



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:10 PM UTC

PDB ID : 1IYJ / pdb_00001iyj
Title : STRUCTURE OF A BRCA2-DSS1 COMPLEX
Authors : Pavletich, N.P.; Jeffrey, P.D.; Yang, H.J.
Deposited on : 2002-08-28
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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

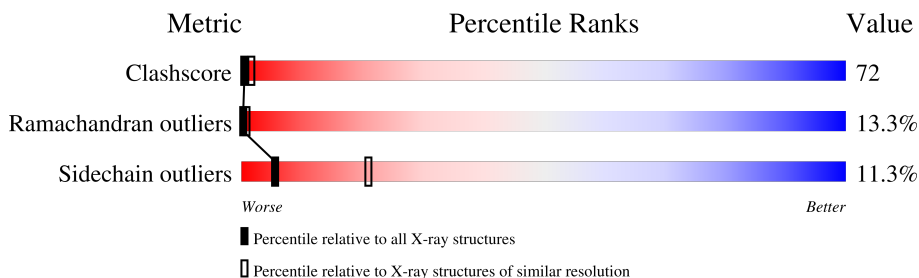
1 Overall quality at a glance

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))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	70	7% 37% 17% • 36%
1	C	70	6% 36% 20% • 36%
2	B	817	13% 44% 14% • 28%
2	D	817	15% 42% 14% • 28%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10092 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 Deleted in split hand/split foot protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	45	Total	C	N	O	0	0	0
			380	235	59	86			
1	C	45	Total	C	N	O	0	0	0
			380	235	59	86			

- Molecule 2 is a protein called breast cancer susceptibility.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	591	Total	C	N	O	S	0	0	0
			4666	2984	805	862	15			
2	D	591	Total	C	N	O	S	0	0	0
			4666	2984	805	862	15			

V2582	P2519	A2456	SER	SER	H3081	L3013	E2949	GLU	LEU	G2767	L2706	SER
L2583	S2520	V2457	GLU	SER	H3082	G3014	W2950	GLU	GLN	S2768	K2707	ASN
L2584	D2521	G2458	ASP	ASN	F3082	L3015	P2951	GLY	ASP	S2769	L2708	V2645
Q2585	D2522	D2459	GLY	GLY	Q3083	A3016	S2952	GLY	ASP	Y2769	S2709	V2646
L2586	G2523	S2460	THR	THR	E3084	P3017	I2953	R2892	ALA	N2772	A2710	D2647
K2587	K2524	V2461	VAL	VAL	E3085	L3018	Q2954	R2893	GLU	N2773	N2711	T2648
L2588	A2525	P2462	ASP	SER	V3086	V3019	L2955	D2894	LEU	E2774	S2712	L2651
R2589	G2526	S2463	ALA	PRO	T3087	L3021	T2956	V2895	TYR	R2775	T2713	L2652
R2590	K2527	A2464	LEU	ARG	N3088	S3022	A2957	S2896	ALA	E2776	R2714	D2653
D2591	E2528	C2465	ARG	SER	M3089	S3023	T2958	T2897	ALA	E2777	P2715	D2654
V2592	E2529	S2466	SER	SER	K3090	D3023	T2959	V2898	VAL	E2778	A2716	G2654
E2593	F2530	P2467	GLU	GLU	H3091	E3024	R2960	V2899	ASP	K2779	R2717	V2655
L2594	Y2531	K2468	ARG	ARG	A3092	C3025	T2961	K2900	GLN	E2780	W2718	V2656
D2595		Q2469	THR	THR	I3093	L3026	L2966	L2901	ALA	A2781	H2719	A2657
N2596	L2534	L2470	ARG	ARG	H3094	H3027	L2967	R2902	SER	L2782	K2720	V2658
S2597	C2535	Y2471	HIS	HIS	N3095	L3028	P2967	V2903	ASP	R2783	K2721	K2659
D2598	D2536	M2472	SER	SER	I3096	L3029	S2968	T2904	PRO	F2784	L2722	A2660
R2599	T2537	S2473	VAL	VAL	D3097	V3031	S2969	S2905	GLU	ALA	G2723	Q2661
S2600	P2538	Q2474	SER	SER	T3098	K3032	S2970	V2906	HIS	GLU	F2724	L2662
A2601	G2539	V2475	ASP	ASP	R3099	K3032	E2971	K2907	LEU	ALA	F2725	D2663
L2602	V2540	S2476	LYS	LYS	Y3100	F3033	T2972	K2908	GLU	GLN	H2726	D2664
K2603	D2541	K2477	SER	SER	K3101	G3034	L2973	R2909	THR	GLN	R2729	P2665
K2604	P2542	A2478	THR	THR	E3102	L3035	L2974	E2910	CYS	LYS	P2730	L2666
I2605	K2543	C2479	LYS	LYS	A3103	D3036	Q2975	K2911	PHE	LYS	P2731	L2667
L2606	L2544	I2480	VAL	VAL	E3104	L3037	L2988	S2912	SER	LEU	F2731	A2668
E2607	I2545	S2481	PHE	PHE	K3105	N3038	Q2978	A2913	GLU	GLU	P2732	L2669
R2608	S2546	V2482	VAL	VAL	R3106	E3039	P2979	L2914	GLU	ALA	P2733	V2670
D2609	S2547	M2483	PRO	PRO	L3107	D3040	R2980	L2915	GLN	LEU	P2734	K2671
D2610	S2484	I2423	PRO	PRO	I3108	L3041	E2981	S2916	LEU	THR	L2735	S2672
T2611	K2485	R2424	PHE	PHE	K3109	K3042	L2982	L2917	ARG	THR	S2736	G2673
A2612	L2425	I2425	LYS	LYS	V3110	P3043	L2983	W2918	ALA	LYS	S2737	R2674
L2613	N2552	A2487	VAL	VAL	L3111	R3044	P2984	R2919	LEU	VAL	L2738	L2675
K2614	H2553	E2488	LYS	LYS	K3112	V3045	F2985	P2920	ASN	HIS	F2739	T2676
T2615	Y2554	K2428	SER	SER	G3113	L3046	S2986	S2921	ASN	THR	D2741	G2678
L2616	R2555	E2429	ARG	ARG	D3114	L3047	K2987	S2922	TYR	GLU	S2740	Q2679
V2620	W2556	Q2491	PHE	PHE	S3115	A3048	S2988	D2923	ARG	LEU	G2742	K2680
S2621	T2557	F2492	HIS	HIS	P3116	A3049	S2989	L2924	GLN	LYS	G2743	K2681
D2622	V2558	A2493	ARG	ARG	K3117	S3050	D2990	P2925	MET	GLU	N2744	L2682
I2623	W2559	I2494	ASP	ASP	TRP	N3051	P2991	S2926	LEU	HIS	V2745	T2683
L2624	E2495	E2495	GLU	GLU	THR	R3055	A2992	L2927	SER	GLU	G2746	T2684
S2625	L2561	D2496	HIS	HIS	PRO	P3056	F2993	L2928	ASP	GLU	C2747	Q2684
L2626	A2562	H2497	PHE	PHE	ASN	E3057	Q2994	T2929	LYS	ASP	V2748	G2685
A2627	L2563	F2498	ASP	ASP	LYS	S3058	P2995	E2930	LYS	ILE	D2749	A2686
S2628	M2564	C2499	SER	SER	ASP	T3059	C2996	Q2931	GLN	ALA	V2750	F2687
E2629	E2565	K2800	LYS	LYS	THR	S3060	S2998	Q2932	ALA	GLN	V2752	L2688
F2630	A2567	E2501	ASN	ASN	PRO	R3061	E2999	R2933	ARG	ARG	Q2753	V2689
S2631	F2638	L2503	VAL	VAL	THR	S3062	V3000	R2935	GLN	VAL	R2754	D2693
K2632	P2569	C2504	ASN	ASN	ARG	R3063	D3001	L2936	SER	LEU	W2755	P2692
L2633	K2570	A2505	GLU	GLU	PRO	V3063	V3002	Y2937	GLU	SER	X2756	A2694
T2634	E2571	G2506	GLY	GLY	TYR	T3064	V3003	H2938	PHE	ARG	P2757	C2695
S2635	K2572	K2507	LYS	LYS	PRO	L3065	L2939	L2939	ARG	ALA	L2758	A2696
A2636	A2573	L2448	ASN	ASN	ALA	F3066	V3005	S2940	LYS	LEU	Q2759	P2697
L2637	L2511	L2449	GLN	GLN	SER	A3067	V3006	V2941	ALA	THR	W2760	L2698
L2638	A2512	P2449	LYS	LYS	THR	G3068	V3007	S2942	LEU	ARG	V2761	A2699
L2639	D2513	R2450	SER	SER	CYS	N3069	S3008	K2943	GLU	GLN	E2762	E2700
S2640	S2514	S2452	ALA	ALA	SER	F3070	V3009	S2944	ALA	VAL	K2763	P2701
L2641	W2516	L2453	ASP	ASP	ALA	V3071	V3010	K2945	ALA	GLU	T2764	V2765
L2642	L2517	Q2454	GLY	GLY	SER	V3072	K3011	N2946	HIS	ALA	L2704	R2705
L2643	R2581	I2518	VAL	VAL	ASP	F3073	P3012		LYS	ALA	S2766	

• Molecule 2: breast cancer susceptibility

Chain D:  15% 42% 14% 28%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	130.31Å 130.31Å 192.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10092	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.48	0/388	1.11	3/526 (0.6%)
1	C	0.48	0/388	1.11	3/526 (0.6%)
2	B	0.53	0/4774	1.11	42/6475 (0.6%)
2	D	0.53	0/4774	1.12	50/6475 (0.8%)
All	All	0.53	0/10324	1.12	98/14002 (0.7%)

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2782	LEU	N-CA-C	-8.58	102.74	113.55
2	D	2782	LEU	N-CA-C	-8.55	102.77	113.55
2	B	2593	GLU	N-CA-C	8.18	120.27	111.36
1	A	49	GLU	N-CA-C	7.99	120.28	108.14
1	C	49	GLU	N-CA-C	7.93	120.19	108.14
2	B	2420	LEU	N-CA-C	-7.75	102.83	111.28
2	D	2593	GLU	N-CA-C	7.67	119.42	111.14
2	D	2547	SER	N-CA-C	-7.56	103.12	111.36
2	B	2547	SER	N-CA-C	-7.40	102.59	111.69
2	D	3069	ASN	N-CA-C	-7.29	104.53	113.50
2	B	3055	ARG	CA-C-N	7.16	128.78	119.84
2	B	3055	ARG	C-N-CA	7.16	128.78	119.84
2	B	2467	PRO	N-CA-CB	6.95	110.54	103.25
2	B	2477	LYS	N-CA-C	-6.88	103.98	112.38
2	D	2467	PRO	N-CA-CB	6.86	110.45	103.25
2	B	2940	SER	N-CA-C	6.79	117.01	108.45
2	B	2696	ALA	CA-C-N	6.79	128.32	119.84
2	B	2696	ALA	C-N-CA	6.79	128.32	119.84
2	D	2966	LEU	CA-C-N	6.78	126.81	119.89
2	D	2966	LEU	C-N-CA	6.78	126.81	119.89
2	D	2477	LYS	N-CA-C	-6.75	104.14	112.38
2	D	2756	TYR	CA-C-N	6.74	127.11	119.83
2	D	2756	TYR	C-N-CA	6.74	127.11	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2673	GLY	N-CA-C	-6.64	105.49	115.32
2	D	2940	SER	N-CA-C	6.63	117.00	108.24
2	D	2695	CYS	N-CA-C	6.63	114.22	108.78
2	D	2594	ILE	N-CA-C	6.53	116.69	110.74
2	D	2434	CYS	N-CA-C	-6.52	100.78	109.84
2	D	2420	LEU	N-CA-C	-6.50	104.20	111.28
1	A	7	PRO	N-CA-CB	6.45	110.03	103.25
2	D	2673	GLY	N-CA-C	-6.45	105.78	115.32
2	B	2756	TYR	CA-C-N	6.44	126.82	119.93
2	B	2756	TYR	C-N-CA	6.44	126.82	119.93
2	B	3069	ASN	N-CA-C	-6.40	105.30	113.23
2	B	2479	CYS	N-CA-C	-6.34	104.45	111.36
2	D	2941	VAL	N-CA-C	-6.33	96.16	109.34
1	C	7	PRO	N-CA-CB	6.33	109.90	103.25
2	D	2501	GLU	N-CA-C	-6.27	97.45	110.80
2	B	2966	LEU	CA-C-N	6.18	126.20	119.89
2	B	2966	LEU	C-N-CA	6.18	126.20	119.89
2	B	2941	VAL	N-CA-C	-6.18	96.48	109.34
2	D	3115	SER	CA-C-N	6.16	126.51	119.92
2	D	3115	SER	C-N-CA	6.16	126.51	119.92
2	B	2436	GLN	CA-C-N	6.11	126.07	119.78
2	B	2436	GLN	C-N-CA	6.11	126.07	119.78
2	D	3055	ARG	CA-C-N	6.01	127.35	119.84
2	D	3055	ARG	C-N-CA	6.01	127.35	119.84
2	D	2479	CYS	N-CA-C	-5.98	104.68	111.14
2	B	2501	GLU	N-CA-C	-5.98	98.07	110.80
2	B	2747	CYS	N-CA-C	5.88	117.63	107.93
2	B	2712	SER	N-CA-C	-5.87	105.88	114.39
2	D	2712	SER	N-CA-C	-5.84	105.92	114.39
2	D	3002	VAL	N-CA-C	5.82	117.09	108.65
2	D	2473	TYR	N-CA-C	-5.82	106.81	114.31
2	B	3057	GLU	N-CA-C	5.81	121.14	112.94
2	B	2453	LEU	N-CA-C	-5.80	104.96	111.28
2	D	3057	GLU	N-CA-C	5.80	121.12	112.94
2	D	2670	VAL	N-CA-C	-5.79	104.69	110.30
2	B	2473	TYR	N-CA-C	-5.75	106.90	114.31
1	A	58	ALA	N-CA-C	-5.74	105.11	111.71
2	B	2482	VAL	N-CA-C	5.70	116.27	107.78
2	D	3062	VAL	CA-C-N	5.64	126.89	119.84
2	D	3062	VAL	C-N-CA	5.64	126.89	119.84
2	D	2729	ARG	CA-C-N	5.62	125.95	119.93
2	D	2729	ARG	C-N-CA	5.62	125.95	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3002	VAL	N-CA-C	5.61	116.78	108.65
2	B	2503	LEU	N-CA-C	-5.59	105.27	111.36
2	B	2584	LEU	N-CA-C	-5.56	105.37	111.82
2	D	2661	GLN	N-CA-C	-5.54	100.15	108.96
2	B	3114	ASP	N-CA-C	-5.54	99.00	110.80
2	B	2670	VAL	N-CA-C	-5.50	104.97	110.30
2	B	2554	TYR	N-CA-C	-5.45	105.37	112.23
2	D	3114	ASP	N-CA-C	-5.43	99.24	110.80
2	D	2747	CYS	N-CA-C	5.42	118.23	108.48
2	B	3062	VAL	CA-C-N	5.42	126.61	119.84
2	B	3062	VAL	C-N-CA	5.42	126.61	119.84
2	B	2661	GLN	N-CA-C	-5.41	100.36	108.96
1	C	58	ALA	N-CA-C	-5.39	105.51	111.71
2	D	2714	ARG	CA-C-N	5.38	125.55	119.90
2	D	2714	ARG	C-N-CA	5.38	125.55	119.90
2	D	2470	LEU	N-CA-C	-5.33	106.04	112.54
2	D	2695	CYS	CB-CA-C	-5.32	109.41	117.07
2	D	2696	ALA	CA-C-N	5.30	126.46	119.84
2	D	2696	ALA	C-N-CA	5.30	126.46	119.84
2	B	2745	VAL	CB-CA-C	-5.30	104.32	111.63
2	D	2482	VAL	N-CA-C	5.29	116.33	107.18
2	D	2695	CYS	CA-C-O	5.28	121.00	117.94
2	B	2470	LEU	N-CA-C	-5.24	106.14	112.54
2	D	2436	GLN	CA-C-N	5.24	125.18	119.78
2	D	2436	GLN	C-N-CA	5.24	125.18	119.78
2	B	3112	LYS	N-CA-C	-5.23	104.19	110.88
2	D	2995	PRO	N-CA-C	5.18	116.12	110.58
2	D	2682	ILE	N-CA-C	-5.17	101.03	108.48
2	D	2554	TYR	N-CA-C	-5.14	105.37	111.69
2	B	2471	TYR	N-CA-C	-5.12	105.77	112.23
2	D	2471	TYR	N-CA-C	-5.08	105.84	112.23
2	B	2682	ILE	N-CA-C	-5.05	101.21	108.48
2	D	2503	LEU	N-CA-C	-5.04	105.86	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	380	0	306	61	0
1	C	380	0	306	68	0
2	B	4666	0	4694	691	0
2	D	4666	0	4694	669	0
All	All	10092	0	10000	1438	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 72.

