:VAL:HG11	1.45	0.97
1:B:1959:THR:HG22	1:B:4341:THR:HA	1.46	0.96
1:B:1554:LEU:HB3	1:B:1609:GLN:HE22	1.29	0.95
1:B:4251:THR:HG23	1:B:4303:LEU:HD21	1.46	0.95
1:B:1928:HIS:CD2	1:B:1933:THR:HG22	2.02	0.95
1:A:4375:LEU:HD11	1:A:4383:VAL:HG23	1.48	0.95
1:B:3673:LEU:HB2	1:B:3781:VAL:HG11	1.44	0.95
1:A:3425:LYS:HD2	1:A:3428:GLU:HG3	1.49	0.94
1:B:2533:VAL:HB	1:B:2581:LEU:HD22	1.51	0.93
1:B:4574:GLN:HE22	1:B:4590:TRP:H	1.15	0.93
1:B:1655:LEU:HB2	1:B:1658:GLU:HB2	1.45	0.93
1:B:4121:ILE:HA	1:B:4125:GLU:HG3	1.48	0.93
1:A:2274:MET:HE3	1:A:2286:TRP:HB3	1.50	0.92
1:B:1972:PRO:HG2	1:B:2076:THR:HG22	1.52	0.92
1:A:4270:ILE:HA	1:A:4273:LEU:HD12	1.52	0.90
1:B:1789:LEU:HD23	1:B:1818:THR:HG23	1.50	0.90
1:A:3837:ALA:HB1	1:A:3850:SER:HB3	1.53	0.89
1:A:2313:LYS:HE3	1:A:2366:ASN:HD21	1.36	0.89
1:A:3018:SER:HB2	1:A:3256:THR:HG21	1.52	0.89
1:A:1639:ILE:HG23	1:A:1672:LEU:HD22	1.53	0.89
1:A:4495:LEU:H	1:A:4495:LEU:HD12	1.38	0.89
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.55	0.89
1:B:3930:LEU:HB3	1:B:3939:ARG:HH21	1.37	0.89
1:B:1813:GLN:HE22	1:B:1940:TYR:HA	1.37	0.88
1:B:2603:THR:HG22	1:B:2604:PRO:HD2	1.54	0.88
1:A:2200:ASN:HD22	1:A:2228:LEU:HD13	1.36	0.88
1:A:1690:GLN:HE22	1:A:1766:ILE:HG21	1.38	0.88
1:A:4046:GLN:HE22	1:A:4057:ILE:H	1.19	0.88
1:A:2447:GLN:HA	1:A:2450:ASN:HD22	1.39	0.88
1:B:4270:ILE:HG22	1:B:4310:ILE:HD13	1.55	0.88
1:B:1524:GLU:HG2	1:B:1580:TYR:HB3	1.57	0.87
1:A:3552:LYS:HA	1:A:3555:ASN:HD22	1.40	0.87
1:A:2570:THR:HG21	1:A:2603:THR:HG21	1.57	0.86
1:B:2381:ASN:HD21	1:B:2383:GLU:HB2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2914:GLN:HB2	1:A:2926:THR:HG21	1.56	0.86
1:A:2200:ASN:HB2	1:A:2228:LEU:HD22	1.56	0.86
1:B:4604:THR:HG23	1:B:4671:TRP:HE1	1.40	0.86
1:B:3271:ILE:HG13	1:B:3592:VAL:HG11	1.57	0.86
1:A:4621:LEU:HD21	1:A:4669:LEU:HD23	1.55	0.86
1:A:2293:ILE:HG22	1:A:2350:ARG:HH22	1.41	0.85
1:B:4109:ASP:HA	1:B:4112:ASN:ND2	1.92	0.85
1:A:4686:LEU:HD21	1:A:4721:VAL:HG11	1.59	0.85
1:A:3809:THR:HA	1:A:3812:LYS:HE2	1.59	0.84
1:A:2560:MET:HG3	1:A:2561:SER:H	1.42	0.84
1:A:4251:THR:HG23	1:A:4303:LEU:HD21	1.58	0.84
1:B:2525:ILE:HD11	1:B:2815:LEU:HB2	1.58	0.84
1:A:4648:VAL:HG12	1:A:4662:THR:HG21	1.60	0.83
1:B:2841:ASN:ND2	1:B:2842:LEU:H	1.75	0.83
1:A:2910:LEU:HD23	1:A:2930:ILE:HD12	1.59	0.83
1:B:3930:LEU:HD11	1:B:3943:LEU:HD21	1.59	0.83
1:B:4548:LYS:HD2	1:B:4549:GLU:N	1.93	0.83
1:A:3718:LEU:HG	1:A:3719:LEU:H	1.42	0.83
1:B:4402:ILE:HD12	1:B:4402:ILE:H	1.42	0.83
1:A:4109:ASP:HA	1:A:4112:ASN:ND2	1.95	0.82
1:A:4190:ILE:HG12	1:A:4219:SER:HB3	1.61	0.82
1:A:3981:ASN:HD22	1:A:4076:ILE:HB	1.44	0.82
1:B:3785:ASN:HD21	1:B:3787:THR:HG23	1.43	0.82
1:B:2250:VAL:HB	1:B:2425:MET:HG3	1.60	0.82
1:B:1926:VAL:HG22	1:B:1935:TYR:CE2	2.15	0.82
1:A:3652:LEU:HD12	1:A:3653:PRO:HD2	1.62	0.82
1:B:1781:LEU:HG	1:B:1814:LEU:HD11	1.61	0.81
1:A:2651:VAL:HG13	1:A:2652:ASP:H	1.44	0.81
1:B:4657:THR:HG22	1:B:4659:ILE:H	1.45	0.81
1:B:2129:VAL:HG22	1:B:2130:PRO:HD3	1.62	0.81
1:A:4185:VAL:HG12	1:A:4186:LEU:H	1.44	0.81
1:B:4335:ARG:HH21	1:B:4365:THR:HG22	1.46	0.81
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	1.61	0.81
1:A:2371:LEU:CB	1:A:2410:ARG:HG3	2.10	0.81
1:A:3238:ILE:HG12	1:A:3601:TYR:CD2	2.16	0.81
1:A:3700:LEU:HD22	1:A:3701:ASP:H	1.43	0.80
1:A:3789:THR:HB	1:A:3790:PRO:HD2	1.63	0.80
1:A:2140:SER:HB2	1:A:2142:GLN:HE22	1.45	0.80
1:A:2857:TYR:HA	1:A:2913:PHE:HE1	1.46	0.80
1:A:2370:LEU:HD21	1:A:2387:LEU:HD13	1.64	0.80
1:A:4654:LEU:HD11	1:A:4705:LEU:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1660:LEU:HA	1:B:1665:ILE:HD11	1.63	0.80
1:A:3694:ILE:HG12	1:A:3717:PRO:HB2	1.63	0.80
1:A:2236:LEU:HD21	1:A:2293:ILE:HD13	1.63	0.80
1:A:4654:LEU:HD13	1:A:4686:LEU:HD23	1.62	0.79
1:B:4270:ILE:HD11	1:B:4329:ILE:HD13	1.65	0.79
1:A:2110:GLN:HG3	1:A:2122:GLU:HA	1.64	0.79
1:B:3607:GLN:HG2	1:B:3657:LEU:HD22	1.65	0.79
1:A:4086:MET:HG3	1:A:4093:ARG:HB2	1.65	0.79
1:A:4349:ASN:HD21	1:A:4351:PHE:HB2	1.46	0.79
1:A:2300:LYS:O	1:A:2349:LYS:HB2	1.81	0.79
1:B:4189:ASN:H	1:B:4218:THR:HG22	1.47	0.79
1:B:3844:ASN:O	1:B:3848:ASP:HB3	1.81	0.79
1:A:4353:MET:HE3	1:A:4356:LEU:HD23	1.64	0.78
1:A:2283:THR:HA	1:A:2286:TRP:HE1	1.48	0.78
1:A:2886:LEU:O	1:A:2890:ILE:HG12	1.84	0.78
1:A:2706:THR:HB	1:A:2707:PRO:HD2	1.65	0.78
1:B:2106:GLU:OE1	1:B:2129:VAL:HG21	1.82	0.78
1:B:4264:PRO:HB3	1:B:4323:ASN:HA	1.64	0.78
1:A:3673:LEU:HB2	1:A:3781:VAL:CG1	2.14	0.78
1:B:2657:VAL:HG13	1:B:2687:THR:HG23	1.64	0.78
1:B:3338:GLN:HG2	1:B:3525:LEU:HD13	1.65	0.78
1:A:2204:ILE:HA	1:A:2207:LEU:HD12	1.65	0.78
1:A:1823:TRP:O	1:A:1827:VAL:HG23	1.84	0.78
1:A:2705:THR:HA	1:A:2709:LEU:HD12	1.66	0.78
1:A:1796:ASP:HB3	1:A:1799:ASP:HB3	1.65	0.77
1:A:4575:LEU:H	1:A:4575:LEU:HD12	1.49	0.77
1:B:2578:MET:HB3	1:B:2597:ILE:HD12	1.65	0.77
1:B:4332:ILE:HD12	1:B:4332:ILE:H	1.48	0.77
1:B:4121:ILE:O	1:B:4125:GLU:HB2	1.85	0.77
1:B:3219:ILE:CB	1:B:3220:PRO:HD3	2.15	0.77
1:A:4318:SER:HA	1:A:4321:ARG:HH21	1.50	0.76
1:A:2766:MET:HB3	1:A:2783:LEU:HD11	1.67	0.76
1:A:3384:LYS:HD3	1:A:3386:LYS:HD3	1.66	0.76
1:B:3230:SER:HA	1:B:3620:ARG:HE	1.51	0.76
1:A:3058:LEU:HD21	1:A:3141:LEU:HD11	1.67	0.76
1:B:3313:LEU:HD13	1:B:3550:SER:HA	1.65	0.76
1:A:2505:TYR:O	1:A:2512:VAL:HG23	1.85	0.76
1:B:3671:TYR:O	1:B:3781:VAL:HG13	1.86	0.76
1:B:4046:GLN:HG3	1:B:4047:PHE:N	2.00	0.76
1:A:1959:THR:HA	1:A:4341:THR:OG1	1.85	0.76
1:B:4531:THR:O	1:B:4535:ARG:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4067:ALA:HB1	1:B:4073:GLN:HG3	1.65	0.76
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.84	0.76
1:B:3639:SER:HB3	1:B:3663:ILE:HD11	1.68	0.76
1:A:3927:ASN:HB3	1:A:3930:LEU:HB2	1.68	0.75
1:A:1813:GLN:HE22	1:A:1940:TYR:HA	1.50	0.75
1:B:1822:VAL:HG22	1:B:1826:GLN:HE21	1.50	0.75
1:A:4122:VAL:HG21	1:A:4216:PHE:CZ	2.20	0.75
1:B:4011:LEU:HD11	1:B:4041:SER:HB2	1.68	0.75
1:A:3731:ASN:H	1:A:3731:ASN:HD22	1.35	0.75
1:A:2273:MET:HB2	1:A:2395:PHE:HB2	1.68	0.75
1:B:3027:ARG:HA	1:B:3037:ILE:HD11	1.68	0.75
1:B:3966:THR:HG22	1:B:4426:MET:HG3	1.68	0.75
1:B:2426:ILE:HD12	1:B:2426:ILE:H	1.51	0.75
1:A:3443:MET:HG3	1:A:3449:ARG:HG3	1.68	0.75
1:A:3358:GLN:HA	1:A:3361:LYS:HE2	1.69	0.75
1:A:3039:THR:HG22	1:A:3040:ILE:H	1.50	0.75
1:A:4648:VAL:HG13	1:A:4657:THR:HG21	1.68	0.75
1:B:3766:THR:HG22	1:B:3768:ASP:H	1.52	0.75
1:A:4622:HIS:HE2	1:A:4678:ILE:HG21	1.50	0.75
1:B:3035:LEU:HD22	1:B:3068:LYS:HB3	1.68	0.75
1:B:1950:THR:HB	1:B:1951:PRO:HD2	1.68	0.75
1:A:2586:GLY:HA2	1:A:2815:LEU:HD13	1.67	0.75
1:A:3015:ILE:HD13	1:A:3147:MET:HG3	1.68	0.74
1:B:2315:GLN:HB3	1:B:2775:THR:HG21	1.69	0.74
1:A:2397:VAL:HG21	1:A:2400:LEU:HD21	1.68	0.74
1:A:3696:LYS:HZ2	1:A:4206:SER:HB3	1.52	0.74
1:B:2638:THR:HG21	1:B:2838:LEU:HD21	1.68	0.74
1:A:1547:ASN:HA	1:A:1553:LYS:HG2	1.70	0.74
1:B:1476:ILE:HG23	1:B:1480:HIS:HB2	1.68	0.74
1:A:2105:ARG:HG2	1:A:2105:ARG:HH11	1.53	0.74
1:B:4278:HIS:HD2	1:B:4343:TYR:OH	1.71	0.73
1:A:4122:VAL:HG21	1:A:4216:PHE:HZ	1.53	0.73
1:A:3774:THR:HB	1:A:3775:PRO:HD2	1.70	0.73
1:A:2309:LYS:HE2	1:A:2756:THR:HG21	1.68	0.73
1:A:4053:VAL:HG12	1:A:4053:VAL:O	1.86	0.73
1:A:3388:LEU:HD23	1:A:3473:ALA:HB1	1.68	0.73
1:A:2793:ASN:HD22	1:A:2793:ASN:N	1.85	0.73
1:A:3725:ASN:HD22	1:A:3725:ASN:H	1.35	0.73
1:A:3281:GLU:HB3	1:A:3581:PHE:HE1	1.54	0.73
1:A:1886:ARG:HG3	1:A:1887:ASP:N	2.04	0.73
1:B:3700:LEU:HD13	1:B:3701:ASP:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3202:PRO:HD2	1:A:3624:VAL:O	1.88	0.73
1:B:3602:ILE:HG23	1:B:3610:ARG:HG2	1.70	0.73
1:A:3453:THR:HA	1:A:3457:LEU:HB2	1.70	0.73
1:B:2572:ARG:HG2	1:B:2617:VAL:HG11	1.69	0.73
1:B:4157:TYR:HB3	1:B:4184:TRP:HB2	1.71	0.73
1:A:2675:PRO:HD2	1:A:2816:VAL:O	1.88	0.73
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	2.04	0.73
1:B:4189:ASN:HD22	1:B:4189:ASN:N	1.85	0.73
1:A:2080:GLY:HA3	1:A:2084:ARG:O	1.89	0.73
1:B:3789:THR:HB	1:B:3790:PRO:HD2	1.70	0.73
1:A:3475:GLY:O	1:A:3478:VAL:HG12	1.88	0.73
1:A:4024:ARG:HD3	1:A:4034:VAL:HG21	1.71	0.73
1:B:3584:GLN:O	1:B:3588:VAL:HG23	1.87	0.73
1:B:2514:LYS:HE2	1:B:2600:ILE:HD11	1.71	0.72
1:A:1655:LEU:HB2	1:A:1658:GLU:HB2	1.69	0.72
1:A:3281:GLU:HB3	1:A:3581:PHE:CE1	2.24	0.72
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	1.70	0.72
1:A:3724:GLU:OE2	1:A:3766:THR:HG23	1.88	0.72
1:B:4136:SER:HB3	1:B:4238:TYR:HB2	1.72	0.72
1:B:4005:ILE:HD13	1:B:4020:LEU:HD23	1.70	0.72
1:B:1899:THR:HB	1:B:1903:ASP:HB2	1.72	0.72
1:B:2938:PHE:O	1:B:2941:VAL:HG12	1.88	0.72
1:B:2841:ASN:HD22	1:B:2842:LEU:H	1.37	0.72
1:A:2042:GLN:HE21	1:A:2059:LEU:HD11	1.54	0.72
1:A:1763:GLY:N	1:A:1764:PRO:HD3	2.04	0.72
1:B:4601:ILE:O	1:B:4604:THR:HG22	1.90	0.71
1:A:3700:LEU:HD13	1:A:3701:ASP:N	2.04	0.71
1:A:2587:LEU:HG	1:A:2817:ASP:HB2	1.72	0.71
1:B:3292:LEU:HD13	1:B:3571:ARG:HA	1.72	0.71
1:A:2626:LEU:HD12	1:A:2626:LEU:H	1.55	0.71
1:A:2042:GLN:NE2	1:A:2059:LEU:HD11	2.06	0.71
1:A:3555:ASN:HB3	1:A:3559:ARG:NH1	2.04	0.71
1:B:2839:LEU:HD13	1:B:2842:LEU:HD12	1.70	0.71
1:A:4347:ILE:HG21	1:A:4353:MET:HG2	1.72	0.71
1:B:4506:GLY:O	1:B:4510:VAL:HG23	1.91	0.71
1:A:1742:ILE:HG22	1:A:1753:THR:HG22	1.71	0.71
1:A:2371:LEU:HB3	1:A:2410:ARG:HG3	1.71	0.71
1:B:3700:LEU:HD22	1:B:3701:ASP:H	1.54	0.71
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.06	0.71
1:A:2208:VAL:HA	1:A:2415:TRP:CD1	2.24	0.71
1:A:1807:VAL:HG13	1:A:1815:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3674:VAL:HG22	1:B:3784:VAL:HB	1.71	0.71
1:A:4242:PRO:HA	1:A:4286:ARG:NH1	2.01	0.71
1:B:3234:ILE:HG23	1:B:3617:TRP:NE1	2.06	0.71
1:A:4553:TYR:H	1:A:4553:TYR:HD1	1.38	0.71
1:A:2258:LYS:HA	1:A:2261:GLN:HG3	1.71	0.71
1:B:4157:TYR:CB	1:B:4184:TRP:HB2	2.21	0.71
1:A:2176:ASP:N	1:A:2179:SER:HG	1.87	0.71
1:A:3859:LYS:O	1:A:3862:THR:HG22	1.90	0.71
1:A:4533:TYR:O	1:A:4537:LEU:HG	1.90	0.71
1:A:4591:LEU:HD21	1:A:4601:ILE:HD11	1.72	0.71
1:A:3037:ILE:H	1:A:3037:ILE:HD13	1.56	0.71
1:A:4029:SER:HB2	1:A:4081:ARG:HH12	1.56	0.71
1:A:2942:ASN:O	1:A:2944:ASP:N	2.24	0.71
1:B:4703:ILE:HD12	1:B:4705:LEU:HD21	1.71	0.71
1:B:2282:LYS:HA	1:B:2416:PHE:CD1	2.26	0.71
1:B:4574:GLN:HE22	1:B:4590:TRP:N	1.89	0.70
1:A:4494:PRO:HG2	1:A:4607:SER:HA	1.73	0.70
1:B:2124:LEU:HD22	1:B:2195:LEU:HD22	1.71	0.70
1:B:1823:TRP:CD1	1:B:1885:GLN:HB3	2.26	0.70
1:A:1879:ILE:O	1:A:1883:VAL:HG23	1.91	0.70
1:A:2371:LEU:HB2	1:A:2410:ARG:HG3	1.71	0.70
1:B:3238:ILE:CG2	1:B:3255:VAL:HG11	2.20	0.70
1:B:1879:ILE:O	1:B:1883:VAL:HG23	1.91	0.70
1:A:2006:LEU:HD23	1:A:2035:ILE:HG23	1.73	0.70
1:A:4540:SER:HB2	1:A:4545:ILE:O	1.91	0.70
1:A:2788:PHE:O	1:A:2789:VAL:HG23	1.90	0.70
1:A:3153:ASP:HA	1:A:3156:ASN:ND2	2.06	0.70
1:A:2113:LEU:HD21	1:A:2156:LEU:HD22	1.74	0.70
1:A:4095:LEU:HD11	1:A:4422:LYS:HB3	1.73	0.70
1:A:3677:PRO:HG3	1:A:3787:THR:HG22	1.72	0.70
1:A:4649:TRP:HA	1:A:4649:TRP:CE3	2.27	0.70
1:A:2106:GLU:CD	1:A:2106:GLU:H	1.95	0.70
1:A:2954:ASN:HD22	1:A:2954:ASN:H	1.39	0.70
1:A:2308:PRO:HD2	1:A:2357:GLY:HA3	1.74	0.70
1:A:4179:ALA:HB1	1:A:4209:PRO:HB3	1.73	0.70
1:A:3812:LYS:O	1:A:3816:LEU:HB3	1.91	0.70
1:A:3380:VAL:HG11	1:A:3435:ILE:HG21	1.72	0.70
1:B:1928:HIS:NE2	1:B:1933:THR:HG22	2.06	0.70
1:A:4086:MET:CG	1:A:4093:ARG:HB2	2.21	0.69
1:A:3331:GLN:HE22	1:A:3533:LYS:HG3	1.56	0.69
1:B:2850:THR:O	1:B:2854:VAL:HG23	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3433:THR:HG22	1:A:3437:ASN:ND2	2.06	0.69
1:B:2540:LEU:HD23	1:B:2576:SER:HA	1.72	0.69
1:B:1687:LEU:HD21	1:B:1706:LEU:HD23	1.74	0.69
1:B:3700:LEU:HD12	1:B:3700:LEU:H	1.58	0.69
1:A:4128:SER:HB2	1:A:4213:PHE:HB3	1.74	0.69
1:B:1739:THR:HB	1:B:1761:ALA:HB2	1.74	0.69
1:A:1846:GLN:HA	1:A:1893:GLN:NE2	2.08	0.69
1:B:2235:GLN:NE2	1:B:2296:VAL:HG13	2.06	0.69
1:B:3238:ILE:HG12	1:B:3601:TYR:CG	2.28	0.69
1:B:1846:GLN:O	1:B:1850:GLN:HG2	1.92	0.69
1:A:3912:SER:HB3	1:A:4231:ARG:HG2	1.75	0.69
1:B:3768:ASP:HB3	1:B:3771:ALA:HB2	1.73	0.69
1:B:3238:ILE:HG21	1:B:3255:VAL:HG11	1.73	0.69
1:B:3256:THR:HB	1:B:3257:PRO:HD2	1.74	0.69
1:A:2028:PHE:HB3	1:A:2075:VAL:HG13	1.72	0.69
1:B:1534:VAL:HG13	1:B:1568:HIS:HD2	1.58	0.69
1:A:2202:THR:HG22	1:A:2265:ILE:HG12	1.74	0.69
1:A:1746:SER:OG	1:A:1750:GLU:HB3	1.93	0.69
1:B:2282:LYS:HA	1:B:2416:PHE:HD1	1.57	0.69
1:B:2200:ASN:HB2	1:B:2228:LEU:HD22	1.75	0.69
1:A:4623:ALA:HB2	1:A:4703:ILE:HD11	1.75	0.69
1:A:1770:LEU:O	1:A:1773:VAL:HG22	1.93	0.69
1:B:4005:ILE:CD1	1:B:4020:LEU:HD23	2.24	0.68
1:A:2748:LEU:HD21	1:A:2800:ARG:NH1	2.09	0.68
1:B:3724:GLU:OE2	1:B:3766:THR:HG23	1.93	0.68
1:B:4362:GLN:HB2	1:B:4714:GLN:NE2	2.08	0.68
1:B:4574:GLN:NE2	1:B:4590:TRP:H	1.87	0.68
1:B:2865:THR:H	1:B:2868:ILE:HD12	1.58	0.68
1:A:1886:ARG:NH1	1:A:1890:ARG:HH22	1.91	0.68
1:B:3652:LEU:HD12	1:B:3653:PRO:HD2	1.74	0.68
1:A:3210:GLU:HG3	1:A:3211:ILE:H	1.57	0.68
1:B:3043:ASN:ND2	1:B:3046:TYR:HB2	2.07	0.68
1:B:1545:LEU:H	1:B:1545:LEU:HD12	1.57	0.68
1:A:1554:LEU:HB3	1:A:1609:GLN:HE21	1.59	0.68
1:A:2010:SER:HB3	1:A:2060:LEU:HD21	1.75	0.68
1:B:1743:GLY:HA2	1:B:1754:PHE:CD1	2.29	0.68
1:B:2320:LEU:HD23	1:B:2320:LEU:O	1.93	0.68
1:A:4200:LEU:HD22	1:A:4204:LEU:HD11	1.75	0.68
1:A:2293:ILE:CG2	1:A:2350:ARG:HH22	2.07	0.68
1:A:1931:ASN:OD1	1:A:1962:GLN:NE2	2.25	0.68
1:B:2400:LEU:HD13	1:B:2408:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1715:ILE:HD11	1:A:1760:ILE:HD13	1.74	0.68
1:A:2742:PHE:HA	1:A:2789:VAL:O	1.94	0.67
1:A:1846:GLN:HA	1:A:1893:GLN:HE22	1.59	0.67
1:A:3961:ASN:O	1:A:3964:LYS:HB2	1.94	0.67
1:A:2699:LEU:HD11	1:A:2713:THR:HG21	1.77	0.67
1:B:2231:ILE:HG21	1:B:2264:GLN:NE2	2.09	0.67
1:A:3013:LEU:HD12	1:A:3145:PHE:HB3	1.74	0.67
1:B:4251:THR:HG23	1:B:4303:LEU:CD2	2.23	0.67
1:A:2212:ILE:HG22	1:A:2213:PRO:HD3	1.77	0.67
1:B:2793:ASN:HB3	1:B:2794:PRO:HD2	1.76	0.67
1:A:3563:LEU:HD11	1:A:3851:VAL:HG22	1.77	0.67
1:A:2447:GLN:HE22	1:A:2492:LEU:HD23	1.58	0.67
1:B:4189:ASN:H	1:B:4218:THR:CG2	2.08	0.67
1:A:1963:ALA:HB1	1:A:2096:ARG:HG3	1.76	0.67
1:A:3397:PRO:HG2	1:A:3419:TRP:CZ2	2.29	0.67
1:B:2815:LEU:HD23	1:B:2816:VAL:N	2.09	0.67
1:B:4189:ASN:H	1:B:4189:ASN:HD22	1.40	0.67
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.30	0.67
1:A:4210:HIS:ND1	1:A:4211:PRO:HD2	2.09	0.67
1:A:4259:ARG:HD3	1:A:4271:TYR:OH	1.95	0.67
1:A:4548:LYS:HG3	1:A:4549:GLU:H	1.60	0.66
1:B:1719:GLN:HA	1:B:1722:PHE:CD2	2.29	0.66
1:A:2014:VAL:HG13	1:A:2065:ILE:HG21	1.78	0.66
1:B:3078:VAL:HG23	1:B:3083:PHE:HB2	1.76	0.66
1:B:3958:THR:HG23	1:B:4235:VAL:HB	1.76	0.66
1:B:2361:PRO:HD3	1:B:2402:TYR:O	1.96	0.66
1:B:2297:ASP:O	1:B:2299:ILE:HG13	1.94	0.66
1:A:4270:ILE:HD13	1:A:4314:VAL:HG21	1.78	0.66
1:B:2423:THR:HG23	1:B:2530:ARG:HD2	1.76	0.66
1:B:2766:MET:HB3	1:B:2783:LEU:HD11	1.75	0.66
1:A:2595:LYS:HE3	1:A:2611:PRO:HG3	1.75	0.66
1:A:3875:VAL:O	1:A:3879:ILE:HG12	1.95	0.66
1:A:3925:ASN:N	1:A:3925:ASN:HD22	1.93	0.66
1:B:2861:GLN:HG3	1:B:2874:TYR:HB2	1.75	0.66
1:A:2108:ILE:O	1:A:2112:MET:HB2	1.96	0.66
1:A:4572:MET:HE1	1:A:4575:LEU:HD11	1.77	0.66
1:A:3245:LEU:HD12	1:A:3249:GLN:HB2	1.78	0.66
1:A:2124:LEU:HD22	1:A:2195:LEU:HD22	1.78	0.66
1:A:2125:ALA:HA	1:A:2128:ILE:HG22	1.78	0.66
1:B:2113:LEU:HD21	1:B:2156:LEU:HD22	1.78	0.66
1:A:2910:LEU:CD2	1:A:2930:ILE:HD12	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1769:TRP:O	1:B:1773:VAL:HG23	1.96	0.66
1:B:2984:LEU:HD22	1:B:2986:VAL:HG22	1.78	0.66
1:A:3309:LYS:O	1:A:3313:LEU:HG	1.96	0.66
1:A:2315:GLN:HB3	1:A:2775:THR:HG21	1.76	0.66
1:B:3785:ASN:ND2	1:B:3787:THR:HG23	2.11	0.66
1:B:1885:GLN:O	1:B:1889:VAL:HG23	1.96	0.66
1:A:3989:ASP:O	1:A:3993:LYS:HB2	1.96	0.66
1:A:3647:TRP:HB3	1:A:3652:LEU:HD23	1.78	0.65
1:A:3410:LEU:HD22	1:A:3452:ILE:HD11	1.78	0.65
1:A:3965:LEU:HG	1:A:4426:MET:HE3	1.77	0.65
1:A:4230:LEU:H	1:A:4230:LEU:HD12	1.61	0.65
1:A:2289:TYR:O	1:A:2293:ILE:HG12	1.95	0.65
1:A:3285:LEU:HD13	1:A:3578:SER:HA	1.78	0.65
1:A:4186:LEU:C	1:A:4187:LEU:HD12	2.17	0.65
1:B:3639:SER:HB3	1:B:3663:ILE:CD1	2.25	0.65
1:A:2535:ASN:HD22	1:A:2668:ARG:HH12	1.45	0.65
1:A:3271:ILE:HG13	1:A:3592:VAL:HG11	1.78	0.65
1:B:2498:CYS:HA	1:B:2501:ILE:HD12	1.77	0.65
1:B:1901:ASN:HD22	1:B:1901:ASN:H	1.43	0.65
1:A:2552:ASN:HD21	1:A:2560:MET:HB2	1.59	0.65
1:A:3700:LEU:CD2	1:A:3701:ASP:H	2.09	0.65
1:A:4054:GLY:O	1:A:4055:GLU:C	2.34	0.65
1:B:2359:VAL:HG13	1:B:2364:VAL:HG21	1.79	0.65
1:B:3813:ARG:O	1:B:3817:LEU:HD13	1.97	0.65
1:B:2339:ILE:HA	1:B:2346:GLU:HG2	1.76	0.65
1:A:2975:ARG:HE	1:A:2975:ARG:HA	1.61	0.65
1:A:3242:ASN:OD1	1:A:3253:ASN:HB3	1.96	0.65
1:A:3015:ILE:HG22	1:A:3149:PRO:HG3	1.77	0.65
1:A:1537:PHE:O	1:A:1541:LEU:HB2	1.97	0.65
1:A:2948:ARG:HH11	1:A:2948:ARG:HG2	1.62	0.65
1:A:4622:HIS:ND1	1:A:4623:ALA:N	2.45	0.65
1:A:4024:ARG:HG3	1:A:4031:SER:HA	1.78	0.65
1:A:2120:THR:O	1:A:2121:ALA:C	2.33	0.65
1:B:3949:SER:HA	1:B:4110:PHE:HE1	1.62	0.65
1:A:3255:VAL:HA	1:A:3259:HIS:HD2	1.61	0.65
1:B:1920:ASN:HD22	1:B:1921:VAL:H	1.44	0.65
1:A:4553:TYR:HB3	1:A:4595:LEU:HD23	1.79	0.65
1:A:4649:TRP:HA	1:A:4649:TRP:HE3	1.60	0.65
1:B:3109:MET:HB3	1:B:3129:LEU:HD23	1.79	0.65
1:A:2305:VAL:HG21	1:A:2769:LYS:HE2	1.79	0.65
1:B:4389:ARG:HG2	1:B:4389:ARG:HH11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1748:GLU:HG2	1:A:1943:ILE:HB	1.79	0.65
1:B:1931:ASN:HB2	1:B:4312:TYR:CZ	2.32	0.64
1:A:2127:LYS:C	1:A:2130:PRO:HD2	2.17	0.64
1:A:2129:VAL:HB	1:A:2130:PRO:HD3	1.78	0.64
1:A:3270:LEU:HB2	1:A:3592:VAL:HG13	1.77	0.64
1:A:4221:ILE:H	1:A:4221:ILE:HD12	1.62	0.64
1:B:4063:ILE:H	1:B:4063:ILE:HD12	1.62	0.64
1:B:3063:GLY:HA2	1:B:3136:GLN:HB3	1.78	0.64
1:A:2968:LEU:O	1:A:2972:VAL:HG23	1.97	0.64
1:A:2704:ALA:HB3	1:A:3085:GLU:HG3	1.77	0.64
1:B:4288:ILE:HG23	1:B:4292:TRP:O	1.97	0.64
1:A:3700:LEU:H	1:A:3700:LEU:HD12	1.62	0.64
1:A:2606:PRO:HD3	1:A:2624:TRP:CD1	2.32	0.64
1:B:1811:PRO:O	1:B:1815:VAL:HG23	1.98	0.64
1:A:2651:VAL:HG13	1:A:2652:ASP:N	2.12	0.64
1:A:3387:HIS:CB	1:A:3473:ALA:HB2	2.27	0.64
1:A:2525:ILE:HG13	1:A:2584:SER:O	1.98	0.64
1:B:2866:PRO:HG3	1:B:2873:ILE:HG22	1.78	0.64
1:A:1921:VAL:HG23	1:A:1922:LEU:HD22	1.79	0.64
1:B:4188:LYS:HA	1:B:4218:THR:HG22	1.80	0.64
1:A:1811:PRO:HD2	1:A:1814:LEU:HD12	1.78	0.64
1:A:3528:SER:O	1:A:3531:THR:HG22	1.98	0.64
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.80	0.64
1:A:4349:ASN:HD22	1:A:4352:ASP:N	1.95	0.64
1:A:2273:MET:CB	1:A:2395:PHE:HB2	2.27	0.64
1:A:2199:ILE:O	1:A:2203:MET:HB2	1.98	0.64
1:A:4050:LYS:O	1:A:4052:GLN:N	2.30	0.64
1:A:2506:PHE:CD1	1:A:2512:VAL:HG21	2.33	0.64
1:B:3991:LEU:O	1:B:4427:ILE:HD12	1.98	0.64
1:A:3897:TYR:HE1	1:A:3913:LEU:HA	1.63	0.64
1:A:3696:LYS:NZ	1:A:4206:SER:HB3	2.13	0.64
1:A:4296:PHE:CE2	1:A:4347:ILE:HD13	2.33	0.64
1:A:1545:LEU:HB3	1:A:1553:LYS:HE2	1.80	0.64
1:A:2979:PHE:CE2	1:A:3028:PHE:HA	2.33	0.64
1:B:3299:VAL:HG11	1:B:3564:LEU:HG	1.78	0.64
1:B:1554:LEU:HD12	1:B:2323:THR:HG22	1.79	0.64
1:B:4548:LYS:HD2	1:B:4549:GLU:H	1.59	0.64
1:B:1694:PHE:HB3	1:B:1697:PHE:CD2	2.33	0.64
1:A:3114:GLU:HG2	1:A:3118:ARG:NH1	2.13	0.64
1:A:4693:ASN:N	1:A:4693:ASN:HD22	1.95	0.64
1:A:2207:LEU:HD13	1:A:2215:ILE:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3293:ARG:HH11	1:A:3293:ARG:HG3	1.63	0.64
1:A:2163:LYS:HB2	1:A:2194:VAL:HG11	1.79	0.64
1:A:3785:ASN:HD22	1:A:3786:PHE:N	1.95	0.64
1:A:4362:GLN:HG3	1:A:4714:GLN:OE1	1.97	0.64
1:B:4351:PHE:CE2	1:B:4689:PRO:HG3	2.32	0.64
1:B:1557:GLY:O	1:B:1561:LEU:HD23	1.98	0.64
1:A:3804:THR:O	1:A:3807:PRO:HD3	1.98	0.64
1:A:2051:LYS:O	1:A:2051:LYS:HD3	1.96	0.64
1:A:1611:ARG:HH11	1:A:1611:ARG:HG3	1.62	0.64
1:A:4396:ILE:O	1:A:4399:LEU:HB2	1.98	0.63
1:A:4296:PHE:CE2	1:A:4347:ILE:HA	2.33	0.63
1:B:3043:ASN:HD22	1:B:3046:TYR:HB2	1.63	0.63
1:B:3087:MET:CE	1:B:3090:LEU:HD23	2.28	0.63
1:A:2490:ALA:O	1:A:2494:VAL:HG23	1.97	0.63
1:A:3387:HIS:HB3	1:A:3473:ALA:HB2	1.80	0.63
1:B:4607:SER:O	1:B:4611:LEU:HG	1.98	0.63
1:A:1811:PRO:O	1:A:1815:VAL:HG23	1.98	0.63
1:A:3416:LYS:HE3	1:A:3418:GLU:HB3	1.80	0.63
1:B:1780:THR:HG22	1:B:1784:LEU:HD12	1.80	0.63
1:B:3563:LEU:HD11	1:B:3845:ILE:HD11	1.79	0.63
1:A:4277:PHE:HB2	1:A:4363:LEU:HD12	1.79	0.63
1:B:1607:ASP:O	1:B:1611:ARG:HG2	1.97	0.63
1:B:1525:ILE:HA	1:B:1528:GLU:HB3	1.80	0.63
1:A:3711:ALA:HA	1:A:3716:CYS:SG	2.39	0.63
1:A:3985:GLU:O	1:A:3989:ASP:HB2	1.97	0.63
1:A:4571:ARG:HA	1:A:4590:TRP:HZ3	1.63	0.63
1:B:1523:GLY:HA3	1:B:1580:TYR:CE2	2.33	0.63
1:B:3238:ILE:HD11	1:B:3617:TRP:HZ2	1.63	0.63
1:A:2995:LEU:HA	1:A:2998:ILE:HD11	1.80	0.63
1:A:4310:ILE:O	1:A:4314:VAL:HB	1.99	0.63
1:A:3482:THR:O	1:A:3486:TYR:HB2	1.99	0.63
1:A:2938:PHE:HB3	1:A:2941:VAL:HG23	1.80	0.63
1:A:3994:GLY:HA3	1:A:4087:LYS:CE	2.29	0.63
1:A:2972:VAL:O	1:A:2976:LEU:HB2	1.98	0.63
1:B:3841:ALA:O	1:B:3842:SER:CB	2.35	0.63
1:A:2995:LEU:HD23	1:A:2998:ILE:HD11	1.80	0.63
1:A:3063:GLY:HA2	1:A:3136:GLN:HB3	1.81	0.63
1:A:4269:ARG:CZ	1:A:4383:VAL:HG11	2.29	0.63
1:A:3445:THR:HG23	1:A:3449:ARG:NH1	2.14	0.63
1:B:3035:LEU:CD2	1:B:3068:LYS:HB3	2.28	0.63
1:A:2000:CYS:SG	1:A:2031:LEU:HD11	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3255:VAL:HA	1:A:3259:HIS:CD2	2.33	0.63
1:B:1592:ASP:O	1:B:1596:ASN:HB2	1.99	0.63
1:B:4133:LEU:HD23	1:B:4230:LEU:HD23	1.79	0.63
1:B:2751:THR:HB	1:B:2756:THR:H	1.63	0.63
1:B:2711:LEU:HD12	1:B:2714:PHE:HD2	1.63	0.63
1:B:2841:ASN:HD22	1:B:2841:ASN:N	1.97	0.62
1:A:3647:TRP:CH2	1:A:3663:ILE:HD12	2.34	0.62
1:A:4049:GLY:O	1:A:4050:LYS:O	2.17	0.62
1:A:3725:ASN:H	1:A:3725:ASN:ND2	1.96	0.62
1:A:2250:VAL:HB	1:A:2425:MET:HE2	1.80	0.62
1:A:3300:LYS:HA	1:A:3564:LEU:HD11	1.81	0.62
1:A:1922:LEU:HD13	1:A:1938:PHE:HD1	1.63	0.62
1:B:3865:ILE:O	1:B:3869:VAL:HG23	1.98	0.62
1:B:4194:PRO:O	1:B:4197:LEU:HB2	1.99	0.62
1:B:2877:ARG:HB3	1:B:2881:ARG:HH12	1.63	0.62
1:A:3599:LEU:HD11	1:A:3638:LEU:HD13	1.80	0.62
1:A:2542:ASN:O	1:A:2546:VAL:HG23	1.99	0.62
1:A:2247:ARG:HB2	1:A:2249:LEU:HG	1.81	0.62
1:A:2205:PRO:HG2	1:A:2265:ILE:HD11	1.81	0.62
1:A:1695:ALA:HB1	1:A:2019:CYS:SG	2.39	0.62
1:A:1975:PRO:HD2	1:A:2101:ILE:HA	1.80	0.62
1:A:2793:ASN:ND2	1:A:2793:ASN:N	2.44	0.62
1:A:1743:GLY:HA3	1:A:1753:THR:HA	1.81	0.62
1:A:2546:VAL:HA	1:A:2549:ILE:HD12	1.80	0.62
1:B:2080:GLY:HA2	1:B:2086:ASN:ND2	2.14	0.62
1:B:3844:ASN:O	1:B:3848:ASP:CB	2.47	0.62
1:B:2277:PRO:HA	1:B:2398:GLN:HG3	1.81	0.62
1:A:3011:HIS:ND1	1:A:3143:VAL:HG23	2.15	0.62
1:A:1927:ILE:HD13	1:A:1991:LEU:HD22	1.79	0.62
1:B:2584:SER:HB3	1:B:2813:ILE:HB	1.82	0.62
1:A:3557:VAL:O	1:A:3561:ILE:HG13	2.00	0.62
1:A:1957:TYR:CD2	1:A:1987:LEU:HD13	2.35	0.62
1:B:2199:ILE:HG23	1:B:2203:MET:HG3	1.81	0.62
1:B:2206:LYS:HB3	1:B:2413:MET:HB3	1.81	0.62
1:A:2645:ASP:O	1:A:2647:VAL:HG23	1.98	0.62
1:A:3634:VAL:HB	1:A:3635:PRO:HD3	1.82	0.62
1:A:3812:LYS:HB3	1:A:3875:VAL:HG22	1.81	0.62
1:A:3452:ILE:HG21	1:A:3485:THR:HG21	1.82	0.62
1:A:4389:ARG:HH11	1:A:4389:ARG:HG2	1.65	0.62
1:A:3408:VAL:HG11	1:A:3477:LEU:HG	1.82	0.62
1:A:4568:PHE:O	1:A:4572:MET:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3566:ASN:HB3	1:A:3855:LEU:HD22	1.82	0.62
1:B:1726:PHE:CD2	1:B:1729:LEU:HD22	2.35	0.62
1:B:4410:LEU:HD22	1:B:4411:PRO:HD2	1.81	0.62
1:A:1967:ARG:HH22	1:A:2069:GLN:HG3	1.63	0.61
1:A:4402:ILE:H	1:A:4402:ILE:HD12	1.65	0.61
1:A:2151:ALA:O	1:A:2155:VAL:HG12	1.99	0.61
1:A:2357:GLY:O	1:A:2397:VAL:HG12	2.00	0.61
1:A:3445:THR:N	1:A:3446:PRO:HD2	2.16	0.61
1:B:2275:VAL:HG13	1:B:2397:VAL:HG13	1.82	0.61
1:A:2954:ASN:H	1:A:2954:ASN:ND2	1.97	0.61
1:A:2912:LEU:C	1:A:2913:PHE:HD2	2.04	0.61
1:A:2090:ASN:HD22	1:A:2090:ASN:C	2.02	0.61
1:B:2212:ILE:N	1:B:2213:PRO:HD2	2.15	0.61
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.35	0.61
1:B:4402:ILE:N	1:B:4402:ILE:HD12	2.14	0.61
1:A:2670:LEU:HG	1:A:2789:VAL:HG22	1.83	0.61
1:A:3271:ILE:O	1:A:3275:ARG:HB2	2.00	0.61
1:B:2704:ALA:HB2	1:B:3085:GLU:OE2	1.98	0.61
1:A:2243:ILE:HD12	1:A:2292:ALA:HB2	1.82	0.61
1:B:3664:MET:O	1:B:3668:PHE:HB3	1.99	0.61
1:B:2208:VAL:HG23	1:B:2211:ASP:HB2	1.81	0.61
1:A:2239:LYS:HA	1:A:2239:LYS:HE3	1.81	0.61
1:A:3731:ASN:N	1:A:3731:ASN:HD22	1.97	0.61
1:A:3260:TYR:O	1:A:3264:ILE:HG12	2.01	0.61
1:B:3673:LEU:HB2	1:B:3781:VAL:CG1	2.26	0.61
1:A:2262:LEU:HD11	1:A:2274:MET:HE2	1.81	0.61
1:A:2258:LYS:HD3	1:A:2261:GLN:HG3	1.83	0.61
1:A:2272:VAL:O	1:A:2394:MET:HA	2.00	0.61
1:A:2869:GLN:HB3	1:A:2872:TYR:CD1	2.36	0.61
1:B:2140:SER:O	1:B:2142:GLN:HG2	1.99	0.61
1:A:4329:ILE:HD12	1:A:4331:TRP:CZ2	2.35	0.61
1:A:2791:ALA:O	1:A:2792:CYS:HB3	2.00	0.61
1:A:4076:ILE:HD11	1:A:4104:SER:O	2.00	0.61
1:A:2948:ARG:HD3	1:A:2950:ILE:HG13	1.82	0.61
1:A:4589:VAL:HG12	1:A:4638:ASN:O	2.01	0.61
1:A:3686:MET:HE2	1:A:3696:LYS:HD2	1.81	0.61
1:A:3474:CYS:HA	1:A:3477:LEU:HD22	1.83	0.61
1:A:2088:PRO:HB2	1:A:2090:ASN:ND2	2.15	0.61
1:B:2732:PRO:HG3	1:B:2739:LEU:HB2	1.83	0.61
1:B:2305:VAL:HG22	1:B:2354:ILE:HB	1.83	0.61
1:A:4600:TYR:O	1:A:4604:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2586:GLY:HA2	1:B:2815:LEU:HD13	1.81	0.61
1:B:4189:ASN:N	1:B:4218:THR:HG22	2.14	0.61
1:B:3291:LYS:HD2	1:B:3835:LEU:HG	1.81	0.61
1:A:3587:THR:HB	1:A:3628:PHE:HA	1.82	0.61
1:A:4624:SER:HB2	1:A:4668:THR:HB	1.83	0.61
1:A:2190:TYR:O	1:A:2194:VAL:HG23	2.01	0.61
1:B:3650:ASN:OD1	1:B:3688:GLN:HA	2.00	0.61
1:A:2985:ASP:O	1:A:2987:PRO:HD3	2.01	0.61
1:A:4396:ILE:HA	1:A:4399:LEU:HD12	1.83	0.60
1:B:2582:GLY:HA2	1:B:2585:MET:HE3	1.81	0.60
1:A:4503:ILE:HG23	1:A:4575:LEU:HB3	1.82	0.60
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.01	0.60
1:A:3385:LYS:O	1:A:3389:ASP:HB2	2.00	0.60
1:B:2869:GLN:HB2	1:B:2872:TYR:CG	2.36	0.60
1:B:4135:CYS:HA	1:B:4219:SER:O	2.00	0.60
1:A:3137:VAL:HG13	1:A:3141:LEU:HD23	1.82	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:HE2	1.83	0.60
1:B:3559:ARG:NE	1:B:3846:LEU:O	2.35	0.60
1:A:4590:TRP:CE3	1:A:4593:GLY:HA3	2.36	0.60
1:A:1687:LEU:HD22	1:A:1705:LEU:HD23	1.83	0.60
1:A:4536:SER:HB2	1:A:4548:LYS:NZ	2.16	0.60
1:A:4636:SER:HB3	1:A:4670:THR:HA	1.83	0.60
1:A:3239:GLY:O	1:A:3243:ILE:HG13	2.00	0.60
1:A:2408:ILE:O	1:A:2409:SER:C	2.38	0.60
1:A:2144:HIS:HB2	1:A:2413:MET:SD	2.40	0.60
1:B:3219:ILE:O	1:B:3221:PRO:HD3	2.00	0.60
1:B:2231:ILE:HG21	1:B:2264:GLN:HE22	1.64	0.60
1:B:2364:VAL:HB	1:B:2407:THR:HG21	1.82	0.60
1:A:2903:ARG:NH2	1:A:2950:ILE:HA	2.16	0.60
1:A:2309:LYS:HG3	1:A:2358:ASP:HB2	1.84	0.60
1:A:2118:PHE:CE1	1:A:2163:LYS:HD2	2.37	0.60
1:A:4690:VAL:O	1:A:4700:LEU:HB2	2.01	0.60
1:A:3345:GLN:O	1:A:3349:ASP:HB2	2.01	0.60
1:A:3718:LEU:HD23	1:A:3762:ILE:HG13	1.84	0.60
1:A:4092:ASP:OD2	1:A:4093:ARG:HG2	2.01	0.60
1:A:1763:GLY:H	1:A:1764:PRO:HD3	1.65	0.60
1:A:3562:ALA:O	1:A:3566:ASN:HB2	2.02	0.60
1:B:3813:ARG:HB3	1:B:3879:ILE:HD13	1.83	0.60
1:A:2250:VAL:HB	1:A:2425:MET:CE	2.31	0.60
1:A:2532:ARG:HG3	1:A:2808:LEU:O	2.01	0.60
1:B:2976:LEU:HD12	1:B:2990:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2917:LEU:HD12	1:A:2923:LYS:HA	1.84	0.60
1:B:1820:GLN:HE22	1:B:1990:GLN:NE2	1.99	0.60
1:A:4182:GLY:HA3	1:A:4212:SER:OG	2.02	0.60
1:A:3075:GLU:O	1:A:3078:VAL:HG12	2.01	0.60
1:A:3598:PHE:CD2	1:A:3634:VAL:HG11	2.36	0.60
1:B:1752:VAL:HG22	1:B:1811:PRO:HG3	1.84	0.60
1:A:4503:ILE:HA	1:A:4575:LEU:HD23	1.84	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:NZ	2.17	0.60
1:B:1908:TYR:CE1	1:B:1958:LEU:HD22	2.37	0.60
1:B:2522:ARG:HD3	1:B:2585:MET:SD	2.42	0.60
1:B:2129:VAL:HG22	1:B:2130:PRO:CD	2.30	0.60
1:A:2730:LEU:HD23	1:A:2783:LEU:HD23	1.83	0.60
1:A:4574:GLN:NE2	1:A:4590:TRP:HB3	2.17	0.60
1:A:2239:LYS:HD3	1:A:2295:GLN:NE2	2.16	0.60
1:B:4153:LEU:HB2	1:B:4155:LYS:HG2	1.83	0.60
1:B:4541:ILE:HA	1:B:4561:LEU:HD11	1.83	0.60
1:A:3040:ILE:HG22	1:A:3042:VAL:HG13	1.82	0.60
1:B:4060:GLU:O	1:B:4064:VAL:HG23	2.02	0.60
1:A:1921:VAL:HG23	1:A:1922:LEU:CD2	2.32	0.60
1:B:3559:ARG:O	1:B:3563:LEU:HB2	2.02	0.60
1:B:1608:VAL:HG21	1:B:1669:MET:HG3	1.83	0.60
1:A:3803:LYS:HE3	1:A:3810:HIS:NE2	2.17	0.60
1:A:3262:ASP:HB2	1:A:3670:ARG:HE	1.67	0.60
1:A:2439:PHE:H	1:A:2495:GLN:HE22	1.48	0.60
1:A:2091:LEU:HD22	1:A:2095:PHE:CE1	2.37	0.60
1:A:1604:VAL:HG11	1:A:1670:GLU:HA	1.84	0.59
1:A:3969:LEU:HD12	1:A:4426:MET:HE2	1.82	0.59
1:B:3017:VAL:HG13	1:B:3174:GLY:O	2.02	0.59
1:A:4004:THR:OG1	1:A:4006:PRO:HD3	2.01	0.59
1:A:3922:ASN:HD22	1:A:3922:ASN:N	2.00	0.59
1:B:3671:TYR:HD2	1:B:3734:LEU:HA	1.67	0.59
1:B:1948:VAL:O	1:B:1950:THR:HG23	2.02	0.59
1:B:4499:PHE:O	1:B:4503:ILE:HB	2.01	0.59
1:A:4691:TYR:CD2	1:A:4696:ARG:HG2	2.36	0.59
1:A:2864:PHE:HB3	1:A:2872:TYR:CD2	2.38	0.59
1:A:3785:ASN:HD22	1:A:3786:PHE:H	1.49	0.59
1:B:2494:VAL:HG11	1:B:2548:VAL:HB	1.84	0.59
1:A:4644:LEU:HD12	1:A:4723:ILE:HG12	1.85	0.59
1:B:3673:LEU:HD22	1:B:3783:PHE:HE1	1.66	0.59
1:B:4124:LYS:O	1:B:4125:GLU:HG2	2.01	0.59
1:A:2273:MET:SD	1:A:2408:ILE:HG22	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4545:ILE:O	1:A:4561:LEU:HD21	2.02	0.59
1:A:3923:LEU:HD22	1:A:3947:ILE:HG12	1.83	0.59
1:B:2616:SER:HB3	1:B:2627:TRP:CE2	2.37	0.59
1:B:4131:PRO:HD2	1:B:4232:MET:O	2.03	0.59
1:B:4137:VAL:HB	1:B:4138:PRO:HD2	1.85	0.59
1:B:2377:LEU:O	1:B:2384:ARG:HA	2.02	0.59
1:A:4715:ASN:O	1:A:4719:ARG:HB2	2.02	0.59
1:A:3672:PRO:HA	1:A:3782:THR:HG23	1.84	0.59
1:A:4190:ILE:HB	1:A:4197:LEU:HD11	1.83	0.59
1:B:2000:CYS:HB3	1:B:2031:LEU:HD13	1.83	0.59
1:A:4371:PRO:HA	1:A:4385:GLU:OE1	2.03	0.59
1:B:1612:TRP:O	1:B:1616:GLU:HB2	2.02	0.59
1:A:3730:LEU:HD11	1:A:3762:ILE:CD1	2.33	0.59
1:A:4157:TYR:OH	1:A:4186:LEU:HD22	2.03	0.59
1:A:3731:ASN:HB2	1:A:3732:PRO:HD3	1.84	0.59
1:A:4597:PRO:HB2	1:A:4700:LEU:HD21	1.85	0.59
1:B:3897:TYR:HE1	1:B:3913:LEU:HA	1.67	0.59
1:B:3024:VAL:HG11	2:B:9010:ADP:H3'	1.83	0.59
1:A:2528:PHE:CE1	1:A:2533:VAL:HG11	2.38	0.59
1:B:3809:THR:HG21	1:B:3882:VAL:HG11	1.84	0.59
1:B:4273:LEU:HD13	1:B:4363:LEU:O	2.02	0.59
1:A:2293:ILE:HG22	1:A:2350:ARG:NH2	2.12	0.59
1:A:2938:PHE:HB3	1:A:2941:VAL:CG2	2.33	0.59
1:A:3924:LEU:HD23	1:A:3943:LEU:CD2	2.32	0.59
1:A:2648:ILE:HG21	1:A:2827:ILE:HA	1.84	0.59
1:B:1625:ILE:HD12	1:B:1628:LEU:HB2	1.83	0.59
1:A:3951:THR:O	1:A:3955:VAL:HG23	2.02	0.59
1:B:2863:ARG:O	1:B:2863:ARG:HD3	2.02	0.59
1:A:4494:PRO:HD3	1:A:4610:GLN:HE22	1.67	0.59
1:A:3190:ARG:HA	1:A:3224:ARG:HH12	1.66	0.59
1:B:1546:VAL:HG22	1:B:1556:ARG:CZ	2.33	0.59
1:B:4207:LEU:O	1:B:4209:PRO:HD3	2.02	0.59
1:B:4424:ARG:NH2	1:B:4558:THR:HG21	2.17	0.59
1:B:2598:GLN:HG2	1:B:2612:LEU:HD23	1.85	0.59
1:B:4332:ILE:O	1:B:4336:THR:HG23	2.02	0.59
1:A:2863:ARG:HD2	1:A:2864:PHE:CE1	2.36	0.59
1:B:1477:LYS:H	1:B:1480:HIS:HD2	1.50	0.59
1:A:3313:LEU:HD13	1:A:3550:SER:OG	2.03	0.59
1:A:4136:SER:O	1:A:4221:ILE:HD12	2.03	0.59
1:B:2273:MET:HG2	1:B:2395:PHE:HB2	1.84	0.59
1:A:1978:THR:CG2	1:A:2103:PRO:HD3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4572:MET:HA	1:A:4575:LEU:HD13	1.85	0.59
1:B:3788:VAL:HG11	1:B:3913:LEU:HD22	1.85	0.59
1:A:2991:PHE:HE1	1:A:2993:GLU:HB2	1.67	0.59
1:A:2598:GLN:CG	1:A:2612:LEU:HB2	2.33	0.59
1:A:1538:TRP:HZ3	1:A:1656:ILE:HD13	1.68	0.59
1:B:4109:ASP:HA	1:B:4112:ASN:HD22	1.67	0.58
1:B:3233:TYR:CD2	1:B:3620:ARG:HG3	2.38	0.58
1:A:1763:GLY:N	1:A:1764:PRO:CD	2.65	0.58
1:A:4066:GLN:NE2	1:A:4081:ARG:HD3	2.18	0.58
1:A:2278:SER:HA	1:A:2806:ARG:HH11	1.68	0.58
1:A:1973:PHE:CE1	1:A:2099:ALA:HA	2.38	0.58
1:A:1797:VAL:CG1	1:A:1855:ILE:HD11	2.33	0.58
1:B:4351:PHE:CD2	1:B:4689:PRO:HG3	2.38	0.58
1:B:2375:LYS:HB3	1:B:2387:LEU:HB3	1.84	0.58
1:A:1735:ASP:OD2	1:A:1737:GLU:HB2	2.03	0.58
1:B:4349:ASN:HB3	1:B:4352:ASP:OD2	2.03	0.58
1:A:4193:ALA:O	1:A:4197:LEU:HD23	2.03	0.58
1:B:3027:ARG:HG2	1:B:3037:ILE:HD12	1.85	0.58
1:A:3723:VAL:HG12	1:A:3766:THR:OG1	2.03	0.58
1:B:4030:PHE:HD1	1:B:4033:LEU:HD22	1.68	0.58
