



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2017 – 10:19 AM EST

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

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

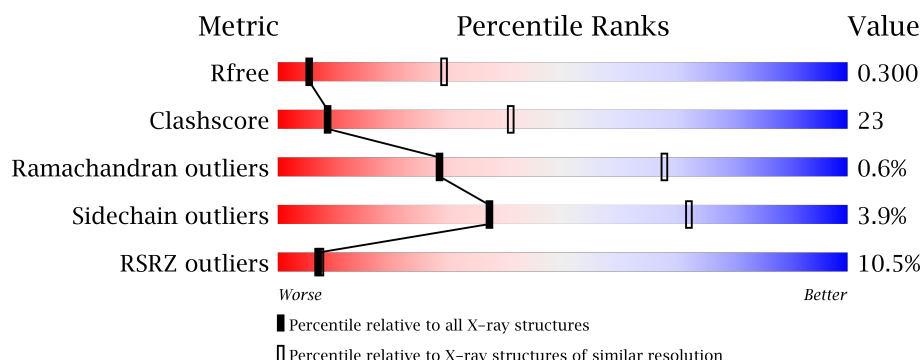
1 Overall quality at a glance

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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>11%</div> <div>66%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>9%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5400	-	-	X	-
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	A	5403	-	-	X	-
4	SO4	B	5403	-	-	X	-

2 Entry composition

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.

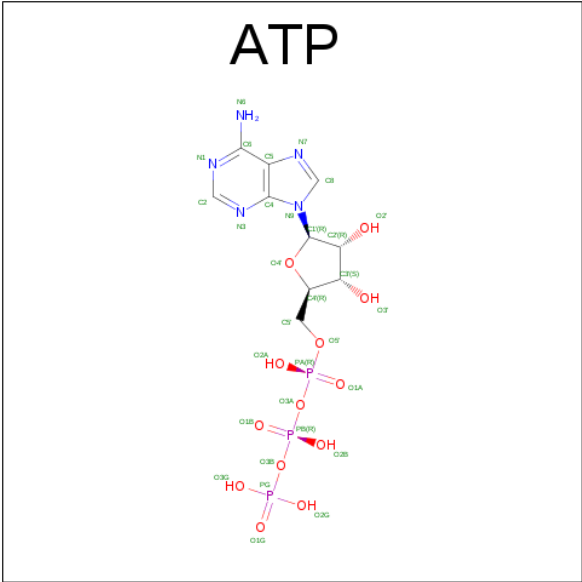
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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:

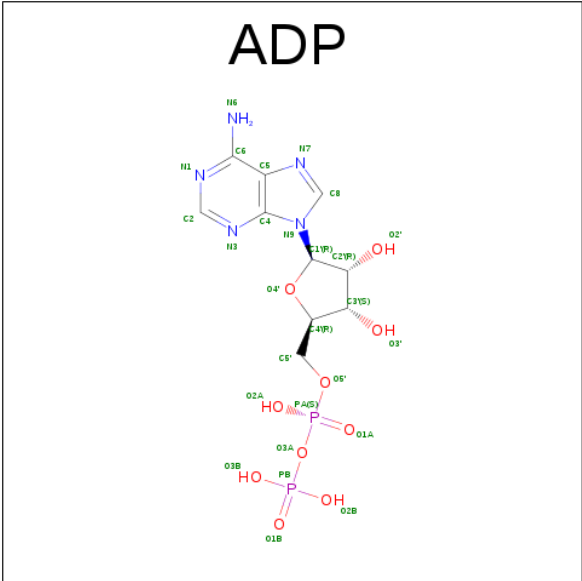
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	LINKER	UNP P36022
A	218	SER	-	LINKER	UNP P36022
A	219	ASP	-	LINKER	UNP P36022
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	217	LYS	-	LINKER	UNP P36022
B	218	SER	-	LINKER	UNP P36022
B	219	ASP	-	LINKER	UNP P36022
B	1630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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



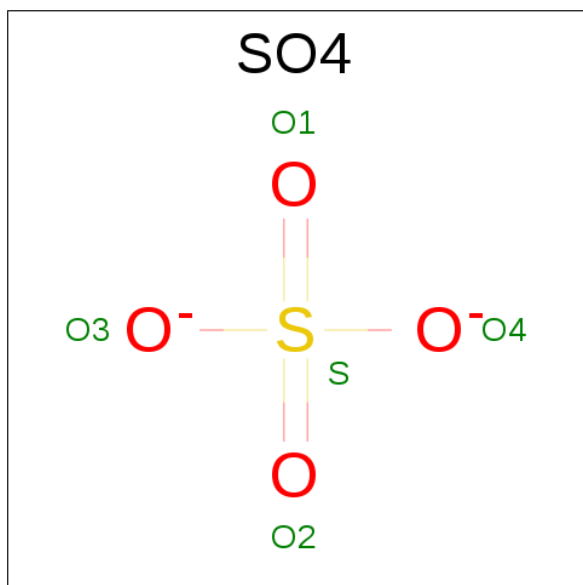
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is SULFATE ION (three-letter code: 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		

