



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:31 PM UTC

PDB ID : 4AI6 / pdb_00004ai6
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

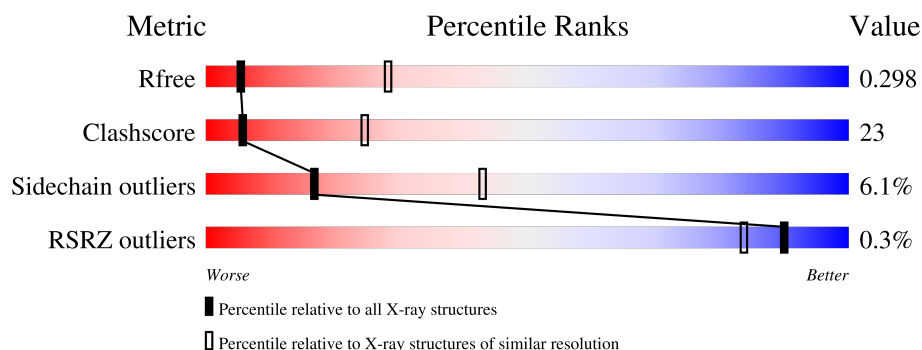
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	 65% 31% . .
1	B	2695	 65% 31% . .

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	B	5403	-	-	X	-

2 Entry composition

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
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 10 discrepancies between the modelled and reference sequences:

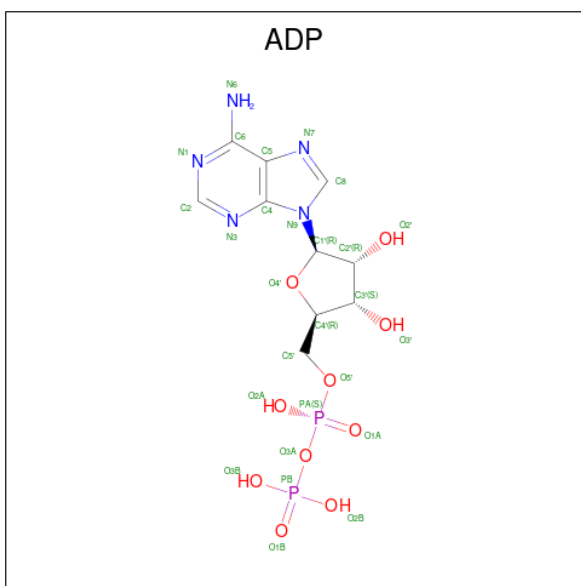
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	linker	UNP P36022
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	217	LYS	-	linker	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630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

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



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

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



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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

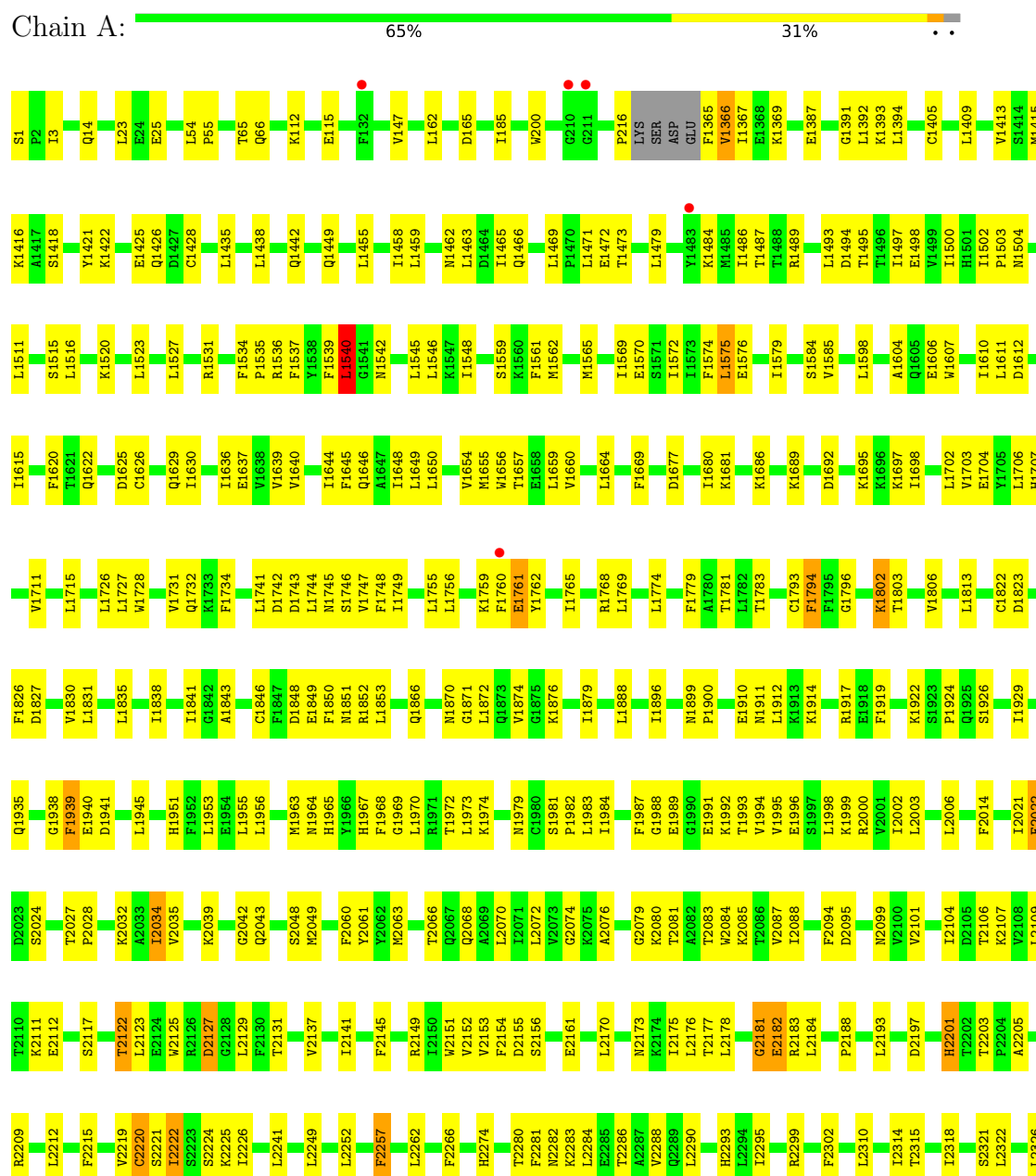
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots

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



I3998	F3915	S3830	D3547	R3439	L3320	N2967	H2886	L2779	N2634	K2512	R2412	G2332
K4002	K3919	K3833	L3548	L3440	I3321	M2980	M2889	K2760	T2635	Q2514	G2413	G2333
L4003	V3923	G3837	K3550	F3649	G3324	G2982	F2889	P2420	P2637	K2517	G2421	S2334
L4004	K3924	K3838	K3555	F3446	I3325	G2983	L2891	T2518	Q2639	T2518	R2424	R2336
C4011	S3925	I3839	K3556	I3452	I3326	V2984	C2892	K2785	T2640	N2521	T2425	T2339
V4014	F3926	L3747	L3557	E3456	S3327	N2986	D2893	K2786	S2643	N2524	M2426	T2340
F4015	Y3927	L3760	L3559	F3457	I3329	R2987	P2894	R2787	L2644	T2525	M2428	S2350
D4019	K3764	L3566	L3566	D3459	Y3330	S2988	M2902	R2788	W2653	L2526	L2431	L2353
N4020	K3765	L3567	L3567	P3460	E3331	P2989	S2904	R2789	R2654	L2527	L2432	D2355
L4021	ARG	L3570	L3570	I3461	E3334	L2989	S2905	F2795	L2655	Y2356	L2437	S2357
L4022	THR	L3578	L3578	S3463	N3338	L2999	L2908	R2799	D2658	A2534	L2437	S2357
I4023	ALA	L3579	L3579	R3464	E3341	L3002	F2909	R2812	V2677	C2535	F2445	V2360
V4024	ALA	N3580	N3580	S3457	R3342	L3010	R2911	R2813	L2686	N2536	S2446	T2361
V4027	ARG	L3583	L3583	N3471	L3346	V3017	W2916	T2816	S2701	R2549	K2447	K2362
R4028	L3674	L3592	L3592	H3472	L3346	L3024	M2917	E2819	D2703	F2550	D2448	K2363
I4029	L3675	E3593	E3593	A3473	K3350	V3017	W2917	S2820	F2704	T2551	T2449	K2365
P4030	W3676	M3594	M3594	V3478	K3355	L3028	W2920	L2828	L2712	R2552	N2463	F2368
Q4031	L3677	K3595	K3595	L3478	G3354	LEU	W2920	E2829	D2707	K2553	L2471	S2369
Q4032	L3678	M3596	M3596	D3483	V3358	VAL	A2929	N2821	N2707	S2563	T2472	C2372
L4033	L3679	E3598	E3598	L3505	Y3360	GLU	M2932	L2822	N2708	G2564	L2473	S2373
L4034	Y3683	L3601	L3601	P3506	D3361	LEU	V2933	N2832	L2712	K2565	K2476	K2375
Q4035	S3687	F3607	F3607	L3509	I3367	ASN	I2936	L2835	D2478	S2566	S2477	V2378
Q4036	K3692	D3612	D3612	R3510	V3371	THR	M2938	D2839	I2479	Q2569	L2482	S2379
Q4037	M3696	K3613	K3613	V3513	T3372	ILE	T2941	T2841	L2485	Y2574	F2485	V2385
E4038	L3697	L3614	L3614	F3518	L3373	LEU	D2942	D2842	E2488	Y2575	M2396	K2396
E4040	M3698	V3615	V3615	V3519	M3377	VAL	ILE	Q2845	N2490	K2577	N2489	V2391
W4062	M3699	E3617	E3617	N3521	K3386	VAL	VAL	G2846	L2491	L2578	L2491	T2392
L4063	L3700	Y3618	Y3618	L3525	L3391	E3302	ASN	E2847	K2496	L2581	K2493	T2393
Q4064	M3702	F3703	F3703	L3534	E3303	K3303	LYS	E2848	L2494	V2582	L2494	T2396
L4065	E3717	G3622	G3622	T3535	E3304	E3304	GLU	L2853	K2497	L2616	D2495	T2397
E4068	A3718	H3624	H3624	E3537	K3306	K3306	LEU	VAL	G2755	R2620	G2498	K2399
S4069	L3709	V3626	V3626	N3538	S3400	L3307	PHE	L2856	M2756	T2623	S2499	E2401
I4070	M3701	K3627	K3627	M3541	D3402	K3308	THR	T2860	A2761	R2624	V2503	L2403
N4071	T3702	L3721	L3721	K3541	F3406	T3310	GLU	L2865	S2762	T2630	L2506	L2407
N4072	M3702	M3722	M3722	E3537	L3407	K3311	PRO	K3312	R2763	T2631	R2507	L2408
Y4073	P3815	G3817	G3817	S3538	L3408	Q3312	ILE	E2870	G2765	A2632	N2409	M2409
E4074	L3816	L3828	L3828	M3541	D3409	F3313	GLN	L2873	T2767	L2633	M2510	K2411
Q4077	L3816	L3828	L3828	M3541	D3409	F3313	GLN	L2873	T2767	L2633	M2510	K2411
A4078	L3816	L3828	L3828	M3541	D3409	F3313	GLN	L2873	T2767	L2633	M2510	K2411
K4079	L3816	L3828	L3828	M3541	D3409	F3313	GLN	L2873	T2767	L2633	M2510	K2411
T4085	L3816	L3828	L3828	M3541	D3409	F3313	GLN	L2873	T2767	L2633	M2510	K2411
M4092	L3816	L3828	L3828	M3541	D3409	F3313	GLN	L2873	T2767	L2633	M2510	K2411