1:A:3331:GLN:NE2	1:A:3533:LYS:HG3	2.18	0.58
1:B:3170:LEU:HD21	1:B:3172:TRP:HE3	1.67	0.58
1:A:2043:ILE:HG23	1:A:2073:ILE:HD12	1.84	0.58
1:A:4251:THR:HG23	1:A:4303:LEU:CD2	2.30	0.58
1:A:4349:ASN:HD22	1:A:4352:ASP:H	1.51	0.58
1:B:1901:ASN:HD22	1:B:1901:ASN:N	2.01	0.58
1:A:3830:LEU:HB3	1:A:3858:LEU:HD13	1.86	0.58
1:B:3182:PHE:O	1:B:3186:SER:HB2	2.03	0.58
1:B:2166:CYS:HA	1:B:2190:TYR:OH	2.03	0.58
1:A:2153:LYS:O	1:A:2157:VAL:HG23	2.03	0.58
1:A:4368:ALA:HA	1:A:4373:PHE:CE1	2.38	0.58
1:A:4003:GLU:HG3	1:B:2842:LEU:CD2	2.34	0.58
1:B:3620:ARG:HH11	1:B:3620:ARG:HG2	1.69	0.58
1:B:1884:HIS:O	1:B:1888:VAL:HG23	2.03	0.58
1:A:3803:LYS:HG3	1:A:3810:HIS:CD2	2.39	0.58
1:A:4032:LYS:HG3	1:A:4069:LEU:HD11	1.83	0.58
1:A:2087:LEU:HB2	1:A:2092:LYS:HG3	1.86	0.58
1:A:2361:PRO:HD3	1:A:2402:TYR:O	2.03	0.58
1:A:2212:ILE:N	1:A:2213:PRO:HD2	2.18	0.58
1:B:2338:ARG:HD2	1:B:2346:GLU:OE1	2.04	0.58
1:B:1821:ILE:HG21	1:B:1914:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1950:THR:HB	1:A:1951:PRO:HD2	1.84	0.58
1:A:1849:GLU:HG3	1:A:1893:GLN:OE1	2.03	0.58
1:B:1719:GLN:HA	1:B:1722:PHE:CE2	2.38	0.58
1:B:4388:THR:HG23	1:B:4391:HIS:HD2	1.68	0.58
1:B:2997:HIS:O	1:B:3001:ILE:HG13	2.03	0.58
1:B:3013:LEU:HD22	1:B:3164:LEU:HD12	1.85	0.58
1:A:4572:MET:HA	1:A:4575:LEU:CD1	2.34	0.58
1:B:1855:ILE:HG22	1:B:1859:LEU:HD12	1.85	0.58
1:B:3923:LEU:HD22	1:B:3947:ILE:HG23	1.85	0.58
1:A:3615:ARG:O	1:A:3619:ILE:HG13	2.03	0.58
1:B:1748:GLU:HB3	1:B:1943:ILE:HD12	1.85	0.58
1:A:1863:VAL:HG21	1:A:2115:SER:O	2.04	0.58
1:A:2135:CYS:HB3	1:A:2147:PHE:CZ	2.38	0.58
1:B:1926:VAL:HG12	1:B:1928:HIS:CD2	2.39	0.58
1:B:3192:LEU:HD11	1:B:3268:VAL:HA	1.84	0.58
1:A:1995:VAL:HA	1:A:2022:TRP:HB2	1.84	0.58
1:B:1643:PHE:CE2	1:B:1647:LEU:HD11	2.39	0.58
1:B:4648:VAL:HA	1:B:4662:THR:HG21	1.85	0.58
1:B:3263:PHE:O	1:B:3267:VAL:HG23	2.03	0.58
1:A:3337:LYS:HA	1:A:3341:ALA:HB3	1.86	0.57
1:A:2838:LEU:O	1:A:2839:LEU:HD23	2.04	0.57
1:B:1813:GLN:NE2	1:B:1941:LEU:H	2.02	0.57
1:B:1939:GLU:O	1:B:1941:LEU:HG	2.03	0.57
1:B:3785:ASN:HD21	1:B:3787:THR:CG2	2.16	0.57
1:A:3255:VAL:O	1:A:3255:VAL:HG13	2.03	0.57
1:A:3595:ALA:HB1	1:A:3638:LEU:HD11	1.85	0.57
1:B:2863:ARG:HG3	1:B:2925:TRP:CE2	2.39	0.57
1:A:4559:ILE:HG23	1:A:4559:ILE:O	2.04	0.57
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.03	0.57
1:B:4189:ASN:ND2	1:B:4189:ASN:N	2.53	0.57
1:A:3487:TYR:O	1:A:3490:ILE:HG12	2.04	0.57
1:A:1982:GLU:HG3	2:A:9001:ADP:H3'	1.86	0.57
1:A:3274:LYS:O	1:A:3278:LEU:HD23	2.04	0.57
1:A:4284:ARG:HG3	1:A:4408:LEU:HB3	1.86	0.57
1:B:3674:VAL:HG13	1:B:3786:PHE:HD2	1.68	0.57
1:B:2869:GLN:HB2	1:B:2872:TYR:CD2	2.39	0.57
1:B:3897:TYR:CE1	1:B:3913:LEU:HA	2.38	0.57
1:B:4255:ILE:HD11	1:B:4307:LEU:HD11	1.85	0.57
1:A:2739:LEU:HD23	1:A:2740:VAL:N	2.19	0.57
1:A:3668:PHE:CD1	1:A:3672:PRO:HD3	2.39	0.57
1:B:2533:VAL:HB	1:B:2581:LEU:CD2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2839:LEU:HD11	1:A:2890:ILE:HD12	1.85	0.57
1:A:2560:MET:HG3	1:A:2561:SER:N	2.16	0.57
1:B:1888:VAL:O	1:B:1892:LEU:HD12	2.04	0.57
1:A:4277:PHE:HB2	1:A:4363:LEU:CD1	2.34	0.57
1:B:2578:MET:HE1	1:B:2612:LEU:HD12	1.86	0.57
1:B:1889:VAL:HA	1:B:1892:LEU:HD13	1.86	0.57
1:B:1687:LEU:HD21	1:B:1706:LEU:CD2	2.33	0.57
1:B:2235:GLN:HE22	1:B:2296:VAL:HG13	1.68	0.57
1:B:2219:LEU:CD1	1:B:2228:LEU:HD11	2.35	0.57
1:A:3909:TYR:OH	1:A:3960:LEU:HG	2.04	0.57
1:B:2417:SER:O	1:B:2420:ILE:HG12	2.03	0.57
1:A:4313:TRP:HB3	1:A:4330:PRO:HG2	1.86	0.57
1:B:4379:ILE:O	1:B:4379:ILE:HG13	2.05	0.57
1:B:2841:ASN:HD22	1:B:2842:LEU:N	2.02	0.57
1:A:2195:LEU:O	1:A:2199:ILE:HG12	2.04	0.57
1:B:3638:LEU:HD12	1:B:3663:ILE:HG21	1.86	0.57
1:A:2053:ASN:O	1:A:2054:SER:C	2.42	0.57
1:A:2252:LYS:O	1:A:2256:VAL:HG23	2.05	0.57
1:B:4318:SER:HB3	1:B:4324:ILE:HD11	1.85	0.57
1:A:3863:THR:O	1:A:3867:LEU:HB3	2.04	0.57
1:B:2835:LEU:HD11	1:B:2890:ILE:HD12	1.85	0.57
1:A:2873:ILE:HD12	1:A:2873:ILE:H	1.68	0.57
1:A:4288:ILE:HG23	1:A:4292:TRP:O	2.04	0.57
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.40	0.57
1:B:2270:HIS:HA	1:B:2392:ARG:HH11	1.70	0.57
1:B:1591:TRP:O	1:B:1595:LEU:HB2	2.05	0.57
1:A:4245:LYS:HD2	1:A:4399:LEU:O	2.04	0.57
1:B:3238:ILE:HG12	1:B:3601:TYR:CD2	2.40	0.57
1:B:2540:LEU:HD12	1:B:2662:ALA:HB3	1.85	0.57
1:A:1718:ILE:HG22	1:A:1722:PHE:CE2	2.40	0.57
1:B:3793:LEU:HD23	1:B:3894:SER:HA	1.86	0.57
1:B:2586:GLY:HA2	1:B:2815:LEU:CD1	2.34	0.57
1:A:4050:LYS:O	1:A:4051:ASP:C	2.42	0.57
1:A:1978:THR:HG22	1:A:2103:PRO:HD3	1.87	0.57
1:B:3912:SER:HB3	1:B:4231:ARG:HG2	1.86	0.57
1:B:4313:TRP:HB3	1:B:4330:PRO:HG2	1.87	0.57
1:A:1681:LYS:O	1:A:1685:GLU:HG3	2.04	0.57
1:A:4415:GLU:OE2	1:A:4415:GLU:HA	2.05	0.57
1:A:4375:LEU:HD11	1:A:4383:VAL:CG2	2.30	0.56
1:A:4132:LEU:HD23	1:A:4236:PHE:HE2	1.70	0.56
1:B:3274:LYS:HE3	1:B:3637:PHE:CE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3266:GLN:HE21	1:A:3270:LEU:CD2	2.18	0.56
1:B:4043:ASP:HB3	1:B:4059:PRO:HB3	1.87	0.56
1:A:3291:LYS:HG3	1:A:3835:LEU:HD22	1.86	0.56
1:B:1537:PHE:O	1:B:1541:LEU:HB2	2.05	0.56
1:A:2989:VAL:HG13	1:A:3187:GLU:CD	2.25	0.56
1:A:3439:ASP:HB3	1:A:3442:LYS:HG2	1.87	0.56
1:B:4543:LYS:HD2	1:B:4545:ILE:HD13	1.87	0.56
1:B:3614:MET:O	1:B:3618:MET:HG3	2.04	0.56
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.69	0.56
1:A:2121:ALA:O	1:A:2122:GLU:C	2.43	0.56
1:A:1978:THR:HG21	1:A:2101:ILE:O	2.05	0.56
1:A:4132:LEU:HD13	1:A:4216:PHE:CE1	2.40	0.56
1:A:4432:LYS:C	1:A:4434:GLN:H	2.08	0.56
1:A:1927:ILE:HD13	1:A:1991:LEU:CD2	2.35	0.56
1:B:4618:ASN:N	1:B:4618:ASN:HD22	2.02	0.56
1:B:1554:LEU:HB3	1:B:1609:GLN:NE2	2.09	0.56
1:A:3813:ARG:HB2	1:A:3813:ARG:CZ	2.34	0.56
1:A:3813:ARG:HB3	1:A:3879:ILE:HD11	1.88	0.56
1:A:2560:MET:CE	1:A:2564:ASN:HD22	2.18	0.56
1:A:2675:PRO:HG2	1:A:2678:SER:HB3	1.88	0.56
1:A:3299:VAL:HG21	1:A:3563:LEU:HD23	1.87	0.56
1:A:3567:LEU:CD2	1:A:3855:LEU:HD11	2.36	0.56
1:A:3195:GLU:OE1	1:A:3224:ARG:HB2	2.04	0.56
1:A:2979:PHE:HE2	1:A:3028:PHE:HA	1.70	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.44	0.56
1:B:1531:LEU:HD13	1:B:1587:GLU:OE2	2.05	0.56
1:B:1956:CYS:SG	1:B:1983:THR:HG21	2.45	0.56
1:A:3598:PHE:HA	1:A:3602:ILE:HG12	1.88	0.56
1:A:3682:MET:SD	1:A:3696:LYS:HE2	2.46	0.56
1:A:3584:GLN:O	1:A:3588:VAL:HG23	2.06	0.56
1:A:4277:PHE:O	1:A:4281:ILE:HG12	2.06	0.56
1:A:2806:ARG:HH12	2:A:9002:ADP:PB	2.28	0.56
1:B:4213:PHE:CZ	1:B:4215:LEU:HB2	2.40	0.56
1:B:2660:LEU:HD21	1:B:2672:LEU:HD21	1.87	0.56
1:A:2229:GLN:HB3	1:A:2230:PRO:HD2	1.86	0.56
1:A:1752:VAL:HG22	1:A:1811:PRO:HG3	1.86	0.56
1:B:2144:HIS:HB3	1:B:2400:LEU:HD12	1.86	0.56
1:B:2739:LEU:HB3	1:B:2786:ILE:HG12	1.87	0.56
1:A:1947:LEU:HD11	1:A:1982:GLU:HB3	1.87	0.56
1:A:4117:ASP:OD1	1:A:4119:ALA:HB3	2.06	0.56
1:A:2087:LEU:O	1:A:2092:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2841:ASN:N	1:B:2841:ASN:ND2	2.54	0.56
1:A:4534:LEU:HA	1:A:4537:LEU:HD12	1.88	0.56
1:A:2284:THR:O	1:A:2288:VAL:HG23	2.06	0.56
1:A:1948:VAL:O	1:A:1950:THR:HG23	2.06	0.56
1:B:2670:LEU:HD11	1:B:2789:VAL:HG13	1.88	0.56
1:B:2560:MET:HG3	1:B:2564:ASN:HB2	1.88	0.56
1:B:2841:ASN:ND2	1:B:2842:LEU:N	2.52	0.56
1:A:3445:THR:HA	1:A:3449:ARG:HD3	1.87	0.56
1:A:2954:ASN:N	1:A:2954:ASN:ND2	2.53	0.56
1:B:3043:ASN:H	1:B:3043:ASN:HD22	1.54	0.56
1:A:3848:ASP:HB3	1:A:3851:VAL:HG12	1.88	0.56
1:B:3758:PRO:HG2	1:B:3759:SER:H	1.71	0.56
1:A:3887:ASN:HB3	1:A:3888:PRO:HD3	1.88	0.56
1:A:2906:ALA:O	1:A:2910:LEU:HG	2.05	0.56
1:A:3813:ARG:HH22	1:A:3817:LEU:CD1	2.18	0.56
1:A:2748:LEU:N	1:A:2749:PRO:CD	2.69	0.56
1:A:4622:HIS:HE2	1:A:4678:ILE:CG2	2.16	0.56
1:A:2941:VAL:HG12	1:A:2942:ASN:N	2.20	0.56
1:A:3376:ALA:O	1:A:3380:VAL:HG23	2.06	0.56
1:B:2081:TYR:O	1:B:2084:ARG:HD2	2.06	0.56
1:A:1687:LEU:HD21	1:A:1706:LEU:HD23	1.88	0.56
1:B:2163:LYS:HB2	1:B:2194:VAL:HG11	1.87	0.56
1:B:1479:ARG:CZ	1:B:1479:ARG:HB2	2.35	0.56
1:A:1862:SER:O	1:A:1865:GLN:HG2	2.06	0.56
1:A:3404:ALA:HA	1:A:3462:PHE:HE1	1.71	0.56
1:B:2276:GLY:O	1:B:2398:GLN:HA	2.06	0.56
1:A:4589:VAL:HG12	1:A:4639:VAL:HA	1.88	0.56
1:A:2381:ASN:OD1	1:A:2383:GLU:HB2	2.06	0.56
1:B:3729:VAL:O	1:B:3729:VAL:HG22	2.05	0.56
1:B:4535:ARG:HG2	1:B:4535:ARG:HH11	1.71	0.55
1:B:4147:ASP:HA	1:B:4157:TYR:OH	2.06	0.55
1:A:3292:LEU:HD22	1:A:3567:LEU:HD22	1.89	0.55
1:B:4389:ARG:HG2	1:B:4389:ARG:NH1	2.21	0.55
1:A:1957:TYR:O	1:A:1961:THR:HG23	2.07	0.55
1:B:4190:ILE:HG12	1:B:4219:SER:HB2	1.86	0.55
1:B:3908:LEU:HD22	1:B:4221:ILE:HG23	1.87	0.55
1:A:3673:LEU:HD13	1:A:3783:PHE:CE1	2.40	0.55
1:A:2910:LEU:HD23	1:A:2930:ILE:CD1	2.33	0.55
1:B:3700:LEU:CD2	1:B:3701:ASP:H	2.18	0.55
1:B:2829:GLY:HA2	1:B:2850:THR:OG1	2.06	0.55
1:A:4005:ILE:HG22	1:A:4008:LEU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4388:THR:O	1:B:4391:HIS:HB2	2.07	0.55
1:A:1800:HIS:HB2	1:A:1858:ASN:HD22	1.71	0.55
1:B:2603:THR:O	1:B:2605:VAL:HG13	2.06	0.55
1:A:2650:THR:H	1:A:2653:THR:HB	1.71	0.55
1:A:2615:TYR:HD1	1:A:2624:TRP:HB3	1.72	0.55
1:A:4590:TRP:CD2	1:A:4593:GLY:HA3	2.42	0.55
1:A:1926:VAL:HG12	1:A:1928:HIS:CD2	2.41	0.55
1:A:2991:PHE:CE1	1:A:2993:GLU:HB2	2.40	0.55
1:A:1699:PHE:HE1	1:A:2015:GLY:HA3	1.71	0.55
1:B:2440:ASP:OD1	1:B:2441:PRO:HD2	2.06	0.55
1:B:2101:ILE:O	1:B:2103:PRO:HD3	2.07	0.55
1:A:3368:LYS:C	1:A:3374:ILE:HD11	2.26	0.55
1:A:3419:TRP:CE3	1:A:3422:ILE:HD11	2.42	0.55
1:A:3066:GLU:HG2	1:A:3136:GLN:HE21	1.71	0.55
1:B:2369:SER:HA	1:B:2372:ASP:OD2	2.07	0.55
1:A:3555:ASN:HB3	1:A:3559:ARG:HH11	1.71	0.55
1:A:2606:PRO:HG2	1:A:2615:TYR:CE1	2.42	0.55
1:A:1625:ILE:HG23	1:A:1626:ASN:H	1.70	0.55
1:B:2774:ARG:HB2	1:B:2781:ILE:CD1	2.37	0.55
1:A:3930:LEU:HG	1:A:3939:ARG:NH1	2.21	0.55
1:A:1875:PHE:O	1:A:1879:ILE:HG12	2.07	0.55
1:A:1763:GLY:H	1:A:1764:PRO:CD	2.19	0.55
1:A:3471:SER:HB3	1:A:3474:CYS:SG	2.47	0.55
1:B:1872:ARG:HH12	1:B:2164:ARG:HD3	1.71	0.55
1:A:4094:VAL:HB	1:A:4423:ALA:HB1	1.88	0.55
1:A:3991:LEU:O	1:A:3991:LEU:HD12	2.07	0.55
1:B:1555:VAL:HG23	1:B:1609:GLN:HE21	1.70	0.55
1:A:2274:MET:CE	1:A:2286:TRP:HB3	2.30	0.55
1:A:1608:VAL:HG13	1:A:1676:LEU:CD1	2.37	0.55
1:A:4319:LYS:H	1:A:4321:ARG:NH2	2.04	0.55
1:B:3018:SER:O	1:B:3256:THR:HB	2.06	0.55
1:A:3453:THR:O	1:A:3458:GLU:HG2	2.06	0.55
1:A:2765:GLN:O	1:A:2769:LYS:HB2	2.07	0.55
1:A:1797:VAL:HG13	1:A:1855:ILE:HD11	1.89	0.55
1:B:4644:LEU:HG	1:B:4664:ILE:HD11	1.88	0.55
1:B:4624:SER:HB2	1:B:4668:THR:HB	1.87	0.55
1:B:3306:LEU:HD22	1:B:3553:VAL:HG13	1.89	0.55
1:B:4132:LEU:HD13	1:B:4216:PHE:CE1	2.42	0.55
1:B:4685:LYS:HE2	1:B:4706:PRO:HD3	1.88	0.55
1:A:2262:LEU:HD11	1:A:2274:MET:CE	2.37	0.55
1:A:2446:GLN:O	1:A:2450:ASN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4571:ARG:O	1:A:4574:GLN:HB3	2.07	0.55
1:B:2612:LEU:HD11	1:B:2624:TRP:CH2	2.42	0.55
1:A:3647:TRP:HH2	1:A:3663:ILE:HD12	1.71	0.55
1:A:2439:PHE:H	1:A:2495:GLN:NE2	2.05	0.55
1:B:2000:CYS:C	1:B:2002:GLU:H	2.10	0.55
1:B:2863:ARG:HD2	1:B:2864:PHE:CE1	2.42	0.55
1:B:2918:VAL:HG13	1:B:3172:TRP:NE1	2.22	0.55
1:B:2779:THR:O	1:B:2781:ILE:HD12	2.06	0.55
1:A:1907:LEU:HA	1:A:1911:ARG:NH1	2.21	0.55
1:B:4095:LEU:HD11	1:B:4422:LYS:CB	2.37	0.55
1:A:4495:LEU:CD1	1:A:4495:LEU:H	2.16	0.55
1:B:4024:ARG:HA	1:B:4030:PHE:O	2.07	0.55
1:A:3965:LEU:HG	1:A:4426:MET:CE	2.37	0.55
1:A:3373:ILE:CD1	1:A:3373:ILE:H	2.06	0.54
1:A:3253:ASN:HB2	1:A:3604:PHE:CE2	2.42	0.54
1:B:2898:LEU:O	1:B:2902:VAL:HG23	2.06	0.54
1:A:2648:ILE:HD13	1:A:2831:PHE:CZ	2.42	0.54
1:B:4101:PHE:O	1:B:4105:VAL:HG23	2.07	0.54
1:A:1755:LYS:HG2	1:A:1780:THR:HG23	1.89	0.54
1:B:4571:ARG:HD3	1:B:4593:GLY:O	2.06	0.54
1:A:2204:ILE:N	1:A:2205:PRO:CD	2.69	0.54
1:A:2275:VAL:HG13	1:A:2415:TRP:CE3	2.42	0.54
1:A:2196:LEU:HD21	1:A:2219:LEU:HD22	1.89	0.54
1:A:1908:TYR:CE1	1:A:1958:LEU:HD13	2.42	0.54
1:B:3652:LEU:HB2	1:B:3684:PHE:CD1	2.43	0.54
1:A:3266:GLN:HE21	1:A:3270:LEU:HD21	1.71	0.54
1:B:1694:PHE:CE1	1:B:1770:LEU:HD13	2.42	0.54
1:B:2832:ASN:HA	1:B:2835:LEU:HB3	1.89	0.54
1:A:3390:GLU:O	1:A:3394:LEU:HG	2.07	0.54
1:A:4413:ASN:ND2	1:A:4660:LEU:HG	2.22	0.54
1:A:3647:TRP:HB3	1:A:3652:LEU:CD2	2.37	0.54
1:A:2431:LEU:HD11	1:A:2506:PHE:CD2	2.42	0.54
1:A:1890:ARG:O	1:A:1894:LYS:HG3	2.07	0.54
1:B:2200:ASN:HA	1:B:2204:ILE:HG12	1.89	0.54
1:A:3830:LEU:HB3	1:A:3858:LEU:CD1	2.37	0.54
1:B:2968:LEU:O	1:B:2972:VAL:HG23	2.07	0.54
1:A:4319:LYS:N	1:A:4321:ARG:NH2	2.55	0.54
1:B:4013:SER:H	1:B:4016:GLN:HE21	1.54	0.54
1:B:2331:LEU:HD21	1:B:2773:TRP:CD1	2.43	0.54
1:B:2283:THR:HA	1:B:2286:TRP:NE1	2.22	0.54
1:A:3086:ARG:HH11	1:A:3096:VAL:CG1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1548:TYR:CD1	1:B:1549:GLN:HG2	2.43	0.54
1:B:1655:LEU:HD22	1:B:1655:LEU:H	1.72	0.54
1:A:3700:LEU:CG	1:A:3701:ASP:H	2.20	0.54
1:B:4323:ASN:ND2	1:B:4323:ASN:N	2.54	0.54
1:A:4121:ILE:O	1:A:4126:VAL:HG12	2.06	0.54
1:A:4553:TYR:CD1	1:A:4553:TYR:N	2.75	0.54
1:B:2498:CYS:SG	1:B:2569:ILE:HG13	2.47	0.54
1:B:2803:LEU:HD12	1:B:2808:LEU:HD21	1.90	0.54
1:B:2990:LEU:HD23	1:B:2994:VAL:HG11	1.90	0.54
1:A:1691:ARG:HD3	1:A:1698:TYR:CD1	2.41	0.54
1:A:3336:ILE:O	1:A:3340:ASP:HB3	2.08	0.54
1:B:2024:CYS:HA	1:B:2074:PHE:O	2.06	0.54
1:A:3602:ILE:O	1:A:3604:PHE:N	2.40	0.54
1:B:2603:THR:CG2	1:B:2604:PRO:HD2	2.31	0.54
1:A:2766:MET:HB3	1:A:2783:LEU:CD1	2.36	0.54
1:A:4122:VAL:HG23	1:A:4214:ARG:HD2	1.89	0.54
1:A:2014:VAL:HG22	1:A:2065:ILE:HD13	1.90	0.54
1:B:2874:TYR:OH	1:B:2916:ARG:HD2	2.08	0.54
1:A:1951:PRO:HG2	1:A:2104:ASP:OD1	2.08	0.54
1:B:1782:ALA:HA	1:B:1938:PHE:CE1	2.42	0.54
1:B:2516:LEU:HD12	1:B:2581:LEU:HD13	1.90	0.54
1:B:2519:ALA:HB2	1:B:2593:PHE:CZ	2.43	0.54
1:A:2121:ALA:O	1:A:2124:LEU:N	2.41	0.54
1:B:4080:PHE:HB2	1:B:4101:PHE:CE1	2.43	0.54
1:A:4254:GLY:O	1:A:4256:PRO:HD3	2.07	0.54
1:A:3423:ARG:O	1:A:3426:ILE:HG22	2.07	0.54
1:A:4348:ASP:OD2	1:A:4349:ASN:N	2.40	0.54
1:B:2641:VAL:HG12	1:B:2642:ALA:N	2.23	0.54
1:A:2031:LEU:HD23	1:A:2035:ILE:HG22	1.89	0.54
1:A:3399:THR:N	1:A:3400:PRO:HD2	2.23	0.54
1:B:4058:ILE:HD12	1:B:4082:LYS:HG2	1.89	0.54
1:A:2751:THR:HB	1:A:2755:GLY:HA2	1.90	0.54
1:A:3263:PHE:O	1:A:3267:VAL:HG23	2.07	0.54
1:A:4013:SER:H	1:A:4016:GLN:HB3	1.73	0.54
1:A:2266:LEU:HD21	1:A:2394:MET:HE3	1.89	0.54
1:A:2447:GLN:HE22	1:A:2492:LEU:CD2	2.21	0.54
1:B:4336:THR:O	1:B:4340:SER:HB3	2.08	0.54
1:A:4547:PRO:HB2	1:A:4550:TRP:CE3	2.43	0.54
1:B:1975:PRO:HD2	1:B:2100:MET:O	2.07	0.54
1:B:2636:VAL:HG21	1:B:2648:ILE:HD11	1.89	0.54
1:B:1982:GLU:HA	1:B:1982:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1724:LYS:HD3	1:A:2382:GLY:O	2.07	0.54
1:B:2929:LYS:O	1:B:2933:VAL:HG23	2.07	0.54
1:B:2500:ALA:HA	1:B:2503:SER:OG	2.08	0.54
1:A:3043:ASN:HD22	1:A:3043:ASN:N	2.05	0.54
1:A:3373:ILE:HD13	1:A:3373:ILE:N	2.12	0.54
1:B:3677:PRO:CD	1:B:3787:THR:HG22	2.38	0.54
1:B:2653:THR:O	1:B:2657:VAL:HG23	2.08	0.54
1:A:4318:SER:CA	1:A:4321:ARG:HH21	2.19	0.54
1:B:3255:VAL:HA	1:B:3259:HIS:CD2	2.43	0.54
1:A:2128:ILE:HG13	1:A:2152:LEU:HD21	1.90	0.54
1:B:4257:ALA:HB2	1:B:4389:ARG:HD3	1.90	0.54
1:A:3760:PHE:CG	1:A:3761:MET:N	2.75	0.54
1:A:3109:MET:O	1:A:3112:CYS:HB2	2.08	0.54
1:A:2819:PRO:HD2	1:A:2876:PRO:HG2	1.89	0.54
1:A:1822:VAL:HG12	1:A:1826:GLN:OE1	2.07	0.54
1:A:2689:ARG:C	1:A:2691:PHE:H	2.12	0.54
1:A:3827:LEU:O	1:A:3831:GLU:HG3	2.08	0.54
1:A:2653:THR:O	1:A:2657:VAL:HG23	2.07	0.53
1:B:4639:VAL:O	1:B:4666:ILE:HD12	2.08	0.53
1:B:1910:MET:CA	1:B:1929:MET:HG3	2.39	0.53
1:A:4375:LEU:CD1	1:A:4383:VAL:HG23	2.32	0.53
1:A:3698:SER:HB2	1:A:3721:GLN:HB2	1.90	0.53
1:A:4553:TYR:N	1:A:4553:TYR:HD1	2.05	0.53
1:B:2863:ARG:HG3	1:B:2925:TRP:CZ2	2.44	0.53
1:A:3218:ALA:O	1:A:3219:ILE:C	2.47	0.53
1:B:1581:TYR:O	1:B:1585:GLU:HB2	2.08	0.53
1:B:1831:LEU:HD13	1:B:1900:GLY:O	2.07	0.53
1:B:1646:ILE:O	1:B:1650:VAL:HG23	2.08	0.53
1:A:2969:ARG:HG3	1:A:2970:GLU:N	2.23	0.53
1:B:3342:ARG:O	1:B:3345:GLN:HB3	2.07	0.53
1:B:1655:LEU:HB2	1:B:1658:GLU:CB	2.31	0.53
1:A:3418:GLU:O	1:A:3422:ILE:HG23	2.08	0.53
1:B:1920:ASN:HD22	1:B:1921:VAL:N	2.06	0.53
1:B:2050:LEU:HG	1:B:2067:LEU:HD21	1.89	0.53
1:A:2825:THR:O	1:A:2829:GLY:HA3	2.08	0.53
1:A:4012:LEU:HD12	1:A:4012:LEU:N	2.23	0.53
1:B:3677:PRO:HG3	1:B:3787:THR:HG22	1.89	0.53
1:A:1827:VAL:O	1:A:1831:LEU:HG	2.08	0.53
1:B:3700:LEU:HD13	1:B:3701:ASP:H	1.71	0.53
1:B:2309:LYS:CE	1:B:2756:THR:HG21	2.39	0.53
1:A:1803:TYR:HE1	1:A:1855:ILE:HD13	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2118:PHE:CE1	1:B:2163:LYS:HG3	2.44	0.53
1:A:1699:PHE:HD1	1:A:1699:PHE:N	2.06	0.53
1:A:4596:ASN:C	1:A:4596:ASN:HD22	2.11	0.53
1:A:4376:VAL:HG12	1:A:4379:ILE:HG22	1.90	0.53
1:B:4671:TRP:C	1:B:4672:LYS:HG2	2.29	0.53
1:A:2704:ALA:O	1:A:2706:THR:HG23	2.08	0.53
1:A:2994:VAL:O	1:A:2998:ILE:HG12	2.08	0.53
1:A:1650:VAL:HG13	1:A:1659:VAL:HG11	1.91	0.53
1:A:2274:MET:HE1	1:A:2286:TRP:HD1	1.73	0.53
1:B:2540:LEU:HD12	1:B:2662:ALA:CB	2.39	0.53
1:B:3109:MET:O	1:B:3129:LEU:HD21	2.09	0.53
1:A:2341:ASP:O	1:A:2343:VAL:N	2.40	0.53
1:B:4098:SER:O	1:B:4102:VAL:HG23	2.09	0.53
1:A:2016:LEU:HD21	1:A:2023:GLY:HA3	1.89	0.53
1:B:3067:GLU:O	1:B:3069:ILE:HG13	2.08	0.53
1:B:2515:VAL:HG11	1:B:2577:LEU:HD13	1.90	0.53
1:A:2397:VAL:HG21	1:A:2400:LEU:CD2	2.38	0.53
1:A:1709:ILE:HA	1:A:1766:ILE:HG12	1.90	0.53
1:A:2745:GLU:HB3	1:A:2748:LEU:HD12	1.91	0.53
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.29	0.53
1:B:1948:VAL:O	1:B:1950:THR:N	2.41	0.53
1:A:1820:GLN:HB3	1:A:1912:TYR:CD2	2.44	0.53
1:B:4260:MET:HG3	1:B:4271:TYR:CD1	2.43	0.53
1:B:4693:ASN:ND2	1:B:4693:ASN:H	2.06	0.53
1:B:4278:HIS:CD2	1:B:4303:LEU:HB2	2.44	0.53
1:A:2274:MET:HE1	1:A:2286:TRP:CD1	2.44	0.53
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.73	0.53
1:A:3700:LEU:HD13	1:A:3701:ASP:H	1.73	0.53
1:B:1558:TRP:CZ3	1:B:1606:ILE:HB	2.44	0.53
1:B:1541:LEU:HD23	1:B:1656:ILE:HG21	1.91	0.53
1:A:4036:HIS:HD2	1:A:4044:TRP:HE1	1.56	0.53
1:B:4597:PRO:HG2	1:B:4692:LEU:HD13	1.90	0.53
1:B:1932:ALA:HB1	1:B:1934:PHE:CE2	2.44	0.53
1:A:2701:PHE:CG	1:A:2705:THR:HG21	2.43	0.53
1:A:4207:LEU:O	1:A:4209:PRO:HD3	2.08	0.53
1:B:2497:GLU:O	1:B:2501:ILE:HG13	2.08	0.53
1:B:2280:GLY:O	1:B:2420:ILE:HD11	2.08	0.53
1:A:3821:GLY:O	1:A:3825:VAL:HG23	2.08	0.53
1:A:2142:GLN:HE21	1:A:2208:VAL:HG11	1.75	0.53
1:A:2359:VAL:CG2	1:A:2397:VAL:HG11	2.38	0.53
1:A:4122:VAL:HG22	1:A:4122:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:TRP:CH2	1:A:1565:LEU:HG	2.44	0.53
1:B:1538:TRP:HZ3	1:B:1656:ILE:HD13	1.73	0.53
1:A:3802:LEU:CD2	1:A:3882:VAL:HG12	2.39	0.53
1:A:4188:LYS:HA	1:A:4218:THR:HB	1.90	0.53
1:B:3895:ARG:HH12	1:B:3977:LYS:HG2	1.73	0.53
1:A:3956:THR:OG1	1:A:3964:LYS:HE3	2.08	0.52
1:A:2598:GLN:HG2	1:A:2612:LEU:HD22	1.90	0.52
1:A:3555:ASN:O	1:A:3559:ARG:HD3	2.09	0.52
1:A:3927:ASN:HB3	1:A:3930:LEU:CB	2.39	0.52
1:A:2017:CYS:HB3	1:A:2067:LEU:HD12	1.90	0.52
1:B:2205:PRO:HA	1:B:2261:GLN:OE1	2.09	0.52
1:B:1525:ILE:HG13	1:B:1529:GLU:HG2	1.91	0.52
1:B:2704:ALA:HB2	1:B:3085:GLU:CD	2.29	0.52
1:B:1612:TRP:CZ2	1:B:1644:ILE:HD11	2.44	0.52
1:B:2818:PHE:HD1	1:B:2876:PRO:HD3	1.74	0.52
1:A:3776:ASP:O	1:A:3780:ARG:HG2	2.09	0.52
1:B:2661:HIS:O	1:B:2665:SER:HB3	2.09	0.52
1:B:1863:VAL:HG21	1:B:2115:SER:O	2.09	0.52
1:A:2142:GLN:HE21	1:A:2208:VAL:CG1	2.22	0.52
1:A:2275:VAL:HB	1:A:2413:MET:HE2	1.90	0.52
1:A:3233:TYR:O	1:A:3237:THR:HG23	2.10	0.52
1:A:2297:ASP:C	1:A:2299:ILE:H	2.12	0.52
1:A:2431:LEU:HD21	1:A:2506:PHE:CE2	2.44	0.52
1:A:4693:ASN:N	1:A:4693:ASN:ND2	2.57	0.52
1:B:3023:SER:HB2	2:B:9010:ADP:O1A	2.09	0.52
1:B:4118:MET:O	1:B:4122:VAL:HG22	2.08	0.52
1:A:3878:GLU:O	1:A:3882:VAL:HG23	2.10	0.52
1:A:2578:MET:CE	1:A:2613:LEU:HA	2.39	0.52
1:B:3059:LEU:HD23	1:B:3137:VAL:HG11	1.92	0.52
1:B:2838:LEU:O	1:B:2840:PRO:HD3	2.10	0.52
1:A:2956:LEU:HD21	1:A:2971:TYR:CG	2.44	0.52
1:B:3681:ALA:HB2	1:B:3786:PHE:CG	2.45	0.52
1:B:2532:ARG:HH11	1:B:2532:ARG:HG2	1.74	0.52
1:B:3082:SER:HA	1:B:3085:GLU:OE1	2.09	0.52
1:B:1930:ALA:HB2	1:B:1958:LEU:HD11	1.91	0.52
1:B:3017:VAL:HG11	1:B:3175:GLU:CD	2.30	0.52
1:A:3439:ASP:C	1:A:3441:LYS:H	2.13	0.52
1:A:4048:PHE:HD1	1:A:4048:PHE:H	1.58	0.52
1:B:2036:LEU:HD23	1:B:2040:SER:HB3	1.90	0.52
1:A:2258:LYS:HE3	1:A:2415:TRP:O	2.10	0.52
1:A:1690:GLN:HE22	1:A:1766:ILE:CG2	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2857:TYR:HA	1:A:2913:PHE:CE1	2.36	0.52
1:B:4323:ASN:HD22	1:B:4323:ASN:N	2.06	0.52
1:B:2144:HIS:HB3	1:B:2400:LEU:CD1	2.40	0.52
1:A:4371:PRO:O	1:A:4372:ASP:HB2	2.09	0.52
1:B:2907:HIS:HA	1:B:2910:LEU:HD12	1.92	0.52
1:A:3225:ASP:O	1:A:3229:SER:HB3	2.08	0.52
1:A:3415:LYS:O	1:A:3417:LEU:HD12	2.09	0.52
1:A:4103:CYS:SG	1:A:4108:GLU:HA	2.50	0.52
1:A:2139:LEU:O	1:A:2140:SER:C	2.48	0.52
1:A:2142:GLN:HG2	1:A:2208:VAL:HG11	1.91	0.52
1:A:2793:ASN:HD22	1:A:2793:ASN:H	1.57	0.52
1:B:2282:LYS:NZ	1:B:2282:LYS:HB2	2.25	0.52
1:B:1600:SER:O	1:B:1604:VAL:HG23	2.10	0.52
1:A:4006:PRO:C	1:A:4008:LEU:H	2.11	0.52
1:A:4413:ASN:HD21	1:A:4660:LEU:HG	1.74	0.52
1:A:2708:GLU:O	1:A:2711:LEU:HB2	2.10	0.52
1:A:2531:LEU:HD12	1:A:2809:ARG:HD2	1.91	0.52
1:B:4156:GLN:O	1:B:4183:THR:HB	2.10	0.52
1:B:2748:LEU:N	1:B:2749:PRO:CD	2.73	0.52
1:A:3373:ILE:HG12	1:A:3374:ILE:H	1.74	0.52
1:B:4270:ILE:CG2	1:B:4310:ILE:HD13	2.34	0.52
1:A:3653:PRO:HB2	1:A:3658:CYS:SG	2.50	0.52
1:B:3233:TYR:O	1:B:3237:THR:HG23	2.09	0.52
1:A:2105:ARG:HG2	1:A:2105:ARG:NH1	2.23	0.52
1:B:2231:ILE:HD11	1:B:2260:LEU:HG	1.91	0.52
1:A:4288:ILE:CG2	1:A:4289:PRO:HA	2.40	0.52
1:A:2528:PHE:HE1	1:A:2533:VAL:HG11	1.73	0.52
1:B:1873:LYS:HB3	1:B:1943:ILE:HG21	1.90	0.52
1:B:1565:LEU:HD23	1:B:1595:LEU:CD1	2.39	0.52
1:B:2506:PHE:CE1	1:B:2512:VAL:HG21	2.43	0.52
1:B:2531:LEU:HD13	1:B:2809:ARG:NH2	2.24	0.52
1:A:2003:GLY:O	1:A:2004:PHE:C	2.49	0.52
1:A:1629:LEU:HD11	1:A:1686:TYR:CD2	2.44	0.52
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.09	0.52
1:A:2408:ILE:O	1:A:2410:ARG:N	2.43	0.52
1:A:3698:SER:C	1:A:3700:LEU:H	2.13	0.52
1:B:4157:TYR:HB2	1:B:4184:TRP:HB2	1.92	0.52
1:A:3924:LEU:HD23	1:A:3943:LEU:HD21	1.91	0.52
1:A:3988:TRP:NE1	1:A:3992:LEU:HD11	2.25	0.52
1:B:2741:VAL:HB	1:B:2788:PHE:CD2	2.44	0.52
1:B:2906:ALA:O	1:B:2909:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2893:MET:HE3	1:A:2896:CYS:HB2	1.92	0.52
1:A:3813:ARG:HG3	1:A:3814:SER:N	2.24	0.52
1:B:4423:ALA:O	1:B:4427:ILE:HG12	2.10	0.52
1:A:2641:VAL:HG12	1:A:2831:PHE:HB3	1.92	0.52
1:A:1964:LEU:HD12	1:A:2074:PHE:HZ	1.75	0.52
1:A:4033:LEU:HD13	1:A:4062:TRP:CE2	2.45	0.52
1:A:2561:SER:OG	1:A:2564:ASN:HB3	2.09	0.51
1:A:1715:ILE:HD11	1:A:1760:ILE:HG21	1.92	0.51
1:B:3563:LEU:HD11	1:B:3845:ILE:CD1	2.40	0.51
1:B:3843:GLY:O	1:B:3845:ILE:N	2.35	0.51
1:B:2910:LEU:O	1:B:2914:GLN:HB3	2.10	0.51
1:B:1957:TYR:O	1:B:1961:THR:HG23	2.10	0.51
1:B:2820:SER:OG	1:B:2823:SER:HB2	2.09	0.51
1:A:4269:ARG:HG2	1:A:4369:PHE:CE1	2.45	0.51
1:A:2898:LEU:CD1	1:A:2941:VAL:HG22	2.40	0.51
1:A:4213:PHE:CZ	1:A:4215:LEU:HB2	2.45	0.51
1:B:1817:LEU:O	1:B:1821:ILE:HG13	2.10	0.51
1:B:4690:VAL:HG21	1:B:4701:PHE:CE1	2.45	0.51
1:B:2764:ARG:HD2	1:B:2806:ARG:O	2.10	0.51
1:A:2271:GLY:O	1:A:2411:CYS:HA	2.10	0.51
1:B:4671:TRP:O	1:B:4672:LYS:HG2	2.11	0.51
1:B:3595:ALA:O	1:B:3598:PHE:HB3	2.11	0.51
1:A:3567:LEU:HD23	1:A:3855:LEU:HD11	1.92	0.51
1:A:2535:ASN:ND2	1:A:2668:ARG:HH12	2.08	0.51
1:A:4136:SER:O	1:A:4220:GLU:HA	2.10	0.51
1:B:1975:PRO:HG2	1:B:1978:THR:HG21	1.91	0.51
1:B:4690:VAL:HG11	1:B:4701:PHE:CZ	2.44	0.51
1:B:1937:GLY:HA3	1:B:1992:GLY:O	2.10	0.51
1:B:2549:ILE:O	1:B:2553:GLN:HB2	2.09	0.51
1:B:3682:MET:SD	1:B:3696:LYS:HE2	2.49	0.51
1:A:2144:HIS:O	1:A:2413:MET:HG2	2.10	0.51
1:A:3730:LEU:HD13	1:A:3734:LEU:HD21	1.91	0.51
1:A:1959:THR:HG21	1:A:2098:MET:HB2	1.92	0.51
1:A:2918:VAL:HG13	1:A:3172:TRP:NE1	2.26	0.51
1:B:2311:ILE:HB	1:B:2315:GLN:HE21	1.76	0.51
1:A:3969:LEU:HD12	1:A:4426:MET:CE	2.41	0.51
1:A:2732:PRO:CG	1:A:2739:LEU:HB2	2.40	0.51
1:B:3902:GLU:C	1:B:3904:SER:H	2.13	0.51
1:B:4636:SER:HA	1:B:4670:THR:HG22	1.91	0.51
1:B:4592:GLY:HA3	1:B:4725:SER:O	2.10	0.51
1:A:3366:LEU:O	1:A:3366:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3670:ARG:O	1:A:3782:THR:HG22	2.10	0.51
1:A:2370:LEU:HD12	1:A:2377:LEU:CB	2.41	0.51
1:A:2586:GLY:HA2	1:A:2815:LEU:CD1	2.37	0.51
1:A:3452:ILE:CG2	1:A:3485:THR:HG21	2.39	0.51
1:B:1920:ASN:ND2	1:B:1921:VAL:H	2.09	0.51
1:A:3114:GLU:HG2	1:A:3118:ARG:HH12	1.74	0.51
1:A:1611:ARG:NH1	1:A:1611:ARG:HG3	2.23	0.51
1:B:3843:GLY:C	1:B:3845:ILE:H	2.13	0.51
1:B:2238:LYS:HA	1:B:2241:GLN:HE21	1.74	0.51
1:A:4025:GLN:HG3	1:B:2899:GLU:OE2	2.10	0.51
1:A:4240:ASN:OD1	1:A:4240:ASN:N	2.38	0.51
1:A:3768:ASP:HB3	1:A:3771:ALA:HB2	1.93	0.51
1:A:3353:LYS:O	1:A:3357:VAL:HG23	2.10	0.51
1:B:3889:MET:CE	1:B:3943:LEU:HB3	2.41	0.51
1:B:2815:LEU:HD23	1:B:2815:LEU:C	2.31	0.51
1:B:1662:ILE:HB	1:B:1665:ILE:CG2	2.40	0.51
1:B:4340:SER:HB2	1:B:4357:TYR:OH	2.10	0.51
1:B:4086:MET:HG3	1:B:4097:TYR:CD2	2.45	0.51
1:B:4222:HIS:CG	1:B:4223:PRO:HD2	2.45	0.51
1:A:4200:LEU:HD22	1:A:4204:LEU:CD1	2.41	0.51
1:A:1625:ILE:HG23	1:A:1626:ASN:OD1	2.11	0.51
1:A:2738:TRP:CE2	1:A:2785:LYS:HG2	2.46	0.51
1:B:1971:ASN:O	1:B:2097:SER:HA	2.11	0.51
1:B:2638:THR:O	1:B:2641:VAL:HG23	2.10	0.51
1:B:3306:LEU:HD13	1:B:3557:VAL:HG22	1.92	0.51
1:A:4384:PRO:HB3	1:A:4395:TRP:CD1	2.45	0.51
1:B:4121:ILE:HA	1:B:4125:GLU:CG	2.32	0.51
1:A:3721:GLN:NE2	1:A:4205:HIS:NE2	2.58	0.51
1:B:2219:LEU:HD13	1:B:2228:LEU:HD11	1.93	0.51
1:B:3063:GLY:HA2	1:B:3136:GLN:CB	2.41	0.51
1:A:3289:LEU:HD13	1:A:3293:ARG:NH2	2.25	0.51
1:B:1556:ARG:HG2	1:B:1557:GLY:N	2.25	0.51
1:B:2877:ARG:HB3	1:B:2881:ARG:NH1	2.26	0.51
1:A:2732:PRO:HG3	1:A:2739:LEU:HB2	1.93	0.51
1:B:2801:VAL:HG12	1:B:2802:GLN:N	2.25	0.51
1:B:3566:ASN:ND2	1:B:3859:LYS:NZ	2.59	0.51
1:B:2643:SER:HB3	1:B:2646:VAL:HG23	1.93	0.51
1:B:2931:ASP:O	1:B:2935:LEU:HG	2.11	0.51
1:B:4550:TRP:O	1:B:4552:TRP:N	2.40	0.51
1:B:1520:ALA:HA	1:B:1580:TYR:CE1	2.46	0.51
1:B:3219:ILE:CB	1:B:3220:PRO:CD	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:LYS:O	1:A:1715:ILE:N	2.44	0.51
1:A:4428:ASN:O	1:A:4432:LYS:HG2	2.10	0.51
1:A:4389:ARG:HH12	1:A:4393:MET:CE	2.24	0.51
1:B:1639:ILE:HG21	1:B:1676:LEU:HG	1.93	0.51
1:B:2849:LEU:HD21	1:B:2886:LEU:HD13	1.93	0.51
1:B:2968:LEU:CD2	1:B:2999:LEU:HD11	2.41	0.51
1:B:2283:THR:HA	1:B:2286:TRP:HE1	1.76	0.51
1:A:2327:TRP:CZ3	1:A:2380:PRO:HD2	2.46	0.51
1:B:2542:ASN:O	1:B:2546:VAL:HG23	2.10	0.51
1:A:2540:LEU:HD23	1:A:2662:ALA:HB3	1.92	0.51
1:A:2138:GLN:NE2	1:A:2218:LEU:HD21	2.26	0.51
1:A:4299:ASN:OD1	1:A:4301:ALA:HB3	2.11	0.51
1:A:2619:ILE:O	1:A:2619:ILE:HG13	2.11	0.51
1:B:2921:GLU:CD	1:B:2921:GLU:H	2.13	0.51
1:A:3425:LYS:HA	1:A:3428:GLU:CG	2.41	0.51
1:A:2204:ILE:HG13	1:A:2205:PRO:HD3	1.92	0.51
1:B:1578:SER:C	1:B:1580:TYR:H	2.14	0.51
1:B:1823:TRP:O	1:B:1827:VAL:HG23	2.10	0.51
1:B:1892:LEU:HA	1:B:1895:CYS:SG	2.51	0.51
1:B:3790:PRO:HA	1:B:3898:PHE:CE2	2.46	0.51
1:A:4222:HIS:ND1	1:A:4223:PRO:HD2	2.26	0.51
1:B:2199:ILE:O	1:B:2203:MET:HB2	2.11	0.51
1:B:3618:MET:HB3	1:B:3628:PHE:CZ	2.46	0.51
1:A:3032:MET:C	1:A:3034:GLY:H	2.15	0.51
1:B:3583:THR:O	1:B:3587:THR:HG23	2.11	0.51
1:A:2839:LEU:HD22	1:A:2896:CYS:HB3	1.93	0.50
1:A:2582:GLY:O	1:A:2585:MET:HB2	2.11	0.50
1:B:1687:LEU:HD11	1:B:1706:LEU:HD21	1.93	0.50
1:B:4288:ILE:HG23	1:B:4289:PRO:HA	1.92	0.50
1:B:4644:LEU:HD13	1:B:4647:ALA:HB3	1.92	0.50
1:B:1573:SER:HA	1:B:1576:LYS:HE2	1.93	0.50
1:A:3116:ALA:HB1	1:A:3121:LEU:O	2.12	0.50
1:B:1527:LEU:HD22	1:B:1575:MET:HB2	1.92	0.50
1:A:2212:ILE:N	1:A:2213:PRO:CD	2.75	0.50
1:A:2856:PHE:CE1	1:A:2930:ILE:HG12	2.46	0.50
1:A:1963:ALA:HB1	1:A:2096:ARG:CG	2.41	0.50
1:B:1534:VAL:HG13	1:B:1568:HIS:CD2	2.42	0.50
1:A:3923:LEU:HD11	1:A:3943:LEU:HA	1.94	0.50
1:B:1479:ARG:O	1:B:1483:ILE:HG13	2.11	0.50
1:B:2729:VAL:HG12	1:B:2782:LYS:HB3	1.94	0.50
1:B:4267:ARG:NH2	1:B:4315:ASP:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3038:TYR:CD2	1:B:3058:LEU:HD13	2.46	0.50
1:A:1776:GLU:HA	1:A:1779:SER:HB3	1.93	0.50
1:B:1951:PRO:HG2	1:B:2104:ASP:OD2	2.10	0.50
1:A:4285:LEU:O	1:A:4288:ILE:HG13	2.10	0.50
1:A:1719:GLN:HA	1:A:1722:PHE:CD2	2.46	0.50
1:B:4686:LEU:HD12	1:B:4687:SER:N	2.27	0.50
1:B:4170:LEU:HD12	1:B:4171:ALA:N	2.26	0.50
1:A:4326:PRO:HB3	1:A:4369:PHE:CD2	2.46	0.50
1:A:3067:GLU:O	1:A:3069:ILE:HD12	2.12	0.50
1:A:4122:VAL:HA	1:A:4126:VAL:HG11	1.91	0.50
1:A:2586:GLY:O	1:A:2590:ARG:HB2	2.10	0.50
1:A:2049:ALA:O	1:A:2054:SER:HB3	2.12	0.50
1:B:2142:GLN:HB2	1:B:2145:TYR:CD1	2.46	0.50
1:A:4044:TRP:CE3	1:A:4048:PHE:HE1	2.29	0.50
1:B:2135:CYS:HB3	1:B:2139:LEU:HD12	1.92	0.50
1:B:1907:LEU:HA	1:B:1911:ARG:NH1	2.26	0.50
1:B:1967:ARG:HG2	1:B:1967:ARG:HH11	1.75	0.50
1:A:4028:PRO:C	1:A:4030:PHE:H	2.15	0.50
1:A:2954:ASN:HD22	1:A:2954:ASN:N	2.02	0.50
1:A:3380:VAL:HG11	1:A:3435:ILE:CG2	2.41	0.50
1:B:2865:THR:N	1:B:2868:ILE:HD12	2.26	0.50
1:A:2533:VAL:HB	1:A:2581:LEU:HA	1.94	0.50
1:A:3834:LEU:HA	1:A:3854:THR:HG21	1.93	0.50
1:A:4118:MET:HB3	1:A:4149:LEU:HD22	1.94	0.50
1:B:1926:VAL:HG22	1:B:1935:TYR:HE2	1.75	0.50
1:A:4052:GLN:C	1:A:4054:GLY:H	2.14	0.50
1:A:2720:TYR:HE1	1:A:2781:ILE:HG21	1.76	0.50
1:B:1862:SER:O	1:B:1867:LEU:HD21	2.12	0.50
1:B:3691:ASP:C	1:B:3693:LYS:H	2.15	0.50
1:B:4111:LEU:N	1:B:4111:LEU:HD12	2.26	0.50
1:B:2367:LEU:HD12	1:B:2367:LEU:N	2.26	0.50
1:A:2913:PHE:CD2	1:A:2913:PHE:N	2.79	0.50
1:B:1662:ILE:HB	1:B:1665:ILE:HG23	1.93	0.50
1:B:4020:LEU:HD11	1:B:4033:LEU:HG	1.93	0.50
1:A:1971:ASN:ND2	1:A:2087:LEU:HD11	2.26	0.50
1:A:2627:TRP:O	1:A:2629:ASN:N	2.45	0.50
1:A:4388:THR:O	1:A:4391:HIS:HB2	2.12	0.50
1:A:2197:ASN:O	1:A:2201:ASP:HB2	2.12	0.50
1:B:2723:THR:CG2	1:B:2727:GLU:HB2	2.42	0.50
1:A:4518:ALA:C	1:A:4520:LEU:H	2.15	0.50
1:B:3105:PHE:O	1:B:3109:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2918:VAL:HG22	1:B:3172:TRP:CD2	2.47	0.50
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.94	0.50
1:A:4185:VAL:HG12	1:A:4186:LEU:N	2.19	0.50
1:A:1889:VAL:HA	1:A:1892:LEU:HD12	1.94	0.50
1:A:3410:LEU:HA	1:A:3414:GLY:O	2.12	0.50
1:A:4078:SER:HA	1:A:4081:ARG:HD2	1.94	0.50
1:A:3433:THR:HG22	1:A:3437:ASN:HD22	1.75	0.50
1:A:3583:THR:O	1:A:3587:THR:HG23	2.11	0.50
1:B:4644:LEU:O	1:B:4661:SER:HB2	2.11	0.50
1:B:2989:VAL:HG13	1:B:3187:GLU:OE2	2.12	0.50
1:A:3977:LYS:O	1:A:3979:THR:HG23	2.12	0.50
1:B:1781:LEU:O	1:B:1814:LEU:HD21	2.12	0.49
1:A:2798:ALA:C	1:A:2800:ARG:H	2.14	0.49
1:B:4339:GLY:HA3	1:B:4360:LEU:HD11	1.93	0.49
1:A:3992:LEU:HD22	1:A:4430:LEU:CB	2.41	0.49
1:A:4278:HIS:CD2	1:A:4343:TYR:OH	2.64	0.49
1:B:1522:GLN:O	1:B:1525:ILE:HG22	2.11	0.49
1:A:1926:VAL:HG12	1:A:1928:HIS:NE2	2.26	0.49
1:B:2976:LEU:HD11	1:B:2990:LEU:HD21	1.94	0.49
1:B:4259:ARG:NH2	1:B:4307:LEU:HB3	2.27	0.49
1:B:4132:LEU:HD13	1:B:4216:PHE:CZ	2.47	0.49
1:B:3061:ARG:HB3	1:B:3067:GLU:OE2	2.12	0.49
1:B:3181:LEU:CB	1:B:3232:VAL:HG13	2.42	0.49
1:B:2504:GLN:HA	1:B:2507:GLU:OE2	2.12	0.49
1:A:3337:LYS:CB	1:A:3525:LEU:HD13	2.24	0.49
1:B:3935:ASP:O	1:B:3939:ARG:HG3	2.12	0.49
1:B:4402:ILE:H	1:B:4402:ILE:CD1	2.21	0.49
1:A:4054:GLY:O	1:A:4055:GLU:O	2.30	0.49
1:A:4055:GLU:HG3	1:A:4093:ARG:NH1	2.27	0.49
1:B:4060:GLU:HA	1:B:4063:ILE:HD13	1.94	0.49
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.94	0.49
1:A:3011:HIS:CE1	1:A:3143:VAL:HG23	2.47	0.49
1:A:3919:ILE:HG21	1:A:3951:THR:HA	1.94	0.49
1:B:4642:MET:HG2	1:B:4725:SER:HA	1.94	0.49
1:B:1494:ILE:HA	1:B:1497:LEU:HD12	1.93	0.49
1:A:2511:LEU:HD11	1:A:2574:LEU:HD21	1.94	0.49
1:A:3059:LEU:HD21	1:A:3090:LEU:HD13	1.94	0.49
1:B:4596:ASN:HD22	1:B:4596:ASN:C	2.15	0.49
1:A:2869:GLN:HG2	1:A:2871:HIS:CE1	2.47	0.49
1:B:3700:LEU:CG	1:B:3701:ASP:H	2.23	0.49