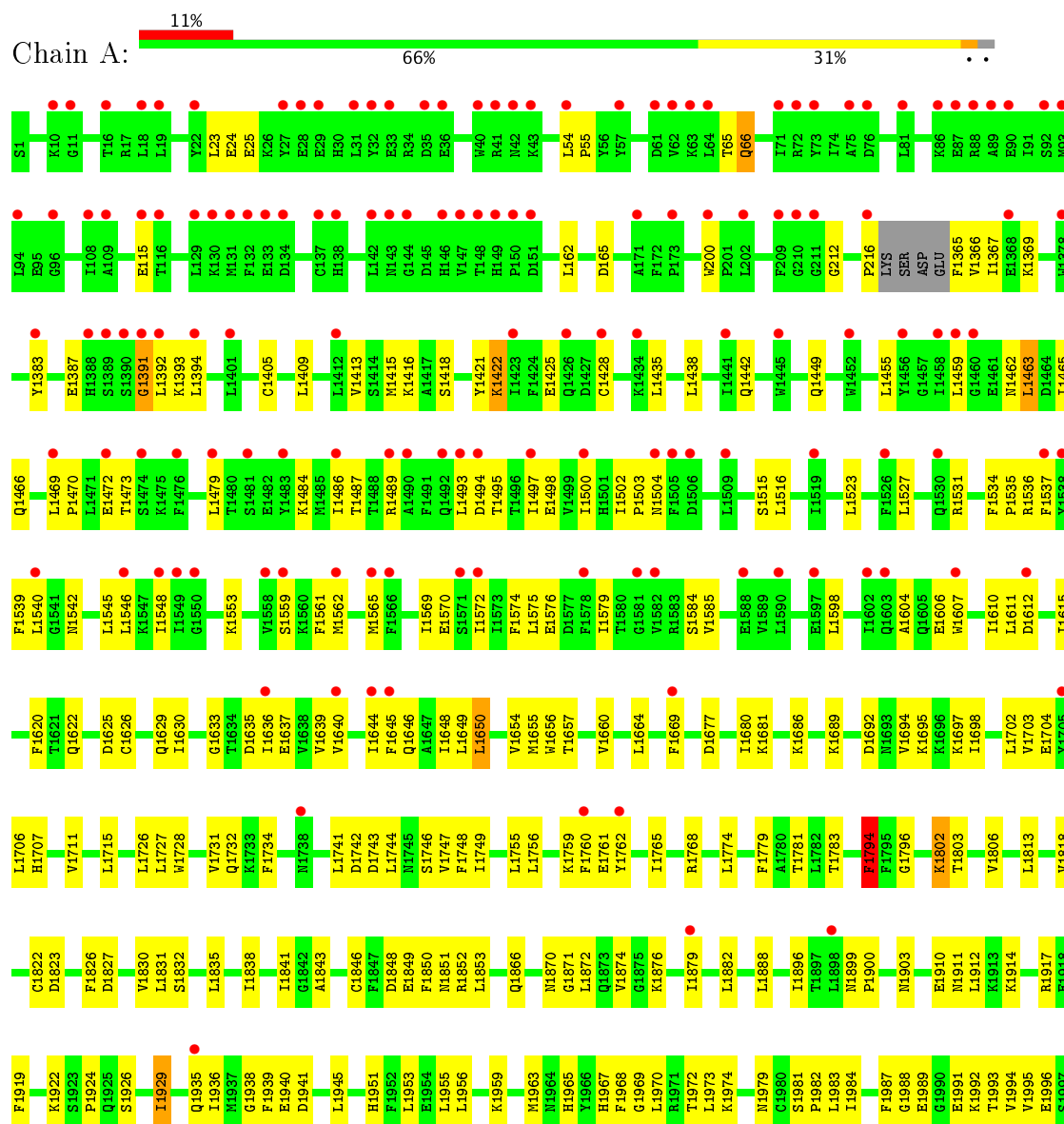
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

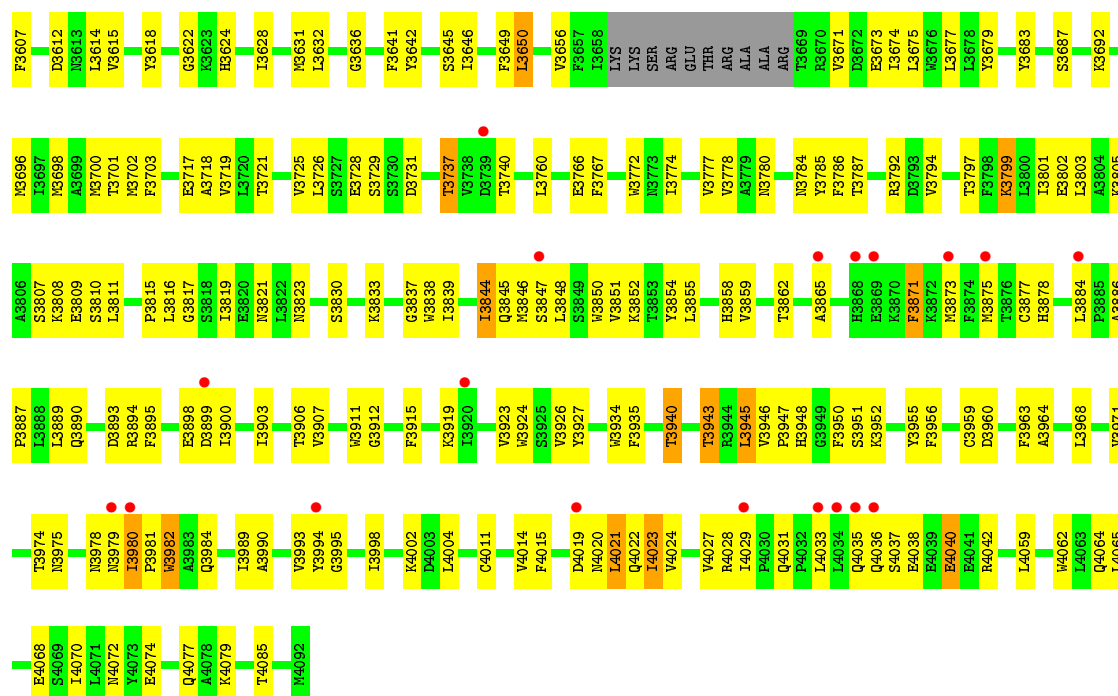
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



