Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 10:06 pm BST

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

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

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

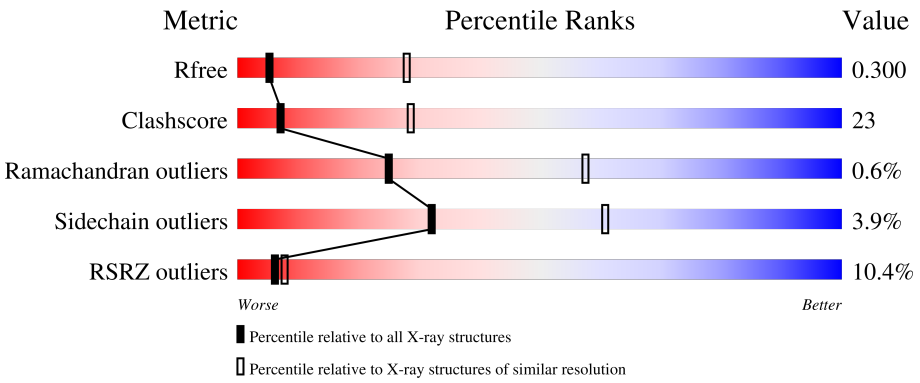
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	11% 66% 31% • •
1	B	2695	9% 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	5400	-	-	X	-
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	A	5403	-	-	X	-
4	SO4	B	5403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

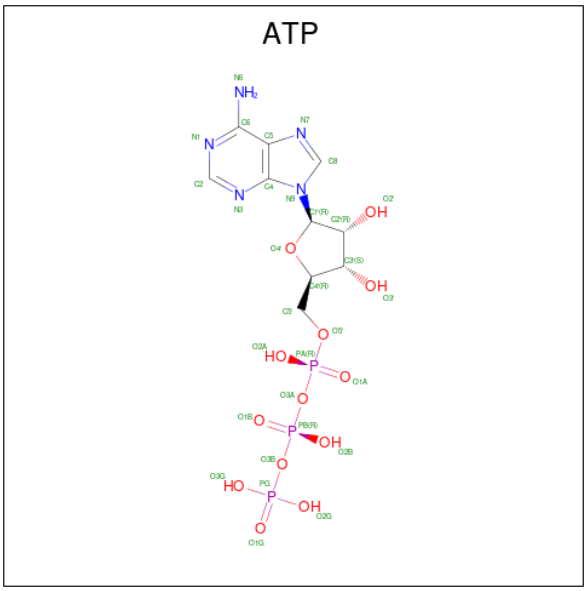
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 10 discrepancies between the modelled and reference sequences:

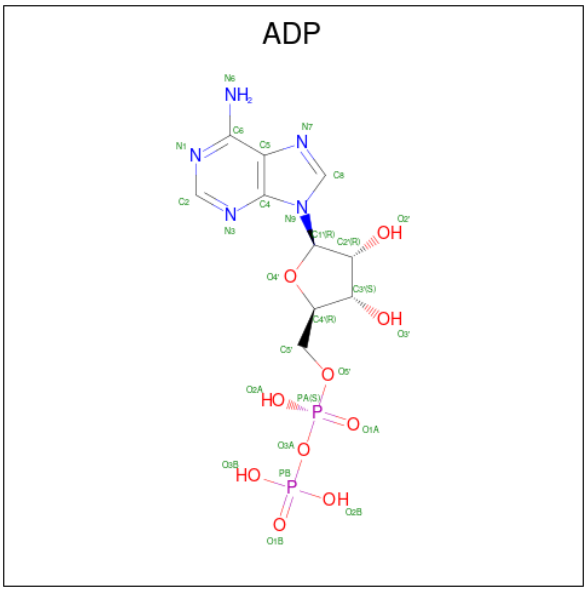
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	linker	UNP P36022
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	217	LYS	-	linker	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630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

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



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

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



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

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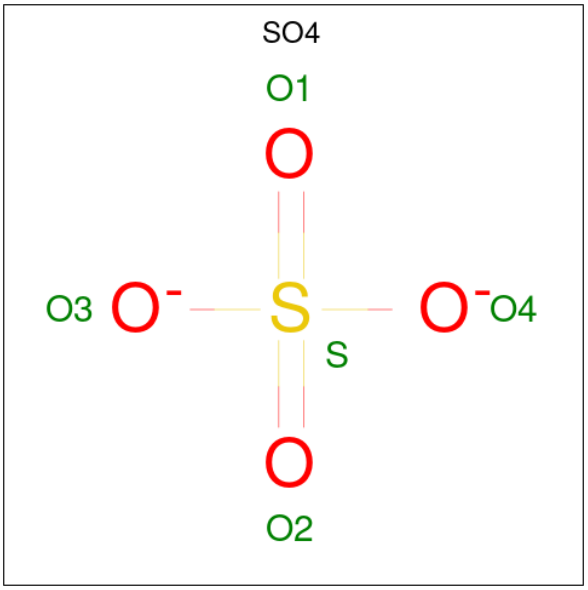
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0

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



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

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

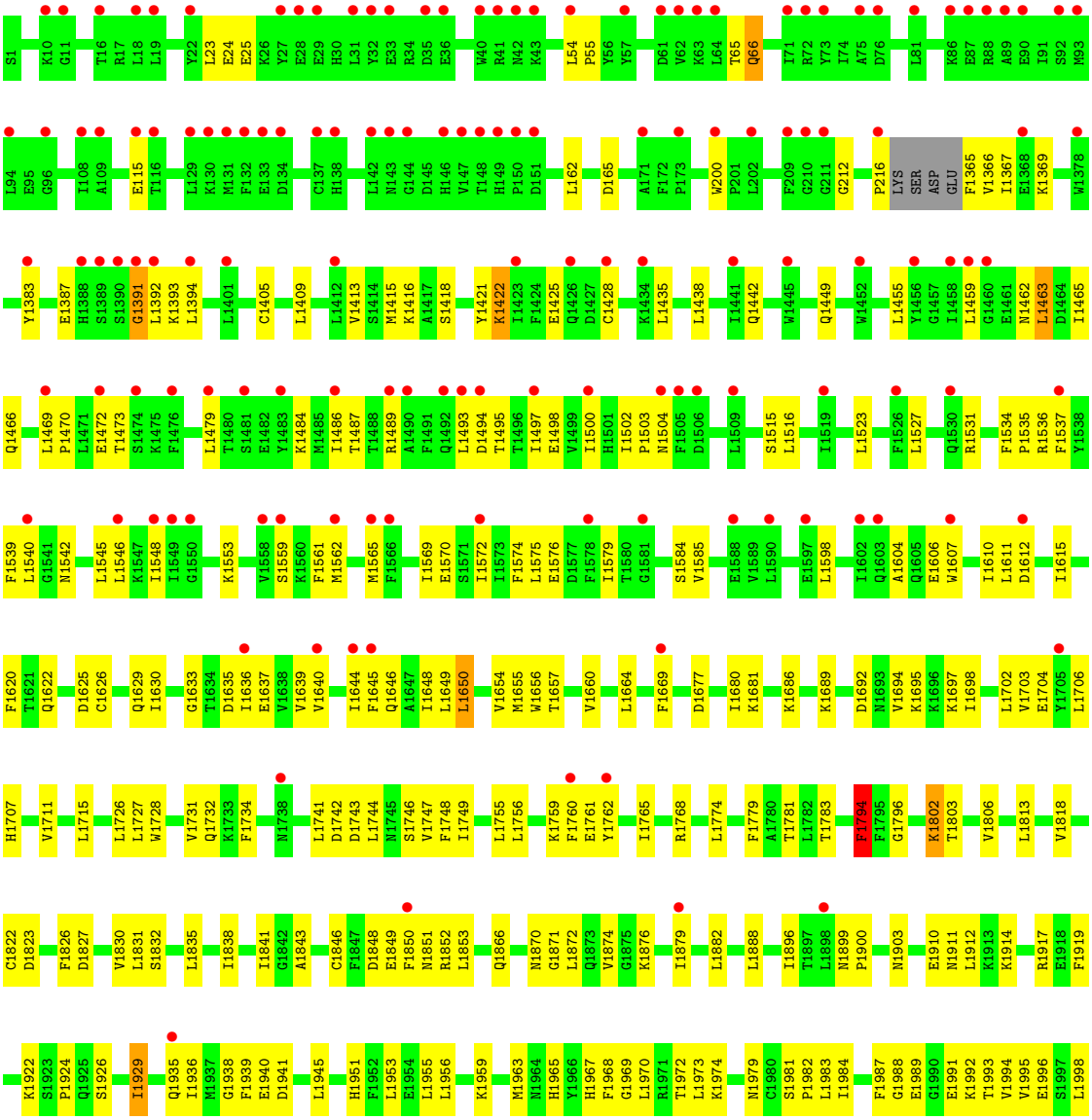
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
			Total	Mg		
5	B	1	1	1	0	0

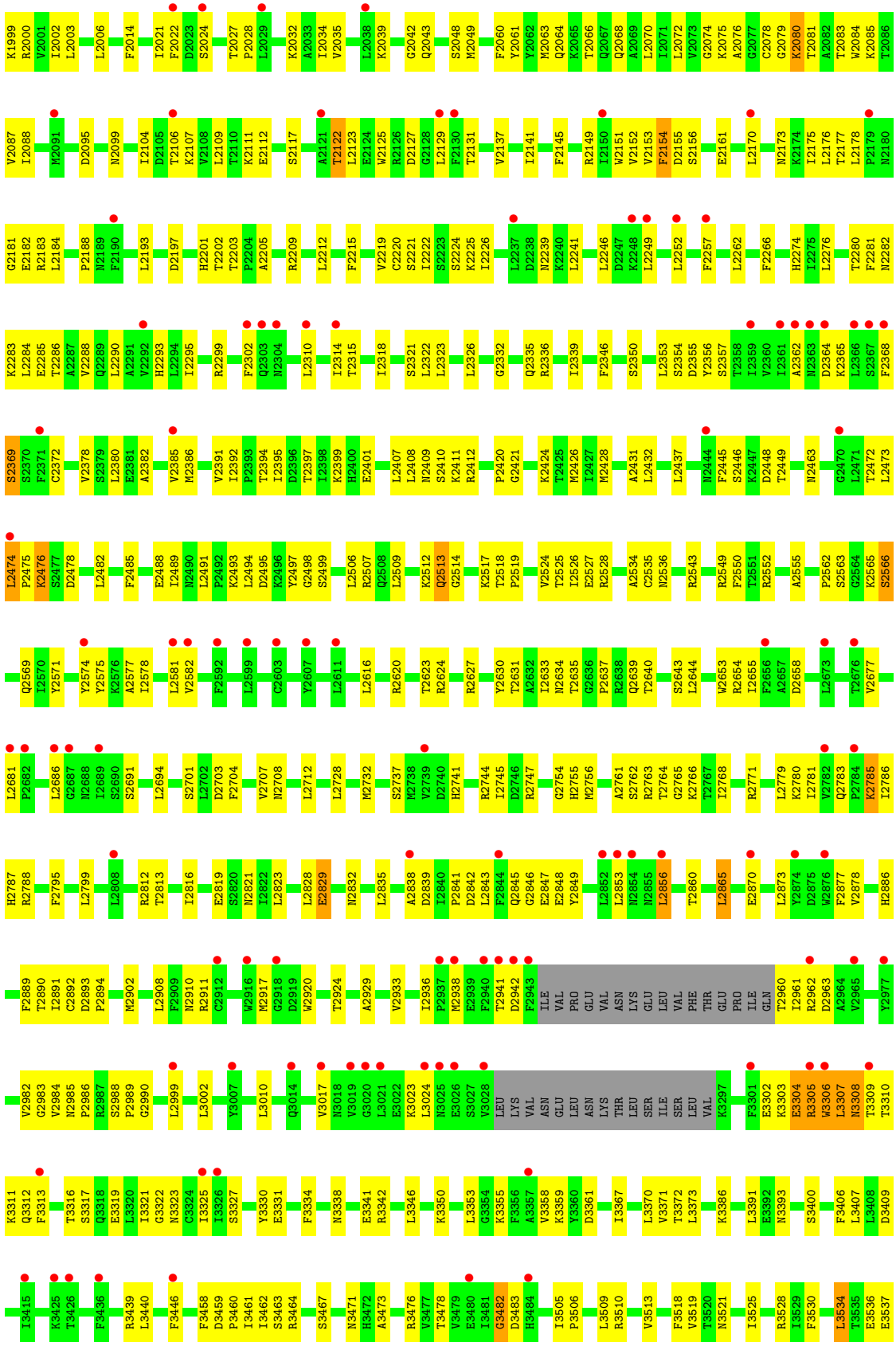
3 Residue-property plots (i)