1:A:3723:VAL:HG23	1:A:3764:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2057:VAL:HG22	1:A:2058:GLU:H	1.78	0.49
1:A:1739:THR:O	1:A:1760:ILE:HG12	2.12	0.49
1:A:2018:GLN:HE21	1:A:2066:SER:HB3	1.77	0.49
1:A:3192:LEU:O	1:A:3224:ARG:NH2	2.46	0.49
1:A:4574:GLN:HE22	1:A:4590:TRP:H	1.60	0.49
1:A:4365:THR:HB	1:A:4366:PRO:HD2	1.93	0.49
1:A:3398:PRO:C	1:A:3400:PRO:HD2	2.33	0.49
1:A:4068:GLN:C	1:A:4070:SER:H	2.15	0.49
1:B:3135:SER:HA	1:B:3138:ARG:HG2	1.95	0.49
1:A:2133:LYS:HD3	1:A:2133:LYS:O	2.12	0.49
1:A:3338:GLN:HA	1:A:3342:ARG:CB	2.42	0.49
1:B:3192:LEU:HD11	1:B:3268:VAL:HG22	1.94	0.49
1:A:4075:THR:HG23	1:A:4076:ILE:N	2.27	0.49
1:A:2374:ASN:O	1:A:2375:LYS:HB2	2.11	0.49
1:A:4122:VAL:HA	1:A:4126:VAL:CG1	2.42	0.49
1:A:3725:ASN:N	1:A:3725:ASN:ND2	2.58	0.49
1:A:1887:ASP:O	1:A:1891:GLN:HG3	2.12	0.49
1:A:4244:VAL:HG23	1:A:4403:SER:CB	2.42	0.49
1:A:2029:ASN:HD22	1:A:2030:ARG:N	2.11	0.49
1:A:2302:GLU:HG2	1:A:2304:HIS:CE1	2.46	0.49
1:A:2370:LEU:HD23	1:A:2387:LEU:HD22	1.95	0.49
1:A:3947:ILE:CG2	1:A:3948:PHE:N	2.76	0.49
1:A:1934:PHE:N	1:A:1934:PHE:CD2	2.81	0.49
1:A:3116:ALA:HB1	1:A:3123:LEU:HD12	1.94	0.49
1:B:2021:ALA:O	1:B:2071:MET:HA	2.13	0.49
1:B:3316:LYS:HD2	1:B:3546:ILE:HD12	1.94	0.49
1:B:2839:LEU:HD22	1:B:2896:CYS:HB3	1.95	0.49
1:B:2315:GLN:HB3	1:B:2775:THR:CG2	2.41	0.49
1:B:4012:LEU:N	1:B:4012:LEU:HD23	2.27	0.49
1:A:3674:VAL:HG13	1:A:3786:PHE:HD2	1.78	0.49
1:B:2832:ASN:HD22	1:B:2835:LEU:HD23	1.77	0.49
1:B:4313:TRP:HB3	1:B:4330:PRO:CG	2.42	0.49
1:A:1699:PHE:N	1:A:1699:PHE:CD1	2.77	0.49
1:A:1907:LEU:HA	1:A:1911:ARG:HH11	1.77	0.49
1:A:3217:MET:O	1:A:3218:ALA:C	2.50	0.49
1:A:1629:LEU:N	1:A:1630:PRO:HD3	2.28	0.49
1:A:2029:ASN:HD22	1:A:2029:ASN:N	2.10	0.49
1:A:3655:ASP:O	1:A:3659:ILE:HG13	2.13	0.49
1:B:2612:LEU:HD11	1:B:2624:TRP:CZ3	2.48	0.49
1:A:2272:VAL:HA	1:A:2412:GLY:H	1.77	0.49
1:A:3039:THR:HG22	1:A:3040:ILE:N	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2848:ASN:HB3	1:A:2938:PHE:HE1	1.77	0.49
1:B:4167:GLY:HA2	1:B:4170:LEU:HD11	1.93	0.49
1:A:3262:ASP:CB	1:A:3670:ARG:HE	2.25	0.49
1:B:4109:ASP:HA	1:B:4112:ASN:HD21	1.72	0.49
1:A:2941:VAL:CG1	1:A:2942:ASN:N	2.76	0.49
1:A:2948:ARG:HG2	1:A:2948:ARG:NH1	2.28	0.49
1:B:3991:LEU:HG	1:B:3992:LEU:HD23	1.94	0.49
1:B:2000:CYS:CB	1:B:2031:LEU:HD13	2.42	0.49
1:A:4068:GLN:N	1:A:4073:GLN:HE21	2.11	0.49
1:A:4072:GLN:OE1	1:A:4077:VAL:HG21	2.11	0.49
1:B:2517:GLU:O	1:B:2521:GLN:HG2	2.13	0.49
1:B:2677:GLY:HA3	1:B:2875:SER:OG	2.12	0.49
1:A:3997:ASN:HD21	1:A:4001:ILE:HD11	1.77	0.49
1:A:4295:PHE:C	1:A:4295:PHE:CD2	2.86	0.49
1:A:2208:VAL:HG22	1:A:2211:ASP:HB2	1.95	0.49
1:A:3981:ASN:HD22	1:A:4076:ILE:CB	2.20	0.49
1:A:3069:ILE:O	1:A:3141:LEU:O	2.30	0.49
1:A:4536:SER:HB2	1:A:4548:LYS:HZ1	1.77	0.49
1:A:4548:LYS:O	1:A:4550:TRP:N	2.46	0.49
1:A:4230:LEU:HB3	1:A:4235:VAL:HG21	1.94	0.49
1:A:2610:ILE:HD12	1:A:2615:TYR:OH	2.13	0.49
1:B:4618:ASN:H	1:B:4618:ASN:ND2	2.11	0.49
1:A:4596:ASN:ND2	1:A:4599:ALA:H	2.11	0.49
1:B:2723:THR:OG1	1:B:2724:PRO:HD2	2.13	0.49
1:A:3689:TYR:CB	1:A:3694:ILE:HD11	2.21	0.49
1:B:1959:THR:HG21	1:B:2098:MET:SD	2.53	0.49
1:A:1639:ILE:HG21	1:A:1676:LEU:HG	1.94	0.49
1:B:1823:TRP:NE1	1:B:1885:GLN:HB3	2.27	0.49
1:A:4402:ILE:N	1:A:4402:ILE:HD12	2.26	0.49
1:A:1565:LEU:HD11	1:A:1598:VAL:HG12	1.94	0.49
1:A:1800:HIS:HB2	1:A:1858:ASN:ND2	2.28	0.49
1:B:4693:ASN:HD22	1:B:4693:ASN:N	2.09	0.49
1:B:1934:PHE:CD2	1:B:1934:PHE:N	2.81	0.49
1:B:2241:GLN:HA	1:B:2244:ALA:HB3	1.93	0.49
1:A:3370:GLU:O	1:A:3372:ALA:N	2.46	0.49
1:B:2655:ARG:O	1:B:2659:VAL:HG23	2.13	0.49
1:A:1603:ASP:O	1:A:1606:ILE:HG22	2.13	0.49
1:B:3929:ASN:HB3	1:B:3942:TYR:CD1	2.47	0.49
1:A:3180:ALA:O	1:A:3184:VAL:HG23	2.12	0.49
1:A:3598:PHE:O	1:A:3602:ILE:HB	2.11	0.48
1:B:1926:VAL:HG12	1:B:1928:HIS:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3017:VAL:HG22	1:A:3018:SER:N	2.27	0.48
1:A:3457:LEU:HD11	1:A:3482:THR:HA	1.95	0.48
1:B:2616:SER:HB3	1:B:2627:TRP:CD2	2.47	0.48
1:A:1820:GLN:HE22	1:A:1990:GLN:HE22	1.60	0.48
1:B:3540:ILE:O	1:B:3544:GLU:HG3	2.13	0.48
1:A:3048:SER:HB2	1:A:3080:GLU:OE1	2.13	0.48
1:A:2572:ARG:O	1:A:2575:TYR:HB3	2.12	0.48
1:B:1813:GLN:NE2	1:B:1940:TYR:HA	2.17	0.48
1:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.95	0.48
1:A:3238:ILE:HG12	1:A:3601:TYR:HD2	1.69	0.48
1:B:4263:GLN:HA	1:B:4264:PRO:C	2.34	0.48
1:A:2720:TYR:CE1	1:A:2781:ILE:HG21	2.48	0.48
1:A:3150:ALA:O	1:A:3151:SER:C	2.51	0.48
1:B:2276:GLY:O	1:B:2282:LYS:HE2	2.13	0.48
1:B:3295:THR:O	1:B:3299:VAL:HG23	2.12	0.48
1:A:4589:VAL:CG1	1:A:4639:VAL:HA	2.43	0.48
1:B:2968:LEU:HG	1:B:2995:LEU:HD22	1.95	0.48
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	1.95	0.48
1:B:1934:PHE:HB3	1:B:1993:ARG:HH22	1.78	0.48
1:B:2229:GLN:O	1:B:2230:PRO:O	2.30	0.48
1:B:4513:ILE:HD12	1:B:4568:PHE:CE2	2.47	0.48
1:A:4083:ILE:HD11	1:A:4098:SER:HA	1.94	0.48
1:B:2604:PRO:O	1:B:2624:TRP:NE1	2.46	0.48
1:A:2088:PRO:C	1:A:2090:ASN:H	2.16	0.48
1:A:4604:THR:OG1	1:A:4671:TRP:HZ3	1.96	0.48
1:A:3007:GLN:NE2	1:A:3008:PRO:HD2	2.29	0.48
1:A:4133:LEU:HD21	1:A:4225:LEU:HD13	1.94	0.48
1:B:4306:ALA:HB1	1:B:4338:LEU:HD13	1.94	0.48
1:B:2720:TYR:CE1	1:B:2730:LEU:HD13	2.48	0.48
1:B:3673:LEU:HD13	1:B:3783:PHE:CE1	2.48	0.48
1:A:3145:PHE:CE2	1:A:3164:LEU:HD21	2.48	0.48
1:A:3920:PHE:O	1:A:3923:LEU:HB3	2.13	0.48
1:B:2080:GLY:HA3	1:B:2084:ARG:O	2.13	0.48
1:B:1910:MET:HA	1:B:1929:MET:HG3	1.95	0.48
1:B:2782:LYS:HB2	1:B:2782:LYS:NZ	2.28	0.48
1:A:4133:LEU:HA	1:A:4217:MET:HB2	1.94	0.48
1:B:2621:ASP:C	1:B:2623:ASN:H	2.16	0.48
1:A:4335:ARG:HD3	1:A:4361:GLU:HA	1.96	0.48
1:A:3425:LYS:HA	1:A:3428:GLU:HG2	1.95	0.48
1:A:2273:MET:HG3	1:A:2413:MET:CE	2.44	0.48
1:A:4190:ILE:HB	1:A:4197:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3677:PRO:HG3	1:B:3769:PRO:HB3	1.94	0.48
1:A:3042:VAL:HB	1:A:3079:LEU:HD11	1.96	0.48
1:B:2641:VAL:CG2	1:B:2887:LEU:HD22	2.43	0.48
1:B:4024:ARG:HG3	1:B:4031:SER:O	2.14	0.48
1:A:3289:LEU:HD13	1:A:3293:ARG:HH22	1.77	0.48
1:A:2752:ASP:C	1:A:2754:TYR:H	2.17	0.48
1:B:2774:ARG:HB2	1:B:2781:ILE:HD13	1.94	0.48
1:A:4047:PHE:HD2	1:A:4048:PHE:CD1	2.32	0.48
1:B:2025:PHE:HB2	1:B:2075:VAL:HG22	1.94	0.48
1:A:4684:SER:O	1:A:4707:TYR:CE2	2.67	0.48
1:A:3664:MET:O	1:A:3668:PHE:HB3	2.13	0.48
1:A:4384:PRO:HB3	1:A:4395:TRP:CG	2.48	0.48
1:A:2204:ILE:CG1	1:A:2205:PRO:HD3	2.44	0.48
1:A:3238:ILE:HD12	1:A:3238:ILE:N	2.28	0.48
1:B:3990:PHE:CE2	1:B:4023:LEU:HD13	2.48	0.48
1:A:4029:SER:CB	1:A:4081:ARG:HH12	2.25	0.48
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.95	0.48
1:A:3924:LEU:C	1:A:3925:ASN:HD22	2.15	0.48
1:A:3408:VAL:HG11	1:A:3477:LEU:CG	2.43	0.48
1:B:4410:LEU:CD2	1:B:4411:PRO:HD2	2.43	0.48
1:A:3487:TYR:O	1:A:3489:GLU:N	2.47	0.48
1:A:3371:PRO:O	1:A:3372:ALA:C	2.52	0.48
1:B:3196:ASN:ND2	1:B:3199:TYR:HB2	2.28	0.48
1:B:3911:PHE:CZ	1:B:3955:VAL:HG13	2.49	0.48
1:B:4653:GLN:OE1	1:B:4708:ASP:HA	2.14	0.48
1:A:2952:TYR:CE1	1:A:2962:PRO:HG3	2.48	0.48
1:B:3677:PRO:HB3	1:B:3769:PRO:HD3	1.94	0.48
1:B:1694:PHE:CE1	1:B:1770:LEU:HB3	2.48	0.48
1:B:1525:ILE:HD12	1:B:1528:GLU:HB3	1.96	0.48
1:A:1973:PHE:HE1	1:A:2099:ALA:CB	2.27	0.48
1:B:4540:SER:HB2	1:B:4545:ILE:O	2.13	0.48
1:A:1960:LEU:O	1:A:1964:LEU:N	2.39	0.48
1:A:1974:GLY:C	1:A:2079:PRO:HD3	2.34	0.48
1:B:3011:HIS:ND1	1:B:3091:LEU:HD22	2.28	0.48
1:B:4400:PRO:HG2	1:B:4407:TRP:CH2	2.49	0.48
1:A:3865:ILE:HA	1:A:3869:VAL:HG23	1.94	0.48
1:A:3323:LYS:HE3	1:A:3539:LEU:HG	1.95	0.48
1:A:3891:LEU:HD21	1:A:3895:ARG:NH2	2.28	0.48
1:B:3887:ASN:N	1:B:3888:PRO:CD	2.77	0.48
1:A:4591:LEU:CD2	1:A:4601:ILE:HD11	2.42	0.48
1:B:2084:ARG:HG2	1:B:2084:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3863:THR:O	1:A:3863:THR:HG22	2.12	0.48
1:B:3955:VAL:HG12	1:B:3959:LEU:HG	1.96	0.48
1:A:1974:GLY:CA	1:A:2079:PRO:HD3	2.44	0.48
1:A:4406:ILE:HB	1:A:4412:GLU:OE2	2.14	0.48
1:B:4070:SER:O	1:B:4071:ASN:C	2.52	0.48
1:A:3987:GLU:HG3	1:A:4027:VAL:CG1	2.44	0.48
1:A:4184:TRP:CD1	1:A:4184:TRP:N	2.82	0.48
1:B:1962:GLN:HB3	1:B:4341:THR:HG21	1.96	0.48
1:A:4655:THR:HG22	1:A:4708:ASP:HB2	1.96	0.48
1:B:3638:LEU:HB2	1:B:3663:ILE:HD12	1.96	0.48
1:A:4132:LEU:HB2	1:A:4216:PHE:HD1	1.79	0.48
1:A:3473:ALA:O	1:A:3476:PRO:HD2	2.13	0.48
1:B:3585:MET:HA	1:B:3588:VAL:HG23	1.96	0.48
1:A:3397:PRO:HG2	1:A:3419:TRP:CE2	2.48	0.48
1:A:1800:HIS:CB	1:A:1858:ASN:HD22	2.26	0.48
1:B:4407:TRP:CD1	1:B:4407:TRP:N	2.82	0.48
1:B:3273:GLU:OE1	1:B:3667:ARG:NH2	2.47	0.48
1:B:3731:ASN:HB2	1:B:3732:PRO:HD3	1.94	0.48
1:A:1701:GLY:HA2	1:A:2011:ARG:NH1	2.29	0.48
1:A:2208:VAL:HA	1:A:2415:TRP:HD1	1.74	0.48
1:A:2375:LYS:HG2	1:A:2387:LEU:HD23	1.95	0.48
1:A:2299:ILE:CG2	1:A:2349:LYS:HA	2.44	0.48
1:A:2704:ALA:HB3	1:A:3085:GLU:CG	2.44	0.48
1:B:4360:LEU:C	1:B:4362:GLN:H	2.17	0.48
1:A:3145:PHE:CD1	1:A:3164:LEU:HD11	2.48	0.48
1:B:4288:ILE:CG2	1:B:4289:PRO:HA	2.44	0.48
1:B:2532:ARG:NH1	1:B:2532:ARG:HG2	2.29	0.48
1:B:4083:ILE:CD1	1:B:4098:SER:HA	2.44	0.48
1:B:3232:VAL:O	1:B:3236:GLN:HG3	2.14	0.48
1:A:4201:GLU:HG3	1:A:4228:ASN:HB2	1.94	0.48
1:A:2813:ILE:HG22	1:A:2814:LEU:N	2.28	0.48
1:A:1535:ARG:HA	1:A:1591:TRP:CZ2	2.49	0.48
1:A:3695:THR:HG21	1:A:3707:ASN:OD1	2.14	0.48
1:B:3350:VAL:HG12	1:B:3354:GLU:OE2	2.13	0.48
1:A:4296:PHE:CZ	1:A:4347:ILE:HD13	2.49	0.47
1:B:2397:VAL:HG22	1:B:2398:GLN:N	2.29	0.47
1:A:3078:VAL:O	1:A:3078:VAL:HG13	2.13	0.47
1:B:2886:LEU:HD23	1:B:2904:LEU:CD2	2.44	0.47
1:A:4048:PHE:N	1:A:4048:PHE:CD1	2.82	0.47
1:B:2613:LEU:HD22	1:B:2655:ARG:NH1	2.29	0.47
1:B:3960:LEU:HD23	1:B:4237:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3699:PHE:CZ	1:A:3726:ILE:HG13	2.49	0.47
1:A:2207:LEU:CD1	1:A:2215:ILE:HG21	2.43	0.47
1:A:3930:LEU:HD11	1:A:3939:ARG:HG2	1.95	0.47
1:A:2128:ILE:HG23	1:A:2129:VAL:N	2.29	0.47
1:B:1568:HIS:O	1:B:1572:ILE:HG13	2.14	0.47
1:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.96	0.47
1:A:3408:VAL:HG23	1:A:3409:CYS:H	1.80	0.47
1:B:2212:ILE:N	1:B:2213:PRO:CD	2.77	0.47
1:A:3903:LEU:HD23	1:A:4433:MET:SD	2.54	0.47
1:A:3074:ASP:H	1:A:3077:ASN:HD22	1.62	0.47
1:B:2918:VAL:HG22	1:B:3172:TRP:CE2	2.49	0.47
1:B:1910:MET:HB2	1:B:1929:MET:HG3	1.95	0.47
1:B:4568:PHE:O	1:B:4572:MET:HG2	2.14	0.47
1:A:4335:ARG:HD3	1:A:4360:LEU:C	2.35	0.47
1:A:4268:SER:OG	1:A:4387:THR:HA	2.14	0.47
1:A:2497:GLU:O	1:A:2501:ILE:HG13	2.13	0.47
1:A:3781:VAL:HG12	1:A:3782:THR:N	2.29	0.47
1:A:2313:LYS:CE	1:A:2366:ASN:HD21	2.17	0.47
1:A:1639:ILE:CD1	1:A:1675:LEU:HB3	2.44	0.47
1:A:3897:TYR:CE1	1:A:3913:LEU:HA	2.47	0.47
1:B:1628:LEU:HD13	1:B:1709:ILE:HG22	1.95	0.47
1:B:3013:LEU:HG	1:B:3013:LEU:O	2.13	0.47
1:A:1934:PHE:HE1	1:A:1964:LEU:HD22	1.78	0.47
1:A:3997:ASN:O	1:A:3999:THR:N	2.47	0.47
1:A:3997:ASN:ND2	1:A:4001:ILE:HD11	2.27	0.47
1:B:1659:VAL:C	1:B:1661:ALA:H	2.18	0.47
1:A:3338:GLN:HG3	1:A:3529:ILE:HD12	1.96	0.47
1:A:2368:ASN:HB3	1:A:2410:ARG:NH1	2.29	0.47
1:B:1811:PRO:HB2	1:B:1814:LEU:HD12	1.95	0.47
1:B:3966:THR:N	1:B:4426:MET:HE2	2.29	0.47
1:B:2309:LYS:O	1:B:2758:ARG:HD2	2.14	0.47
1:B:2754:TYR:O	1:B:2755:GLY:C	2.52	0.47
1:A:3804:THR:C	1:A:3806:ARG:H	2.18	0.47
1:B:2363:TRP:CH2	1:B:2395:PHE:HE1	2.32	0.47
1:A:2598:GLN:HG3	1:A:2612:LEU:HB2	1.96	0.47
1:A:2616:SER:OG	1:A:2617:VAL:N	2.47	0.47
1:B:1591:TRP:HA	1:B:1591:TRP:CE3	2.49	0.47
1:A:3219:ILE:CB	1:A:3220:PRO:CD	2.93	0.47
1:B:1971:ASN:HA	1:B:2075:VAL:O	2.14	0.47
1:B:2427:PHE:O	1:B:2431:LEU:HG	2.14	0.47
1:A:3480:TRP:HE1	1:A:3484:GLN:HE21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2595:LYS:HE3	1:B:2611:PRO:HG3	1.96	0.47
1:A:3730:LEU:CD2	1:A:3733:VAL:HB	2.44	0.47
1:A:2010:SER:O	1:A:2060:LEU:HD11	2.14	0.47
1:A:4200:LEU:HD22	1:A:4204:LEU:CG	2.45	0.47
1:B:1920:ASN:ND2	1:B:1921:VAL:N	2.62	0.47
1:B:1603:ASP:O	1:B:1606:ILE:HG22	2.15	0.47
1:A:2282:LYS:HB2	2:A:9002:ADP:O3B	2.15	0.47
1:A:4313:TRP:HB3	1:A:4330:PRO:CG	2.45	0.47
1:A:1628:LEU:C	1:A:1630:PRO:HD3	2.35	0.47
1:A:3648:HIS:CE1	1:A:3654:SER:HA	2.49	0.47
1:A:1592:ASP:O	1:A:1596:ASN:HB2	2.14	0.47
1:B:3605:PHE:HB3	1:B:3609:PHE:HB3	1.95	0.47
1:A:4326:PRO:HB3	1:A:4369:PHE:HD2	1.79	0.47
1:A:2204:ILE:HA	1:A:2207:LEU:CD1	2.42	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:HG23	1.96	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:CG2	2.45	0.47
1:B:1766:ILE:HG23	1:B:1767:HIS:N	2.30	0.47
1:A:2250:VAL:HG21	1:A:2425:MET:HA	1.97	0.47
1:B:2532:ARG:CZ	1:B:2813:ILE:HD12	2.45	0.47
1:B:4618:ASN:H	1:B:4618:ASN:HD22	1.60	0.47
1:B:4596:ASN:C	1:B:4596:ASN:ND2	2.68	0.47
1:A:3794:GLN:HG3	1:A:3891:LEU:HA	1.96	0.47
1:B:2667:HIS:HA	1:B:2787:GLN:OE1	2.14	0.47
1:A:4109:ASP:O	1:A:4112:ASN:HB2	2.15	0.47
1:A:2273:MET:HB3	1:A:2395:PHE:CD1	2.50	0.47
1:B:2125:ALA:O	1:B:2129:VAL:HG13	2.14	0.47
1:A:2196:LEU:HA	1:A:2199:ILE:HG12	1.97	0.47
1:A:4344:GLY:HA2	1:A:4347:ILE:HG13	1.95	0.47
1:A:3036:SER:N	1:A:3068:LYS:O	2.48	0.47
1:B:3698:SER:HB3	1:B:3700:LEU:CD1	2.44	0.47
1:B:2540:LEU:HB3	1:B:2576:SER:OG	2.14	0.47
1:B:4359:PHE:O	1:B:4362:GLN:HB3	2.15	0.47
1:B:2231:ILE:HG12	1:B:2260:LEU:HD23	1.96	0.47
1:A:4430:LEU:O	1:A:4434:GLN:HB2	2.15	0.47
1:B:2335:THR:O	1:B:2339:ILE:HG13	2.14	0.47
1:B:4059:PRO:O	1:B:4063:ILE:HD12	2.15	0.47
1:B:2676:PRO:HG3	1:B:2873:ILE:HD12	1.96	0.47
1:B:1547:ASN:HD21	1:B:1550:ARG:H	1.63	0.47
1:B:1611:ARG:O	1:B:1615:LEU:HD23	2.14	0.47
1:A:2990:LEU:HD23	1:A:2994:VAL:HG11	1.97	0.47
1:A:1927:ILE:C	1:A:1928:HIS:HD2	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:PRO:HB2	1:A:2090:ASN:HD21	1.80	0.47
1:B:3650:ASN:O	1:B:3651:SER:HB2	2.15	0.47
1:A:4690:VAL:HG21	1:A:4701:PHE:CE1	2.50	0.47
1:A:3074:ASP:H	1:A:3077:ASN:ND2	2.13	0.47
1:B:2882:TRP:CZ2	1:B:2909:ALA:HB2	2.48	0.47
1:B:1782:ALA:HB2	1:B:1922:LEU:HD23	1.96	0.47
1:B:2512:VAL:HA	1:B:2515:VAL:HG12	1.95	0.47
1:A:4043:ASP:OD2	1:A:4043:ASP:N	2.45	0.47
1:A:3032:MET:O	1:A:3034:GLY:N	2.47	0.47
1:A:3370:GLU:O	1:A:3371:PRO:C	2.51	0.47
1:B:4119:ALA:HA	1:B:4149:LEU:HD11	1.96	0.47
1:B:4673:ASP:C	1:B:4675:ASP:H	2.18	0.47
1:B:4429:ASP:O	1:B:4433:MET:HG3	2.15	0.47
1:A:4269:ARG:HA	1:A:4392:PHE:CZ	2.50	0.47
1:A:4162:ILE:HG13	1:A:4187:LEU:HD23	1.97	0.47
1:A:2766:MET:CB	1:A:2783:LEU:HD11	2.42	0.47
1:A:2127:LYS:HB3	1:A:2222:VAL:HG13	1.97	0.47
1:B:3043:ASN:HD22	1:B:3043:ASN:N	2.10	0.47
1:A:3563:LEU:O	1:A:3567:LEU:HG	2.14	0.47
1:A:3988:TRP:O	1:A:3992:LEU:HG	2.14	0.47
1:A:2641:VAL:O	1:A:2646:VAL:HG11	2.15	0.47
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.49	0.47
1:A:4244:VAL:HG23	1:A:4403:SER:HB3	1.96	0.47
1:B:3849:ASP:HA	1:B:3852:ILE:HG22	1.97	0.47
1:A:2370:LEU:CD2	1:A:2387:LEU:HD22	2.45	0.47
1:B:3601:TYR:O	1:B:3602:ILE:C	2.53	0.47
1:B:4005:ILE:HG21	1:B:4008:LEU:HD12	1.96	0.47
1:A:3776:ASP:HB3	1:A:3780:ARG:HH12	1.80	0.47
1:A:4295:PHE:HD2	1:A:4295:PHE:C	2.18	0.47
1:A:1868:SER:O	1:A:1872:ARG:HB2	2.15	0.47
1:B:2252:LYS:HE2	1:B:2254:GLU:HG2	1.96	0.47
1:B:2556:SER:C	1:B:2558:PHE:H	2.17	0.47
1:B:2587:LEU:HD12	1:B:2817:ASP:HB3	1.96	0.47
1:B:3930:LEU:O	1:B:3931:VAL:C	2.53	0.47
1:B:3677:PRO:CG	1:B:3787:THR:HG22	2.45	0.47
1:B:4157:TYR:HB2	1:B:4184:TRP:C	2.35	0.47
1:B:2309:LYS:HE2	1:B:2756:THR:HG21	1.96	0.47
1:B:4136:SER:O	1:B:4220:GLU:HA	2.15	0.47
1:B:2669:PRO:HG2	1:B:2810:HIS:O	2.14	0.47
1:B:2660:LEU:O	1:B:2664:LEU:HB2	2.15	0.47
1:A:4376:VAL:HB	1:A:4381:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4650:ASN:O	1:B:4653:GLN:HG3	2.15	0.47
1:B:2701:PHE:CE2	1:B:2759:VAL:HG11	2.50	0.47
1:A:2424:GLN:HG3	1:A:2508:PRO:HG3	1.97	0.47
1:A:2905:TRP:CZ3	1:A:2934:ALA:HB2	2.50	0.47
1:A:2316:LEU:HD23	1:A:2363:TRP:HB2	1.97	0.47
1:A:3639:SER:HB2	1:A:3643:GLU:OE1	2.15	0.46
1:A:2651:VAL:CG1	1:A:2652:ASP:H	2.23	0.46
1:A:3040:ILE:O	1:A:3040:ILE:HG22	2.14	0.46
1:A:3452:ILE:O	1:A:3457:LEU:HD23	2.15	0.46
1:A:4537:LEU:HD23	1:A:4548:LYS:HE3	1.97	0.46
1:A:2065:ILE:HG22	1:A:2066:SER:N	2.30	0.46
1:A:3285:LEU:HD22	1:A:3578:SER:HB2	1.97	0.46
1:A:3270:LEU:CB	1:A:3592:VAL:HG13	2.44	0.46
1:B:2270:HIS:HB3	1:B:2392:ARG:NH1	2.29	0.46
1:B:2774:ARG:HG2	1:B:2776:SER:OG	2.15	0.46
1:B:1576:LYS:HG2	1:B:1585:GLU:OE2	2.14	0.46
1:B:1642:GLU:O	1:B:1646:ILE:HG12	2.16	0.46
1:A:4599:ALA:O	1:A:4602:THR:HG22	2.15	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CZ	2.49	0.46
1:A:4099:HIS:ND1	1:A:4111:LEU:HD12	2.30	0.46
1:B:3973:ILE:HG13	1:B:3988:TRP:CZ3	2.50	0.46
1:B:1555:VAL:H	1:B:1609:GLN:NE2	2.12	0.46
1:B:4604:THR:HG23	1:B:4671:TRP:NE1	2.21	0.46
1:A:2101:ILE:N	1:A:2101:ILE:HD13	2.30	0.46
1:B:3027:ARG:HA	1:B:3037:ILE:CD1	2.43	0.46
1:A:1886:ARG:CZ	1:A:1890:ARG:HH22	2.28	0.46
1:B:2532:ARG:HG3	1:B:2808:LEU:O	2.14	0.46
1:B:4128:SER:HB2	1:B:4213:PHE:HB3	1.96	0.46
1:A:4067:ALA:C	1:A:4073:GLN:HE21	2.19	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CE2	2.50	0.46
1:A:1969:GLY:N	1:A:2047:GLN:NE2	2.64	0.46
1:A:2415:TRP:HA	1:A:2415:TRP:CE3	2.51	0.46
1:A:2720:TYR:CE1	1:A:2730:LEU:HD13	2.50	0.46
1:B:4030:PHE:HE1	1:B:4085:LEU:HG	1.80	0.46
1:A:4220:GLU:O	1:A:4222:HIS:N	2.49	0.46
1:B:4190:ILE:HG12	1:B:4219:SER:CB	2.44	0.46
1:A:2956:LEU:HD21	1:A:2971:TYR:CD2	2.50	0.46
1:A:3975:SER:C	1:A:3977:LYS:H	2.18	0.46
1:A:3021:GLY:O	1:A:3025:LEU:HB2	2.14	0.46
1:B:1601:LEU:HA	1:B:1666:GLN:OE1	2.16	0.46
1:A:3283:LEU:HD23	1:A:3283:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1809:ASN:HD22	1:A:1809:ASN:HA	1.60	0.46
1:A:2492:LEU:HG	1:A:2496:LYS:NZ	2.31	0.46
1:A:4087:LYS:HG2	1:A:4087:LYS:O	2.15	0.46
1:A:2903:ARG:HB2	1:A:2945:ALA:O	2.15	0.46
1:A:4589:VAL:HG22	1:A:4590:TRP:N	2.29	0.46
1:B:2529:THR:OG1	1:B:2532:ARG:HB2	2.15	0.46
1:B:2191:GLU:HA	1:B:2194:VAL:HG23	1.98	0.46
1:A:3219:ILE:CB	1:A:3220:PRO:HD3	2.46	0.46
1:A:1630:PRO:O	1:A:1634:THR:HG23	2.15	0.46
1:A:2882:TRP:CZ2	1:A:2905:TRP:NE1	2.83	0.46
1:B:3288:GLY:HA3	1:B:3574:TRP:CZ3	2.49	0.46
1:B:3773:PHE:HB3	1:B:3777:LEU:HD23	1.98	0.46
1:B:2937:HIS:C	1:B:2939:PRO:HD3	2.35	0.46
1:A:3071:PHE:HE2	1:A:3087:MET:HE3	1.79	0.46
1:B:1555:VAL:H	1:B:1609:GLN:HE22	1.64	0.46
1:A:2257:GLU:O	1:A:2261:GLN:HG2	2.16	0.46
1:A:2856:PHE:CZ	1:A:2930:ILE:HG12	2.49	0.46
1:A:3733:VAL:C	1:A:3735:ASN:H	2.19	0.46
1:B:2127:LYS:C	1:B:2130:PRO:HD2	2.35	0.46
1:B:1846:GLN:O	1:B:1849:GLU:HB3	2.16	0.46
1:A:1948:VAL:O	1:A:1950:THR:N	2.49	0.46
1:B:2907:HIS:HB2	1:B:2950:ILE:HG21	1.96	0.46
1:A:3998:LEU:HD13	1:A:3998:LEU:O	2.15	0.46
1:A:3324:LEU:HD12	1:A:3539:LEU:CD2	2.46	0.46
1:A:2435:SER:HB3	1:A:2496:LYS:HG2	1.97	0.46
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	1.98	0.46
1:A:3387:HIS:HB2	1:A:3473:ALA:HB2	1.95	0.46
1:A:3725:ASN:N	1:A:3725:ASN:HD22	1.99	0.46
1:A:2832:ASN:ND2	1:A:2883:ASP:OD2	2.49	0.46
1:A:4044:TRP:HE3	1:A:4048:PHE:HE1	1.62	0.46
1:A:4044:TRP:CE2	1:A:4059:PRO:HG3	2.51	0.46
1:B:3891:LEU:HD21	1:B:3895:ARG:NH2	2.31	0.46
1:B:2748:LEU:HD11	1:B:3162:PRO:HG2	1.97	0.46
1:A:3113:LYS:HG3	1:A:3123:LEU:O	2.15	0.46
1:A:3007:GLN:O	1:A:3142:HIS:HE1	1.99	0.46
1:B:1799:ASP:OD1	1:B:1801:SER:HB3	2.15	0.46
1:A:2376:LEU:HA	1:A:2385:LEU:O	2.15	0.46
1:A:1786:SER:HB2	1:A:1914:TYR:OH	2.16	0.46
1:B:1721:HIS:C	1:B:1725:MET:HE2	2.36	0.46
1:B:4296:PHE:HB3	1:B:4346:ARG:HD2	1.98	0.46
1:B:1962:GLN:CB	1:B:4341:THR:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2841:ASN:ND2	1:B:2842:LEU:HG	2.31	0.46
1:A:4318:SER:HA	1:A:4321:ARG:NH2	2.23	0.46
1:B:4222:HIS:ND1	1:B:4223:PRO:HD2	2.31	0.46
1:B:4020:LEU:HG	1:B:4034:VAL:HG22	1.98	0.46
1:A:3990:PHE:HD2	1:A:4084:LEU:HD22	1.81	0.46
1:B:2532:ARG:NH1	1:B:2813:ILE:HD12	2.31	0.46
1:A:2243:ILE:HG21	1:A:2288:VAL:HG13	1.96	0.46
1:B:3788:VAL:HG11	1:B:3913:LEU:CD2	2.46	0.46
1:A:3830:LEU:HD12	1:A:3858:LEU:HD13	1.96	0.46
1:A:2578:MET:HE1	1:A:2613:LEU:HA	1.96	0.46
1:B:2749:PRO:O	1:B:2757:GLN:HG2	2.16	0.46
1:B:4645:GLU:HG3	1:B:4722:SER:OG	2.15	0.46
1:B:4281:ILE:HG13	1:B:4282:GLN:N	2.31	0.46
1:A:2205:PRO:HG3	1:A:2261:GLN:OE1	2.16	0.46
1:A:2603:THR:HG22	1:A:2604:PRO:HD2	1.97	0.46
1:A:2059:LEU:HG	1:A:2060:LEU:HG	1.97	0.46
1:A:4719:ARG:HH11	1:A:4719:ARG:HG3	1.81	0.46
1:A:2360:ASP:HB2	1:A:2361:PRO:HD2	1.96	0.46
1:A:1904:PHE:C	1:A:1906:TRP:H	2.17	0.46
1:A:2829:GLY:HA2	1:A:2850:THR:OG1	2.16	0.46
1:B:4597:PRO:HG2	1:B:4692:LEU:CD1	2.46	0.46
1:A:4022:CYS:O	1:A:4026:GLN:HB2	2.16	0.46
1:A:4681:ASN:ND2	1:A:4685:LYS:HE3	2.30	0.46
1:A:2443:GLU:OE2	1:A:2489:PRO:HB2	2.15	0.46
1:B:3993:LYS:O	1:B:3994:GLY:C	2.54	0.46
1:A:4395:TRP:CZ3	1:A:4399:LEU:HD11	2.51	0.46
1:A:3925:ASN:N	1:A:3925:ASN:ND2	2.63	0.46
1:B:1683:LEU:O	1:B:1683:LEU:HD12	2.16	0.46
1:B:3715:GLY:HA3	1:B:3758:PRO:HG2	1.98	0.46
1:A:4596:ASN:ND2	1:A:4596:ASN:C	2.69	0.46
1:A:1530:PHE:CZ	1:A:1571:SER:HB2	2.51	0.46
1:A:1745:SER:OG	1:A:1751:THR:HG22	2.16	0.46
1:B:4331:TRP:CZ2	1:B:4369:PHE:HE2	2.34	0.46
1:B:4284:ARG:NH2	1:B:4355:LEU:HD21	2.31	0.46
1:A:3017:VAL:HG21	1:A:3257:PRO:HD3	1.98	0.46
1:A:2864:PHE:HB3	1:A:2872:TYR:HD2	1.81	0.46
1:B:3789:THR:H	1:B:3792:SER:HB3	1.81	0.46
1:A:4278:HIS:HD2	1:A:4343:TYR:OH	1.99	0.46
1:A:2641:VAL:O	1:A:2643:SER:N	2.49	0.46
1:A:4402:ILE:CD1	1:A:4402:ILE:H	2.28	0.46
1:A:1911:ARG:HD3	1:A:1911:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4095:LEU:HD11	1:B:4422:LYS:HB3	1.97	0.46
1:B:4274:LEU:HD11	1:B:4306:ALA:HB1	1.98	0.46
1:A:2952:TYR:CZ	1:A:2962:PRO:HG3	2.51	0.46
1:B:4400:PRO:HG2	1:B:4407:TRP:HH2	1.81	0.46
1:B:2044:GLN:O	1:B:2048:VAL:HG23	2.16	0.46
1:A:4263:GLN:NE2	1:A:4322:SER:HA	2.30	0.46
1:A:1662:ILE:HG22	1:A:1663:GLU:N	2.32	0.46
1:B:4574:GLN:NE2	1:B:4590:TRP:HB3	2.31	0.45
1:B:1822:VAL:HG13	1:B:1823:TRP:N	2.31	0.45
1:B:2275:VAL:HG11	1:B:2400:LEU:HG	1.97	0.45
1:B:1534:VAL:HG22	1:B:1568:HIS:CD2	2.50	0.45
1:B:2873:ILE:O	1:B:2873:ILE:HG13	2.14	0.45
1:B:4434:GLN:HE21	1:B:4434:GLN:HB3	1.55	0.45
1:A:2249:LEU:HB3	2:A:9002:ADP:N6	2.30	0.45
1:A:2980:TYR:OH	1:A:2987:PRO:HA	2.15	0.45
1:B:1604:VAL:O	1:B:1608:VAL:HG23	2.16	0.45
1:B:3912:SER:HB3	1:B:4231:ARG:CG	2.45	0.45
1:B:4122:VAL:HG11	1:B:4216:PHE:HZ	1.81	0.45
1:B:1985:LYS:HD3	1:B:1997:VAL:HG21	1.98	0.45
1:A:2851:ASP:HB3	1:A:2937:HIS:CE1	2.51	0.45
1:A:1642:GLU:O	1:A:1646:ILE:HG13	2.16	0.45
1:A:4726:TRP:CH2	1:A:4728:SER:HB2	2.51	0.45
1:A:2338:ARG:HH11	1:A:2338:ARG:HG2	1.81	0.45
1:B:1931:ASN:HD21	1:B:1962:GLN:HE22	1.64	0.45
1:A:3015:ILE:CG2	1:A:3149:PRO:HG3	2.45	0.45
1:B:2309:LYS:HZ3	1:B:2756:THR:HG21	1.77	0.45
1:A:3271:ILE:HG12	1:A:3592:VAL:HG21	1.97	0.45
1:B:4379:ILE:HG23	1:B:4381:LEU:HG	1.98	0.45
1:B:2331:LEU:HD21	1:B:2773:TRP:CG	2.51	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:O	2.16	0.45
1:A:4309:SER:O	1:A:4312:TYR:HB3	2.16	0.45
1:A:4039:GLN:HB3	1:A:4040:ASN:H	1.57	0.45
1:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.16	0.45
1:A:3551:SER:O	1:A:3554:LYS:HB2	2.16	0.45
1:A:3814:SER:C	1:A:3818:LYS:HD3	2.37	0.45
1:A:4653:GLN:O	1:A:4655:THR:HG23	2.17	0.45
1:A:4337:ILE:O	1:A:4341:THR:HG22	2.16	0.45
1:A:3481:ALA:O	1:A:3485:THR:HG23	2.16	0.45
1:A:3190:ARG:C	1:A:3192:LEU:H	2.20	0.45
1:A:4281:ILE:HG13	1:A:4282:GLN:N	2.31	0.45
1:A:3798:LEU:O	1:A:3802:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2745:GLU:HG2	1:B:2748:LEU:HD11	1.98	0.45
1:A:4026:GLN:HB3	1:A:4027:VAL:H	1.60	0.45
1:B:4431:GLN:HG2	1:B:4431:GLN:O	2.16	0.45
1:A:2896:CYS:SG	1:A:2897:THR:N	2.90	0.45
1:B:4335:ARG:NH2	1:B:4365:THR:HG22	2.22	0.45
1:B:4047:PHE:HE1	1:B:4086:MET:HE1	1.81	0.45
1:B:3990:PHE:HD2	1:B:4084:LEU:HD22	1.82	0.45
1:A:2845:PHE:O	1:A:2848:ASN:HB2	2.16	0.45
1:A:2976:LEU:HD12	1:A:3028:PHE:CE1	2.51	0.45
1:A:2398:GLN:NE2	1:A:2806:ARG:HG2	2.31	0.45
1:B:3015:ILE:HD12	1:B:3170:LEU:HD11	1.98	0.45
1:B:2849:LEU:HD13	1:B:2901:LEU:HD11	1.99	0.45
1:B:3306:LEU:HD13	1:B:3557:VAL:CG2	2.46	0.45
1:A:2738:TRP:CZ3	1:A:2785:LYS:HA	2.51	0.45
1:B:3536:TYR:O	1:B:3540:ILE:HD13	2.16	0.45
1:A:3792:SER:OG	1:A:3793:LEU:N	2.50	0.45
1:A:3893:CYS:HB3	1:A:3916:PHE:HZ	1.81	0.45
1:A:2323:THR:O	1:A:2324:THR:HG23	2.16	0.45
1:A:4279:ALA:O	1:A:4283:GLU:HB2	2.17	0.45
1:B:3930:LEU:HD22	1:B:3939:ARG:HE	1.81	0.45
1:A:4648:VAL:HG23	1:A:4655:THR:OG1	2.16	0.45
1:A:3686:MET:CE	1:A:3696:LYS:HB2	2.46	0.45
1:A:4349:ASN:O	1:A:4352:ASP:HB2	2.16	0.45
1:A:3459:ASP:HB3	1:A:3462:PHE:CB	2.47	0.45
1:B:4012:LEU:HA	1:B:4016:GLN:NE2	2.31	0.45
1:A:3549:GLU:O	1:A:3553:VAL:HG23	2.17	0.45
1:B:2630:LYS:CB	1:B:2654:THR:HG21	2.47	0.45
1:B:3673:LEU:HD22	1:B:3783:PHE:CE1	2.48	0.45
1:A:2603:THR:CB	1:A:2604:PRO:HD2	2.46	0.45
1:A:3897:TYR:HD2	1:A:3898:PHE:CD2	2.34	0.45
1:A:1784:LEU:HB3	1:A:1814:LEU:HD13	1.99	0.45
1:A:1842:GLN:OE1	1:A:1893:GLN:HG2	2.17	0.45
1:B:4714:GLN:O	1:B:4718:GLN:HG3	2.16	0.45
1:A:3011:HIS:C	1:A:3168:CYS:HB3	2.36	0.45
1:A:3919:ILE:HD13	1:A:3951:THR:HA	1.98	0.45
1:A:1973:PHE:C	1:A:1973:PHE:CD1	2.89	0.45
1:B:4693:ASN:ND2	1:B:4693:ASN:N	2.64	0.45
1:A:1964:LEU:HD12	1:A:2074:PHE:CZ	2.51	0.45
1:A:1968:MET:HB3	1:A:2094:LEU:O	2.16	0.45
1:B:4404:THR:HB	1:B:4405:PRO:HD2	1.99	0.45
1:B:2819:PRO:HB2	1:B:2824:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1726:PHE:HB2	1:A:1729:LEU:HB3	1.98	0.45
1:A:3350:VAL:O	1:A:3350:VAL:HG12	2.15	0.45
1:A:4249:LEU:O	1:A:4253:ILE:HG13	2.17	0.45
1:A:2435:SER:CB	1:A:2496:LYS:HG2	2.47	0.45
1:A:3234:ILE:O	1:A:3238:ILE:HD13	2.17	0.45
1:A:2124:LEU:HD22	1:A:2195:LEU:CD2	2.46	0.45
1:A:3388:LEU:CD2	1:A:3473:ALA:HB1	2.44	0.45
1:B:2825:THR:HG23	1:B:2854:VAL:HG21	1.98	0.45
1:A:1907:LEU:HD22	1:A:1911:ARG:NH1	2.31	0.45
1:B:4666:ILE:HG13	1:B:4667:ALA:N	2.32	0.45
1:B:3696:LYS:HG3	1:B:3719:LEU:HD23	1.99	0.45
1:B:3542:GLU:O	1:B:3546:ILE:HG12	2.16	0.45
1:A:3463:ASP:O	1:A:3467:VAL:HG23	2.17	0.45
1:B:3004:VAL:O	1:B:3010:GLY:HA3	2.17	0.45
1:A:3022:LYS:HA	1:A:3173:PHE:CE1	2.52	0.45
1:A:4384:PRO:HG2	1:A:4392:PHE:CD1	2.51	0.45
1:A:4668:THR:C	1:A:4669:LEU:HD12	2.37	0.45
1:B:3990:PHE:CZ	1:B:4023:LEU:HD13	2.52	0.45
1:A:2902:VAL:HG21	1:A:2941:VAL:CG2	2.47	0.45
1:A:1922:LEU:HD13	1:A:1938:PHE:CD1	2.48	0.45
1:B:1618:ILE:HD13	1:B:1683:LEU:HD21	1.99	0.45
1:B:4197:LEU:HB3	1:B:4226:PRO:HG2	1.98	0.45
1:A:4329:ILE:HB	1:A:4331:TRP:CE2	2.51	0.45
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.52	0.45
1:B:4618:ASN:N	1:B:4618:ASN:ND2	2.65	0.45
1:A:1800:HIS:CD2	1:A:1858:ASN:HB3	2.52	0.45
1:B:2091:LEU:HD22	1:B:2095:PHE:CE2	2.51	0.45
1:B:1740:THR:HG22	1:B:1759:SER:HA	1.98	0.45
1:A:3602:ILE:O	1:A:3603:GLY:C	2.54	0.45
1:A:2140:SER:HB2	1:A:2211:ASP:OD2	2.15	0.45
1:A:4046:GLN:NE2	1:A:4057:ILE:HG22	2.32	0.45
1:A:3639:SER:OG	1:A:3663:ILE:HD11	2.17	0.45
1:B:4657:THR:HG22	1:B:4658:ASP:N	2.32	0.45
1:A:2196:LEU:HA	1:A:2199:ILE:CG1	2.46	0.45
1:A:4347:ILE:CG2	1:A:4353:MET:HG2	2.43	0.45
1:B:2204:ILE:N	1:B:2205:PRO:CD	2.80	0.45
1:A:3145:PHE:CG	1:A:3164:LEU:HD11	2.52	0.45
1:A:2526:MET:O	1:A:2527:ASP:C	2.55	0.45
1:B:3992:LEU:HD12	1:B:4434:GLN:NE2	2.31	0.45
1:A:2052:GLU:O	1:A:2053:ASN:CB	2.64	0.45
1:A:4032:LYS:HA	1:A:4032:LYS:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2270:HIS:HB3	1:B:2392:ARG:HH11	1.82	0.45
1:B:4095:LEU:HD11	1:B:4422:LYS:HB2	1.99	0.45
1:A:3218:ALA:O	1:A:3220:PRO:N	2.49	0.45
1:A:4311:ASP:O	1:A:4315:ASP:HB3	2.17	0.45
1:B:3254:TYR:CD2	1:B:3775:PRO:HA	2.52	0.45
1:B:4621:LEU:HG	1:B:4622:HIS:H	1.82	0.45
1:A:1925:LEU:HD23	1:A:1936:TYR:HB2	1.98	0.45
1:B:1548:TYR:HD2	1:B:1554:LEU:HD11	1.82	0.45
1:A:2272:VAL:HB	1:A:2394:MET:HE2	1.97	0.45
1:A:3813:ARG:HA	1:A:3875:VAL:HG11	1.99	0.45
1:A:3696:LYS:HZ3	1:A:3721:GLN:CD	2.21	0.45
1:B:2641:VAL:HG13	1:B:2831:PHE:HB3	1.98	0.45
1:B:4220:GLU:O	1:B:4222:HIS:N	2.50	0.45
1:A:3912:SER:HB3	1:A:4231:ARG:CG	2.45	0.45
1:B:3078:VAL:O	1:B:3078:VAL:HG13	2.16	0.45
1:B:4197:LEU:HD13	1:B:4226:PRO:HD3	1.99	0.45
1:A:3903:LEU:HD13	1:A:3959:LEU:HD21	1.99	0.45
1:A:4116:LEU:HB3	1:A:4117:ASP:H	1.52	0.45
1:A:3540:ILE:N	1:A:3540:ILE:HD12	2.32	0.45
1:B:1764:PRO:HB2	1:B:1768:GLU:CB	2.47	0.45
1:A:3542:GLU:O	1:A:3546:ILE:HG13	2.17	0.45
1:B:2998:ILE:CG2	1:B:3025:LEU:HD22	2.47	0.45
1:A:4455:SER:C	1:A:4457:SER:H	2.20	0.45
1:A:3908:LEU:HD21	1:A:4237:SER:OG	2.16	0.45
1:A:3027:ARG:HH11	1:A:3027:ARG:HB2	1.81	0.45
1:B:4253:ILE:HG22	1:B:4253:ILE:O	2.17	0.45
1:B:2381:ASN:ND2	1:B:2383:GLU:HB2	2.20	0.44
1:A:4076:ILE:HD12	1:A:4105:VAL:HG22	1.99	0.44
1:A:3682:MET:CE	1:A:3721:GLN:HE21	2.31	0.44
1:A:2730:LEU:HD22	1:A:2772:PHE:CZ	2.52	0.44
1:A:1958:LEU:O	1:A:1962:GLN:HB2	2.16	0.44
1:B:2774:ARG:C	1:B:2776:SER:H	2.20	0.44
1:B:1869:ALA:HA	1:B:1872:ARG:HB3	1.99	0.44
1:A:3825:VAL:HA	1:A:3828:ARG:HD3	1.99	0.44
1:A:3776:ASP:HB3	1:A:3780:ARG:NH1	2.31	0.44
1:B:2705:THR:HG22	1:B:2759:VAL:HG21	1.98	0.44
1:B:1629:LEU:HD22	1:B:1632:GLU:HG2	1.98	0.44
1:A:1777:MET:CE	1:A:1939:GLU:HA	2.48	0.44
1:A:2142:GLN:NE2	1:A:2208:VAL:HG21	2.32	0.44
1:A:2359:VAL:HG11	1:A:2400:LEU:HD22	1.99	0.44
1:B:3233:TYR:CG	1:B:3620:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4121:ILE:HG22	1:A:4122:VAL:N	2.32	0.44
1:A:2898:LEU:HD13	1:A:2898:LEU:O	2.17	0.44
1:A:1609:GLN:O	1:A:1613:VAL:HG23	2.17	0.44
1:B:2263:HIS:HB2	1:B:2289:TYR:CE1	2.52	0.44
1:A:1748:GLU:HB3	1:A:1943:ILE:HD12	1.99	0.44
1:B:4192:LEU:C	1:B:4194:PRO:HD3	2.38	0.44
1:A:3408:VAL:HG23	1:A:3409:CYS:N	2.32	0.44
1:A:3490:ILE:O	1:A:3490:ILE:HG13	2.18	0.44
1:A:3974:ILE:O	1:A:3977:LYS:HB2	2.17	0.44
1:A:2302:GLU:HG2	1:A:2304:HIS:HE1	1.81	0.44
1:B:3088:ASN:OD1	1:B:3163:ALA:HB3	2.17	0.44
1:A:2433:THR:HG23	1:A:2437:GLU:HG3	1.99	0.44
1:B:2955:TRP:HZ2	1:B:3002:ASP:OD1	2.00	0.44
1:A:3809:THR:HG22	1:A:3812:LYS:NZ	2.32	0.44
1:A:2502:ILE:HD12	1:A:2506:PHE:HE2	1.82	0.44
1:A:3361:LYS:HE2	1:A:3361:LYS:HB3	1.84	0.44
1:A:2056:GLU:O	1:A:2056:GLU:HG3	2.17	0.44
1:A:4691:TYR:HA	1:A:4699:LEU:HA	1.99	0.44
1:B:2660:LEU:HD21	1:B:2672:LEU:CD2	2.48	0.44
1:A:2016:LEU:HD21	1:A:2023:GLY:CA	2.47	0.44
1:B:4686:LEU:HD12	1:B:4687:SER:H	1.83	0.44
1:A:3055:LEU:O	1:A:3059:LEU:HD23	2.17	0.44
1:A:2340:ILE:HD11	1:A:2386:ALA:O	2.17	0.44
1:B:4266:GLU:HG3	1:B:4369:PHE:CE1	2.52	0.44
1:A:3670:ARG:NH1	1:A:3781:VAL:O	2.51	0.44
1:A:2399:ASP:O	1:A:2400:LEU:HD23	2.16	0.44
1:B:2381:ASN:ND2	1:B:2381:ASN:C	2.71	0.44
1:A:3731:ASN:H	1:A:3731:ASN:ND2	2.09	0.44
1:B:3601:TYR:O	1:B:3603:GLY:N	2.50	0.44
1:A:2046:ILE:HD11	1:A:2059:LEU:HD22	2.00	0.44
1:A:2902:VAL:HG22	1:A:2938:PHE:CD2	2.53	0.44
1:A:2742:PHE:HD1	1:A:2789:VAL:HG12	1.83	0.44
1:B:3958:THR:CG2	1:B:4235:VAL:HB	2.47	0.44
1:A:2641:VAL:HG21	1:A:2887:LEU:HD13	1.99	0.44
1:B:1640:ASN:ND2	1:B:1644:ILE:HG12	2.32	0.44
1:B:4693:ASN:HD22	1:B:4693:ASN:H	1.64	0.44
1:B:3316:LYS:HD2	1:B:3546:ILE:CD1	2.47	0.44
1:B:3011:HIS:CE1	1:B:3091:LEU:HA	2.53	0.44
1:B:4244:VAL:HG23	1:B:4403:SER:OG	2.18	0.44
1:B:4405:PRO:HD3	1:B:4415:GLU:HG2	1.98	0.44
1:A:3805:GLU:HB3	1:A:3886:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3675:ILE:O	1:A:3675:ILE:HG22	2.17	0.44
1:B:4087:LYS:HG2	1:B:4087:LYS:O	2.17	0.44
1:A:3338:GLN:NE2	1:A:3525:LEU:HB2	2.32	0.44
1:A:2200:ASN:O	1:A:2204:ILE:HG12	2.18	0.44
1:A:2200:ASN:ND2	1:A:2228:LEU:HD13	2.18	0.44
1:B:3602:ILE:HG23	1:B:3610:ARG:CG	2.43	0.44
1:A:4513:ILE:HA	1:A:4550:TRP:HE1	1.82	0.44
1:A:3154:PHE:C	1:A:3156:ASN:H	2.21	0.44
1:B:1828:ASP:OD2	1:B:1901:ASN:HB2	2.17	0.44
1:A:3293:ARG:HG3	1:A:3293:ARG:NH1	2.27	0.44
1:A:3902:GLU:O	1:A:3905:GLN:HG2	2.17	0.44
1:B:2976:LEU:CD1	1:B:2990:LEU:HD11	2.48	0.44
1:A:3274:LYS:HA	1:A:3274:LYS:HD3	1.77	0.44
1:B:2886:LEU:O	1:B:2890:ILE:HG13	2.18	0.44
1:A:1719:GLN:OE1	1:A:1732:LEU:N	2.50	0.44
1:B:2301:SER:HA	1:B:2350:ARG:O	2.18	0.44
1:A:2339:ILE:HG21	1:A:2391:VAL:CG2	2.48	0.44
1:A:3727:ASP:CB	1:A:3729:VAL:HG12	2.48	0.44
1:A:4673:ASP:O	1:A:4677:PRO:HD2	2.18	0.44
1:A:4075:THR:HG23	1:A:4076:ILE:H	1.82	0.44