Chain B: 65% 31% 4%



L4088	P3981	L3884	S3807	S3687	K3471	L3353	V3028	I2936	V2837	M2756	T2635
W3962	W3885	P3886	K3808	A3688	H3472	K3359	LEU	I2937	A2838	M2757	G2636
Q3984	A3886	P3887	L3811	L3690	A3473	Y3360	VAL	M2938	D2839	L2758	P2637
L3992	L3888	L3887	K3812	D3691	R3477	D3361	ASN	T2941	P2841	Q2760	Q2639
W3993	L3813	L3889	L3813	K3692	V3476	L3367	GLU	D2942	D2842	A2761	T2640
Y3994	L3814	Q3890	L3815	L3693	T3478	I3367	LEU	F2943	L2843	S2762	L2641
L3998	F3816	R3894	F3816	F3694	T3481	V3371	ASN	I2944	F2844	R2763	R2642
K4002	G3816	F3895	G3816	M3698	D3483	T3372	THR	VAL	G2846	T2764	S2643
D4003	L3817	G3896	G3817	A3594	D3483	L3380	THR	PRO	Y2849	G2766	R2646
L4004	L3818	W3897	L3818	M3595	V3488	L3391	SER	VAL	L2852	T2767	Y2653
E4005	E3820	M3700	E3820	M3596	V3488	L3392	ILE	ASN	L2853	L2768	Y2654
W4006	L3821	T3701	L3821	M3702	S3502	N3393	SER	GLU	L2770	T2771	K2664
V4014	L3822	M3702	L3822	E3605	S3502	N3393	VAL	LEU	L2856	R2779	L2673
G4017	F3708	F3708	N3823	D3612	T3506	S3400	VAL	VAL	T2860	L2779	L2677
S4018	L3720	L3720	Q3826	N3613	P3506	Q3401	PHE	THR	T2860	L2781	L2686
D4019	V3725	V3725	K3831	L3507	F3508	D3402	THR	GLU	L2865	V2782	L2686
N4020	S3832	S3832	K3832	F3509	S3510	A3403	PRO	PRO	L2866	Q2783	L2686
L4021	K3833	S3729	K3833	S3511	R3512	F3406	GLN	GLN	L2867	K2785	L2689
Q4022	G3836	S3730	G3836	S3512	L3407	L3408	L2960	L2961	E2870	L2786	S2691
L4023	G3837	D3731	G3837	V3513	V3417	D3409	L2962	L2963	L2873	L2795	L2702
V4024	F3838	T3737	F3838	F3518	H3413	H3413	K3311	D2963	F2877	M2797	V2707
V4027	L3839	T3740	L3839	M3631	M3414	M3414	Q3312	A2964	V2878	L2798	K2709
R4028	N3843	T3744	N3843	E3632	V3417	V3417	Q3313	V2965	H2886	D2795	L2799
L4029	L3844	L3744	L3844	K3634	L3429	L3429	S3314	V2966	F2889	F2796	L2702
P4030	Q3845	T3757	Q3845	F3641	V3437	V3437	K3315	N2967	L2891	M2797	L2712
L4034	S3847	L3760	S3847	F3641	R3438	R3438	S3317	F2972	C2892	L2815	L2713
S4037	L3848	L3760	L3848	I3644	L3439	L3439	N3323	M2980	D2893	C2814	L2728
E4038	Q3849	F3767	Q3849	I3645	L3440	L3440	C3324	K2981	P2894	L2816	L2732
E4039	V3851	F3768	V3851	I3646	L3440	L3440	I3325	P2986	L2903	S2905	V2733
E4040	K3852	V3769	K3852	V3656	A3443	A3443	I3326	R2987	S2906	L2817	L2734
S4060	L3853	W3772	L3853	F3657	F3446	F3446	Q3329	S2988	A2907	D2818	S2737
P3947	Y3854	L3774	Y3854	L3658	V3450	V3450	Y3330	P2989	N2910	L2822	V2738
H3948	H3858	V3777	H3858	ARG	D3454	D3454	F3334	G2990	R2911	L2823	D2740
G3949	V3859	V3778	V3859	ARG	G3455	G3455	N3338	I2993	C2912	E2824	H2741
F3950	T3862	A3779	T3862	THR	E3456	E3456	E3339	K3001	L2913	T2825	L2742
Y3955	A3865	N3780	A3865	ALA	K3550	K3550	E3341	V3003	L2914	A2826	L2743
F3956	L3865	N3784	L3865	ALA	L3551	L3551	R3340	L3010	N2915	R2830	L2745
F3963	E3869	Y3785	E3869	ARG	E3554	E3554	L3346	Q3011	W2917	M2831	Q2761
A3964	K3870	F3786	K3870	T3669	Y3555	Y3555	L3347	L3010	N2917	N2832	V2752
S3965	F3871	T3787	F3871	V3671	S3463	S3463	E3012	L3010	W2920	L2833	Q2753
L3968	K3872	R3792	K3872	L3674	R3464	R3464	L3348	L3010	T2924	L2834	G2754
L3968	L3873	L3792	L3873	L3674	L3465	L3465	L3349	V3017	L2932	A2836	
N3978	H3874	K3799	H3874	L3677	L3567	L3567	L3350	L3024			
N3979	L3875	L3800	L3875	L3677	L3570	L3570	L3352				
T4085	H3876	L3803	H3876	Y3683							
	H3878		H3878								

4 Data and refinement statistics

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 49.29 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.29-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.303 (Not available) , 0.298	Depositor DCC
R_{free} test set	5512 reflections (4.69%)	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)	0.31 , 149.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SO4, MG, 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	0.72	3/21146 (0.0%)	1.15	76/28618 (0.3%)
1	B	0.71	3/21146 (0.0%)	1.13	68/28618 (0.2%)
All	All	0.72	6/42292 (0.0%)	1.14	144/57236 (0.3%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLU	N-CA	6.86	1.55	1.46
1	B	2765	GLY	C-N	-6.46	1.25	1.33
1	A	3980	ILE	CA-C	5.60	1.58	1.52
1	B	2755	HIS	CA-C	-5.59	1.46	1.52
1	B	2464	TYR	N-CA	5.21	1.52	1.46
1	A	115	GLU	CA-CB	5.12	1.62	1.53

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SER	CA-C-N	10.93	133.50	119.84
1	A	1	SER	C-N-CA	10.93	133.50	119.84
1	B	2479	ILE	N-CA-C	10.34	121.17	110.62
1	B	1422	LYS	N-CA-C	9.36	121.09	111.07
1	B	3920	ILE	N-CA-C	-8.72	105.43	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2333	GLU	N-CA-C	-8.28	102.33	111.36
1	B	2840	ILE	CA-C-N	8.25	127.82	119.24
1	B	2840	ILE	C-N-CA	8.25	127.82	119.24
1	B	144	GLY	N-CA-C	8.19	123.47	111.76
1	B	1540	LEU	N-CA-C	8.04	119.82	111.14
1	A	2984	VAL	N-CA-C	8.04	118.20	106.55
1	A	200	TRP	CA-C-N	8.01	146.22	127.00
1	A	200	TRP	C-N-CA	8.01	146.22	127.00
1	A	2127	ASP	N-CA-C	7.96	119.59	111.07
1	B	2182	GLU	N-CA-C	7.95	120.21	108.60
1	B	2471	LEU	CB-CA-C	-7.61	107.80	116.63
1	A	3459	ASP	CA-C-N	7.59	127.98	119.32
1	A	3459	ASP	C-N-CA	7.59	127.98	119.32
1	B	200	TRP	CA-C-N	7.46	144.89	127.00
1	B	200	TRP	C-N-CA	7.46	144.89	127.00
1	A	3900	ILE	CB-CA-C	-7.43	102.23	110.78
1	B	2257	PHE	N-CA-C	7.43	121.03	108.02
1	A	4029	ILE	N-CA-C	7.35	115.46	107.60
1	B	2127	ASP	N-CA-C	7.33	119.27	111.28
1	A	3772	TRP	N-CA-C	7.29	120.83	109.96
1	A	3308	ASN	N-CA-C	7.09	119.62	111.11
1	A	2479	ILE	N-CA-C	7.09	117.85	110.62
1	A	3900	ILE	N-CA-C	7.00	115.61	107.77
1	A	3402	ASP	N-CA-C	-6.94	104.81	113.28
1	A	1939	PHE	N-CA-C	6.94	118.49	111.07
1	A	3616	GLU	N-CA-C	6.93	118.84	111.28
1	A	3621	ILE	CB-CA-C	-6.93	102.79	112.14
1	B	1575	LEU	N-CA-C	-6.87	104.02	112.88
1	B	1	SER	CA-C-N	6.84	128.39	119.84
1	B	1	SER	C-N-CA	6.84	128.39	119.84
1	B	2390	ILE	CB-CA-C	6.84	118.20	110.41
1	B	2375	ILE	N-CA-C	6.76	115.26	107.89
1	A	2333	GLU	N-CA-C	-6.75	104.00	111.36
1	A	1575	LEU	N-CA-C	-6.68	104.26	112.88
1	A	3521	ASN	N-CA-C	6.47	119.27	110.35
1	B	3920	ILE	CB-CA-C	-6.31	104.70	110.63
1	A	1540	LEU	N-CA-C	6.30	117.94	111.14
1	A	2375	ILE	N-CA-C	6.24	115.04	107.61
1	B	3413	HIS	N-CA-C	-6.24	105.71	113.38
1	B	3459	ASP	CA-C-N	6.19	126.66	119.47
1	B	3459	ASP	C-N-CA	6.19	126.66	119.47
1	A	200	TRP	N-CA-C	6.19	113.79	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1794	PHE	N-CA-C	6.14	118.53	108.52
1	B	2027	THR	CA-C-N	6.12	127.49	119.84
1	B	2027	THR	C-N-CA	6.12	127.49	119.84
1	A	3727	SER	CA-C-N	-6.09	112.92	122.73
1	A	3727	SER	C-N-CA	-6.09	112.92	122.73
1	A	1794	PHE	N-CA-CB	6.05	120.09	110.65
1	A	4027	VAL	N-CA-CB	-6.04	103.75	110.99
1	A	2101	VAL	N-CA-C	6.02	116.97	108.36
1	B	3848	LEU	N-CA-C	6.02	118.33	111.11
1	A	3	ILE	N-CA-C	6.01	116.77	108.12
1	A	2564	GLY	N-CA-C	-6.00	107.38	115.36
1	A	2182	GLU	N-CA-C	5.98	117.63	108.42
1	B	2101	VAL	N-CA-C	5.96	117.17	108.58
1	A	1458	ILE	N-CA-C	5.96	116.13	110.53
1	B	2564	GLY	N-CA-C	-5.93	107.57	115.40
1	A	3303	LYS	CA-C-N	-5.91	112.36	120.28
1	A	3303	LYS	C-N-CA	-5.91	112.36	120.28
1	B	2001	VAL	CB-CA-C	-5.84	104.91	111.80
1	A	1794	PHE	N-CA-C	5.82	117.90	108.41
1	B	2418	GLY	CA-C-N	5.81	126.36	120.38
1	B	2418	GLY	C-N-CA	5.81	126.36	120.38
1	A	3452	ILE	N-CA-C	5.81	116.16	107.51
1	B	1458	ILE	N-CA-C	5.78	116.42	110.82
1	B	2905	SER	CA-C-N	5.78	124.98	118.97
1	B	2905	SER	C-N-CA	5.78	124.98	118.97
1	A	185	ILE	CA-C-N	5.77	127.05	119.84
1	A	185	ILE	C-N-CA	5.77	127.05	119.84
1	A	2022	PHE	N-CA-C	5.76	118.05	108.13
1	A	2257	PHE	N-CA-C	5.73	118.30	109.07
1	A	2916	TRP	N-CA-C	5.70	117.69	108.41
1	A	1964	ASN	N-CA-C	5.68	118.20	111.33
1	B	2938	MET	N-CA-C	5.68	118.03	110.53
1	B	3982	TRP	N-CA-C	5.67	119.30	112.38
1	A	2372	CYS	N-CA-C	5.67	118.46	109.50
1	A	3461	ILE	N-CA-C	5.66	116.39	110.62
1	A	3980	ILE	N-CA-C	5.65	121.09	108.88
1	A	2983	GLY	N-CA-C	-5.65	104.61	112.18
1	B	3980	ILE	N-CA-C	5.65	121.08	108.88
1	B	2752	VAL	CB-CA-C	-5.63	104.77	111.81
1	A	3766	GLU	N-CA-C	-5.62	106.38	113.18
1	A	2034	ILE	CB-CA-C	-5.61	104.56	112.14
1	A	2521	ASN	N-CA-C	5.59	119.42	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2094	PHE	N-CA-C	5.59	118.22	111.40
1	A	2980	MET	N-CA-C	5.56	118.53	111.69
1	B	1938	GLY	N-CA-C	-5.55	100.03	113.18
1	B	2373	SER	N-CA-C	5.54	119.34	111.92
1	A	3951	SER	N-CA-C	5.48	117.96	111.33
1	A	4029	ILE	CB-CA-C	-5.47	104.89	111.18
1	A	3794	VAL	N-CA-C	5.46	116.78	108.80
1	B	3325	ILE	N-CA-C	5.46	116.09	110.36
1	A	2471	LEU	CB-CA-C	-5.45	108.72	116.34
1	B	3461	ILE	N-CA-C	5.44	116.21	110.72
1	B	2491	LEU	CA-C-N	-5.44	114.36	119.85
1	B	2491	LEU	C-N-CA	-5.44	114.36	119.85
1	A	2360	VAL	N-CA-C	5.44	115.72	108.11
1	B	2988	SER	CA-C-N	5.42	126.62	119.84
1	B	2988	SER	C-N-CA	5.42	126.62	119.84
1	B	1542	ASN	N-CA-C	5.41	116.86	111.07
1	B	2837	ASN	N-CA-C	-5.40	102.20	110.14
1	B	2434	ASN	N-CA-C	5.40	118.33	111.69
1	B	2394	THR	N-CA-C	-5.40	101.20	109.41
1	A	2373	SER	N-CA-C	5.39	119.27	111.56
1	A	2503	VAL	N-CA-C	5.36	115.99	110.36
1	B	2811	SER	N-CA-C	5.33	117.17	111.36
1	A	2222	ILE	N-CA-CB	5.32	116.42	110.51
1	A	112	LYS	N-CA-C	-5.31	106.30	112.89
1	B	3339	GLU	CA-C-N	5.31	127.40	120.28
1	B	3339	GLU	C-N-CA	5.31	127.40	120.28
1	A	14	GLN	N-CA-C	5.31	120.15	113.25
1	A	2220	CYS	N-CA-C	5.31	117.25	109.24
1	A	2181	GLY	N-CA-C	5.30	122.64	115.00
1	A	2941	THR	CA-C-N	5.27	127.60	120.38
1	A	2941	THR	C-N-CA	5.27	127.60	120.38
1	A	2761	ALA	CB-CA-C	-5.27	110.07	117.23
1	B	2580	LYS	N-CA-C	-5.25	106.38	112.89
1	B	2522	LYS	N-CA-C	5.24	117.82	109.81
1	A	2201	HIS	N-CA-C	5.23	117.06	111.36
1	A	3764	LYS	N-CA-C	-5.22	105.27	111.69
1	B	2739	VAL	N-CA-C	-5.22	105.62	110.53
1	B	2837	ASN	CA-C-N	-5.19	115.43	123.17
1	B	2837	ASN	C-N-CA	-5.19	115.43	123.17
1	A	147	VAL	N-CA-C	5.15	116.33	109.37
1	B	1793	CYS	CA-C-N	-5.15	115.84	123.05
1	B	1793	CYS	C-N-CA	-5.15	115.84	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2980	MET	N-CA-C	5.14	118.02	111.69
1	A	2403	ILE	N-CA-C	5.14	115.36	110.42
1	B	1794	PHE	N-CA-CB	5.13	118.61	110.55
1	B	2124	GLU	N-CA-C	-5.10	100.85	109.07
1	B	3507	ILE	N-CA-C	5.10	116.43	110.62
1	A	1793	CYS	CA-C-N	-5.09	115.82	123.00
1	A	1793	CYS	C-N-CA	-5.09	115.82	123.00
1	B	2220	CYS	N-CA-C	5.09	117.54	109.50
1	B	3454	ASP	N-CA-C	5.08	116.87	108.49
1	A	1761	GLU	N-CA-C	5.07	117.45	110.35
1	B	1939	PHE	N-CA-C	5.06	116.61	111.14
1	A	3975	ASN	N-CA-C	5.04	117.92	110.46
1	A	3626	VAL	N-CA-CB	5.04	117.01	110.57