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: 11% 66% 31%

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V2087 I2088 M2091 D2095 N2099 I2104 D2105 T2106 K2107 V2108 L2109 T2110 K2111 E2112 S2117 A2121 T2122 L2123 E2124 W2125 R2126 D2127 G2128 L2129 F2130 T2131 V2137 I2141 F2145 R2149 I2150 W2151 V2152 V2153 F2154 D2155 S2156 E2161 L2170 N2173 K2174 I2175 L2176 T2177 L2178 P2179 N2180
G2181 E2182 R2183 L2184 P2188 N2189 F2190 L2193 D2197 H2201 T2202 T2203 P2204 A2205 R2209 L2212 F2215 V2219 C2220 S2221 I2222 S2223 S2224 K2225 I2226 L2237 D2238 N2239 K2240 L2241 L2246 D2247 K2248 L2249 L2252 F2257 L2262 F2266 H2274 T2275 L2276 T2280 F2281 N2282
K2283 L2284 E2285 T2286 A2287 V2288 Q2289 L2290 A2291 V2292 H2293 L2294 I2295 R2299 F2302 Q2303 N2304 L2310 I2314 T2315 I2318 S2321 L2322 L2323 L2326 G2332 Q2335 R2336 I2339 F2346 S2350 L2353 S2354 D2355 Y2356 S2357 T2358 I2359 V2360 I2361 A2362 N2363 D2364 K2365 L2366 S2367 F2368
S2369 S2370 F2371 C2372 V2378 S2379 L2380 E2381 A2382 V2385 M2386 V2391 I2392 P2393 T2394 I2395 D2396 T2397 I2398 K2399 H2400 E2401 L2407 L2408 N2409 S2410 K2411 R2412 P2420 G2421 K2424 T2425 M2426 I2427 M2428 A2431 L2432 L2437 N2444 F2445 S2446 K2447 D2448 T2449 N2463 G2470 L2471 T2472 L2473
L2474 P2475 K2476 S2477 D2478 L2482 F2485 E2488 I2489 N2490 L2491 P2492 K2493 L2494 D2495 K2496 Y2497 G2498 S2499 L2506 R2507 Q2508 L2509 K2512 Q2513 G2514 K2517 T2518 P2519 V2524 T2525 I2526 E2527 R2528 A2534 C2535 N2536 R2543 R2549 F2550 T2551 R2552 A2555 P2562 S2563 G2564 K2565 S2566
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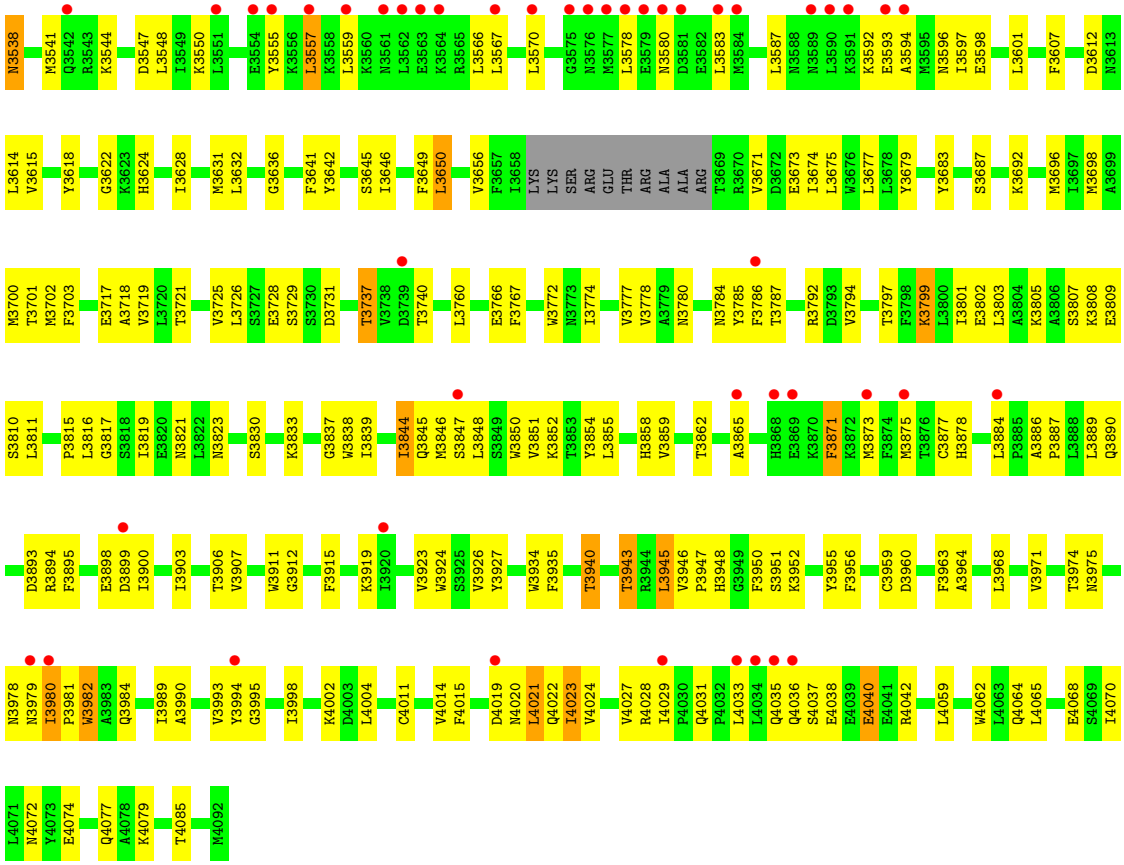
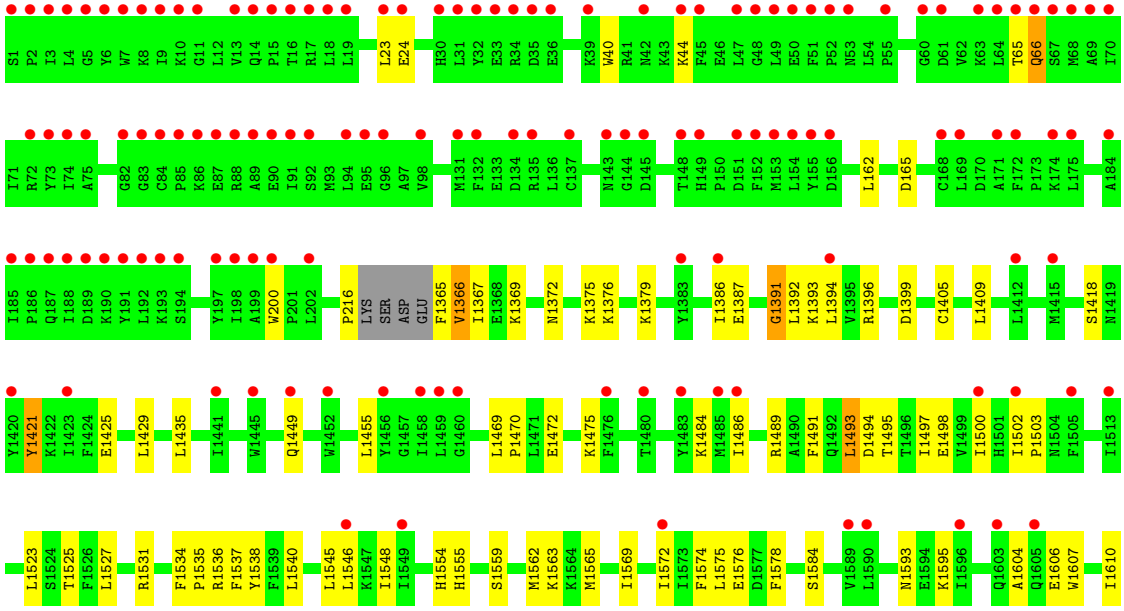
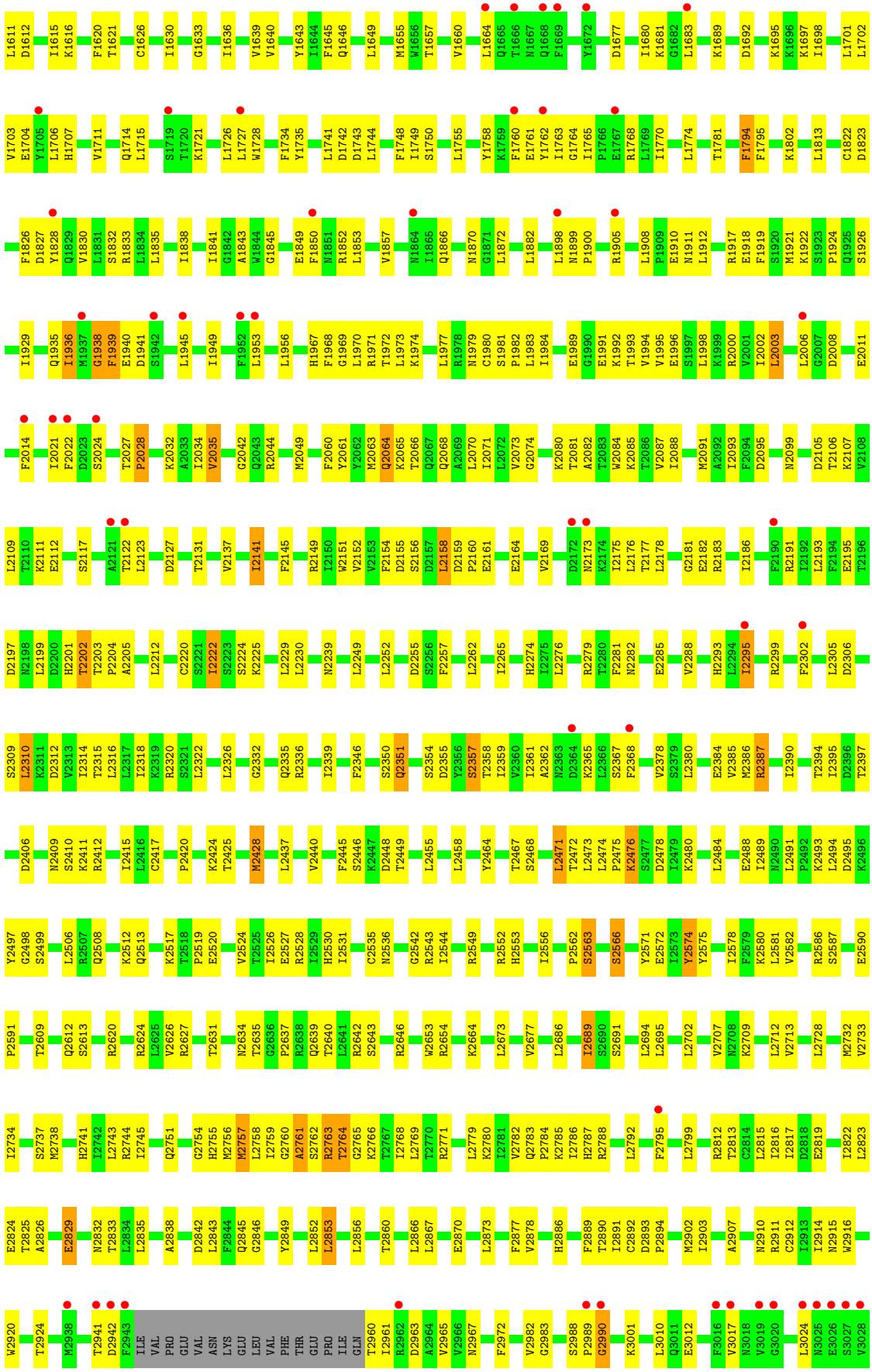
L2681 P2682 L2686 G2687 N2688 I2689 S2690 S2691 L2694 S2701 L2702 D2703 F2704 V2707 N2708 L2712 L2728 M2732 S2737 M2738 V2739 D2740 H2741 R2744 I2745 D2746 R2747 G2754 H2755 M2756 A2761 S2762 R2763 T2764 G2765 K2766 T2767 I2768 R2771 L2779 K2780 I2781 V2782 Q2783 P2784 K2785 I2786
H2787 R2788 F2795 L2799 L2808 R2812 T2813 I2816 E2819 S2820 N2821 I2822 L2823 L2828 E2829 N2832 L2835 A2838 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 E2847 E2848 Y2849 L2852 L2853 N2854 N2855 L2856 T2860 L2865 E2870 L2873 Y2874 D2875 W2876 F2877 V2878 H2886
F2889 T2890 I2891 C2892 D2893 P2894 M2902 L2908 F2909 N2910 R2911 C2912 W2916 M2917 G2918 D2919 W2920 T2924 A2929 V2933 I2936 P2937 M2938 E2939 F2940 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 A2964 V2965 Y2977
V2982 G2983 V2984 N2985 P2986 R2987 S2988 P2989 G2990 L2999 L3002 Y3007 L3010 Q3014 V3017 N3018 V3019 G3020 L3021 E3022 K3023 L3024 N3025 E3026 S3027 V3028 LEU LYS VAL ASN GLU LEU ASN LYS THR LEU SER ILE SER LEU VAL K3297 E3301 E3302 K3303 E3304 R3305 W3306 L3307 N3308 T3309 T3310
K3311 Q3312 F3313 T3316 S3317 Q3318 E3319 L3320 I3321 G3322 N3323 C3324 I3325 I3326 S3327 Y3330 E3331 F3334 N3338 E3341 R3342 L3346 K3350 L3353 G3354 K3355 F3356 A3357 V3358 K3359 Y3360 D3361 I3367 L3370 V3371 T3372 L3373 K3386 L3391 E3392 N3393 S3400 F3406 L3407 L3408 D3409
I3415 K3425 T3426 F3436 R3439 L3440 F3446 F3458 D3459 P3460 I3461 I3462 S3463 R3464 S3467 N3471 H3472 A3473 R3476 V3477 T3478 V3479 E3480 I3481 G3482 D3483 H3484 I3505 P3506 L3509 R3510 V3513 F3518 V3519 T3520 N3521 I3525 R3528 I3529 F3530 L3534 T3535 E3536 E3537



