Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 01:00 pm GMT

PDB ID	:	4AKH
Title	:	Dynein Motor Domain - AMPPNP complex
Authors	:	Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on	:	2012-02-22
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

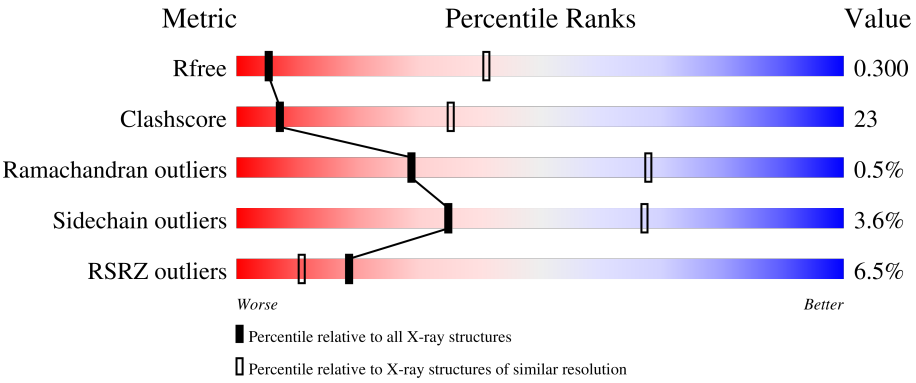
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	3% 65% 31%
1	B	2695	10% 67% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5093	-	-	X	-
4	SO4	A	5095	-	-	X	-
4	SO4	B	5096	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

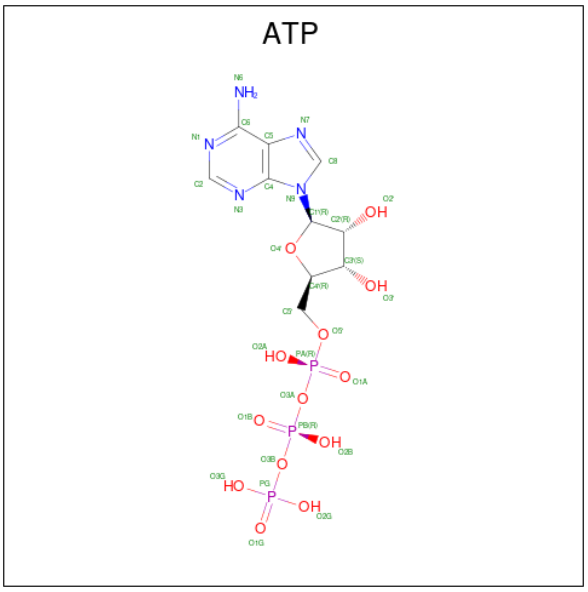
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 8 discrepancies between the modelled and reference sequences:

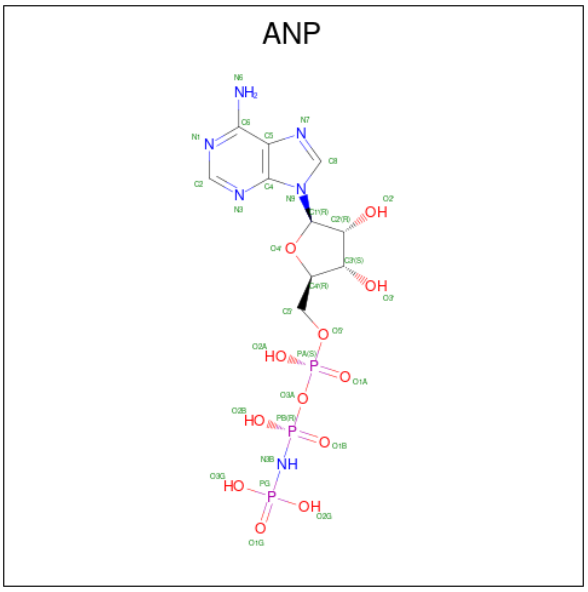
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP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

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



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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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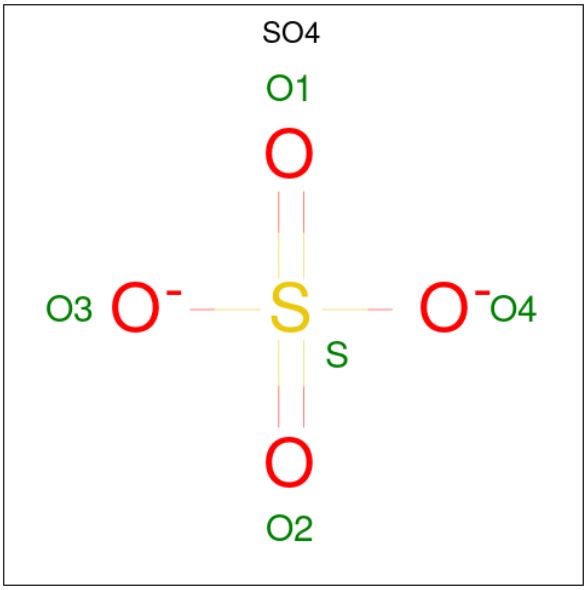
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

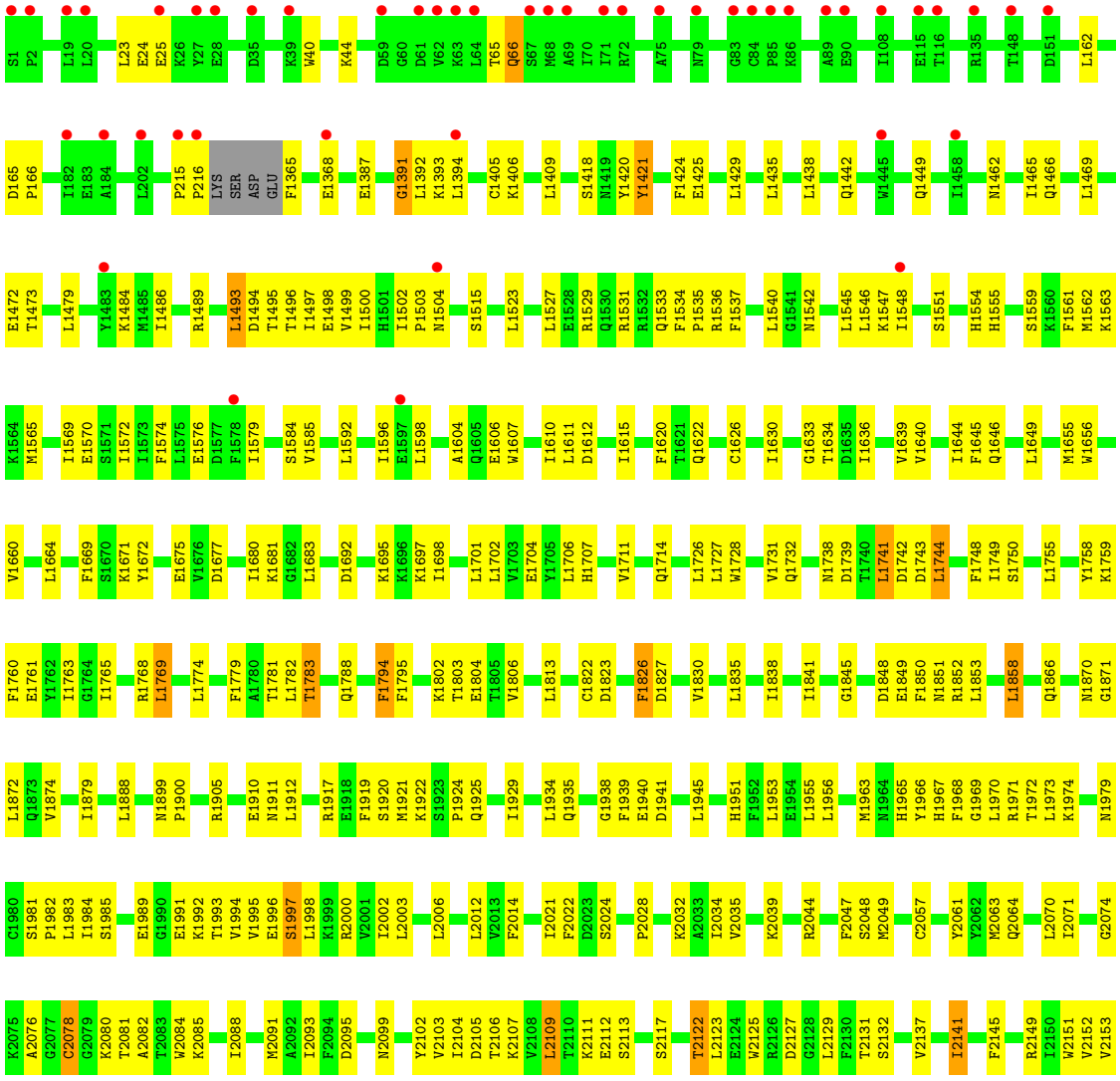
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

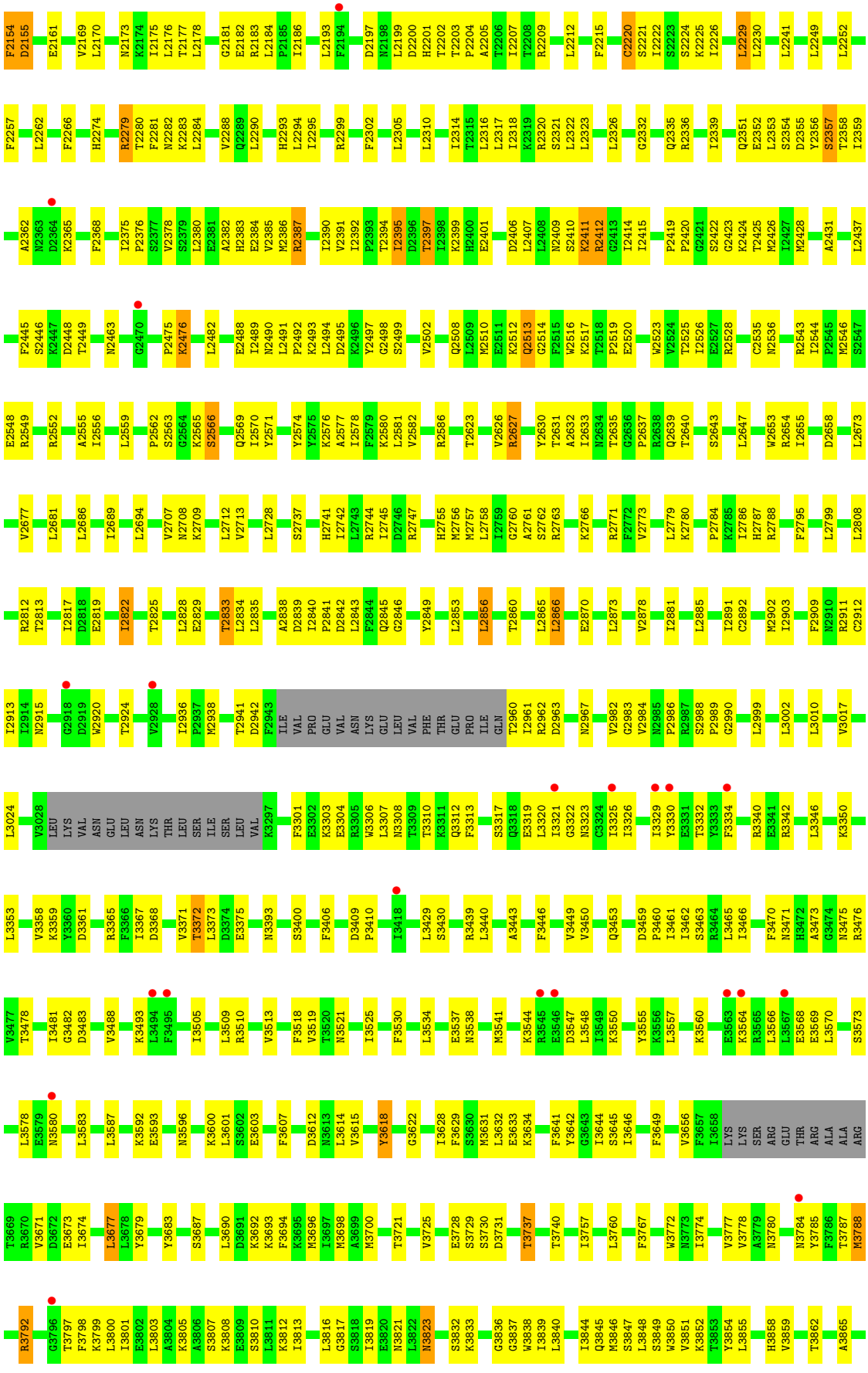
3 Residue-property plots (i)

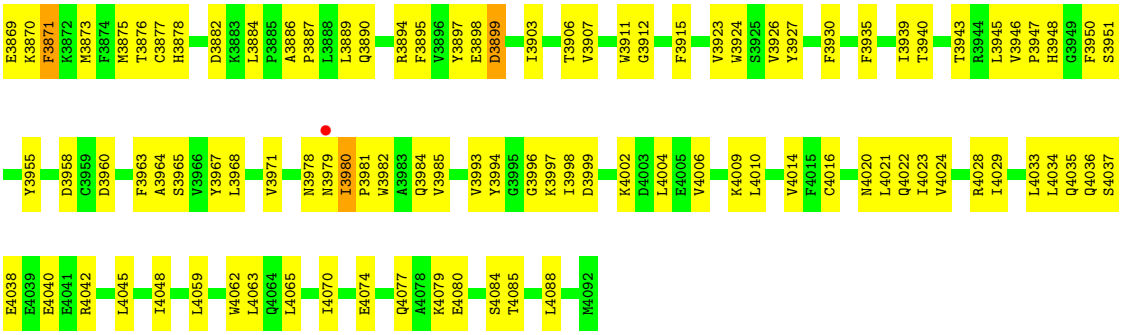
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

Chain A:

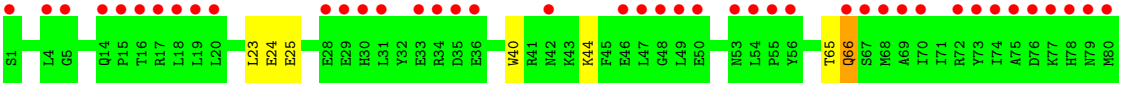


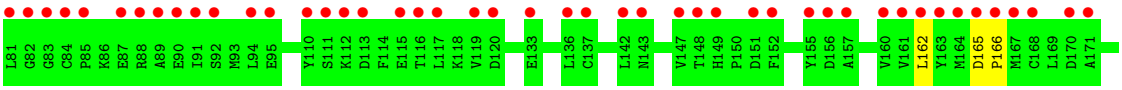

F2154 D2155 E2161 V2169 L2170 N2173 K2174 I2175 L2176 T2177 L2178 G2181 E2182 R2183 L2184 P2185 I2186 L2193 F2194 D2197 N2198 L2199 D2200 H2201 T2202 T2203 P2204 A2205 T2206 I2207 T2208 R2209 L2212 F2215 G2220 S2221 I2222 S2223 S2224 K2225 I2226 L2229 L2230 L2241 L2249 L2252
F2257 L2262 F2266 H2274 R2279 T2280 F2281 N2282 K2283 L2284 V2288 Q2289 L2290 H2293 L2294 I2295 R2299 F2302 L2305 L2310 I2314 T2315 L2316 L2317 I2318 K2319 R2320 S2321 L2322 L2323 L2326 G2332 Q2335 R2336 I2339 Q2351 E2352 L2353 S2354 D2355 Y2356 S2357 T2358 I2359
A2362 N2363 D2364 K2365 F2368 I2375 P2376 S2377 V2378 S2379 L2380 E2381 A2382 H2383 E2384 V2385 M2386 R2387 I2390 V2391 I2392 P2393 T2394 I2395 D2396 T2397 I2398 K2399 H2400 E2401 D2406 L2407 L2408 N2409 S2410 K2411 R2412 G2413 I2414 I2415 P2419 P2420 G2421 S2422 G2423 K2424 T2425 M2426 I2427 M2428 A2431 L2437
F2445 S2446 K2447 D2448 T2449 N2463 G2470 P2475 K2476 L2482 E2488 I2489 N2490 L2491 P2492 K2493 L2494 D2495 K2496 Y2497 G2498 S2499 V2502 Q2508 L2509 M2510 E2511 K2512 Q2513 G2514 F2515 W2516 K2517 T2518 P2519 E2520 W2523 V2524 T2525 I2526 E2527 R2528 C2535 N2536 R2543 I2544 P2545 M2546 S2547
E2548 R2549 R2552 A2555 I2556 L2559 P2562 S2563 G2564 K2565 S2566 Q2569 I2570 Y2571 Y2574 Y2575 K2576 A2577 I2578 F2579 K2580 L2581 V2582 R2586 T2623 V2626 R2627 Y2630 T2631 A2632 I2633 N2634 T2635 G2636 P2637 R2638 Q2639 T2640 S2643 L2647 W2653 R2654 I2655 D2658 L2673
V2677 L2681 L2686 I2689 L2694 V2707 N2708 K2709 L2712 V2713 L2728 S2737 H2741 I2742 L2743 R2744 I2745 D2746 R2747 H2755 M2756 M2757 L2758 I2759 G2760 A2761 S2762 R2763 K2766 R2771 F2772 V2773 L2779 K2780 P2784 K2785 I2786 H2787 R2788 F2795 L2799 L2808
R2812 T2813 I2817 D2818 E2819 I2822 T2825 L2828 E2829 T2833 L2834 L2835 A2838 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 Y2849 L2853 L2856 T2860 L2865 L2866 E2870 L2873 V2878 I2881 L2885 I2891 C2892 M2902 I2903 F2909 M2910 R2911 C2912
I2913 I2914 N2915 G2918 D2919 W2920 T2924 V2928 I2936 P2937 M2938 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 N2967 V2982 G2983 V2984 N2985 P2986 R2987 S2988 P2989 G2990 L2999 L3002 L3010 V3017
L3024 V3028 LEU LYS VAL ASN GLU LEU ASN LYS THR LEU SER ILE SER LEU VAL K3297 F3301 E3302 K3303 E3304 R3305 W3306 L3307 N3308 T3309 T3310 K3311 Q3312 F3313 S3317 Q3318 E3319 L3320 I3321 G3322 N3323 C3324 I3325 I3326 I3329 Y3330 E3331 T3332 Y3333 F3334 R3340 E3341 R3342 L3346 K3350
L3353 V3358 K3359 Y3360 D3361 R3365 F3366 I3367 D3368 V3371 T3372 L3373 D3374 E3375 N3393 S3400 F3406 D3409 P3410 I3418 L3429 S3430 R3439 L3440 A3443 F3446 V3449 V3450 Q3453 D3459 P3460 I3461 I3462 S3463 R3464 L3465 I3466 F3470 N3471 H3472 A3473 G3474 N3475 R3476
V3477 T3478 I3481 G3482 D3483 V3488 K3493 L3494 F3495 I3505 L3509 R3510 V3513 F3518 V3519 T3520 N3521 I3525 F3530 L3534 E3537 N3538 M3541 K3544 R3545 E3546 D3547 L3548 I3549 K3550 Y3555 K3556 L3557 K3560 E3563 K3564 R3566 L3566 L3567 E3568 E3569 L3570 S3573
L3578 E3579 N3580 L3583 L3587 K3592 E3593 N3596 K3600 L3601 S3602 E3603 F3607 D3612 N3613 L3614 V3615 Y3618 G3622 I3628 F3629 S3630 M3631 L3632 E3633 K3634 F3641 Y3642 G3643 I3644 S3645 I3646 F3649 V3656 F3657 I3658 LYS LYS SER ARG GLU THR ARG ALA ALA ARG
T3669 R3670 V3671 D3672 E3673 I3674 L3677 L3678 Y3679 Y3683 S3687 L3690 D3691 K3692 K3693 F3694 K3695 M3696 I3697 M3698 A3699 M3700 T3721 V3725 E3728 S3729 S3730 D3731 T3737 T3740 I3757 L3760 F3767 W3772 N3773 I3774 T3853 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 M3788
R3792 G3796 T3797 F3798 K3799 L3800 I3801 E3802 L3803 A3804 K3805 A3806 S3807 K3808 E3809 S3810 L3811 K3812 I3813 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823 S3832 K3833 G3836 G3837 W3838 I3839 L3840 I3844 Q3845 M3846 S3847 L3848 S3849 W3850 V3851 K3852 T3853 Y3854 L3855 H3858 V3859 T3862 A3865