All (1438) 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)
2:D:2683:THR:HG22	2:D:2713:THR:HB	1.22	1.16
2:D:2750:VAL:HG11	2:D:2903:VAL:HB	1.18	1.16
2:B:2683:THR:HG22	2:B:2713:THR:HB	1.20	1.13
2:B:2750:VAL:HG11	2:B:2903:VAL:HB	1.19	1.12
2:B:2942:SER:HB3	2:B:2953:ILE:HD11	1.39	1.03
2:B:2483:ASN:H	2:B:2486:ASN:ND2	1.56	1.02
2:B:2483:ASN:N	2:B:2486:ASN:HD21	1.58	1.02
2:D:2483:ASN:H	2:D:2486:ASN:ND2	1.57	1.01
2:B:2404:PRO:HB2	2:B:2410:LEU:HD22	1.37	1.01
2:B:3061:ARG:HG3	2:B:3062:VAL:HG12	1.41	1.01
2:D:2950:TRP:H	2:D:2951:PRO:HD2	1.26	1.00
2:D:2430:ARG:HG3	2:D:2430:ARG:HH11	1.27	1.00
2:D:2483:ASN:N	2:D:2486:ASN:HD21	1.59	0.99
2:B:2430:ARG:HG3	2:B:2430:ARG:HH11	1.28	0.99
2:B:2750:VAL:CG1	2:B:2903:VAL:HB	1.92	0.99
2:D:3061:ARG:HG3	2:D:3062:VAL:HG12	1.45	0.99
2:B:2950:TRP:H	2:B:2951:PRO:HD2	1.26	0.98
2:D:2483:ASN:H	2:D:2486:ASN:HD21	1.03	0.98
2:D:2750:VAL:CG1	2:D:2903:VAL:HB	1.92	0.98
2:D:2773:ASN:H	2:D:2776:GLU:HB2	1.29	0.97
2:D:2773:ASN:ND2	2:D:2776:GLU:HG3	1.80	0.96
2:B:2608:ARG:HH11	2:B:2608:ARG:HB2	1.30	0.95
2:B:2959:LYS:H	2:B:2959:LYS:HD3	1.32	0.95
2:D:2665:PRO:HG3	2:D:2742:GLY:HA2	1.44	0.95
2:B:2773:ASN:H	2:B:2776:GLU:HB2	1.32	0.94
2:D:2942:SER:HB3	2:D:2953:ILE:HD11	1.45	0.94
2:D:2758:LEU:HD21	2:D:2897:THR:HB	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2403:PHE:HA	2:B:2503:LEU:HD11	1.52	0.92
2:D:2959:LYS:H	2:D:2959:LYS:HD3	1.30	0.91
2:B:2483:ASN:H	2:B:2486:ASN:HD21	0.99	0.91
2:D:2608:ARG:HH11	2:D:2608:ARG:HB2	1.34	0.91
2:B:2608:ARG:HH22	2:B:2688:LEU:HD23	1.37	0.90
2:B:2758:LEU:HD21	2:B:2897:THR:HB	1.50	0.90
2:D:2552:ASN:HD21	2:D:2556:TRP:NE1	1.70	0.90
2:B:2773:ASN:ND2	2:B:2776:GLU:HG3	1.85	0.90
2:B:2665:PRO:HG3	2:B:2742:GLY:HA2	1.53	0.89
2:B:2552:ASN:HD21	2:B:2556:TRP:NE1	1.70	0.88
2:D:2709:SER:O	2:D:2713:THR:HG22	1.72	0.88
2:D:2917:ILE:HG22	2:D:2920:PRO:HG3	1.56	0.87
2:B:2917:ILE:HD13	2:B:2924:LEU:HD21	1.54	0.87
2:D:2656:TYR:CD2	2:D:2697:PRO:HB2	2.10	0.87
2:B:2750:VAL:HG11	2:B:2903:VAL:CB	2.04	0.87
2:B:2709:SER:O	2:B:2713:THR:HG22	1.76	0.86
2:D:2750:VAL:HG11	2:D:2903:VAL:CB	2.03	0.86
2:D:2552:ASN:HD21	2:D:2556:TRP:HE1	1.23	0.86
2:D:2944:SER:HB2	2:D:2954:GLN:HE21	1.41	0.85
2:D:2426:LYS:HG3	2:D:2430:ARG:HH22	1.41	0.85
2:B:2430:ARG:HG3	2:B:2430:ARG:NH1	1.88	0.85
2:B:2608:ARG:HH11	2:B:2608:ARG:CB	1.88	0.85
2:B:2552:ASN:HD21	2:B:2556:TRP:HE1	1.21	0.85
2:B:3116:PRO:O	2:B:3117:LYS:HG2	1.77	0.85
2:D:2608:ARG:HH11	2:D:2608:ARG:CB	1.89	0.85
2:D:2917:ILE:HD13	2:D:2924:LEU:HD21	1.57	0.84
2:B:2944:SER:HB2	2:B:2954:GLN:HE21	1.41	0.84
2:D:3048:ALA:HB1	2:D:3082:PHE:CD2	2.12	0.84
2:B:2414:LEU:HD23	2:B:2506:GLY:HA2	1.59	0.84
2:D:2430:ARG:HG3	2:D:2430:ARG:NH1	1.89	0.84
2:D:2953:ILE:HG13	2:D:2954:GLN:H	1.41	0.84
2:B:2656:TYR:CD2	2:B:2697:PRO:HB2	2.13	0.83
2:B:3048:ALA:HB1	2:B:3082:PHE:CD2	2.13	0.83
2:D:2733:LEU:HD23	2:D:2733:LEU:H	1.43	0.83
2:B:2744:ASN:HB2	2:B:2940:SER:CB	2.09	0.83
2:D:2608:ARG:HH22	2:D:2688:LEU:HD23	1.43	0.83
2:B:3007:VAL:HB	2:B:3104:GLU:CD	2.03	0.83
2:D:2904:THR:OG1	2:D:2910:GLU:HB2	1.79	0.83
2:B:2902:ARG:HH11	2:B:2902:ARG:HB2	1.42	0.83
2:D:2414:LEU:HD23	2:D:2506:GLY:HA2	1.59	0.82
2:D:2739:PHE:HB2	2:D:2742:GLY:HA3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2426:LYS:HG3	2:B:2430:ARG:HH22	1.45	0.82
2:D:2902:ARG:HH11	2:D:2902:ARG:HB2	1.43	0.82
2:D:2421:GLN:HB2	2:D:2424:ARG:NH2	1.95	0.82
2:D:2683:THR:HG22	2:D:2713:THR:CB	2.09	0.82
2:B:2953:ILE:HG13	2:B:2954:GLN:H	1.44	0.81
2:B:2764:THR:HB	2:B:2767:GLY:O	1.80	0.81
2:B:2752:VAL:HA	2:B:2903:VAL:HG12	1.62	0.81
2:B:2404:PRO:HG2	2:B:2504:CYS:HA	1.63	0.81
2:B:2683:THR:CG2	2:B:2713:THR:HB	2.06	0.81
2:B:2904:THR:OG1	2:B:2910:GLU:HB2	1.81	0.81
2:D:3007:VAL:HB	2:D:3104:GLU:CD	2.05	0.81
2:D:2980:ARG:HH21	2:D:3051:ASN:HD21	1.29	0.81
2:D:3030:VAL:HG23	2:D:3062:VAL:HG22	1.62	0.80
2:B:2683:THR:HG22	2:B:2713:THR:CB	2.06	0.80
2:B:2713:THR:O	2:B:2714:ARG:HD3	1.81	0.80
2:B:2490:PHE:CZ	2:B:2577:LEU:HD21	2.16	0.80
2:B:2739:PHE:HB2	2:B:2742:GLY:HA3	1.63	0.80
2:D:2750:VAL:HG12	2:D:2751:ILE:H	1.46	0.80
2:D:2437:PRO:HG2	2:D:2442:LEU:HD11	1.63	0.79
2:B:2950:TRP:H	2:B:2951:PRO:CD	1.95	0.79
2:B:2479:CYS:O	2:B:2482:VAL:HG12	1.82	0.79
2:B:2744:ASN:HB2	2:B:2940:SER:HB3	1.64	0.79
2:D:3009:VAL:HG22	2:D:3019:VAL:HG22	1.61	0.79
2:B:2917:ILE:HG22	2:B:2920:PRO:HG3	1.64	0.79
2:B:3030:VAL:HG23	2:B:3062:VAL:HG22	1.64	0.79
2:D:2764:THR:HB	2:D:2767:GLY:O	1.82	0.79
2:D:2933:ARG:HB3	2:D:2966:LEU:O	1.83	0.79
2:B:2773:ASN:HD21	2:B:2776:GLU:HG3	1.46	0.78
2:D:2501:GLU:C	2:D:2503:LEU:H	1.90	0.78
2:D:2589:ARG:HG2	2:D:2655:TRP:CH2	2.18	0.78
2:B:2687:GLU:HB2	2:B:2707:LYS:HB3	1.63	0.78
2:D:2744:ASN:HB2	2:D:2940:SER:HB3	1.66	0.78
2:D:2744:ASN:HB2	2:D:2940:SER:CB	2.13	0.78
2:B:2589:ARG:HG3	2:B:2589:ARG:HH11	1.49	0.78
2:D:2404:PRO:HB2	2:D:2410:LEU:HD22	1.64	0.78
2:D:2675:LEU:HD21	2:D:2681:ILE:HD11	1.64	0.78
2:D:2683:THR:CG2	2:D:2713:THR:HB	2.09	0.78
2:B:2733:LEU:HD23	2:B:2733:LEU:H	1.48	0.78
2:D:2950:TRP:H	2:D:2951:PRO:CD	1.95	0.78
2:D:2427:ASN:HA	2:D:2430:ARG:CZ	2.14	0.77
2:B:2610:ASP:C	2:B:2612:ALA:H	1.91	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2479:CYS:O	2:D:2482:VAL:HG12	1.84	0.77
2:D:2484:SER:HB2	2:D:2559:TRP:CZ2	2.19	0.77
2:B:2558:VAL:HG13	2:B:2577:LEU:HD11	1.64	0.77
2:D:2614:LYS:CG	2:D:2615:THR:H	1.98	0.77
2:D:2666:LEU:HG	2:D:2710:ALA:HB2	1.67	0.76
2:B:2772:ARG:HA	2:B:2776:GLU:OE1	1.85	0.76
2:D:2610:ASP:C	2:D:2612:ALA:H	1.94	0.76
2:D:2426:LYS:O	2:D:2430:ARG:NH1	2.19	0.76
2:D:2761:VAL:C	2:D:2895:VAL:HG23	2.11	0.76
2:D:2773:ASN:HD21	2:D:2776:GLU:HG3	1.47	0.76
2:B:2750:VAL:HG12	2:B:2751:ILE:H	1.51	0.76
2:D:2980:ARG:NH2	2:D:3051:ASN:HD21	1.84	0.76
2:B:2501:GLU:C	2:B:2503:LEU:H	1.91	0.76
2:B:2909:ARG:O	2:B:2910:GLU:HG2	1.86	0.76
2:D:2713:THR:O	2:D:2714:ARG:HD3	1.84	0.75
2:B:2738:LEU:HD13	2:B:2745:VAL:HG21	1.69	0.75
2:B:2427:ASN:HA	2:B:2430:ARG:CZ	2.15	0.75
2:B:2980:ARG:HH21	2:B:3051:ASN:HD21	1.33	0.75
2:B:2761:VAL:C	2:B:2895:VAL:HG23	2.11	0.75
1:A:56:LEU:H	2:B:2462:PRO:HG2	1.51	0.75
2:B:3113:GLY:O	2:B:3114:ASP:HB2	1.87	0.75
2:D:2589:ARG:HG3	2:D:2589:ARG:HH11	1.52	0.75
2:D:2909:ARG:O	2:D:2910:GLU:HG2	1.86	0.75
2:D:3048:ALA:HB1	2:D:3082:PHE:HD2	1.52	0.75
2:B:2413:SER:HB2	2:B:2506:GLY:HA3	1.69	0.75
1:A:54:ASN:O	1:A:55:GLN:HB2	1.85	0.74
2:B:2933:ARG:HB3	2:B:2966:LEU:O	1.86	0.74
2:D:3029:LEU:C	2:D:3029:LEU:HD23	2.12	0.74
1:C:54:ASN:O	1:C:55:GLN:HB2	1.87	0.74
1:A:62:LYS:HE3	2:B:2676:THR:HG21	1.70	0.74
2:D:2780:GLU:HA	2:D:2783:ARG:HB3	1.70	0.74
2:B:2985:PHE:HD1	2:B:2985:PHE:H	1.36	0.74
2:D:3017:PRO:O	2:D:3018:LEU:HD23	1.87	0.74
2:D:3083:GLN:HA	2:D:3086:VAL:HG12	1.70	0.73
2:B:2944:SER:HB2	2:B:2954:GLN:NE2	2.02	0.73
2:B:2940:SER:O	2:B:2941:VAL:HG23	1.87	0.73
2:D:2494:ILE:HD12	2:D:2495:GLU:H	1.53	0.73
2:D:3033:PHE:HA	2:D:3067:ALA:HB3	1.71	0.73
2:B:2614:LYS:CG	2:B:2615:THR:H	1.99	0.73
2:B:3009:VAL:HG22	2:B:3019:VAL:HG22	1.70	0.73
2:B:2450:ARG:NH1	2:B:2450:ARG:HB3	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3083:GLN:HA	2:B:3086:VAL:HG12	1.68	0.73
2:D:2534:LEU:HD22	2:D:2540:VAL:HG21	1.68	0.73
2:B:3048:ALA:HB1	2:B:3082:PHE:HD2	1.52	0.73
1:A:43:TRP:HZ3	2:B:2713:THR:HG23	1.53	0.73
2:B:3030:VAL:HG23	2:B:3062:VAL:CG2	2.19	0.73
2:B:3010:VAL:HG12	2:B:3012:PRO:HD3	1.70	0.72
2:D:2404:PRO:HG2	2:D:2504:CYS:HA	1.71	0.72
2:D:2558:VAL:HG13	2:D:2577:LEU:HD11	1.70	0.72
2:B:2534:LEU:HD22	2:B:2540:VAL:HG21	1.70	0.72
2:B:3029:LEU:C	2:B:3029:LEU:HD23	2.15	0.72
2:D:2687:GLU:HB2	2:D:2707:LYS:HB3	1.70	0.72
2:D:2944:SER:HB2	2:D:2954:GLN:NE2	2.03	0.72
2:B:3002:VAL:HG22	2:B:3049:ALA:HB3	1.70	0.72
2:D:2413:SER:HB2	2:D:2506:GLY:HA3	1.71	0.72
2:D:2494:ILE:HG21	2:D:2519:PRO:HG3	1.72	0.72
2:B:2780:GLU:HA	2:B:2783:ARG:HB3	1.71	0.72
2:D:2512:ALA:CB	2:D:2584:LEU:HG	2.20	0.71
2:B:2666:LEU:HG	2:B:2710:ALA:HB2	1.71	0.71
2:D:2490:PHE:CZ	2:D:2577:LEU:HD21	2.25	0.71
2:D:2772:ARG:HA	2:D:2776:GLU:OE1	1.90	0.71
2:D:2940:SER:O	2:D:2941:VAL:HG23	1.91	0.71
2:D:2733:LEU:HD23	2:D:2733:LEU:N	2.05	0.71
2:D:2922:SER:O	2:D:2925:PRO:HD2	1.91	0.71
2:B:2604:LYS:HB3	2:B:2610:ASP:HB3	1.72	0.71
2:D:2620:VAL:HG23	2:D:2678:GLY:H	1.54	0.71
2:B:2494:ILE:HD12	2:B:2495:GLU:H	1.54	0.71
2:B:2494:ILE:HG21	2:B:2519:PRO:HG3	1.71	0.71
2:B:2483:ASN:N	2:B:2486:ASN:ND2	2.27	0.71
2:B:2620:VAL:HG23	2:B:2678:GLY:H	1.55	0.71
2:B:3028:LEU:HD12	2:B:3111:LEU:HD22	1.71	0.70
2:B:3033:PHE:HA	2:B:3067:ALA:HB3	1.73	0.70
1:C:39:TRP:HE1	2:D:2733:LEU:HD22	1.57	0.70
2:D:2567:ALA:C	2:D:2569:PRO:HD3	2.17	0.70
2:B:2403:PHE:HA	2:B:2503:LEU:CD1	2.20	0.70
2:B:2484:SER:HB2	2:B:2559:TRP:CZ2	2.27	0.70
2:D:3030:VAL:HG23	2:D:3062:VAL:CG2	2.21	0.70
2:B:2421:GLN:HB2	2:B:2424:ARG:NH2	2.06	0.70
2:D:2483:ASN:N	2:D:2486:ASN:ND2	2.26	0.70
2:D:2756:TYR:HD2	2:D:3070:PHE:HB3	1.57	0.69
2:D:3002:VAL:HG22	2:D:3049:ALA:HB3	1.74	0.69
2:B:3005:VAL:HG22	2:B:3046:LEU:HD11	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2620:VAL:HG23	2:D:2678:GLY:N	2.06	0.69
2:B:2476:SER:OG	2:B:2478:ALA:HB3	1.92	0.69
2:B:2610:ASP:O	2:B:2612:ALA:N	2.25	0.69
2:B:2733:LEU:HD23	2:B:2733:LEU:N	2.08	0.69
2:D:2752:VAL:HA	2:D:2903:VAL:HG12	1.73	0.69
2:D:2476:SER:OG	2:D:2478:ALA:HB3	1.92	0.69
2:D:2918:TRP:C	2:D:2920:PRO:HD3	2.18	0.69
2:B:2663:ASP:OD2	2:B:2666:LEU:HB2	1.91	0.69
2:D:2604:LYS:HB3	2:D:2610:ASP:HB3	1.74	0.69
2:D:2747:CYS:SG	2:D:2937:TYR:HE1	2.15	0.69
2:D:2758:LEU:HD23	2:D:2759:GLN:N	2.07	0.69
2:D:2985:PHE:HD1	2:D:2985:PHE:H	1.40	0.69
2:B:2922:SER:O	2:B:2925:PRO:HD2	1.92	0.69
2:D:2646:VAL:HB	2:D:2671:LYS:HE3	1.74	0.69
2:D:2663:ASP:OD2	2:D:2666:LEU:HB2	1.93	0.69
2:D:2936:ILE:CG2	2:D:2939:LEU:HB2	2.23	0.68
2:B:2620:VAL:HG23	2:B:2678:GLY:N	2.08	0.68
2:D:2450:ARG:NH1	2:D:2450:ARG:HB3	2.07	0.68
2:D:3055:ARG:O	2:D:3057:GLU:HG2	1.94	0.68
2:B:2672:SER:HB2	2:B:2674:ARG:HG2	1.75	0.68
2:D:2936:ILE:HG22	2:D:2939:LEU:HB2	1.74	0.68
2:D:3028:LEU:HD12	2:D:3111:LEU:HD22	1.74	0.68
2:B:2915:LEU:HD12	2:B:2916:SER:N	2.09	0.68
2:D:3111:LEU:O	2:D:3112:LYS:HD3	1.94	0.68
2:B:2567:ALA:C	2:B:2569:PRO:HD3	2.18	0.68
2:B:2512:ALA:CB	2:B:2584:LEU:HG	2.24	0.67
2:B:2475:VAL:HG12	2:B:2480:ILE:HG13	1.76	0.67
2:B:2662:LEU:HD22	2:B:2666:LEU:HD13	1.76	0.67
2:B:2494:ILE:HG22	2:B:2498:PHE:CE1	2.30	0.67
2:B:2589:ARG:HG2	2:B:2655:TRP:CH2	2.29	0.67
2:D:2601:ALA:O	2:D:2605:ILE:HG12	1.94	0.67
2:D:2729:ARG:HD3	2:D:2730:PRO:HD2	1.77	0.67
2:B:2520:SER:OG	2:B:2524:LYS:HB2	1.94	0.67
2:B:2430:ARG:HH11	2:B:2430:ARG:CG	2.04	0.67
1:A:39:TRP:HE1	2:B:2733:LEU:HD22	1.59	0.67
2:B:2450:ARG:HB3	2:B:2450:ARG:HH11	1.60	0.67
2:D:2610:ASP:O	2:D:2612:ALA:N	2.27	0.66
2:D:2756:TYR:HB3	2:D:2757:PRO:HD2	1.76	0.66
2:D:3010:VAL:HG12	2:D:3012:PRO:HD3	1.76	0.66
1:C:56:LEU:H	2:D:2462:PRO:HG2	1.59	0.66
2:B:3107:LEU:HD23	2:B:3108:ILE:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2413:SER:CB	2:B:2506:GLY:HA3	2.25	0.66
2:B:2441:TYR:O	2:B:2445:SER:HB3	1.96	0.66
2:B:2919:ARG:N	2:B:2920:PRO:HD3	2.11	0.66
2:D:2441:TYR:O	2:D:2445:SER:HB3	1.95	0.66
1:A:50:ASP:CG	1:A:51:ASP:H	2.04	0.66
2:D:2953:ILE:HG13	2:D:2954:GLN:N	2.11	0.66
2:D:2534:LEU:O	2:D:2537:THR:HB	1.96	0.66
2:D:2565:GLU:CD	2:D:2574:ASN:HA	2.21	0.66
1:A:51:ASP:HB3	2:B:2717:ARG:HG3	1.78	0.65
2:B:2541:ASP:OD1	2:B:2543:LYS:HB2	1.95	0.65
2:D:2541:ASP:OD1	2:D:2543:LYS:HB2	1.95	0.65
2:D:2466:SER:O	2:D:2468:LYS:N	2.29	0.65
2:B:2426:LYS:O	2:B:2430:ARG:NH1	2.29	0.65
2:D:2425:ILE:HG23	2:D:2542:PRO:HG2	1.78	0.65
2:D:3037:LEU:O	2:D:3039:GLU:N	2.24	0.65
2:B:2646:VAL:HB	2:B:2671:LYS:HE3	1.78	0.65
2:D:2413:SER:CB	2:D:2506:GLY:HA3	2.26	0.65
2:D:2764:THR:HG22	2:D:2765:VAL:H	1.62	0.65
2:D:2404:PRO:HD3	2:D:2503:LEU:CD1	2.27	0.65
2:B:2918:TRP:C	2:B:2920:PRO:HD3	2.22	0.65
2:D:2484:SER:HB2	2:D:2559:TRP:CE2	2.31	0.65
2:D:2672:SER:HB2	2:D:2674:ARG:HG2	1.76	0.65
2:D:2919:ARG:N	2:D:2920:PRO:HD3	2.11	0.65
2:B:2927:LEU:HD11	2:B:2934:TYR:HE1	1.62	0.65
2:B:2675:LEU:HD21	2:B:2681:ILE:HD11	1.78	0.65
2:B:2758:LEU:HD23	2:B:2759:GLN:N	2.12	0.65
2:B:3017:PRO:O	2:B:3018:LEU:HD23	1.96	0.65
2:B:3111:LEU:O	2:B:3112:LYS:HD3	1.96	0.65
2:D:2614:LYS:CG	2:D:2615:THR:N	2.60	0.65
2:B:2980:ARG:NH2	2:B:3051:ASN:HD21	1.94	0.64
2:D:2667:LEU:O	2:D:2667:LEU:HD23	1.96	0.64
2:D:2714:ARG:HG3	2:D:2715:PRO:HD2	1.79	0.64
2:B:2466:SER:O	2:B:2468:LYS:N	2.30	0.64
2:B:2978:GLN:HG2	2:B:2996:PRO:HG2	1.79	0.64
2:D:2747:CYS:SG	2:D:2937:TYR:CE1	2.91	0.64
1:C:50:ASP:CG	1:C:51:ASP:H	2.04	0.64
2:D:2512:ALA:O	2:D:2513:ASP:HB2	1.95	0.64
2:D:3031:VAL:HA	2:D:3065:LEU:O	1.97	0.64
1:A:13:LEU:HD12	2:B:2451:ILE:O	1.96	0.64
2:B:2410:LEU:O	2:B:2414:LEU:HG	1.96	0.64
2:B:2428:LYS:HD3	2:B:2542:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2959:LYS:H	2:B:2959:LYS:CD	2.09	0.64
2:D:3110:VAL:C	2:D:3112:LYS:H	2.04	0.64
2:B:2736:SER:HB3	2:B:2909:ARG:HH21	1.63	0.64
2:D:2662:LEU:HD22	2:D:2666:LEU:HD13	1.79	0.64
2:D:3094:GLU:C	2:D:3096:ILE:H	2.05	0.64
2:B:2526:GLY:H	2:B:2529:GLU:HB2	1.62	0.64
2:D:2738:LEU:HD13	2:D:2745:VAL:HG21	1.80	0.64
2:B:2902:ARG:HB2	2:B:2902:ARG:NH1	2.10	0.63
2:B:2764:THR:HG22	2:B:2765:VAL:H	1.63	0.63
2:D:2620:VAL:HG21	2:D:2676:THR:O	1.98	0.63
2:D:3058:SER:O	2:D:3059:THR:HB	1.97	0.63
2:B:2984:PRO:HG2	2:B:2987:LYS:CG	2.27	0.63
2:B:2489:TYR:O	2:B:2490:PHE:HB3	1.96	0.63
2:D:2736:SER:HB3	2:D:2909:ARG:HH21	1.63	0.63
2:D:3087:THR:HG22	2:D:3088:ASN:N	2.12	0.63
2:B:2620:VAL:HG21	2:B:2676:THR:O	1.99	0.63
2:B:2893:ARG:O	2:B:2894:ASP:HB3	1.99	0.63
2:D:2450:ARG:HB3	2:D:2450:ARG:HH11	1.61	0.63
2:B:2616:LEU:HD13	2:B:2724:PHE:CD2	2.34	0.63
2:D:3107:LEU:HD23	2:D:3108:ILE:N	2.14	0.63
2:B:2738:LEU:CD1	2:B:2745:VAL:HG21	2.28	0.62
2:B:2939:LEU:HG	2:B:2939:LEU:O	1.99	0.62
2:B:3058:SER:O	2:B:3059:THR:HB	1.99	0.62
2:B:3061:ARG:HG2	2:B:3061:ARG:HH11	1.64	0.62
2:B:3094:GLU:C	2:B:3096:ILE:H	2.06	0.62
2:B:3110:VAL:C	2:B:3112:LYS:H	2.07	0.62
2:B:2404:PRO:HD3	2:B:2503:LEU:CD1	2.29	0.62
2:B:2747:CYS:SG	2:B:2937:TYR:HE1	2.21	0.62
1:A:16:ASP:OD2	1:A:57:ARG:NH2	2.32	0.62
2:B:3100:TYR:O	2:B:3102:GLU:N	2.33	0.62
2:D:2520:SER:OG	2:D:2524:LYS:HB2	1.99	0.62
2:B:2437:PRO:HG2	2:B:2442:LEU:HD11	1.82	0.62
2:D:2503:LEU:HD13	2:D:2503:LEU:O	1.99	0.62
2:D:2939:LEU:O	2:D:2939:LEU:HG	1.98	0.62
2:B:3037:LEU:O	2:B:3039:GLU:N	2.29	0.62
2:B:3097:ASP:C	2:B:3099:PHE:H	2.07	0.62
2:D:2751:ILE:HG23	2:D:2751:ILE:O	1.99	0.62
2:B:2414:LEU:CD2	2:B:2506:GLY:HA2	2.29	0.62
1:C:43:TRP:C	1:C:45:ASP:H	2.07	0.62
1:A:56:LEU:O	1:A:57:ARG:CB	2.48	0.62
2:B:2973:LEU:C	2:B:2975:GLN:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:O	1:C:57:ARG:CB	2.48	0.62
2:D:2902:ARG:HB2	2:D:2902:ARG:NH1	2.14	0.62
2:D:2915:LEU:HD12	2:D:2916:SER:N	2.14	0.62
2:B:2745:VAL:HG12	2:B:2746:GLY:N	2.15	0.62
2:D:2500:LYS:HD3	2:D:2503:LEU:HD12	1.81	0.62
2:D:2973:LEU:C	2:D:2975:GLN:H	2.06	0.62
2:D:2995:PRO:HD2	2:D:3054:TRP:CZ3	2.35	0.62
2:B:2425:ILE:HG23	2:B:2542:PRO:HG2	1.82	0.61
2:B:2614:LYS:CG	2:B:2615:THR:N	2.62	0.61
2:D:2972:THR:O	2:D:2975:GLN:HB3	2.00	0.61
2:D:2987:LYS:C	2:D:2989:SER:H	2.08	0.61
2:B:2693:ASP:O	2:B:2694:ALA:HB3	2.00	0.61
2:B:2936:ILE:CG2	2:B:2939:LEU:HB2	2.30	0.61
2:D:2944:SER:HB3	2:D:2952:SER:O	1.99	0.61
2:D:2475:VAL:HG12	2:D:2480:ILE:HG13	1.82	0.61
2:B:2468:LYS:C	2:B:2470:LEU:H	2.09	0.61
2:B:2537:THR:HG23	2:B:2538:PRO:HD2	1.82	0.61
2:B:2552:ASN:ND2	2:B:2556:TRP:NE1	2.46	0.61
2:D:2667:LEU:HD23	2:D:2667:LEU:C	2.25	0.61
2:D:2755:VAL:HG13	2:D:2899:TRP:HE1	1.64	0.61
2:B:2936:ILE:HG22	2:B:2939:LEU:HB2	1.80	0.61
2:B:3116:PRO:O	2:B:3117:LYS:CG	2.48	0.61
2:B:2763:LYS:HB2	2:B:2894:ASP:OD2	2.00	0.61
2:B:3002:VAL:CG2	2:B:3049:ALA:HB3	2.31	0.61
2:D:2404:PRO:HD3	2:D:2503:LEU:HD12	1.82	0.61
2:D:2893:ARG:O	2:D:2894:ASP:HB3	2.01	0.61
2:D:2985:PHE:CE2	2:D:3029:LEU:HD13	2.36	0.61
2:B:3026:LEU:HD21	2:B:3104:GLU:HA	1.81	0.61
2:D:2714:ARG:NH2	2:D:2733:LEU:HD12	2.16	0.61
1:A:43:TRP:C	1:A:45:ASP:H	2.08	0.61
2:B:2751:ILE:HG22	2:B:2904:THR:O	2.00	0.61
2:D:2407:ASN:O	2:D:2411:MET:HG3	2.01	0.61
2:D:2984:PRO:HG2	2:D:2987:LYS:CG	2.30	0.61
2:B:2972:THR:O	2:B:2975:GLN:HB3	2.00	0.61
2:B:2984:PRO:HG2	2:B:2987:LYS:HG2	1.82	0.61
1:C:62:LYS:HE3	2:D:2676:THR:HG21	1.81	0.61
2:D:2430:ARG:HH11	2:D:2430:ARG:CG	2.04	0.61
2:D:2997:CYS:O	2:D:2999:GLU:HG3	2.01	0.61
2:D:3061:ARG:HG2	2:D:3061:ARG:HH11	1.65	0.61
2:B:2406:PHE:O	2:B:2408:LYS:N	2.34	0.61