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

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	966	0
1	B	20748	0	20207	946	0
2	A	31	0	12	6	0
2	B	31	0	12	22	0
3	A	54	0	24	31	0
3	B	54	0	24	29	0
4	A	5	0	0	1	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	1915	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 (1915) 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:B:2732:MET:HE1	1:B:2768:ILE:CG2	1.41	1.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1826:PHE:CE2	1:A:1831:LEU:HB2	1.86	1.10
1:B:2732:MET:CB	3:B:5402:ADP:C6	2.34	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:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.34	1.07
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.37	1.06
1:B:2732:MET:HE1	1:B:2768:ILE:HG21	1.26	1.06
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:2732:MET:HE1	1:A:2768:ILE:HG21	1.09	1.05
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:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.39	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:3307:LEU:C	1:A:3307:LEU:HD12	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2732:MET:HE1	1:B:2768:ILE:HG23	1.06	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2412:ARG:NH1	1:B:2553:HIS:HA	1.82	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:A:3307:LEU:HD12	1:A:3307:LEU:O	1.67	0.94
1:B:2080:LYS:HD2	1:B:2195:GLU:HB2	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2732:MET:HE1	1:A:2768:ILE:CG2	2.00	0.88
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:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1421:TYR:HE1	1:A:1425:GLU:CD	1.83	0.85
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.23	0.85
1:A:1535:PRO:C	1:A:1841:ILE:HD11	2.02	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:B:2732:MET:CE	1:B:2768:ILE:HG23	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:PRO:C	1:A:1365:PHE:HA	2.04	0.82
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: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: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:2745:ILE:CG2	1:A:2756:MET:HE1	2.09	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: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: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: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: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:1421:TYR:CE1	1:A:1425:GLU:CD	2.61	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3307:LEU:C	1:A:3307:LEU:CD1	2.57	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
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:B:2762:SER:C	1:B:2764:THR:H	1.94	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:A:3306:TRP:CZ3	1:A:3595:MET:HE3	2.20	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:B:1392:LEU:HD13	1:B:1392:LEU:C	2.11	0.76
1:B:2732:MET:HE2	1:B:2768:ILE:HG21	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1392:LEU:HD13	1:A:1392:LEU:C	2.14	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:A:3979:ASN:C	1:A:3981:PRO:HD2	2.14	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:2428:MET:HE2	1:B:2432:LEU:HD12	1.69	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:2745:ILE:HG12	1:A:2756:MET:HE1	1.72	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
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: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:A:3631:MET:HE1	1:A:3698:MET:HG3	1.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1967:HIS:C	1:A:1968:PHE:HD1	2.00	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:1640:VAL:HB	1:A:1686:LYS:HZ1	1.57	0.69
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2448:ASP:HB2	1:B:2829:GLU:CD	2.18	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:3401:GLN:C	1:B:3403:ALA:H	2.00	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: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: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:B:2760:GLY:O	1:B:2761:ALA:C	2.38	0.66
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.77	0.66
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.25	0.66
1:B:1967:HIS:C	1:B:1968:PHE:HD1	2.04	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:2428:MET:HE2	1:A:2432:LEU:HD12	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3308:ASN:C	1:A:3310:THR:N	2.54	0.65
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:A:2932:MET:HE1	1:A:2993:ILE:HG23	1.78	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.62	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
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:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.56	0.64
1:A:1527:LEU:HD22	1:A:1545:LEU:HD22	1.80	0.63
1:A:1637:GLU:O	1:A:1686:LYS:NZ	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.27	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:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.57	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: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:2413:GLY:HA3	1:B:2510:MET:HE3	1.81	0.62
1:B:3461:ILE:C	1:B:3463:SER:H	2.07	0.62
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.57	0.62
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:1392:LEU:HD13	1:A:1393:LYS:C	2.24	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:A:1967:HIS:O	1:A:1968:PHE:HD1	1.81	0.62
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:2095:ASP:CG	1:B:2149:ARG:NH2	2.58	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: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:2032:LYS:O	1:B:2035:VAL:HG12	1.99	0.61
1:B:2745:ILE:CG2	1:B:2756:MET:HE1	2.22	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:B:2745:ILE:HG23	1:B:2756:MET:CE	2.25	0.61
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4065:LEU:HD12	1:A:4065:LEU:C	2.26	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:2426:MET:HE1	3:A:5401:ADP:C5	2.35	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
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:B:2762:SER:C	1:B:2764:THR:N	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.31	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:B:1392:LEU:HD13	1:B:1393:LYS:C	2.26	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:3303:LYS:C	1:B:3306:TRP:HD1	2.09	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
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:2769:LEU:HD12	1:B:2917:MET:HE1	1.85	0.59
1:B:3401:GLN:C	1:B:3403:ALA:N	2.61	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:3919:LYS:HZ3	1:B:4038:GLU:CG	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:3979:ASN:C	1:A:3981:PRO:CD	2.76	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:1650:LEU:O	1:A:1654:VAL:HG23	2.03	0.58
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.38	0.58
1:A:4065:LEU:HD12	1:A:4065:LEU:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.69	0.58
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.29	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:B:1365:PHE:C	1:B:1367:ILE:N	2.59	0.57
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.29	0.57
1:A:4020:ASN:HB3	1:A:4028:ARG:NH2	2.18	0.57
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:B:3979:ASN:C	1:B:3981:PRO:HD2	2.30	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:2563:SER:CB	1:B:2566:SER:OG	2.53	0.57
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2488:GLU:CD	1:A:2491:LEU:HD11	2.30	0.56
1:A:2495:ASP:O	1:A:2498:GLY:N	2.38	0.56
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.04	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: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:1822:CYS:SG	1:B:1849:GLU:C	2.89	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2413:GLY:HA3	1:A:2510:MET:HE3	1.88	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:3308:ASN:C	1:A:3310:THR:H	2.12	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:A:2984:VAL:C	1:A:2986:PRO:HD3	2.32	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
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:A:1910:GLU:HB2	1:A:3846:MET:HB2	1.89	0.54
1:A:3461:ILE:C	1:A:3463:SER:H	2.16	0.54
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2426:MET:HE1	3:A:5401:ADP:C6	2.42	0.54
1:A:3306:TRP:CH2	1:A:3595:MET:HE3	2.42	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:A:1637:GLU:C	1:A:1686:LYS:HZ2	2.15	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:1535:PRO:C	1:B:1841:ILE:HD11	2.33	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
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.33	0.54
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:2476:LYS:HZ2	1:B:2528:ARG:HD2	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: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:1531:ARG:HG2	1:B:1537:PHE:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:B:3946:VAL:HA	1:B:3947:PRO:C	2.32	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:B:1770:ILE:HD11	1:B:1936:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1967:HIS:C	1:A:1968:PHE:CD1	2.87	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:1967:HIS:C	1:B:1968:PHE:CD1	2.85	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:1392:LEU:C	1:B:1392:LEU:CD1	2.80	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
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:2122:THR:O	1:B:2123:LEU:C	2.53	0.52
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2745:ILE:CG1	1:A:2756:MET:HE1	2.37	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:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.75	0.52
1:A:3330:TYR:HH	1:A:3346:LEU:HD22	1.75	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:B:2473:LEU:HD23	1:B:2473:LEU:C	2.34	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
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.86	0.51
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3414:MET:HE3	1:A:3518:PHE:CD1	2.45	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: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
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:1655:MET:HE3	1:B:1659:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1575:LEU:O	1:B:1576:GLU:HB3	2.10	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: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:1392:LEU:C	1:A:1392:LEU:CD1	2.84	0.50
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.58	0.50
1:B:2932:MET:HE1	1:B:2993:ILE:HG23	1.94	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
1:A:1637:GLU:HA	1:A:1686:LYS:NZ	2.27	0.50
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:2424:LYS:NZ	3:A:5401:ADP:O2B	2.32	0.50
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3461:ILE:C	1:B:3463:SER:N	2.65	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: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
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:2181:GLY:C	1:B:2182:GLU:HG3	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1637:GLU:CA	1:A:1686:LYS:HZ2	2.26	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: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:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.27	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:2122:THR:O	1:A:2123:LEU:C	2.55	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:3979:ASN:C	1:B:3981:PRO:CD	2.85	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:A:1849:GLU:CD	1:A:1899:ASN:ND2	2.70	0.48
1:A:2368:PHE:O	1:A:2369:SER:OG	2.27	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3722:MET:HE1	1:A:3744:LEU:HG	1.95	0.48
1:B:1365:PHE:O	1:B:1366:VAL:C	2.56	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:4074:GLU:HA	1:A:4077:GLN:HE21	1.78	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: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
1:A:3797:THR:O	1:A:3801:ILE:HG12	2.13	0.48
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.96	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:2175:ILE:HG13	1:A:2184:LEU:C	2.39	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: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:2428:MET:HE1	1:B:2440:VAL:CG1	2.43	0.47
1:B:2732:MET:CB	3:B:5402:ADP:C4	2.97	0.47
1:B:3414:MET:HE3	1:B:3518:PHE:CD1	2.48	0.47
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.62	0.47
1:B:3848:LEU:O	1:B:3849:SER:C	2.57	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3330:TYR:HH	1:B:3346:LEU:HD22	1.81	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:O	1:B:1826:PHE:CG	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:2095:ASP:CG	1:A:2149:ARG:HH21	2.23	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:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	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:1535:PRO:C	1:A:1841:ILE:CD1	2.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.30	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:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.74	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:B:3304:GLU:O	1:B:3305:ARG:C	2.59	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2476:LYS:HE3	1:B:2528:ARG:CB	2.47	0.45
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.98	0.45
1:A:1822:CYS:SG	1:A:1849:GLU:C	3.00	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:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3002:LEU:HD21	1:A:3370:LEU:HD11	1.99	0.45
1:A:3461:ILE:C	1:A:3463:SER:N	2.71	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:2732:MET:HE2	3:A:5402:ADP:H2'	1.99	0.44
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:2745:ILE:CB	1:A:2756:MET:HE1	2.46	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:A:3980:ILE:C	1:A:3982:TRP:H	2.24	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:A:3428:LEU:HD23	1:A:3428:LEU:C	2.42	0.44
1:B:3946:VAL:HB	1:B:3947:PRO:HA	2.00	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:2354:SER:OG	1:A:2357:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2380:LEU:HD12	1:A:2380:LEU:C	2.42	0.44
1:A:2623:THR:HG21	3:A:5401:ADP:O2'	2.17	0.44
1:A:2745:ILE:HG12	1:A:2756:MET:CE	2.44	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:3708:PHE:HZ	1:B:3720:LEU:HD21	1.82	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: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:B:2984:VAL:C	1:B:2986:PRO:HD3	2.43	0.44
1:A:1612:ASP:C	1:A:1615:ILE:HG12	2.43	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: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
1:B:1645:PHE:HZ	1:B:1768:ARG:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2091:MET:HE3	1:B:2149:ARG:NH1	2.33	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:B:4034:LEU:HD23	1:B:4034:LEU:C	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:B:4018:SER:O	1:B:4019:ASP:HB2	2.17	0.43
1:A:1425:GLU:O	1:A:1428:CYS:SG	2.74	0.43
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:3869:GLU:O	1:B:3870:LYS:C	2.62	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:3612:ASP:C	1:B:3615:VAL:HG22	2.43	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:1655:MET:HE3	1:A:1659:LEU:CD1	2.49	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:A:3848:LEU:O	1:A:3849:SER:C	2.61	0.42
1:B:1770:ILE:HD13	1:B:1770:ILE:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:23:LEU:C	1:A:25:GLU:N	2.77	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:2494:LEU:C	1:B:2494:LEU:HD12	2.45	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: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:2563:SER:C	1:B:2565:LYS:H	2.27	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:2563:SER:C	1:A:2565:LYS:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2060:PHE:CZ	1:A:2193:LEU:HD21	2.54	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
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:1425:GLU:O	1:A:1426:GLN:C	2.61	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:A:2904:SER:O	1:A:2905:SER:C	2.62	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:2166:MET:HE1	1:B:2192:ILE:HD13	2.01	0.42
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.01	0.42
1:B:3948:HIS:NE2	1:B:4072:ASN:CG	2.77	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:1637:GLU:HA	1:A:1686:LYS:HZ2	1.85	0.41
1:A:2701:SER:HB2	1:A:2703:ASP:O	2.20	0.41
1:A:2754:GLY:HA3	1:A:2886:HIS:HD1	1.85	0.41
1:A:2889:PHE:CD1	1:A:2902:MET:HE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1664:LEU:O	1:B:1721:LYS:HE3	2.19	0.41
1:B:2095:ASP:CG	1:B:2149:ARG:HH22	2.27	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
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:3330:TYR:CE1	1:A:3334:PHE:CE2	3.08	0.41
1:A:4023:ILE:HD13	1:A:4023:ILE:HG21	1.70	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: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: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:2817:ILE:HG13	1:B:2831:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.50	0.41
1:A:4033:LEU:HD12	1:A:4033:LEU:C	2.45	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
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:1743:ASP:C	1:A:1745:ASN:N	2.79	0.41
1:A:2765:GLY:CA	3:A:5402:ADP:O2A	2.59	0.41
1:A:3303:LYS:O	1:A:3304:GLU:C	2.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:23:LEU:C	1:A:25:GLU:H	2.29	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:3631:MET:HE2	1:A:3632:LEU:HG	2.02	0.41
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.34	0.41
1:B:2387:ARG:C	1:B:2389:ASP:H	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:2428:MET:HE1	1:B:2440:VAL:CG2	2.51	0.40
1:B:2446:SER:O	1:B:2447:LYS:C	2.64	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
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:2902:MET:HE3	1:A:2902:MET:HB3	1.88	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: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](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1197/2453 (49%)	1117 (93%)	80 (7%)	15	41
1	B	2218/2453 (90%)	2089 (94%)	129 (6%)	18	45
All	All	3415/4906 (70%)	3206 (94%)	209 (6%)	17	43