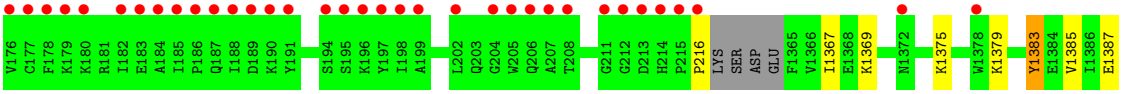


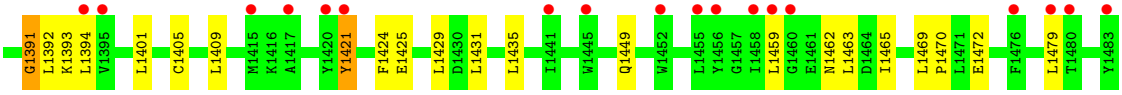
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC

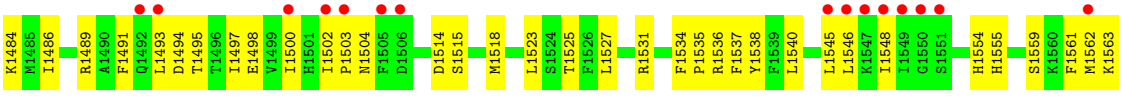
Chain B:

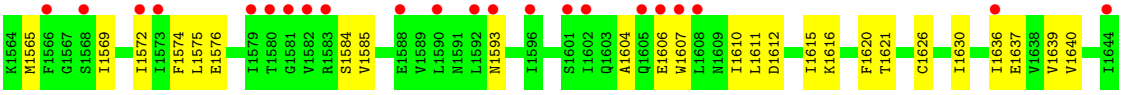


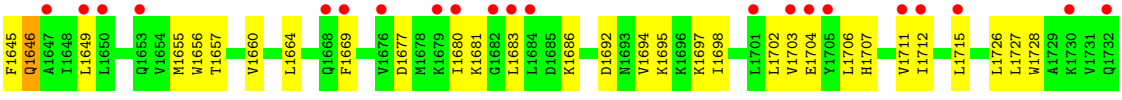


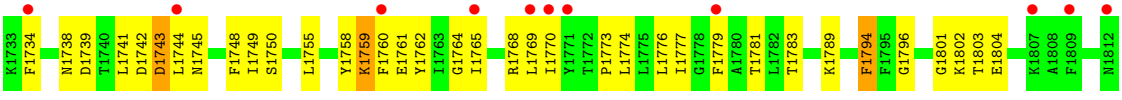


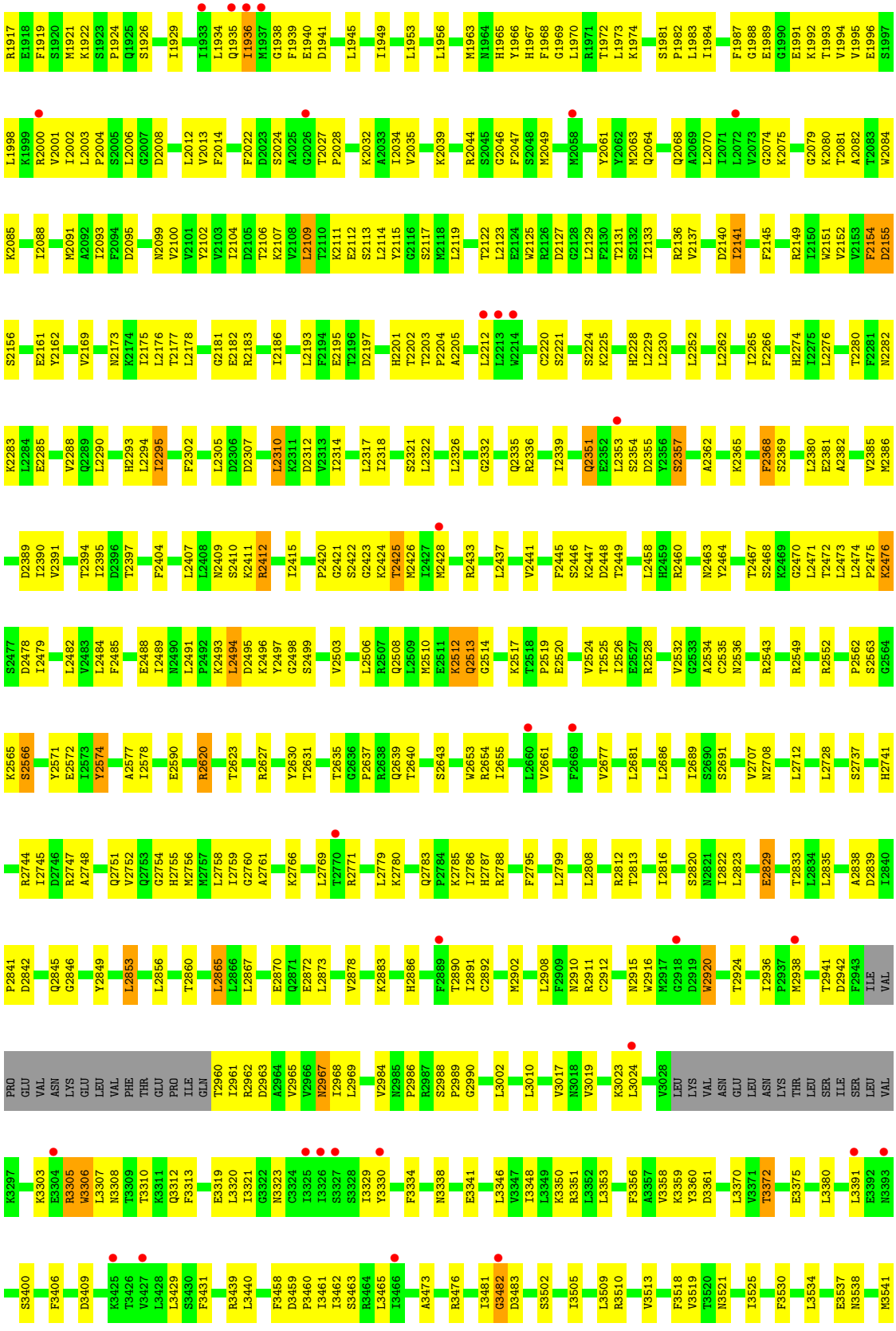


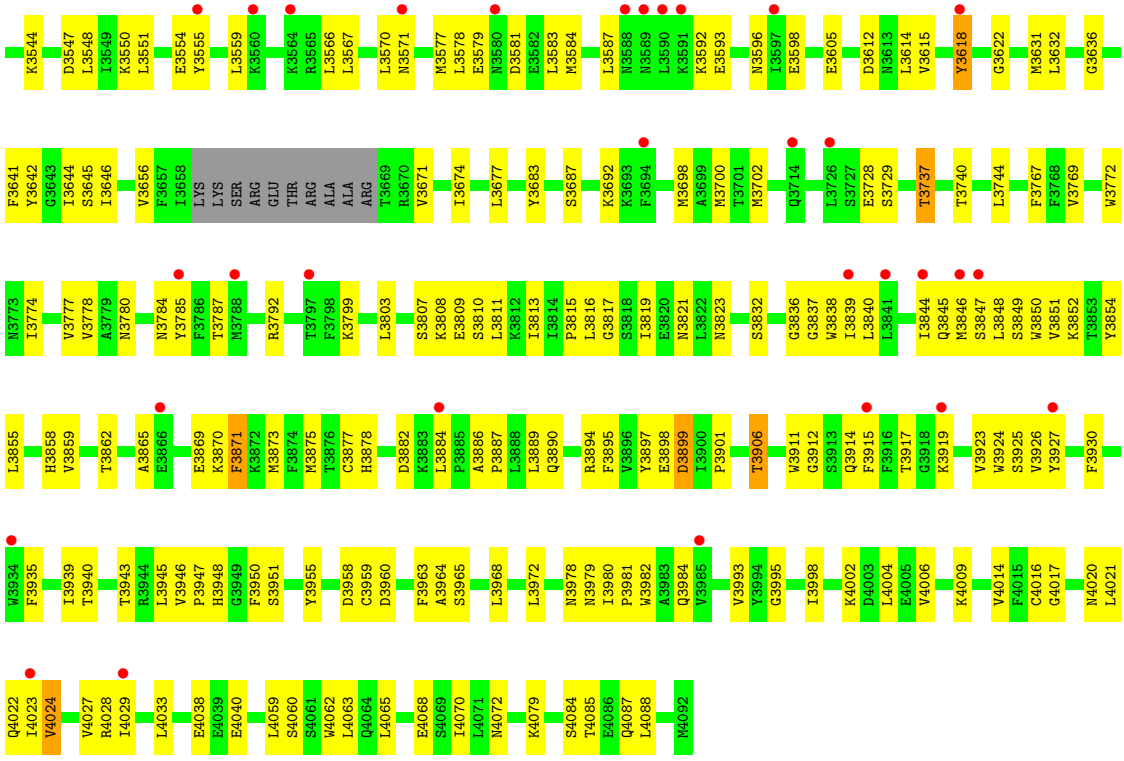











K3544
D3547 L3548 I3549 K3550 L3551
E3554 Y3555
L3559 K3560
K3564 R3565 L3566 L3567
L3570 N3571
M3577 L3578 E3579 N3580 D3581 E3582 L3583 M3584
L3587 N3588 N3589 L3590 K3591 K3592 E3593
N3596 I3597 E3598
E3605
D3612 N3613 L3614 V3615
Y3618
G3622
M3631 L3632
G3636
F3641 Y3642 G3643 I3644 S3645 I3646
V3656 F3657 I3658
LYS LYS SER ARG GLU THR ARG ALA ALA ARG
T3669 R3670 V3671
I3674
L3677
Y3683
S3687
K3692 K3693 F3694
M3698 A3699 M3700 T3701 M3702
Q3714
L3726 S3727 E3728 S3729
T3737
T3740
L3744
F3767 F3768 V3769
W3772
N3773 I3774
V3777 V3778 A3779 N3780
N3784 Y3785 F3786 T3787 M3788
R3792
T3797 F3798 K3799
L3803
S3807 K3808 E3809 S3810 L3811 K3812 I3813 T3814 P3815 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823
S3832
G3836 G3837 W3838 I3839 L3840 L3841
I3844 Q3845 M3846 S3847 L3848 S3849 W3850 V3851 K3852 T3853 Y3854
L3855 H3858 V3859
T3862
A3865 E3866
E3869 K3870 F3871 K3872 M3873 F3874 M3875 T3876 C3877 H3878
D3882 K3883 L3884 P3885 A3886 P3887 L3888 L3889 Q3890
R3894 F3895 V3896 Y3897 E3898 D3899 I3900 P3901
T3906
W3911 G3912 S3913 Q3914 F3915 F3916 T3917 G3918 K3919
V3923 W3924 S3925 V3926 Y3927
F3930
W3934 F3935
I3939 T3940
T3943 R3944 L3945 V3946 P3947 H3948 G3949 F3950 S3951
Y3955
D3958 C3959 D3960
F3963 A3964 S3965
L3968
L3972
N3978 N3979 I3980 P3981 W3982 A3983 Q3984 V3985
V3993 Y3994 G3995
I3998
K4002 D4003 L4004 E4005 V4006
K4009
V4014 F4015 C4016 G4017
N4020 L4021
Q4022 I4023 V4024
V4027 R4028 I4029
L4033
E4038 E4039 E4040
L4059 S4060 S4061 W4062 L4063 Q4064 L4065
E4068 S4069 I4070 L4071 N4072
K4079
S4084 T4085 E4086 Q4087 L4088
M4092