2:B:2714:ARG:HG3	2:B:2715:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2428:LYS:C	2:D:2430:ARG:H	2.08	0.61
2:D:2468:LYS:C	2:D:2470:LEU:H	2.09	0.61
2:D:2501:GLU:C	2:D:2503:LEU:N	2.58	0.61
2:D:3100:TYR:O	2:D:3102:GLU:N	2.34	0.60
2:B:2601:ALA:O	2:B:2605:ILE:HG12	2.00	0.60
2:D:2565:GLU:HG2	2:D:2572:PHE:O	2.01	0.60
2:B:2732:PRO:HB3	2:B:2747:CYS:SG	2.42	0.60
2:B:2747:CYS:SG	2:B:2937:TYR:CE1	2.94	0.60
2:D:2719:HIS:CG	2:D:2720:SER:H	2.20	0.60
2:D:2982:LEU:O	2:D:2984:PRO:HD3	2.00	0.60
2:B:2995:PRO:HD2	2:B:3054:TRP:CZ3	2.37	0.60
1:C:49:GLU:C	1:C:53:SER:OG	2.45	0.60
2:D:2614:LYS:HG2	2:D:2615:THR:N	2.16	0.60
2:D:2750:VAL:HG12	2:D:2751:ILE:N	2.15	0.60
2:D:3015:LEU:O	2:D:3016:ALA:HB3	2.01	0.60
2:B:2501:GLU:C	2:B:2503:LEU:N	2.59	0.60
2:B:2457:VAL:HG11	2:B:2568:PHE:CE2	2.37	0.60
2:B:2500:LYS:HD3	2:B:2503:LEU:HD12	1.83	0.60
2:B:2756:TYR:HD2	2:B:3070:PHE:HB3	1.65	0.60
2:D:2410:LEU:O	2:D:2414:LEU:HG	2.02	0.60
2:B:2717:ARG:HH11	2:B:2717:ARG:HG2	1.65	0.60
2:B:2945:LYS:HD2	2:B:2945:LYS:C	2.26	0.60
2:D:2754:ARG:HA	2:D:2930:GLU:OE2	2.01	0.60
2:B:2484:SER:HB2	2:B:2559:TRP:CE2	2.37	0.60
2:B:2751:ILE:HG23	2:B:2751:ILE:O	2.01	0.60
2:B:2953:ILE:HG13	2:B:2954:GLN:N	2.13	0.60
2:B:3055:ARG:O	2:B:3057:GLU:HG2	2.01	0.60
2:D:2494:ILE:HG22	2:D:2498:PHE:CE1	2.36	0.60
2:D:2526:GLY:H	2:D:2529:GLU:HB2	1.65	0.60
2:D:2655:TRP:C	2:D:2656:TYR:CD1	2.79	0.60
2:D:2693:ASP:O	2:D:2694:ALA:HB3	2.00	0.60
2:D:2589:ARG:HG2	2:D:2655:TRP:CZ3	2.36	0.60
2:D:2917:ILE:CG2	2:D:2920:PRO:HG3	2.32	0.60
2:D:3001:ASP:OD1	2:D:3050:SER:HA	2.02	0.60
2:B:2421:GLN:HE21	2:B:2536:ASP:CG	2.10	0.59
2:B:2503:LEU:HD13	2:B:2503:LEU:O	2.00	0.59
2:B:2564:MET:HE2	2:B:2572:PHE:CE2	2.37	0.59
2:B:3087:THR:HG22	2:B:3088:ASN:N	2.16	0.59
2:D:2580:GLU:O	2:D:2584:LEU:HB2	2.02	0.59
2:D:2761:VAL:HG13	2:D:2761:VAL:O	2.01	0.59
2:D:3097:ASP:C	2:D:3099:PHE:H	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2414:LEU:HD23	2:B:2506:GLY:CA	2.29	0.59
2:B:2614:LYS:HG2	2:B:2615:THR:N	2.17	0.59
2:B:2744:ASN:HB2	2:B:2940:SER:HB2	1.84	0.59
1:C:56:LEU:O	1:C:57:ARG:HB2	2.01	0.59
2:D:3005:VAL:HG22	2:D:3046:LEU:HD11	1.83	0.59
2:B:2534:LEU:O	2:B:2537:THR:HB	2.02	0.59
2:B:2602:LEU:HB2	2:B:2653:ASP:OD2	2.02	0.59
2:D:2500:LYS:HA	2:D:2503:LEU:HB3	1.84	0.59
1:A:43:TRP:CH2	2:B:2666:LEU:HD21	2.37	0.59
2:B:2592:VAL:HG12	2:B:2593:GLU:N	2.18	0.59
2:D:2754:ARG:HB2	2:D:2756:TYR:CE1	2.38	0.59
2:D:2949:GLU:HB3	2:D:2951:PRO:HD2	1.85	0.59
2:B:2494:ILE:HD11	2:B:2523:GLY:C	2.28	0.59
2:D:2945:LYS:HD2	2:D:2945:LYS:C	2.27	0.59
2:B:3031:VAL:HA	2:B:3065:LEU:O	2.03	0.59
1:A:48:VAL:C	1:A:49:GLU:HG3	2.28	0.59
2:B:2949:GLU:HB3	2:B:2951:PRO:HD2	1.85	0.59
2:B:2997:CYS:O	2:B:2999:GLU:HG3	2.03	0.59
2:B:3015:LEU:O	2:B:3016:ALA:HB3	2.02	0.59
1:C:51:ASP:HB3	2:D:2717:ARG:HG3	1.84	0.59
2:B:2756:TYR:HB3	2:B:2757:PRO:HD2	1.84	0.59
2:D:2738:LEU:CD1	2:D:2745:VAL:HG21	2.33	0.59
2:B:3028:LEU:HD12	2:B:3111:LEU:CD2	2.32	0.58
2:D:2984:PRO:HG2	2:D:2987:LYS:HG2	1.84	0.58
2:D:2933:ARG:NH1	2:D:2966:LEU:HB3	2.18	0.58
1:C:48:VAL:C	1:C:49:GLU:HG3	2.28	0.58
2:D:2756:TYR:N	2:D:2756:TYR:CD1	2.70	0.58
2:D:3005:VAL:HG23	2:D:3089:MET:HE3	1.86	0.58
2:B:2404:PRO:HD3	2:B:2503:LEU:HD12	1.84	0.58
2:B:2414:LEU:O	2:B:2416:ASN:N	2.36	0.58
2:B:2933:ARG:NH1	2:B:2966:LEU:HB3	2.18	0.58
2:D:2428:LYS:O	2:D:2430:ARG:N	2.36	0.58
2:D:2494:ILE:HD12	2:D:2494:ILE:N	2.18	0.58
2:D:2602:LEU:HB2	2:D:2653:ASP:OD2	2.03	0.58
2:D:2616:LEU:HD13	2:D:2724:PHE:CD2	2.38	0.58
2:B:2506:GLY:O	2:B:2507:LYS:C	2.47	0.58
2:B:2565:GLU:CD	2:B:2574:ASN:HA	2.27	0.58
2:B:2720:SER:OG	2:B:2721:LYS:N	2.36	0.58
2:D:3023:ASP:OD1	2:D:3027:HIS:HB2	2.04	0.58
2:B:3001:ASP:OD1	2:B:3050:SER:HA	2.02	0.58
1:C:37:HIS:O	1:C:38:VAL:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3089:MET:C	2:D:3091:HIS:N	2.61	0.58
2:D:2927:LEU:HD11	2:D:2934:TYR:HE1	1.67	0.58
2:D:3002:VAL:CG2	2:D:3049:ALA:HB3	2.33	0.58
2:B:2500:LYS:HA	2:B:2503:LEU:HB3	1.84	0.58
1:C:15:GLU:HB2	1:C:18:GLU:HG3	1.85	0.58
2:D:3055:ARG:HG2	2:D:3056:PRO:HD2	1.86	0.58
1:A:56:LEU:C	1:A:56:LEU:HD23	2.28	0.58
2:B:2616:LEU:HD13	2:B:2724:PHE:HD2	1.68	0.58
2:B:2667:LEU:O	2:B:2667:LEU:HD23	2.04	0.58
2:D:2512:ALA:HB1	2:D:2584:LEU:HG	1.86	0.58
2:B:2483:ASN:ND2	2:B:2486:ASN:HD22	2.02	0.58
2:B:3089:MET:C	2:B:3091:HIS:N	2.60	0.58
1:A:56:LEU:O	1:A:57:ARG:HB2	2.04	0.57
2:B:2418:ARG:O	2:B:2421:GLN:N	2.37	0.57
2:B:2756:TYR:N	2:B:2756:TYR:CD1	2.72	0.57
2:B:3090:LYS:O	2:B:3094:GLU:HG3	2.04	0.57
1:C:16:ASP:OD2	1:C:57:ARG:NH2	2.37	0.57
2:D:2479:CYS:C	2:D:2481:SER:H	2.12	0.57
2:D:2717:ARG:HH11	2:D:2717:ARG:HG2	1.68	0.57
2:D:2732:PRO:HB3	2:D:2747:CYS:SG	2.44	0.57
2:D:2908:LYS:O	2:D:2909:ARG:C	2.47	0.57
2:B:2512:ALA:O	2:B:2513:ASP:HB2	2.04	0.57
2:B:2754:ARG:HB2	2:B:2756:TYR:CE1	2.38	0.57
2:B:2982:LEU:O	2:B:2984:PRO:HD3	2.04	0.57
2:D:2506:GLY:O	2:D:2507:LYS:C	2.47	0.57
2:D:2720:SER:OG	2:D:2721:LYS:N	2.37	0.57
1:A:56:LEU:HD23	1:A:57:ARG:HB2	1.86	0.57
2:B:2664:PRO:HB2	2:B:2741:ASP:OD2	2.04	0.57
2:B:2719:HIS:CG	2:B:2720:SER:H	2.21	0.57
2:B:2939:LEU:HD11	2:B:2955:LEU:HB3	1.85	0.57
2:B:2987:LYS:C	2:B:2989:SER:H	2.12	0.57
2:B:3005:VAL:HG23	2:B:3089:MET:HE3	1.86	0.57
2:D:3007:VAL:HB	2:D:3104:GLU:OE2	2.03	0.57
2:B:2479:CYS:SG	2:B:2480:ILE:N	2.78	0.57
1:C:21:GLU:HG3	1:C:22:PHE:CD2	2.39	0.57
2:D:2465:CYS:SG	2:D:2466:SER:N	2.76	0.57
2:D:2763:LYS:HB2	2:D:2894:ASP:OD2	2.04	0.57
1:A:19:PHE:CD1	1:A:19:PHE:C	2.83	0.57
2:D:2537:THR:HG23	2:D:2538:PRO:HD2	1.86	0.57
2:D:2665:PRO:HG3	2:D:2742:GLY:CA	2.29	0.57
2:D:2953:ILE:CG1	2:D:2954:GLN:H	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2489:TYR:O	2:D:2490:PHE:HB3	2.04	0.57
2:B:2428:LYS:C	2:B:2430:ARG:H	2.13	0.57
2:B:2750:VAL:HG12	2:B:2751:ILE:N	2.18	0.57
2:B:3018:LEU:HD21	2:B:3032:LYS:HG2	1.86	0.57
2:B:3055:ARG:HG2	2:B:3056:PRO:HD2	1.86	0.57
2:D:2745:VAL:HG12	2:D:2746:GLY:N	2.20	0.57
2:D:3090:LYS:O	2:D:3094:GLU:HG3	2.04	0.57
1:A:8:VAL:O	1:A:10:LEU:N	2.38	0.57
2:B:2469:GLN:O	2:B:2472:MET:HB3	2.05	0.57
2:B:2665:PRO:HG3	2:B:2742:GLY:CA	2.31	0.57
2:B:2978:GLN:HG2	2:B:2996:PRO:CG	2.34	0.57
1:C:49:GLU:C	1:C:53:SER:HG	2.13	0.57
1:C:38:VAL:O	1:C:38:VAL:HG22	2.03	0.57
2:B:2565:GLU:HG2	2:B:2572:PHE:O	2.05	0.56
2:B:2944:SER:HB3	2:B:2952:SER:O	2.05	0.56
2:B:2953:ILE:CG1	2:B:2954:GLN:H	2.17	0.56
2:D:2906:TYR:CD1	2:D:2933:ARG:NE	2.72	0.56
2:B:2624:ILE:CD1	2:B:2659:LYS:HE3	2.35	0.56
2:D:2414:LEU:HD23	2:D:2506:GLY:CA	2.31	0.56
2:D:2483:ASN:ND2	2:D:2486:ASN:HD22	2.04	0.56
2:B:2655:TRP:C	2:B:2656:TYR:CD1	2.83	0.56
2:B:2945:LYS:HD2	2:B:2945:LYS:O	2.05	0.56
2:D:2552:ASN:ND2	2:D:2556:TRP:NE1	2.47	0.56
1:A:49:GLU:C	1:A:53:SER:OG	2.48	0.56
1:A:21:GLU:HG3	1:A:22:PHE:CD2	2.41	0.56
1:A:15:GLU:HB2	1:A:18:GLU:HG3	1.87	0.56
2:D:2945:LYS:HD2	2:D:2945:LYS:O	2.05	0.56
2:B:2761:VAL:HG13	2:B:2761:VAL:O	2.05	0.56
1:A:18:GLU:OE1	2:B:2450:ARG:NH2	2.39	0.56
2:B:2479:CYS:C	2:B:2481:SER:H	2.13	0.56
2:B:2541:ASP:OD1	2:B:2541:ASP:C	2.49	0.56
1:C:19:PHE:CD1	1:C:19:PHE:C	2.82	0.56
2:D:2494:ILE:O	2:D:2498:PHE:HD1	1.89	0.56
2:B:2745:VAL:HB	2:B:2940:SER:OG	2.06	0.56
2:D:2564:MET:HE2	2:D:2572:PHE:CE2	2.41	0.56
2:D:2761:VAL:HG12	2:D:2896:SER:O	2.06	0.56
2:D:2937:TYR:O	2:D:2961:THR:HA	2.06	0.56
2:B:2666:LEU:HA	2:B:2669:LEU:HD12	1.87	0.55
2:B:2693:ASP:O	2:B:2694:ALA:CB	2.54	0.55
2:B:2745:VAL:CG1	2:B:2746:GLY:N	2.69	0.55
2:D:2744:ASN:HB2	2:D:2940:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3026:LEU:HD21	2:D:3104:GLU:HA	1.88	0.55
2:B:2782:LEU:C	2:B:2784:PHE:N	2.63	0.55
2:D:2693:ASP:O	2:D:2694:ALA:CB	2.54	0.55
2:D:2745:VAL:HB	2:D:2940:SER:OG	2.06	0.55
2:D:3089:MET:C	2:D:3091:HIS:H	2.14	0.55
2:B:2729:ARG:HD3	2:B:2730:PRO:HD2	1.89	0.55
2:B:3018:LEU:CD2	2:B:3032:LYS:HG2	2.36	0.55
2:B:2937:TYR:O	2:B:2961:THR:HA	2.07	0.55
2:D:2783:ARG:HG3	2:D:2783:ARG:HH11	1.71	0.55
2:D:3058:SER:C	2:D:3060:SER:H	2.13	0.55
2:B:2667:LEU:HD23	2:B:2667:LEU:C	2.32	0.55
2:B:2494:ILE:HD12	2:B:2494:ILE:N	2.22	0.55
2:B:2669:LEU:O	2:B:2674:ARG:HB2	2.06	0.55
2:B:2758:LEU:HD22	2:B:2760:TRP:CZ3	2.42	0.55
2:B:3007:VAL:HB	2:B:3104:GLU:OE2	2.06	0.55
1:C:56:LEU:C	1:C:56:LEU:HD23	2.31	0.55
2:D:2939:LEU:HD11	2:D:2955:LEU:HB3	1.87	0.55
2:B:2600:SER:O	2:B:2603:LYS:HB3	2.06	0.55
2:B:2755:VAL:HG13	2:B:2899:TRP:HE1	1.70	0.55
2:B:3023:ASP:OD1	2:B:3027:HIS:HB2	2.06	0.55
2:B:3093:ILE:HG23	2:B:3094:GLU:N	2.20	0.55
2:D:2441:TYR:CZ	2:D:2596:ASN:ND2	2.75	0.55
2:D:2751:ILE:HG22	2:D:2904:THR:O	2.07	0.55
1:C:48:VAL:HG23	1:C:49:GLU:HG3	1.88	0.55
2:D:2469:GLN:O	2:D:2472:MET:HB3	2.06	0.55
2:D:2479:CYS:SG	2:D:2480:ILE:N	2.80	0.55
2:D:2664:PRO:N	2:D:2665:PRO:HD2	2.21	0.55
2:D:2780:GLU:O	2:D:2780:GLU:HG3	2.06	0.55
2:B:2738:LEU:HD13	2:B:2745:VAL:CG2	2.36	0.55
2:D:2669:LEU:HB3	2:D:2674:ARG:HB2	1.89	0.55
2:B:2531:TYR:CD1	2:B:2531:TYR:C	2.83	0.55
2:B:3089:MET:C	2:B:3091:HIS:H	2.13	0.55
2:D:2418:ARG:O	2:D:2421:GLN:N	2.39	0.55
2:D:2915:LEU:HD13	2:D:2939:LEU:HD13	1.88	0.55
2:B:2908:LYS:O	2:B:2909:ARG:C	2.50	0.54
2:D:2782:LEU:C	2:D:2784:PHE:N	2.63	0.54
2:D:3014:GLY:O	2:D:3015:LEU:HG	2.07	0.54
1:A:38:VAL:HG22	1:A:38:VAL:O	2.07	0.54
2:B:2406:PHE:C	2:B:2408:LYS:H	2.15	0.54
2:B:3014:GLY:O	2:B:3015:LEU:HG	2.08	0.54
2:D:2428:LYS:HD3	2:D:2542:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2580:GLU:O	2:B:2584:LEU:HB2	2.07	0.54
2:B:2666:LEU:HD23	2:B:2669:LEU:HD12	1.88	0.54
2:B:2780:GLU:O	2:B:2780:GLU:HG3	2.07	0.54
2:B:3058:SER:C	2:B:3060:SER:H	2.14	0.54
2:B:3107:LEU:HD23	2:B:3107:LEU:C	2.33	0.54
2:D:2419:ASP:O	2:D:2423:ILE:HG13	2.07	0.54
2:D:2755:VAL:CG1	2:D:2899:TRP:HE1	2.21	0.54
2:B:2437:PRO:HA	2:B:2591:ASP:OD1	2.08	0.54
2:B:2537:THR:HG23	2:B:2538:PRO:CD	2.36	0.54
2:D:2997:CYS:O	2:D:2999:GLU:N	2.40	0.54
2:B:2494:ILE:HD11	2:B:2523:GLY:CA	2.37	0.54
2:B:2906:TYR:CD1	2:B:2933:ARG:NE	2.73	0.54
2:D:3018:LEU:CD2	2:D:3032:LYS:HG2	2.37	0.54
2:B:2558:VAL:HG13	2:B:2577:LEU:CD1	2.36	0.54
1:C:22:PHE:O	1:C:23:PRO:C	2.50	0.54
2:D:3107:LEU:HD23	2:D:3107:LEU:C	2.31	0.54
2:B:2666:LEU:HD11	2:B:2708:ILE:HG22	1.90	0.54
2:B:3026:LEU:CD2	2:B:3104:GLU:HA	2.38	0.54
1:C:43:TRP:HZ3	2:D:2713:THR:HG23	1.71	0.54
2:D:2663:ASP:C	2:D:2665:PRO:HD2	2.33	0.54
2:D:2666:LEU:HA	2:D:2669:LEU:HD12	1.90	0.54
2:B:2491:GLN:HA	2:B:2525:ALA:O	2.08	0.54
2:B:2929:THR:O	2:B:2930:GLU:O	2.26	0.54
2:B:3099:PHE:CD2	2:B:3099:PHE:N	2.75	0.54
2:B:2476:SER:C	2:B:2478:ALA:N	2.62	0.54
2:D:2689:VAL:HG21	2:D:2707:LYS:HE3	1.90	0.54
2:B:2516:TRP:HB2	2:B:2536:ASP:OD1	2.08	0.53
2:D:2409:ASP:O	2:D:2413:SER:N	2.34	0.53
2:B:2441:TYR:CZ	2:B:2596:ASN:ND2	2.76	0.53
2:B:2927:LEU:O	2:B:2929:THR:HG23	2.08	0.53
2:D:2476:SER:C	2:D:2478:ALA:N	2.65	0.53
1:A:54:ASN:O	1:A:55:GLN:CB	2.53	0.53
2:B:2406:PHE:C	2:B:2408:LYS:N	2.66	0.53
2:B:2501:GLU:O	2:B:2502:ALA:HB3	2.08	0.53
1:C:19:PHE:C	1:C:19:PHE:HD1	2.15	0.53
2:B:2409:ASP:O	2:B:2412:SER:N	2.40	0.53
2:B:3095:ASN:HD22	2:B:3095:ASN:N	2.05	0.53
2:D:2600:SER:O	2:D:2603:LYS:HB3	2.08	0.53
2:D:2932:GLN:HA	2:D:2932:GLN:OE1	2.08	0.53
2:D:2987:LYS:C	2:D:2989:SER:N	2.64	0.53
1:A:19:PHE:C	1:A:19:PHE:HD1	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG23	1:A:49:GLU:HG3	1.89	0.53
2:B:2589:ARG:HG2	2:B:2655:TRP:CZ3	2.43	0.53
2:B:3116:PRO:O	2:B:3117:LYS:CB	2.57	0.53
2:D:2587:LYS:O	2:D:2590:TYR:HB3	2.08	0.53
2:B:2676:THR:HG23	2:B:2679:GLN:HG3	1.89	0.53
2:B:3015:LEU:O	2:B:3016:ALA:CB	2.56	0.53
1:C:8:VAL:O	1:C:10:LEU:N	2.42	0.53
2:D:2592:VAL:HG12	2:D:2593:GLU:N	2.24	0.53
2:B:2552:ASN:O	2:B:2555:ARG:HB3	2.08	0.53
2:D:2414:LEU:O	2:D:2416:ASN:N	2.42	0.53
2:D:2537:THR:HG23	2:D:2538:PRO:CD	2.38	0.53
2:D:3099:PHE:N	2:D:3099:PHE:CD2	2.74	0.53
2:B:2568:PHE:N	2:B:2569:PRO:HD3	2.24	0.53
2:D:2414:LEU:CD2	2:D:2506:GLY:HA2	2.33	0.53
2:D:2764:THR:HG22	2:D:2765:VAL:N	2.24	0.53
2:D:3015:LEU:O	2:D:3016:ALA:CB	2.56	0.53
1:A:56:LEU:N	2:B:2462:PRO:HG2	2.24	0.53
2:B:2704:LEU:C	2:B:2704:LEU:HD23	2.34	0.53
2:B:2750:VAL:HG13	2:B:2904:THR:C	2.34	0.53
2:B:2772:ARG:HB3	2:B:2776:GLU:HB2	1.91	0.53
2:B:2778:GLU:O	2:B:2781:ALA:HB3	2.09	0.53
2:B:3050:SER:O	2:B:3051:ASN:HB2	2.09	0.53
2:D:2457:VAL:HG11	2:D:2568:PHE:CE2	2.44	0.53
2:D:2928:LEU:HA	2:D:2934:TYR:CZ	2.43	0.53
2:D:3100:TYR:HD1	2:D:3101:LYS:HD2	1.74	0.53
2:B:2531:TYR:CE1	2:B:2535:CYS:SG	3.02	0.53
2:B:2933:ARG:NH1	2:B:2966:LEU:CB	2.72	0.53
2:D:2494:ILE:HD12	2:D:2495:GLU:N	2.22	0.53
2:D:2531:TYR:CD1	2:D:2531:TYR:C	2.85	0.53
2:D:2624:ILE:CD1	2:D:2659:LYS:HE3	2.39	0.53
2:B:2409:ASP:O	2:B:2413:SER:N	2.34	0.52
2:D:3097:ASP:C	2:D:3099:PHE:N	2.66	0.52
2:B:2479:CYS:C	2:B:2481:SER:N	2.65	0.52
2:B:2494:ILE:HD11	2:B:2523:GLY:O	2.09	0.52
2:B:2711:ASN:HD21	2:B:2739:PHE:H	1.56	0.52
2:D:2503:LEU:HD13	2:D:2503:LEU:C	2.35	0.52
2:D:3028:LEU:HD12	2:D:3111:LEU:CD2	2.39	0.52
2:B:2475:VAL:O	2:B:2476:SER:C	2.53	0.52
2:B:2483:ASN:OD1	2:B:2485:LYS:N	2.42	0.52
2:B:2568:PHE:O	2:B:2570:LYS:N	2.42	0.52
2:B:2772:ARG:NH2	2:B:2780:GLU:HG2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2915:LEU:HD13	2:B:2939:LEU:CD1	2.39	0.52
2:D:2541:ASP:OD1	2:D:2541:ASP:C	2.51	0.52
2:B:2424:ARG:NH1	2:B:2536:ASP:OD1	2.42	0.52
2:B:2426:LYS:HG3	2:B:2430:ARG:NH2	2.19	0.52
2:B:2755:VAL:CG1	2:B:2899:TRP:HE1	2.22	0.52
2:B:2764:THR:HG22	2:B:2765:VAL:N	2.24	0.52
2:D:2656:TYR:CD2	2:D:2697:PRO:CB	2.90	0.52
2:D:2973:LEU:C	2:D:2975:GLN:N	2.67	0.52
2:B:2503:LEU:HD13	2:B:2503:LEU:C	2.34	0.52
2:B:2616:LEU:HD11	2:B:2724:PHE:CE2	2.44	0.52
2:D:2606:LEU:CD1	2:D:2704:LEU:HD11	2.39	0.52
2:D:3091:HIS:O	2:D:3093:ILE:N	2.43	0.52
2:D:3093:ILE:HG23	2:D:3094:GLU:N	2.25	0.52
1:A:39:TRP:HA	1:A:39:TRP:CE3	2.45	0.52
2:B:2608:ARG:NH2	2:B:2688:LEU:HD23	2.16	0.52
2:B:2783:ARG:HG3	2:B:2783:ARG:HH11	1.75	0.52
2:B:2915:LEU:HD13	2:B:2939:LEU:HD13	1.90	0.52
2:B:2973:LEU:C	2:B:2975:GLN:N	2.68	0.52
1:C:59:GLU:OE1	2:D:2464:ALA:N	2.43	0.52
2:D:2426:LYS:HG3	2:D:2430:ARG:NH2	2.18	0.52
2:D:2758:LEU:HD22	2:D:2760:TRP:CZ3	2.43	0.52
2:D:2494:ILE:HD11	2:D:2523:GLY:C	2.34	0.52
2:D:2763:LYS:HG2	2:D:2769:TYR:HD2	1.73	0.52
2:D:2778:GLU:O	2:D:2781:ALA:HB3	2.10	0.52
2:B:2754:ARG:HA	2:B:2930:GLU:OE2	2.09	0.52
2:B:2983:LEU:HD11	2:B:2988:LEU:HG	1.92	0.52
2:D:2648:THR:HG21	2:D:2705:ARG:HH12	1.75	0.52
2:D:2669:LEU:O	2:D:2674:ARG:HB2	2.10	0.52
2:D:3109:GLN:NE2	2:D:3109:GLN:C	2.67	0.52
2:B:2412:SER:O	2:B:2413:SER:C	2.51	0.52
2:B:2717:ARG:HG2	2:B:2717:ARG:NH1	2.25	0.52
2:B:2969:SER:O	2:B:2970:SER:C	2.52	0.52
2:B:3030:VAL:HG12	2:B:3031:VAL:N	2.24	0.52
2:B:3097:ASP:C	2:B:3099:PHE:N	2.64	0.52
2:D:2665:PRO:CG	2:D:2742:GLY:HA2	2.30	0.52
2:D:2898:VAL:HG22	2:D:2918:TRP:CZ3	2.44	0.52
2:D:2941:VAL:HG12	2:D:2943:LYS:HG3	1.92	0.52
2:D:2969:SER:O	2:D:2970:SER:C	2.53	0.52
2:D:2624:ILE:HG22	2:D:2647:ASP:HB3	1.92	0.52
2:D:2927:LEU:O	2:D:2934:TYR:OH	2.28	0.52
2:B:2666:LEU:O	2:B:2669:LEU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2494:ILE:HD11	2:D:2523:GLY:CA	2.39	0.51
2:D:2516:TRP:HB2	2:D:2536:ASP:OD1	2.10	0.51
2:D:2676:THR:HG23	2:D:2679:GLN:HG3	1.92	0.51
2:D:2915:LEU:HD13	2:D:2939:LEU:CD1	2.39	0.51
2:D:2483:ASN:OD1	2:D:2485:LYS:N	2.43	0.51
2:D:2487:ALA:C	2:D:2489:TYR:H	2.19	0.51
2:B:2465:CYS:SG	2:B:2466:SER:N	2.79	0.51
2:B:2749:ASP:OD1	2:B:2933:ARG:NH2	2.43	0.51
1:C:54:ASN:O	1:C:55:GLN:CB	2.54	0.51
2:D:3018:LEU:HD21	2:D:3032:LYS:HG2	1.93	0.51
2:B:2664:PRO:N	2:B:2665:PRO:HD2	2.24	0.51
1:C:43:TRP:CH2	2:D:2666:LEU:HD21	2.45	0.51
2:D:2437:PRO:CG	2:D:2442:LEU:HD11	2.36	0.51
2:D:3093:ILE:HD11	2:D:3100:TYR:CE1	2.46	0.51
2:B:2421:GLN:NE2	2:B:2536:ASP:OD1	2.37	0.51
2:B:2624:ILE:CG2	2:B:2626:LEU:HG	2.40	0.51
2:B:2763:LYS:HG2	2:B:2769:TYR:HD2	1.75	0.51
2:B:3109:GLN:NE2	2:B:3110:VAL:HG12	2.25	0.51
2:D:2685:GLY:H	2:D:2712:SER:HB3	1.74	0.51
2:D:3010:VAL:C	2:D:3012:PRO:HD3	2.36	0.51
2:B:2772:ARG:HB3	2:B:2776:GLU:CB	2.41	0.51
1:C:62:LYS:O	1:C:63:HIS:C	2.54	0.51
2:D:3060:SER:C	2:D:3062:VAL:N	2.67	0.51
2:D:3116:PRO:O	2:D:3117:LYS:HB2	2.09	0.51
2:B:2622:ASP:OD2	2:B:2623:ILE:N	2.44	0.51
2:D:2552:ASN:O	2:D:2555:ARG:HB3	2.10	0.51
2:D:2614:LYS:HG2	2:D:2615:THR:H	1.75	0.51
2:D:2901:LEU:HD11	2:D:2928:LEU:HD13	1.93	0.51
2:D:3095:ASN:HD22	2:D:3095:ASN:N	2.08	0.51
1:A:37:HIS:O	1:A:38:VAL:HG12	2.09	0.51
2:B:2494:ILE:O	2:B:2498:PHE:HD1	1.94	0.51
2:D:2763:LYS:HG2	2:D:2769:TYR:CD2	2.45	0.51
2:D:3058:SER:O	2:D:3059:THR:CB	2.58	0.51
2:B:2414:LEU:C	2:B:2416:ASN:N	2.68	0.51