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

Chain B: 9% 67% 30%

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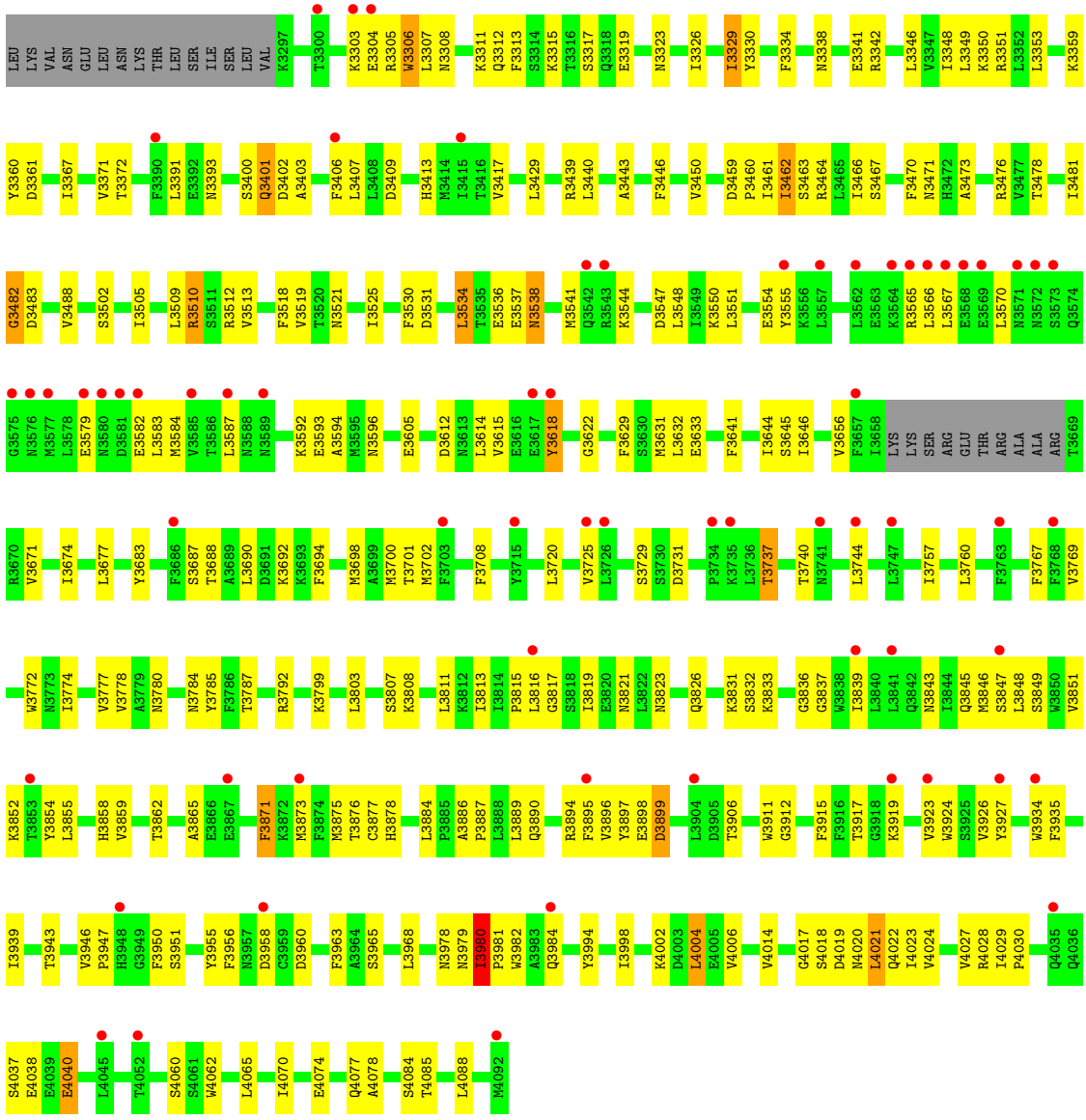
W2920 T2924 M2938 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 A2964 V2965 V2966 N2967 F2972 V2982 G2983 S2988 P2989 G2990 K3001 L3010 Q3011 E3012 F3016 V3017 N3018 V3019 G3020 L3024 N3025 E3026 S3027 V3028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G3575 N3576 M3577 L3578 E3579 N3580 D3581 E3582 L3583 M3584 V3585 T3586 L3587 N3588 N3589 K3592 E3593 A3594 M3595 N3596 E3605 D3612 N3613 L3614 V3615 E3616 E3617 Y3618 G3622 F3629 S3630 M3631 L3632 E3633 F3641 I3644 S3645 I3646 V3656 F3657 I3658 LYS LYS SER ARG GLU THR ARG ALA ALA ARG T3669
R3670 V3671 I3674 L3677 Y3683 F3686 S3687 T3688 A3689 L3690 D3691 K3692 K3693 F3694 M3698 A3699 M3700 T3701 M3702 F3703 F3708 Y3715 L3720 V3725 L3726 S3729 S3730 D3731 P3734 K3735 L3736 T3737 T3740 M3741 L3744 L3747 I3757 L3760 F3763 F3767 F3768 V3769
W3772 N3773 I3774 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 R3792 K3799 L3803 S3807 K3808 L3811 K3812 I3813 I3814 P3815 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823 Q3826 K3831 S3832 K3833 G3836 G3837 W3838 I3839 L3840 L3841 Q3842 N3843 I3844 Q3845 M3846 S3847 L3848 S3849 W3850 V3851
K3852 T3853 Y3854 L3855 H3858 V3859 T3862 A3865 E3866 E3867 F3871 K3872 M3873 F3874 M3875 T3876 C3877 H3878 L3884 P3885 A3886 P3887 L3888 L3889 Q3890 R3894 F3895 V3896 Y3897 E3898 D3899 L3904 D3905 T3906 W3911 G3912 F3915 F3916 T3917 G3918 K3919 V3923 W3924 S3925 V3926 Y3927 W3934 F3935
I3939 T3943 V3946 P3947 H3948 G3949 F3950 S3951 Y3955 F3956 N3957 D3958 C3959 D3960 F3963 A3964 S3965 L3968 N3978 N3979 I3980 P3981 W3982 A3983 Q3984 Y3994 I3998 K4002 D4003 L4004 E4005 V4006 V4014 G4017 S4018 D4019 N4020 L4021 Q4022 I4023 V4024 V4027 R4028 I4029 P4030 Q4035 Q4036
S4037 E4038 E4039 E4040 L4045 T4052 S4060 S4061 W4062 L4065 I4070 E4074 Q4077 A4078 S4084 T4085 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	174.89Å 119.17Å 193.97Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	49.29 – 3.40 49.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.24-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.303 0.236 , 0.300	Depositor DCC
R_{free} test set	5512 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	133.4	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 132.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41678	wwPDB-VP
Average B, all atoms (Å^2)	190.0	wwPDB-VP