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 70.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (70.46-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4767 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 117.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	0/21146	0.77	7/28618 (0.0%)
1	B	0.46	2/21146 (0.0%)	0.68	5/28618 (0.0%)
All	All	0.49	2/42292 (0.0%)	0.73	12/57236 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3306	TRP	CE3-CZ3	-6.25	1.27	1.38
1	B	3306	TRP	CE2-CZ2	-5.22	1.30	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2012	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	1741	LEU	CB-CG-CD1	6.69	122.38	111.00
1	A	3792	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	1782	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	2460	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	2865	LEU	CB-CG-CD1	-5.47	101.69	111.00
1	A	2866	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	2494	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	A	2220	CYS	CA-CB-SG	-5.22	104.60	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2279	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	B	3306	TRP	N-CA-C	-5.02	97.43	111.00
1	B	1463	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2119	LEU	Peptide
1	B	2620	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	952	0
1	B	20748	0	20206	909	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	7	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1861	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1861) 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:216:PRO:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23
1:A:2061:TYR:CE1	1:A:2091:MET:SD	2.35	1.20
1:A:2061:TYR:HE1	1:A:2091:MET:SD	1.65	1.19
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.80	1.16
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.25	1.16
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.58	1.16
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.18	1.14
1:B:3023:LYS:CD	1:B:3567:LEU:HD21	1.77	1.14
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.14
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.27	1.14
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.61	1.13
1:A:215:PRO:CB	1:A:3475:ASN:HD22	1.61	1.13
1:B:2470:GLY:HA3	1:B:2473:LEU:HD21	1.29	1.13
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.84	1.12
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	1.77	1.12
1:B:2404:PHE:CZ	1:B:2428:MET:SD	2.43	1.12
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.49	1.12
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.22	1.11
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.13	1.11
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.51	1.10
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.68	1.10
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.10
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.13	1.10
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.09	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.88	1.09
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.83	1.09
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.50	1.08
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.33	1.08
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.28	1.08
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.36	1.08
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.18	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.22	1.08
1:B:3023:LYS:CD	1:B:3567:LEU:CD2	2.31	1.08
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.83	1.08
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.36	1.08
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.96	1.07
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.37	1.07
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.10	1.07
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.84	1.07
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.85	1.06
1:B:2467:THR:HB	1:B:2473:LEU:HD12	1.32	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.34	1.06
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.05
1:B:2467:THR:CB	1:B:2473:LEU:HD12	1.86	1.05
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.43	1.05
1:B:2061:TYR:HE1	1:B:2091:MET:CE	1.70	1.05
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.86	1.05
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.86	1.05
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.86	1.04
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.90	1.04
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.36	1.03
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.88	1.03
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.58	1.03
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.41	1.03
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.73	1.03
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.35	1.03
1:A:2476:LYS:CD	1:A:2476:LYS:H	1.66	1.02
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.41	1.02
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.60	1.02
1:B:3023:LYS:HD3	1:B:3567:LEU:HD21	1.37	1.02
1:B:2061:TYR:CE1	1:B:2091:MET:SD	2.53	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.03	1.02
1:B:2386:MET:CB	1:B:2627:ARG:HD3	1.90	1.02
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	0.87	1.02
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.77	1.01
1:B:2391:VAL:HG23	1:B:2426:MET:SD	2.00	1.01
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.36	1.01
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.40	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.91	1.01
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.58	1.01
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.43	1.00
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.02	1.00
1:B:1421:TYR:CE2	1:B:1425:GLU:CG	2.45	1.00
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.89	1.00
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.03	1.00
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.41	1.00
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.61	0.99
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:THR:HB	2:B:5093:ATP:O2A	1.60	0.99
1:A:215:PRO:CB	1:A:3475:ASN:ND2	2.24	0.99
1:B:3023:LYS:HD2	1:B:3567:LEU:CD2	1.92	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.46	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.97	0.99
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.44	0.99
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.92	0.99
1:B:1421:TYR:CE2	1:B:1425:GLU:HG3	1.97	0.99
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.75	0.98
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.00	0.98
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.26	0.97
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.46	0.97
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.46	0.97
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.26	0.97
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.93	0.97
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.94	0.97
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.94	0.97
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.98	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.64	0.97
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.65	0.97
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.95	0.96
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.43	0.96
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.31	0.96
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.66	0.96
1:B:1992:LYS:CG	1:B:2024:SER:HB2	1.94	0.96
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	1.95	0.95
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.45	0.95
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.43	0.95
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.47	0.95
1:B:3023:LYS:HE2	1:B:3567:LEU:HG	1.49	0.95
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.85	0.94
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.66	0.94
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.79	0.94
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.32	0.94
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.50	0.93
1:B:2380:LEU:HD12	1:B:2577:ALA:HB1	1.49	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:2380:LEU:HD12	1:A:2577:ALA:CB	1.98	0.93
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.93
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.69	0.93
1:B:3023:LYS:HD2	1:B:3567:LEU:HD21	1.51	0.92
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.31	0.92
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.52	0.92
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.23	0.92
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.52	0.92
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.04	0.92
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.03	0.92
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.90	0.92
1:A:2787:HIS:HA	1:A:3460:PRO:CD	1.99	0.91
1:B:2061:TYR:HE1	1:B:2091:MET:SD	1.91	0.91
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.52	0.91
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.85	0.91
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.24	0.91
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.06	0.91
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.00	0.91
1:B:1421:TYR:CZ	1:B:1425:GLU:HG3	2.05	0.91
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.01	0.91
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.01	0.90
1:B:2380:LEU:CD1	1:B:2577:ALA:CB	2.49	0.90
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.00	0.90
1:B:2380:LEU:HD12	1:B:2577:ALA:CB	2.01	0.90
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.72	0.90
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.60	0.90
1:B:2061:TYR:HE1	1:B:2091:MET:HE1	1.37	0.90
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.60	0.90
1:B:3303:LYS:CD	1:B:3306:TRP:HD1	1.82	0.90
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.02	0.89
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.89
1:B:2404:PHE:HZ	1:B:2428:MET:SD	1.94	0.89
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.55	0.89
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.54	0.89
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.89
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.71	0.89
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.37	0.89
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.00	0.89
1:B:2404:PHE:CE1	1:B:2428:MET:SD	2.66	0.89
1:B:2467:THR:HB	1:B:2473:LEU:HD11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:A:2757:MET:CE	1:A:2912:CYS:HB2	2.01	0.89
1:B:3303:LYS:CD	1:B:3306:TRP:CD1	2.54	0.89
1:A:2563:SER:HB3	1:A:2566:SER:H	1.37	0.88
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.04	0.88
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.88
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.72	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.53	0.88
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.53	0.88
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.04	0.88
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.09	0.88
1:A:1979:ASN:O	1:A:1983:LEU:HD13	1.73	0.87
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:B:2224:SER:O	2:B:5093:ATP:H2	1.57	0.87
1:A:1535:PRO:C	1:A:1841:ILE:HD11	1.94	0.87
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.74	0.87
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.03	0.87
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.11	0.86
1:B:2563:SER:HB3	1:B:2566:SER:H	1.38	0.86
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.05	0.86
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.04	0.86
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.04	0.86
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.10	0.86
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.39	0.86
1:A:2412:ARG:HB2	1:A:2412:ARG:HH11	1.41	0.86
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.06	0.85
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.10	0.85
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.06	0.85
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.57	0.85
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.58	0.85
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.76	0.85
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.07	0.85
1:A:1368:GLU:HG2	1:A:1424:PHE:HZ	1.36	0.85
1:A:2380:LEU:HD12	1:A:2577:ALA:HB1	1.56	0.85
1:A:2380:LEU:CD1	1:A:2577:ALA:CB	2.54	0.85
1:B:1425:GLU:OE2	1:B:1429:LEU:HG	1.76	0.85
1:A:166:PRO:CB	1:A:3476:ARG:HD3	2.06	0.84
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.57	0.84
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.59	0.84
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.77	0.84
1:A:2446:SER:H	1:A:2449:THR:CG2	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.17	0.84
1:A:216:PRO:CB	1:A:1365:PHE:CZ	2.59	0.84
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.22	0.84
1:A:2061:TYR:CE1	1:A:2091:MET:CE	2.60	0.84
1:B:1425:GLU:OE2	1:B:1429:LEU:CG	2.24	0.84
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.84
1:A:1368:GLU:CG	1:A:1424:PHE:CZ	2.58	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.57	0.83
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.61	0.83
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.08	0.83
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.78	0.83
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.06	0.83
1:B:2623:THR:HG21	3:B:5094:ANP:O3'	1.78	0.83
1:A:2476:LYS:HD3	1:A:2476:LYS:N	1.90	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.13	0.83
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.26	0.83
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.61	0.83
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.60	0.83
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.58	0.83
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.07	0.83
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.93	0.83
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.61	0.83
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.26	0.83
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.04	0.83
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.59	0.83
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.61	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.59	0.83
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.60	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.94	0.82
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.77	0.82
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.08	0.82
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.82
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.61	0.82
1:B:1421:TYR:CE2	1:B:1425:GLU:HG2	2.13	0.82
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.45	0.82
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.95	0.82
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.82
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.78	0.82
1:A:1365:PHE:CZ	1:A:1420:TYR:CD1	2.68	0.82
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.82
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.10	0.82
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.14	0.81
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.80	0.81
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.61	0.81
1:A:1779:PHE:O	1:A:1783:THR:HG22	1.80	0.81
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.96	0.81
1:A:2224:SER:O	2:A:5093:ATP:H2	1.63	0.81
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.81	0.81
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.81
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.08	0.81
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.61	0.81
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.57	0.80
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.45	0.80
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.59	0.80
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.80	0.80
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.62	0.80
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.29	0.80
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.96	0.80
1:A:2225:LYS:HA	2:A:5093:ATP:C2	2.16	0.80
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.82	0.80
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.64	0.80
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.62	0.80
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.97	0.80
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.12	0.79
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.12	0.79
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.22	0.79
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.09	0.79
1:B:3023:LYS:HD2	1:B:3567:LEU:HD23	1.64	0.79
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.03	0.79
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.13	0.78
1:A:2513:GLN:O	1:A:2526:ILE:HG13	1.82	0.78
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.99	0.78
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.18	0.78
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.64	0.78
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.82	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.61	0.78
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.83	0.78
1:A:2631:THR:O	1:A:2635:THR:HG22	1.81	0.78
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.70	0.78
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.64	0.78
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.84	0.78
1:B:2061:TYR:CE1	1:B:2091:MET:HE1	2.18	0.78
1:A:2552:ARG:HG2	1:A:2552:ARG:HH11	1.48	0.78
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.77
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.88	0.77
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.14	0.77
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	1.99	0.77
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.87	0.77
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.66	0.77
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.64	0.77
1:A:2757:MET:HE3	1:A:2912:CYS:HB2	1.64	0.77
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.20	0.77
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.83	0.77
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.77
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.84	0.77
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.77
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.66	0.77
1:A:2061:TYR:CD1	1:A:2091:MET:SD	2.78	0.77
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.66	0.77
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.20	0.77
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.32	0.76
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.50	0.76
1:A:2103:VAL:CG1	1:A:2155:ASP:OD1	2.33	0.76
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.87	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.59	0.76
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.33	0.76
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.67	0.76
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.84	0.76
1:A:216:PRO:CB	1:A:1365:PHE:CD1	2.69	0.76
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.49	0.76
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.85	0.76
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.66	0.76
1:A:2766:LYS:HE3	1:A:2892:CYS:SG	2.26	0.76
1:B:2380:LEU:HD11	1:B:2577:ALA:CB	2.15	0.76
1:B:3019:VAL:O	1:B:3023:LYS:HG3	1.86	0.76
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.76
1:A:2061:TYR:CD1	1:A:2091:MET:CE	2.69	0.76
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.14	0.76
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.01	0.76
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.75
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2467:THR:CB	1:B:2473:LEU:CD1	2.50	0.75
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.11	0.75
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.68	0.75
1:B:2446:SER:H	1:B:2449:THR:HG23	1.52	0.75
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.16	0.75
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.66	0.75
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.66	0.75
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.52	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.87	0.75
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.75
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.64	0.75
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.87	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB1	2.15	0.74
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.27	0.74
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.54	0.74
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.68	0.74
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.52	0.74
1:B:3023:LYS:HE2	1:B:3567:LEU:CG	2.16	0.74
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.69	0.74
1:B:2081:THR:CB	2:B:5093:ATP:O2A	2.28	0.74
1:B:2517:LYS:HE2	1:B:2520:GLU:OE1	1.88	0.74
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.88	0.74
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.87	0.74
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.74	0.74
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.15	0.74
1:B:2220:CYS:CB	2:B:5093:ATP:C6	2.71	0.74
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.51	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.53	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB2	2.18	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.73
1:B:3618:TYR:N	1:B:3618:TYR:CD1	2.51	0.73
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.70	0.73
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.73
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.36	0.73
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.18	0.73
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.86	0.73
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.23	0.73
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.04	0.73
1:A:2425:THR:CG2	3:A:5094:ANP:O3G	2.37	0.73
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.18	0.72
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.18	0.72
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.88	0.72
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.10	0.72
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.71	0.72
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.89	0.72
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.03	0.72
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.29	0.72
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.70	0.72
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.20	0.72
1:B:2446:SER:H	1:B:2449:THR:CG2	2.01	0.72
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.72	0.72
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.90	0.72
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.71	0.72
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.60	0.72
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.36	0.71
1:A:2380:LEU:CD1	1:A:2577:ALA:HB2	2.20	0.71
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.72	0.71
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.04	0.71
1:A:2061:TYR:CE1	1:A:2091:MET:HE1	2.24	0.71
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.38	0.71
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.91	0.71
1:B:3618:TYR:N	1:B:3618:TYR:HD1	1.87	0.71
1:B:2061:TYR:CE1	1:B:2091:MET:CE	2.63	0.71
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.73	0.71
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.26	0.71
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.25	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.72	0.71
1:B:1852:ARG:O	1:B:1852:ARG:HG3	1.91	0.71
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.31	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.13	0.71
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.72	0.71
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.26	0.71
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.10	0.71
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.11	0.71
1:A:2103:VAL:HG13	1:A:2155:ASP:OD1	1.91	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71
1:B:1738:ASN:O	1:B:1739:ASP:OD1	2.09	0.71
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.20	0.71
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.17	0.70
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.91	0.70
1:B:2420:PRO:HB2	1:B:2620:ARG:NH2	2.06	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.25	0.70
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.22	0.70
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.92	0.70
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.21	0.70
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.73	0.70
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.53	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.74	0.70
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.92	0.70
1:B:3577:MET:O	1:B:3579:GLU:N	2.24	0.70
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.73	0.70
1:B:2064:GLN:OE1	1:B:2151:TRP:HH2	1.74	0.70
1:A:216:PRO:CB	1:A:1365:PHE:HE1	1.99	0.70
1:A:2225:LYS:HA	2:A:5093:ATP:N3	2.07	0.70
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.73	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.81	0.69
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.72	0.69
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.92	0.69
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.22	0.69
1:B:3645:SER:CB	1:B:3890:GLN:HE21	2.03	0.69
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.57	0.69
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.92	0.69
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.74	0.69
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.81	0.69
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.71	0.69
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.23	0.69
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.73	0.69
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.92	0.69
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.57	0.69
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.57	0.69
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.75	0.69
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.73	0.69
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.21	0.69
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.57	0.69
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.13	0.69
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.93	0.69
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1802:LYS:NZ	4:A:5095:SO4:O2	2.26	0.69
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.14	0.69
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.21	0.68
1:B:2061:TYR:CD1	1:B:2091:MET:SD	2.86	0.68
1:A:1368:GLU:HG2	1:A:1424:PHE:CE2	2.25	0.68
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.22	0.68
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.75	0.68
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.73	0.68
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:B:3023:LYS:CD	1:B:3567:LEU:HD23	2.19	0.68
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.57	0.68
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.75	0.68
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.22	0.68
1:B:3819:ILE:O	1:B:3823:ASN:HB2	1.93	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.76	0.68
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.93	0.68
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.93	0.68
1:A:2476:LYS:NZ	1:A:2528:ARG:HD3	2.09	0.68
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.93	0.68
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.93	0.68
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.59	0.68
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.93	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.76	0.68
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.64	0.68
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.92	0.68
1:B:3612:ASP:O	1:B:3615:VAL:HG22	1.93	0.68
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.24	0.67
1:B:2620:ARG:HH12	1:B:2910:ASN:CG	1.97	0.67
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.47	0.67
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.24	0.67
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.29	0.67
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.67
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.75	0.67
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.29	0.67
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.82	0.67
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.10	0.67
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.28	0.67
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.94	0.67
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.94	0.67
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.77	0.67
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.72	0.67
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.15	0.67
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.09	0.67
1:A:2380:LEU:HD12	1:A:2577:ALA:HB2	1.75	0.67
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.59	0.67
1:B:2394:THR:H	1:B:2397:THR:HB	1.59	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:2757:MET:HE2	1:A:2912:CYS:HB2	1.75	0.67
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.09	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.29	0.67
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.77	0.67
1:A:2224:SER:O	2:A:5093:ATP:C2	2.48	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.10	0.67
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.30	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.25	0.67
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.10	0.66
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.58	0.66
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.25	0.66
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.77	0.66
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.77	0.66
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.25	0.66
1:A:1527:LEU:HD23	1:A:1545:LEU:HD22	1.77	0.66
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.25	0.66
1:B:2936:ILE:HG22	1:B:2962:ARG:HD3	1.78	0.66
1:A:2081:THR:O	1:A:2085:LYS:HB2	1.96	0.66
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.76	0.66
1:A:2425:THR:HG23	3:A:5094:ANP:O3G	1.95	0.66
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.26	0.66
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.26	0.66
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.77	0.66
1:A:2495:ASP:O	1:A:2498:GLY:N	2.29	0.66
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.59	0.66
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.25	0.66
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.26	0.65
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.77	0.65
1:B:3023:LYS:CE	1:B:3567:LEU:HG	2.25	0.65
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.00	0.65
1:A:3618:TYR:N	1:A:3618:TYR:HD1	1.94	0.65
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.76	0.65
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.36	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.30	0.65
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.12	0.65
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.77	0.65
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.27	0.65
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.79	0.65
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.96	0.65
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.96	0.65
1:A:2766:LYS:CE	1:A:2892:CYS:SG	2.84	0.65
1:B:2508:GLN:HG3	1:B:2512:LYS:HG3	1.77	0.65
1:B:3460:PRO:O	1:B:3463:SER:HB3	1.97	0.65
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.11	0.65
1:B:2391:VAL:CG2	1:B:2426:MET:SD	2.83	0.65
1:B:2513:GLN:O	1:B:2526:ILE:CG1	2.45	0.65
1:B:1425:GLU:OE2	1:B:1429:LEU:CD2	2.45	0.65
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.32	0.65
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.78	0.64
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.62	0.64
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	1.79	0.64
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.16	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.27	0.64
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.78	0.64
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.98	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.12	0.64
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.62	0.64
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.86	0.64
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.62	0.64
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.75	0.64
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.62	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.78	0.64
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.98	0.64
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.56	0.64
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.80	0.64
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.79	0.64
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.13	0.64
1:A:1365:PHE:CZ	1:A:1420:TYR:CE1	2.86	0.63
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.98	0.63
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	1.81	0.63
1:B:2623:THR:HB	3:B:5094:ANP:O2'	1.99	0.63
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.29	0.63
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.61	0.63
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.28	0.63
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.33	0.63
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.28	0.63
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.64	0.63
1:A:2552:ARG:HG2	1:A:2552:ARG:NH1	2.14	0.63
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.64	0.63
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.80	0.63
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.34	0.63
1:B:2508:GLN:CG	1:B:2512:LYS:HG3	2.28	0.63
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.53	0.63
1:B:1421:TYR:O	1:B:1425:GLU:N	2.32	0.63
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.13	0.62
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.11	0.62
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.74	0.62