2:B:2735:LEU:HD13	2:B:2748:VAL:HG11	1.93	0.51
1:C:12:LEU:O	2:D:2450:ARG:NH1	2.44	0.51
2:D:2404:PRO:HD3	2:D:2500:LYS:HE2	1.91	0.51
2:D:2412:SER:O	2:D:2413:SER:C	2.53	0.51
2:D:2568:PHE:N	2:D:2569:PRO:HD3	2.25	0.51
2:B:2441:TYR:O	2:B:2441:TYR:CD2	2.63	0.51
2:B:2978:GLN:CG	2:B:2996:PRO:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3007:VAL:O	2:B:3008:SER:HB3	2.10	0.51
2:B:3019:VAL:HG12	2:B:3021:LEU:HD21	1.93	0.51
2:D:2437:PRO:HA	2:D:2591:ASP:OD1	2.10	0.51
2:D:2465:CYS:O	2:D:2466:SER:CB	2.59	0.51
2:D:2479:CYS:C	2:D:2481:SER:N	2.65	0.51
2:D:2987:LYS:O	2:D:2989:SER:N	2.44	0.51
2:D:2898:VAL:HG22	2:D:2918:TRP:CE3	2.46	0.50
2:D:2933:ARG:NH1	2:D:2966:LEU:CB	2.74	0.50
2:D:3050:SER:O	2:D:3051:ASN:HB2	2.11	0.50
2:B:2937:TYR:C	2:B:2939:LEU:N	2.67	0.50
2:B:2984:PRO:HG2	2:B:2987:LYS:HG3	1.92	0.50
2:B:3081:HIS:CD2	2:B:3082:PHE:HD1	2.28	0.50
2:B:3109:GLN:NE2	2:B:3109:GLN:C	2.69	0.50
2:D:2548:VAL:O	2:D:2551:SER:HB2	2.12	0.50
2:D:2733:LEU:N	2:D:2733:LEU:CD2	2.74	0.50
2:D:3043:PRO:O	2:D:3044:ARG:HB2	2.10	0.50
2:B:2414:LEU:O	2:B:2417:ALA:N	2.44	0.50
2:B:2465:CYS:O	2:B:2466:SER:CB	2.59	0.50
2:B:2602:LEU:O	2:B:2606:LEU:HB2	2.11	0.50
2:B:2620:VAL:HG22	2:B:2679:GLN:O	2.11	0.50
2:B:2663:ASP:C	2:B:2665:PRO:HD2	2.35	0.50
2:D:2408:LYS:O	2:D:2409:ASP:HB2	2.10	0.50
2:D:2491:GLN:HA	2:D:2525:ALA:O	2.11	0.50
2:D:2616:LEU:HD11	2:D:2724:PHE:CE2	2.47	0.50
2:B:2900:LYS:C	2:B:2901:LEU:HD23	2.37	0.50
2:B:3005:VAL:HG22	2:B:3046:LEU:CD1	2.39	0.50
2:B:3021:LEU:HB2	2:B:3029:LEU:HD22	1.92	0.50
2:D:2407:ASN:C	2:D:2411:MET:HG3	2.36	0.50
2:D:2501:GLU:O	2:D:2503:LEU:N	2.41	0.50
2:D:2531:TYR:CE1	2:D:2535:CYS:SG	3.05	0.50
2:D:3057:GLU:OE2	2:D:3064:THR:HB	2.11	0.50
1:A:13:LEU:HD11	2:B:2453:LEU:HA	1.94	0.50
2:B:2761:VAL:HG12	2:B:2896:SER:O	2.11	0.50
2:B:2777:GLU:O	2:B:2781:ALA:N	2.44	0.50
2:B:3010:VAL:C	2:B:3012:PRO:HD3	2.36	0.50
2:D:2589:ARG:O	2:D:2593:GLU:HB3	2.12	0.50
2:D:2704:LEU:O	2:D:2705:ARG:HD3	2.12	0.50
2:B:2704:LEU:HD23	2:B:2704:LEU:O	2.11	0.50
2:D:2738:LEU:HD13	2:D:2745:VAL:CG2	2.42	0.50
1:A:46:ASP:CG	2:B:2674:ARG:HH12	2.20	0.50
2:B:2955:LEU:CD1	2:B:2955:LEU:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2414:LEU:O	2:D:2417:ALA:N	2.44	0.50
2:D:2421:GLN:NE2	2:D:2536:ASP:OD1	2.39	0.50
2:D:2927:LEU:O	2:D:2929:THR:HG23	2.11	0.50
2:D:3019:VAL:HG12	2:D:3021:LEU:HD21	1.94	0.50
2:B:2419:ASP:O	2:B:2423:ILE:HG13	2.12	0.50
2:B:2616:LEU:CD1	2:B:2724:PHE:CD2	2.94	0.50
2:B:2667:LEU:CD2	2:B:2671:LYS:HD3	2.41	0.50
1:C:46:ASP:CG	2:D:2674:ARG:HH12	2.20	0.50
2:D:2427:ASN:O	2:D:2428:LYS:C	2.54	0.50
2:D:2602:LEU:O	2:D:2606:LEU:HB2	2.12	0.50
2:D:3111:LEU:C	2:D:3112:LYS:HD3	2.36	0.50
1:A:61:GLU:C	1:A:63:HIS:H	2.19	0.50
2:D:2622:ASP:OD2	2:D:2623:ILE:N	2.45	0.50
2:D:2745:VAL:CG1	2:D:2746:GLY:N	2.75	0.50
2:D:2900:LYS:C	2:D:2901:LEU:HD23	2.36	0.50
2:B:2428:LYS:O	2:B:2430:ARG:N	2.45	0.49
2:D:2447:THR:HG22	2:D:2448:LEU:N	2.27	0.49
2:D:2667:LEU:CD2	2:D:2671:LYS:HD3	2.42	0.49
2:D:2676:THR:HG22	2:D:2679:GLN:CD	2.36	0.49
2:D:2704:LEU:O	2:D:2704:LEU:HD23	2.12	0.49
2:D:3081:HIS:CD2	2:D:3082:PHE:HD1	2.30	0.49
1:A:39:TRP:HA	1:A:39:TRP:HE3	1.77	0.49
2:B:2606:LEU:CD1	2:B:2704:LEU:HD11	2.41	0.49
2:B:2745:VAL:N	2:B:2940:SER:OG	2.45	0.49
2:D:2572:PHE:O	2:D:2573:ALA:C	2.55	0.49
2:B:2754:ARG:HB2	2:B:2756:TYR:HE1	1.77	0.49
2:D:2955:LEU:N	2:D:2955:LEU:CD1	2.74	0.49
2:B:2548:VAL:O	2:B:2551:SER:HB2	2.12	0.49
2:B:2666:LEU:O	2:B:2667:LEU:C	2.55	0.49
2:B:2585:GLN:O	2:B:2588:TYR:HB3	2.13	0.49
2:B:2941:VAL:HG12	2:B:2943:LYS:HG3	1.95	0.49
2:B:3102:GLU:OE1	2:B:3102:GLU:HA	2.13	0.49
2:D:2406:PHE:O	2:D:2411:MET:HG2	2.13	0.49
2:D:2419:ASP:HA	2:D:2422:ASP:HB2	1.94	0.49
2:D:2936:ILE:HG21	2:D:2939:LEU:HD22	1.94	0.49
2:D:3026:LEU:CD2	2:D:3104:GLU:HA	2.43	0.49
2:B:2408:LYS:O	2:B:2409:ASP:HB2	2.13	0.49
2:B:2501:GLU:O	2:B:2503:LEU:N	2.45	0.49
2:B:2676:THR:HG22	2:B:2679:GLN:CD	2.37	0.49
2:B:3111:LEU:C	2:B:3112:LYS:HD3	2.37	0.49
1:C:39:TRP:NE1	2:D:2733:LEU:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2421:GLN:HE21	2:D:2536:ASP:CG	2.21	0.49
2:D:2439:SER:HB3	2:D:2584:LEU:HD21	1.94	0.49
2:D:2773:ASN:N	2:D:2776:GLU:HB2	2.13	0.49
2:B:2730:PRO:HB2	2:B:2747:CYS:HB2	1.94	0.49
2:B:3043:PRO:O	2:B:3044:ARG:HB2	2.12	0.49
1:C:39:TRP:HA	1:C:39:TRP:CE3	2.47	0.49
2:D:2489:TYR:O	2:D:2491:GLN:N	2.45	0.49
2:D:2555:ARG:CZ	2:D:2556:TRP:CH2	2.95	0.49
2:D:2616:LEU:HD13	2:D:2724:PHE:HD2	1.74	0.49
2:D:2953:ILE:O	2:D:2954:GLN:HB2	2.12	0.49
1:C:37:HIS:ND1	1:C:38:VAL:HG12	2.27	0.49
2:D:2726:HIS:ND1	2:D:2726:HIS:N	2.61	0.49
2:D:3035:ILE:HG23	2:D:3068:GLY:O	2.12	0.49
2:D:2772:ARG:NH2	2:D:2780:GLU:HG2	2.27	0.49
2:B:2985:PHE:CE2	2:B:3029:LEU:HD13	2.48	0.49
2:D:2552:ASN:ND2	2:D:2552:ASN:C	2.69	0.49
2:D:2777:GLU:O	2:D:2781:ALA:N	2.46	0.49
2:D:3004:GLY:HA2	2:D:3089:MET:HE1	1.95	0.49
2:D:3030:VAL:HG12	2:D:3031:VAL:N	2.27	0.49
2:B:2763:LYS:HG2	2:B:2769:TYR:CD2	2.49	0.48
2:B:3057:GLU:OE2	2:B:3064:THR:HB	2.13	0.48
2:D:2754:ARG:HB2	2:D:2756:TYR:HE1	1.78	0.48
2:D:2919:ARG:N	2:D:2920:PRO:CD	2.76	0.48
2:D:3102:GLU:OE1	2:D:3102:GLU:HA	2.13	0.48
1:C:39:TRP:HZ3	2:D:2682:ILE:HB	1.77	0.48
2:D:2501:GLU:O	2:D:2502:ALA:HB3	2.13	0.48
2:B:2458:GLY:O	2:B:2459:ASP:HB2	2.14	0.48
2:B:2476:SER:C	2:B:2478:ALA:H	2.21	0.48
2:D:2664:PRO:HB2	2:D:2741:ASP:OD2	2.13	0.48
2:D:2956:THR:O	2:D:2957:ALA:C	2.55	0.48
2:D:3016:ALA:H	2:D:3017:PRO:HD3	1.79	0.48
2:B:2608:ARG:CB	2:B:2608:ARG:NH1	2.68	0.48
2:B:2719:HIS:O	2:B:2720:SER:C	2.56	0.48
2:B:3058:SER:O	2:B:3059:THR:CB	2.61	0.48
1:A:48:VAL:C	1:A:49:GLU:CG	2.86	0.48
2:B:2762:GLU:OE2	2:B:2893:ARG:NH1	2.47	0.48
2:B:2919:ARG:N	2:B:2920:PRO:CD	2.76	0.48
2:B:2927:LEU:O	2:B:2934:TYR:OH	2.31	0.48
2:B:2929:THR:O	2:B:2930:GLU:C	2.55	0.48
2:B:3093:ILE:HD11	2:B:3100:TYR:CE1	2.48	0.48
1:C:48:VAL:C	1:C:49:GLU:CG	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2500:LYS:O	2:D:2501:GLU:HB3	2.13	0.48
2:D:2751:ILE:HD11	2:D:2973:LEU:HD13	1.96	0.48
2:D:2761:VAL:HG11	2:D:2918:TRP:CZ3	2.49	0.48
2:D:3094:GLU:C	2:D:3096:ILE:N	2.72	0.48
2:B:2610:ASP:O	2:B:2610:ASP:CG	2.56	0.48
2:D:2409:ASP:O	2:D:2412:SER:N	2.40	0.48
2:D:2545:ILE:HG13	2:D:2545:ILE:O	2.13	0.48
2:D:2717:ARG:HG2	2:D:2717:ARG:NH1	2.28	0.48
2:D:2745:VAL:N	2:D:2940:SER:OG	2.47	0.48
2:B:2915:LEU:HD12	2:B:2915:LEU:C	2.38	0.48
1:C:50:ASP:O	1:C:52:PHE:N	2.46	0.48
2:D:2761:VAL:O	2:D:2895:VAL:HG23	2.13	0.48
2:B:2717:ARG:O	2:B:2718:TRP:C	2.56	0.48
1:C:56:LEU:O	1:C:56:LEU:HD23	2.13	0.48
2:D:2437:PRO:HG2	2:D:2442:LEU:CD1	2.39	0.48
2:D:2493:ALA:O	2:D:2496:ASP:N	2.46	0.48
2:D:2558:VAL:HG13	2:D:2577:LEU:CD1	2.40	0.48
2:D:2756:TYR:N	2:D:2756:TYR:HD1	2.12	0.48
2:B:2403:PHE:HD1	2:B:2503:LEU:CD1	2.26	0.48
2:B:2692:PRO:HG2	2:B:2693:ASP:N	2.29	0.48
2:B:2933:ARG:CB	2:B:2968:VAL:HG22	2.43	0.48
1:C:60:LEU:HD11	2:D:2562:ALA:HB1	1.96	0.48
2:D:2487:ALA:C	2:D:2489:TYR:N	2.69	0.48
2:B:3057:GLU:HA	2:B:3057:GLU:OE1	2.14	0.48
2:D:2599:ARG:HH22	2:D:2609:ASP:CB	2.27	0.48
2:D:2616:LEU:CD1	2:D:2724:PHE:CD2	2.96	0.48
2:D:2983:LEU:HD11	2:D:2988:LEU:HG	1.95	0.48
2:B:2752:VAL:HG12	2:B:2930:GLU:HA	1.96	0.47
2:D:2458:GLY:O	2:D:2459:ASP:HB2	2.14	0.47
2:D:3100:TYR:C	2:D:3102:GLU:N	2.71	0.47
1:A:62:LYS:O	1:A:63:HIS:C	2.57	0.47
2:B:2447:THR:HG22	2:B:2448:LEU:N	2.29	0.47
2:B:2669:LEU:HB3	2:B:2674:ARG:HB2	1.95	0.47
2:B:2714:ARG:NH2	2:B:2733:LEU:HD12	2.29	0.47
2:B:2917:ILE:HD13	2:B:2924:LEU:CD2	2.36	0.47
2:B:2928:LEU:HA	2:B:2934:TYR:CZ	2.49	0.47
2:B:2987:LYS:O	2:B:2989:SER:N	2.47	0.47
2:D:2620:VAL:HG22	2:D:2679:GLN:O	2.14	0.47
1:A:37:HIS:ND1	1:A:38:VAL:HG12	2.28	0.47
2:B:2744:ASN:OD1	2:B:2744:ASN:C	2.57	0.47
2:B:3007:VAL:HB	2:B:3104:GLU:OE1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3010:VAL:HG12	2:B:3012:PRO:CD	2.43	0.47
1:C:43:TRP:C	1:C:45:ASP:N	2.71	0.47
2:D:2585:GLN:O	2:D:2588:TYR:HB3	2.13	0.47
2:D:2589:ARG:HG3	2:D:2589:ARG:NH1	2.26	0.47
2:D:2610:ASP:O	2:D:2610:ASP:CG	2.55	0.47
2:D:2937:TYR:O	2:D:2961:THR:HG23	2.14	0.47
2:D:2937:TYR:C	2:D:2939:LEU:N	2.69	0.47
2:D:3007:VAL:O	2:D:3008:SER:HB3	2.13	0.47
2:D:3024:GLU:OE2	2:D:3085:ARG:NH2	2.47	0.47
2:B:2733:LEU:N	2:B:2733:LEU:CD2	2.76	0.47
2:B:2932:GLN:HA	2:B:2932:GLN:OE1	2.13	0.47
1:C:13:LEU:HD12	2:D:2451:ILE:O	2.15	0.47
2:D:2939:LEU:CD1	2:D:2955:LEU:HB3	2.45	0.47
2:D:2984:PRO:HG2	2:D:2987:LYS:HG3	1.96	0.47
2:D:3100:TYR:O	2:D:3101:LYS:C	2.57	0.47
2:D:3101:LYS:O	2:D:3105:LYS:HG3	2.15	0.47
1:A:56:LEU:O	1:A:56:LEU:HD23	2.14	0.47
2:B:2407:ASN:O	2:B:2411:MET:HG3	2.13	0.47
2:B:2427:ASN:O	2:B:2428:LYS:C	2.57	0.47
2:B:2493:ALA:O	2:B:2496:ASP:N	2.47	0.47
2:B:2541:ASP:OD1	2:B:2543:LYS:N	2.47	0.47
2:B:2761:VAL:HG11	2:B:2918:TRP:CZ3	2.50	0.47
2:B:2773:ASN:OD1	2:B:2776:GLU:OE1	2.32	0.47
2:B:3108:ILE:HG12	2:B:3112:LYS:HE3	1.95	0.47
2:D:2498:PHE:HB2	2:D:2503:LEU:HD23	1.97	0.47
2:D:2557:ILE:O	2:D:2561:LEU:HD12	2.14	0.47
2:D:2772:ARG:HB3	2:D:2776:GLU:HB2	1.96	0.47
2:D:3109:GLN:HE21	2:D:3110:VAL:N	2.12	0.47
2:B:2755:VAL:HG23	2:B:2930:GLU:HG2	1.97	0.47
2:B:2911:LYS:O	2:B:2912:SER:C	2.57	0.47
2:B:2956:THR:O	2:B:2957:ALA:C	2.58	0.47
2:B:2987:LYS:C	2:B:2989:SER:N	2.66	0.47
2:B:2997:CYS:O	2:B:2999:GLU:N	2.47	0.47
1:C:38:VAL:O	1:C:38:VAL:HG13	2.14	0.47
1:C:56:LEU:HD23	1:C:57:ARG:HB2	1.95	0.47
2:D:2441:TYR:O	2:D:2441:TYR:CD2	2.68	0.47
2:D:2553:HIS:O	2:D:2557:ILE:HG13	2.15	0.47
2:D:2565:GLU:OE1	2:D:2574:ASN:HA	2.13	0.47
2:D:2704:LEU:HD23	2:D:2704:LEU:C	2.40	0.47
1:A:51:ASP:CB	2:B:2717:ARG:HG3	2.45	0.47
2:B:2489:TYR:O	2:B:2491:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2511:LEU:O	2:B:2512:ALA:C	2.58	0.47
2:B:2534:LEU:CD2	2:B:2540:VAL:HG21	2.41	0.47
2:B:2689:VAL:HG21	2:B:2707:LYS:HE3	1.96	0.47
2:B:2939:LEU:CD1	2:B:2955:LEU:HB3	2.45	0.47
2:B:3062:VAL:HG22	2:B:3062:VAL:O	2.14	0.47
2:B:3100:TYR:O	2:B:3103:ALA:N	2.48	0.47
1:C:46:ASP:OD2	2:D:2674:ARG:NH1	2.48	0.47
2:D:2782:LEU:C	2:D:2784:PHE:H	2.23	0.47
2:D:3061:ARG:HG2	2:D:3061:ARG:NH1	2.29	0.47
2:D:2424:ARG:NH1	2:D:2536:ASP:OD1	2.48	0.47
2:D:2777:GLU:OE2	2:D:2893:ARG:NH2	2.46	0.47
2:D:2779:LYS:C	2:D:2781:ALA:H	2.23	0.47
2:D:2909:ARG:O	2:D:2910:GLU:CG	2.60	0.47
2:D:2918:TRP:C	2:D:2920:PRO:CD	2.88	0.47
2:D:2997:CYS:O	2:D:2998:SER:C	2.58	0.47
2:B:2403:PHE:CA	2:B:2503:LEU:HD11	2.36	0.47
2:B:3108:ILE:CG1	2:B:3112:LYS:HE3	2.44	0.47
2:D:2597:SER:O	2:D:2598:SER:C	2.58	0.47
2:D:2983:LEU:HB3	2:D:3002:VAL:HG12	1.97	0.47
2:B:2434:CYS:SG	2:B:2435:PRO:N	2.86	0.47
2:B:2512:ALA:HB1	2:B:2584:LEU:HG	1.93	0.47
2:B:2545:ILE:HG13	2:B:2545:ILE:O	2.15	0.47
2:B:2685:GLY:H	2:B:2712:SER:HB3	1.80	0.47
2:B:3083:GLN:HA	2:B:3086:VAL:CG1	2.43	0.47
2:D:2414:LEU:C	2:D:2416:ASN:N	2.72	0.47
2:D:2568:PHE:O	2:D:2570:LYS:N	2.48	0.47
2:D:2600:SER:HB2	2:D:2655:TRP:HB2	1.97	0.47
2:B:2937:TYR:O	2:B:2961:THR:HG23	2.14	0.46
2:B:3024:GLU:OE2	2:B:3085:ARG:NH2	2.48	0.46
2:B:3060:SER:C	2:B:3062:VAL:N	2.69	0.46
1:C:39:TRP:HA	1:C:39:TRP:HE3	1.79	0.46
2:D:2554:TYR:O	2:D:2558:VAL:HG23	2.15	0.46
2:D:2719:HIS:O	2:D:2720:SER:C	2.58	0.46
2:D:2738:LEU:HD22	2:D:2745:VAL:CG2	2.45	0.46
1:A:60:LEU:HD11	2:B:2562:ALA:HB1	1.97	0.46
2:B:2446:SER:OG	2:B:2448:LEU:HD12	2.15	0.46
2:B:2487:ALA:C	2:B:2489:TYR:H	2.22	0.46
2:B:2719:HIS:CG	2:B:2720:SER:N	2.83	0.46
1:C:20:GLU:O	1:C:21:GLU:C	2.59	0.46
2:D:2403:PHE:HA	2:D:2503:LEU:HD11	1.96	0.46
2:D:2428:LYS:C	2:D:2430:ARG:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2563:ALA:O	2:D:2566:PHE:N	2.49	0.46
2:D:3109:GLN:NE2	2:D:3110:VAL:HG12	2.30	0.46
1:A:51:ASP:O	2:B:2717:ARG:HA	2.16	0.46
2:B:2777:GLU:O	2:B:2778:GLU:C	2.58	0.46
2:B:2927:LEU:HD12	2:B:2927:LEU:C	2.40	0.46
2:B:2935:ARG:HD3	2:B:2937:TYR:OH	2.15	0.46
2:D:2525:ALA:HA	2:D:2529:GLU:OE1	2.16	0.46
2:D:2624:ILE:CG2	2:D:2626:LEU:HG	2.46	0.46
2:D:3108:ILE:CG1	2:D:3112:LYS:HE3	2.46	0.46
2:B:3062:VAL:HB	2:B:3111:LEU:HD21	1.96	0.46
2:D:2500:LYS:O	2:D:2501:GLU:CB	2.64	0.46
2:D:2765:VAL:HG23	2:D:2766:SER:N	2.31	0.46
2:B:2403:PHE:CA	2:B:2500:LYS:HE2	2.45	0.46
2:B:2455:ALA:O	2:B:2456:ALA:C	2.58	0.46
2:B:2553:HIS:O	2:B:2557:ILE:HG13	2.15	0.46
2:B:2681:ILE:HG22	2:B:2683:THR:HG23	1.97	0.46
2:B:2761:VAL:O	2:B:2895:VAL:HG23	2.16	0.46
2:B:3100:TYR:HD1	2:B:3101:LYS:HD2	1.80	0.46
2:D:2414:LEU:O	2:D:2415:GLN:C	2.58	0.46
2:D:2933:ARG:CB	2:D:2968:VAL:HG22	2.46	0.46
2:D:3062:VAL:HB	2:D:3111:LEU:HD21	1.96	0.46
2:B:2653:ASP:C	2:B:2722:LEU:HD13	2.41	0.46
2:B:2782:LEU:C	2:B:2784:PHE:H	2.23	0.46
2:B:3020:TYR:CD2	2:B:3030:VAL:HG22	2.51	0.46
2:D:2475:VAL:O	2:D:2476:SER:C	2.58	0.46
2:D:2482:VAL:HA	2:D:2486:ASN:HD21	1.80	0.46
2:D:2773:ASN:OD1	2:D:2776:GLU:OE1	2.34	0.46
2:B:2500:LYS:O	2:B:2501:GLU:HB3	2.15	0.46
2:B:2711:ASN:OD1	2:B:2738:LEU:HA	2.16	0.46
2:B:2773:ASN:N	2:B:2776:GLU:HB2	2.15	0.46
2:D:2534:LEU:CD2	2:D:2540:VAL:HG21	2.41	0.46
2:B:2701:PRO:O	2:B:2704:LEU:HB3	2.15	0.46
2:D:2729:ARG:HD3	2:D:2730:PRO:CD	2.46	0.46
2:B:2418:ARG:O	2:B:2421:GLN:HB3	2.16	0.46
2:B:2447:THR:O	2:B:2448:LEU:O	2.34	0.46
2:B:2487:ALA:C	2:B:2489:TYR:N	2.73	0.46
2:B:2565:GLU:OE1	2:B:2574:ASN:HA	2.16	0.46
2:B:2744:ASN:CB	2:B:2940:SER:HB2	2.46	0.46
2:B:2918:TRP:O	2:B:2919:ARG:C	2.58	0.46
2:B:3004:GLY:HA2	2:B:3089:MET:HE1	1.98	0.46
2:D:2461:VAL:HB	2:D:2462:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3020:TYR:CD2	2:D:3030:VAL:HG22	2.51	0.46
1:A:8:VAL:HG12	1:A:10:LEU:HD23	1.98	0.46
2:B:2761:VAL:HG11	2:B:2918:TRP:CH2	2.51	0.46
2:B:2765:VAL:HG23	2:B:2766:SER:N	2.31	0.46
2:B:3016:ALA:H	2:B:3017:PRO:HD3	1.80	0.46
2:B:3100:TYR:C	2:B:3102:GLU:N	2.71	0.46
1:C:61:GLU:C	1:C:63:HIS:H	2.23	0.46
2:D:2608:ARG:CB	2:D:2608:ARG:NH1	2.70	0.46
2:D:2701:PRO:O	2:D:2704:LEU:HB3	2.16	0.46
2:D:2969:SER:HB2	2:D:2972:THR:HG23	1.98	0.46
1:A:12:LEU:O	2:B:2450:ARG:NH1	2.49	0.45
1:A:46:ASP:OD2	2:B:2674:ARG:NH1	2.49	0.45
2:B:2587:LYS:O	2:B:2590:TYR:HB3	2.16	0.45
2:B:2614:LYS:HG2	2:B:2615:THR:H	1.74	0.45
2:B:2909:ARG:O	2:B:2910:GLU:CG	2.60	0.45
2:B:3107:LEU:O	2:B:3108:ILE:C	2.59	0.45
2:B:3109:GLN:HE21	2:B:3110:VAL:N	2.13	0.45
2:D:3109:GLN:C	2:D:3109:GLN:HE21	2.23	0.45
2:B:2416:ASN:O	2:B:2420:LEU:HB2	2.16	0.45
2:B:2428:LYS:CD	2:B:2542:PRO:HD3	2.46	0.45
2:B:2554:TYR:O	2:B:2558:VAL:HG23	2.16	0.45
2:B:2779:LYS:C	2:B:2781:ALA:H	2.24	0.45
2:B:3100:TYR:O	2:B:3101:LYS:C	2.58	0.45
2:D:2621:SER:O	2:D:2622:ASP:HB2	2.17	0.45
2:D:2666:LEU:O	2:D:2667:LEU:C	2.57	0.45
2:D:2985:PHE:C	2:D:2987:LYS:N	2.74	0.45
1:A:22:PHE:O	1:A:23:PRO:C	2.59	0.45
2:B:2563:ALA:O	2:B:2566:PHE:N	2.49	0.45
2:B:3095:ASN:N	2:B:3095:ASN:ND2	2.64	0.45
2:B:3110:VAL:C	2:B:3112:LYS:N	2.72	0.45
1:C:9:ASP:O	1:C:11:GLY:N	2.50	0.45
2:D:2666:LEU:O	2:D:2669:LEU:N	2.43	0.45
2:D:2927:LEU:HG	2:D:2928:LEU:N	2.32	0.45
2:B:2494:ILE:HD12	2:B:2495:GLU:N	2.25	0.45
2:B:2750:VAL:HG11	2:B:2903:VAL:CG2	2.47	0.45
2:B:2911:LYS:O	2:B:2912:SER:O	2.34	0.45
2:D:2448:LEU:O	2:D:2449:PRO:C	2.58	0.45
2:D:2468:LYS:C	2:D:2470:LEU:N	2.74	0.45
2:D:3029:LEU:C	2:D:3029:LEU:CD2	2.84	0.45
2:D:3091:HIS:O	2:D:3094:GLU:N	2.50	0.45
2:D:3100:TYR:CD1	2:D:3101:LYS:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TRP:HZ3	2:B:2682:ILE:HB	1.81	0.45
2:B:2656:TYR:CD2	2:B:2697:PRO:CB	2.93	0.45
2:B:2917:ILE:CG2	2:B:2920:PRO:HG3	2.40	0.45
2:D:2541:ASP:O	2:D:2542:PRO:C	2.60	0.45
2:D:2719:HIS:CG	2:D:2720:SER:N	2.82	0.45
2:D:2749:ASP:O	2:D:2906:TYR:HB2	2.17	0.45
2:D:3021:LEU:HB2	2:D:3029:LEU:HD22	1.97	0.45
1:A:57:ARG:HG2	2:B:2559:TRP:CZ2	2.52	0.45
2:B:2555:ARG:CZ	2:B:2556:TRP:CH2	2.99	0.45
2:B:2675:LEU:HD23	2:B:2675:LEU:HA	1.72	0.45
2:B:2726:HIS:ND1	2:B:2726:HIS:N	2.62	0.45
1:C:50:ASP:CG	1:C:51:ASP:N	2.74	0.45
2:D:3005:VAL:HG22	2:D:3046:LEU:CD1	2.47	0.45
1:A:15:GLU:HB2	1:A:18:GLU:CG	2.47	0.45
2:B:2552:ASN:O	2:B:2555:ARG:N	2.49	0.45
2:D:2772:ARG:HB3	2:D:2776:GLU:CB	2.46	0.45
2:D:2911:LYS:O	2:D:2912:SER:C	2.59	0.45
2:D:2978:GLN:HG2	2:D:2996:PRO:HG2	1.99	0.45
1:A:20:GLU:O	1:A:21:GLU:C	2.59	0.45
2:D:2554:TYR:CE1	2:D:2582:VAL:HG11	2.51	0.45
2:D:2666:LEU:HD11	2:D:2708:ILE:HG22	1.99	0.45
2:D:2744:ASN:OD1	2:D:2744:ASN:C	2.60	0.45
2:D:2772:ARG:NE	2:D:2780:GLU:HG2	2.32	0.45
2:D:3097:ASP:HA	2:D:3100:TYR:HB2	1.99	0.45
2:B:2440:LEU:C	2:B:2442:LEU:N	2.72	0.45
2:B:2483:ASN:CG	2:B:2485:LYS:H	2.25	0.45
2:B:2500:LYS:O	2:B:2501:GLU:CB	2.65	0.45
2:B:2901:LEU:HD11	2:B:2928:LEU:HD13	1.99	0.45
2:B:2997:CYS:O	2:B:2998:SER:C	2.60	0.45
2:B:3035:ILE:HG23	2:B:3068:GLY:O	2.17	0.45