1:A:4296:PHE:HE2	1:A:4347:ILE:HA	1.77	0.44
1:B:4265:ALA:H	1:B:4323:ASN:HB3	1.83	0.44
1:A:3410:LEU:C	1:A:3410:LEU:HD23	2.38	0.44
1:A:2125:ALA:HA	1:A:2128:ILE:CG2	2.46	0.44
1:A:2152:LEU:HD13	1:A:2152:LEU:O	2.18	0.44
1:B:2986:VAL:O	1:B:2988:LEU:HG	2.17	0.44
1:B:4304:ARG:HA	1:B:4307:LEU:HD12	1.99	0.44
1:B:4330:PRO:O	1:B:4333:ALA:HB3	2.17	0.44
1:A:1628:LEU:O	1:A:1628:LEU:HD23	2.18	0.44
1:A:3521:THR:O	1:A:3525:LEU:HD12	2.18	0.44
1:A:3603:GLY:HA2	1:A:3664:MET:CE	2.48	0.44
1:A:2056:GLU:HB2	1:A:2065:ILE:O	2.18	0.44
1:A:2991:PHE:O	1:A:2992:ASN:C	2.55	0.44
1:B:3013:LEU:HD13	1:B:3145:PHE:HB3	2.00	0.44
1:B:3164:LEU:C	1:B:3166:ASN:H	2.22	0.44
1:B:3715:GLY:HA2	1:B:3760:PHE:HB2	2.00	0.44
1:A:1904:PHE:C	1:A:1906:TRP:N	2.71	0.44
1:B:4686:LEU:HD22	1:B:4716:TRP:HB3	2.00	0.44
1:B:2694:PHE:HA	1:B:2738:TRP:O	2.18	0.44
1:B:1530:PHE:CZ	1:B:1571:SER:HB2	2.53	0.44
1:A:1674:ASP:OD1	1:A:1678:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4374:PRO:HB3	1:B:4377:PRO:HG3	1.98	0.44
1:A:2077:MET:HE2	1:A:2077:MET:HB3	1.81	0.44
1:B:2612:LEU:O	1:B:2612:LEU:HD13	2.18	0.44
1:A:2926:THR:O	1:A:2930:ILE:HG13	2.18	0.44
1:A:2289:TYR:CE1	1:A:2293:ILE:HD11	2.53	0.44
1:A:3812:LYS:HB3	1:A:3875:VAL:CG2	2.47	0.44
1:A:3813:ARG:HH22	1:A:3817:LEU:HD13	1.83	0.44
1:B:2766:MET:HB3	1:B:2783:LEU:CD1	2.43	0.44
1:A:2903:ARG:HD2	1:A:2945:ALA:O	2.18	0.44
1:B:4289:PRO:HB2	1:B:4696:ARG:HD2	2.00	0.44
1:B:4689:PRO:HD2	1:B:4721:VAL:O	2.18	0.44
1:A:1695:ALA:CB	1:A:2019:CYS:SG	3.06	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HA	1.81	0.44
1:B:3553:VAL:O	1:B:3557:VAL:HG23	2.18	0.44
1:A:3869:VAL:O	1:A:3869:VAL:HG12	2.18	0.44
1:A:1535:ARG:HA	1:A:1591:TRP:HZ2	1.83	0.44
1:A:2376:LEU:HD12	1:A:2385:LEU:C	2.38	0.44
1:A:3205:PHE:CE2	1:A:3221:PRO:HB3	2.52	0.44
1:B:2828:TYR:HE1	1:B:2880:SER:HA	1.83	0.44
1:B:3872:THR:O	1:B:3876:MET:HG2	2.18	0.44
1:B:3552:LYS:NZ	1:B:3552:LYS:HB2	2.33	0.44
1:B:2839:LEU:CD2	1:B:2896:CYS:HB3	2.48	0.44
1:A:3700:LEU:CD1	1:A:3701:ASP:H	2.31	0.44
1:A:2913:PHE:HD2	1:A:2913:PHE:N	2.15	0.44
1:A:4257:ALA:C	1:A:4259:ARG:H	2.21	0.44
1:A:3190:ARG:HA	1:A:3224:ARG:NH1	2.32	0.44
1:A:2903:ARG:HH22	1:A:2950:ILE:HA	1.82	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HB2	1.83	0.44
1:A:2361:PRO:HD2	1:A:2754:TYR:CE1	2.53	0.44
1:B:1869:ALA:O	1:B:1872:ARG:HB3	2.17	0.44
1:B:3903:LEU:HD11	1:B:3967:PHE:CD1	2.53	0.44
1:B:2112:MET:O	1:B:2116:GLN:HG2	2.17	0.44
1:B:2965:ARG:HG3	1:B:2965:ARG:HH11	1.82	0.44
1:A:2255:TRP:CH2	1:A:2259:ILE:HD11	2.53	0.43
1:A:2560:MET:HE3	1:A:2564:ASN:HD22	1.81	0.43
1:A:3652:LEU:HD12	1:A:3653:PRO:CD	2.41	0.43
1:B:2426:ILE:H	1:B:2426:ILE:CD1	2.27	0.43
1:B:2902:VAL:HG21	1:B:2941:VAL:HG21	2.00	0.43
1:B:3046:TYR:CE1	1:B:3050:ASP:HB2	2.53	0.43
1:A:3585:MET:HA	1:A:3588:VAL:HG23	2.00	0.43
1:B:2714:PHE:HE1	1:B:2741:VAL:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2249:LEU:HD22	2:A:9002:ADP:C5	2.53	0.43
1:A:4690:VAL:HG11	1:A:4701:PHE:CE2	2.53	0.43
1:A:2091:LEU:HD22	1:A:2095:PHE:HE1	1.80	0.43
1:A:2617:VAL:HG13	1:A:2617:VAL:O	2.18	0.43
1:B:3038:TYR:HE2	1:B:3058:LEU:HD22	1.82	0.43
1:A:1591:TRP:HA	1:A:1591:TRP:CE3	2.53	0.43
1:B:3961:ASN:HA	1:B:3964:LYS:HE2	2.00	0.43
1:A:1756:LYS:HB2	1:A:1756:LYS:NZ	2.32	0.43
1:B:2522:ARG:NH1	1:B:2593:PHE:HD1	2.16	0.43
1:A:2650:THR:OG1	1:A:2651:VAL:N	2.50	0.43
1:A:3462:PHE:CE2	1:A:3478:VAL:HG23	2.53	0.43
1:B:4024:ARG:O	1:B:4024:ARG:HG2	2.17	0.43
1:B:4153:LEU:HB2	1:B:4155:LYS:CG	2.46	0.43
1:B:1674:ASP:O	1:B:1678:LYS:HG3	2.18	0.43
1:B:2265:ILE:HD12	1:B:2414:VAL:HG22	1.99	0.43
1:A:2547:ASN:O	1:A:2551:TYR:HB2	2.17	0.43
1:B:4691:TYR:HA	1:B:4698:GLU:O	2.18	0.43
1:A:2400:LEU:HB3	1:A:2403:ALA:HB3	2.00	0.43
1:A:2408:ILE:HG13	1:A:2409:SER:H	1.83	0.43
1:A:4319:LYS:O	1:A:4321:ARG:NH1	2.52	0.43
1:A:1958:LEU:HD23	1:A:4341:THR:HB	1.99	0.43
1:B:2282:LYS:HZ2	1:B:2282:LYS:HB2	1.83	0.43
1:A:1922:LEU:CD1	1:A:1938:PHE:HD1	2.31	0.43
1:A:2053:ASN:N	1:A:2053:ASN:ND2	2.65	0.43
1:B:4225:LEU:HD23	1:B:4230:LEU:HD21	2.00	0.43
1:A:3470:ALA:O	1:A:3471:SER:HB2	2.17	0.43
1:A:1755:LYS:HA	1:A:1755:LYS:HD2	1.80	0.43
1:B:2773:TRP:CZ3	1:B:2780:TRP:HB2	2.53	0.43
1:B:1497:LEU:HD22	1:B:1501:SER:HB2	1.99	0.43
1:A:3019:GLY:HA2	2:A:9004:ADP:H5'2	2.00	0.43
1:A:4091:SER:O	1:A:4420:SER:HA	2.18	0.43
1:B:3686:MET:HA	1:B:3694:ILE:HG21	2.00	0.43
1:A:1604:VAL:O	1:A:1608:VAL:HG23	2.18	0.43
1:A:2359:VAL:HB	1:A:2397:VAL:HG11	2.00	0.43
1:B:3192:LEU:HD22	1:B:3271:ILE:HG21	2.00	0.43
1:A:4052:GLN:O	1:A:4054:GLY:N	2.43	0.43
1:A:3062:ALA:HB2	1:A:3069:ILE:HD13	1.99	0.43
1:B:3634:VAL:HB	1:B:3635:PRO:HD3	1.99	0.43
1:B:3635:PRO:C	1:B:3637:PHE:H	2.21	0.43
1:B:4012:LEU:HD11	1:B:4020:LEU:HD22	2.01	0.43
1:A:3990:PHE:CE2	1:A:4023:LEU:HG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3681:ALA:HB2	1:A:3786:PHE:CD2	2.53	0.43
1:A:4182:GLY:HA3	1:A:4212:SER:HG	1.84	0.43
1:B:1975:PRO:HG2	1:B:1978:THR:CG2	2.48	0.43
1:B:1831:LEU:HA	1:B:1841:ILE:HG23	1.99	0.43
1:B:2964:ASN:HD21	1:B:2967:ASP:CG	2.22	0.43
1:B:4022:CYS:HB3	1:B:4026:GLN:HE21	1.84	0.43
1:A:1835:THR:O	1:A:1836:LEU:CB	2.67	0.43
1:A:3933:LYS:HB3	1:A:3933:LYS:HZ3	1.84	0.43
1:B:3041:LYS:N	1:B:3041:LYS:HD2	2.33	0.43
1:B:4574:GLN:HE22	1:B:4590:TRP:HB3	1.82	0.43
1:A:1830:ALA:O	1:A:1841:ILE:HG23	2.18	0.43
1:A:4132:LEU:HB2	1:A:4216:PHE:CD1	2.52	0.43
1:A:3445:THR:HA	1:A:3449:ARG:HB2	2.00	0.43
1:B:3234:ILE:HG23	1:B:3617:TRP:CD1	2.54	0.43
1:B:3289:LEU:HA	1:B:3292:LEU:HD12	1.99	0.43
1:B:1639:ILE:HG23	1:B:1672:LEU:HD22	2.01	0.43
1:B:2352:TRP:CD1	1:B:2392:ARG:HB2	2.54	0.43
1:A:3096:VAL:HB	1:A:3099:LEU:HB2	2.00	0.43
1:B:1653:ALA:HB1	1:B:1658:GLU:HG2	2.01	0.43
1:A:2200:ASN:ND2	1:A:2228:LEU:HB3	2.33	0.43
1:A:4337:ILE:HG22	1:A:4338:LEU:HD12	1.99	0.43
1:A:3015:ILE:HG21	1:A:3172:TRP:CH2	2.54	0.43
1:A:2057:VAL:HG22	1:A:2058:GLU:N	2.34	0.43
1:A:4066:GLN:HE22	1:A:4081:ARG:HD3	1.81	0.43
1:A:3638:LEU:HD22	1:A:3667:ARG:HD3	2.01	0.43
1:A:3078:VAL:O	1:A:3078:VAL:HG22	2.19	0.43
1:B:2882:TRP:O	1:B:2886:LEU:HG	2.18	0.43
1:A:2012:ILE:HG22	1:A:2016:LEU:CD1	2.49	0.43
1:B:3160:THR:O	1:B:3162:PRO:HD3	2.18	0.43
1:B:3902:GLU:C	1:B:3904:SER:N	2.71	0.43
1:A:3357:VAL:O	1:A:3357:VAL:HG12	2.18	0.43
1:B:3181:LEU:HB3	1:B:3232:VAL:HG13	2.00	0.43
1:B:4407:TRP:H	1:B:4407:TRP:HD1	1.64	0.43
1:B:3993:LYS:HG3	1:B:4431:GLN:HG3	1.99	0.43
1:B:4728:SER:OG	1:B:4729:ASP:N	2.51	0.43
1:B:1744:MET:SD	1:B:1777:MET:HG3	2.59	0.43
1:A:1955:ARG:HB2	1:A:1955:ARG:NH1	2.33	0.43
1:A:2145:TYR:OH	1:A:2207:LEU:HA	2.18	0.43
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.54	0.43
1:A:4648:VAL:HG13	1:A:4657:THR:CG2	2.44	0.43
1:A:2748:LEU:HD21	1:A:2800:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3238:ILE:HD11	1:B:3617:TRP:CZ2	2.48	0.43
1:A:2678:SER:HB2	1:A:2817:ASP:O	2.18	0.43
1:A:4179:ALA:HA	1:A:4213:PHE:CD1	2.53	0.43
1:B:1766:ILE:HD12	1:B:1769:TRP:HE1	1.84	0.43
1:B:1546:VAL:O	1:B:1553:LYS:HA	2.19	0.43
1:A:4389:ARG:NH1	1:A:4389:ARG:HG2	2.32	0.43
1:A:4288:ILE:HG23	1:A:4289:PRO:HA	2.01	0.43
1:B:4293:THR:HG23	1:B:4352:ASP:OD1	2.19	0.43
1:A:1906:TRP:CZ2	1:A:1911:ARG:HG2	2.54	0.43
1:B:2968:LEU:HD22	1:B:2999:LEU:HD11	2.00	0.43
1:A:3451:ALA:O	1:A:3455:GLY:N	2.51	0.43
1:A:2270:HIS:ND1	1:A:2270:HIS:N	2.66	0.43
1:A:4280:ILE:HG21	1:A:4359:PHE:CE1	2.53	0.43
1:B:2840:PRO:O	1:B:2843:ARG:HB2	2.19	0.43
1:A:1658:GLU:O	1:A:1661:ALA:HB3	2.19	0.43
1:B:4028:PRO:O	1:B:4031:SER:N	2.52	0.43
1:B:3289:LEU:O	1:B:3293:ARG:HG3	2.19	0.43
1:A:3862:THR:C	1:A:3864:GLU:H	2.22	0.43
1:A:3416:LYS:HE3	1:A:3418:GLU:CB	2.48	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CG	2.54	0.43
1:B:1780:THR:HG22	1:B:1784:LEU:CD1	2.48	0.43
1:B:1606:ILE:HG23	1:B:1607:ASP:N	2.33	0.43
1:B:4058:ILE:CD1	1:B:4082:LYS:HG2	2.48	0.43
1:A:4379:ILE:HG23	1:A:4381:LEU:HD13	2.00	0.43
1:A:2327:TRP:CZ2	1:A:2379:LEU:HD22	2.54	0.43
1:A:2304:HIS:N	1:A:2352:TRP:O	2.51	0.43
1:A:3324:LEU:HD12	1:A:3539:LEU:HD23	2.00	0.43
1:B:4331:TRP:HZ2	1:B:4369:PHE:CE2	2.37	0.43
1:A:3197:PRO:HG2	1:A:3198:GLN:OE1	2.18	0.43
1:A:2290:LEU:HD23	1:A:2301:SER:O	2.19	0.43
1:B:3065:LYS:O	1:B:3066:GLU:C	2.57	0.43
1:B:3725:ASN:ND2	1:B:3725:ASN:N	2.67	0.43
1:B:3675:ILE:HG22	1:B:3675:ILE:O	2.19	0.43
1:B:3139:ARG:HH11	1:B:3139:ARG:HG3	1.84	0.43
1:A:2269:ASN:O	1:A:2272:VAL:HG23	2.19	0.43
1:A:2774:ARG:CZ	1:A:2781:ILE:HD11	2.48	0.43
1:B:3620:ARG:NH1	1:B:3620:ARG:HG2	2.34	0.43
1:A:1892:LEU:C	1:A:1894:LYS:H	2.22	0.43
1:B:4023:LEU:O	1:B:4027:VAL:HB	2.18	0.43
1:A:3859:LYS:C	1:A:3859:LYS:HD3	2.39	0.43
1:A:3588:VAL:O	1:A:3592:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2339:ILE:HG21	1:B:2391:VAL:CG2	2.49	0.43
1:A:2645:ASP:O	1:A:2646:VAL:C	2.57	0.43
1:A:3902:GLU:HB3	1:A:4433:MET:HG2	2.00	0.43
1:B:4185:VAL:O	1:B:4215:LEU:HD12	2.19	0.43
1:B:4079:ASN:O	1:B:4082:LYS:HB2	2.18	0.43
1:B:3895:ARG:NH1	1:B:3977:LYS:HG2	2.34	0.43
1:B:4282:GLN:O	1:B:4285:LEU:HB2	2.19	0.43
1:B:3202:PRO:HG3	1:B:3623:SER:O	2.19	0.43
1:A:1578:SER:HA	1:A:1579:PRO:HD3	1.92	0.43
1:B:2304:HIS:NE2	1:B:2351:HIS:HD2	2.17	0.43
1:A:4565:ILE:HG22	1:A:4566:SER:N	2.34	0.43
1:B:3272:ASN:HD22	1:B:3272:ASN:HA	1.61	0.43
1:A:2211:ASP:C	1:A:2213:PRO:HD2	2.38	0.43
1:A:4708:ASP:C	1:A:4710:SER:H	2.22	0.43
1:A:3953:ASN:O	1:A:3956:THR:HG22	2.19	0.43
1:A:4432:LYS:C	1:A:4434:GLN:N	2.72	0.43
1:A:1927:ILE:O	1:A:1928:HIS:HD2	2.01	0.43
1:A:3391:ILE:HD11	1:A:3471:SER:OG	2.19	0.43
1:B:4324:ILE:HG13	1:B:4324:ILE:H	1.52	0.43
1:B:4617:GLU:HG2	1:B:4618:ASN:N	2.34	0.43
1:B:4638:ASN:HB3	1:B:4666:ILE:HD11	2.00	0.43
1:A:4335:ARG:HG2	1:A:4360:LEU:HG	2.01	0.43
1:A:2362:GLU:C	1:A:2364:VAL:H	2.22	0.43
1:B:4075:THR:HG23	1:B:4076:ILE:N	2.34	0.43
1:A:4659:ILE:HD12	1:A:4659:ILE:N	2.34	0.43
1:A:1963:ALA:HA	1:A:2096:ARG:HH11	1.83	0.42
1:B:3722:ASP:HA	1:B:3724:GLU:OE1	2.19	0.42
1:A:4024:ARG:HA	1:A:4030:PHE:O	2.19	0.42
1:A:1967:ARG:NH1	1:A:2053:ASN:HA	2.34	0.42
1:A:3716:CYS:H	1:A:3760:PHE:HB2	1.84	0.42
1:B:2849:LEU:CD1	1:B:2901:LEU:HD11	2.49	0.42
1:B:3723:VAL:HG23	1:B:3764:LEU:HD22	2.01	0.42
1:B:2368:ASN:O	1:B:2410:ARG:NH1	2.52	0.42
1:B:2196:LEU:HD11	1:B:2223:PHE:CD2	2.54	0.42
1:A:4354:ARG:HD3	1:A:4717:TYR:CD2	2.53	0.42
1:B:2271:GLY:HA2	1:B:2393:VAL:O	2.19	0.42
1:A:3782:THR:HG23	1:A:3782:THR:O	2.18	0.42
1:A:2560:MET:CG	1:A:2565:GLN:HB2	2.49	0.42
1:B:2423:THR:HA	1:B:2426:ILE:HD13	2.00	0.42
1:A:4678:ILE:O	1:A:4678:ILE:HG22	2.19	0.42
1:B:3234:ILE:HG23	1:B:3617:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3598:PHE:CD2	1:B:3634:VAL:HG11	2.55	0.42
1:B:3676:ASP:CB	1:B:3681:ALA:HB3	2.49	0.42
1:B:3647:TRP:HB3	1:B:3652:LEU:CD2	2.49	0.42
1:A:1554:LEU:HD22	1:A:1609:GLN:HG3	2.00	0.42
1:B:2109:ALA:HA	1:B:2156:LEU:CD1	2.49	0.42
1:A:3992:LEU:CD1	1:A:4434:GLN:HG3	2.48	0.42
1:A:4358:SER:O	1:A:4362:GLN:HB2	2.19	0.42
1:A:2425:MET:HE2	1:A:2425:MET:HB3	1.81	0.42
1:B:2886:LEU:HD23	1:B:2904:LEU:HD22	2.01	0.42
1:A:1907:LEU:HD22	1:A:1911:ARG:CZ	2.49	0.42
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.18	0.42
1:B:4673:ASP:OD1	1:B:4674:LYS:N	2.52	0.42
1:B:2991:PHE:CE1	1:B:2993:GLU:HB2	2.54	0.42
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	2.02	0.42
1:A:3718:LEU:HG	1:A:3719:LEU:N	2.21	0.42
1:B:2129:VAL:N	1:B:2130:PRO:CD	2.82	0.42
1:A:3067:GLU:HG2	1:A:3068:LYS:N	2.34	0.42
1:A:2870:ALA:C	1:A:2872:TYR:H	2.21	0.42
1:B:3030:ALA:HB3	1:B:3037:ILE:HD11	2.00	0.42
1:B:3698:SER:HB3	1:B:3700:LEU:HD12	2.00	0.42
1:A:2832:ASN:CG	1:A:2849:LEU:HD23	2.39	0.42
1:A:3156:ASN:C	1:A:3158:SER:H	2.21	0.42
1:B:3078:VAL:O	1:B:3078:VAL:HG22	2.18	0.42
1:A:2525:ILE:HD12	1:A:2526:MET:N	2.33	0.42
1:B:2669:PRO:HA	1:B:2788:PHE:O	2.19	0.42
1:A:3096:VAL:HB	1:A:3099:LEU:HD22	2.01	0.42
1:B:1960:LEU:HD13	1:B:2074:PHE:CE1	2.54	0.42
1:A:1816:LEU:HD23	1:A:1878:LEU:CD1	2.49	0.42
1:B:3962:ASP:C	1:B:3964:LYS:H	2.23	0.42
1:B:1505:SER:O	1:B:1506:ASP:C	2.57	0.42
1:B:2017:CYS:SG	1:B:2046:ILE:HD13	2.59	0.42
1:A:4000:SER:O	1:B:2940:SER:HB3	2.19	0.42
1:A:4109:ASP:CA	1:A:4112:ASN:HD22	2.11	0.42
1:A:3018:SER:O	1:A:3257:PRO:HD2	2.18	0.42
1:A:1639:ILE:HG12	1:A:1675:LEU:HD23	2.01	0.42
1:A:2142:GLN:HB2	1:A:2145:TYR:CD1	2.54	0.42
1:A:2266:LEU:HD21	1:A:2394:MET:CE	2.49	0.42
1:B:1811:PRO:HB2	1:B:1814:LEU:CD1	2.49	0.42
1:B:2125:ALA:C	1:B:2127:LYS:H	2.21	0.42
1:A:3700:LEU:CD1	1:A:3701:ASP:N	2.80	0.42
1:A:4134:LEU:HD23	1:A:4236:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1752:VAL:CG2	1:A:1811:PRO:HG3	2.48	0.42
1:A:3993:LYS:O	1:A:3995:GLY:N	2.53	0.42
1:A:2615:TYR:N	1:A:2615:TYR:CD2	2.87	0.42
1:A:4289:PRO:HA	1:A:4292:TRP:O	2.20	0.42
1:B:2272:VAL:HG12	1:B:2273:MET:N	2.34	0.42
1:A:1973:PHE:HD1	1:A:1973:PHE:O	2.02	0.42
1:A:1732:LEU:HD13	1:A:1741:ILE:HD12	2.01	0.42
1:A:2819:PRO:HB2	1:A:2824:LEU:CD2	2.50	0.42
1:B:3057:MET:O	1:B:3061:ARG:HG3	2.19	0.42
1:A:1816:LEU:O	1:A:1820:GLN:HG3	2.19	0.42
1:B:3181:LEU:HB2	1:B:3232:VAL:HG13	2.01	0.42
1:B:2591:GLU:HA	1:B:2613:LEU:HD12	2.01	0.42
1:B:3960:LEU:CD2	1:B:4237:SER:HB2	2.50	0.42
1:A:3209:ALA:CB	1:A:3221:PRO:HG3	2.49	0.42
1:B:3039:THR:HG22	1:B:3072:ILE:HB	2.01	0.42
1:A:4168:PHE:O	1:A:4172:GLU:HG3	2.19	0.42
1:A:3262:ASP:OD2	1:A:3670:ARG:NE	2.52	0.42
1:B:2528:PHE:HE1	1:B:2533:VAL:HG11	1.85	0.42
1:A:2408:ILE:O	1:A:2411:CYS:HB2	2.20	0.42
1:A:2502:ILE:CG2	1:A:2573:LEU:HD12	2.48	0.42
1:B:3598:PHE:O	1:B:3602:ILE:HB	2.20	0.42
1:A:2587:LEU:CG	1:A:2817:ASP:HB2	2.45	0.42
1:A:3192:LEU:HD11	1:A:3271:ILE:HG22	2.01	0.42
1:A:2051:LYS:C	1:A:2051:LYS:HD3	2.39	0.42
1:A:1967:ARG:CB	1:A:2051:LYS:HA	2.50	0.42
1:B:3084:LEU:O	1:B:3087:MET:N	2.52	0.42
1:A:4373:PHE:CD1	1:A:4374:PRO:HD2	2.54	0.42
1:B:2706:THR:HA	1:B:2759:VAL:HG22	2.01	0.42
1:A:2905:TRP:HZ3	1:A:2934:ALA:HB2	1.83	0.42
1:A:3536:TYR:O	1:A:3540:ILE:HD13	2.20	0.42
1:B:2112:MET:SD	1:B:2153:LYS:HG2	2.59	0.42
1:A:2534:LEU:HB3	1:A:2538:PHE:CE2	2.55	0.42
1:A:1708:ILE:HD11	1:A:1721:HIS:HB3	2.01	0.42
1:A:2415:TRP:HA	1:A:2415:TRP:HE3	1.83	0.42
1:A:1766:ILE:HG23	1:A:1767:HIS:N	2.35	0.42
1:A:2910:LEU:HB3	1:A:2911:ARG:HH12	1.85	0.42
1:A:2370:LEU:HD23	1:A:2370:LEU:O	2.19	0.42
1:B:1598:VAL:HG22	1:B:1660:LEU:HD22	2.01	0.42
1:A:3061:ARG:O	1:A:3067:GLU:HB3	2.18	0.42
1:A:2106:GLU:CD	1:A:2106:GLU:N	2.69	0.42
1:A:4128:SER:CB	1:A:4213:PHE:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3043:ASN:ND2	1:B:3043:ASN:N	2.68	0.42
1:B:1914:TYR:CZ	1:B:1924:LYS:HB3	2.54	0.42
1:B:3160:THR:C	1:B:3162:PRO:HD3	2.40	0.42
1:B:2230:PRO:HB3	1:B:2237:ARG:HH22	1.84	0.42
1:A:1777:MET:HE3	1:A:1939:GLU:HA	2.02	0.42
1:B:2610:ILE:HD12	1:B:2615:TYR:OH	2.20	0.42
1:A:3108:LEU:HD11	1:A:3133:PHE:CZ	2.54	0.42
1:A:1979:GLY:O	1:A:1980:LYS:C	2.58	0.42
1:A:3009:GLN:HG2	1:A:3138:ARG:O	2.20	0.42
1:A:4178:ALA:HA	1:A:4183:THR:OG1	2.20	0.42
1:A:3915:ALA:O	1:A:3918:ASP:HB2	2.19	0.42
1:A:3954:ARG:HD3	1:A:3954:ARG:O	2.19	0.42
1:B:2327:TRP:CH2	1:B:2380:PRO:HD2	2.55	0.42
1:A:2269:ASN:O	1:A:2271:GLY:N	2.53	0.42
1:A:2701:PHE:HB2	1:A:2745:GLU:O	2.20	0.42
1:A:2573:LEU:C	1:A:2573:LEU:HD23	2.40	0.42
1:A:3457:LEU:HD12	1:A:3486:TYR:CE1	2.55	0.42
1:B:3990:PHE:CD2	1:B:4084:LEU:HD22	2.55	0.42
1:A:2126:GLY:O	1:A:2130:PRO:HG2	2.19	0.42
1:B:2290:LEU:HD22	1:B:2352:TRP:CZ3	2.55	0.42
1:B:2773:TRP:CH2	1:B:2780:TRP:HB2	2.54	0.42
1:B:3061:ARG:O	1:B:3067:GLU:HB3	2.19	0.42
1:A:2270:HIS:HB2	1:A:2392:ARG:HD2	2.02	0.42
1:A:2426:ILE:CD1	1:A:2530:ARG:HD3	2.50	0.42
1:B:2588:VAL:HG23	1:B:2589:GLU:N	2.34	0.42
1:A:3602:ILE:HG22	1:A:3603:GLY:N	2.34	0.42
1:B:2528:PHE:CE1	1:B:2533:VAL:HG11	2.54	0.42
1:A:2561:SER:HA	1:A:2562:PRO:HD3	1.95	0.42
1:A:1952:LEU:HD22	1:A:2103:PRO:HA	2.01	0.42
1:B:3259:HIS:NE2	1:B:3779:SER:HA	2.34	0.42
1:A:2057:VAL:HB	1:A:2067:LEU:HD13	2.01	0.42
1:A:2849:LEU:HA	1:A:2938:PHE:HZ	1.85	0.42
1:B:2825:THR:CG2	1:B:2854:VAL:HG21	2.50	0.42
1:B:2084:ARG:CZ	1:B:4295:PHE:CD2	3.03	0.42
1:B:1608:VAL:HG13	1:B:1676:LEU:CD1	2.50	0.42
1:A:4313:TRP:CD1	1:A:4334:VAL:HG22	2.55	0.42
1:B:1907:LEU:HD22	1:B:1911:ARG:NH2	2.34	0.42
1:B:2513:HIS:O	1:B:2517:GLU:HG3	2.19	0.42
1:B:4280:ILE:HG23	1:B:4408:LEU:HA	2.01	0.42
1:B:4284:ARG:CG	1:B:4408:LEU:HB3	2.49	0.42
1:B:4036:HIS:CD2	1:B:4044:TRP:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1791:HIS:HD2	1:A:1806:TRP:HD1	1.66	0.42
1:A:3268:VAL:HG13	1:A:3269:LEU:N	2.35	0.42
1:A:2842:LEU:HD11	1:A:2897:THR:C	2.40	0.42
1:A:3449:ARG:NH1	1:A:3449:ARG:HB3	2.35	0.42
1:A:2585:MET:O	1:A:2815:LEU:HD13	2.19	0.42
1:B:3256:THR:CG2	1:B:3779:SER:HB3	2.50	0.42
1:B:2540:LEU:HB3	1:B:2576:SER:CB	2.49	0.42
1:A:3224:ARG:HB2	1:A:3224:ARG:HE	1.73	0.42
1:A:3075:GLU:C	1:A:3077:ASN:H	2.23	0.42
1:A:2989:VAL:HG13	1:A:3187:GLU:OE2	2.20	0.42
1:B:3976:VAL:O	1:B:3979:THR:HG23	2.20	0.42
1:A:2009:MET:HE3	1:A:2012:ILE:HB	2.02	0.42
1:B:2989:VAL:HG21	1:B:3184:VAL:HA	2.02	0.42
1:B:3039:THR:CG2	1:B:3072:ILE:HB	2.50	0.42
1:B:2856:PHE:HE2	1:B:2913:PHE:CD2	2.37	0.42
1:A:2071:MET:HG3	1:A:2071:MET:O	2.20	0.42
1:A:1792:PHE:CD2	1:A:1792:PHE:C	2.92	0.42
1:B:3235:HIS:CE1	1:B:3260:TYR:HB2	2.55	0.42
1:A:4575:LEU:H	1:A:4575:LEU:CD1	2.26	0.42
1:A:1746:SER:HB3	1:A:1940:TYR:CZ	2.55	0.42
1:A:3148:ASN:HA	1:A:3149:PRO:HD3	1.93	0.42
1:A:4418:LEU:HD11	1:A:4422:LYS:HZ3	1.84	0.42
1:B:4434:GLN:HG2	1:B:4434:GLN:O	2.19	0.42
1:B:1615:LEU:HD13	1:B:1618:ILE:HD12	2.01	0.42
1:B:3017:VAL:HG11	1:B:3175:GLU:HA	2.01	0.42
1:A:1973:PHE:HE1	1:A:2099:ALA:CA	2.33	0.42
1:A:4065:ALA:O	1:A:4069:LEU:HB2	2.20	0.42
1:A:1818:THR:O	1:A:1822:VAL:HG23	2.20	0.42
1:A:4070:SER:C	1:A:4072:GLN:N	2.72	0.42
1:B:4070:SER:O	1:B:4072:GLN:N	2.53	0.42
1:B:1952:LEU:HA	1:B:1955:ARG:NH2	2.35	0.42
1:A:3315:VAL:O	1:A:3319:GLN:HB2	2.19	0.42
1:A:2833:ARG:HA	1:A:2846:ALA:HB1	2.02	0.42
1:A:1556:ARG:HG2	1:A:1557:GLY:N	2.35	0.42
1:A:1929:MET:O	1:A:1930:ALA:HB3	2.20	0.42
1:B:2684:LEU:HD13	1:B:2684:LEU:C	2.40	0.42
1:A:2140:SER:HB2	1:A:2142:GLN:NE2	2.23	0.41
1:A:2204:ILE:HG13	1:A:2205:PRO:CD	2.50	0.41
1:B:4191:HIS:CD2	1:B:4220:GLU:HG2	2.54	0.41
1:A:2898:LEU:HD11	1:A:2941:VAL:HG22	2.01	0.41
1:B:2292:ALA:O	1:B:2296:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2370:LEU:HD12	1:B:2377:LEU:HB2	2.02	0.41
1:B:2272:VAL:O	1:B:2394:MET:HA	2.20	0.41
1:B:3923:LEU:HD22	1:B:3947:ILE:CG2	2.47	0.41
1:B:1565:LEU:HD23	1:B:1595:LEU:HD12	2.00	0.41
1:B:2579:TRP:HZ2	1:B:2655:ARG:HD2	1.84	0.41
1:A:3889:MET:SD	1:A:3889:MET:C	2.99	0.41
1:A:4370:ASN:N	1:A:4370:ASN:HD22	2.16	0.41
1:A:3256:THR:HB	1:A:3257:PRO:HD2	2.01	0.41
1:A:2258:LYS:HA	1:A:2261:GLN:CG	2.44	0.41
1:A:3808:ASP:CG	1:A:3809:THR:N	2.73	0.41
1:B:1785:LEU:HB2	1:B:1814:LEU:HD23	2.00	0.41
1:A:2370:LEU:HA	1:A:2375:LYS:HA	2.02	0.41
1:A:1831:LEU:HA	1:A:1841:ILE:HG12	2.02	0.41
1:A:2745:GLU:CB	1:A:2748:LEU:HD12	2.50	0.41
1:A:2783:LEU:HD22	1:A:2786:ILE:HB	2.01	0.41
1:A:4337:ILE:O	1:A:4341:THR:CG2	2.68	0.41
1:A:4623:ALA:HB2	1:A:4703:ILE:CD1	2.48	0.41
1:B:3700:LEU:CD1	1:B:3701:ASP:H	2.30	0.41
1:A:3990:PHE:O	1:A:3994:GLY:HA2	2.20	0.41
1:B:4277:PHE:HZ	1:B:4356:LEU:HD21	1.84	0.41
1:A:1973:PHE:HD1	1:A:1973:PHE:C	2.23	0.41
1:B:1960:LEU:HD13	1:B:2074:PHE:HE1	1.85	0.41
1:A:4684:SER:O	1:A:4707:TYR:HE2	2.02	0.41
1:B:3877:GLN:O	1:B:3881:GLU:HB2	2.20	0.41
1:B:3573:ARG:HH11	1:B:3573:ARG:HG2	1.84	0.41
1:A:2893:MET:O	1:A:2895:GLY:N	2.46	0.41
1:B:2578:MET:O	1:B:2582:GLY:HA3	2.19	0.41
1:A:1959:THR:O	1:A:1963:ALA:CB	2.69	0.41
1:A:3443:MET:HE3	1:A:3449:ARG:HA	2.02	0.41
1:A:3148:ASN:OD1	1:A:3150:ALA:N	2.45	0.41
1:B:2231:ILE:CG2	1:B:2264:GLN:HE22	2.31	0.41
1:A:3994:GLY:O	1:A:3995:GLY:C	2.58	0.41
1:B:3563:LEU:CD1	1:B:3845:ILE:HD11	2.49	0.41
1:A:4278:HIS:O	1:A:4282:GLN:HB2	2.20	0.41
1:B:2208:VAL:HG12	1:B:2415:TRP:NE1	2.36	0.41
1:A:1719:GLN:HA	1:A:1722:PHE:CE2	2.56	0.41
1:B:3910:GLN:HB3	1:B:4231:ARG:HD3	2.03	0.41
1:B:2670:LEU:HD12	1:B:2670:LEU:O	2.20	0.41
1:A:1625:ILE:HG23	1:A:1626:ASN:N	2.33	0.41
1:B:1872:ARG:NH2	1:B:2164:ARG:NE	2.68	0.41
1:B:3566:ASN:HD21	1:B:3859:LYS:HZ2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3960:LEU:HB3	1:B:4239:GLU:OE2	2.21	0.41
1:B:4284:ARG:HG2	1:B:4408:LEU:HB3	2.02	0.41
1:A:3206:ILE:HA	1:A:3221:PRO:HG2	2.03	0.41
1:B:4201:GLU:HG3	1:B:4228:ASN:HB2	2.03	0.41
1:B:1590:HIS:NE2	1:B:1594:ARG:NH1	2.68	0.41
1:B:3886:TYR:CE2	1:B:3940:LEU:HD23	2.56	0.41
1:A:4270:ILE:HG22	1:A:4310:ILE:HD13	2.01	0.41
1:A:4314:VAL:O	1:A:4314:VAL:CG1	2.68	0.41
1:A:4648:VAL:CG1	1:A:4662:THR:HG21	2.41	0.41
1:A:3652:LEU:HD21	1:A:3662:ALA:HB2	2.02	0.41
1:A:4349:ASN:ND2	1:A:4352:ASP:N	2.65	0.41
1:A:2749:PRO:HG2	1:A:2759:VAL:HG11	2.01	0.41
1:A:2774:ARG:HH21	1:A:2779:THR:HB	1.85	0.41
1:A:2586:GLY:CA	1:A:2815:LEU:HD13	2.43	0.41
1:B:3602:ILE:O	1:B:3603:GLY:C	2.59	0.41
1:A:2127:LYS:O	1:A:2130:PRO:HD2	2.20	0.41
1:A:3164:LEU:HA	1:A:3164:LEU:HD12	1.81	0.41
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	2.01	0.41
1:A:3553:VAL:O	1:A:3557:VAL:HG23	2.21	0.41
1:A:1697:PHE:CD2	1:A:1705:LEU:HD11	2.55	0.41
1:A:4692:LEU:HD12	1:A:4700:LEU:HD21	2.02	0.41
1:A:2612:LEU:HD12	1:A:2612:LEU:O	2.21	0.41
1:A:4012:LEU:H	1:A:4012:LEU:HD12	1.84	0.41
1:A:3819:ILE:C	1:A:3821:GLY:H	2.23	0.41
1:B:2036:LEU:O	1:B:2036:LEU:HD23	2.20	0.41
1:B:4068:GLN:C	1:B:4070:SER:H	2.24	0.41
1:A:1701:GLY:HA2	1:A:2011:ARG:CZ	2.50	0.41
1:B:2556:SER:C	1:B:2558:PHE:N	2.73	0.41
1:A:2376:LEU:HD12	1:A:2386:ALA:N	2.35	0.41
1:A:2868:ILE:HG21	1:A:2922:GLU:OE2	2.21	0.41
1:B:4371:PRO:O	1:B:4372:ASP:HB2	2.20	0.41
1:A:4283:GLU:OE2	1:A:4286:ARG:NH1	2.54	0.41
1:A:2204:ILE:CA	1:A:2207:LEU:HD12	2.44	0.41
1:B:3606:ASP:O	1:B:3610:ARG:HG3	2.21	0.41
1:B:4006:PRO:C	1:B:4008:LEU:H	2.24	0.41
1:A:2832:ASN:HA	1:A:2835:LEU:HB3	2.01	0.41
1:A:2222:VAL:C	1:A:2224:PRO:HD3	2.40	0.41
1:A:2606:PRO:HG2	1:A:2615:TYR:CD1	2.56	0.41
1:A:1782:ALA:HA	1:A:1938:PHE:CZ	2.55	0.41
1:A:4401:GLU:HB2	1:A:4402:ILE:HD12	2.01	0.41
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1817:LEU:HD11	1:B:1936:TYR:CD2	2.55	0.41
1:A:4012:LEU:HD21	1:A:4020:LEU:HD22	2.02	0.41
1:B:1493:ILE:O	1:B:1497:LEU:HG	2.21	0.41
1:A:2376:LEU:HD21	1:A:2384:ARG:HB3	2.02	0.41
1:B:2223:PHE:C	1:B:2225:GLY:H	2.23	0.41
1:B:4553:TYR:O	1:B:4555:VAL:HG22	2.20	0.41
1:A:2275:VAL:HG23	1:A:2397:VAL:HG23	2.03	0.41
1:A:1766:ILE:HG23	1:A:1767:HIS:H	1.84	0.41
1:A:2748:LEU:CD2	1:A:2800:ARG:HD3	2.51	0.41
1:B:4184:TRP:NE1	1:B:4214:ARG:HB2	2.35	0.41
1:A:4537:LEU:CD2	1:A:4548:LYS:HE3	2.50	0.41
1:B:3087:MET:HE2	1:B:3090:LEU:HD23	2.03	0.41
1:A:4278:HIS:HD2	1:A:4343:TYR:CE1	2.39	0.41
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.67	0.41
1:B:2711:LEU:HD12	1:B:2711:LEU:HA	1.89	0.41
1:A:4670:THR:HG22	1:A:4671:TRP:N	2.36	0.41
1:A:4006:PRO:O	1:A:4008:LEU:N	2.52	0.41
1:A:3439:ASP:OD2	1:A:3442:LYS:HE2	2.21	0.41
1:A:3571:ARG:HB3	1:A:3571:ARG:NH1	2.35	0.41
1:B:2670:LEU:C	1:B:2670:LEU:HD12	2.41	0.41
1:B:1910:MET:CB	1:B:1929:MET:HG3	2.50	0.41
1:A:4240:ASN:HA	1:A:4241:PRO:HD2	1.89	0.41
1:A:2694:PHE:CD2	1:A:2738:TRP:HB2	2.56	0.41
1:A:4001:ILE:HB	1:A:4018:LYS:HD3	2.02	0.41
1:A:1888:VAL:HG22	1:A:1909:HIS:CE1	2.56	0.41
1:A:2579:TRP:HZ2	1:A:2655:ARG:HD2	1.85	0.41
1:A:4535:ARG:HG2	1:A:4535:ARG:HH11	1.84	0.41
1:B:4535:ARG:HG2	1:B:4535:ARG:NH1	2.34	0.41
1:B:4023:LEU:HG	1:B:4030:PHE:CD1	2.56	0.41
1:A:2057:VAL:HG13	1:A:2059:LEU:H	1.86	0.41
1:B:2278:SER:H	1:B:2398:GLN:NE2	2.17	0.41
1:B:2400:LEU:HD13	1:B:2408:ILE:CD1	2.48	0.41
1:A:2615:TYR:HD2	1:A:2615:TYR:N	2.18	0.41
1:B:2363:TRP:C	1:B:2365:GLU:H	2.24	0.41
1:B:2853:MET:HA	1:B:2882:TRP:CZ3	2.56	0.41
1:B:1483:ILE:HG22	1:B:1517:VAL:HG22	2.02	0.41
1:B:4644:LEU:HD23	1:B:4723:ILE:HG12	2.02	0.41
1:B:1497:LEU:HB3	1:B:1501:SER:CB	2.51	0.41
1:B:4509:LEU:HD23	1:B:4568:PHE:CE1	2.55	0.41
1:B:3903:LEU:O	1:B:3909:TYR:HB2	2.21	0.41
1:B:2239:LYS:O	1:B:2243:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1500:GLY:O	1:B:1504:ASP:N	2.50	0.41
1:A:2855:GLU:OE2	1:A:2933:VAL:HG22	2.21	0.41
1:A:2696:VAL:HG22	1:A:2697:VAL:N	2.36	0.41
1:B:3567:LEU:HD23	1:B:3567:LEU:HA	1.94	0.41
1:B:3781:VAL:HG12	1:B:3782:THR:N	2.34	0.41
1:B:3930:LEU:O	1:B:3932:ASP:N	2.54	0.41
1:A:2269:ASN:C	1:A:2271:GLY:H	2.24	0.41
1:A:3652:LEU:HB2	1:A:3684:PHE:CD1	2.55	0.41
1:B:3258:ARG:HD2	1:B:3779:SER:HB2	2.01	0.41
1:A:2000:CYS:O	1:A:2001:ASP:C	2.58	0.41
1:A:2028:PHE:CB	1:A:2075:VAL:HG13	2.44	0.41
1:A:3567:LEU:HD23	1:A:3567:LEU:HA	1.91	0.41
1:A:4426:MET:O	1:A:4430:LEU:HG	2.21	0.41
1:A:4033:LEU:HD13	1:A:4062:TRP:CZ2	2.55	0.41
1:A:2579:TRP:CE3	1:A:2659:VAL:HG21	2.56	0.41
1:A:2890:ILE:HD13	1:A:2893:MET:CE	2.51	0.41
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.43	0.41
1:A:1712:SER:HB3	1:A:1766:ILE:HB	2.03	0.41
1:B:2381:ASN:HD22	1:B:2381:ASN:C	2.25	0.41
1:A:3597:ALA:O	1:A:3601:TYR:HD1	2.04	0.41
1:B:2887:LEU:O	1:B:2891:GLN:HG3	2.21	0.41
1:A:1886:ARG:HG3	1:A:1887:ASP:H	1.81	0.41
1:B:4157:TYR:HB2	1:B:4184:TRP:CB	2.50	0.41
1:A:4024:ARG:CG	1:A:4031:SER:HA	2.49	0.41
1:B:4145:LYS:HE2	1:B:4238:TYR:CE1	2.55	0.41
1:B:3571:ARG:O	1:B:3575:GLU:HG3	2.19	0.41
1:A:2848:ASN:HB3	1:A:2938:PHE:CE1	2.55	0.41
1:B:1739:THR:O	1:B:1760:ILE:N	2.54	0.41
1:B:3647:TRP:HB3	1:B:3652:LEU:HD22	2.02	0.41
1:A:3844:ASN:O	1:A:3848:ASP:HB2	2.20	0.41
1:B:4094:VAL:HB	1:B:4423:ALA:HB1	2.02	0.41
1:B:2084:ARG:HG2	1:B:2084:ARG:NH1	2.36	0.41
1:A:2088:PRO:C	1:A:2090:ASN:N	2.75	0.41
1:A:3078:VAL:HG23	1:A:3083:PHE:HB2	2.02	0.41
1:B:4503:ILE:HD11	1:B:4575:LEU:O	2.21	0.41
1:B:4277:PHE:HB2	1:B:4363:LEU:HD12	2.03	0.41
1:B:2420:ILE:HG13	1:B:2421:LEU:N	2.36	0.41
1:B:2270:HIS:CA	1:B:2392:ARG:HH11	2.33	0.41
1:B:1831:LEU:HB3	1:B:1900:GLY:HA2	2.02	0.41
1:B:4509:LEU:O	1:B:4513:ILE:HG13	2.20	0.41
1:B:4306:ALA:HA	1:B:4338:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1726:PHE:CD2	1:A:1729:LEU:HD22	2.55	0.41
1:B:4022:CYS:HB3	1:B:4026:GLN:NE2	2.36	0.41
1:B:2236:LEU:O	1:B:2240:ILE:HG13	2.21	0.41
1:A:4592:GLY:CA	1:A:4725:SER:HB2	2.50	0.41
1:B:2151:ALA:O	1:B:2154:SER:N	2.52	0.41
1:A:4060:GLU:O	1:A:4064:VAL:HG23	2.21	0.41
1:B:1844:GLN:O	1:B:1847:SER:HB2	2.21	0.41
1:B:4056:PRO:HD2	1:B:4093:ARG:NH2	2.36	0.41
1:B:4162:ILE:HG22	1:B:4163:GLY:N	2.35	0.41
1:B:3228:VAL:HA	1:B:3231:LEU:HD12	2.03	0.41
1:B:2029:ASN:N	1:B:2029:ASN:HD22	2.18	0.41
1:B:2492:LEU:O	1:B:2493:LYS:C	2.59	0.41
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.36	0.41
1:B:4141:ASP:OD2	1:B:4143:SER:HB2	2.21	0.41
1:A:3093:GLY:O	1:A:3095:GLU:N	2.54	0.41
1:A:3230:SER:HA	1:A:3620:ARG:HE	1.86	0.41
1:B:1734:LEU:HA	1:B:1742:ILE:HG12	2.03	0.41
1:B:3539:LEU:HA	1:B:3539:LEU:HD12	1.92	0.41
1:B:4649:TRP:HA	1:B:4649:TRP:CE3	2.55	0.41
1:A:3606:ASP:O	1:A:3610:ARG:HG3	2.21	0.41
1:A:2359:VAL:HG23	1:A:2397:VAL:HG11	2.03	0.41
1:A:3698:SER:C	1:A:3700:LEU:HD12	2.41	0.41
1:A:4122:VAL:HB	1:A:4132:LEU:CD2	2.51	0.41
1:B:2260:LEU:O	1:B:2263:HIS:HB3	2.21	0.41
1:B:3017:VAL:HG13	1:B:3174:GLY:C	2.41	0.41
1:B:3015:ILE:O	1:B:3173:PHE:N	2.51	0.41
1:B:1947:LEU:HD21	1:B:1982:GLU:CG	2.51	0.41
1:B:4711:THR:OG1	1:B:4716:TRP:NE1	2.54	0.41
1:B:1909:HIS:O	1:B:1911:ARG:HD3	2.22	0.41
1:A:1939:GLU:O	1:A:1941:LEU:HG	2.21	0.41
1:A:4606:GLN:HA	1:A:4609:SER:OG	2.21	0.41
1:A:4063:ILE:HD13	1:A:4082:LYS:NZ	2.36	0.41
1:A:2332:PHE:HA	1:A:2335:THR:OG1	2.20	0.41
1:B:3685:LEU:O	1:B:3689:TYR:HB2	2.20	0.41
1:A:2269:ASN:C	1:A:2271:GLY:N	2.74	0.40
1:A:4647:ALA:HA	1:A:4657:THR:HG22	2.02	0.40
1:A:3720:VAL:HG21	1:A:3762:ILE:HD11	2.03	0.40
1:A:3237:THR:OG1	1:A:3238:ILE:HD12	2.21	0.40
1:A:4090:HIS:C	1:A:4092:ASP:H	2.24	0.40
1:A:4086:MET:HG2	1:A:4093:ARG:HB2	1.99	0.40
1:B:3234:ILE:O	1:B:3238:ILE:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2754:TYR:O	1:B:2756:THR:HG22	2.21	0.40
1:B:2120:THR:HB	1:B:2124:LEU:HG	2.03	0.40
1:B:3046:TYR:CZ	1:B:3050:ASP:HB2	2.55	0.40
1:A:2439:PHE:HZ	1:A:2542:ASN:OD1	2.03	0.40
1:B:4499:PHE:HA	1:B:4502:GLU:HB2	2.03	0.40
1:B:3976:VAL:HG13	1:B:4105:VAL:HG11	2.01	0.40
1:A:3025:LEU:HD23	1:A:3025:LEU:HA	1.86	0.40
1:A:3022:LYS:HB2	1:A:3022:LYS:NZ	2.36	0.40
1:A:3199:TYR:OH	1:A:3226:ALA:HB2	2.21	0.40
1:A:1633:SER:O	1:A:1637:LYS:HG2	2.21	0.40
1:A:2877:ARG:HD2	1:A:2881:ARG:NH2	2.36	0.40
1:A:2935:LEU:C	1:A:2935:LEU:HD23	2.41	0.40
1:B:1928:HIS:CG	1:B:1933:THR:HG22	2.52	0.40
1:A:2212:ILE:O	1:A:2215:ILE:HG22	2.22	0.40
1:A:3698:SER:O	1:A:3704:PHE:HB2	2.22	0.40
1:B:4264:PRO:HA	1:B:4322:SER:O	2.21	0.40
1:B:3218:ALA:O	1:B:3219:ILE:C	2.60	0.40
1:A:2005:ASP:OD1	1:A:2006:LEU:N	2.55	0.40
1:B:1546:VAL:HG12	1:B:1547:ASN:N	2.36	0.40
1:B:2081:TYR:O	1:B:2082:ALA:HB3	2.21	0.40
1:B:1820:GLN:NE2	1:B:1990:GLN:NE2	2.66	0.40
1:A:4117:ASP:C	1:A:4119:ALA:H	2.25	0.40
1:B:4083:ILE:HD11	1:B:4098:SER:HA	2.03	0.40
1:A:3225:ASP:O	1:A:3229:SER:CB	2.69	0.40
1:A:3997:ASN:O	1:A:3998:LEU:C	2.60	0.40
1:A:3727:ASP:C	1:A:3729:VAL:H	2.25	0.40
1:B:4493:ASP:OD1	1:B:4494:PRO:HD2	2.21	0.40
1:A:4245:LYS:HE2	1:A:4249:LEU:HD11	2.03	0.40
1:A:3256:THR:HB	1:A:3257:PRO:CD	2.51	0.40
1:B:2379:LEU:HD12	1:B:2383:GLU:HG2	2.03	0.40
1:B:4402:ILE:N	1:B:4402:ILE:CD1	2.81	0.40
1:B:3966:THR:HG23	1:B:4426:MET:HE3	2.02	0.40
1:A:2793:ASN:HB3	1:A:2794:PRO:HD2	2.04	0.40
1:B:3700:LEU:CD1	1:B:3701:ASP:N	2.80	0.40
1:B:3256:THR:N	1:B:3259:HIS:HD2	2.19	0.40
1:B:4703:ILE:CD1	1:B:4705:LEU:HD21	2.45	0.40
1:A:4418:LEU:HD11	1:A:4422:LYS:NZ	2.36	0.40
1:B:4428:ASN:O	1:B:4432:LYS:HG3	2.21	0.40
1:A:2995:LEU:CD2	1:A:2998:ILE:HD11	2.48	0.40
1:B:1696:ARG:HH21	1:B:1726:PHE:HA	1.86	0.40
1:B:4403:SER:HB2	1:B:4407:TRP:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1726:PHE:CB	1:A:1729:LEU:HB3	2.51	0.40
1:A:4130:SER:HA	1:A:4131:PRO:HD3	1.88	0.40
1:A:2986:VAL:O	1:A:2988:LEU:HG	2.20	0.40
1:A:4189:ASN:HA	1:A:4191:HIS:CD2	2.57	0.40
1:A:1898:LEU:HA	1:A:1898:LEU:HD23	1.89	0.40
1:A:1853:GLN:HE22	1:A:1886:ARG:HH11	1.68	0.40
1:B:2258:LYS:HD3	1:B:2261:GLN:OE1	2.21	0.40
1:A:3947:ILE:HD13	1:A:3947:ILE:O	2.21	0.40
1:A:4247:ASN:HD21	1:A:4282:GLN:NE2	2.19	0.40
1:B:2135:CYS:O	1:B:2139:LEU:HB2	2.21	0.40
1:B:1867:LEU:HD12	1:B:1867:LEU:H	1.86	0.40
1:B:3002:ASP:HA	1:B:3029:VAL:HG11	2.04	0.40
1:A:2529:THR:O	1:A:2530:ARG:C	2.60	0.40
1:B:2029:ASN:HD22	1:B:2030:ARG:N	2.20	0.40
1:A:2536:SER:HB2	1:A:2580:GLY:O	2.21	0.40
1:B:2688:LEU:HD13	1:B:2696:VAL:HB	2.04	0.40
1:B:1928:HIS:NE2	1:B:1933:THR:CG2	2.81	0.40
1:B:3927:ASN:HB3	1:B:3930:LEU:HD12	2.02	0.40
1:B:1813:GLN:HE22	1:B:1941:LEU:H	1.69	0.40
1:B:2519:ALA:HB2	1:B:2593:PHE:CE1	2.57	0.40
1:A:4057:ILE:HA	1:A:4057:ILE:HD12	1.96	0.40
1:B:3271:ILE:HA	1:B:3592:VAL:HG21	2.03	0.40
1:A:2236:LEU:HD21	1:A:2293:ILE:CD1	2.44	0.40
1:A:1831:LEU:HD22	1:A:1898:LEU:HD13	2.04	0.40
1:B:2309:LYS:HG3	1:B:2358:ASP:HB2	2.02	0.40
1:A:3459:ASP:HA	1:A:3460:PRO:HD3	1.97	0.40
1:A:3296:GLU:HG3	1:A:3567:LEU:HD13	2.04	0.40
1:A:2591:GLU:OE1	1:A:2611:PRO:HG2	2.22	0.40
1:A:1778:LYS:HB3	1:A:1922:LEU:HD11	2.04	0.40
1:B:4432:LYS:C	1:B:4434:GLN:H	2.25	0.40
1:A:3066:GLU:HG2	1:A:3136:GLN:NE2	2.36	0.40
1:A:4284:ARG:CG	1:A:4408:LEU:HB3	2.49	0.40
1:B:2270:HIS:CB	1:B:2392:ARG:HH11	2.34	0.40
1:B:2745:GLU:HG2	1:B:2748:LEU:CD1	2.51	0.40
1:B:1906:TRP:CZ2	1:B:1911:ARG:HG2	2.57	0.40
1:B:2799:GLY:HA3	1:B:3159:ALA:HB1	2.04	0.40
1:A:2710:LEU:HD23	1:A:2762:PHE:CE2	2.57	0.40
1:A:3845:ILE:HG13	1:A:3845:ILE:H	1.57	0.40
1:B:2645:ASP:OD2	1:B:2645:ASP:N	2.54	0.40
1:A:2036:LEU:O	1:A:2036:LEU:HD12	2.21	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	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	3 34
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	8 51
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	4 42