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1366	VAL
1	A	1463	LEU
1	A	1471	LEU
1	A	1486	ILE
1	A	1504	ASN
1	A	1511	LEU
1	A	1520	LYS
1	A	1540	LEU
1	A	1769	LEU
1	A	1802	LYS
1	A	2122	THR
1	A	2155	ASP
1	A	2397	THR
1	A	2472	THR
1	A	2474	LEU
1	A	2476	LYS
1	A	2482	LEU
1	A	2544	ILE
1	A	2822	ILE
1	A	2829	GLU
1	A	2853	LEU
1	A	2873	LEU
1	A	2967	ASN
1	A	3304	GLU
1	A	3305	ARG
1	A	3306	TRP
1	A	3307	LEU

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Mol	Chain	Res	Type
1	A	3312	GLN
1	A	3316	THR
1	A	3329	ILE
1	A	3355	LYS
1	A	3371	VAL
1	A	3372	THR
1	A	3377	MET
1	A	3386	LYS
1	A	3391	LEU
1	A	3400	SER
1	A	3439	ARG
1	A	3456	GLU
1	A	3483	ASP
1	A	3534	LEU
1	A	3536	GLU
1	A	3538	ASN
1	A	3548	LEU
1	A	3549	ILE
1	A	3557	LEU
1	A	3559	LEU
1	A	3566	LEU
1	A	3567	LEU
1	A	3578	LEU
1	A	3598	GLU
1	A	3601	LEU
1	A	3618	TYR
1	A	3646	ILE
1	A	3677	LEU
1	A	3717	GLU
1	A	3729	SER
1	A	3737	THR
1	A	3744	LEU
1	A	3747	LEU
1	A	3794	VAL
1	A	3802	GLU
1	A	3805	LYS
1	A	3811	LEU
1	A	3844	ILE
1	A	3899	ASP
1	A	3900	ILE
1	A	3906	THR
1	A	3939	ILE

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Mol	Chain	Res	Type
1	A	3940	THR
1	A	3943	THR
1	A	3952	LYS
1	A	3966	VAL
1	A	3980	ILE
1	A	3982	TRP
1	A	3992	ILE
1	A	3998	ILE
1	A	4040	GLU
1	A	4064	GLN
1	A	4068	GLU
1	B	1366	VAL
1	B	1421	TYR
1	B	1455	LEU
1	B	1475	LYS
1	B	1486	ILE
1	B	1493	LEU
1	B	1495	THR
1	B	1511	LEU
1	B	1525	THR
1	B	1589	VAL
1	B	1644	ILE
1	B	1646	GLN
1	B	1689	LYS
1	B	1720	THR
1	B	1749	ILE
1	B	1767	GLU
1	B	1768	ARG
1	B	1770	ILE
1	B	1788	GLN
1	B	1832	SER
1	B	1936	ILE
1	B	1971	ARG
1	B	1992	LYS
1	B	2003	LEU
1	B	2035	VAL
1	B	2064	GLN
1	B	2107	LYS
1	B	2109	LEU
1	B	2141	ILE
1	B	2155	ASP
1	B	2186	ILE

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Mol	Chain	Res	Type
1	B	2202	THR
1	B	2218	ASP
1	B	2222	ILE
1	B	2276	LEU
1	B	2295	ILE
1	B	2310	LEU
1	B	2318	ILE
1	B	2322	LEU
1	B	2323	LEU
1	B	2351	GLN
1	B	2352	GLU
1	B	2357	SER
1	B	2361	ILE
1	B	2395	ILE
1	B	2397	THR
1	B	2476	LYS
1	B	2510	MET
1	B	2544	ILE
1	B	2563	SER
1	B	2566	SER
1	B	2576	LYS
1	B	2587	SER
1	B	2613	SER
1	B	2616	LEU
1	B	2626	VAL
1	B	2664	LYS
1	B	2689	ILE
1	B	2694	LEU
1	B	2702	LEU
1	B	2751	GLN
1	B	2753	GLN
1	B	2757	MET
1	B	2797	MET
1	B	2829	GLU
1	B	2833	THR
1	B	2843	LEU
1	B	2853	LEU
1	B	2856	LEU
1	B	2865	LEU
1	B	2873	LEU
1	B	2914	ILE
1	B	2936	ILE

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Mol	Chain	Res	Type
1	B	2967	ASN
1	B	3001	LYS
1	B	3003	VAL
1	B	3012	GLU
1	B	3302	GLU
1	B	3316	THR
1	B	3329	ILE
1	B	3360	TYR
1	B	3371	VAL
1	B	3372	THR
1	B	3380	LEU
1	B	3391	LEU
1	B	3400	SER
1	B	3437	VAL
1	B	3456	GLU
1	B	3466	ILE
1	B	3502	SER
1	B	3510	ARG
1	B	3512	ARG
1	B	3534	LEU
1	B	3536	GLU
1	B	3538	ASN
1	B	3548	LEU
1	B	3549	ILE
1	B	3565	ARG
1	B	3566	LEU
1	B	3567	LEU
1	B	3584	MET
1	B	3605	GLU
1	B	3618	TYR
1	B	3634	LYS
1	B	3677	LEU
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3800	LEU
1	B	3811	LEU
1	B	3813	ILE
1	B	3831	LYS
1	B	3844	ILE
1	B	3862	THR
1	B	3876	THR

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Mol	Chain	Res	Type
1	B	3884	LEU
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3943	THR
1	B	3980	ILE
1	B	3982	TRP
1	B	3992	ILE
1	B	3998	ILE
1	B	4003	ASP
1	B	4004	LEU
1	B	4021	LEU
1	B	4040	GLU
1	B	4068	GLU