2:B:3097:ASP:HA	2:B:3100:TYR:HB2	1.99	0.45
2:D:2783:ARG:HG3	2:D:2783:ARG:NH1	2.32	0.45
2:D:2900:LYS:HD2	2:D:3070:PHE:CE2	2.51	0.45
2:D:3095:ASN:N	2:D:3095:ASN:ND2	2.65	0.45
2:D:3107:LEU:O	2:D:3108:ILE:C	2.57	0.45
2:B:2572:PHE:O	2:B:2573:ALA:C	2.60	0.45
2:B:2648:THR:HG21	2:B:2705:ARG:HH12	1.81	0.45
2:B:2772:ARG:NE	2:B:2780:GLU:HG2	2.32	0.45
2:B:3048:ALA:HB1	2:B:3082:PHE:CE2	2.52	0.45
2:D:2936:ILE:HG21	2:D:2939:LEU:HB2	1.97	0.45
1:A:43:TRP:C	1:A:45:ASP:N	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2498:PHE:HB2	2:B:2503:LEU:HD23	1.98	0.44
2:B:2509:PHE:O	2:B:2517:LEU:N	2.48	0.44
2:B:3109:GLN:HE22	2:B:3110:VAL:HG12	1.80	0.44
2:D:2461:VAL:HB	2:D:2462:PRO:CD	2.47	0.44
2:B:3091:HIS:O	2:B:3093:ILE:N	2.51	0.44
2:D:2765:VAL:HG23	2:D:2766:SER:H	1.82	0.44
2:D:2777:GLU:O	2:D:2778:GLU:C	2.60	0.44
2:D:3060:SER:C	2:D:3062:VAL:H	2.24	0.44
2:D:2569:PRO:O	2:D:2573:ALA:HA	2.18	0.44
2:D:2667:LEU:C	2:D:2667:LEU:CD2	2.89	0.44
2:D:2761:VAL:HG11	2:D:2918:TRP:CH2	2.52	0.44
2:D:2921:SER:O	2:D:2924:LEU:HB2	2.17	0.44
2:D:2959:LYS:H	2:D:2959:LYS:CD	2.09	0.44
2:D:2995:PRO:HD2	2:D:3054:TRP:CE3	2.52	0.44
2:D:3095:ASN:C	2:D:3096:ILE:HG13	2.42	0.44
1:A:43:TRP:CZ3	2:B:2713:THR:HG23	2.41	0.44
2:B:2403:PHE:C	2:B:2500:LYS:HE2	2.42	0.44
2:B:2589:ARG:HG3	2:B:2589:ARG:NH1	2.25	0.44
2:B:3061:ARG:HG2	2:B:3061:ARG:NH1	2.29	0.44
2:D:2603:LYS:O	2:D:2604:LYS:C	2.60	0.44
2:D:2620:VAL:HG23	2:D:2677:VAL:HA	2.00	0.44
2:D:2717:ARG:O	2:D:2718:TRP:C	2.60	0.44
2:D:3105:LYS:O	2:D:3109:GLN:HB2	2.17	0.44
2:B:2751:ILE:HD11	2:B:2973:LEU:HD13	1.99	0.44
2:D:2421:GLN:HA	2:D:2424:ARG:NE	2.33	0.44
2:D:2480:ILE:O	2:D:2480:ILE:CG2	2.65	0.44
2:D:2680:LYS:NZ	2:D:2719:HIS:O	2.50	0.44
2:D:2929:THR:O	2:D:2930:GLU:C	2.61	0.44
2:B:2419:ASP:HA	2:B:2422:ASP:HB2	2.00	0.44
2:B:2704:LEU:O	2:B:2705:ARG:HD3	2.17	0.44
2:B:2745:VAL:H	2:B:2940:SER:CB	2.30	0.44
2:B:2756:TYR:N	2:B:2756:TYR:HD1	2.15	0.44
2:B:2772:ARG:CZ	2:B:2780:GLU:HG2	2.48	0.44
2:B:2588:TYR:O	2:B:2589:ARG:C	2.59	0.44
2:B:2744:ASN:HB2	2:B:2941:VAL:N	2.33	0.44
2:B:2950:TRP:N	2:B:2951:PRO:CD	2.68	0.44
2:B:3058:SER:C	2:B:3060:SER:N	2.76	0.44
2:D:2541:ASP:OD1	2:D:2543:LYS:N	2.50	0.44
2:D:2620:VAL:CG2	2:D:2677:VAL:HA	2.46	0.44
2:D:2911:LYS:O	2:D:2912:SER:O	2.36	0.44
2:D:3110:VAL:C	2:D:3112:LYS:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2750:VAL:CG1	2:B:2904:THR:N	2.81	0.44
2:B:2765:VAL:HG23	2:B:2766:SER:H	1.82	0.44
1:C:39:TRP:HE1	2:D:2733:LEU:HB3	1.83	0.44
2:D:2752:VAL:HG12	2:D:2930:GLU:HA	2.00	0.44
2:D:3107:LEU:C	2:D:3109:GLN:N	2.76	0.44
2:D:3060:SER:O	2:D:3063:PRO:HD3	2.18	0.44
2:B:2744:ASN:CB	2:B:2940:SER:HB3	2.41	0.43
1:C:56:LEU:N	2:D:2462:PRO:HG2	2.29	0.43
2:D:2494:ILE:HD11	2:D:2523:GLY:O	2.18	0.43
2:D:2745:VAL:H	2:D:2940:SER:CB	2.31	0.43
2:D:2924:LEU:HB3	2:D:2925:PRO:HD3	1.99	0.43
2:D:2990:ASP:O	2:D:2991:PRO:C	2.61	0.43
2:D:3058:SER:C	2:D:3060:SER:N	2.76	0.43
1:A:50:ASP:CG	1:A:51:ASP:N	2.75	0.43
2:B:2410:LEU:HD13	2:B:2504:CYS:O	2.18	0.43
2:B:2940:SER:O	2:B:2941:VAL:CG2	2.61	0.43
1:C:12:LEU:HD21	2:D:2443:THR:HG23	2.00	0.43
1:C:60:LEU:HD12	2:D:2563:ALA:N	2.33	0.43
2:D:2418:ARG:O	2:D:2421:GLN:HB3	2.18	0.43
2:D:2666:LEU:HD23	2:D:2669:LEU:HD12	2.00	0.43
2:D:2675:LEU:HA	2:D:2675:LEU:HD23	1.79	0.43
1:A:21:GLU:HG3	1:A:22:PHE:CG	2.53	0.43
2:B:2557:ILE:O	2:B:2561:LEU:HD12	2.19	0.43
2:B:2744:ASN:CB	2:B:2940:SER:CB	2.88	0.43
2:B:2762:GLU:CB	2:B:2772:ARG:HH12	2.32	0.43
1:C:21:GLU:HG3	1:C:22:PHE:CG	2.53	0.43
2:D:2476:SER:C	2:D:2478:ALA:H	2.24	0.43
2:D:2479:CYS:O	2:D:2481:SER:N	2.51	0.43
2:D:2492:PHE:CE2	2:D:2578:ASN:HA	2.52	0.43
2:D:2676:THR:HG22	2:D:2679:GLN:NE2	2.34	0.43
2:D:3029:LEU:HD23	2:D:3030:VAL:N	2.32	0.43
2:B:2667:LEU:HD23	2:B:2671:LYS:HD3	2.00	0.43
2:B:2778:GLU:HA	2:B:2781:ALA:HB3	2.01	0.43
2:B:2933:ARG:HB3	2:B:2968:VAL:HG22	2.00	0.43
2:B:3058:SER:O	2:B:3060:SER:N	2.46	0.43
1:C:39:TRP:CD1	2:D:2733:LEU:HB3	2.53	0.43
2:D:2608:ARG:HH11	2:D:2608:ARG:CA	2.30	0.43
2:D:2730:PRO:HB2	2:D:2747:CYS:HB2	1.99	0.43
2:D:3111:LEU:HD12	2:D:3111:LEU:HA	1.84	0.43
1:A:43:TRP:O	1:A:45:ASP:N	2.47	0.43
2:B:2468:LYS:C	2:B:2470:LEU:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2592:VAL:HG11	2:B:2655:TRP:CH2	2.54	0.43
2:B:2745:VAL:N	2:B:2940:SER:CB	2.81	0.43
2:B:2991:PRO:O	2:B:2993:PHE:N	2.51	0.43
2:B:3105:LYS:O	2:B:3109:GLN:HB2	2.18	0.43
2:D:2688:LEU:HD12	2:D:2688:LEU:HA	1.77	0.43
2:D:2756:TYR:HD2	2:D:3070:PHE:CB	2.30	0.43
2:D:2762:GLU:CB	2:D:2772:ARG:HH12	2.31	0.43
2:D:2773:ASN:C	2:D:2775:ARG:N	2.73	0.43
2:D:2902:ARG:NH1	2:D:2914:LEU:HD13	2.33	0.43
2:D:2927:LEU:HD12	2:D:2927:LEU:C	2.42	0.43
2:D:3042:LYS:O	2:D:3045:VAL:HG23	2.18	0.43
2:D:3048:ALA:HB1	2:D:3082:PHE:CE2	2.52	0.43
2:B:2672:SER:CB	2:B:2674:ARG:HG2	2.46	0.43
2:B:2898:VAL:HG22	2:B:2918:TRP:CZ3	2.53	0.43
2:B:2953:ILE:O	2:B:2954:GLN:HB2	2.17	0.43
2:B:2985:PHE:C	2:B:2987:LYS:N	2.75	0.43
2:B:3117:LYS:HA	2:B:3117:LYS:HD3	1.72	0.43
2:D:2903:VAL:O	2:D:2913:ALA:N	2.48	0.43
2:D:3057:GLU:O	2:D:3060:SER:HB2	2.19	0.43
1:A:50:ASP:O	1:A:52:PHE:N	2.51	0.43
1:A:60:LEU:HA	2:B:2566:PHE:CE2	2.54	0.43
2:B:2436:GLN:HA	2:B:2437:PRO:HD2	1.88	0.43
2:B:2440:LEU:C	2:B:2442:LEU:H	2.26	0.43
2:B:2492:PHE:CE2	2:B:2578:ASN:HA	2.53	0.43
2:B:2589:ARG:HH11	2:B:2589:ARG:CG	2.22	0.43
2:B:2597:SER:O	2:B:2598:SER:C	2.61	0.43
1:C:46:ASP:O	1:C:47:ASN:O	2.37	0.43
2:D:2511:LEU:O	2:D:2512:ALA:C	2.60	0.43
2:D:2552:ASN:O	2:D:2555:ARG:N	2.52	0.43
2:D:2943:LYS:O	2:D:2944:SER:O	2.36	0.43
2:D:3083:GLN:HA	2:D:3086:VAL:CG1	2.45	0.43
2:B:2552:ASN:ND2	2:B:2552:ASN:C	2.75	0.43
2:B:2568:PHE:C	2:B:2570:LYS:H	2.25	0.43
2:B:2606:LEU:HD21	2:B:2658:VAL:HG11	2.00	0.43
2:D:2520:SER:O	2:D:2521:ASP:C	2.60	0.43
1:A:43:TRP:CZ3	2:B:2713:THR:O	2.71	0.43
2:B:2520:SER:O	2:B:2521:ASP:C	2.62	0.43
2:B:2666:LEU:CD1	2:B:2708:ILE:HG22	2.48	0.43
2:B:2943:LYS:O	2:B:2944:SER:O	2.36	0.43
2:D:2782:LEU:O	2:D:2784:PHE:N	2.51	0.43
1:A:60:LEU:HD12	2:B:2563:ALA:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2465:CYS:HB3	2:B:2566:PHE:CE1	2.54	0.43
2:B:2479:CYS:O	2:B:2481:SER:N	2.52	0.43
2:B:2501:GLU:O	2:B:2501:GLU:HG3	2.19	0.43
2:B:2541:ASP:O	2:B:2542:PRO:C	2.58	0.43
2:B:2687:GLU:CD	2:B:2707:LYS:HD2	2.43	0.43
2:B:3093:ILE:CG2	2:B:3094:GLU:N	2.82	0.43
1:C:37:HIS:O	1:C:37:HIS:ND1	2.52	0.43
2:D:2483:ASN:CG	2:D:2485:LYS:H	2.26	0.43
2:D:2599:ARG:HH22	2:D:2609:ASP:HB3	1.83	0.43
2:D:2611:THR:O	2:D:2612:ALA:C	2.62	0.43
2:D:2745:VAL:N	2:D:2940:SER:CB	2.82	0.43
2:D:2772:ARG:CZ	2:D:2780:GLU:HG2	2.49	0.43
2:B:2412:SER:C	2:B:2414:LEU:N	2.76	0.42
2:B:2448:LEU:O	2:B:2449:PRO:C	2.61	0.42
2:B:2937:TYR:C	2:B:2939:LEU:H	2.26	0.42
2:D:2720:SER:O	2:D:2721:LYS:HB2	2.19	0.42
2:B:2421:GLN:HA	2:B:2424:ARG:NE	2.34	0.42
2:B:3089:MET:O	2:B:3091:HIS:N	2.52	0.42
2:B:3107:LEU:C	2:B:3109:GLN:N	2.75	0.42
2:D:2439:SER:HB3	2:D:2584:LEU:CD2	2.49	0.42
2:D:2551:SER:O	2:D:2554:TYR:HB3	2.19	0.42
2:D:2648:THR:OG1	2:D:2649:ILE:N	2.51	0.42
2:D:2653:ASP:C	2:D:2653:ASP:OD1	2.62	0.42
2:D:2908:LYS:O	2:D:2910:GLU:N	2.52	0.42
2:D:3085:ARG:O	2:D:3086:VAL:C	2.62	0.42
2:D:3096:ILE:O	2:D:3099:PHE:HD2	2.02	0.42
2:B:2990:ASP:O	2:B:2991:PRO:C	2.62	0.42
1:C:60:LEU:HA	2:D:2566:PHE:CE2	2.54	0.42
1:C:60:LEU:HA	2:D:2566:PHE:CD2	2.54	0.42
2:D:2447:THR:O	2:D:2448:LEU:O	2.36	0.42
2:D:2492:PHE:CE2	2:D:2578:ASN:CA	3.02	0.42
2:D:3100:TYR:CD1	2:D:3101:LYS:N	2.87	0.42
1:A:39:TRP:NE1	2:B:2733:LEU:HB3	2.35	0.42
2:B:2582:VAL:O	2:B:2586:LEU:HD12	2.19	0.42
2:B:3101:LYS:O	2:B:3105:LYS:HG3	2.19	0.42
2:D:2655:TRP:HB3	2:D:2656:TYR:CE1	2.54	0.42
2:D:2687:GLU:O	2:D:2706:LEU:HD22	2.19	0.42
2:B:2492:PHE:CE2	2:B:2578:ASN:CA	3.03	0.42
2:B:3028:LEU:HD11	2:B:3108:ILE:HB	2.02	0.42
2:D:2689:VAL:HG12	2:D:2690:GLY:N	2.35	0.42
2:D:2783:ARG:HD2	2:D:2783:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3115:SER:HB2	2:D:3116:PRO:HD2	2.01	0.42
2:B:2439:SER:HB3	2:B:2584:LEU:HD21	2.01	0.42
2:B:2582:VAL:O	2:B:2582:VAL:HG12	2.20	0.42
2:B:2941:VAL:O	2:B:2942:SER:O	2.37	0.42
2:B:3109:GLN:C	2:B:3109:GLN:HE21	2.26	0.42
1:C:18:GLU:OE1	2:D:2450:ARG:NH2	2.52	0.42
1:C:60:LEU:HD12	2:D:2563:ALA:CA	2.50	0.42
2:B:2564:MET:HE2	2:B:2572:PHE:CD2	2.55	0.42
2:B:3060:SER:C	2:B:3062:VAL:H	2.28	0.42
2:B:3060:SER:O	2:B:3063:PRO:HD3	2.20	0.42
2:B:3115:SER:OG	2:B:3116:PRO:HD2	2.19	0.42
1:C:9:ASP:C	1:C:11:GLY:N	2.78	0.42
2:D:2425:ILE:HG23	2:D:2542:PRO:CG	2.49	0.42
2:D:2684:GLN:HE21	2:D:2684:GLN:HB2	1.54	0.42
2:D:2895:VAL:HG22	2:D:2896:SER:N	2.33	0.42
2:D:2933:ARG:HB2	2:D:2968:VAL:HG22	2.01	0.42
1:A:60:LEU:HD12	2:B:2563:ALA:N	2.34	0.42
2:B:2414:LEU:O	2:B:2415:GLN:C	2.63	0.42
2:B:2414:LEU:C	2:B:2416:ASN:H	2.28	0.42
2:B:2611:THR:O	2:B:2612:ALA:C	2.63	0.42
2:B:2669:LEU:O	2:B:2674:ARG:N	2.48	0.42
1:C:12:LEU:C	2:D:2450:ARG:NH1	2.77	0.42
2:D:2465:CYS:HB3	2:D:2566:PHE:CE1	2.55	0.42
2:D:2483:ASN:HD22	2:D:2486:ASN:HD22	1.68	0.42
2:D:2995:PRO:HA	2:D:2996:PRO:HD3	1.89	0.42
2:B:2782:LEU:O	2:B:2784:PHE:N	2.52	0.42
2:B:2783:ARG:HD2	2:B:2783:ARG:O	2.20	0.42
2:B:3057:GLU:C	2:B:3058:SER:O	2.61	0.42
2:D:3057:GLU:OE1	2:D:3057:GLU:HA	2.19	0.42
2:D:3109:GLN:HE22	2:D:3110:VAL:HG12	1.84	0.42
2:B:2955:LEU:N	2:B:2955:LEU:HD12	2.35	0.42
2:B:3109:GLN:NE2	2:B:3110:VAL:CG1	2.83	0.42
1:C:13:LEU:HD11	2:D:2453:LEU:HA	2.01	0.42
2:D:2749:ASP:OD1	2:D:2933:ARG:NH2	2.53	0.42
2:D:2762:GLU:OE2	2:D:2893:ARG:NH1	2.53	0.42
2:D:2953:ILE:CG1	2:D:2954:GLN:N	2.74	0.42
1:A:38:VAL:O	1:A:38:VAL:HG13	2.19	0.41
2:B:2490:PHE:HE2	2:B:2492:PHE:CZ	2.37	0.41
2:B:2525:ALA:HA	2:B:2529:GLU:OE1	2.20	0.41
2:B:2621:SER:HB3	2:B:2652:THR:HG22	2.02	0.41
2:B:2918:TRP:C	2:B:2920:PRO:CD	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3029:LEU:C	2:B:3029:LEU:CD2	2.86	0.41
2:B:3095:ASN:C	2:B:3096:ILE:HG13	2.45	0.41
1:C:43:TRP:O	1:C:45:ASP:N	2.44	0.41
2:D:2421:GLN:C	2:D:2423:ILE:N	2.75	0.41
2:D:2424:ARG:HH12	2:D:2516:TRP:CD1	2.38	0.41
2:D:2906:TYR:CE1	2:D:2933:ARG:NE	2.88	0.41
2:D:3046:LEU:HD22	2:D:3090:LYS:HB2	2.02	0.41
2:D:3100:TYR:O	2:D:3103:ALA:N	2.53	0.41
2:B:2488:GLU:HG2	2:B:2527:LYS:HD2	2.02	0.41
2:B:2688:LEU:HD13	2:B:2706:LEU:HD23	2.02	0.41
2:B:2958:THR:O	2:B:2961:THR:HB	2.19	0.41
2:B:3066:PHE:CD1	2:B:3066:PHE:C	2.98	0.41
1:C:45:ASP:O	1:C:45:ASP:OD2	2.39	0.41
2:D:2455:ALA:O	2:D:2456:ALA:C	2.63	0.41
2:D:2735:LEU:HD13	2:D:2748:VAL:HG11	2.02	0.41
2:D:2750:VAL:HG11	2:D:2903:VAL:CG2	2.48	0.41
2:B:2457:VAL:HG21	2:B:2568:PHE:CE2	2.56	0.41
2:B:2461:VAL:HB	2:B:2462:PRO:HD2	2.01	0.41
2:B:2710:ALA:HA	2:B:2713:THR:HG23	2.01	0.41
2:B:2908:LYS:O	2:B:2910:GLU:N	2.53	0.41
2:B:3047:ILE:HA	2:B:3047:ILE:HD13	1.80	0.41
2:B:3091:HIS:O	2:B:3094:GLU:N	2.53	0.41
2:D:2667:LEU:HD23	2:D:2671:LYS:HD3	2.03	0.41
2:D:2750:VAL:HG13	2:D:2904:THR:C	2.45	0.41
2:D:2937:TYR:C	2:D:2939:LEU:H	2.27	0.41
2:D:2969:SER:HB2	2:D:2972:THR:CG2	2.50	0.41
2:D:2997:CYS:C	2:D:2999:GLU:N	2.77	0.41
2:B:2412:SER:O	2:B:2414:LEU:N	2.53	0.41
2:B:2624:ILE:HG22	2:B:2647:ASP:HB3	2.01	0.41
2:B:2692:PRO:HG2	2:B:2693:ASP:H	1.84	0.41
2:B:3030:VAL:CG1	2:B:3031:VAL:N	2.84	0.41
2:D:2610:ASP:C	2:D:2612:ALA:N	2.62	0.41
2:D:2778:GLU:HA	2:D:2781:ALA:HB3	2.02	0.41
2:D:3060:SER:O	2:D:3062:VAL:N	2.54	0.41
2:B:2530:PHE:HD2	2:B:2583:LEU:HD23	1.86	0.41
2:B:2608:ARG:HH11	2:B:2608:ARG:CA	2.30	0.41
2:B:2773:ASN:C	2:B:2775:ARG:N	2.78	0.41
2:B:2909:ARG:HH11	2:B:2909:ARG:HG3	1.86	0.41
2:B:2985:PHE:CD1	2:B:2985:PHE:N	2.81	0.41
2:B:3081:HIS:O	2:B:3084:GLU:HB3	2.20	0.41
2:D:2568:PHE:C	2:D:2570:LYS:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2929:THR:O	2:D:2930:GLU:O	2.38	0.41
2:B:2476:SER:HG	2:B:2478:ALA:HB3	1.84	0.41
2:D:2900:LYS:HD2	2:D:3070:PHE:CZ	2.55	0.41
2:D:3108:ILE:HG12	2:D:3112:LYS:HE3	2.01	0.41
2:B:2480:ILE:O	2:B:2480:ILE:CG2	2.68	0.41
2:B:2651:LEU:HD12	2:B:2660:ALA:HB2	2.03	0.41
2:B:2676:THR:HG22	2:B:2679:GLN:NE2	2.36	0.41
2:B:2755:VAL:HG23	2:B:2930:GLU:CG	2.50	0.41
2:B:2902:ARG:NH1	2:B:2914:LEU:HD13	2.36	0.41
2:B:2924:LEU:HB3	2:B:2925:PRO:HD3	2.02	0.41
2:B:3097:ASP:O	2:B:3099:PHE:N	2.52	0.41
2:D:2692:PRO:O	2:D:2694:ALA:N	2.43	0.41
2:D:2950:TRP:O	2:D:2952:SER:N	2.49	0.41
2:D:3047:ILE:HA	2:D:3047:ILE:HD13	1.83	0.41
2:B:2753:GLN:HB2	2:B:2902:ARG:O	2.20	0.41
2:B:3068:GLY:N	2:B:3071:SER:OG	2.54	0.41
2:B:3096:ILE:O	2:B:3099:PHE:HD2	2.03	0.41
2:D:2552:ASN:C	2:D:2552:ASN:HD22	2.28	0.41
2:D:2578:ASN:O	2:D:2582:VAL:HG23	2.20	0.41
2:D:2709:SER:C	2:D:2713:THR:HG22	2.43	0.41
2:D:2991:PRO:O	2:D:2993:PHE:N	2.54	0.41
2:B:2403:PHE:HD1	2:B:2503:LEU:HD13	1.85	0.41
2:B:2554:TYR:CE1	2:B:2582:VAL:HG11	2.56	0.41
2:B:2600:SER:HB2	2:B:2655:TRP:HB2	2.03	0.41
2:B:2620:VAL:HG23	2:B:2677:VAL:HA	2.02	0.41
2:B:2735:LEU:HD11	2:B:2955:LEU:HD11	2.02	0.41
2:B:2921:SER:O	2:B:2924:LEU:HB2	2.21	0.41
2:B:2981:GLU:HG3	2:B:2982:LEU:N	2.36	0.41
1:C:51:ASP:O	2:D:2717:ARG:HA	2.21	0.41
2:D:2440:LEU:C	2:D:2442:LEU:N	2.79	0.41
2:D:2511:LEU:HD12	2:D:2517:LEU:HB2	2.02	0.41
2:D:2600:SER:HB3	2:D:2603:LYS:HB2	2.02	0.41
2:D:2602:LEU:HA	2:D:2605:ILE:HB	2.03	0.41
2:D:2621:SER:HB3	2:D:2652:THR:HG22	2.03	0.41
2:D:2663:ASP:OD1	2:D:2710:ALA:N	2.39	0.41
2:D:2748:VAL:HG21	2:D:2939:LEU:HD23	2.03	0.41
2:D:2762:GLU:HB3	2:D:2772:ARG:HH12	1.85	0.41
2:D:2909:ARG:HH11	2:D:2909:ARG:HG3	1.85	0.41
2:D:3068:GLY:O	2:D:3071:SER:OG	2.39	0.41
2:B:2413:SER:HB2	2:B:2506:GLY:CA	2.45	0.41
2:B:2428:LYS:C	2:B:2430:ARG:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2621:SER:O	2:B:2622:ASP:HB2	2.20	0.41
2:B:2700:ALA:HA	2:B:2701:PRO:HD3	1.91	0.41
2:B:2772:ARG:HD3	2:B:2776:GLU:O	2.20	0.41
2:B:2995:PRO:HD2	2:B:3054:TRP:CE3	2.56	0.41
2:B:3081:HIS:CD2	2:B:3082:PHE:N	2.89	0.41
2:D:2623:ILE:HA	2:D:2649:ILE:HG22	2.02	0.41
2:D:2738:LEU:HD22	2:D:2745:VAL:HG22	2.03	0.41
2:D:2755:VAL:HG13	2:D:2899:TRP:NE1	2.33	0.41
2:B:2550:VAL:O	2:B:2554:TYR:HB2	2.22	0.40
2:B:2612:ALA:O	2:B:2613:ALA:C	2.64	0.40
2:B:2615:THR:O	2:B:2615:THR:HG23	2.21	0.40
2:B:2676:THR:HG23	2:B:2679:GLN:CG	2.50	0.40
2:B:2676:THR:CG2	2:B:2679:GLN:CD	2.94	0.40
2:B:2969:SER:HB2	2:B:2972:THR:HG23	2.03	0.40
2:D:2480:ILE:O	2:D:2480:ILE:HG22	2.20	0.40
2:D:2490:PHE:O	2:D:2491:GLN:HB2	2.22	0.40
2:D:2758:LEU:HD23	2:D:2758:LEU:C	2.45	0.40
2:D:2918:TRP:O	2:D:2919:ARG:C	2.61	0.40
2:B:2403:PHE:CD1	2:B:2503:LEU:HD13	2.56	0.40
2:B:2588:TYR:O	2:B:2591:ASP:N	2.53	0.40
2:B:2599:ARG:HH22	2:B:2609:ASP:CB	2.34	0.40
2:B:2667:LEU:C	2:B:2667:LEU:CD2	2.95	0.40
2:B:2762:GLU:HB3	2:B:2772:ARG:HH12	1.86	0.40
2:B:2936:ILE:HG21	2:B:2939:LEU:HB2	2.03	0.40
2:B:3072:VAL:CG1	2:B:3073:PHE:N	2.82	0.40
1:C:57:ARG:HG2	2:D:2559:TRP:CZ2	2.56	0.40
2:D:2719:HIS:O	2:D:2720:SER:OG	2.39	0.40
2:D:2903:VAL:O	2:D:2912:SER:HA	2.21	0.40
2:B:2568:PHE:C	2:B:2570:LYS:N	2.79	0.40
2:B:2687:GLU:O	2:B:2707:LYS:N	2.54	0.40
2:D:2488:GLU:HG2	2:D:2527:LYS:HD2	2.04	0.40
2:D:2490:PHE:HE2	2:D:2492:PHE:CZ	2.38	0.40
2:D:2553:HIS:ND1	2:D:2589:ARG:HD3	2.37	0.40
2:D:2915:LEU:HD12	2:D:2915:LEU:C	2.47	0.40
2:D:3091:HIS:C	2:D:3093:ILE:N	2.79	0.40
1:A:59:GLU:O	1:A:60:LEU:C	2.64	0.40
2:B:2427:ASN:OD1	2:B:2430:ARG:HD2	2.21	0.40
2:B:2461:VAL:HB	2:B:2462:PRO:CD	2.51	0.40
2:B:2482:VAL:HA	2:B:2486:ASN:HD21	1.86	0.40
2:B:2602:LEU:CB	2:B:2653:ASP:OD2	2.69	0.40
2:B:2610:ASP:C	2:B:2612:ALA:N	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2939:LEU:HD21	2:B:2955:LEU:HD23	2.04	0.40
2:B:3042:LYS:O	2:B:3045:VAL:HG23	2.21	0.40
2:B:3108:ILE:HA	2:B:3111:LEU:CB	2.52	0.40
1:C:59:GLU:O	1:C:60:LEU:C	2.65	0.40
2:D:2676:THR:CG2	2:D:2679:GLN:CD	2.94	0.40
2:D:2917:ILE:HD13	2:D:2924:LEU:CD2	2.41	0.40
2:D:2983:LEU:C	2:D:2983:LEU:HD13	2.47	0.40
2:B:2494:ILE:HD11	2:B:2523:GLY:HA3	2.03	0.40
2:B:2569:PRO:O	2:B:2573:ALA:HA	2.21	0.40
2:B:2738:LEU:HD22	2:B:2745:VAL:CG2	2.52	0.40
2:B:2903:VAL:O	2:B:2912:SER:HA	2.22	0.40
2:B:2906:TYR:CE1	2:B:2933:ARG:NE	2.89	0.40
2:B:3100:TYR:CD1	2:B:3101:LYS:N	2.90	0.40
2:D:2499:GLY:O	2:D:2501:GLU:HG2	2.22	0.40
2:D:2501:GLU:O	2:D:2501:GLU:HG3	2.21	0.40
2:D:2719:HIS:CD2	2:D:2720:SER:H	2.40	0.40
2:D:2950:TRP:N	2:D:2951:PRO:CD	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	41/70 (59%)	18 (44%)	11 (27%)	12 (29%)	0	0
1	C	41/70 (59%)	18 (44%)	11 (27%)	12 (29%)	0	0
2	B	585/817 (72%)	387 (66%)	128 (22%)	70 (12%)	0	2
2	D	585/817 (72%)	391 (67%)	122 (21%)	72 (12%)	0	1
All	All	1252/1774 (71%)	814 (65%)	272 (22%)	166 (13%)	0	1