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1836	LEU
1	A	2121	ALA
1	A	2409	SER
1	A	2560	MET
1	A	2617	VAL
1	A	2641	VAL
1	A	2646	VAL
1	A	2943	LEU
1	A	2992	ASN
1	A	3033	ASN
1	A	3219	ILE
1	A	3370	GLU
1	A	3371	PRO
1	A	3372	ALA
1	A	3603	GLY
1	A	4050	LYS
1	A	4051	ASP
1	A	4117	ASP
1	A	4121	ILE
1	A	4207	LEU
1	A	4548	LYS
1	A	4549	GLU
1	A	4660	LEU
1	B	1949	GLN
1	B	1975	PRO

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Mol	Chain	Res	Type
1	B	1980	LYS
1	B	2071	MET
1	B	3602	ILE
1	B	3931	VAL
1	B	4207	LEU
1	A	1714	ASP
1	A	1949	GLN
1	A	2004	PHE
1	A	2080	GLY
1	A	2101	ILE
1	A	2342	ASN
1	A	2527	ASP
1	A	2530	ARG
1	A	2628	LYS
1	A	2642	ALA
1	A	2645	ASP
1	A	2727	GLU
1	A	2776	SER
1	A	2789	VAL
1	A	2792	CYS
1	A	3218	ALA
1	A	3430	ASN
1	A	3440	THR
1	A	3488	SER
1	A	3715	GLY
1	A	3719	LEU
1	A	3841	ALA
1	A	3926	ASN
1	A	3994	GLY
1	A	3998	LEU
1	A	4000	SER
1	A	4014	THR
1	A	4053	VAL
1	A	4116	LEU
1	A	4123	GLU
1	A	4125	GLU
1	A	4158	LYS
1	A	4221	ILE
1	A	4342	ILE
1	A	4594	LEU
1	A	4666	ILE
1	A	4672	LYS