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

Mol	Chain	Res	Type
1	A	1442	GLN
1	A	1449	GLN
1	A	2383	HIS
1	A	2634	ASN
1	A	2777	ASN
1	A	2910	ASN
1	A	2927	GLN
1	A	3008	GLN
1	A	3323	ASN
1	A	3336	HIS
1	A	3338	ASN
1	A	3363	ASN
1	A	3420	ASN
1	A	3521	ASN
1	A	3542	GLN
1	A	3561	ASN
1	A	3588	ASN
1	A	3780	ASN
1	A	3890	GLN
1	A	3914	GLN
1	A	4020	ASN
1	A	4031	GLN
1	A	4036	GLN
1	A	4051	ASN

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Mol	Chain	Res	Type
1	A	4077	GLN
1	A	4087	GLN
1	B	1444	ASN
1	B	1449	GLN
1	B	1501	HIS
1	B	1605	GLN
1	B	1622	GLN
1	B	1629	GLN
1	B	1646	GLN
1	B	1707	HIS
1	B	1714	GLN
1	B	1717	ASN
1	B	1736	GLN
1	B	1745	ASN
1	B	1899	ASN
1	B	1951	HIS
1	B	2099	ASN
1	B	2228	HIS
1	B	2239	ASN
1	B	2270	ASN
1	B	2282	ASN
1	B	2293	HIS
1	B	2335	GLN
1	B	2383	HIS
1	B	2409	ASN
1	B	2513	GLN
1	B	2536	ASN
1	B	2598	HIS
1	B	2601	ASN
1	B	2634	ASN
1	B	2683	ASN
1	B	2688	ASN
1	B	2896	ASN
1	B	2927	GLN
1	B	3008	GLN
1	B	3025	ASN
1	B	3323	ASN
1	B	3336	HIS
1	B	3338	ASN
1	B	3413	HIS
1	B	3453	GLN
1	B	3521	ASN

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Mol	Chain	Res	Type
1	B	3538	ASN
1	B	3542	GLN
1	B	3624	HIS
1	B	3637	GLN
1	B	3843	ASN
1	B	3890	GLN
1	B	4020	ASN
1	B	4036	GLN
1	B	4077	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	ADP	B	5401	-	28,29,29	1.77	6 (21%)	43,45,45	1.75	9 (20%)
2	ATP	A	5400	-	32,33,33	1.49	7 (21%)	48,52,52	1.73	10 (20%)
3	ADP	A	5401	-	28,29,29	1.64	6 (21%)	43,45,45	1.77	10 (23%)
4	SO4	B	5403	-	4,4,4	0.43	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	5402	-	28,29,29	1.48	5 (17%)	43,45,45	1.83	10 (23%)
4	SO4	A	5403	-	4,4,4	0.42	0	6,6,6	0.70	0
2	ATP	B	5400	-	32,33,33	1.42	5 (15%)	48,52,52	1.73	10 (20%)
3	ADP	A	5402	-	28,29,29	1.49	5 (17%)	43,45,45	1.94	11 (25%)

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	5401	-	-	7/16/32/32	0/3/3/3
2	ATP	A	5400	-	-	4/22/38/38	0/3/3/3
3	ADP	A	5401	-	-	8/16/32/32	0/3/3/3
3	ADP	B	5402	-	-	0/16/32/32	0/3/3/3
2	ATP	B	5400	-	-	4/22/38/38	0/3/3/3
3	ADP	A	5402	-	-	6/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5401	ADP	C5-C4	5.35	1.48	1.39
3	B	5401	ADP	C5-C4	4.93	1.47	1.39
3	B	5402	ADP	C5-C4	4.88	1.47	1.39
2	B	5400	ATP	C5-C4	4.67	1.47	1.39
3	A	5402	ADP	C5-C4	4.62	1.47	1.39
2	A	5400	ATP	C5-C4	4.57	1.47	1.39
3	B	5401	ADP	C4-N9	-3.78	1.29	1.37
3	B	5401	ADP	PA-O3A	3.28	1.63	1.59
3	B	5401	ADP	C8-N7	3.00	1.37	1.31
3	A	5402	ADP	PA-O3A	2.89	1.62	1.59
2	B	5400	ATP	C5-C6	2.81	1.48	1.41
3	B	5401	ADP	C5-N7	-2.81	1.34	1.39
3	A	5401	ADP	C5-N7	-2.79	1.34	1.39
3	A	5402	ADP	C5-C6	2.73	1.48	1.41
2	A	5400	ATP	C5-C6	2.71	1.48	1.41
3	B	5402	ADP	C5-C6	2.69	1.48	1.41
3	A	5401	ADP	C5-C6	2.68	1.48	1.41
3	B	5401	ADP	C5-C6	2.64	1.48	1.41
3	A	5401	ADP	C4-N9	-2.56	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5402	ADP	PA-O3A	2.51	1.62	1.59
2	B	5400	ATP	C5-N7	-2.47	1.34	1.39
2	A	5400	ATP	C5-N7	-2.46	1.34	1.39
2	A	5400	ATP	C4-N9	-2.37	1.32	1.37
3	A	5401	ADP	C8-N7	2.33	1.36	1.31
3	A	5402	ADP	C8-N7	2.28	1.36	1.31
2	A	5400	ATP	PA-O3A	2.24	1.61	1.59
3	A	5401	ADP	PA-O3A	2.19	1.61	1.59
3	A	5402	ADP	C5-N7	-2.16	1.35	1.39
3	B	5402	ADP	C5-N7	-2.13	1.35	1.39
2	A	5400	ATP	PB-O3B	2.10	1.61	1.59
2	A	5400	ATP	C8-N7	2.09	1.35	1.31
2	B	5400	ATP	PB-O3B	2.07	1.61	1.59
2	B	5400	ATP	C4-N9	-2.04	1.33	1.37
3	B	5402	ADP	C8-N7	2.04	1.35	1.31

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5402	ADP	C5-C4-N3	-5.82	118.71	126.72
3	B	5402	ADP	C5-C4-N3	-5.71	118.86	126.72
3	A	5401	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	5400	ATP	C5-C4-N3	-5.63	118.97	126.72
2	B	5400	ATP	C5-C4-N3	-5.50	119.14	126.72
3	B	5401	ADP	C5-C4-N3	-5.12	119.66	126.72
3	B	5402	ADP	N3-C4-N9	4.70	135.16	127.17
3	A	5402	ADP	N3-C4-N9	4.58	134.95	127.17
3	A	5401	ADP	N3-C4-N9	4.49	134.81	127.17
2	B	5400	ATP	N3-C4-N9	4.36	134.58	127.17
2	A	5400	ATP	N3-C4-N9	4.34	134.54	127.17
3	A	5402	ADP	C2-N3-C4	4.06	121.75	111.83
3	A	5402	ADP	N3-C2-N1	-3.94	122.61	128.58
3	B	5401	ADP	C2-N3-C4	3.80	121.11	111.83
3	B	5401	ADP	N3-C2-N1	-3.78	122.86	128.58
3	B	5402	ADP	C2-N3-C4	3.78	121.05	111.83
2	B	5400	ATP	C2-N3-C4	3.64	120.73	111.83
2	A	5400	ATP	C2-N3-C4	3.57	120.54	111.83
3	A	5402	ADP	C4-C5-N7	-3.55	106.53	110.58
2	A	5400	ATP	C4-C5-N7	-3.50	106.58	110.58
3	B	5402	ADP	N3-C2-N1	-3.50	123.28	128.58
2	B	5400	ATP	C4-C5-N7	-3.49	106.59	110.58
3	A	5401	ADP	C2-N3-C4	3.43	120.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5401	ADP	N3-C4-N9	3.26	132.72	127.17
2	B	5400	ATP	N3-C2-N1	-3.18	123.77	128.58
3	B	5402	ADP	C4-C5-N7	-3.16	106.97	110.58
2	A	5400	ATP	N3-C2-N1	-3.16	123.80	128.58
3	B	5401	ADP	C4-C5-N7	-2.97	107.18	110.58
3	A	5402	ADP	C3'-C2'-C1'	2.95	107.04	101.46
3	A	5401	ADP	C4-C5-N7	-2.93	107.23	110.58
3	A	5402	ADP	C5-N7-C8	2.70	107.69	103.45
3	A	5401	ADP	N3-C2-N1	-2.67	124.55	128.58
2	B	5400	ATP	C3'-C2'-C1'	2.64	106.46	101.46
3	A	5402	ADP	C6-C5-N7	2.60	137.11	132.09
2	A	5400	ATP	C3'-C2'-C1'	2.59	106.36	101.46
3	B	5402	ADP	C4-N9-C8	2.55	108.41	105.74
3	B	5402	ADP	C3'-C2'-C1'	2.54	106.28	101.46
2	B	5400	ATP	C5-N7-C8	2.54	107.44	103.45
3	A	5402	ADP	C4-N9-C8	2.54	108.40	105.74
3	A	5401	ADP	C2'-C3'-C4'	2.50	107.43	102.61
2	A	5400	ATP	C4-N9-C8	2.48	108.34	105.74
3	B	5401	ADP	C6-C5-N7	2.32	136.57	132.09
3	B	5402	ADP	O3B-PB-O2B	2.27	116.31	107.80
2	A	5400	ATP	C5-N7-C8	2.26	107.00	103.45
2	B	5400	ATP	O3G-PG-O2G	2.25	116.24	107.80
2	B	5400	ATP	C6-C5-N7	2.22	136.38	132.09
3	B	5402	ADP	C5-N7-C8	2.22	106.94	103.45
3	B	5401	ADP	O4'-C1'-N9	2.21	112.34	108.09
3	A	5401	ADP	O2A-PA-O1A	2.18	122.58	112.44
3	A	5401	ADP	N6-C6-N1	2.15	123.16	118.38
3	A	5401	ADP	C4-N9-C8	2.14	107.99	105.74
3	B	5401	ADP	C2-N1-C6	2.14	122.24	118.73
2	B	5400	ATP	C4-N9-C8	2.13	107.98	105.74
3	A	5401	ADP	O4'-C1'-C2'	2.12	111.14	106.62
2	A	5400	ATP	C6-C5-N7	2.09	136.13	132.09
3	B	5402	ADP	C2-N1-C6	2.05	122.09	118.73
3	A	5402	ADP	N9-C8-N7	-2.05	111.03	113.94
3	A	5402	ADP	O3B-PB-O2B	2.04	115.44	107.80
3	B	5401	ADP	O2'-C2'-C3'	-2.02	105.35	111.82
2	A	5400	ATP	O3G-PG-O2G	2.01	115.34	107.80

There are no chirality outliers.