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

[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 (i)

5.1 Standard geometry (i)

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

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

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

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

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3308	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	934	0
1	B	20748	0	20207	930	0
2	A	31	0	12	6	0
2	B	31	0	12	22	0
3	A	54	0	24	28	0
3	B	54	0	24	29	0
4	A	5	0	0	2	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41678	0	40485	1867	0

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

All (1867) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:SER:O	1:A:1421:TYR:CE2	2.62	0.53
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.08	0.53
1:A:1826:PHE:CZ	1:A:1830:VAL:HG13	2.44	0.53
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.43	0.53
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.09	0.53
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.96	0.53
1:B:3342:ARG:NH1	1:B:3393:ASN:OD1	2.38	0.53
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.09	0.53
1:B:3760:LEU:HD21	1:B:4078:ALA:HA	1.91	0.53
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.39	0.53
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.73	0.53
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.41	0.53
1:A:2220:CYS:SG	1:A:2221:SER:N	2.82	0.53
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.29	0.53
1:B:1770:ILE:HD11	1:B:1936:ILE:HD11	1.90	0.53
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.32	0.53
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.91	0.53
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.90	0.53
1:A:2380:LEU:CD1	1:A:2577:ALA:CB	2.86	0.53
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.74	0.53
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.38	0.53
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.08	0.53
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.57	0.53
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.43	0.52
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.44	0.52
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.39	0.52
1:B:2080:LYS:HZ1	1:B:2549:ARG:NE	2.07	0.52
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.09	0.52
1:B:3737:THR:CB	1:B:3740:THR:CB	2.87	0.52
1:B:3862:THR:HB	1:B:3865:ALA:HB2	1.91	0.52
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.24	0.52
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.74	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	1.90	0.52
1:A:2941:THR:HG22	1:A:2942:ASP:N	2.22	0.52
1:A:4024:VAL:CG2	1:A:4027:VAL:HB	2.40	0.52
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.10	0.52
1:B:1866:GLN:O	1:B:1870:ASN:HB2	2.08	0.52
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.10	0.52
1:B:2081:THR:HB	2:B:5400:ATP:O1A	2.09	0.52
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.52
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	1.91	0.52
1:B:2891:ILE:HD11	1:B:2903:ILE:HD11	1.90	0.52
1:A:1416:LYS:O	1:A:1421:TYR:OH	2.25	0.52
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.91	0.52
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.54	0.52
1:A:3701:THR:OG1	1:A:4085:THR:HG22	2.08	0.52
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.45	0.52
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.74	0.52
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.92	0.52
1:A:2473:LEU:HD22	1:A:2527:GLU:HG2	1.91	0.52
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.44	0.52
1:A:1416:LYS:O	1:A:1421:TYR:CE2	2.63	0.52
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.44	0.52
1:A:3304:GLU:O	1:A:3307:LEU:HB3	2.10	0.52
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.50	0.52
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.91	0.52
1:B:2624:ARG:NH2	1:B:2910:ASN:O	2.43	0.52
1:B:3934:TRP:CB	1:B:4023:ILE:HD13	2.40	0.52
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.44	0.52
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.91	0.52
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.10	0.52
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.30	0.52
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.90	0.52
1:A:1970:LEU:CD2	1:A:1974:LYS:HE2	2.40	0.52
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.50	0.52
1:B:23:LEU:O	1:B:24:GLU:CB	2.57	0.52
1:B:2073:VAL:HG21	1:B:2199:LEU:HD11	1.92	0.52
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.91	0.52
1:A:1956:LEU:CB	1:A:1968:PHE:CE2	2.87	0.52
1:B:2044:ARG:NH2	1:B:2093:ILE:HD11	2.24	0.52
1:A:1527:LEU:HD21	1:A:1546:LEU:HD21	1.91	0.52
1:A:1706:LEU:HD22	1:A:1935:GLN:CG	2.38	0.52
1:A:2076:ALA:CB	1:A:2549:ARG:HG2	2.40	0.52
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.57	0.52
1:A:3304:GLU:HG3	1:A:3307:LEU:CD2	2.32	0.52
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.50	0.52
1:B:2728:LEU:CG	1:B:2771:ARG:HH22	2.22	0.52
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.09	0.51
1:B:2080:LYS:HG2	2:B:5400:ATP:O1B	2.07	0.51
1:A:2421:GLY:H	3:A:5401:ADP:PB	2.33	0.51