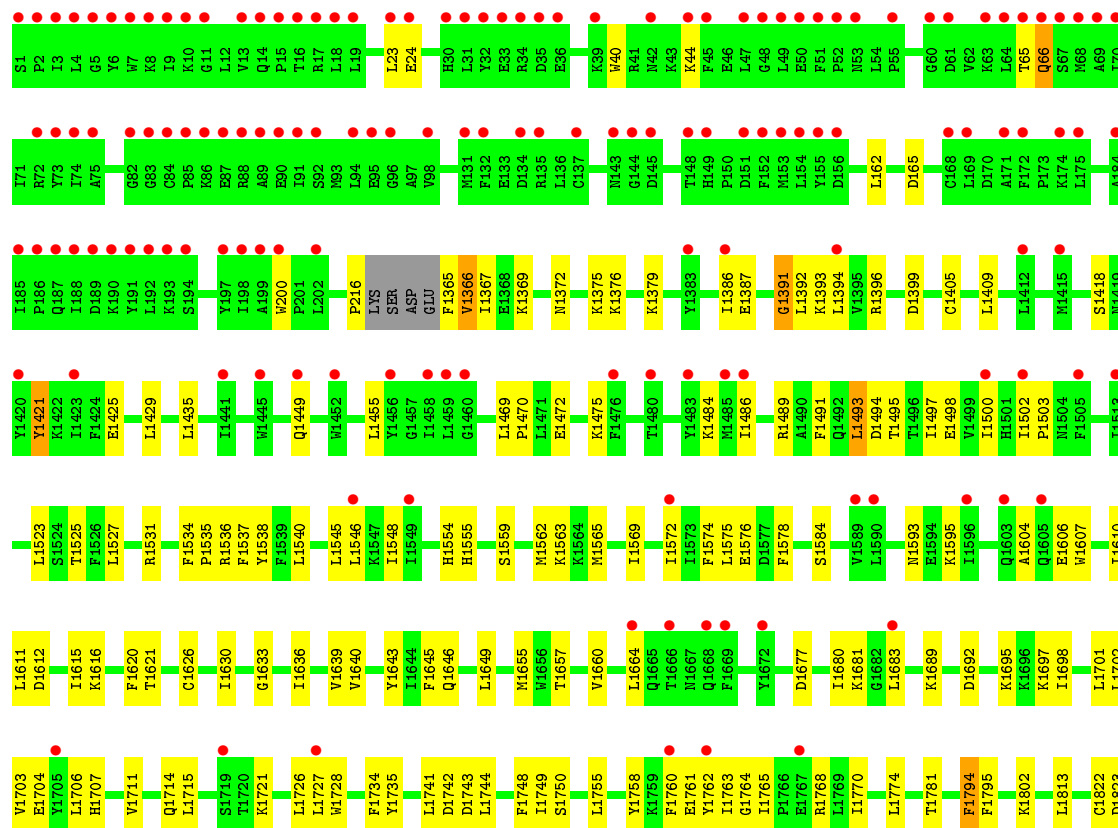
L3534	L3535	E3536	E3537	N3538	N3541	Q3542	R3543	K3544	D3547	L3548	L3549	L3551	E3554	E3555	K3556	K3557	L3558	L3559	K3560	K3561	L3562	E3563	K3564	L3565	L3566	L3567	L3570	G3575	K3576	K3577	L3578	E3579	K3580	D3581	E3582	L3583	N3584	L3587	N3588	L3589	L3590	K3591	K3592	E3593	N3594	L3595	N3596	L3597	E3598	L3601																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
I3408	D3409	I3415	K3425	T3426	F3436	R3439	L3440	F3446	G3447	S3448	F3458	D3459	P3460	I3461	S3462	S3463	R3464	S3467	N3471	H3472	R3476	V3477	V3478	E3481	G3482	H3484	I3505	P3506	L3509	R3510	V3513	F3518	V3519	T3520	N3521	L3525	R3528	L3529	F3530	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
T3309	T3310	Q3311	Q3312	F3313	T3316	S3317	T3318	E3319	L3320	I3321	G3322	N3323	G3324	L3325	L3326	S3327	Y3330	E3331	F3334	N3338	E3341	R3342	L3346	K3350	L3353	G3354	K3355	F3356	A3357	V3358	K3359	D3361	I3367	I3370	V3371	T3372	L3373	K3386	L3391	E3392	N3393	L3395	R3396	L3397	E3398	L3400	F3406	L3407																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
H2886	F2889	T2890	T2891	C2892	D2893	T2894	M2902	R2812	T2813	L2816	E2819	C2912	V2916	H2917	D2918	N2919	T2924	A2929	V2933	L2936	F2937	M2938	E2939	F2940	T2941	D2942	L2943	I2944	V2945	I2946	V2947	V2948	V2949	V2950	V2951	V2952	V2953	V2954	V2955	V2956	V2957	V2958	V2959	V2960	V2961	V2962	V2963	V2964	V2965																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
Y2977	V2982	G2983	V2984	N2985	P2986	R2987	S2988	P2989	G2990	L2999	L3002	Y3007	L3010	Q3014	V3017	N3018	V3019	L3021	E3022	K3023	L3024	N3025	E3026	V3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259	L3260	L3261	L3262	L3263	L3264	L3265	L3266	L3267	L3268	L3269	L3270	L3271	L3272	L3273	L3274	L3275	L3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293	L3294	L3295	L3296	L3297	L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413	L3414	L3415	L3416	L3417	L3418	L3419	L3420	L3421	L3422	L3423	L3424	L3425	L3426	L3427	L3428	L3429	L3430	L3431	L3432	L3433	L3434	L3435	L3436	L3437	L3438	L3439	L3440	L3441	L3442	L3443	L3444	L3445	L3446	L3447	L3448	L3449	L3450	L3451	L3452	L3453	L3454	L3455	L3456	L3457	L3458	L3459	L3460	L3461	L3462	L3463	L3464	L3465	L3466	L3467	L3468	L3469	L3470	L3471	L3472	L3473	L3474	L3475	L3476	L3477	L3478	L3479	L3480	L3481	L3482	L3483	L3484	L3485	L3486	L3487	L3488	L3489	L3490	L3491	L3492	L3493	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601
T2472	L2473	L2474	P2475	K2476	S2477	D2478	L2482	F2485	E2488	L2489	N2490	L2491	P2492	K2493	L2494	D2495	Y2497	G2498	S2499	L2506	Q2508	L2509	K2512	Q2513	Q2514	K2517	T2518	P2519	V2524	T2525	L2526	E2527	R2528	A2534	C2535	N2536	R2543	R2549	F2550	L2551	R2552	F2553	D2554	A2555	P2562	S2563	G2564																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
K2565	S2566	Q2569	L2570	Y2571	Y2574	Y2575	L2576	A2577	L2578	L2581	V2582	F2582	L2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	L2639	L2640	L2641	L2642	L2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2822	L2823	L2824	L2825	L2826	L2827	L2828	L2829	L2830	L2831	L2832	L2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	L2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933	L2934	L2935	L2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3																																																																																																																																																		