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	47	ASN
1	A	51	ASP
1	A	53	SER
1	A	57	ARG
2	B	2429	GLU
2	B	2448	LEU
2	B	2465	CYS
2	B	2466	SER
2	B	2467	PRO
2	B	2501	GLU
2	B	2512	ALA
2	B	2573	ALA
2	B	2610	ASP
2	B	2611	THR
2	B	2647	ASP
2	B	2686	ALA
2	B	2692	PRO
2	B	2737	SER
2	B	2752	VAL
2	B	2907	LYS
2	B	2909	ARG
2	B	2912	SER
2	B	2930	GLU
2	B	2941	VAL
2	B	2942	SER
2	B	2944	SER
2	B	2946	ASN
2	B	2950	TRP
2	B	3016	ALA
2	B	3038	ASN
2	B	3099	PHE
2	B	3101	LYS
2	B	3114	ASP
1	C	9	ASP
1	C	41	ASP
1	C	47	ASN
1	C	51	ASP
1	C	53	SER
1	C	57	ARG
2	D	2429	GLU
2	D	2448	LEU
2	D	2465	CYS

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Mol	Chain	Res	Type
2	D	2466	SER
2	D	2467	PRO
2	D	2501	GLU
2	D	2512	ALA
2	D	2573	ALA
2	D	2610	ASP
2	D	2611	THR
2	D	2647	ASP
2	D	2686	ALA
2	D	2692	PRO
2	D	2737	SER
2	D	2752	VAL
2	D	2907	LYS
2	D	2909	ARG
2	D	2912	SER
2	D	2941	VAL
2	D	2942	SER
2	D	2944	SER
2	D	2946	ASN
2	D	2950	TRP
2	D	2998	SER
2	D	3016	ALA
2	D	3038	ASN
2	D	3099	PHE
2	D	3101	LYS
2	D	3114	ASP
1	A	9	ASP
1	A	39	TRP
1	A	55	GLN
2	B	2407	ASN
2	B	2415	GLN
2	B	2460	SER
2	B	2507	LYS
2	B	2605	ILE
2	B	2694	ALA
2	B	2721	LYS
2	B	2893	ARG
2	B	2945	LYS
2	B	2979	PRO
2	B	2992	ALA
2	B	2998	SER
2	B	3040	ASP