All (29) torsion outliers are listed below:

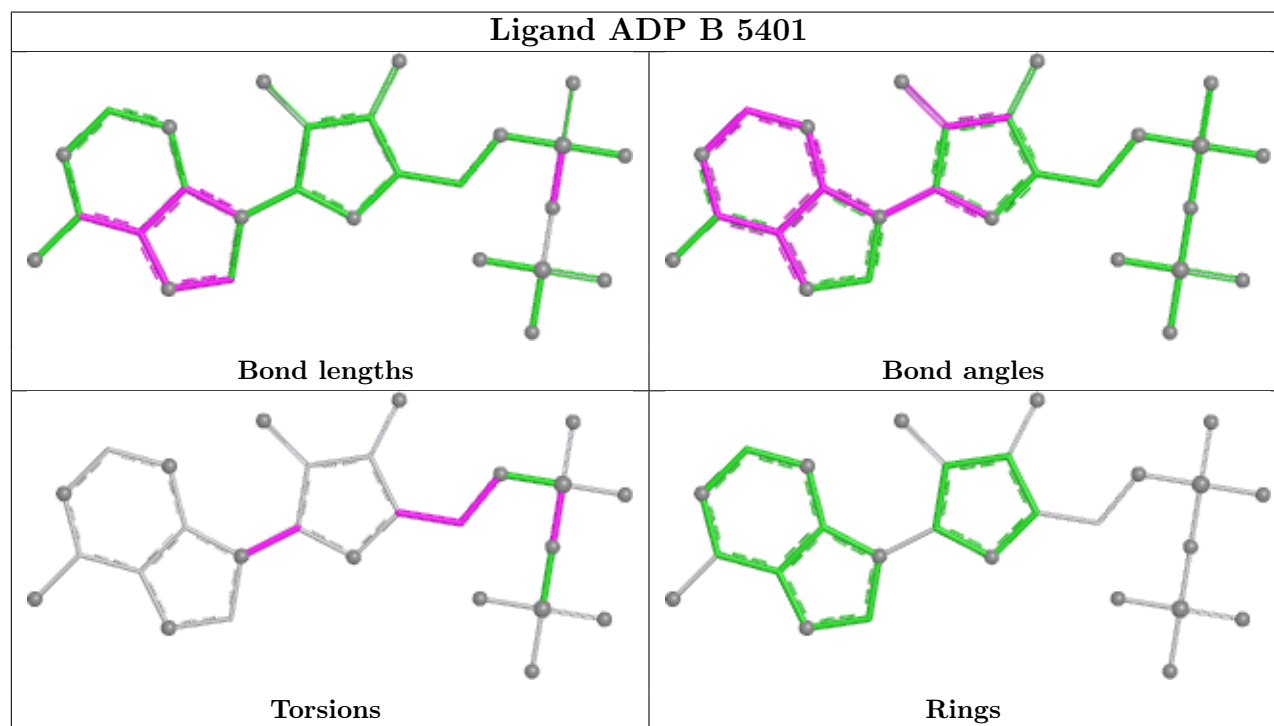
Mol	Chain	Res	Type	Atoms
2	A	5400	ATP	C5'-O5'-PA-O2A
2	B	5400	ATP	C5'-O5'-PA-O2A
3	A	5401	ADP	PA-O3A-PB-O2B
3	A	5401	ADP	C5'-O5'-PA-O1A
3	A	5401	ADP	C5'-O5'-PA-O2A
3	A	5401	ADP	C5'-O5'-PA-O3A
3	A	5401	ADP	O4'-C4'-C5'-O5'
3	A	5402	ADP	O4'-C4'-C5'-O5'
3	A	5401	ADP	C3'-C4'-C5'-O5'
3	B	5401	ADP	C3'-C4'-C5'-O5'
2	A	5400	ATP	O4'-C4'-C5'-O5'
2	B	5400	ATP	O4'-C4'-C5'-O5'
3	A	5402	ADP	C3'-C4'-C5'-O5'
2	A	5400	ATP	C3'-C4'-C5'-O5'
2	B	5400	ATP	C3'-C4'-C5'-O5'
3	B	5401	ADP	O4'-C4'-C5'-O5'
3	B	5401	ADP	C2'-C1'-N9-C4
3	B	5401	ADP	C2'-C1'-N9-C8
3	A	5401	ADP	C2'-C1'-N9-C4
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	A	5402	ADP	C5'-O5'-PA-O3A
3	A	5401	ADP	C2'-C1'-N9-C8
3	B	5401	ADP	PB-O3A-PA-O2A
3	B	5401	ADP	C4'-C5'-O5'-PA
3	B	5401	ADP	PB-O3A-PA-O1A
3	A	5402	ADP	PB-O3A-PA-O2A

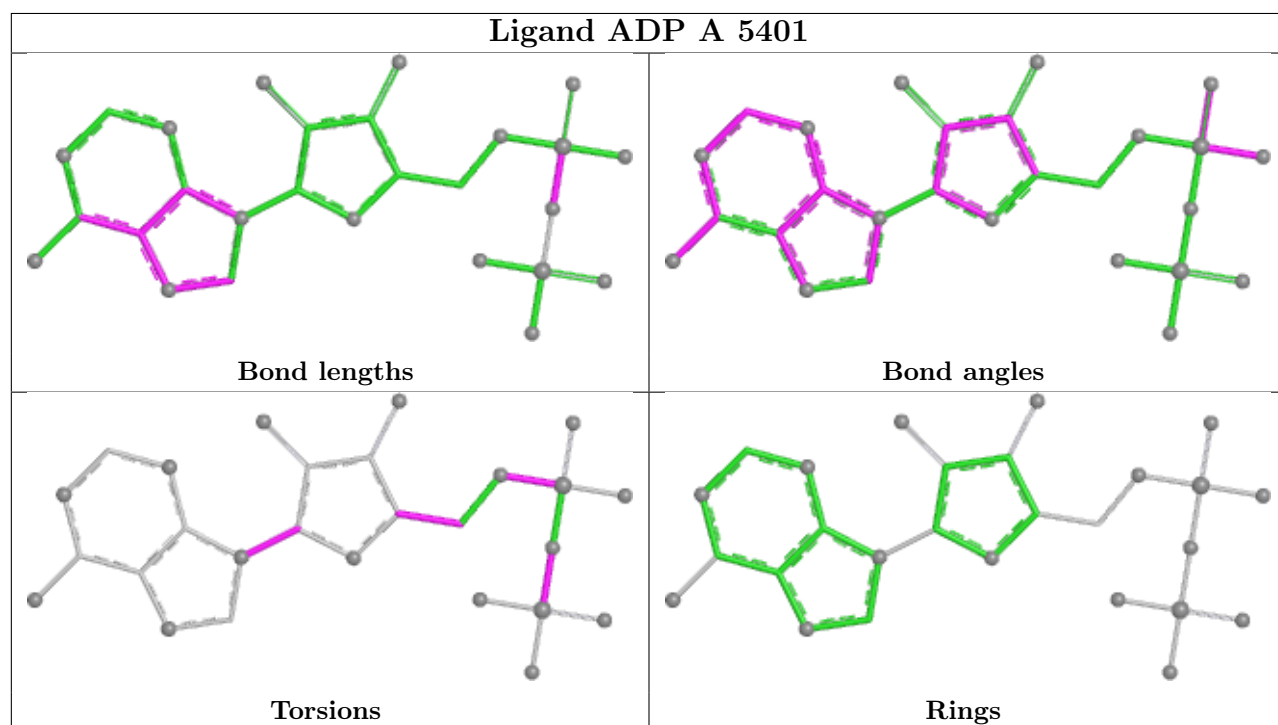
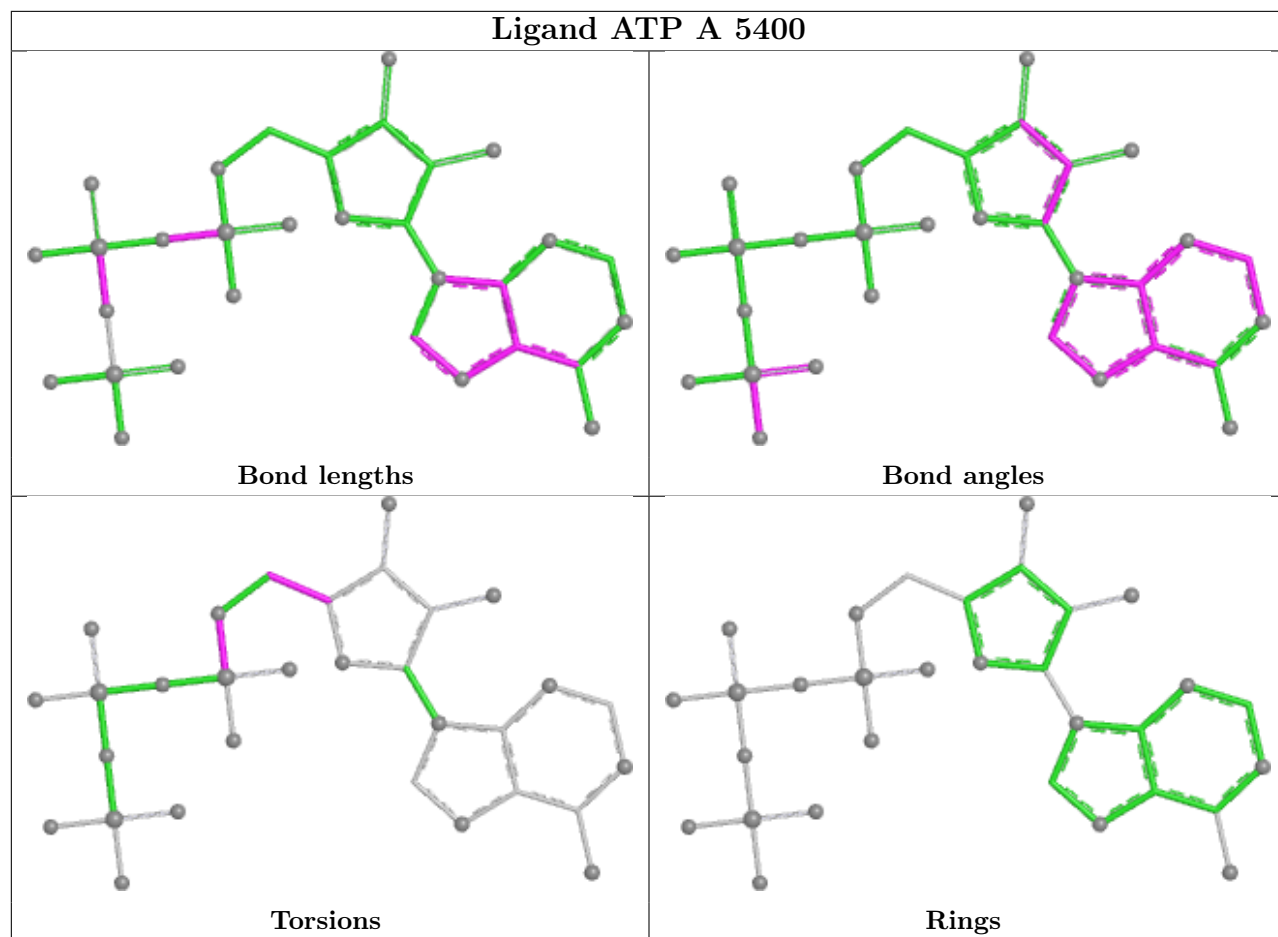
There are no ring outliers.