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.13	0.62
1:B:2220:CYS:SG	2:B:5093:ATP:C6	2.92	0.62
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.81	0.62
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.87	0.62
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.29	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.52	0.62
1:B:1425:GLU:OE2	1:B:1429:LEU:HD21	1.98	0.62
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.99	0.62
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.80	0.62
1:B:2428:MET:SD	1:B:2532:VAL:HG11	2.39	0.62
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.81	0.62
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.33	0.62
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.81	0.62
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.30	0.62
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.81	0.62
1:B:2467:THR:OG1	1:B:2473:LEU:HD12	1.99	0.62
1:B:2677:VAL:HG11	1:B:2686:LEU:HD21	1.82	0.62
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.63	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.63	0.62
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.80	0.62
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.98	0.62
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.29	0.62
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.81	0.62
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.82	0.62
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.81	0.62
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.65	0.61
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.65	0.61
1:B:2631:THR:O	1:B:2635:THR:HG22	1.99	0.61
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.82	0.61
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.81	0.61
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.82	0.61
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.63	0.61
1:B:3737:THR:HB	1:B:3740:THR:CB	2.29	0.61
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.61
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.82	0.61
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.30	0.61
1:A:2380:LEU:HD11	1:A:2577:ALA:CB	2.30	0.61
1:B:3023:LYS:HD3	1:B:3567:LEU:CD2	2.10	0.61
1:A:1469:LEU:HD13	1:A:1523:LEU:CD2	2.30	0.61
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.83	0.61
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.41	0.61
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.66	0.61
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.61
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.82	0.61
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.82	0.61
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.00	0.61
1:B:3023:LYS:CE	1:B:3567:LEU:CD2	2.79	0.61
1:A:2394:THR:H	1:A:2397:THR:HB	1.65	0.61
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.36	0.60
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.31	0.60
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.16	0.60
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.77	0.60
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.60
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.34	0.60
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.55	0.60
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.36	0.60
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.60
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.30	0.60
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.84	0.60
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.18	0.60
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.83	0.60
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.60
1:B:1991:GLU:O	1:B:1995:VAL:HG23	2.01	0.60
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.90	0.60
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.01	0.60
1:A:2757:MET:HE1	1:A:2909:PHE:HA	1.83	0.60
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.84	0.60
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.32	0.60
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.01	0.60
1:B:1983:LEU:CG	1:B:1993:THR:HG23	2.25	0.60
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.38	0.60
1:B:2476:LYS:H	1:B:2476:LYS:HD2	1.67	0.60
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.37	0.60
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.82	0.60
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.64	0.59
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.50	0.59
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.02	0.59
1:A:3819:ILE:O	1:A:3823:ASN:HB2	2.01	0.59
1:A:2446:SER:H	1:A:2449:THR:HG21	1.66	0.59
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.02	0.59
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.84	0.59
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.02	0.59
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.67	0.59
1:A:2757:MET:CE	1:A:2912:CYS:CB	2.77	0.59
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.84	0.59
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.03	0.59
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.32	0.59
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.50	0.59
1:B:3631:MET:HE3	1:B:3698:MET:HG3	1.82	0.59
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.01	0.59
1:A:1802:LYS:NZ	4:A:5095:SO4:S	2.75	0.59
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.84	0.59
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.83	0.59
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.37	0.59
1:A:1534:PHE:HD2	1:A:1537:PHE:CE1	2.20	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.01	0.59
1:B:2423:GLY:N	3:B:5094:ANP:O1B	2.29	0.59
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.41	0.59
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.86	0.59
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.51	0.59
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.50	0.59
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.84	0.59
1:A:2080:LYS:HG2	1:A:2215:PHE:CD1	2.38	0.59
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.38	0.59
1:A:2757:MET:HE2	1:A:2912:CYS:CB	2.32	0.59
1:B:166:PRO:CB	1:B:1369:LYS:HB3	2.32	0.59
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.84	0.59
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.67	0.59
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.84	0.59
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.03	0.59
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.38	0.59
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.01	0.59
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.03	0.59
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.51	0.59
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.83	0.59
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.19	0.59
1:A:2425:THR:HG21	3:A:5094:ANP:O3G	2.02	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.84	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.32	0.58
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.03	0.58
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.24	0.58
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.84	0.58
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.58
1:A:1425:GLU:C	1:A:1425:GLU:OE1	2.42	0.58
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.83	0.58
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.06	0.58
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.82	0.58
1:A:1368:GLU:CG	1:A:1424:PHE:CE2	2.86	0.58
1:B:2517:LYS:CE	1:B:2520:GLU:OE1	2.50	0.58
1:B:3948:HIS:NE2	1:B:4072:ASN:CG	2.57	0.58
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.24	0.58
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.85	0.58
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.04	0.58
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.68	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:A:1774:LEU:HD21	1:A:1922:LYS:O	2.03	0.58
1:A:2563:SER:CB	1:A:2566:SER:OG	2.51	0.58
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.85	0.58
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.30	0.58
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.58
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.34	0.58
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.22	0.58
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.49	0.58
1:A:2755:HIS:O	1:A:2913:ILE:HG13	2.03	0.58
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.39	0.58
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.39	0.58
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.02	0.58
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.34	0.58
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.69	0.58
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.04	0.58
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.19	0.58
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.04	0.58
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.24	0.57
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.39	0.57
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.33	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.85	0.57
1:B:2224:SER:C	2:B:5093:ATP:H2	2.07	0.57
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.51	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.57	0.57
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.86	0.57
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.57	0.57
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.68	0.57
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.69	0.57
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.04	0.57
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.57
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.33	0.57
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.05	0.57
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.86	0.57
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.23	0.57
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.86	0.57
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.52	0.57
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.20	0.57
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.87	0.57
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.05	0.57
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.87	0.57
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.87	0.57
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.34	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.86	0.57
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.47	0.57
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.87	0.57
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.87	0.57
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.70	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57
1:B:2620:ARG:O	1:B:2623:THR:HG22	2.04	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.70	0.57
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.38	0.57
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.20	0.57
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.39	0.57
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.85	0.57
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.40	0.57
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.51	0.57
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.25	0.57
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.35	0.57
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.66	0.57
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.70	0.57
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.05	0.56
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.69	0.56
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.86	0.56
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.86	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.47	0.56
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.40	0.56
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.93	0.56
1:B:3810:SER:O	1:B:3838:TRP:HB2	2.04	0.56
1:A:2517:LYS:HG2	1:A:2520:GLU:HB2	1.87	0.56
1:A:3618:TYR:O	1:A:3622:GLY:N	2.37	0.56
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.05	0.56
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.20	0.56
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.69	0.56
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.20	0.56
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.86	0.56
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.71	0.56
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.20	0.56
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.39	0.56
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.41	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.87	0.56
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.87	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.05	0.56
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.71	0.56
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.21	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.56
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.56
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.88	0.56
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.41	0.56
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.84	0.56
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.88	0.56
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.87	0.56
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.87	0.56
1:A:2513:GLN:O	1:A:2526:ILE:CG1	2.50	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.87	0.56
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.87	0.56
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.87	0.56
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.21	0.56
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.70	0.56
1:A:3481:ILE:O	1:A:3483:ASP:N	2.35	0.56
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.06	0.56
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.19	0.55
1:A:2380:LEU:CD1	1:A:2577:ALA:HB1	2.30	0.55
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.70	0.55
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.71	0.55
1:B:216:PRO:CB	1:B:1424:PHE:CG	2.89	0.55
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.24	0.55
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.55
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.54	0.55
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.87	0.55
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.06	0.55
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.88	0.55
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.40	0.55
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.07	0.55
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	2.21	0.55
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.55
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.71	0.55
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.55
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.30	0.55
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.55
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2472:THR:CB	1:B:2524:VAL:HG22	2.37	0.55
1:A:1365:PHE:CE2	1:A:1420:TYR:CE2	2.94	0.55
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.18	0.55
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.42	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.87	0.55
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.89	0.55
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.71	0.55
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.39	0.55
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.06	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.35	0.55
1:B:2220:CYS:SG	2:B:5093:ATP:N1	2.79	0.55
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.87	0.55
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.42	0.55
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.37	0.55
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.25	0.55
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.90	0.55
1:B:2420:PRO:HB2	1:B:2620:ARG:HH21	1.69	0.55
1:B:2495:ASP:O	1:B:2498:GLY:N	2.39	0.55
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.35	0.55
1:A:1365:PHE:CD1	1:A:1365:PHE:N	2.74	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.89	0.55
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.07	0.55
1:A:2825:THR:O	1:A:2829:GLU:HG2	2.06	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.72	0.55
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.40	0.55
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.88	0.55
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.55	0.55
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.55
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.37	0.55
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:HE2	1.78	0.55
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.88	0.55
1:B:2891:ILE:HG21	1:B:2902:MET:HG3	1.89	0.55
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.35	0.55
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.34	0.55
1:A:1970:LEU:HD12	1:A:1970:LEU:C	2.27	0.55
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.41	0.55
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.37	0.55
1:A:3945:LEU:O	1:A:3948:HIS:O	2.24	0.55
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.89	0.55
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.36	0.55
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.42	0.54
1:A:3460:PRO:O	1:A:3463:SER:CB	2.55	0.54
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.72	0.54
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.88	0.54
1:B:1802:LYS:NZ	4:B:5096:SO4:O4	2.40	0.54
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.37	0.54
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.66	0.54
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.54
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.37	0.54
1:B:3023:LYS:HE2	1:B:3567:LEU:CD2	2.37	0.54
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.86	0.54
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.07	0.54
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.72	0.54
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.60	0.54
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.72	0.54
1:A:1969:GLY:O	1:A:1972:THR:HB	2.07	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.88	0.54
1:A:4084:SER:O	1:A:4088:LEU:HG	2.07	0.54
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.06	0.54
1:B:2424:LYS:HE2	1:B:2534:ALA:HB1	1.88	0.54
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.65	0.54
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.07	0.54
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.38	0.54
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.90	0.54
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.07	0.54
1:A:2064:GLN:HE22	1:A:2091:MET:HG3	1.73	0.54
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	2.08	0.54
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.07	0.54
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.54
1:A:2566:SER:O	1:A:2570:ILE:HD12	2.08	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.95	0.54
1:B:3945:LEU:O	1:B:3948:HIS:O	2.25	0.54
1:A:1826:PHE:CG	1:A:1826:PHE:O	2.61	0.54
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.38	0.54
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.42	0.54
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.90	0.54
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.86	0.54
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.08	0.54
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2412:ARG:HH11	1:A:2412:ARG:CB	2.16	0.54
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.90	0.54
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.91	0.54
1:B:2412:ARG:HH11	1:B:2412:ARG:HB2	1.73	0.54
1:B:2420:PRO:CB	1:B:2620:ARG:NH2	2.71	0.54
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.42	0.54
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.07	0.53
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.73	0.53
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	1.90	0.53
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.42	0.53
1:B:2425:THR:HG23	1:B:2485:PHE:HE2	1.71	0.53
1:B:2514:GLY:HA3	1:B:2525:THR:HA	1.90	0.53
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.89	0.53
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.71	0.53
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.28	0.53
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.37	0.53
1:B:3509:LEU:HD11	1:B:3513:VAL:HG21	1.90	0.53
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.90	0.53
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.29	0.53
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.90	0.53
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.91	0.53
1:A:2391:VAL:HG23	1:A:2426:MET:SD	2.47	0.53
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.83	0.53
1:A:2154:PHE:N	1:A:2154:PHE:HD1	2.05	0.53
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.53
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.44	0.53
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	1.91	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.09	0.53
1:A:2410:SER:O	1:A:2411:LYS:CG	2.57	0.53
1:A:2640:THR:HG23	1:A:2643:SER:H	1.74	0.53
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.55	0.53
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.44	0.53
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.24	0.53
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.09	0.53
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.21	0.53
1:A:1365:PHE:CE2	1:A:1420:TYR:CZ	2.97	0.53
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.44	0.53
1:A:2154:PHE:N	1:A:2154:PHE:CD1	2.74	0.53
1:A:2410:SER:O	1:A:2411:LYS:HG3	2.08	0.53
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.57	0.53
1:B:2467:THR:O	1:B:2471:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.08	0.53
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.44	0.53
1:A:2424:LYS:HE2	3:A:5094:ANP:O1G	2.08	0.53
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.91	0.53
1:B:1759:LYS:HE3	1:B:1761:GLU:OE2	2.09	0.53
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.89	0.53
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.48	0.53
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.57	0.53
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.20	0.53
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.70	0.53
1:A:2220:CYS:SG	1:A:2221:SER:N	2.82	0.53
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.30	0.53
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.39	0.53
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.73	0.53
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.72	0.53
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.90	0.53
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.74	0.53
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.09	0.53
1:B:2224:SER:O	2:B:5093:ATP:C2	2.53	0.53
1:B:4021:LEU:HD23	1:B:4023:ILE:HG12	1.91	0.53
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.09	0.52
1:B:2472:THR:HG21	1:B:2524:VAL:CG2	2.39	0.52
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.37	0.52
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.10	0.52
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.57	0.52
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.09	0.52
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.52
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.10	0.52
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.91	0.52
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.44	0.52
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.74	0.52
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.24	0.52
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.57	0.52
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.39	0.52
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.52
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.44	0.52
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.92	0.52
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.92	0.52
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.90	0.52
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.09	0.52
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3632:LEU:HD13	1:B:3644:ILE:HD13	1.92	0.52
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.91	0.52
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.75	0.52
1:A:1535:PRO:O	1:A:1841:ILE:CD1	2.58	0.52
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.89	0.52
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.91	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.10	0.52
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.45	0.52
1:B:2476:LYS:H	1:B:2476:LYS:CD	2.23	0.52
1:B:3737:THR:CB	1:B:3740:THR:CB	2.87	0.52
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.44	0.52
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.31	0.52
1:B:3460:PRO:O	1:B:3463:SER:CB	2.58	0.52
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.40	0.52
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.44	0.52
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.09	0.52
1:A:2494:LEU:HD12	1:A:2494:LEU:O	2.10	0.52
1:A:2834:LEU:HD21	1:A:2885:LEU:HD21	1.92	0.52
1:A:3631:MET:HE3	1:A:3698:MET:HG3	1.91	0.52
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.82	0.52
1:A:65:THR:O	1:A:66:GLN:CB	2.57	0.52
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.10	0.52
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.56	0.52
1:B:3618:TYR:O	1:B:3622:GLY:N	2.38	0.52
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.74	0.51
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	2.98	0.51
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	2.99	0.51
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.41	0.51
1:B:1826:PHE:CE1	1:B:1853:LEU:HD22	2.45	0.51
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.39	0.51
1:B:2220:CYS:HB2	2:B:5093:ATP:C6	2.45	0.51
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.92	0.51
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.92	0.51
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.43	0.51
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.11	0.51
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.91	0.51
1:A:1992:LYS:HG2	1:A:2024:SER:CB	2.38	0.51
1:B:65:THR:O	1:B:66:GLN:CB	2.58	0.51
1:B:2428:MET:HE2	1:B:2485:PHE:HD1	1.74	0.51
1:B:2428:MET:HE2	1:B:2485:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.10	0.51
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.75	0.51
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.92	0.51
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.93	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.38	0.51
1:B:1968:PHE:HD1	1:B:1968:PHE:N	2.08	0.51
1:B:2154:PHE:N	1:B:2154:PHE:CD1	2.78	0.51
1:B:2425:THR:HG23	1:B:2485:PHE:CE2	2.45	0.51
1:B:2470:GLY:CA	1:B:2473:LEU:HD21	2.20	0.51
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.93	0.51
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.76	0.51
1:B:1826:PHE:HE1	1:B:1853:LEU:HD22	1.76	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.45	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.91	0.51
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.83	0.51
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.40	0.51
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.41	0.51
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.91	0.51
1:B:3737:THR:CB	1:B:3740:THR:HB	2.41	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.88	0.51
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.93	0.51
1:B:2368:PHE:CD1	1:B:2368:PHE:N	2.77	0.51
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.11	0.51
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.41	0.51
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.76	0.51
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.51
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.43	0.51
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.51
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.58	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.91	0.51
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.94	0.51
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.46	0.51
1:B:3023:LYS:CE	1:B:3567:LEU:HD23	2.41	0.51
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.44	0.51
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.46	0.51
1:B:2472:THR:HB	1:B:2524:VAL:HG22	1.92	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:B:1462:ASN:CB	1:B:1465:ILE:HG22	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.94	0.50
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.30	0.50
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.46	0.50
1:A:3569:GLU:O	1:A:3573:SER:OG	2.22	0.50
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.11	0.50
1:B:1929:ILE:H	1:B:1929:ILE:HD12	1.75	0.50
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.93	0.50
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.59	0.50
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.12	0.50
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.32	0.50
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.95	0.50
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.92	0.50
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.69	0.50
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.41	0.50
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.93	0.50
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.50
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.91	0.50
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.47	0.50
1:A:2048:SER:H	2:A:5093:ATP:N6	2.08	0.50
1:A:2410:SER:O	1:A:2411:LYS:CB	2.57	0.50
1:A:2514:GLY:HA3	1:A:2525:THR:HA	1.93	0.50
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.41	0.50
1:B:1939:PHE:H	1:B:1939:PHE:HD1	1.58	0.50
1:B:1968:PHE:N	1:B:1968:PHE:CD1	2.79	0.50
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.51	0.50
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.25	0.50
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.27	0.50
1:A:162:LEU:HA	1:A:165:ASP:O	2.11	0.50
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.59	0.50
1:A:1822:CYS:SG	1:A:1850:PHE:CA	2.97	0.50
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.50
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.25	0.50
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.12	0.50
1:A:2201:HIS:CE1	1:A:2497:TYR:HB3	2.47	0.50
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.35	0.50
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.94	0.50
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.94	0.50
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.45	0.50
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.93	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.94	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.11	0.49
1:B:2620:ARG:HH12	1:B:2910:ASN:ND2	2.10	0.49
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.93	0.49
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.47	0.49
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.93	0.49
1:A:2003:LEU:HD23	1:A:2006:LEU:HD12	1.93	0.49
1:A:2492:PRO:HB2	1:A:2502:VAL:HG11	1.93	0.49
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.25	0.49
1:A:3848:LEU:CD2	1:A:3852:LYS:HE3	2.41	0.49
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	2.13	0.49
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.77	0.49
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.29	0.49
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.42	0.49
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.27	0.49
1:A:2249:LEU:HD21	1:A:2302:PHE:HD2	1.77	0.49
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.12	0.49
1:A:3737:THR:CB	1:A:3740:THR:HB	2.43	0.49
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.11	0.49
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.42	0.49
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.12	0.49
1:A:2563:SER:C	1:A:2565:LYS:H	2.15	0.49
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.12	0.49
1:B:1983:LEU:HD11	1:B:2000:ARG:HH21	1.76	0.49
1:B:3461:ILE:C	1:B:3463:SER:H	2.15	0.49
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.33	0.49
1:B:1535:PRO:O	1:B:1841:ILE:HD11	2.13	0.49
1:B:2421:GLY:C	3:B:5094:ANP:O1B	2.51	0.49
1:B:2640:THR:HG23	1:B:2643:SER:H	1.77	0.49
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.12	0.49
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.93	0.49
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.48	0.49
1:A:2853:LEU:HD21	1:A:2870:GLU:HG3	1.94	0.49
1:A:2941:THR:HG22	1:A:2942:ASP:N	2.24	0.49
1:B:2380:LEU:HD11	1:B:2577:ALA:HB2	1.88	0.49
1:B:2620:ARG:NH1	1:B:2910:ASN:CG	2.65	0.49
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.12	0.49
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.94	0.49
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.95	0.49
1:A:2936:ILE:HG22	1:A:2962:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.95	0.49
1:B:4084:SER:O	1:B:4088:LEU:HG	2.13	0.49
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.94	0.49
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.78	0.49
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	2.47	0.49
1:A:2080:LYS:O	1:A:2084:TRP:CD1	2.65	0.49
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	1.95	0.49
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.49
1:B:2136:ARG:O	1:B:2140:ASP:O	2.30	0.49
1:B:2154:PHE:N	1:B:2154:PHE:HD1	2.10	0.49
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.94	0.49
1:A:2988:SER:CB	1:A:2989:PRO:CD	2.66	0.49
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.95	0.49
1:A:3693:LYS:HE3	1:A:4080:GLU:HB3	1.94	0.49
1:B:162:LEU:HA	1:B:165:ASP:O	2.12	0.49
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.94	0.49
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.95	0.49
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.39	0.48
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	1.94	0.48
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.95	0.48
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.42	0.48
1:B:1801:GLY:N	4:B:5096:SO4:O4	2.46	0.48
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.48
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.95	0.48
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.94	0.48
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.94	0.48
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.48