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Mol	Chain	Res	Type
2	B	3092	ALA
1	C	39	TRP
1	C	55	GLN
2	D	2415	GLN
2	D	2460	SER
2	D	2507	LYS
2	D	2694	ALA
2	D	2721	LYS
2	D	2893	ARG
2	D	2930	GLU
2	D	2945	LYS
2	D	2979	PRO
2	D	2992	ALA
2	D	3040	ASP
2	D	3088	ASN
2	D	3092	ALA
2	B	2406	PHE
2	B	2519	PRO
2	B	2564	MET
2	B	2569	PRO
2	B	2710	ALA
2	B	2738	LEU
2	B	2970	SER
2	B	2988	LEU
2	B	3095	ASN
2	D	2519	PRO
2	D	2564	MET
2	D	2697	PRO
2	D	2710	ALA
2	D	2910	GLU
2	D	2954	GLN
2	D	2970	SER
2	D	2988	LEU
2	D	3095	ASN
1	A	44	ASP
2	B	2697	PRO
2	B	2764	THR
2	B	2910	GLU
2	B	2954	GLN
2	B	3008	SER
2	B	3088	ASN
1	C	10	LEU

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Mol	Chain	Res	Type
1	C	44	ASP
2	D	2407	ASN
2	D	2464	ALA
2	D	2490	PHE
2	D	2569	PRO
2	D	2605	ILE
2	D	2672	SER
2	D	2738	LEU
2	D	2764	THR
2	B	2490	PHE
2	D	2779	LYS
2	D	2985	PHE
2	D	3008	SER
2	D	3039	GLU
2	B	2447	THR
2	B	2685	GLY
2	B	2779	LYS
2	B	2991	PRO
2	D	2447	THR
2	D	2991	PRO
2	B	2462	PRO
1	C	48	VAL
2	D	2919	ARG
1	A	7	PRO
1	A	48	VAL
2	B	2592	VAL
2	B	3035	ILE
1	C	7	PRO
2	D	2462	PRO
2	D	2480	ILE
2	D	3035	ILE
1	A	8	VAL
2	D	2685	GLY
2	B	2474	GLY
2	B	3063	PRO
2	D	2592	VAL
2	D	2953	ILE
2	B	2480	ILE
2	B	2953	ILE