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Mol	Chain	Res	Type
1	A	4709	GLN
1	B	1919	GLU
1	B	2141	ALA
1	B	2230	PRO
1	B	2384	ARG
1	B	2600	ILE
1	B	2641	VAL
1	B	2755	GLY
1	B	2775	THR
1	B	3092	ALA
1	B	3603	GLY
1	B	3842	SER
1	B	3844	ASN
1	B	4113	THR
1	B	4221	ILE
1	B	4297	GLU
1	B	4340	SER
1	B	4464	ALA
1	B	4551	LYS
1	A	1663	GLU
1	A	1697	PHE
1	A	1703	GLU
1	A	1727	ALA
1	A	1923	HIS
1	A	2001	ASP
1	A	2089	ASP
1	A	2140	SER
1	A	2282	LYS
1	A	2329	ASP
1	A	2374	ASN
1	A	2705	THR
1	A	2871	HIS
1	A	2990	LEU
1	A	3082	SER
1	A	3671	TYR
1	A	3693	LYS
1	A	3843	GLY
1	A	3933	LYS
1	A	4007	GLN
1	A	4055	GLU
1	A	4118	MET
1	A	4131	PRO

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Mol	Chain	Res	Type
1	A	4163	GLY
1	A	4168	PHE
1	A	4318	SER
1	A	4401	GLU
1	A	4412	GLU
1	B	1663	GLU
1	B	2001	ASP
1	B	2527	ASP
1	B	2915	ASP
1	B	3080	GLU
1	B	3094	GLY
1	B	3248	ARG
1	B	3692	LYS
1	B	4071	ASN
1	B	4692	LEU
1	A	1799	ASP
1	A	1837	GLN
1	A	2002	GLU
1	A	2054	SER
1	A	2122	GLU
1	A	2177	ALA
1	A	2270	HIS
1	A	2370	LEU
1	A	2653	THR
1	A	2690	ALA
1	A	2744	ASP
1	A	2891	GLN
1	A	3094	GLY
1	A	3166	ASN
1	A	3444	MET
1	A	3699	PHE
1	A	3907	HIS
1	A	4026	GLN
1	A	4029	SER
1	A	4259	ARG
1	A	4519	ASN
1	B	1506	ASP
1	B	2165	LYS
1	B	2308	PRO
1	B	2401	LYS
1	B	2749	PRO
1	B	2947	LYS