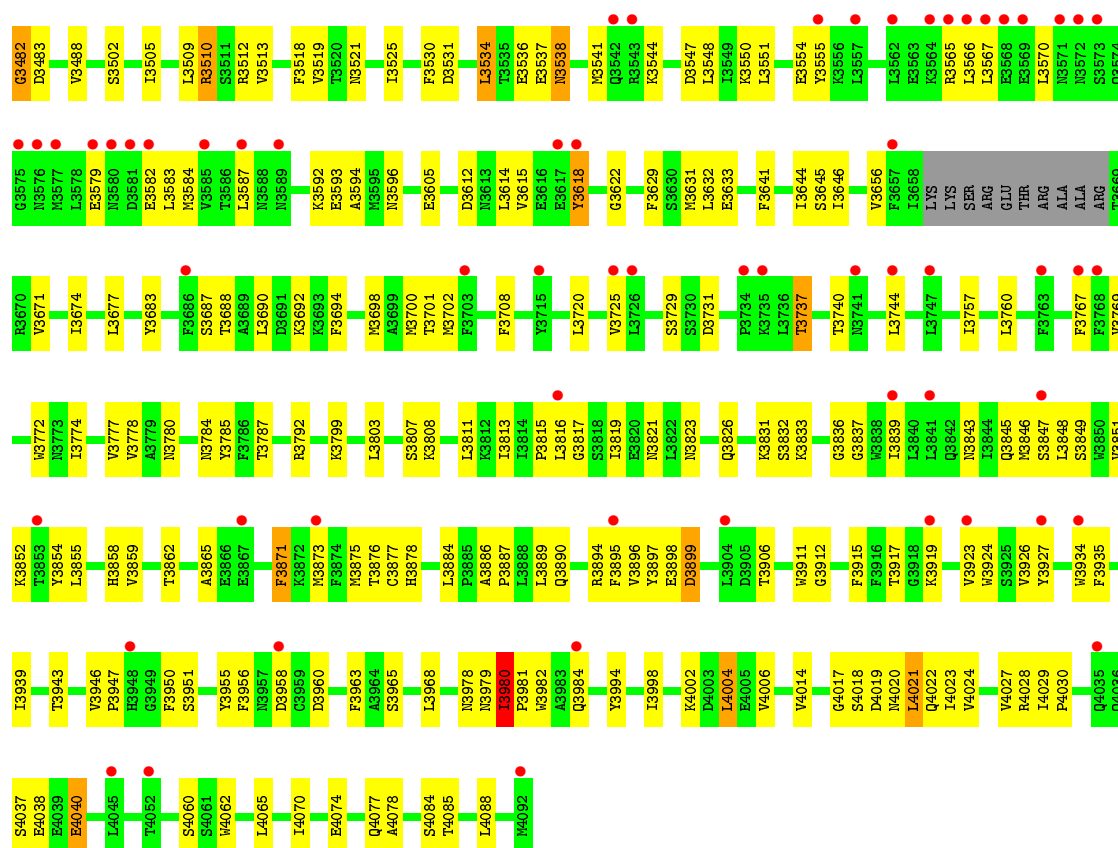
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



Chain B:



Y3360	D3361	I3367	V3371	T3372	F3390	L3391	E3392	N3393	S3400	Q3401	D3402	A3403	F3406	L3407	D3408	D3409	H3413	H3414	T3415	V3417	L3429	R3439	L3440	A3443	F3446	V3450	D3459	P3460	I3461	I3462	S3463	L3464	L3465	S3466	S3467	F3470	N3471	H3472	A3473	R3476	V3477	T3478	I3481					
LEU	VAL	ASN	GLU	LEU	ASN	THR	LEU	VAL	PRO	GLU	VAL	VAL	K3297	T3300	K3303	E3304	R3305	H3306	L3307	M3308	K3311	Q3312	F3313	S3314	K3315	S3317	Q3318	E3319	M3323	I3326	S3329	Y3330	F3334	M3338	E3341	R3342	L3346	V3347	L3348	L3349	K3350	R3351	L3352	L3353	V3356	T3357		
E2824	T2825	A2826	E2829	N2832	T2833	L2834	L2835	A2838	D2842	L2843	F2844	Q2845	G2846	Y2849	L2852	L2853	L2856	T2860	L2866	L2867	E2870	L2873	F2877	L2878	H2886	F2889	T2890	L2891	C2892	D2893	P2894	M2902	L2903	A2907	N2910	R2911	C2912	T2913	L2914	N2915	W2916							
W2920	T2924	H2938	T2941	D2942	L2943	ILE	VAL	PRO	GLU	VAL	ASN	LYS	GLU	LEU	VAL	PHE	THR	GLU	PRO	ILE	T2960	T2961	T2962	T2963	T2964	T2965	T2966	T2972	T2982	T2983	S2988	P2989	G2990	K3001	L3010	Q3011	E3012	F3016	V3017	N3018	V3019	G3020	L3024	N3025	E3026	L3027	N3028	
L2734	S2737	M2738	H2741	L2742	L2743	L2744	L2745	Q2751	G2754	H2755	M2756	F2757	L2758	L2759	G2760	A2761	S2762	R2763	L2764	T2765	K2766	L2779	T2780	L2781	Q2782	Q2783	P2784	K2785	H2787	R2788	L2792	F2795	L2799	R2812	T2813	C2814	L2815	L2816	L2817	L2818	E2819	L2822	L2823					
Y2497	G2498	S2499	L2506	R2507	Q2508	K2512	Q2513	K2517	P2519	E2520	V2524	T2525	L2526	E2527	L2528	L2529	H2530	I2531	C2535	N2536	G2542	L2543	L2544	R2549	R2552	H2553	L2556	P2562	S2563	S2566	Y2571	E2572	L2573	Y2574	Y2575	L2578	F2579	K2580	L2581	L2582	V2582	R2586	S2587	E2590				
D2406	N2409	S2410	K2411	R2412	I2415	L2416	C2417	P2420	K2424	T2425	M2428	L2437	V2440	F2445	S2446	K2447	D2448	T2449	L2455	L2458	Y2464	T2467	S2468	L2471	T2472	L2473	L2474	P2475	K2476	S2477	D2478	K2480	L2484	E2488	R2489	R2490	L2491	P2492	K2493	L2494	D2495	K2496						
S2309	L2310	K2311	D2312	V2313	L2314	T2315	L2316	L2317	K2318	R2319	R2320	S2321	L2322	L2326	G2332	Q2335	R2336	I2339	F2346	S2350	Q2351	S2354	S2355	Y2356	S2357	T2358	L2359	L2361	A2362	N2363	D2364	K2365	L2366	S2367	F2368	V2378	S2379	L2380	E2384	R2385	R2386	R2387	L2390	T2394	L2395	D2396	T2397	
D2197	F2198	L2199	H2201	T2202	T2203	T2204	A2205	L2212	C2220	S2221	T2222	S2223	S2224	K2225	L2229	L2230	N2239	V2261	V2262	V2263	F2264	D2265	S2266	F2267	L2268	T2269	L2272	H2274	L2275	L2276	R2279	T2280	F2281	N2282	E2285	V2288	H2293	L2294	T2295	R2299	F2302	L2305	D2306					
L2109	T2110	E2112	S2117	K2121	T2122	L2123	D2127	K2132	T2131	V2137	I2141	F2145	R2149	V2151	V2152	V2153	F2154	D2155	S2156	D2157	L2158	D2159	E2161	E2164	V2169	D2172	K2174	L2175	L2176	T2177	L2178	G2181	E2182	R2183	T2186	F2190	R2192	L2193	E2194	E2195	T2196							
F1826	D1827	Y1828	Q1829	V1830	H1831	L1832	S1833	L1834	L1835	I1838	I1841	G1842	L1843	H1844	G1845	E1849	F1850	N1851	L1852	L1853	V1857	N1864	I1865	Q1866	N1870	G1871	L1872	L1882	L1888	N1889	P1900	R1905	L1908	P1909	E1910	N1911	L1912	R1917	E1918	F1919	S1920	M1921	K1922	S1923	Q1924	S1926		
I1929	Q1935	H1936	H1937	G1938	F1939	E1940	D1941	S1942	L1945	I1949	F1952	L1953	L1956	H1967	F1968	G1969	L1970	R1971	T1972	L1973	K1974	L1977	R1978	N1979	C1980	S1981	P1982	L1983	L1988	E1989	G1990	E1991	K1992	T1993	V1994	V1995	E1996	S1997	L1998	K1999	R2000	V2001	T2002	L2003	L2006	G2007	D2008	E2011
F2014	I2021	D2023	S2024	T2027	P2028	K2032	L2033	I2034	V2035	G2042	D2043	R2044	P2049	F2060	V2061	V2062	K2063	K2064	T2066	D2067	K2068	K2069	L2070	L2071	L2072	V2073	G2074	K2080	T2081	A2082	T2083	K2084	K2085	T2086	V2087	L2088	K2091	K2092	I2093	F2094	D2095	N2099	D2105	T2106	V2108			



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 49.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.24-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.303 0.236 , 0.300	Depositor DCC
R_{free} test set	5512 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	133.4	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 132.2	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	0.94	EDS
Total number of atoms	41678	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