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	41/63 (65%)	33 (80%)	8 (20%)	1	5
1	C	41/63 (65%)	33 (80%)	8 (20%)	1	5
2	B	517/721 (72%)	464 (90%)	53 (10%)	7	24
2	D	517/721 (72%)	460 (89%)	57 (11%)	6	22
All	All	1116/1568 (71%)	990 (89%)	126 (11%)	5	21

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	19	PHE
1	A	22	PHE
1	A	23	PRO
1	A	39	TRP
1	A	49	GLU
1	A	56	LEU
1	A	60	LEU
2	B	2419	ASP
2	B	2430	ARG
2	B	2433	LEU
2	B	2434	CYS
2	B	2442	LEU
2	B	2443	THR
2	B	2450	ARG
2	B	2453	LEU
2	B	2483	ASN
2	B	2485	LYS
2	B	2494	ILE
2	B	2527	LYS
2	B	2534	LEU
2	B	2537	THR
2	B	2548	VAL
2	B	2583	LEU

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Mol	Chain	Res	Type
2	B	2584	LEU
2	B	2586	LEU
2	B	2598	SER
2	B	2608	ARG
2	B	2609	ASP
2	B	2614	LYS
2	B	2658	VAL
2	B	2675	LEU
2	B	2684	GLN
2	B	2698	LEU
2	B	2706	LEU
2	B	2713	THR
2	B	2714	ARG
2	B	2726	HIS
2	B	2733	LEU
2	B	2736	SER
2	B	2744	ASN
2	B	2748	VAL
2	B	2750	VAL
2	B	2756	TYR
2	B	2773	ASN
2	B	2901	LEU
2	B	2915	LEU
2	B	2968	VAL
2	B	2985	PHE
2	B	3007	VAL
2	B	3026	LEU
2	B	3029	LEU
2	B	3047	ILE
2	B	3056	PRO
2	B	3058	SER
2	B	3062	VAL
2	B	3063	PRO
2	B	3072	VAL
2	B	3087	THR
2	B	3099	PHE
2	B	3109	GLN
1	C	14	GLU
1	C	19	PHE
1	C	22	PHE
1	C	23	PRO
1	C	39	TRP

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Mol	Chain	Res	Type
1	C	49	GLU
1	C	56	LEU
1	C	60	LEU
2	D	2405	GLN
2	D	2419	ASP
2	D	2430	ARG
2	D	2433	LEU
2	D	2434	CYS
2	D	2442	LEU
2	D	2443	THR
2	D	2450	ARG
2	D	2453	LEU
2	D	2483	ASN
2	D	2485	LYS
2	D	2494	ILE
2	D	2527	LYS
2	D	2534	LEU
2	D	2537	THR
2	D	2548	VAL
2	D	2583	LEU
2	D	2584	LEU
2	D	2586	LEU
2	D	2598	SER
2	D	2608	ARG
2	D	2609	ASP
2	D	2614	LYS
2	D	2658	VAL
2	D	2675	LEU
2	D	2684	GLN
2	D	2698	LEU
2	D	2706	LEU
2	D	2713	THR
2	D	2714	ARG
2	D	2726	HIS
2	D	2733	LEU
2	D	2736	SER
2	D	2744	ASN
2	D	2748	VAL
2	D	2750	VAL
2	D	2756	TYR
2	D	2773	ASN
2	D	2901	LEU

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Mol	Chain	Res	Type
2	D	2915	LEU
2	D	2941	VAL
2	D	2944	SER
2	D	2955	LEU
2	D	2968	VAL
2	D	2985	PHE
2	D	3007	VAL
2	D	3026	LEU
2	D	3029	LEU
2	D	3047	ILE
2	D	3056	PRO
2	D	3058	SER
2	D	3062	VAL
2	D	3063	PRO
2	D	3087	THR
2	D	3099	PHE
2	D	3109	GLN
2	D	3117	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	B	2421	GLN
2	B	2436	GLN
2	B	2454	GLN
2	B	2486	ASN
2	B	2497	HIS
2	B	2552	ASN
2	B	2574	ASN
2	B	2596	ASN
2	B	2954	GLN
2	B	2962	GLN
2	B	2965	GLN
2	B	3051	ASN
2	B	3053	GLN
2	B	3081	HIS
2	B	3083	GLN
2	B	3095	ASN
2	B	3109	GLN
1	C	54	ASN
2	D	2405	GLN

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Mol	Chain	Res	Type
2	D	2436	GLN
2	D	2454	GLN
2	D	2486	ASN
2	D	2497	HIS
2	D	2552	ASN
2	D	2574	ASN
2	D	2596	ASN
2	D	2684	GLN
2	D	2954	GLN
2	D	2962	GLN
2	D	2965	GLN
2	D	3051	ASN
2	D	3053	GLN
2	D	3081	HIS
2	D	3083	GLN
2	D	3095	ASN
2	D	3109	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.