1:A:2226:ILE:HG23	1:A:2288:VAL:HG21	1.95	0.48
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.48	0.48
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.95	0.48
1:B:1802:LYS:NZ	4:B:5096:SO4:S	2.86	0.48
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.13	0.48
1:B:2441:VAL:HB	1:B:2484:LEU:HD23	1.95	0.48
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	1.95	0.48
1:B:2046:GLY:O	1:B:2228:HIS:HB2	2.13	0.48
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.94	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:CD2	2.92	0.48
1:A:2822:ILE:O	1:A:2822:ILE:HG13	2.14	0.48
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.14	0.48
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.94	0.48
1:B:2122:THR:O	1:B:2123:LEU:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.94	0.48
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.78	0.48
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.48
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.48
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.48
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.79	0.48
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.48	0.48
1:B:2623:THR:CB	3:B:5094:ANP:O2'	2.61	0.48
1:B:2833:THR:CG2	1:B:2841:PRO:HD2	2.43	0.48
1:B:3023:LYS:NZ	1:B:3571:ASN:HD21	2.11	0.48
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.67	0.48
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.13	0.48
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.96	0.48
1:A:2314:ILE:HG22	1:A:2318:ILE:HD12	1.96	0.48
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.13	0.48
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.94	0.48
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.47	0.48
1:B:2102:TYR:HB2	1:B:2152:VAL:HG22	1.95	0.48
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.96	0.48
1:B:2473:LEU:CD2	1:B:2525:THR:HB	2.43	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.86	0.48
1:A:2425:THR:OG1	3:A:5094:ANP:O2A	2.31	0.48
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.73	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.96	0.48
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.49	0.48
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.94	0.48
1:B:3348:ILE:HA	1:B:3351:ARG:HG2	1.95	0.48
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.75	0.48
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.96	0.48
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.41	0.48
1:B:23:LEU:O	1:B:25:GLU:N	2.47	0.48
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.81	0.48
1:B:2106:THR:HG1	1:B:2154:PHE:HD2	1.61	0.48
1:B:4022:GLN:O	1:B:4022:GLN:HG2	2.14	0.48
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.94	0.47
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.96	0.47
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.34	0.47
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.95	0.47
1:B:3566:LEU:HD13	1:B:3570:LEU:HD12	1.96	0.47
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:PHE:CD2	1:A:1537:PHE:CE1	3.02	0.47
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.96	0.47
1:A:2354:SER:OG	1:A:2357:SER:CB	2.62	0.47
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.14	0.47
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.54	0.47
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	1.95	0.47
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.45	0.47
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.14	0.47
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.96	0.47
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.14	0.47
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.95	0.47
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.14	0.47
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	1.96	0.47
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.95	0.47
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.97	0.47
1:A:3911:TRP:HH2	1:A:3926:VAL:HG13	1.79	0.47
1:B:40:TRP:O	1:B:44:LYS:N	2.48	0.47
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.96	0.47
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.96	0.47
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.25	0.47
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.47
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.62	0.47
1:A:1495:THR:CG2	1:A:1497:ILE:HG22	2.41	0.47
1:A:1527:LEU:HD21	1:A:1546:LEU:HD23	1.96	0.47
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.95	0.47
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.44	0.47
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.97	0.47
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.14	0.47
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.14	0.47
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.96	0.47
1:A:2463:ASN:O	1:A:2475:PRO:HD2	2.15	0.47
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.15	0.47
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.97	0.47
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.47
1:A:1365:PHE:HE2	1:A:1420:TYR:CZ	2.33	0.47
1:A:2122:THR:O	1:A:2123:LEU:C	2.53	0.47
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.15	0.47
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.15	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.97	0.47
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.79	0.47
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.49	0.47
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.93	0.47
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	1.97	0.47
1:B:2061:TYR:O	1:B:2064:GLN:HG2	2.14	0.47
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.15	0.47
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.49	0.47
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.15	0.47
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.47
1:B:2472:THR:CG2	1:B:2524:VAL:CG2	2.86	0.47
1:A:1750:SER:HA	1:A:1755:LEU:HD23	1.96	0.47
1:A:2422:SER:N	3:A:5094:ANP:O1B	2.47	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.97	0.47
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	1.97	0.47
1:B:2276:LEU:CD2	1:B:2415:ILE:HG21	2.45	0.47
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.96	0.47
1:B:4020:ASN:ND2	1:B:4028:ARG:HD3	2.30	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.98	0.46
1:A:2757:MET:HE3	1:A:2912:CYS:CB	2.38	0.46
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	1.96	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.96	0.46
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.81	0.46
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.94	0.46
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.46	0.46
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.46
1:B:2441:VAL:HG21	1:B:2482:LEU:HD21	1.96	0.46
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.96	0.46
1:B:3307:LEU:HA	1:B:3310:THR:HB	1.97	0.46
1:A:1592:LEU:CD1	1:A:1596:ILE:HD12	2.45	0.46
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	1.97	0.46
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.51	0.46
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.96	0.46
1:B:2354:SER:OG	1:B:2357:SER:CB	2.63	0.46
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.15	0.46
1:B:2938:MET:SD	1:B:3321:ILE:HG21	2.55	0.46
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.97	0.46
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.98	0.46
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.63	0.46
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.16	0.46
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.97	0.46
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	1.97	0.46
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.45	0.46
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.16	0.46
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.15	0.46
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.51	0.46
1:A:3869:GLU:O	1:A:3870:LYS:C	2.54	0.46
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.84	0.46
1:B:1367:ILE:H	1:B:1367:ILE:HD12	1.80	0.46
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.29	0.46
1:B:2220:CYS:HG	1:B:2224:SER:HB3	1.80	0.46
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.73	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.96	0.46
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.97	0.46
1:A:1744:LEU:HA	1:A:1760:PHE:HE2	1.75	0.46
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.46
1:A:3911:TRP:CH2	1:A:3926:VAL:HG13	2.50	0.46
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.46	0.46
1:B:1983:LEU:HD13	1:B:2000:ARG:HE	1.80	0.46
1:B:2137:VAL:O	1:B:2141:ILE:HG23	2.16	0.46
1:A:2061:TYR:CD1	1:A:2091:MET:HE3	2.47	0.46
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD3	1.81	0.46
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.51	0.46
1:B:1421:TYR:O	1:B:1425:GLU:CA	2.63	0.46
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.43	0.46
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.14	0.46
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.80	0.46
1:B:2493:LYS:HG3	1:B:2494:LEU:N	2.30	0.46
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.97	0.46
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.50	0.46
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.45	0.46
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.15	0.46
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.51	0.46
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.98	0.46
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.46
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.46
1:A:1802:LYS:NZ	4:A:5095:SO4:O1	2.40	0.46
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.97	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.98	0.46
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.98	0.46
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3473:ALA:HB3	1:A:3476:ARG:HG3	1.97	0.46
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.97	0.46
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.46	0.46
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.50	0.46
1:B:2563:SER:C	1:B:2565:LYS:H	2.18	0.46
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.97	0.46
1:B:1969:GLY:O	1:B:1972:THR:HB	2.15	0.46
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	1.97	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.94	0.46
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.45	0.46
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.90	0.46
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.16	0.46
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.97	0.46
1:A:215:PRO:C	1:A:3475:ASN:ND2	2.69	0.45
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.16	0.45
1:A:1802:LYS:O	1:A:1806:VAL:HG23	2.16	0.45
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.56	0.45
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.98	0.45
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.45	0.45
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.64	0.45
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.96	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.15	0.45
1:A:3322:GLY:HA2	1:A:3325:ILE:HD12	1.98	0.45
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.98	0.45
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.45
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.50	0.45
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.97	0.45
1:B:2380:LEU:HD12	1:B:2577:ALA:HB2	1.85	0.45
1:B:2420:PRO:CB	1:B:2620:ARG:HH21	2.29	0.45
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.98	0.45
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.81	0.45
1:A:1365:PHE:CZ	1:A:1420:TYR:CG	3.05	0.45
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.98	0.45
1:A:2490:ASN:HB3	1:A:2546:MET:HE1	1.98	0.45
1:A:2563:SER:CB	1:A:2566:SER:H	2.19	0.45
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.45
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.98	0.45
1:A:1365:PHE:HZ	1:A:1420:TYR:CE1	2.31	0.45
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.17	0.45
1:A:1563:LYS:HE2	1:A:1585:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2081:THR:HG22	1:A:2085:LYS:HD2	1.98	0.45
1:A:3592:LYS:O	1:A:3596:ASN:N	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:3832:SER:O	1:A:3836:GLY:N	2.43	0.45
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.17	0.45
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.49	0.45
1:B:2471:LEU:O	1:B:2473:LEU:HG	2.16	0.45
1:B:3965:SER:HA	1:B:3968:LEU:HD12	1.98	0.45
1:A:23:LEU:O	1:A:25:GLU:N	2.50	0.45
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.99	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.50	0.45
1:A:3342:ARG:NH2	1:A:3393:ASN:OD1	2.47	0.45
1:A:3926:VAL:HG11	1:A:4042:ARG:HG2	1.97	0.45
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.99	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HB3	2.52	0.45
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.17	0.45
1:B:2839:ASP:O	1:B:2841:PRO:HD3	2.17	0.45
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.98	0.45
1:A:1919:PHE:CD1	1:A:3996:GLY:HA2	2.51	0.45
1:A:2412:ARG:HD3	1:A:2555:ALA:HB2	1.99	0.45
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.57	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.37	0.45
1:B:1495:THR:HB	1:B:1498:GLU:CG	2.47	0.45
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.18	0.45
1:B:3461:ILE:C	1:B:3463:SER:N	2.68	0.45
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.22	0.45
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.52	0.45
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.47	0.45
1:B:3946:VAL:HB	1:B:3947:PRO:HA	1.98	0.45
1:A:1750:SER:HB2	1:A:1755:LEU:CD2	2.47	0.45
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.17	0.45
1:A:1934:LEU:HD22	1:A:1945:LEU:HD12	1.98	0.45
1:A:1984:ILE:CG2	1:A:1989:GLU:HG3	2.46	0.45
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.82	0.45
1:A:2755:HIS:O	1:A:2913:ILE:N	2.48	0.45
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.98	0.45
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.46	0.45
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.82	0.45
1:A:3903:ILE:O	1:A:3907:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3994:TYR:O	1:A:3998:ILE:HD12	2.16	0.45
1:A:4022:GLN:O	1:A:4023:ILE:C	2.56	0.45
1:B:2155:ASP:OD1	1:B:2195:GLU:OE2	2.34	0.45
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.99	0.45
1:B:2354:SER:H	1:B:2357:SER:HB2	1.81	0.45
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.45	0.45
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	1.99	0.45
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.46	0.45
1:A:1469:LEU:HD13	1:A:1523:LEU:HD21	1.99	0.45
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.82	0.45
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.52	0.45
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.52	0.45
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.82	0.45
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.52	0.45
1:A:1365:PHE:CE2	1:A:1420:TYR:CD2	3.04	0.45
1:A:1970:LEU:HD12	1:A:1971:ARG:CA	2.47	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CE2	3.04	0.45
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.99	0.45
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.52	0.45
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.16	0.45
1:B:2203:THR:HG23	1:B:2204:PRO:HD2	1.99	0.45
1:B:2294:LEU:HB3	1:B:2317:LEU:HD22	1.98	0.45
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.98	0.45
1:B:2508:GLN:HG2	1:B:2512:LYS:HG3	1.97	0.45
1:B:2755:HIS:HD2	1:B:2911:ARG:HB3	1.82	0.45
1:B:3862:THR:HB	1:B:3865:ALA:HB2	1.99	0.45
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.82	0.44
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.50	0.44
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.51	0.44
1:B:1421:TYR:CD2	1:B:1425:GLU:CG	2.98	0.44
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.81	0.44
1:A:1527:LEU:HD22	1:A:1545:LEU:HD22	1.97	0.44
1:A:2424:LYS:HA	1:A:2559:LEU:HD12	1.99	0.44
1:A:2745:ILE:HG12	1:A:2756:MET:CE	2.42	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.99	0.44
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.47	0.44
1:B:2109:LEU:HB3	1:B:2113:SER:HB2	2.00	0.44
1:B:3481:ILE:O	1:B:3483:ASP:N	2.46	0.44
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.29	0.44
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.87	0.44
1:A:2356:TYR:CE1	1:A:2399:LYS:HD2	2.52	0.44
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.51	0.44
1:B:1995:VAL:HG22	1:B:2022:PHE:CD2	2.52	0.44
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.00	0.44
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	1.99	0.44
1:A:1392:LEU:C	1:A:1392:LEU:CD1	2.83	0.44
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.47	0.44
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.20	0.44
1:A:1982:PRO:O	1:A:1985:SER:HB2	2.18	0.44
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.32	0.44
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.46	0.44
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.99	0.44
1:B:3636:GLY:CA	1:B:3642:TYR:O	2.66	0.44
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.17	0.44
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	2.00	0.44
1:B:1779:PHE:O	1:B:1783:THR:HG22	2.18	0.44
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.17	0.44
1:B:3998:ILE:HG22	1:B:4004:LEU:HG	1.97	0.44
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.32	0.44
1:B:2421:GLY:CA	3:B:5094:ANP:O1B	2.66	0.44
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.00	0.44
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.53	0.44
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.47	0.44
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.82	0.44
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.17	0.44
1:A:2423:GLY:N	3:A:5094:ANP:O1B	2.39	0.44
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	2.00	0.44
1:A:3798:PHE:HA	1:A:3801:ILE:HG12	2.00	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.71	0.44
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.44
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	2.00	0.44
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	2.00	0.44
1:A:3473:ALA:CB	1:A:3476:ARG:HG3	2.48	0.44
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.31	0.44
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.18	0.44
1:B:2389:ASP:HB3	1:B:2433:ARG:HH11	1.83	0.44
1:B:2572:GLU:CG	1:B:2590:GLU:HG3	2.47	0.44
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.58	0.44
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.53	0.43
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.53	0.43
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.25	0.43
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.18	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	2.00	0.43
1:B:3911:TRP:CH2	1:B:3926:VAL:CG1	3.01	0.43
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.33	0.43
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.53	0.43
1:A:2201:HIS:CE1	1:A:2497:TYR:O	2.71	0.43
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.19	0.43
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.33	0.43
1:A:3845:GLN:NE2	1:A:3882:ASP:O	2.51	0.43
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.39	0.43
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.18	0.43
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.43
1:A:2099:ASN:HB3	1:A:2151:TRP:HE1	1.83	0.43
1:A:2203:THR:HG23	1:A:2204:PRO:HD2	1.99	0.43
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.43
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	2.00	0.43
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.17	0.43
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.83	0.43
1:B:1540:LEU:HD23	1:B:1540:LEU:HA	1.72	0.43
1:B:3592:LYS:O	1:B:3596:ASN:N	2.51	0.43
1:B:3832:SER:O	1:B:3836:GLY:N	2.46	0.43
1:B:3848:LEU:O	1:B:3849:SER:C	2.57	0.43
1:A:1536:ARG:CD	1:A:1841:ILE:HD13	2.48	0.43
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.18	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.31	0.43
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.65	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:HE1	1.83	0.43
1:B:2201:HIS:CE1	1:B:2497:TYR:CA	3.01	0.43
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.83	0.43
1:B:3886:ALA:N	1:B:3887:PRO:CD	2.78	0.43
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.65	0.43
1:A:1934:LEU:HD13	1:A:1945:LEU:HB2	2.01	0.43
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.43
1:A:3800:LEU:HA	1:A:3803:LEU:HD12	1.99	0.43
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.83	0.43
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.19	0.43
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:B:4065:LEU:C	1:B:4065:LEU:HD12	2.39	0.43
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.43
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	2.00	0.43
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.71	0.43
1:B:2517:LYS:HD2	1:B:2524:VAL:CG2	2.49	0.43
1:B:3462:ILE:O	1:B:3465:LEU:N	2.51	0.43
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.18	0.43
1:A:1872:LEU:HG	1:A:1888:LEU:HD21	2.00	0.43
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.65	0.43
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.99	0.43
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	2.01	0.43
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.43
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.49	0.43
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.18	0.43
1:B:2425:THR:CG2	1:B:2485:PHE:HE2	2.32	0.43
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.19	0.43
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	2.01	0.43
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	2.01	0.43
1:A:3788:MET:O	1:A:3788:MET:HG3	2.19	0.43
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ3	1.81	0.43
1:B:2220:CYS:SG	1:B:2221:SER:N	2.92	0.43
1:B:2510:MET:O	1:B:2513:GLN:NE2	2.52	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.51	0.43
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.51	0.43
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	2.01	0.43
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.54	0.43
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.19	0.43
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.19	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:CE1	2.54	0.43
1:B:2446:SER:H	1:B:2449:THR:HG21	1.80	0.43
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.52	0.43
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.19	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.19	0.43
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.80	0.43
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.67	0.43
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.02	0.43
1:B:2368:PHE:O	1:B:2369:SER:OG	2.25	0.43
1:A:1469:LEU:CD1	1:A:1523:LEU:CD2	2.97	0.42
1:A:1645:PHE:CZ	1:A:1768:ARG:HD2	2.52	0.42
1:A:2170:LEU:HB3	1:A:2209:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2220:CYS:SG	1:A:2224:SER:HB3	2.59	0.42
1:A:4023:ILE:HG13	1:A:4029:ILE:HD12	2.01	0.42
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	2.01	0.42
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.85	0.42
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.54	0.42
1:A:3326:ILE:HG22	1:A:3330:TYR:CE2	2.54	0.42
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.20	0.42
1:A:3930:PHE:HE2	1:A:4029:ILE:HD13	1.83	0.42
1:B:2001:VAL:O	1:B:2004:PRO:HD2	2.19	0.42
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.42
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.42
1:B:2220:CYS:SG	2:B:5093:ATP:N6	2.93	0.42
1:B:2220:CYS:HB2	2:B:5093:ATP:N6	2.33	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	2.00	0.42
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.42
1:A:2742:ILE:HG23	1:A:2773:VAL:HG22	2.00	0.42
1:A:3409:ASP:HA	1:A:3410:PRO:HD3	1.93	0.42
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.54	0.42
1:B:1630:ILE:HG21	1:B:1655:MET:SD	2.57	0.42
1:B:1870:ASN:O	1:B:1874:VAL:HG23	2.19	0.42
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.31	0.42
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.01	0.42
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.19	0.42
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.27	0.42
1:A:4022:GLN:O	1:A:4022:GLN:HG2	2.19	0.42
1:B:2224:SER:C	2:B:5093:ATP:C2	2.92	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:B:3431:PHE:CZ	1:B:3458:PHE:HD1	2.38	0.42
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	2.01	0.42
1:A:1365:PHE:N	1:A:1365:PHE:HD1	2.17	0.42
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.50	0.42
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	2.00	0.42
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.42
1:A:4006:VAL:HG13	1:A:4009:LYS:HE2	2.01	0.42
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	2.01	0.42
1:B:4033:LEU:HD23	1:B:4033:LEU:HA	1.84	0.42
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.19	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:B:1656:TRP:O	1:B:1660:VAL:HG12	2.18	0.42
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	2.01	0.42
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.34	0.42
1:A:2737:SER:HB2	1:A:2924:THR:HG21	2.01	0.42
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.40	0.42
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.80	0.42
1:B:23:LEU:C	1:B:25:GLU:N	2.73	0.42
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	2.02	0.42
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.55	0.42
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.23	0.42
1:B:2467:THR:HG22	1:B:2468:SER:N	2.34	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.53	0.42
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.90	0.42
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.40	0.42
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.55	0.42
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.01	0.42
1:B:1531:ARG:HD2	1:B:1538:TYR:HA	2.01	0.42
1:B:1660:VAL:CG1	1:B:1728:TRP:CH2	3.02	0.42
1:B:2114:LEU:HA	1:B:2129:LEU:HB3	2.02	0.42
1:A:1769:LEU:HD11	1:A:1804:GLU:HB3	2.01	0.42
1:A:2354:SER:H	1:A:2357:SER:HB2	1.85	0.42
1:A:2799:LEU:HD13	1:A:2840:ILE:CD1	2.49	0.42
1:A:3304:GLU:C	1:A:3306:TRP:H	2.23	0.42
1:A:3462:ILE:O	1:A:3465:LEU:N	2.48	0.42
1:A:3509:LEU:HG	1:A:3513:VAL:HG21	2.02	0.42
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.20	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.42
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.50	0.42
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	2.02	0.42
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.42
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.55	0.42
1:A:3600:LYS:HA	1:A:3603:GLU:HG2	2.01	0.42
1:A:3671:VAL:CA	1:A:3674:ILE:HG22	2.49	0.42
1:B:1593:ASN:ND2	1:B:1621:THR:OG1	2.47	0.42
1:B:2336:ARG:HG2	1:B:2355:ASP:OD1	2.19	0.42
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:A:3725:VAL:HA	1:A:3730:SER:O	2.19	0.41
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.80	0.41
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.19	0.41
1:B:1983:LEU:CD1	1:B:2000:ARG:HH21	2.33	0.41
1:B:1992:LYS:CG	1:B:2024:SER:CB	2.83	0.41
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.76	0.41
1:B:2754:GLY:HA3	1:B:2886:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.41
1:B:3002:LEU:HD21	1:B:3370:LEU:HD11	2.02	0.41
1:B:3303:LYS:O	1:B:3306:TRP:HD1	2.03	0.41
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.19	0.41
1:A:1823:ASP:HB3	1:A:1852:ARG:O	2.15	0.41
1:A:2034:ILE:HG13	1:A:2061:TYR:CE2	2.55	0.41
1:A:2226:ILE:HG23	1:A:2288:VAL:CG2	2.49	0.41
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.35	0.41
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.60	0.41
1:A:3373:LEU:HD13	1:A:3557:LEU:HD13	2.02	0.41
1:A:3979:ASN:OD1	1:A:3979:ASN:N	2.51	0.41
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.02	0.41
1:B:3901:PRO:HG2	1:B:3906:THR:HG23	2.01	0.41
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.20	0.41
1:A:1671:LYS:HA	1:A:1671:LYS:HD3	1.96	0.41
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.55	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.02	0.41
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.56	0.41
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	2.02	0.41
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.02	0.41
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	2.01	0.41
1:B:1939:PHE:CD1	1:B:1939:PHE:N	2.88	0.41
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.31	0.41
1:A:1697:LYS:O	1:A:1701:LEU:HG	2.20	0.41
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.49	0.41
1:A:2279:ARG:HH11	1:A:2279:ARG:HD2	1.66	0.41
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.77	0.41
1:B:1536:ARG:NE	1:B:1841:ILE:HD13	2.35	0.41
1:B:2661:VAL:HG12	1:B:2916:TRP:CD2	2.55	0.41
1:B:2938:MET:SD	1:B:3321:ILE:CG2	3.09	0.41
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.35	0.41
1:A:2099:ASN:HB3	1:A:2151:TRP:NE1	2.34	0.41
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	2.02	0.41
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.20	0.41
1:B:2080:LYS:O	1:B:2081:THR:C	2.59	0.41
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.41
1:B:4022:GLN:O	1:B:4023:ILE:C	2.58	0.41
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.36	0.41
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.41
1:A:3367:ILE:O	1:A:3371:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3930:PHE:CE2	1:A:4029:ILE:HD13	2.55	0.41
1:B:1774:LEU:HA	1:B:1777:ILE:HD12	2.02	0.41
1:B:1832:SER:HB3	1:B:1882:LEU:HD22	2.03	0.41
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.40	0.41
1:B:3584:MET:HA	1:B:3587:LEU:HD12	2.03	0.41
1:A:1496:THR:O	1:A:1499:VAL:HG23	2.21	0.41
1:A:1866:GLN:O	1:A:1870:ASN:HB2	2.21	0.41
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.85	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.69	0.41
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.35	0.41
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	2.03	0.41
1:B:2034:ILE:CD1	1:B:2061:TYR:CZ	3.03	0.41
1:B:2290:LEU:HD13	1:B:2407:LEU:HD23	2.02	0.41
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.55	0.41
1:B:3924:TRP:CD1	1:B:3924:TRP:C	2.94	0.41
1:A:215:PRO:C	1:A:3475:ASN:HD21	2.24	0.41
1:A:1406:LYS:HE2	1:A:1406:LYS:HB3	1.95	0.41
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.20	0.41
1:A:1795:PHE:CE1	1:A:1920:SER:HB3	2.55	0.41
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	2.02	0.41
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	2.01	0.41
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.03	0.41
1:B:1826:PHE:CE1	1:B:1853:LEU:CD2	3.04	0.41
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.85	0.41
1:B:2079:GLY:HA2	2:B:5093:ATP:H5'2	2.02	0.41
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	2.03	0.41
1:B:2428:MET:HG2	1:B:2485:PHE:CE1	2.55	0.41
1:B:3846:MET:HG3	1:B:3847:SER:N	2.35	0.41
1:A:2938:MET:HG2	1:A:3321:ILE:HG12	2.03	0.41
1:A:3430:SER:HB2	1:A:3453:GLN:HB3	2.02	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:ND2	2.19	0.41
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	2.02	0.41
1:B:1702:LEU:O	1:B:1706:LEU:HG	2.21	0.41
1:B:2000:ARG:O	1:B:2004:PRO:HG2	2.21	0.41
1:B:2295:ILE:HG12	1:B:2314:ILE:HD12	2.02	0.41
1:B:2422:SER:N	3:B:5094:ANP:O1B	2.54	0.41
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.78	0.41
1:B:2572:GLU:HG3	1:B:2590:GLU:HG3	2.02	0.41
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.50	0.41
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.46	0.41
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.21	0.41
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	2.02	0.41
1:A:1535:PRO:C	1:A:1841:ILE:CD1	2.79	0.41
1:A:1620:PHE:CE1	1:A:1743:ASP:HB3	2.55	0.41
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.88	0.41
1:A:2320:ARG:O	1:A:2323:LEU:HB3	2.20	0.41
1:A:3642:TYR:N	1:A:3642:TYR:CD1	2.87	0.41
1:B:1637:GLU:HG2	1:B:1686:LYS:HG3	2.03	0.41
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.41	0.41
1:A:1704:GLU:O	1:A:1707:HIS:HB3	2.21	0.40
1:A:1838:ILE:HD11	1:A:1845:GLY:N	2.37	0.40
1:A:1853:LEU:HB2	1:A:1858:LEU:HD12	2.03	0.40
1:A:2199:LEU:O	1:A:2200:ASP:C	2.59	0.40
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.40
1:A:3848:LEU:O	1:A:3849:SER:C	2.57	0.40
1:A:3862:THR:HB	1:A:3865:ALA:HB2	2.03	0.40
1:A:4065:LEU:HD12	1:A:4065:LEU:O	2.21	0.40
1:B:2039:LYS:HG2	1:B:2049:MET:HG3	2.02	0.40
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.28	0.40
1:B:2178:LEU:HB2	1:B:2182:GLU:H	1.86	0.40
1:B:2476:LYS:CD	1:B:2476:LYS:N	2.84	0.40
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.03	0.40
1:A:1592:LEU:HD13	1:A:1596:ILE:CD1	2.50	0.40
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.86	0.40
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.40
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.89	0.40
1:A:3978:ASN:O	1:A:3981:PRO:HD2	2.19	0.40
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.86	0.40
1:B:1743:ASP:C	1:B:1745:ASN:N	2.74	0.40
1:B:1987:PHE:HB3	1:B:1988:GLY:H	1.73	0.40
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.50	0.40
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.54	0.40
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.81	0.40
1:A:2125:TRP:CE2	1:A:2178:LEU:HD13	2.56	0.40
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.54	0.40
1:A:4033:LEU:HD13	1:A:4035:GLN:H	1.87	0.40
1:B:23:LEU:C	1:B:25:GLU:H	2.25	0.40
1:B:1734:PHE:CD2	1:B:1749:ILE:HG12	2.56	0.40
1:B:2012:LEU:HD12	1:B:2013:VAL:N	2.36	0.40
1:B:2820:SER:O	1:B:2823:LEU:HD12	2.21	0.40
1:A:2071:ILE:HB	1:A:2212:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3443:ALA:HB1	1:A:3450:VAL:CG2	2.50	0.40
1:A:3564:LYS:O	1:A:3568:GLU:HG2	2.21	0.40
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	2.03	0.40
1:B:1826:PHE:O	1:B:1826:PHE:CD1	2.75	0.40
1:B:2759:ILE:HG21	1:B:2916:TRP:CZ2	2.56	0.40
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.51	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.02	0.40
1:A:3939:ILE:CG1	1:A:4010:LEU:CD2	2.99	0.40
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	2.03	0.40
1:B:1796:GLY:O	1:B:1900:PRO:HD3	2.22	0.40
1:B:1832:SER:O	1:B:1836:VAL:HG23	2.21	0.40
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.21	0.40
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.35	0.40
1:B:3566:LEU:HA	1:B:3583:LEU:HD23	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2640/2695 (98%)	2518 (95%)	110 (4%)	12 (0%)	29	68
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	29	68
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	29	68