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

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

5.1 Standard geometry

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

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

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

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

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3308	ASN	Peptide

5.2 Too-close contacts ⓘ

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2620:ARG:NH2	3:A:5401:ADP:PA	2.64	0.70
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.74	0.70
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.72	0.70
1:B:2631:THR:O	1:B:2635:THR:HG22	1.92	0.70
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.32	0.70
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	2.27	0.70
1:A:2763:ARG:HE	3:A:5402:ADP:C4'	2.04	0.70
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.65	0.70
1:A:1455:LEU:HD12	1:A:1516:LEU:HD23	1.74	0.70
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.19	0.70
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.21	0.70
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.22	0.70
1:A:3304:GLU:O	1:A:3307:LEU:CB	2.40	0.70
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.78	0.70
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.55	0.70
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.73	0.70
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	2.07	0.70
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	1.91	0.70
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.74	0.70
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.92	0.70
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.90	0.69
1:A:3307:LEU:CD1	1:A:3307:LEU:C	2.57	0.69
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.74	0.69
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.69	0.69
1:B:2080:LYS:HE2	2:B:5400:ATP:PB	2.32	0.69
1:B:2378:VAL:CG2	1:B:2380:LEU:HD11	2.23	0.69
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.19	0.69
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.51	0.69
1:B:2728:LEU:HD12	1:B:2771:ARG:HH22	1.57	0.69
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.27	0.69
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.22	0.69
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.74	0.69
1:A:1415:MET:O	1:A:1421:TYR:CD2	2.46	0.69
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.73	0.69
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.91	0.69
1:B:2732:MET:CE	1:B:2768:ILE:HG23	1.99	0.69
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.75	0.69
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.58	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.52
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	1.91	0.52
1:B:2891:ILE:HD11	1:B:2903:ILE:HD11	1.90	0.52
1:A:1416:LYS:O	1:A:1421:TYR:OH	2.25	0.52
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.91	0.52
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.54	0.52
1:A:3701:THR:OG1	1:A:4085:THR:HG22	2.08	0.52
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.45	0.52
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.74	0.52
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.92	0.52
1:A:2473:LEU:HD22	1:A:2527:GLU:HG2	1.91	0.52
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.44	0.52
1:A:1416:LYS:O	1:A:1421:TYR:CE2	2.63	0.52
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.44	0.52
1:A:3304:GLU:O	1:A:3307:LEU:HB3	2.10	0.52
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.91	0.52
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.50	0.52
1:B:2624:ARG:NH2	1:B:2910:ASN:O	2.43	0.52
1:B:3934:TRP:CB	1:B:4023:ILE:HD13	2.40	0.52
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.44	0.52
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.91	0.52
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.10	0.52
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.30	0.52
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.90	0.52
1:A:1970:LEU:CD2	1:A:1974:LYS:HE2	2.40	0.52
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.50	0.52
1:B:2073:VAL:HG21	1:B:2199:LEU:HD11	1.92	0.52
1:B:23:LEU:O	1:B:24:GLU:CB	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.86	0.51
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.46	0.51
1:B:2080:LYS:HG3	2:B:5400:ATP:O1B	2.11	0.51
1:B:2080:LYS:HG3	1:B:2195:GLU:OE1	2.10	0.51
1:B:2386:MET:HB2	1:B:2627:ARG:CD	2.37	0.51
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.29	0.51
1:B:3934:TRP:HB3	1:B:4023:ILE:HD13	1.93	0.51
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.11	0.51
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.92	0.51
1:A:2633:ILE:HD11	1:A:2644:LEU:CD2	2.41	0.51
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.89	0.51
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.92	0.51
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	1.92	0.51
1:A:2517:LYS:HG3	1:A:2524:VAL:HG23	1.93	0.51
1:A:3303:LYS:HA	1:A:3306:TRP:HB2	1.92	0.51
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.40	0.51
1:B:2257:PHE:HD1	1:B:2262:LEU:HD11	1.75	0.51
1:B:3911:TRP:HH2	1:B:3926:VAL:HG13	1.76	0.51
1:A:3460:PRO:O	1:A:3463:SER:CB	2.59	0.51
1:B:1910:GLU:CB	1:B:3846:MET:HB3	2.41	0.51
1:B:2506:LEU:HD22	1:B:2531:ILE:HD12	1.91	0.51
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.92	0.51
1:B:2786:ILE:HD12	1:B:3460:PRO:HG2	1.92	0.51
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.91	0.51
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.30	0.51
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.11	0.51
1:A:2154:PHE:CD1	1:A:2154:PHE:N	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4074:GLU:HA	1:B:4077:GLN:HE21	1.80	0.46
1:A:2856:LEU:HD21	1:A:2877:PHE:HB2	1.97	0.46
1:A:3304:GLU:O	1:A:3307:LEU:N	2.48	0.46
1:A:3509:LEU:O	1:A:3513:VAL:HG23	2.16	0.46
1:A:3624:HIS:ND1	1:A:3675:LEU:HD11	2.30	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.97	0.46
1:A:3945:LEU:HD21	1:A:4070:ILE:CD1	2.45	0.46
1:B:1563:LYS:HA	1:B:1569:ILE:O	2.15	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG23	2.15	0.46
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.15	0.46