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3797:THR:O	1:A:3801:ILE:HG12	2.13	0.48
1:B:1386:ILE:HG22	1:B:1396:ARG:HG2	1.95	0.48
1:B:1714:GLN:HB3	1:B:1727:LEU:HD11	1.96	0.48
1:B:2642:ARG:O	1:B:2646:ARG:HG3	2.14	0.48
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.77	0.48
1:A:1455:LEU:HD12	1:A:1516:LEU:CD2	2.41	0.48
1:A:2463:ASN:O	1:A:2475:PRO:HD2	2.13	0.48
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.96	0.48
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.85	0.48
1:A:1969:GLY:O	1:A:1972:THR:HB	2.14	0.48
1:A:2771:ARG:HG2	1:A:2781:ILE:HG21	1.96	0.48
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	1.96	0.48
1:B:2295:ILE:HG12	1:B:2314:ILE:HD12	1.96	0.48
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.43	0.48
1:A:1941:ASP:O	1:A:1945:LEU:HG	2.13	0.47
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	1.91	0.47
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.39	0.47
1:B:2754:GLY:HA3	1:B:2886:HIS:CE1	2.49	0.47
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	2.97	0.47
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	1.94	0.47
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.29	0.47
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.49	0.47
1:B:2467:THR:HG22	1:B:2468:SER:N	2.28	0.47
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.44	0.47
1:A:2201:HIS:CE1	1:A:2497:TYR:HB3	2.48	0.47
1:A:3628:ILE:HG22	1:A:3649:PHE:CE2	2.49	0.47
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.96	0.47
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.14	0.47
1:B:2122:THR:O	1:B:2123:LEU:C	2.53	0.47
1:B:2220:CYS:SG	2:B:5400:ATP:C6	3.07	0.47
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.63	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.97	0.47
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.14	0.47
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.80	0.47
1:B:2732:MET:CB	3:B:5402:ADP:C4	2.97	0.47
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.62	0.47
1:A:2889:PHE:CD1	1:A:2902:MET:HE1	2.50	0.47
1:A:3940:THR:O	1:A:3943:THR:HB	2.14	0.47
1:B:1979:ASN:OD1	1:B:2066:THR:HG21	2.15	0.47
1:B:2106:THR:H	1:B:2156:SER:HB2	1.79	0.47
1:B:2757:MET:HG2	1:B:2914:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.14	0.47
1:A:1938:GLY:HA3	1:A:1989:GLU:HG2	1.96	0.47
1:A:3979:ASN:O	1:A:3981:PRO:CD	2.57	0.47
1:B:2473:LEU:HD23	1:B:2473:LEU:C	2.34	0.47
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	1.97	0.47
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.45	0.47
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.49	0.47
1:B:2891:ILE:CD1	1:B:2903:ILE:HD11	2.44	0.47
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.50	0.47
1:A:1422:LYS:HA	1:A:1422:LYS:HD3	1.63	0.47
1:A:1992:LYS:HG2	1:A:2024:SER:CB	2.43	0.47
1:A:2368:PHE:O	1:A:2369:SER:CB	2.62	0.47
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.97	0.47
1:B:1534:PHE:CD2	1:B:1537:PHE:CE2	3.02	0.47
1:B:2361:ILE:HG22	1:B:2367:SER:O	2.15	0.47
1:B:2734:ILE:HD12	1:B:2734:ILE:H	1.80	0.47
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.30	0.47
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.79	0.47
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.25	0.47
1:B:2424:LYS:N	3:B:5401:ADP:O1B	2.48	0.47
1:B:3326:ILE:HA	1:B:3349:LEU:HD21	1.96	0.47
1:B:3994:TYR:O	1:B:3998:ILE:HD12	2.15	0.47
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.80	0.47
1:A:3302:GLU:O	1:A:3305:ARG:CA	2.63	0.47
1:A:3718:ALA:O	1:A:3721:THR:HG22	2.15	0.47
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.96	0.47
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.18	0.47
1:B:1910:GLU:HB2	1:B:3846:MET:HB2	1.97	0.47
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.79	0.47
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.96	0.47
1:B:2354:SER:OG	1:B:2357:SER:CB	2.63	0.47
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.97	0.47
1:B:4037:SER:HB3	1:B:4040:GLU:HB2	1.97	0.47
1:A:1970:LEU:HD23	1:A:1974:LYS:HE3	1.97	0.46
1:A:3956:PHE:CD1	1:A:3994:TYR:HD1	2.33	0.46
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.45	0.46
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.97	0.46
1:B:2819:GLU:O	1:B:2822:ILE:HG13	2.15	0.46
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.97	0.46
1:B:1828:TYR:HB2	1:B:1857:VAL:HG13	1.98	0.46
1:B:2152:VAL:HG12	1:B:2154:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4074:GLU:HA	1:B:4077:GLN:HE21	1.80	0.46
1:A:2856:LEU:HD21	1:A:2877:PHE:HB2	1.97	0.46
1:A:3304:GLU:O	1:A:3307:LEU:N	2.48	0.46
1:A:3509:LEU:O	1:A:3513:VAL:HG23	2.16	0.46
1:A:3624:HIS:ND1	1:A:3675:LEU:HD11	2.30	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.97	0.46
1:A:3945:LEU:HD21	1:A:4070:ILE:CD1	2.45	0.46
1:B:1563:LYS:HA	1:B:1569:ILE:O	2.15	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG23	2.15	0.46
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.15	0.46
1:B:2080:LYS:CE	1:B:2549:ARG:HH21	2.28	0.46
1:B:4023:ILE:CD1	1:B:4029:ILE:HD11	2.45	0.46
1:A:1970:LEU:HD21	1:A:1974:LYS:HE2	1.97	0.46
1:A:3990:ALA:HB2	1:A:4011:CYS:SG	2.56	0.46
1:B:1386:ILE:CG2	1:B:1396:ARG:HG2	2.46	0.46
1:B:2081:THR:HG22	1:B:2085:LYS:HD2	1.97	0.46
1:B:2732:MET:SD	3:B:5402:ADP:N7	2.89	0.46
1:B:2786:ILE:HD12	1:B:3460:PRO:CG	2.46	0.46
1:B:2824:GLU:HG2	1:B:2825:THR:H	1.80	0.46
1:B:2961:ILE:O	1:B:2965:VAL:HG23	2.14	0.46
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.28	0.46
1:A:2068:GLN:HE22	1:A:2188:PRO:HA	1.81	0.46
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.81	0.46
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.69	0.46
1:A:4019:ASP:H	1:A:4031:GLN:HE21	1.64	0.46
3:A:5401:ADP:H2'	3:A:5401:ADP:N3	2.31	0.46
1:B:1826:PHE:CG	1:B:1826:PHE:O	2.68	0.46
1:B:2064:GLN:OE1	1:B:2065:LYS:HG3	2.15	0.46
1:B:2424:LYS:HE2	1:B:2424:LYS:HB2	1.55	0.46
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.97	0.46
1:A:2420:PRO:CG	1:A:2616:LEU:HD21	2.45	0.46
1:A:2938:MET:SD	1:A:3321:ILE:CG2	3.03	0.46
1:A:2999:LEU:HD11	1:A:3325:ILE:HG12	1.97	0.46
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.50	0.46
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.55	0.46
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.98	0.46
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.63	0.46
1:B:3911:TRP:CH2	1:B:3926:VAL:HG13	2.51	0.46
1:A:1418:SER:O	1:A:1421:TYR:CD2	2.68	0.46
1:A:2219:VAL:HG21	2:A:5400:ATP:N7	2.31	0.46
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.45	0.46
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.97	0.46
1:B:3701:THR:OG1	1:B:4085:THR:HG22	2.15	0.46
1:B:2081:THR:HB	2:B:5400:ATP:O2A	2.15	0.46
1:B:3725:VAL:HG22	1:B:3731:ASP:HA	1.96	0.46
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.46	0.46
1:B:2080:LYS:HZ1	1:B:2549:ARG:CZ	2.26	0.46
1:B:3367:ILE:O	1:B:3371:VAL:HG22	2.16	0.46
1:A:23:LEU:O	1:A:25:GLU:N	2.49	0.46
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.16	0.46
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.16	0.46
1:A:2754:GLY:HA3	1:A:2886:HIS:CE1	2.51	0.46
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	1.97	0.46
1:B:1838:ILE:HD11	1:B:1845:GLY:CA	2.46	0.46
1:B:2394:THR:H	1:B:2397:THR:HB	1.81	0.46
1:A:1644:ILE:O	1:A:1648:ILE:HG22	2.16	0.45
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.16	0.45
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.97	0.45
1:B:2358:THR:HG22	1:B:2359:ILE:N	2.31	0.45
1:A:2763:ARG:HA	3:A:5402:ADP:C4'	2.47	0.45
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.64	0.45
1:B:1366:VAL:CG1	1:B:1369:LYS:HE3	2.45	0.45
1:B:2856:LEU:HD21	1:B:2877:PHE:HB2	1.98	0.45
1:A:2072:LEU:HB3	1:A:2215:PHE:HE1	1.80	0.45
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.16	0.45
1:A:3373:LEU:HD13	1:A:3557:LEU:CD1	2.47	0.45
1:B:65:THR:O	1:B:66:GLN:CB	2.64	0.45
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.81	0.45
1:B:2088:ILE:HG12	1:B:2151:TRP:CZ2	2.51	0.45
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.63	0.45
1:B:2473:LEU:HD21	1:B:2475:PRO:CG	2.47	0.45
1:A:1392:LEU:C	1:A:1392:LEU:CD1	2.84	0.45
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.84	0.45
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.51	0.45
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.16	0.45
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.97	0.45
1:A:2853:LEU:HD21	1:A:2870:GLU:HG3	1.98	0.45
1:A:2893:ASP:HA	1:A:2894:PRO:HD2	1.89	0.45
1:A:3636:GLY:CA	1:A:3642:TYR:O	2.64	0.45
1:B:40:TRP:O	1:B:44:LYS:N	2.50	0.45
1:B:216:PRO:HA	1:B:1365:PHE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.29	0.45
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	1.99	0.45
1:B:2068:GLN:HA	1:B:2191:ARG:HG2	1.98	0.45
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.38	0.45
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.98	0.45
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.47	0.45
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.99	0.45
1:A:2982:VAL:CG1	1:A:2983:GLY:H	2.29	0.45
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.94	0.45
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.00	0.45
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	1.98	0.45
1:B:2249:LEU:HA	1:B:2252:LEU:HD12	1.99	0.45
1:B:2467:THR:O	1:B:2471:LEU:N	2.48	0.45
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.16	0.45
1:B:4084:SER:O	1:B:4088:LEU:HG	2.17	0.45
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.73	0.45
1:A:1995:VAL:HG22	1:A:2022:PHE:HD2	1.80	0.45
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.99	0.45
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.36	0.45
1:B:2476:LYS:HE3	1:B:2528:ARG:CB	2.47	0.45
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.97	0.45
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.98	0.45
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.99	0.45
1:A:1956:LEU:HB3	1:A:1968:PHE:CD2	2.51	0.45
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.45
1:A:2241:LEU:HD21	1:A:2249:LEU:HD12	1.99	0.45
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.17	0.45
1:A:3306:TRP:CH2	1:A:3594:ALA:HB1	2.45	0.45
1:B:2609:THR:HA	1:B:2612:GLN:O	2.17	0.45
1:B:2695:LEU:HD23	1:B:2743:LEU:HD11	1.99	0.45
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.51	0.45
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.81	0.45
1:B:2941:THR:CG2	1:B:2942:ASP:H	2.29	0.45
1:B:3470:PHE:CE1	1:B:3488:VAL:HG21	2.52	0.45
1:A:1416:LYS:CA	1:A:1421:TYR:OH	2.65	0.45
1:A:1646:GLN:OE1	1:A:1762:TYR:HD1	2.00	0.45
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.51	0.45
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.31	0.45
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.50	0.45
1:A:3592:LYS:O	1:A:3596:ASN:N	2.50	0.45
1:B:1536:ARG:HD3	1:B:1841:ILE:HD13	1.98	0.45

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:THR:HB	1:A:1498:GLU:HB2	2.01	0.41
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.02	0.41
1:A:1726:LEU:HD13	1:A:3984:GLN:HB3	2.01	0.41
1:A:2476:LYS:HB3	1:A:2482:LEU:HB2	2.02	0.41
1:A:2640:THR:HG23	1:A:2643:SER:H	1.85	0.41
1:A:2821:ASN:O	1:A:2823:LEU:HD13	2.21	0.41
1:A:3692:LYS:HG3	1:A:3898:GLU:HG3	2.02	0.41
1:A:3786:PHE:CD1	1:A:3893:ASP:HB2	2.56	0.41
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.21	0.41
1:B:1626:CYS:HB2	1:B:1643:TYR:CD2	2.56	0.41
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.35	0.41
1:B:3896:VAL:HG12	1:B:3898:GLU:HG2	2.02	0.41
1:A:2765:GLY:CA	3:A:5402:ADP:O2A	2.59	0.41
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.81	0.41
1:B:1578:PHE:HB3	1:B:1595:LYS:HB2	2.02	0.41
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.51	0.41
1:B:2285:GLU:CB	1:B:2412:ARG:NH2	2.83	0.41
1:B:2732:MET:CG	3:B:5402:ADP:C6	3.02	0.41
1:B:2788:ARG:H	1:B:3459:ASP:HB2	1.85	0.41
1:B:3950:PHE:HE1	1:B:4006:VAL:HB	1.86	0.41
1:A:1409:LEU:O	1:A:1413:VAL:HG23	2.20	0.41
1:A:1744:LEU:CD2	1:A:1760:PHE:CD2	3.03	0.41
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.50	0.41
1:A:2728:LEU:HB2	1:A:2771:ARG:HH12	1.86	0.41
1:A:2982:VAL:HG12	1:A:2983:GLY:H	1.85	0.41
1:A:3971:VAL:HA	1:A:3974:THR:HG22	2.03	0.41
1:B:1697:LYS:O	1:B:1701:LEU:HG	2.20	0.41
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.97	0.41
1:B:3304:GLU:O	1:B:3305:ARG:C	2.59	0.41
1:B:3409:ASP:HB3	1:B:3518:PHE:CB	2.47	0.41
1:B:3757:ILE:HD11	1:B:4074:GLU:HG2	2.02	0.41
1:B:3826:GLN:HB2	1:B:3854:TYR:CZ	2.56	0.41
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.42	0.41
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.99	0.41
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.61	0.41
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.56	0.41
1:A:2226:ILE:HG23	1:A:2288:VAL:CG2	2.46	0.41
1:A:2485:PHE:CZ	1:A:2534:ALA:HB2	2.56	0.41
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.48	0.41
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.83	0.41
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3528:ARG:HH11	1:A:3650:LEU:HD11	1.86	0.41
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.21	0.41
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	2.02	0.41
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.86	0.41
1:A:3703:PHE:HE2	1:A:3719:VAL:HG21	1.86	0.41
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.74	0.41
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	2.02	0.41
1:B:1830:VAL:HG23	1:B:1833:ARG:NH2	2.36	0.41
1:B:1838:ILE:HD11	1:B:1845:GLY:HA3	2.03	0.41
1:B:2099:ASN:HD22	1:B:2151:TRP:HE1	1.68	0.41
1:B:2590:GLU:N	1:B:2591:PRO:HD2	2.36	0.41
1:B:2782:VAL:HB	1:B:2815:LEU:HD12	2.02	0.41
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.45	0.41
1:A:1664:LEU:HD21	1:A:1715:LEU:HD22	2.03	0.41
1:A:2266:PHE:CD1	1:A:2326:LEU:HD21	2.53	0.41
1:A:2408:LEU:HD13	1:A:2432:LEU:HD21	2.03	0.41
1:A:2985:ASN:N	1:A:2986:PRO:CD	2.84	0.41
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.34	0.41
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.56	0.40
1:A:2332:GLY:HA2	1:A:2335:GLN:CG	2.50	0.40
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.40
1:B:2225:LYS:HD2	1:B:2281:PHE:CZ	2.55	0.40
1:B:2299:ARG:HA	1:B:2302:PHE:CD2	2.56	0.40
1:B:2320:ARG:NH1	1:B:2406:ASP:OD2	2.40	0.40
1:B:2766:LYS:HD2	1:B:2890:THR:HG22	2.02	0.40
1:B:3629:PHE:O	1:B:3633:GLU:HB2	2.20	0.40
1:B:3833:LYS:HZ3	1:B:3862:THR:HG21	1.85	0.40
1:B:3839:ILE:HG22	1:B:3871:PHE:HE1	1.86	0.40
1:A:1392:LEU:HD21	1:A:1487:THR:HG21	2.02	0.40
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	2.02	0.40
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.91	0.40
1:A:2060:PHE:HZ	1:A:2193:LEU:HD21	1.86	0.40
1:A:2380:LEU:HD12	1:A:2380:LEU:C	2.42	0.40
1:A:3458:PHE:HD2	1:A:3506:PRO:HG2	1.86	0.40
1:A:3844:ILE:HD11	1:A:3855:LEU:HD22	2.03	0.40
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.03	0.40
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.21	0.40
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.40
1:A:1637:GLU:C	1:A:1686:LYS:HZ2	2.20	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.03	0.40
1:B:2306:ASP:HB2	1:B:2309:SER:HB3	2.03	0.40