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU

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Mol	Chain	Res	Type
1	A	1633	GLY
1	A	2513	GLN
1	A	3482	GLY
1	B	24	GLU
1	B	2513	GLN
1	B	2990	GLY
1	B	3482	GLY
1	A	2990	GLY
1	A	66	GLN
1	A	1744	LEU
1	A	2519	PRO
1	B	66	GLN
1	B	3914	GLN
1	B	2519	PRO
1	B	2562	PRO
1	B	3809	GLU
1	A	3980	ILE
1	B	3305	ARG
1	A	2028	PRO
1	B	3980	ILE
1	A	2562	PRO
1	B	1470	PRO

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	2218/2453 (90%)	2138 (96%)	80 (4%)	35	67
1	B	2218/2453 (90%)	2137 (96%)	81 (4%)	34	66
All	All	4436/4906 (90%)	4275 (96%)	161 (4%)	35	67

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1421	TYR

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Mol	Chain	Res	Type
1	A	1486	ILE
1	A	1493	LEU
1	A	1504	ASN
1	A	1769	LEU
1	A	1783	THR
1	A	1788	GLN
1	A	1794	PHE
1	A	1826	PHE
1	A	1858	LEU
1	A	1925	GLN
1	A	1997	SER
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2122	THR
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2202	THR
1	A	2229	LEU
1	A	2295	ILE
1	A	2352	GLU
1	A	2357	SER
1	A	2387	ARG
1	A	2395	ILE
1	A	2397	THR
1	A	2411	LYS
1	A	2412	ARG
1	A	2428	MET
1	A	2476	LYS
1	A	2482	LEU
1	A	2544	ILE
1	A	2548	GLU
1	A	2566	SER
1	A	2576	LYS
1	A	2623	THR
1	A	2626	VAL
1	A	2627	ARG
1	A	2681	LEU
1	A	2689	ILE
1	A	2694	LEU
1	A	2822	ILE

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Mol	Chain	Res	Type
1	A	2833	THR
1	A	2843	LEU
1	A	2856	LEU
1	A	2866	LEU
1	A	2967	ASN
1	A	2999	LEU
1	A	3002	LEU
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3340	ARG
1	A	3372	THR
1	A	3400	SER
1	A	3560	LYS
1	A	3578	LEU
1	A	3601	LEU
1	A	3618	TYR
1	A	3634	LYS
1	A	3673	GLU
1	A	3677	LEU
1	A	3729	SER
1	A	3737	THR
1	A	3788	MET
1	A	3805	LYS
1	A	3823	ASN
1	A	3871	PHE
1	A	3876	THR
1	A	3899	ASP
1	A	3906	THR
1	A	3940	THR
1	A	3943	THR
1	A	3958	ASP
1	A	3960	ASP
1	A	3980	ILE
1	A	3982	TRP
1	A	3997	LYS
1	A	4016	CYS
1	B	1383	TYR
1	B	1421	TYR
1	B	1486	ILE
1	B	1504	ASN
1	B	1525	THR

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Mol	Chain	Res	Type
1	B	1646	GLN
1	B	1694	VAL
1	B	1743	ASP
1	B	1759	LYS
1	B	1794	PHE
1	B	1826	PHE
1	B	1858	LEU
1	B	1936	ILE
1	B	2008	ASP
1	B	2068	GLN
1	B	2075	LYS
1	B	2109	LEU
1	B	2141	ILE
1	B	2154	PHE
1	B	2155	ASP
1	B	2202	THR
1	B	2229	LEU
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2310	LEU
1	B	2351	GLN
1	B	2357	SER
1	B	2368	PHE
1	B	2381	GLU
1	B	2390	ILE
1	B	2395	ILE
1	B	2412	ARG
1	B	2425	THR
1	B	2476	LYS
1	B	2479	ILE
1	B	2496	LYS
1	B	2512	LYS
1	B	2566	SER
1	B	2574	TYR
1	B	2681	LEU
1	B	2689	ILE
1	B	2769	LEU
1	B	2822	ILE
1	B	2829	GLU
1	B	2853	LEU
1	B	2920	TRP

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Mol	Chain	Res	Type
1	B	2967	ASN
1	B	2969	LEU
1	B	3305	ARG
1	B	3329	ILE
1	B	3360	TYR
1	B	3372	THR
1	B	3380	LEU
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3559	LEU
1	B	3581	ASP
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3811	LEU
1	B	3844	ILE
1	B	3871	PHE
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3940	THR
1	B	3943	THR
1	B	3958	ASP
1	B	3960	ASP
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL
1	B	4040	GLU
1	B	4068	GLU
1	B	4087	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1533	GLN
1	A	1605	GLN
1	A	1622	GLN
1	A	1646	GLN

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Mol	Chain	Res	Type
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	2064	GLN
1	A	2068	GLN
1	A	2099	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2351	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2444	ASN
1	A	2459	HIS
1	A	2536	ASN
1	A	2601	ASN
1	A	2634	ASN
1	A	2688	ASN
1	A	2896	ASN
1	A	3323	ASN
1	A	3420	ASN
1	A	3475	ASN
1	A	3521	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	3962	GLN
1	A	3970	ASN
1	A	4020	ASN
1	A	4077	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1707	HIS
1	B	1736	GLN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN

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Mol	Chain	Res	Type
1	B	1951	HIS
1	B	2068	GLN
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2409	ASN
1	B	2444	ASN
1	B	2536	ASN
1	B	2598	HIS
1	B	2634	ASN
1	B	2751	GLN
1	B	2753	GLN
1	B	2755	HIS
1	B	2896	ASN
1	B	2910	ASN
1	B	3323	ASN
1	B	3338	ASN
1	B	3471	ASN
1	B	3521	ASN
1	B	3542	GLN
1	B	3571	ASN
1	B	3624	HIS
1	B	3685	GLN
1	B	3780	ASN
1	B	3783	ASN
1	B	3890	GLN
1	B	3962	GLN
1	B	3970	ASN
1	B	4020	ASN
1	B	4077	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	5095	-	4,4,4	0.33	0	6,6,6	0.46	0
3	ANP	A	5094	-	29,33,33	2.43	5 (17%)	31,52,52	1.56	7 (22%)
4	SO4	B	5096	-	4,4,4	0.35	0	6,6,6	0.20	0
4	SO4	A	5095	-	4,4,4	0.52	0	6,6,6	0.69	0
4	SO4	A	5096	-	4,4,4	0.45	0	6,6,6	0.24	0
2	ATP	A	5093	5	26,33,33	1.01	1 (3%)	31,52,52	1.65	5 (16%)
3	ANP	B	5094	-	29,33,33	2.48	5 (17%)	31,52,52	1.52	4 (12%)
2	ATP	B	5093	5	26,33,33	1.02	2 (7%)	31,52,52	1.65	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	5094	-	-	8/14/38/38	0/3/3/3
2	ATP	B	5093	5	-	7/18/38/38	0/3/3/3
2	ATP	A	5093	5	-	5/18/38/38	0/3/3/3
3	ANP	B	5094	-	-	6/14/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O1G	9.66	1.61	1.46
3	A	5094	ANP	PG-O1G	9.47	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-N3B	4.66	1.75	1.63
3	A	5094	ANP	PG-N3B	4.66	1.75	1.63
3	B	5094	ANP	PB-N3B	4.60	1.75	1.63
3	A	5094	ANP	PB-N3B	4.34	1.74	1.63
3	B	5094	ANP	PG-O3G	-3.08	1.48	1.56
3	A	5094	ANP	PG-O3G	-3.04	1.48	1.56
2	A	5093	ATP	C5-C4	2.73	1.48	1.40
2	B	5093	ATP	C5-C4	2.62	1.47	1.40
3	B	5094	ANP	C5-C4	2.52	1.47	1.40
3	A	5094	ANP	C5-C4	2.43	1.47	1.40
2	B	5093	ATP	O4'-C1'	2.24	1.44	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5093	ATP	C3'-C2'-C1'	3.97	106.96	100.98
2	B	5093	ATP	C3'-C2'-C1'	3.77	106.65	100.98
2	B	5093	ATP	PB-O3B-PG	-3.71	120.08	132.83
2	B	5093	ATP	PA-O3A-PB	-3.69	120.16	132.83
2	A	5093	ATP	PB-O3B-PG	-3.60	120.49	132.83
3	B	5094	ANP	C3'-C2'-C1'	3.55	106.32	100.98
2	A	5093	ATP	PA-O3A-PB	-3.45	120.98	132.83
3	B	5094	ANP	PB-O3A-PA	-3.43	120.54	132.62
3	A	5094	ANP	N3-C2-N1	-3.36	123.42	128.68
3	A	5094	ANP	PB-O3A-PA	-3.30	120.99	132.62
3	B	5094	ANP	N3-C2-N1	-3.15	123.75	128.68
2	A	5093	ATP	N3-C2-N1	-3.14	123.77	128.68
2	B	5093	ATP	N3-C2-N1	-3.06	123.89	128.68
3	A	5094	ANP	C4-C5-N7	-2.82	106.46	109.40
3	B	5094	ANP	C4-C5-N7	-2.71	106.57	109.40
3	A	5094	ANP	C2'-C3'-C4'	2.70	107.90	102.64
2	B	5093	ATP	C4-C5-N7	-2.68	106.60	109.40
2	A	5093	ATP	C4-C5-N7	-2.63	106.66	109.40
3	A	5094	ANP	C3'-C2'-C1'	2.39	104.57	100.98
3	A	5094	ANP	O2A-PA-O1A	2.09	122.58	112.24
3	A	5094	ANP	O3G-PG-O1G	-2.08	108.23	113.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	5094	ANP	PB-N3B-PG-O1G
3	A	5094	ANP	C5'-O5'-PA-O2A
3	B	5094	ANP	PB-N3B-PG-O1G
3	B	5094	ANP	C5'-O5'-PA-O1A
3	B	5094	ANP	C5'-O5'-PA-O2A
3	B	5094	ANP	O4'-C4'-C5'-O5'
2	A	5093	ATP	O4'-C4'-C5'-O5'
2	A	5093	ATP	C3'-C4'-C5'-O5'
2	B	5093	ATP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C3'-C4'-C5'-O5'
3	B	5094	ANP	C3'-C4'-C5'-O5'
3	A	5094	ANP	PB-O3A-PA-O1A
3	A	5094	ANP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C5'-O5'-PA-O3A
3	A	5094	ANP	C5'-O5'-PA-O3A
2	B	5093	ATP	PA-O3A-PB-O1B
3	A	5094	ANP	C5'-O5'-PA-O1A
3	A	5094	ANP	PB-O3A-PA-O2A
2	A	5093	ATP	PA-O3A-PB-O1B
2	A	5093	ATP	C5'-O5'-PA-O3A
3	B	5094	ANP	C5'-O5'-PA-O3A
3	A	5094	ANP	C3'-C4'-C5'-O5'
2	B	5093	ATP	PA-O3A-PB-O2B
2	A	5093	ATP	C5'-O5'-PA-O1A
2	B	5093	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