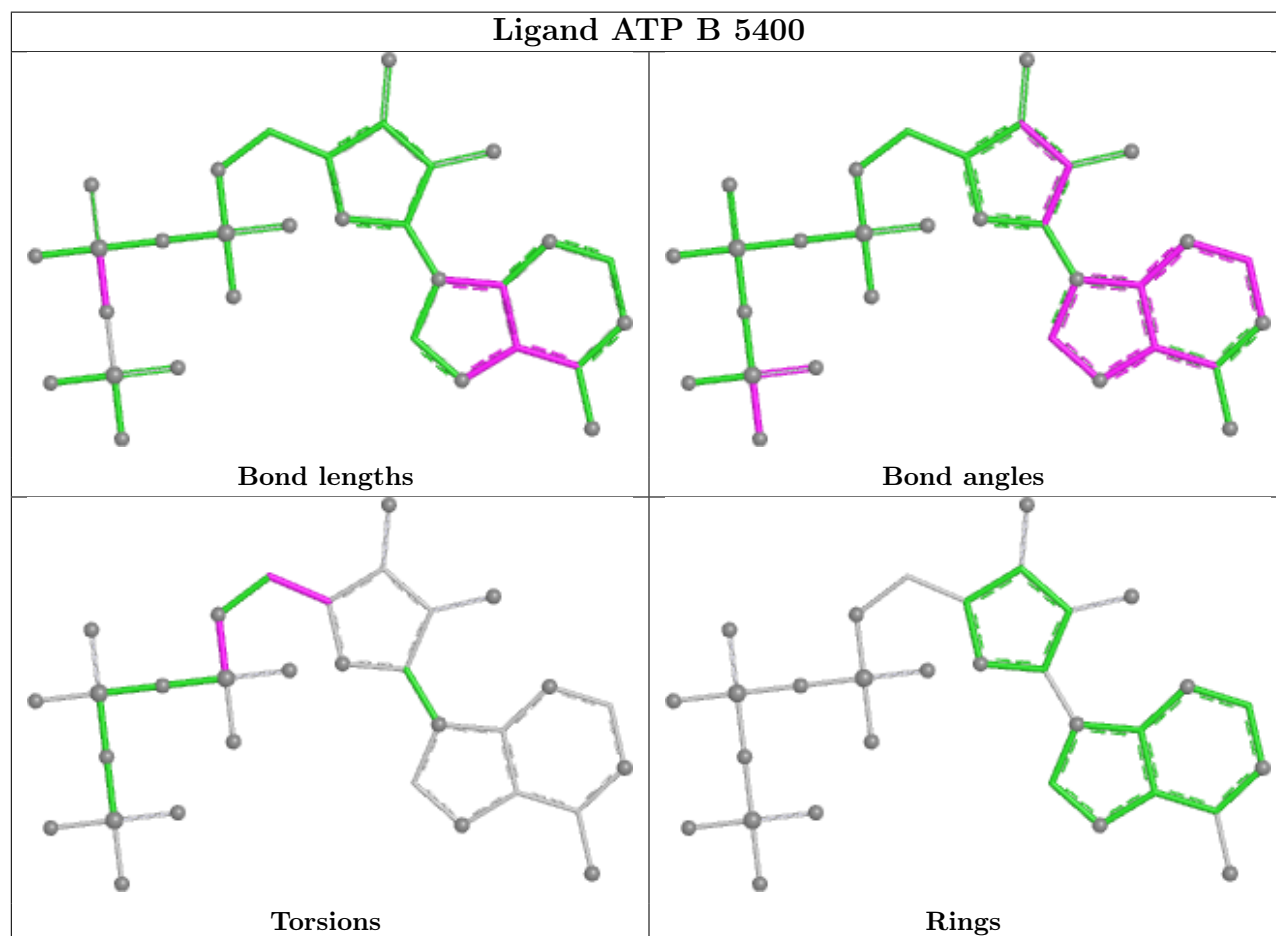
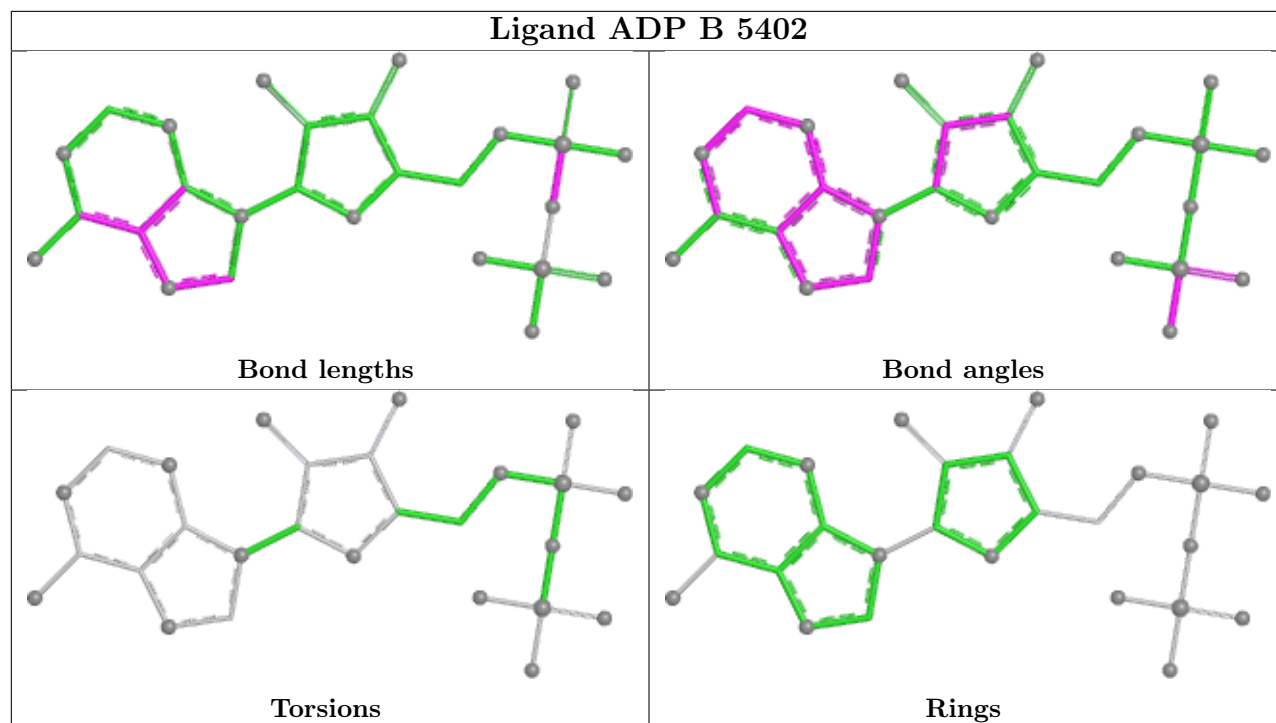
8 monomers are involved in 91 short contacts:

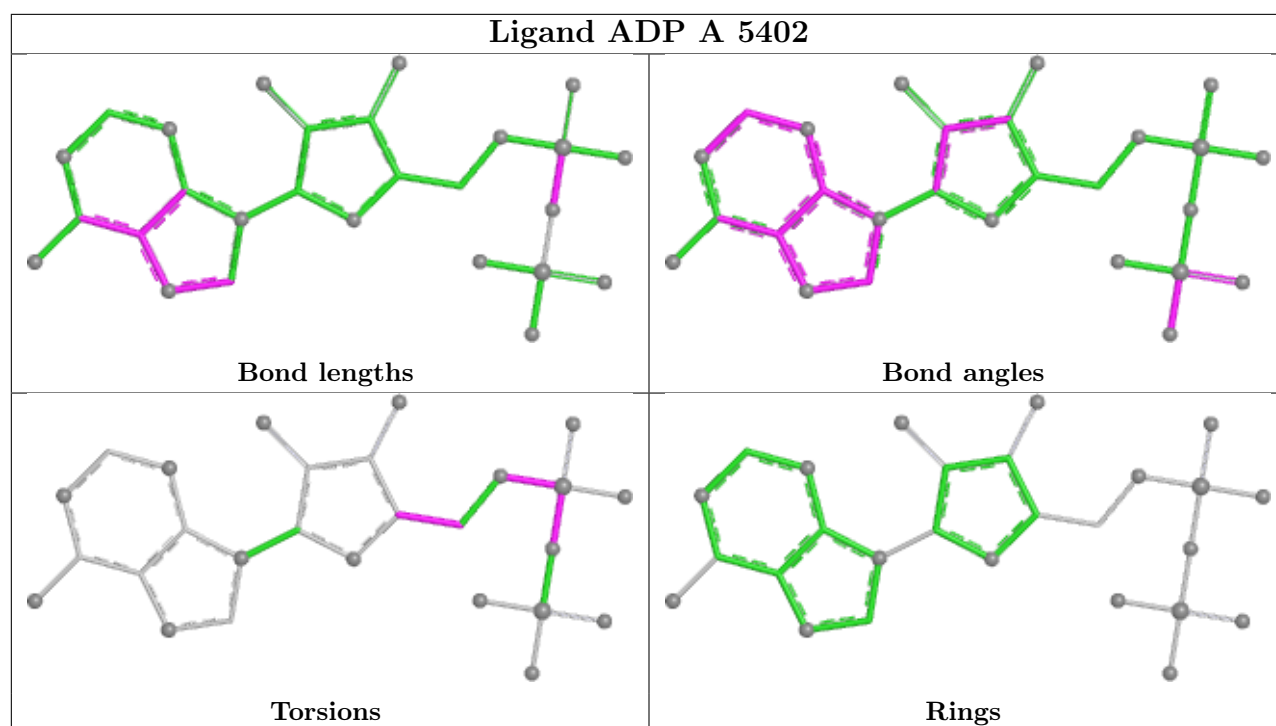
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5401	ADP	6	0
2	A	5400	ATP	6	0
3	A	5401	ADP	13	0
4	B	5403	SO4	2	0
3	B	5402	ADP	23	0
4	A	5403	SO4	1	0
2	B	5400	ATP	22	0
3	A	5402	ADP	18	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.48	6 (0%) 91 87	88, 185, 310, 500	1 (0%)
1	B	2650/2695 (98%)	-0.50	8 (0%) 90 84	96, 180, 317, 500	1 (0%)
All	All	5300/5390 (98%)	-0.49	14 (0%) 90 84	88, 183, 311, 500	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	3.5
1	B	152	PHE	3.3
1	B	2106	THR	2.9
1	A	132	PHE	2.9
1	A	1483	TYR	2.9
1	A	211	GLY	2.7
1	B	15	PRO	2.6
1	B	155	TYR	2.4
1	A	3895	PHE	2.3
1	B	1762	TYR	2.3
1	A	1760	PHE	2.2
1	B	51	PHE	2.1
1	B	151	ASP	2.1
1	B	3811	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

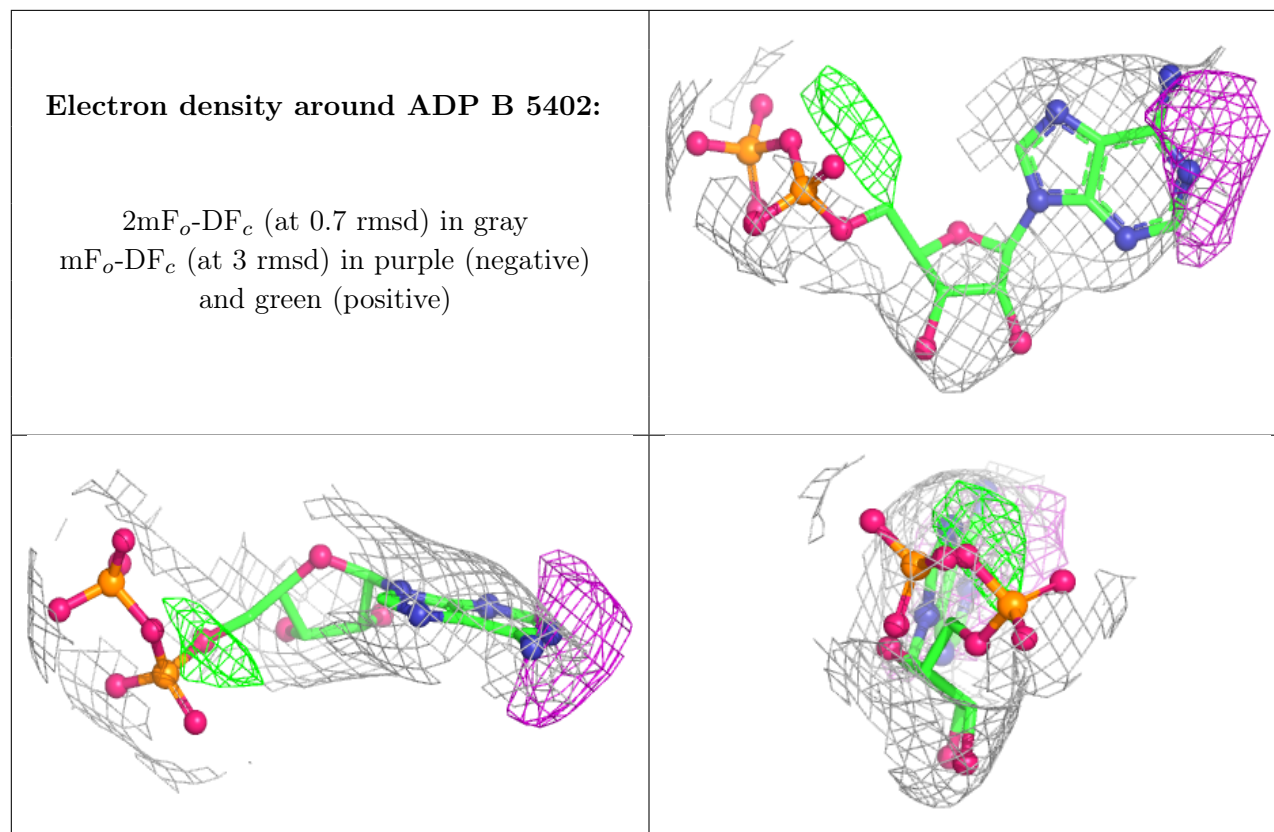
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