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2640/2695 (98%)	2503 (95%)	121 (5%)	16 (1%)	25 57
1	B	2640/2695 (98%)	2506 (95%)	116 (4%)	18 (1%)	22 55
All	All	5280/5390 (98%)	5009 (95%)	237 (4%)	34 (1%)	25 57

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	1391	GLY
1	A	2369	SER
1	A	3309	THR
1	B	1391	GLY
1	B	2761	ALA
1	B	3306	TRP
1	A	212	GLY
1	A	1633	GLY
1	B	2763	ARG
1	B	2764	THR
1	B	2990	GLY
1	B	3482	GLY
1	A	2562	PRO
1	A	2990	GLY
1	A	3980	ILE
1	A	115	GLU
1	A	2513	GLN
1	A	2519	PRO
1	A	3809	GLU
1	B	66	GLN
1	B	2519	PRO
1	B	3402	ASP
1	A	66	GLN
1	B	2562	PRO
1	A	3482	GLY
1	B	1366	VAL
1	B	3462	ILE
1	B	3980	ILE
1	B	1633	GLY
1	B	2028	PRO
1	B	1470	PRO
1	B	2141	ILE
1	A	1470	PRO

5.3.2 Protein sidechains (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%)	2128 (96%)	90 (4%)	30	59
1	B	2218/2453 (90%)	2133 (96%)	85 (4%)	33	61
All	All	4436/4906 (90%)	4261 (96%)	175 (4%)	32	61

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

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

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

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

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

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

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

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	5403	-	4,4,4	0.34	0	6,6,6	0.45	0
3	ADP	B	5402	-	24,29,29	0.98	1 (4%)	29,45,45	1.53	5 (17%)
3	ADP	A	5402	-	24,29,29	1.02	1 (4%)	29,45,45	1.58	5 (17%)
2	ATP	A	5400	-	26,33,33	1.02	1 (3%)	31,52,52	1.62	6 (19%)
2	ATP	B	5400	-	26,33,33	1.02	1 (3%)	31,52,52	1.61	6 (19%)
4	SO4	A	5403	-	4,4,4	0.36	0	6,6,6	0.74	0
3	ADP	B	5401	-	24,29,29	1.22	2 (8%)	29,45,45	1.56	6 (20%)
3	ADP	A	5401	-	24,29,29	1.20	2 (8%)	29,45,45	1.46	7 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	5402	-	-	1/12/32/32	0/3/3/3

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

All (8) bond length outliers are listed below:

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

All (35) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

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

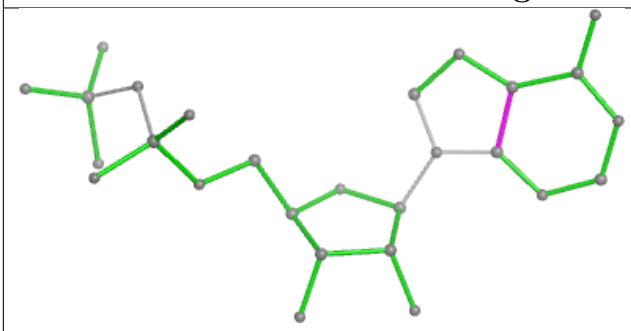
There are no ring outliers.

8 monomers are involved in 89 short contacts:

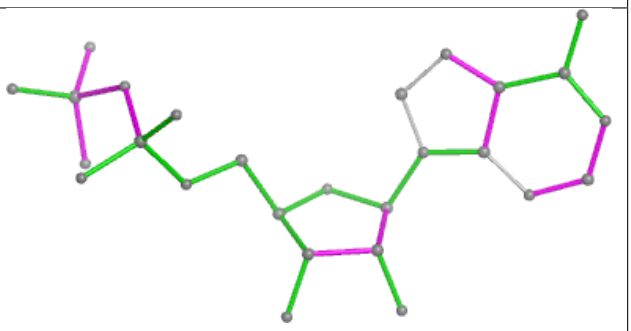
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5403	SO4	2	0
3	B	5402	ADP	23	0
3	A	5402	ADP	17	0
2	A	5400	ATP	6	0
2	B	5400	ATP	22	0
4	A	5403	SO4	2	0
3	B	5401	ADP	6	0
3	A	5401	ADP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