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Mol	Chain	Res	Type
1	B	3932	ASP
1	B	4003	GLU
1	B	4051	ASP
1	B	4053	VAL
1	B	4189	ASN
1	B	4674	LYS
1	A	2363	TRP
1	A	2601	ALA
1	A	2987	PRO
1	A	3140	ASN
1	A	3142	HIS
1	A	3471	SER
1	A	3712	LEU
1	A	3999	THR
1	A	4011	LEU
1	A	4169	GLU
1	A	4579	SER
1	A	4691	TYR
1	A	4712	SER
1	B	1498	THR
1	B	2069	GLN
1	B	2140	SER
1	B	2210	ASP
1	B	2558	PHE
1	B	3693	LYS
1	B	3849	ASP
1	B	3963	ASP
1	B	4412	GLU
1	A	1868	SER
1	A	1944	GLY
1	A	2966	SER
1	A	3164	LEU
1	A	3716	CYS
1	A	3845	ILE
1	B	1582	LYS
1	B	1630	PRO
1	B	1727	ALA
1	B	4459	GLU
1	B	4621	LEU
1	A	3395	PRO
1	A	3806	ARG
1	A	3976	VAL

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Mol	Chain	Res	Type
1	B	4131	PRO
1	A	4056	PRO
1	B	3093	GLY
1	B	4556	PRO
1	A	2644	PRO
1	A	2755	GLY
1	A	3602	ILE
1	A	3677	PRO
1	B	1579	PRO
1	B	2380	PRO
1	A	2208	VAL
1	B	4094	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2457/3028 (81%)	2249 (92%)	208 (8%)	13	52
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	23	65
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	17	58