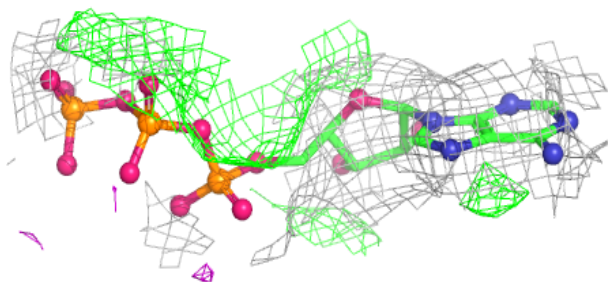
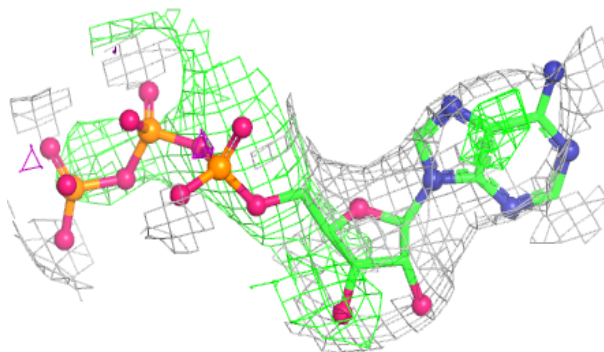
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	5404	1/1	0.86	0.09	97,97,97,97	0
3	ADP	B	5402	27/27	0.93	0.08	108,145,183,194	0
2	ATP	B	5400	31/31	0.93	0.10	124,160,195,221	0
5	MG	B	5404	1/1	0.93	0.06	107,107,107,107	0
3	ADP	A	5401	27/27	0.95	0.06	126,146,191,198	0
3	ADP	A	5402	27/27	0.96	0.05	134,176,208,218	0
4	SO4	B	5403	5/5	0.96	0.06	139,143,171,171	0
3	ADP	B	5401	27/27	0.97	0.06	98,121,138,153	0
2	ATP	A	5400	31/31	0.97	0.08	122,147,224,246	0
4	SO4	A	5403	5/5	0.97	0.04	101,136,142,145	0

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

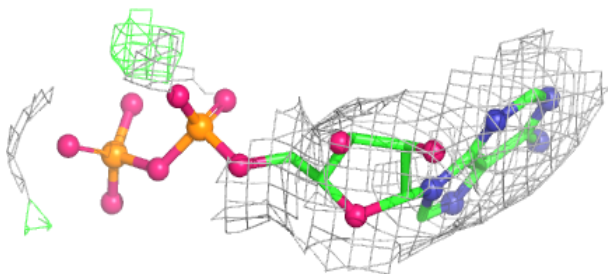
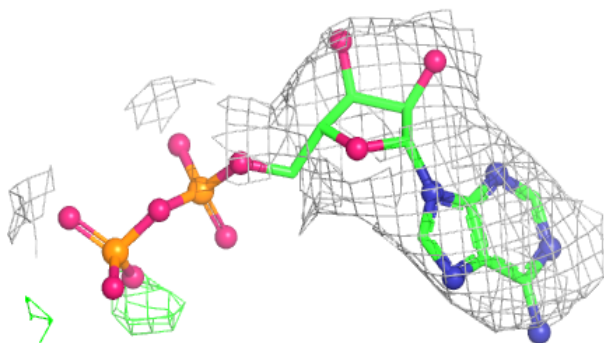


Electron density around ATP B 5400:

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

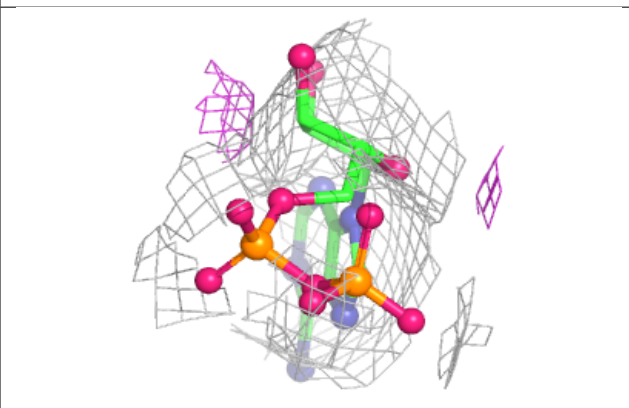
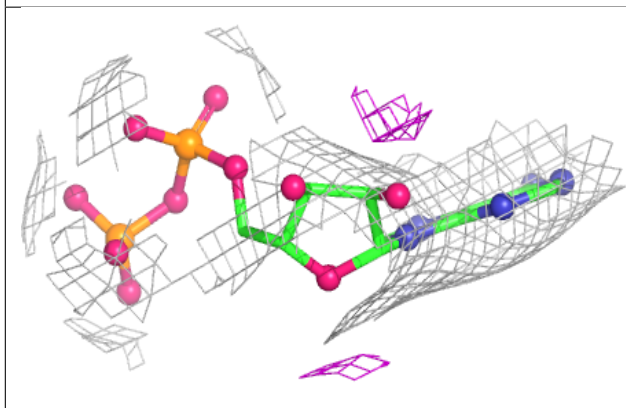
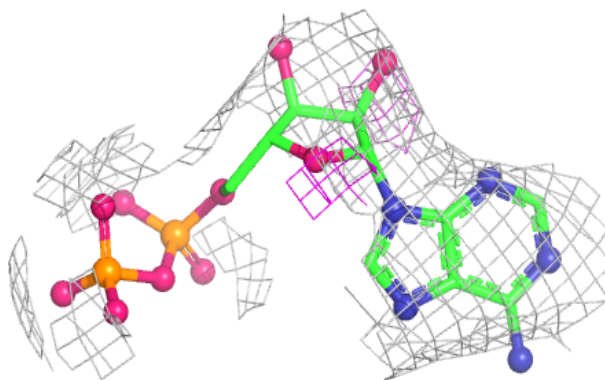
**Electron density around ADP A 5401:**

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

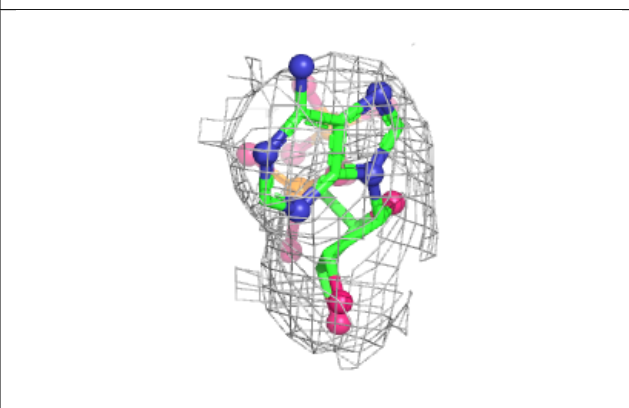
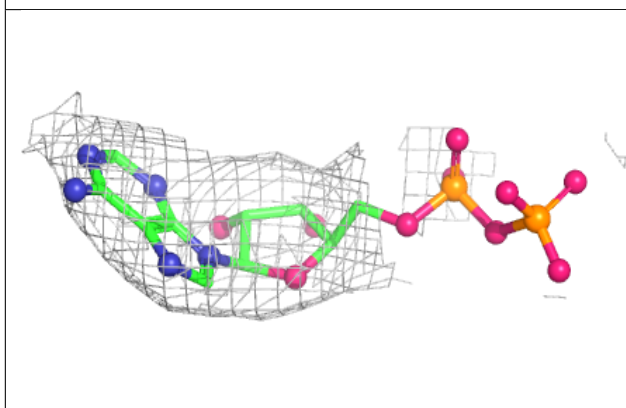
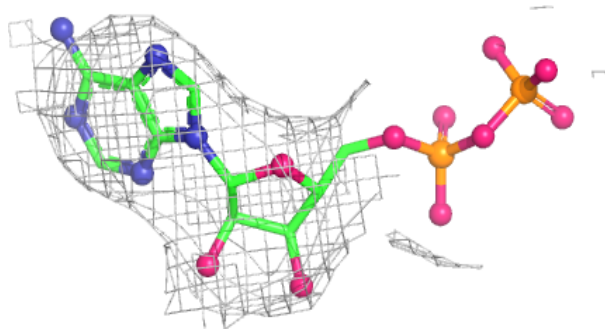


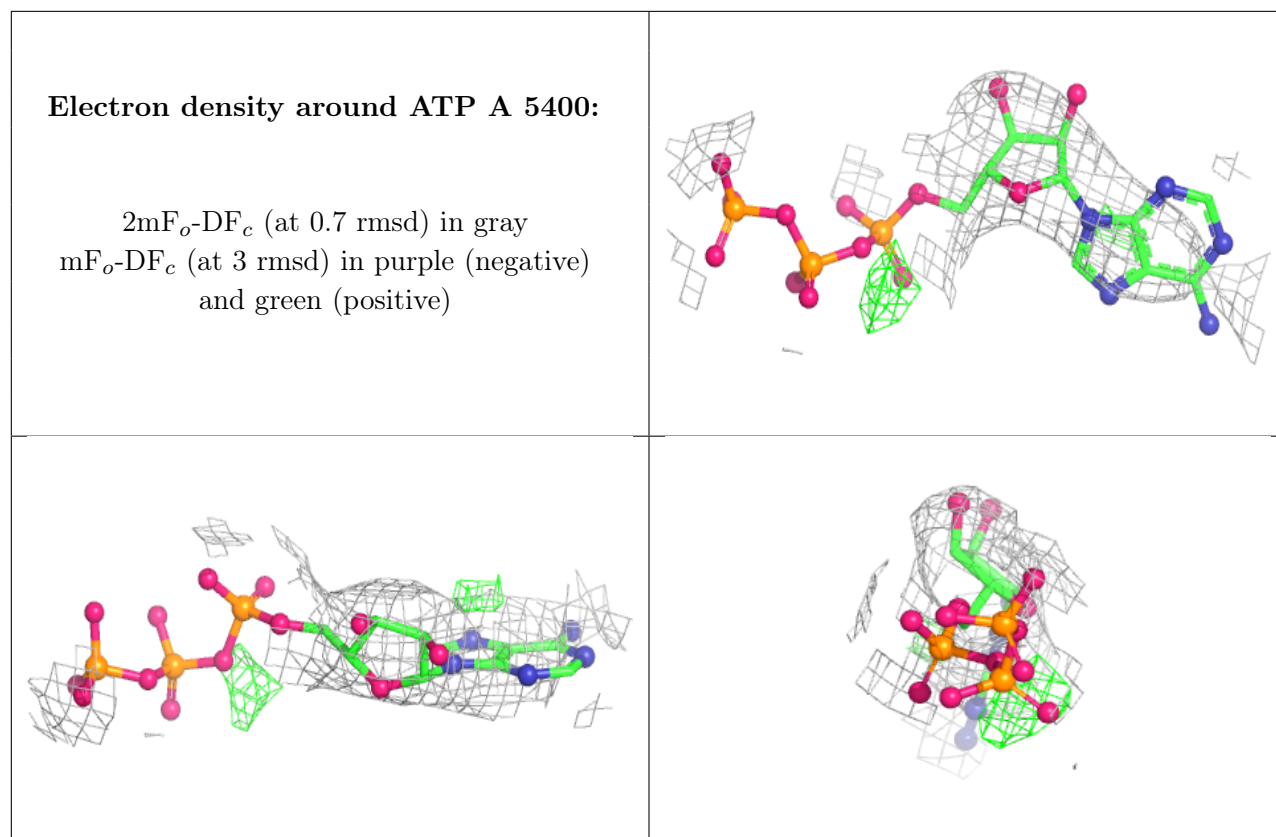
Electron density around ADP A 5402:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.