1:B:2080:LYS:CE	1:B:2549:ARG:HH21	2.28	0.46
1:B:4023:ILE:CD1	1:B:4029:ILE:HD11	2.45	0.46
1:A:1970:LEU:HD21	1:A:1974:LYS:HE2	1.97	0.46
1:A:3990:ALA:HB2	1:A:4011:CYS:SG	2.56	0.46
1:B:1386:ILE:CG2	1:B:1396:ARG:HG2	2.46	0.46
1:B:2081:THR:HG22	1:B:2085:LYS:HD2	1.97	0.46
1:B:2732:MET:SD	3:B:5402:ADP:N7	2.89	0.46
1:B: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:2786:ILE:HD12	1:B:3460:PRO:CG	2.46	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:2339:ILE:HG23	1:A:2353:LEU:HB3	1.97	0.46
1:A:2420:PRO:CG	1:A:2616:LEU:HD21	2.45	0.46
1:A:2938:MET:SD	1:A:3321:ILE:CG2	3.03	0.46
1:A:2999:LEU:HD11	1:A:3325:ILE:HG12	1.97	0.46
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.50	0.46
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.55	0.46
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.98	0.46
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.63	0.46
1:B:3911:TRP:CH2	1:B:3926:VAL:HG13	2.51	0.46
1:A:1418:SER:O	1:A:1421:TYR:CD2	2.68	0.46
1:A: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.97	0.46
1:A:2219:VAL:HG21	2:A:5400:ATP:N7	2.31	0.46
1:B:3701:THR:OG1	1:B:4085:THR:HG22	2.15	0.46
1:B:3725:VAL:HG22	1:B:3731:ASP:HA	1.96	0.46
1:B:2081:THR:HB	2:B:5400:ATP:O2A	2.15	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: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:23:LEU:O	1:A:25:GLU:N	2.49	0.46
1:A:2754:GLY:HA3	1:A:2886:HIS:CE1	2.51	0.46
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	1.97	0.46
1:B:1838:ILE:HD11	1:B:1845:GLY:CA	2.46	0.46
1:B:2394:THR:H	1:B:2397:THR:HB	1.81	0.46
1:A:1644:ILE:O	1:A:1648:ILE:HG22	2.16	0.45
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.16	0.45
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.97	0.45
1:B:2358:THR:HG22	1:B:2359:ILE:N	2.31	0.45
1:A:2763:ARG:HA	3:A:5402:ADP:C4'	2.47	0.45
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.64	0.45
1:B:1366:VAL:CG1	1:B:1369:LYS:HE3	2.45	0.45
1:B:2856:LEU:HD21	1:B:2877:PHE:HB2	1.98	0.45
1:A:2072:LEU:HB3	1:A:2215:PHE:HE1	1.80	0.45
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.16	0.45
1:A:3373:LEU:HD13	1:A:3557:LEU:CD1	2.47	0.45
1:B: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:B:65:THR:O	1:B:66:GLN:CB	2.64	0.45
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.84	0.45
1:A:1968:PHE:N	1:A:1968:PHE:CD1	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:216:PRO:HA	1:B:1365:PHE:HA	1.98	0.45
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.29	0.45
1:B: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:B:40:TRP:O	1:B:44:LYS:N	2.50	0.45
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.98	0.45
1:A:2982:VAL:CG1	1:A:2983:GLY:H	2.29	0.45
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.99	0.45
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.47	0.45
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.94	0.45
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.00	0.45
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	1.98	0.45
1:B:2249:LEU:HA	1:B:2252:LEU:HD12	1.99	0.45
1:B:2467:THR:O	1:B:2471:LEU:N	2.48	0.45
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.16	0.45
1:B:4084:SER:O	1:B:4088:LEU:HG	2.17	0.45
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.73	0.45
1:A:1995:VAL:HG22	1:A:2022:PHE:HD2	1.80	0.45
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.99	0.45
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.36	0.45
1:B:2476:LYS:HE3	1:B:2528:ARG:CB	2.47	0.45
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.97	0.45
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.98	0.45
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.99	0.45
1:A:1956:LEU:HB3	1:A:1968:PHE:CD2	2.51	0.45
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.45
1:A:2241:LEU:HD21	1:A:2249:LEU:HD12	1.99	0.45
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.17	0.45
1:A:3306:TRP:CH2	1:A:3594:ALA:HB1	2.45	0.45
1:B:2609:THR:HA	1:B:2612:GLN:O	2.17	0.45
1:B:2695:LEU:HD23	1:B:2743:LEU:HD11	1.99	0.45
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.51	0.45
1:B:2941:THR:CG2	1:B:2942:ASP:H	2.29	0.45
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.81	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3799:LYS:HG3	1:A:3803:LEU:HD11	2.02	0.42
1:A:1914:LYS:HD3	1:A:3959:CYS:SG	2.60	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:1622:GLN:HE22	1:A:1644:ILE:H	1.67	0.42
1:A:216:PRO:CB	1:A:1365:PHE:N	2.83	0.42
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.20	0.42
1:B:2034:ILE:HD12	1:B:2061:TYR:CE2	2.54	0.42
1:B:2071:ILE:HB	1:B:2212:LEU:HD12	2.01	0.42
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.01	0.42
1:A:1874:VAL:HG21	1:A:1876:LYS:NZ	2.34	0.42
1:A:2081:THR:HG22	1:A:2085:LYS:HD2	2.01	0.42
1:A:2412:ARG:HH11	1:A:2555:ALA:HB2	1.85	0.42
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.42
1:A:2847:GLU:HG3	1:A:2848:GLU:N	2.34	0.42
1:A:3302:GLU:O	1:A:3306:TRP:N	2.49	0.42
1:A:3327:SER:O	1:A:3331:GLU:HG3	2.20	0.42
1:A:3636:GLY:HA2	1:A:3642:TYR:O	2.20	0.42
1:A:3830:SER:HA	1:A:3833:LYS:HE3	2.02	0.42
1:A:3839:ILE:HG22	1:A:3873:MET:HA	2.02	0.42
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	2.01	0.42
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	2.02	0.42
1:B: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:B:2082:ALA:N	2:B:5400:ATP:O2A	2.53	0.42
1:A:1625:ASP:O	1:A:1629:GLN:HG3	2.19	0.41
1:A:2701:SER:HB2	1:A:2703:ASP:O	2.20	0.41
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.99	0.41
1:A:3555:TYR:HB3	1:A:3597:ILE:HD11	2.02	0.41
1:A:3903:ILE:O	1:A:3907:VAL:HG23	2.20	0.41
1:B:1664:LEU:O	1:B:1721:LYS:HE3	2.19	0.41
1:B:2222:ILE:H	1:B:2222:ILE:HG13	1.67	0.41
1:B:2852:LEU:O	1:B:2856:LEU:HB2	2.20	0.41
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.20	0.41
1:B:4019:ASP:O	1:B:4030:PRO:HA	2.19	0.41
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.20	0.41
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	2.02	0.41
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.85	0.41
1:A:2828:LEU:HD11	1:A:2908:LEU:HD11	2.01	0.41
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.20	0.41
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.35	0.41