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1516	GLU
1	A	1559	ASP
1	A	1593	ASP
1	A	1594	ARG
1	A	1665	ILE
1	A	1699	PHE
1	A	1719	GLN
1	A	1744	MET
1	A	1753	THR
1	A	1756	LYS
1	A	1803	TYR

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Mol	Chain	Res	Type
1	A	1809	ASN
1	A	1844	GLN
1	A	1849	GLU
1	A	1865	GLN
1	A	1874	LYS
1	A	1882	LEU
1	A	1911	ARG
1	A	1922	LEU
1	A	1934	PHE
1	A	1962	GLN
1	A	1973	PHE
1	A	1978	THR
1	A	2006	LEU
1	A	2029	ASN
1	A	2051	LYS
1	A	2053	ASN
1	A	2069	GLN
1	A	2071	MET
1	A	2073	ILE
1	A	2090	ASN
1	A	2096	ARG
1	A	2105	ARG
1	A	2107	MET
1	A	2120	THR
1	A	2136	GLN
1	A	2142	GLN
1	A	2149	LEU
1	A	2152	LEU
1	A	2221	ASP
1	A	2234	ASP
1	A	2239	LYS
1	A	2274	MET
1	A	2297	ASP
1	A	2324	THR
1	A	2329	ASP
1	A	2346	GLU
1	A	2350	ARG
1	A	2359	VAL
1	A	2369	SER
1	A	2384	ARG
1	A	2392	ARG
1	A	2408	ILE

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Mol	Chain	Res	Type
1	A	2409	SER
1	A	2415	TRP
1	A	2424	GLN
1	A	2435	SER
1	A	2442	GLN
1	A	2450	ASN
1	A	2511	LEU
1	A	2512	VAL
1	A	2527	ASP
1	A	2529	THR
1	A	2572	ARG
1	A	2587	LEU
1	A	2603	THR
1	A	2613	LEU
1	A	2614	ASP
1	A	2615	TYR
1	A	2626	LEU
1	A	2645	ASP
1	A	2650	THR
1	A	2685	THR
1	A	2694	PHE
1	A	2728	THR
1	A	2747	ASN
1	A	2761	THR
1	A	2793	ASN
1	A	2809	ARG
1	A	2817	ASP
1	A	2863	ARG
1	A	2873	ILE
1	A	2880	SER
1	A	2883	ASP
1	A	2897	THR
1	A	2926	THR
1	A	2944	ASP
1	A	2954	ASN
1	A	2998	ILE
1	A	3007	GLN
1	A	3026	SER
1	A	3027	ARG
1	A	3037	ILE
1	A	3043	ASN
1	A	3052	ASP

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Mol	Chain	Res	Type
1	A	3084	LEU
1	A	3123	LEU
1	A	3141	LEU
1	A	3143	VAL
1	A	3145	PHE
1	A	3158	SER
1	A	3168	CYS
1	A	3175	GLU
1	A	3179	GLU
1	A	3186	SER
1	A	3195	GLU
1	A	3200	ILE
1	A	3216	LEU
1	A	3240	GLU
1	A	3269	LEU
1	A	3278	LEU
1	A	3330	ASP
1	A	3337	LYS
1	A	3365	ASP
1	A	3366	LEU
1	A	3373	ILE
1	A	3381	SER
1	A	3399	THR
1	A	3405	MET
1	A	3432	ILE
1	A	3457	LEU
1	A	3468	ASN
1	A	3516	ASP
1	A	3536	TYR
1	A	3564	LEU
1	A	3566	ASN
1	A	3569	SER
1	A	3571	ARG
1	A	3583	THR
1	A	3584	GLN
1	A	3612	ASP
1	A	3623	SER
1	A	3630	SER
1	A	3663	ILE
1	A	3676	ASP
1	A	3678	SER
1	A	3691	ASP

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Mol	Chain	Res	Type
1	A	3695	THR
1	A	3700	LEU
1	A	3707	ASN
1	A	3719	LEU
1	A	3725	ASN
1	A	3730	LEU
1	A	3731	ASN
1	A	3759	SER
1	A	3760	PHE
1	A	3776	ASP
1	A	3785	ASN
1	A	3791	SER
1	A	3799	HIS
1	A	3806	ARG
1	A	3813	ARG
1	A	3817	LEU
1	A	3830	LEU
1	A	3865	ILE
1	A	3867	LEU
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3947	ILE
1	A	3974	ILE
1	A	3998	LEU
1	A	4007	GLN
1	A	4023	LEU
1	A	4026	GLN
1	A	4034	VAL
1	A	4039	GLN
1	A	4043	ASP
1	A	4048	PHE
1	A	4055	GLU
1	A	4069	LEU
1	A	4079	ASN
1	A	4100	SER
1	A	4200	LEU
1	A	4206	SER
1	A	4232	MET
1	A	4240	ASN
1	A	4259	ARG
1	A	4267	ARG

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Mol	Chain	Res	Type
1	A	4282	GLN
1	A	4286	ARG
1	A	4290	LEU
1	A	4295	PHE
1	A	4321	ARG
1	A	4337	ILE
1	A	4353	MET
1	A	4360	LEU
1	A	4362	GLN
1	A	4385	GLU
1	A	4388	THR
1	A	4404	THR
1	A	4428	ASN
1	A	4434	GLN
1	A	4503	ILE
1	A	4550	TRP
1	A	4553	TYR
1	A	4565	ILE
1	A	4566	SER
1	A	4596	ASN
1	A	4606	GLN
1	A	4638	ASN
1	A	4649	TRP
1	A	4671	TRP
1	A	4692	LEU
1	A	4693	ASN
1	A	4694	GLU
1	A	4711	THR
1	A	4714	GLN
1	B	1479	ARG
1	B	1490	THR
1	B	1545	LEU
1	B	1547	ASN
1	B	1555	VAL
1	B	1596	ASN
1	B	1629	LEU
1	B	1640	ASN
1	B	1658	GLU
1	B	1671	ARG
1	B	1712	SER
1	B	1734	LEU
1	B	1736	ASP

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Mol	Chain	Res	Type
1	B	1762	ASN
1	B	1793	ASN
1	B	1809	ASN
1	B	1817	LEU
1	B	1828	ASP
1	B	1867	LEU
1	B	1901	ASN
1	B	1911	ARG
1	B	1920	ASN
1	B	1946	ARG
1	B	2029	ASN
1	B	2071	MET
1	B	2106	GLU
1	B	2129	VAL
1	B	2149	LEU
1	B	2166	CYS
1	B	2185	GLN
1	B	2189	GLN
1	B	2197	ASN
1	B	2211	ASP
1	B	2235	GLN
1	B	2236	LEU
1	B	2239	LYS
1	B	2253	GLN
1	B	2254	GLU
1	B	2260	LEU
1	B	2290	LEU
1	B	2313	LYS
1	B	2320	LEU
1	B	2342	ASN
1	B	2352	TRP
1	B	2374	ASN
1	B	2381	ASN
1	B	2423	THR
1	B	2425	MET
1	B	2432	ASP
1	B	2504	GLN
1	B	2541	MET
1	B	2550	GLU
1	B	2581	LEU
1	B	2587	LEU
1	B	2603	THR

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Mol	Chain	Res	Type
1	B	2612	LEU
1	B	2613	LEU
1	B	2699	LEU
1	B	2745	GLU
1	B	2797	ASP
1	B	2821	THR
1	B	2825	THR
1	B	2841	ASN
1	B	2843	ARG
1	B	2883	ASP
1	B	2897	THR
1	B	2899	GLU
1	B	2927	ASP
1	B	2928	LYS
1	B	2929	LYS
1	B	2946	LEU
1	B	2966	SER
1	B	2977	LYS
1	B	2984	LEU
1	B	2996	ASP
1	B	3018	SER
1	B	3026	SER
1	B	3043	ASN
1	B	3050	ASP
1	B	3059	LEU
1	B	3087	MET
1	B	3140	ASN
1	B	3151	SER
1	B	3164	LEU
1	B	3195	GLU
1	B	3284	HIS
1	B	3302	LEU
1	B	3322	GLN
1	B	3560	SER
1	B	3563	LEU
1	B	3566	ASN
1	B	3619	ILE
1	B	3620	ARG
1	B	3623	SER
1	B	3676	ASP
1	B	3700	LEU
1	B	3725	ASN

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Mol	Chain	Res	Type
1	B	3780	ARG
1	B	3833	SER
1	B	3867	LEU
1	B	3954	ARG
1	B	3998	LEU
1	B	4005	ILE
1	B	4012	LEU
1	B	4029	SER
1	B	4046	GLN
1	B	4091	SER
1	B	4105	VAL
1	B	4157	TYR
1	B	4185	VAL
1	B	4189	ASN
1	B	4200	LEU
1	B	4206	SER
1	B	4218	THR
1	B	4219	SER
1	B	4232	MET
1	B	4258	THR
1	B	4309	SER
1	B	4318	SER
1	B	4323	ASN
1	B	4324	ILE
1	B	4327	ASP
1	B	4334	VAL
1	B	4356	LEU
1	B	4402	ILE
1	B	4413	ASN
1	B	4425	LYS
1	B	4434	GLN
1	B	4500	GLU
1	B	4503	ILE
1	B	4548	LYS
1	B	4555	VAL
1	B	4558	THR
1	B	4573	GLN
1	B	4576	SER
1	B	4596	ASN
1	B	4607	SER
1	B	4618	ASN
1	B	4644	LEU

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Mol	Chain	Res	Type
1	B	4693	ASN
1	B	4698	GLU
1	B	4709	GLN
1	B	4715	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1512	ASN
1	A	1522	GLN
1	A	1549	GLN
1	A	1563	ASN
1	A	1609	GLN
1	A	1690	GLN
1	A	1791	HIS
1	A	1798	ASN
1	A	1809	ASN
1	A	1813	GLN
1	A	1844	GLN
1	A	1853	GLN
1	A	1857	ASN
1	A	1858	ASN
1	A	1865	GLN
1	A	1877	HIS
1	A	1971	ASN
1	A	1990	GLN
1	A	2018	GLN
1	A	2029	ASN
1	A	2042	GLN
1	A	2044	GLN
1	A	2047	GLN
1	A	2053	ASN
1	A	2086	ASN
1	A	2090	ASN
1	A	2136	GLN
1	A	2138	GLN
1	A	2142	GLN
1	A	2167	GLN
1	A	2197	ASN
1	A	2200	ASN
1	A	2295	GLN
1	A	2351	HIS

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Mol	Chain	Res	Type
1	A	2366	ASN
1	A	2368	ASN
1	A	2428	GLN
1	A	2436	ASN
1	A	2447	GLN
1	A	2450	ASN
1	A	2495	GLN
1	A	2535	ASN
1	A	2552	ASN
1	A	2553	GLN
1	A	2564	ASN
1	A	2565	GLN
1	A	2598	GLN
1	A	2656	HIS
1	A	2747	ASN
1	A	2787	GLN
1	A	2793	ASN
1	A	2810	HIS
1	A	2826	GLN
1	A	2869	GLN
1	A	2907	HIS
1	A	2942	ASN
1	A	2954	ASN
1	A	2961	GLN
1	A	3007	GLN
1	A	3009	GLN
1	A	3033	ASN
1	A	3043	ASN
1	A	3077	ASN
1	A	3156	ASN
1	A	3223	HIS
1	A	3253	ASN
1	A	3266	GLN
1	A	3277	GLN
1	A	3286	ASN
1	A	3331	GLN
1	A	3338	GLN
1	A	3377	GLN
1	A	3437	ASN
1	A	3555	ASN
1	A	3566	ASN
1	A	3607	GLN

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Mol	Chain	Res	Type
1	A	3646	ASN
1	A	3687	ASN
1	A	3721	GLN
1	A	3725	ASN
1	A	3731	ASN
1	A	3785	ASN
1	A	3794	GLN
1	A	3820	GLN
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3981	ASN
1	A	4017	GLN
1	A	4046	GLN
1	A	4066	GLN
1	A	4073	GLN
1	A	4079	ASN
1	A	4112	ASN
1	A	4191	HIS
1	A	4210	HIS
1	A	4234	ASN
1	A	4263	GLN
1	A	4278	HIS
1	A	4282	GLN
1	A	4349	ASN
1	A	4362	GLN
1	A	4370	ASN
1	A	4413	ASN
1	A	4573	GLN
1	A	4574	GLN
1	A	4596	ASN
1	A	4610	GLN
1	A	4653	GLN
1	A	4693	ASN
1	A	4715	ASN
1	A	4718	GLN
1	B	1480	HIS
1	B	1522	GLN
1	B	1547	ASN
1	B	1568	HIS
1	B	1589	ASN
1	B	1609	GLN

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Mol	Chain	Res	Type
1	B	1640	ASN
1	B	1690	GLN
1	B	1793	ASN
1	B	1813	GLN
1	B	1820	GLN
1	B	1826	GLN
1	B	1857	ASN
1	B	1891	GLN
1	B	1901	ASN
1	B	1920	ASN
1	B	1931	ASN
1	B	1990	GLN
1	B	2029	ASN
1	B	2044	GLN
1	B	2086	ASN
1	B	2110	GLN
1	B	2235	GLN
1	B	2241	GLN
1	B	2264	GLN
1	B	2315	GLN
1	B	2342	ASN
1	B	2351	HIS
1	B	2368	ASN
1	B	2381	ASN
1	B	2398	GLN
1	B	2504	GLN
1	B	2542	ASN
1	B	2547	ASN
1	B	2564	ASN
1	B	2571	ASN
1	B	2793	ASN
1	B	2826	GLN
1	B	2832	ASN
1	B	2841	ASN
1	B	2861	GLN
1	B	2937	HIS
1	B	2992	ASN
1	B	3043	ASN
1	B	3196	ASN
1	B	3223	HIS
1	B	3235	HIS
1	B	3272	ASN

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Mol	Chain	Res	Type
1	B	3322	GLN
1	B	3338	GLN
1	B	3555	ASN
1	B	3566	ASN
1	B	3577	GLN
1	B	3687	ASN
1	B	3725	ASN
1	B	3731	ASN
1	B	3785	ASN
1	B	3794	GLN
1	B	3799	HIS
1	B	3925	ASN
1	B	3926	ASN
1	B	3953	ASN
1	B	3981	ASN
1	B	4016	GLN
1	B	4026	GLN
1	B	4036	HIS
1	B	4038	GLN
1	B	4040	ASN
1	B	4052	GLN
1	B	4112	ASN
1	B	4152	GLN
1	B	4189	ASN
1	B	4199	GLN
1	B	4263	GLN
1	B	4278	HIS
1	B	4323	ASN
1	B	4391	HIS
1	B	4413	ASN
1	B	4434	GLN
1	B	4573	GLN
1	B	4574	GLN
1	B	4596	ASN
1	B	4618	ASN
1	B	4651	ASN
1	B	4693	ASN
1	B	4709	GLN

5.3.3 RNA

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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	9001	-	22,29,29	1.30	3 (13%)	27,45,45	2.22	6 (22%)
2	ADP	A	9002	-	22,29,29	1.27	3 (13%)	27,45,45	2.17	5 (18%)
2	ADP	A	9003	-	22,29,29	1.30	3 (13%)	27,45,45	2.20	5 (18%)
2	ADP	A	9004	-	22,29,29	1.26	3 (13%)	27,45,45	2.23	6 (22%)
2	ADP	B	9007	-	22,29,29	1.26	3 (13%)	27,45,45	2.21	6 (22%)
2	ADP	B	9008	-	22,29,29	1.26	3 (13%)	27,45,45	2.18	6 (22%)
2	ADP	B	9009	-	22,29,29	1.29	3 (13%)	27,45,45	2.20	6 (22%)
2	ADP	B	9010	-	22,29,29	1.27	3 (13%)	27,45,45	2.21	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	9001	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9008	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	0/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	O4'-C1'	2.01	1.43	1.41
2	B	9008	ADP	O4'-C1'	2.11	1.43	1.41
2	B	9007	ADP	O4'-C1'	2.14	1.43	1.41
2	A	9004	ADP	O4'-C1'	2.18	1.44	1.41
2	B	9010	ADP	O4'-C1'	2.23	1.44	1.41
2	B	9009	ADP	O4'-C1'	2.35	1.44	1.41
2	A	9003	ADP	O4'-C1'	2.38	1.44	1.41
2	A	9004	ADP	C2-N3	2.41	1.36	1.32
2	B	9007	ADP	C2-N3	2.44	1.36	1.32
2	A	9003	ADP	C2-N3	2.47	1.36	1.32
2	B	9009	ADP	C2-N3	2.47	1.36	1.32
2	B	9010	ADP	C2-N3	2.47	1.36	1.32
2	A	9002	ADP	C2-N3	2.48	1.36	1.32
2	A	9001	ADP	O4'-C1'	2.48	1.44	1.41
2	B	9008	ADP	C2-N3	2.48	1.36	1.32
2	A	9001	ADP	C2-N3	2.54	1.36	1.32
2	A	9001	ADP	C5-C4	3.59	1.48	1.40
2	B	9007	ADP	C5-C4	3.60	1.48	1.40
2	B	9010	ADP	C5-C4	3.61	1.48	1.40
2	A	9004	ADP	C5-C4	3.61	1.48	1.40
2	A	9003	ADP	C5-C4	3.62	1.48	1.40
2	B	9009	ADP	C5-C4	3.63	1.48	1.40
2	B	9008	ADP	C5-C4	3.65	1.48	1.40
2	A	9002	ADP	C5-C4	3.70	1.48	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	9004	ADP	N3-C2-N1	-9.13	121.91	128.89
2	A	9003	ADP	N3-C2-N1	-9.06	121.96	128.89
2	B	9007	ADP	N3-C2-N1	-9.04	121.97	128.89
2	B	9010	ADP	N3-C2-N1	-9.01	122.00	128.89
2	A	9001	ADP	N3-C2-N1	-9.01	122.00	128.89
2	B	9009	ADP	N3-C2-N1	-8.96	122.03	128.89
2	A	9002	ADP	N3-C2-N1	-8.86	122.11	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9008	ADP	N3-C2-N1	-8.82	122.14	128.89
2	A	9002	ADP	PA-O3A-PB	-3.25	121.77	132.67
2	B	9008	ADP	PA-O3A-PB	-3.18	122.01	132.67
2	A	9001	ADP	PA-O3A-PB	-3.15	122.11	132.67
2	B	9007	ADP	C4-C5-N7	-3.04	106.68	109.48
2	B	9010	ADP	C4-C5-N7	-3.04	106.69	109.48
2	B	9009	ADP	PA-O3A-PB	-3.03	122.49	132.67
2	A	9001	ADP	C4-C5-N7	-3.01	106.71	109.48
2	A	9004	ADP	C4-C5-N7	-3.01	106.71	109.48
2	A	9002	ADP	C4-C5-N7	-3.01	106.71	109.48
2	B	9009	ADP	C4-C5-N7	-3.01	106.71	109.48
2	A	9003	ADP	C4-C5-N7	-3.00	106.72	109.48
2	B	9008	ADP	C4-C5-N7	-3.00	106.72	109.48
2	A	9003	ADP	PA-O3A-PB	-3.00	122.61	132.67
2	B	9010	ADP	PA-O3A-PB	-3.00	122.61	132.67
2	A	9004	ADP	PA-O3A-PB	-2.96	122.73	132.67
2	B	9007	ADP	PA-O3A-PB	-2.86	123.08	132.67
2	A	9001	ADP	C2'-C1'-N9	-2.49	110.49	114.29
2	B	9010	ADP	C2'-C1'-N9	-2.26	110.84	114.29
2	B	9007	ADP	C2'-C1'-N9	-2.25	110.86	114.29
2	A	9004	ADP	C2'-C1'-N9	-2.25	110.86	114.29
2	B	9008	ADP	C2'-C1'-N9	-2.24	110.88	114.29
2	B	9009	ADP	C2'-C1'-N9	-2.09	111.10	114.29
2	A	9001	ADP	C4'-O4'-C1'	2.04	111.96	109.72
2	A	9004	ADP	C4'-O4'-C1'	2.07	112.00	109.72
2	A	9002	ADP	C2-N1-C6	2.08	122.49	118.77
2	B	9008	ADP	C4'-O4'-C1'	2.09	112.02	109.72
2	B	9010	ADP	C4'-O4'-C1'	2.10	112.03	109.72
2	B	9008	ADP	C2-N1-C6	2.10	122.53	118.77
2	B	9009	ADP	C2-N1-C6	2.11	122.54	118.77
2	B	9010	ADP	C2-N1-C6	2.12	122.56	118.77
2	A	9003	ADP	C2-N1-C6	2.12	122.56	118.77
2	A	9001	ADP	C2-N1-C6	2.13	122.57	118.77
2	B	9007	ADP	C2-N1-C6	2.14	122.58	118.77
2	A	9004	ADP	C2-N1-C6	2.18	122.66	118.77
2	A	9002	ADP	C4'-O4'-C1'	2.19	112.13	109.72
2	B	9007	ADP	C4'-O4'-C1'	2.19	112.13	109.72
2	A	9003	ADP	C4'-O4'-C1'	2.20	112.14	109.72
2	B	9009	ADP	C4'-O4'-C1'	2.26	112.20	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	A	9002	ADP	4	0
2	A	9004	ADP	2	0
2	B	9009	ADP	1	0
2	B	9010	ADP	2	0

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^{th} 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	3042/3367 (90%)	-0.11	64 (2%)	67	51	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.15	30 (1%)	84	72	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.13	94 (1%)	74	60	64, 133, 209, 335	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.6
1	B	1517	VAL	4.8
1	A	1652	GLY	4.8
1	A	4187	LEU	4.4
1	A	1651	SER	4.4
1	A	3516	ASP	4.1
1	A	1555	VAL	4.0
1	A	3718	LEU	3.8
1	A	4550	TRP	3.7
1	A	4122	VAL	3.7
1	A	1545	LEU	3.6
1	B	1484	LEU	3.6
1	A	1650	VAL	3.6
1	A	4165	PRO	3.4
1	A	4509	LEU	3.4
1	A	4217	MET	3.4
1	A	4162	ILE	3.3
1	A	3512	LYS	3.3
1	A	3842	SER	3.3
1	A	3515	GLN	3.3
1	A	3518	ILE	3.1
1	B	3356	ALA	3.1
1	A	1657	LEU	3.1
1	A	3334	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	2335	THR	2.9
1	B	2720	TYR	2.9
1	A	3328	VAL	2.9
1	A	4168	PHE	2.9
1	A	3513	LEU	2.9
1	B	4517	LEU	2.9
1	A	4215	LEU	2.9
1	B	2304	HIS	2.9
1	A	4185	VAL	2.8
1	A	1575	MET	2.8
1	A	3846	LEU	2.8
1	A	1554	LEU	2.7
1	A	1538	TRP	2.7
1	A	1584	PHE	2.7
1	B	4541	ILE	2.7
1	B	1495	THR	2.7
1	A	3866	ALA	2.6
1	A	1656	ILE	2.6
1	A	3360	VAL	2.6
1	B	1575	MET	2.5
1	A	3536	TYR	2.5
1	A	1639	ILE	2.5
1	A	4118	MET	2.5
1	B	2620	ASP	2.5
1	A	3359	LYS	2.5
1	A	1527	LEU	2.5
1	A	3330	ASP	2.4
1	B	1543	LEU	2.4
1	B	3112	CYS	2.4
1	A	1544	ASP	2.4
1	B	2574	LEU	2.4
1	A	2060	LEU	2.3
1	A	4131	PRO	2.3
1	A	4186	LEU	2.3
1	A	3762	ILE	2.3
1	A	1549	GLN	2.3
1	A	3764	LEU	2.3
1	B	1514	TYR	2.3
1	A	1565	LEU	2.3
1	B	1511	GLU	2.3
1	B	1656	ILE	2.3
1	A	4635	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	3341	ALA	2.3
1	A	4192	LEU	2.2
1	A	2353	ILE	2.2
1	A	3319	GLN	2.2
1	A	4142	ALA	2.2
1	B	4550	TRP	2.2
1	B	1497	LEU	2.2
1	B	3341	ALA	2.2
1	A	1551	LYS	2.2
1	A	2452	ASN	2.2
1	B	4215	LEU	2.2
1	A	3346	VAL	2.2
1	B	3544	GLU	2.1
1	B	3842	SER	2.1
1	B	1510	ASN	2.1
1	A	3533	LYS	2.1
1	A	3388	LEU	2.1
1	B	1515	ARG	2.1
1	B	3324	LEU	2.1
1	A	3474	CYS	2.1
1	B	3332	GLN	2.0
1	A	3763	PHE	2.0
1	B	4537	LEU	2.0
1	A	3321	ASN	2.0
1	A	4030	PHE	2.0
1	B	4502	GLU	2.0
1	B	3328	VAL	2.0
1	A	2990	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	A	9001	27/27	0.94	0.39	2.68	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	2.41	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	1.87	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	1.86	129,129,129,129	0
2	ADP	B	9008	27/27	0.85	0.40	1.80	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	1.32	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.30	0.79	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	0.07	129,129,129,129	0

6.5 Other polymers (i)

There are no such residues in this entry.