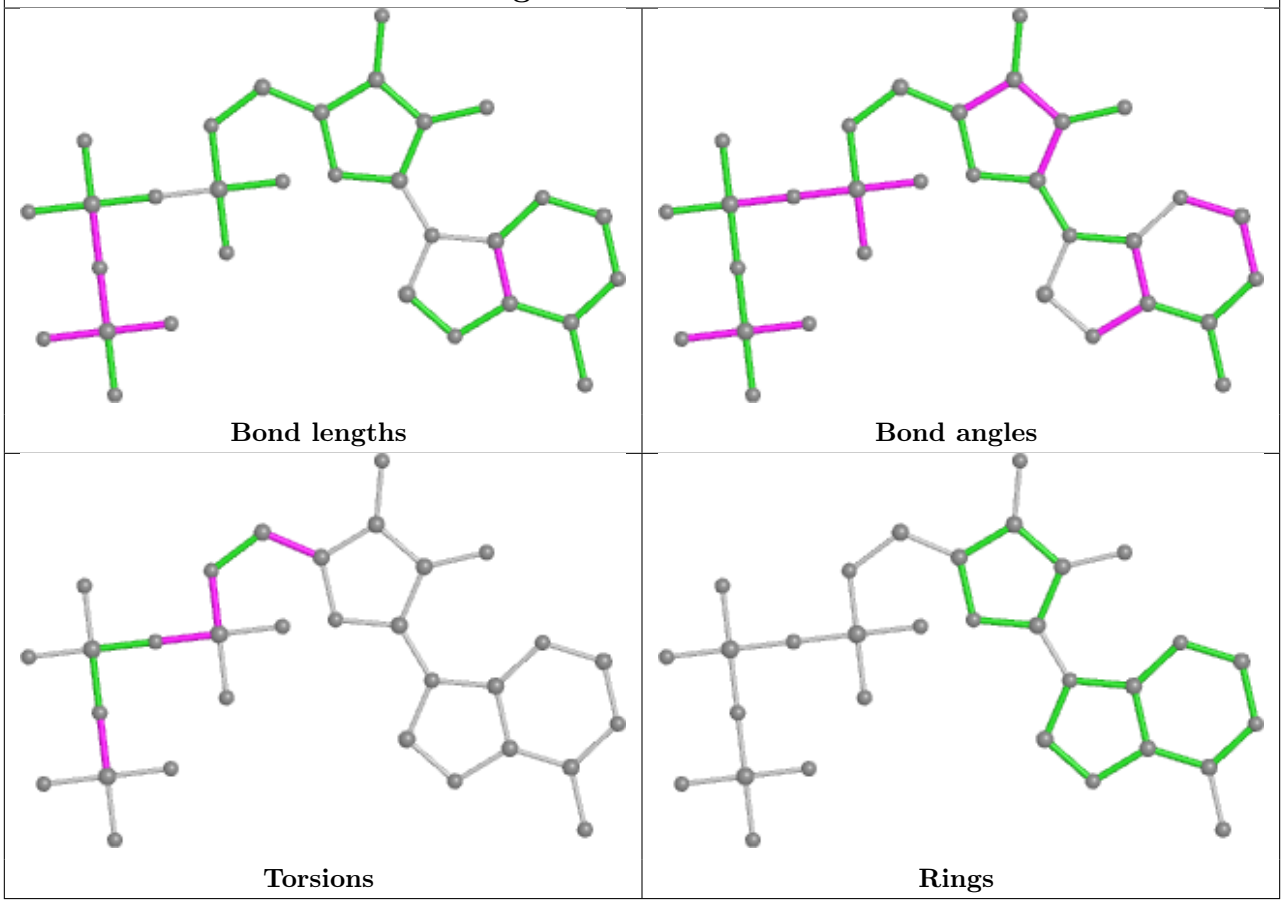
6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5094	ANP	7	0
4	B	5096	SO4	3	0
4	A	5095	SO4	3	0
2	A	5093	ATP	8	0
3	B	5094	ANP	7	0
2	B	5093	ATP	17	0

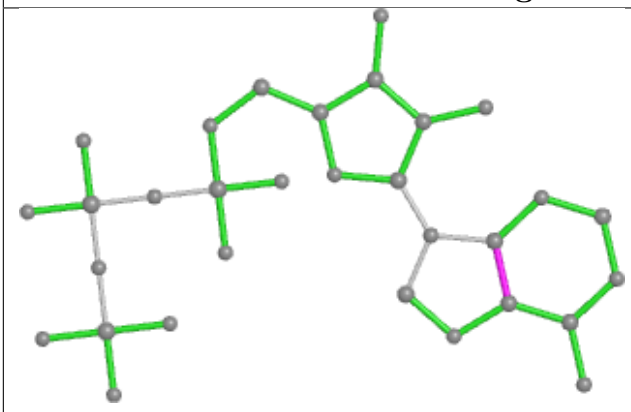
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

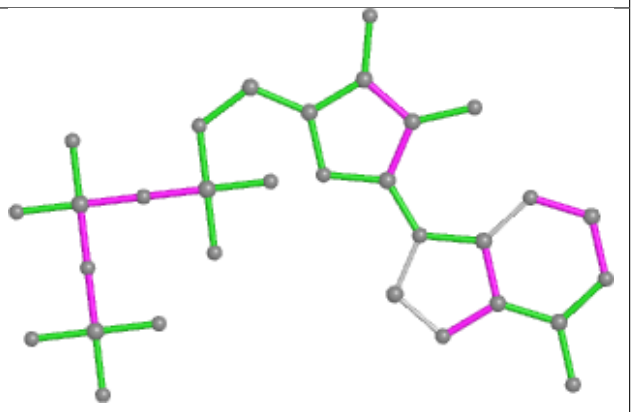
Ligand ANP A 5094



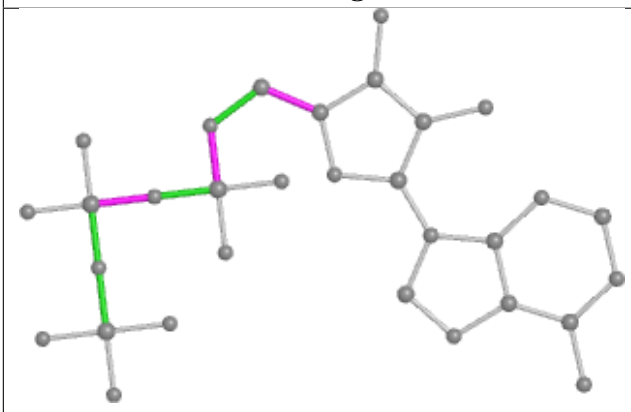
Ligand ATP A 5093



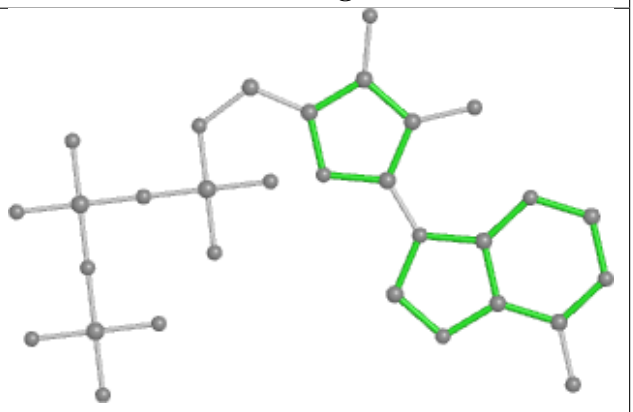
Bond lengths



Bond angles

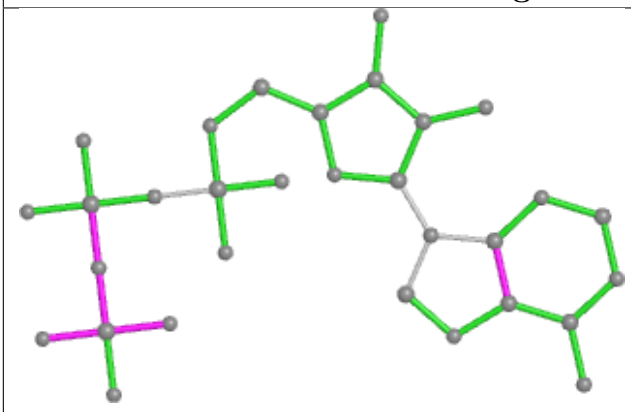


Torsions

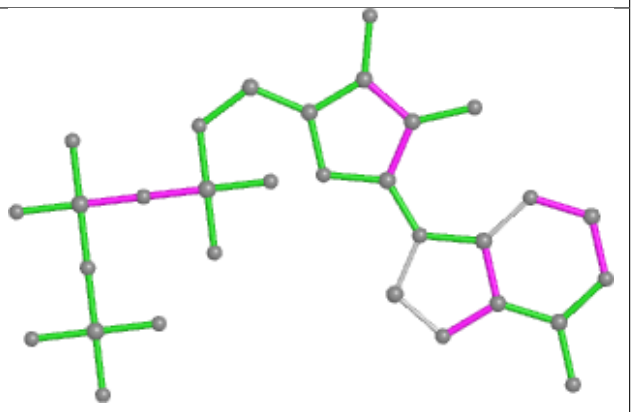


Rings

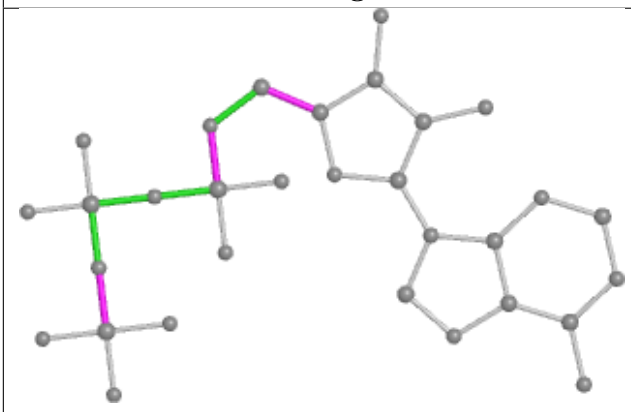
Ligand ANP B 5094



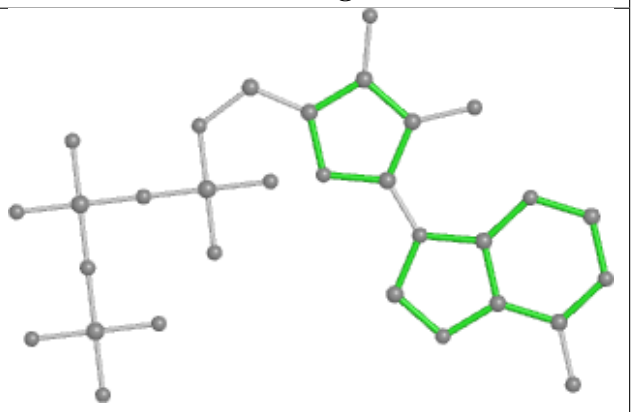
Bond lengths



Bond angles

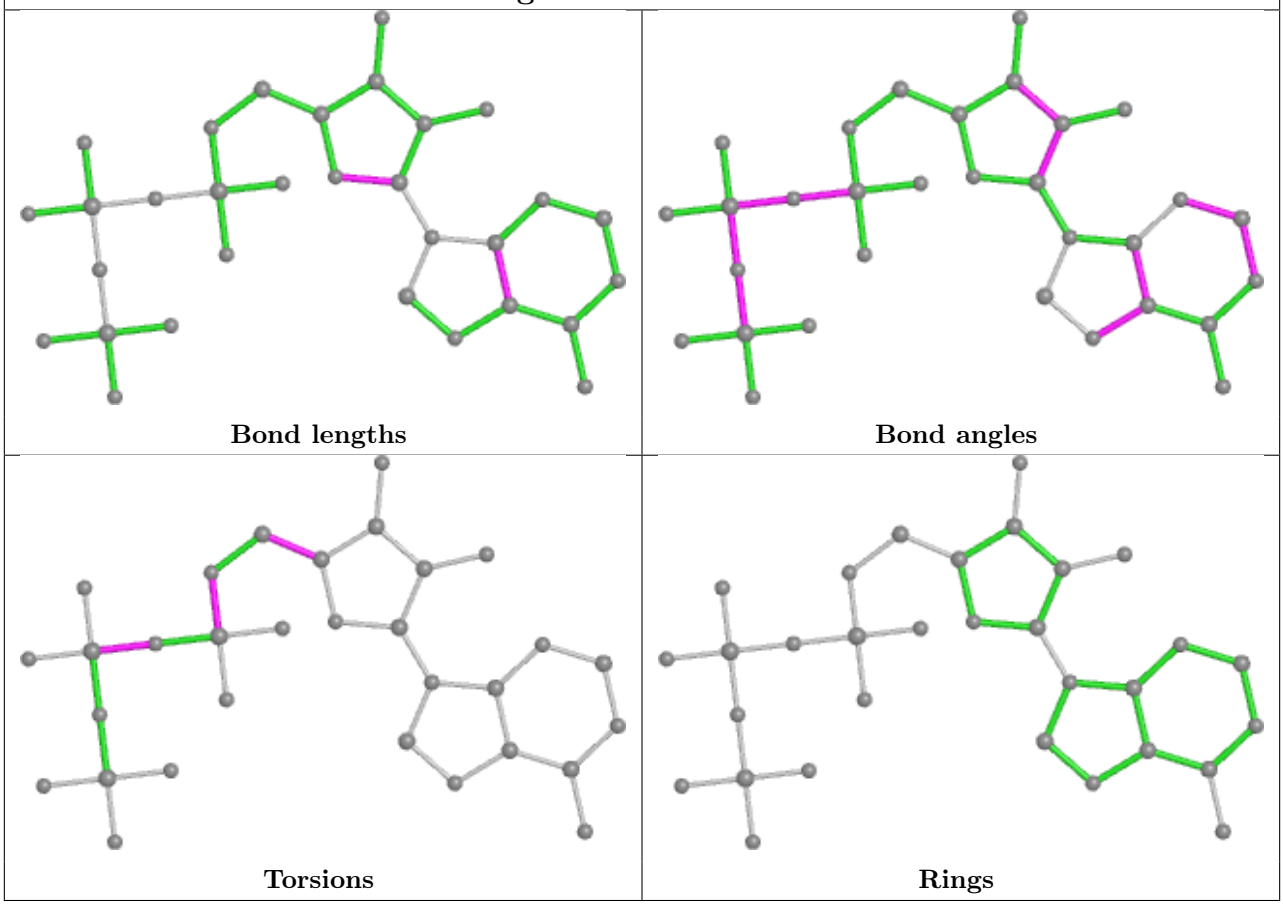


Torsions



Rings

Ligand ATP B 5093



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	2650/2695 (98%)	0.11	69 (2%) 56 40	69, 151, 281, 423	0
1	B	2650/2695 (98%)	0.64	277 (10%) 6 3	92, 193, 357, 500	0
All	All	5300/5390 (98%)	0.37	346 (6%) 18 11	69, 172, 321, 500	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	24.7
1	B	164	MET	22.6
1	B	213	ASP	20.8
1	B	29	GLU	19.9
1	B	163	TYR	19.7
1	B	161	VAL	19.2
1	B	84	CYS	18.3
1	B	49	LEU	16.9
1	B	214	HIS	16.0
1	B	142	LEU	15.4
1	B	206	GLN	14.4
1	B	166	PRO	14.2
1	B	48	GLY	14.0
1	B	80	MET	14.0
1	B	143	ASN	13.1
1	A	2	PRO	12.6
1	B	168	CYS	12.6
1	B	19	LEU	12.5
1	B	162	LEU	12.3
1	B	69	ALA	12.2
1	B	18	LEU	12.1
1	B	83	GLY	11.9
1	B	151	ASP	11.8
1	B	53	ASN	11.1