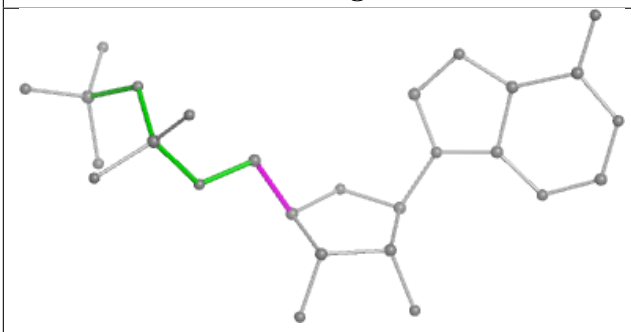
Ligand ADP B 5402



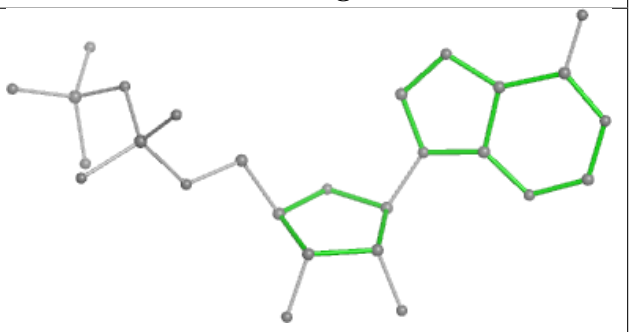
Bond lengths



Bond angles

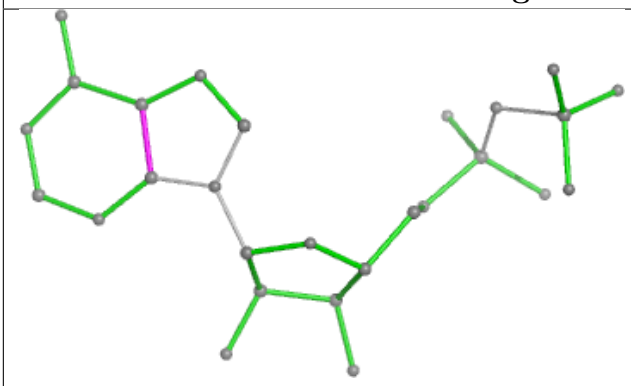


Torsions

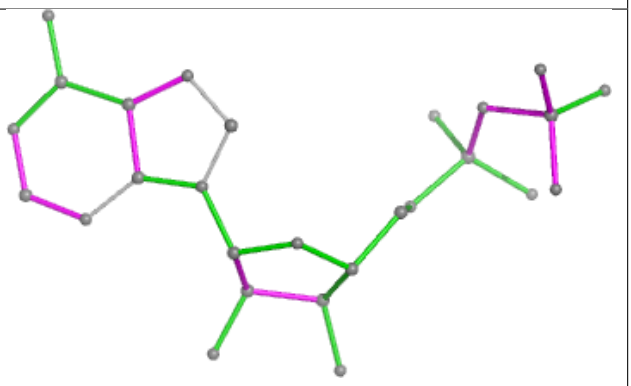


Rings

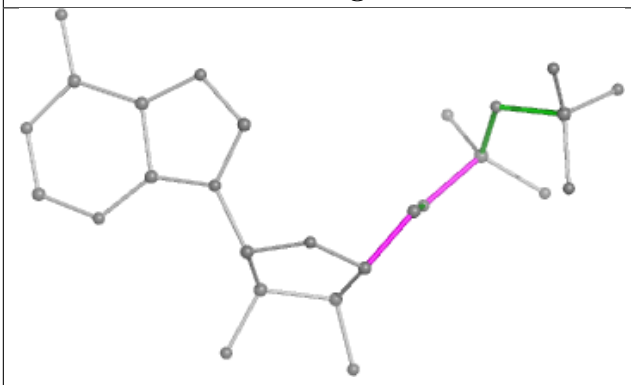
Ligand ADP A 5402



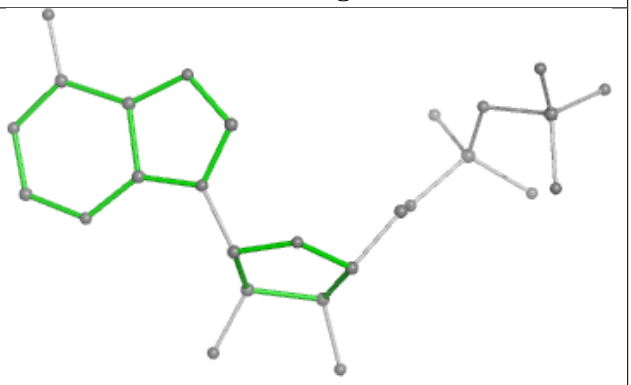
Bond lengths



Bond angles

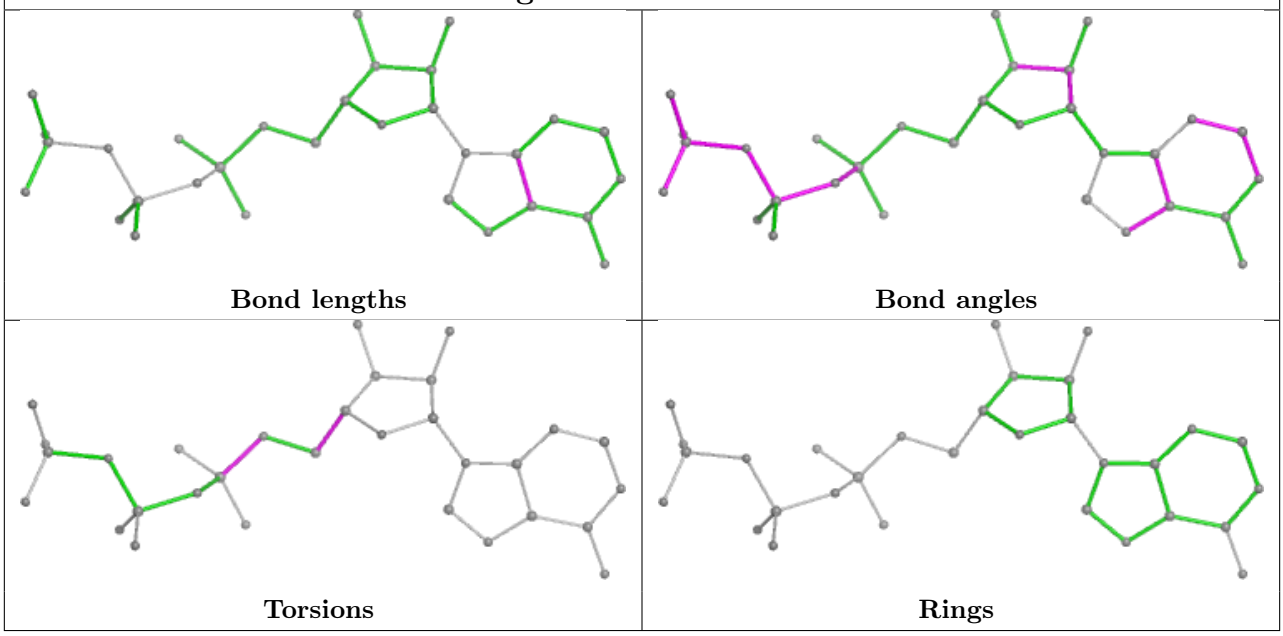


Torsions

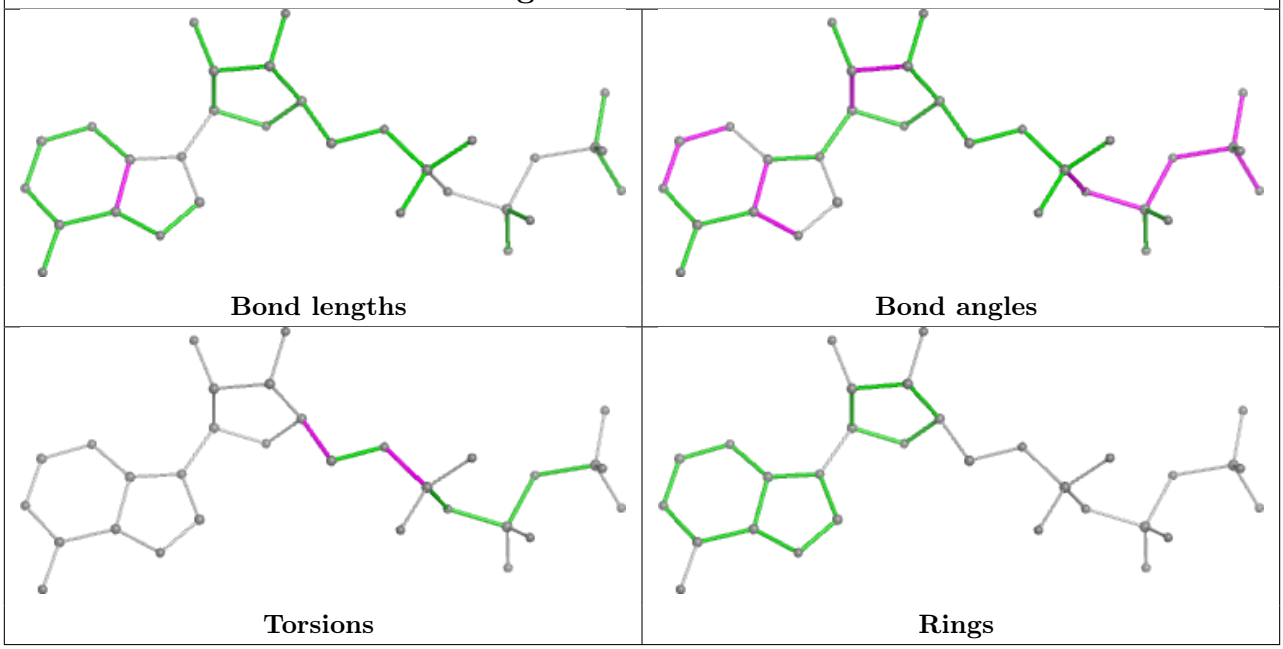


Rings

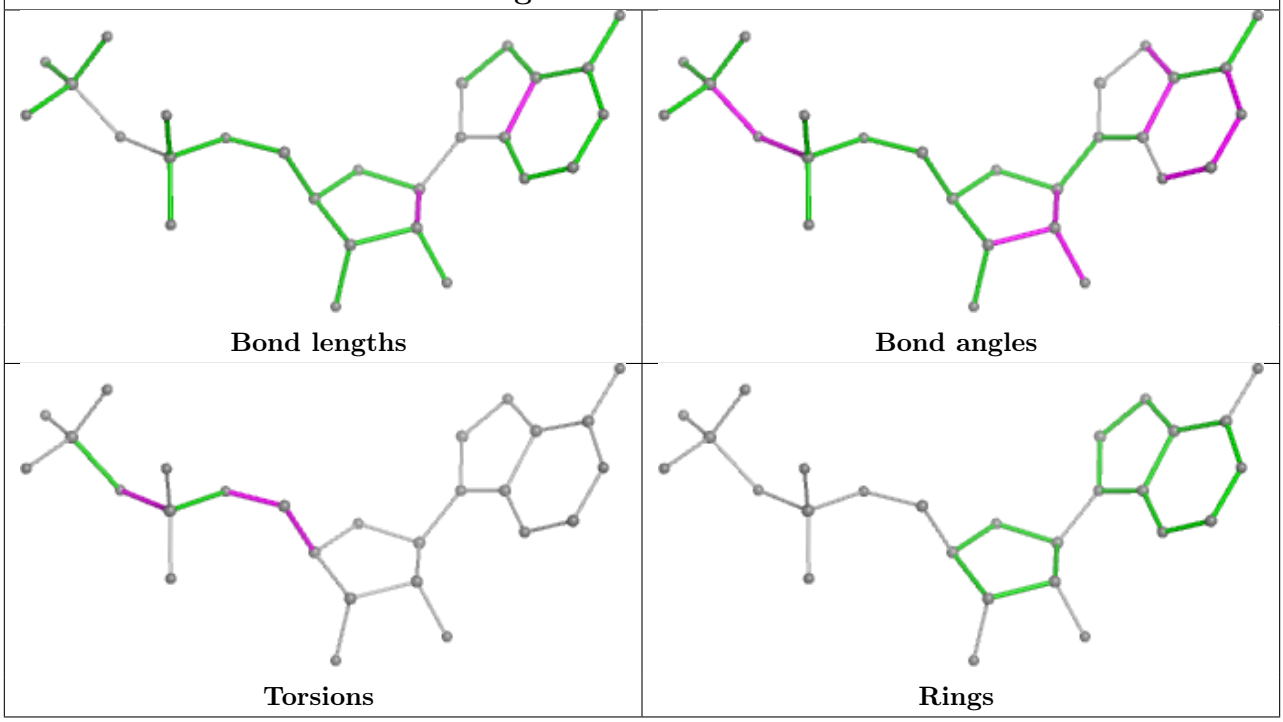
Ligand ATP A 5400



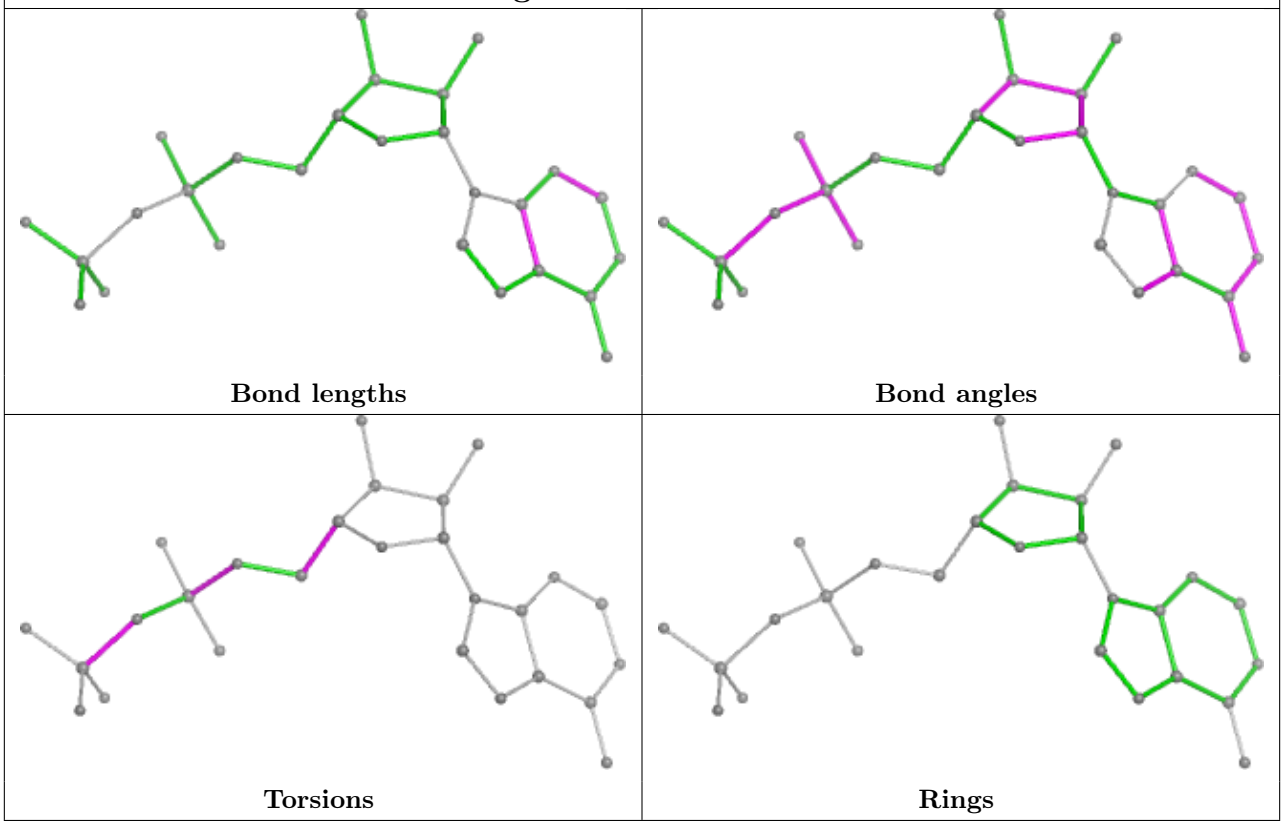
Ligand ATP B 5400



Ligand ADP B 5401



Ligand ADP A 5401



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

All (552) RSRZ outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

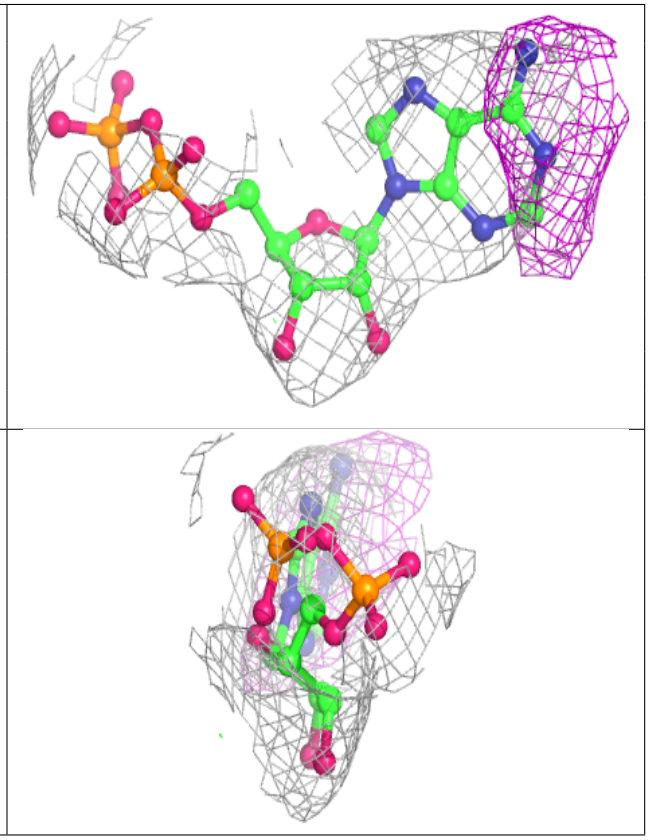
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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