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Mol	Chain	Res	Type	RSRZ
1	B	215	PRO	10.9
1	B	70	ILE	10.9
1	B	76	ASP	10.6
1	B	78	HIS	10.6
1	B	212	GLY	10.1
1	B	4	LEU	9.8
1	B	1683	LEU	9.5
1	B	30	HIS	9.3
1	A	2364	ASP	8.9
1	B	1572	ILE	8.7
1	B	184	ALA	8.6
1	B	167	MET	8.2
1	B	120	ASP	8.2
1	B	90	GLU	8.1
1	B	197	TYR	8.1
1	A	63	LYS	8.1
1	B	185	ILE	8.0
1	B	73	TYR	7.9
1	B	188	ILE	7.8
1	B	1549	ILE	7.8
1	B	208	THR	7.7
1	B	115	GLU	7.7
1	B	148	THR	7.7
1	A	1	SER	7.5
1	B	1644	ILE	7.4
1	B	216	PRO	7.4
1	B	205	TRP	7.3
1	B	1937	MET	7.3
1	A	1483	TYR	7.2
1	A	115	GLU	7.2
1	B	74	ILE	7.1
1	B	14	GLN	7.1
1	B	186	PRO	7.1
1	B	68	MET	7.0
1	B	92	SER	6.9
1	B	79	ASN	6.8
1	B	1459	LEU	6.7
1	B	160	VAL	6.6
1	A	71	ILE	6.5
1	B	189	ASP	6.5
1	B	133	GLU	6.5
1	B	1680	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	6.4
1	A	28	GLU	6.3
1	B	1590	LEU	6.3
1	B	1582	VAL	6.3
1	B	1679	LYS	6.3
1	B	171	ALA	6.3
1	B	1732	GLN	6.2
1	B	157	ALA	6.1
1	B	50	GLU	6.1
1	B	116	THR	6.0
1	B	67	SER	5.9
1	B	46	GLU	5.9
1	B	33	GLU	5.8
1	B	1550	GLY	5.8
1	B	1684	LEU	5.8
1	B	1581	GLY	5.7
1	B	1669	PHE	5.7
1	B	190	LYS	5.7
1	B	147	VAL	5.7
1	B	177	CYS	5.6
1	B	82	GLY	5.6
1	B	91	ILE	5.6
1	B	111	SER	5.4
1	B	34	ARG	5.4
1	A	86	LYS	5.4
1	B	207	ALA	5.4
1	A	85	PRO	5.4
1	A	27	TYR	5.3
1	B	75	ALA	5.3
1	B	1458	ILE	5.3
1	B	3580	ASN	5.3
1	B	180	LYS	5.3
1	B	77	LYS	5.2
1	B	194	SER	5.2
1	B	3555	TYR	5.1
1	B	1601	SER	5.1
1	B	1596	ILE	5.0
1	B	1730	LYS	4.9
1	B	119	VAL	4.9
1	B	1705	TYR	4.9
1	B	195	SER	4.9
1	B	196	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	3563	GLU	4.9
1	B	1545	LEU	4.8
1	B	16	THR	4.8
1	B	1649	LEU	4.8
1	B	35	ASP	4.7
1	B	66	GLN	4.7
1	A	216	PRO	4.7
1	B	1606	GLU	4.7
1	B	1483	TYR	4.7
1	B	1566	PHE	4.7
1	B	3866	GLU	4.7
1	B	1452	TRP	4.6
1	A	215	PRO	4.6
1	B	1456	TYR	4.6
1	B	47	LEU	4.5
1	B	54	LEU	4.5
1	B	204	GLY	4.4
1	B	1771	TYR	4.4
1	B	85	PRO	4.4
1	B	1415	MET	4.4
1	B	17	ARG	4.3
1	B	1647	ALA	4.3
1	B	170	ASP	4.3
1	B	179	LYS	4.3
1	A	25	GLU	4.3
1	A	3580	ASN	4.1
1	B	1770	ILE	4.1
1	A	35	ASP	4.1
1	B	1476	PHE	4.1
1	B	117	LEU	4.1
1	B	1548	ILE	4.1
1	B	1893	ALA	4.0
1	B	3482	GLY	4.0
1	A	62	VAL	3.9
1	B	1894	VAL	3.9
1	B	28	GLU	3.8
1	B	3304	GLU	3.8
1	B	3393	ASN	3.8
1	B	1394	LEU	3.8
1	A	151	ASP	3.7
1	B	211	GLY	3.7
1	B	1701	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	3588	ASN	3.7
1	B	15	PRO	3.7
1	A	116	THR	3.6
1	B	2938	MET	3.6
1	A	148	THR	3.6
1	B	1460	GLY	3.6
1	B	1546	LEU	3.6
1	A	84	CYS	3.6
1	B	3846	MET	3.5
1	B	183	GLU	3.5
1	A	83	GLY	3.4
1	B	56	TYR	3.4
1	A	1394	LEU	3.4
1	A	3979	ASN	3.4
1	B	112	LYS	3.4
1	B	1933	ILE	3.4
1	B	1734	PHE	3.4
1	B	187	GLN	3.4
1	A	69	ALA	3.3
1	A	20	LEU	3.3
1	B	1441	ILE	3.3
1	A	1597	GLU	3.3
1	A	61	ASP	3.2
1	B	178	PHE	3.2
1	B	152	PHE	3.2
1	B	4023	ILE	3.2
1	B	1	SER	3.2
1	A	3330	TYR	3.2
1	A	2918	GLY	3.2
1	B	89	ALA	3.1
1	A	72	ARG	3.1
1	B	1835	LEU	3.1
1	B	1636	ILE	3.1
1	B	1812	ASN	3.1
1	B	1653	GLN	3.1
1	A	90	GLU	3.1
1	A	64	LEU	3.1
1	B	191	TYR	3.1
1	B	198	ILE	3.1
1	B	2000	ARG	3.0
1	B	1445	TRP	3.0
1	B	1935	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	202	LEU	3.0
1	B	1760	PHE	3.0
1	B	1676	VAL	3.0
1	B	1845	GLY	3.0
1	B	1608	LEU	3.0
1	B	5	GLY	3.0
1	B	2213	LEU	3.0
1	B	1602	ILE	3.0
1	B	1372	ASN	3.0
1	B	1579	ILE	2.9
1	B	1650	LEU	2.9
1	B	3726	LEU	2.9
1	B	42	ASN	2.9
1	B	1395	VAL	2.9
1	B	3391	LEU	2.9
1	B	1744	LEU	2.9
1	B	155	TYR	2.8
1	B	1715	LEU	2.8
1	B	2669	PHE	2.8
1	B	1605	GLN	2.8
1	B	3326	ILE	2.8
1	B	113	ASP	2.8
1	B	1813	LEU	2.8
1	B	1765	ILE	2.8
1	A	3334	PHE	2.8
1	B	1703	VAL	2.8
1	B	1936	ILE	2.8
1	A	79	ASN	2.7
1	B	87	GLU	2.7
1	B	110	TYR	2.7
1	B	1562	MET	2.7
1	A	3418	ILE	2.7
1	B	1682	GLY	2.7
1	B	1704	GLU	2.7
1	A	1548	ILE	2.7
1	B	3325	ILE	2.7
1	A	2194	PHE	2.7
1	B	36	GLU	2.7
1	B	2770	THR	2.7
1	B	1378	TRP	2.7
1	B	3919	LYS	2.7
1	B	1506	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1420	TYR	2.7
1	A	3564	LYS	2.7
1	A	202	LEU	2.7
1	B	3841	LEU	2.7
1	A	1368	GLU	2.7
1	B	72	ARG	2.6
1	B	1493	LEU	2.6
1	B	1607	TRP	2.6
1	B	3589	ASN	2.6
1	A	59	ASP	2.6
1	B	1592	LEU	2.6
1	B	1593	ASN	2.6
1	B	3788	MET	2.6
1	B	1568	SER	2.6
1	A	1458	ILE	2.6
1	B	55	PRO	2.6
1	A	67	SER	2.6
1	A	3495	PHE	2.6
1	A	75	ALA	2.5
1	B	199	ALA	2.5
1	B	156	ASP	2.5
1	B	3847	SER	2.5
1	B	20	LEU	2.5
1	B	1711	VAL	2.5
1	B	2353	LEU	2.5
1	B	3839	ILE	2.5
1	B	1505	PHE	2.5
1	B	2428	MET	2.5
1	A	3567	LEU	2.5
1	B	4029	ILE	2.5
1	B	94	LEU	2.5
1	A	89	ALA	2.5
1	A	68	MET	2.5
1	B	1479	LEU	2.4
1	A	3784	ASN	2.4
1	B	3714	GLN	2.4
1	B	3024	LEU	2.4
1	A	135	ARG	2.4
1	B	1809	PHE	2.4
1	B	31	LEU	2.4
1	B	1492	GLN	2.4
1	B	136	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	3590	LEU	2.4
1	B	2026	GLY	2.3
1	B	2918	GLY	2.3
1	A	182	ILE	2.3
1	B	182	ILE	2.3
1	B	2072	LEU	2.3
1	A	108	ILE	2.3
1	B	1421	TYR	2.3
1	A	2928	VAL	2.3
1	B	3425	LYS	2.3
1	B	3785	TYR	2.3
1	B	1547	LYS	2.3
1	B	2058	MET	2.3
1	B	1500	ILE	2.3
1	B	3597	ILE	2.3
1	B	1551	SER	2.3
1	B	3618	TYR	2.3
1	B	1417	ALA	2.3
1	B	3560	LYS	2.3
1	B	1503	PRO	2.3
1	B	3694	PHE	2.3
1	B	1712	ILE	2.3
1	A	1445	TRP	2.2
1	B	1573	ILE	2.2
1	A	184	ALA	2.2
1	A	3321	ILE	2.2
1	B	1580	THR	2.2
1	B	2214	TRP	2.2
1	B	1583	ARG	2.2
1	B	137	CYS	2.2
1	B	176	VAL	2.2
1	B	3571	ASN	2.2
1	B	1807	LYS	2.2
1	B	3466	ILE	2.2
1	B	3591	LYS	2.2
1	B	149	HIS	2.2
1	A	1504	ASN	2.2
1	B	3427	VAL	2.2
1	B	3915	PHE	2.2
1	A	3494	LEU	2.2
1	B	88	ARG	2.2
1	B	1769	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3927	TYR	2.1
1	B	95	GLU	2.1
1	B	1588	GLU	2.1
1	B	2212	LEU	2.1
1	A	1578	PHE	2.1
1	A	19	LEU	2.1
1	B	1502	ILE	2.1
1	B	2660	LEU	2.1
1	B	3884	LEU	2.1
1	B	3564	LYS	2.1
1	B	3934	TRP	2.1
1	B	2889	PHE	2.1
1	B	3985	VAL	2.1
1	A	39	LYS	2.1
1	A	3329	ILE	2.1
1	B	3327	SER	2.0
1	B	1480	THR	2.0
1	A	2470	GLY	2.0
1	B	3330	TYR	2.0
1	B	3844	ILE	2.0
1	A	3545	ARG	2.0
1	B	1668	GLN	2.0
1	B	1455	LEU	2.0
1	B	1779	PHE	2.0
1	A	3325	ILE	2.0
1	B	3797	THR	2.0
1	A	3546	GLU	2.0
1	A	3796	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

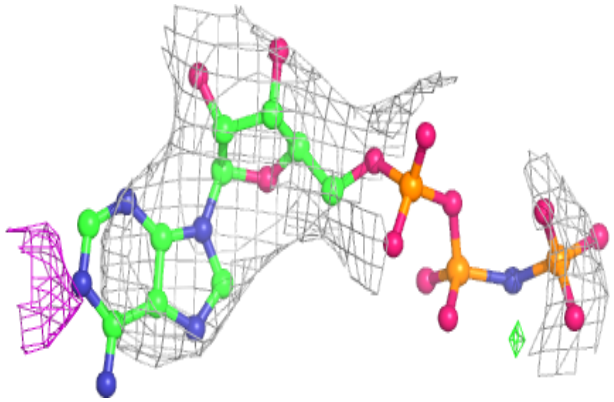
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

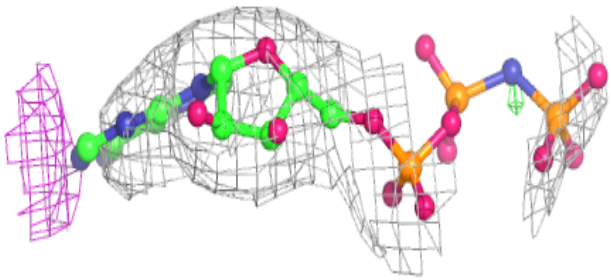
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	5095	5/5	0.84	0.18	152,154,166,167	0
3	ANP	B	5094	31/31	0.89	0.29	112,145,237,257	0
2	ATP	B	5093	31/31	0.92	0.24	99,141,184,200	0
3	ANP	A	5094	31/31	0.94	0.27	111,140,238,248	0
2	ATP	A	5093	31/31	0.95	0.29	88,123,185,204	0
4	SO4	B	5096	5/5	0.95	0.14	155,168,174,176	0
4	SO4	A	5095	5/5	0.96	0.25	84,98,104,105	0
4	SO4	A	5096	5/5	0.96	0.20	115,130,143,145	0
5	MG	B	5097	1/1	0.97	0.18	66,66,66,66	0
5	MG	A	5097	1/1	0.99	0.22	62,62,62,62	0

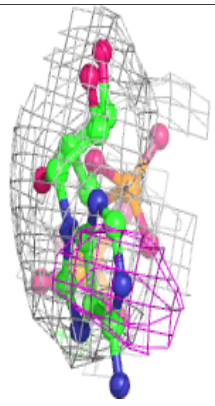
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 5094:

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

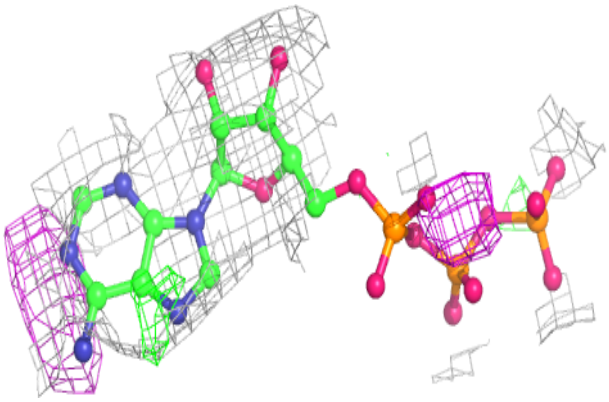


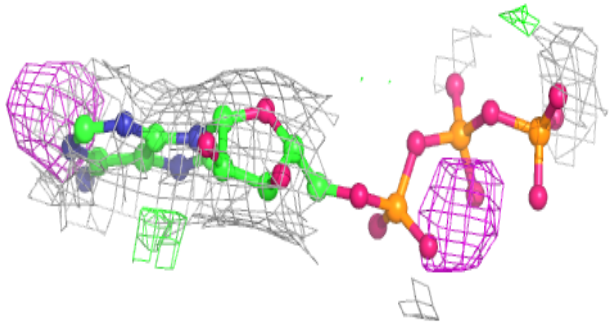


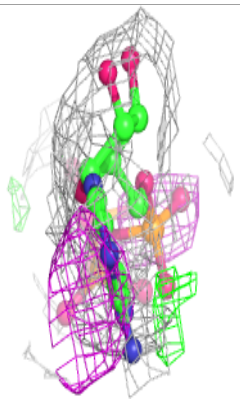


Electron density around ATP B 5093:

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

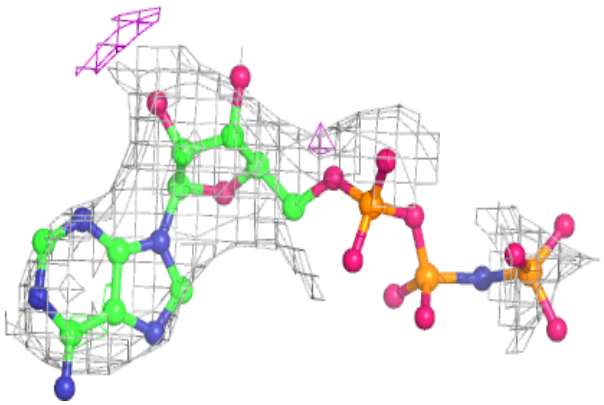


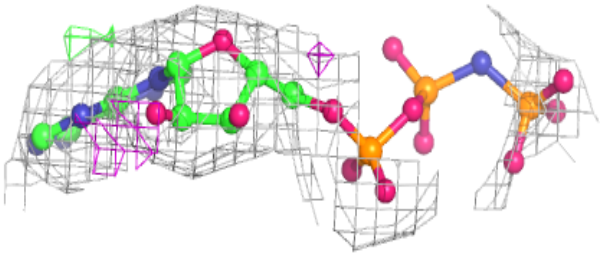


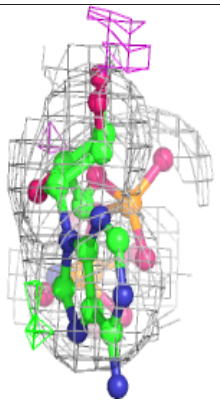


Electron density around ANP A 5094:

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

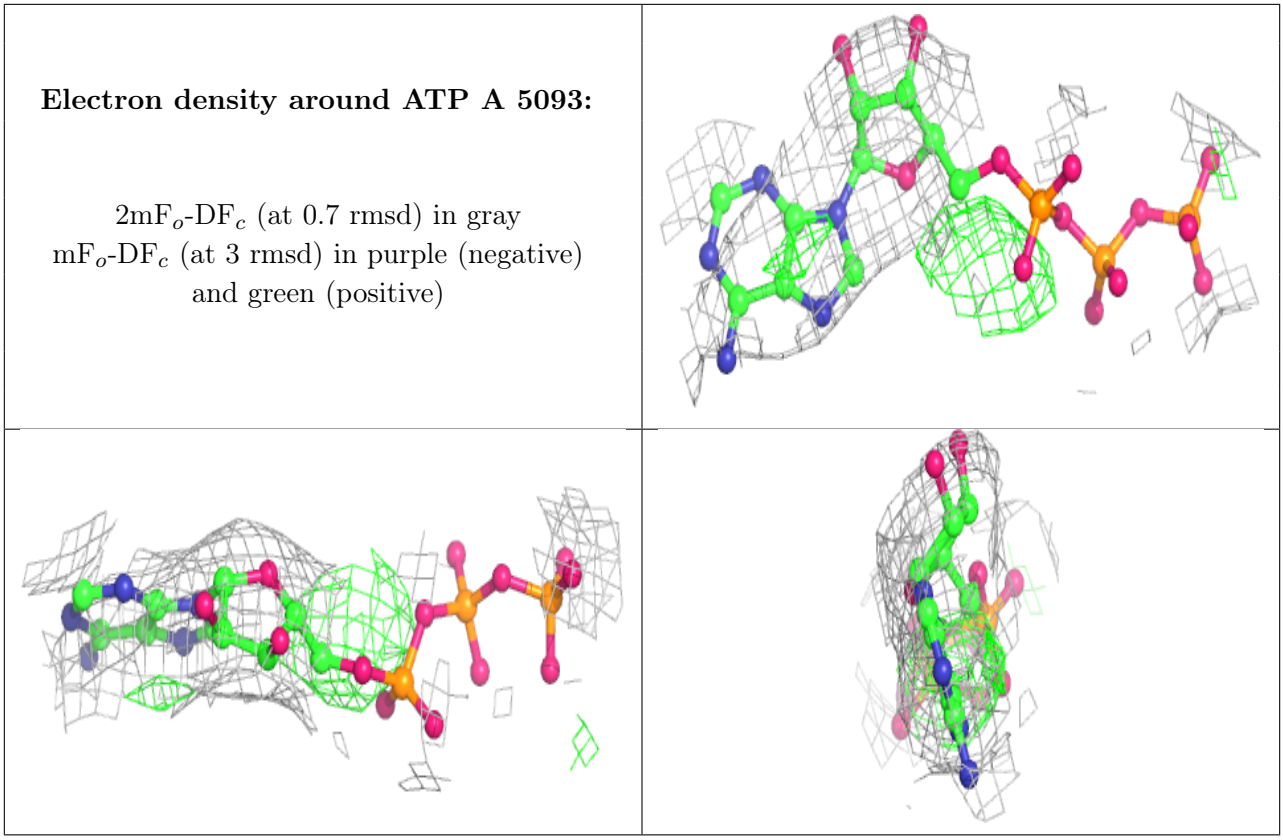






Electron density around ATP A 5093:

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



6.5 Other polymers (i)

There are no such residues in this entry.