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

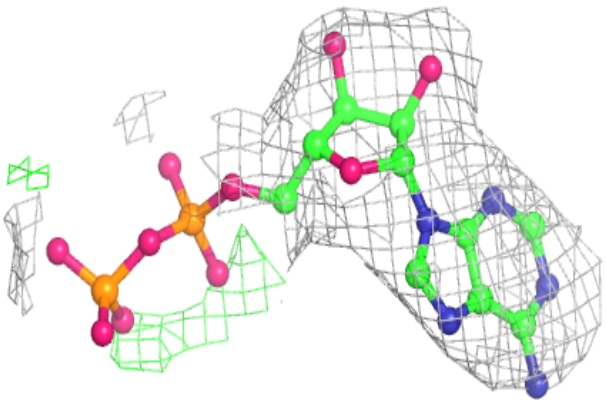
Electron density around ADP B 5402:

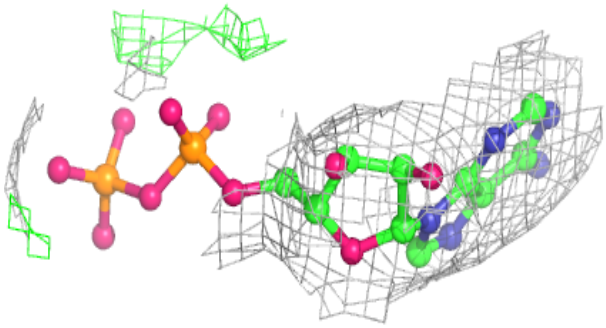
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

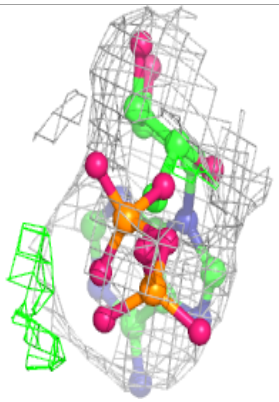


Electron density around ADP A 5401:

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

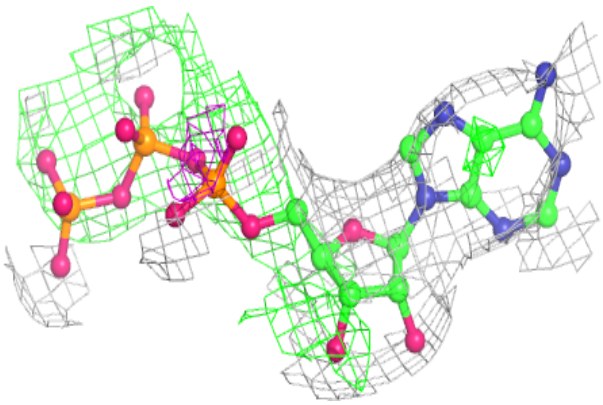


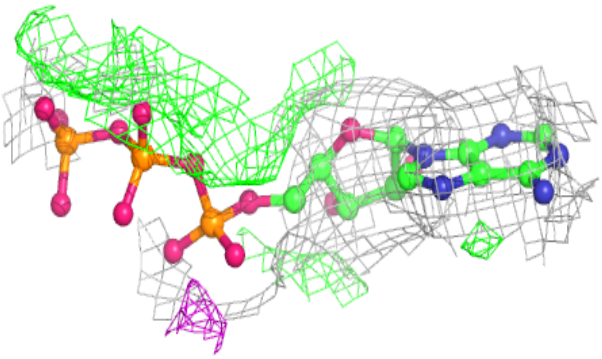




Electron density around ATP B 5400:

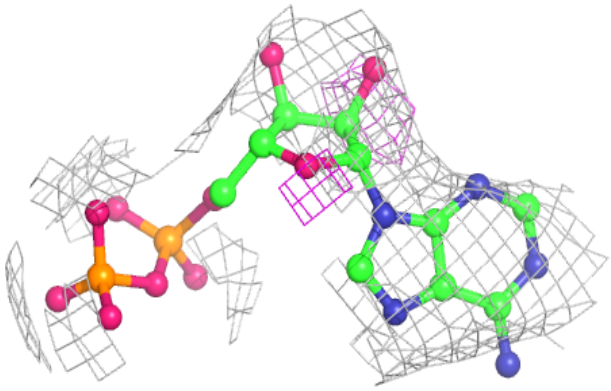
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

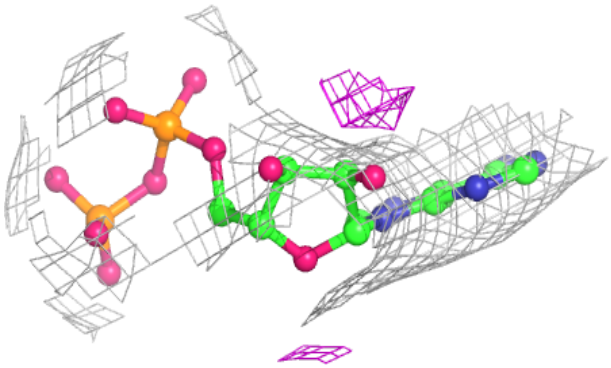


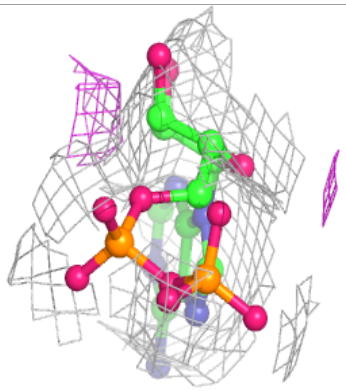


Electron density around ADP A 5402:

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

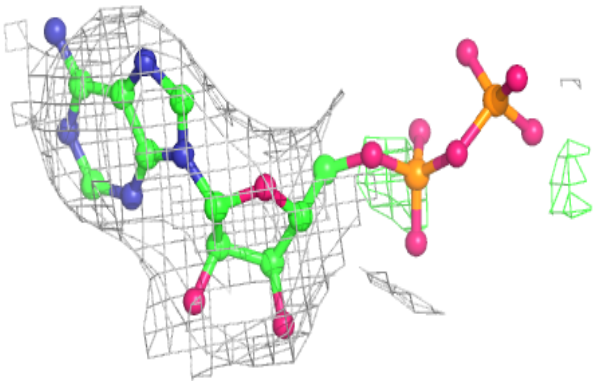


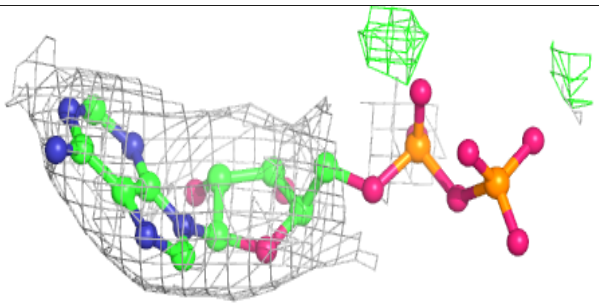


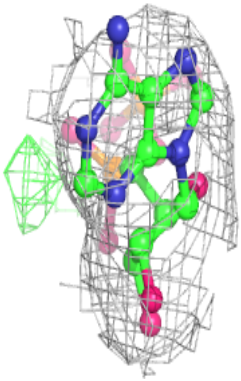


Electron density around ADP B 5401:

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

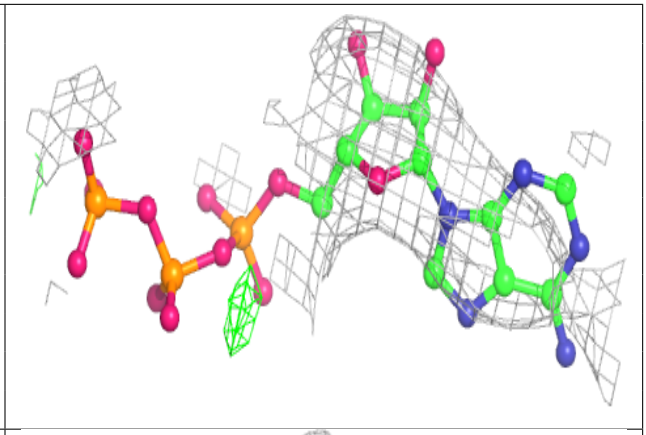


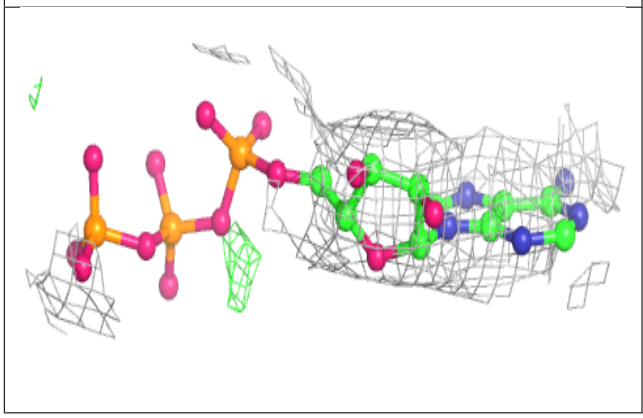


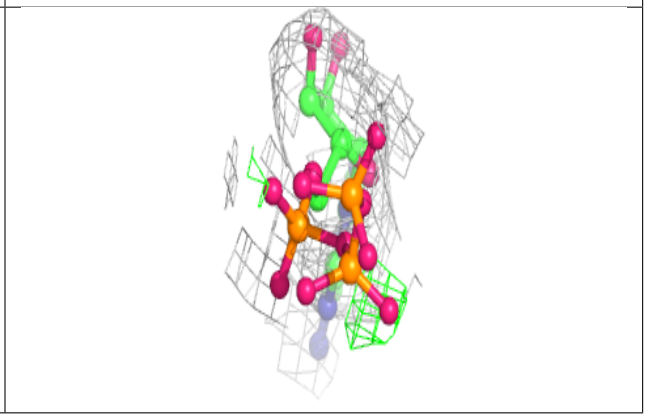


Electron density around ATP A 5400:

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







6.5 Other polymers (i)

There are no such residues in this entry.