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:THR:HB	1:A:1498:GLU:HB2	2.01	0.41
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.02	0.41
1:A: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:3786:PHE:CD1	1:A:3893:ASP:HB2	2.56	0.41
1:A:3692:LYS:HG3	1:A:3898:GLU:HG3	2.02	0.41
1:A:1726:LEU:HD13	1:A:3984:GLN:HB3	2.01	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:3886:ALA:N	1:A:3887:PRO:CD	2.81	0.41
1:A:2765:GLY:CA	3:A:5402:ADP:O2A	2.59	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: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:B:2732:MET:CG	3:B:5402:ADP:C6	3.02	0.41
1:A:1409:LEU:O	1:A:1413:VAL:HG23	2.20	0.41
1:A:1744:LEU:CD2	1:A:1760:PHE:CD2	3.03	0.41
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.50	0.41
1:A:2728:LEU:HB2	1:A:2771:ARG:HH12	1.86	0.41
1:A:2982:VAL:HG12	1:A:2983:GLY:H	1.85	0.41
1:A:3971:VAL:HA	1:A:3974:THR:HG22	2.03	0.41
1:B:1697:LYS:O	1:B:1701:LEU:HG	2.20	0.41
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.97	0.41
1:B:3304:GLU:O	1:B:3305:ARG:C	2.59	0.41
1:B:3409:ASP:HB3	1:B:3518:PHE:CB	2.47	0.41
1:B:3826:GLN:HB2	1:B:3854:TYR:CZ	2.56	0.41
1:B:3757:ILE:HD11	1:B:4074:GLU:HG2	2.02	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:2226:ILE:HG23	1:A:2288:VAL:CG2	2.46	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: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:3948:HIS:NE2	1:A:4072:ASN:CG	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	2.02	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:4065:LEU:HD11	1:B:4070:ILE:CD1	2.45	0.41
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.42	0.41
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.56	0.41
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.48	0.41
1:A:2485:PHE:CZ	1:A:2534:ALA:HB2	2.56	0.41
1:A:3528:ARG:HH11	1:A:3650:LEU:HD11	1.86	0.41
1:A:3703:PHE:HE2	1:A:3719:VAL:HG21	1.86	0.41
1:B:1830:VAL:HG23	1:B:1833:ARG:NH2	2.36	0.41
1:B:2782:VAL:HB	1:B:2815:LEU:HD12	2.02	0.41
1:A:1664:LEU:HD21	1:A:1715:LEU:HD22	2.03	0.41
1:A:2266:PHE:CD1	1:A:2326:LEU:HD21	2.53	0.41
1:A:2408:LEU:HD13	1:A:2432:LEU:HD21	2.03	0.41
1:A:2985:ASN:N	1:A:2986:PRO:CD	2.84	0.41
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.34	0.41
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.56	0.40
1:A:2332:GLY:HA2	1:A:2335:GLN:CG	2.50	0.40
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.40
1:B:2225:LYS:HD2	1:B:2281:PHE:CZ	2.55	0.40
1:B:2299:ARG:HA	1:B:2302:PHE:CD2	2.56	0.40
1:B:2320:ARG:NH1	1:B:2406:ASP:OD2	2.40	0.40
1:B:2766:LYS:HD2	1:B:2890:THR:HG22	2.02	0.40
1:B:3629:PHE:O	1:B:3633:GLU:HB2	2.20	0.40
1:B:3833:LYS:HZ3	1:B:3862:THR:HG21	1.85	0.40
1:B:3839:ILE:HG22	1:B:3871:PHE:HE1	1.86	0.40
1:A:1392:LEU:HD21	1:A:1487:THR:HG21	2.02	0.40
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	2.02	0.40
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.91	0.40
1:A:2060:PHE:HZ	1:A:2193:LEU:HD21	1.86	0.40
1:A:2380:LEU:HD12	1:A:2380:LEU:C	2.42	0.40
1:A:3458:PHE:HD2	1:A:3506:PRO:HG2	1.86	0.40
1:A:3844:ILE:HD11	1:A:3855:LEU:HD22	2.03	0.40
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.03	0.40
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.21	0.40
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.40
1:A:1637:GLU:C	1:A:1686:LYS:HZ2	2.20	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.03	0.40
1:B:2306:ASP:HB2	1:B:2309:SER:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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	2640/2695 (98%)	2503 (95%)	121 (5%)	16 (1%)	28	68
1	B	2640/2695 (98%)	2506 (95%)	116 (4%)	18 (1%)	25	65
All	All	5280/5390 (98%)	5009 (95%)	237 (4%)	34 (1%)	28	68

All (34) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2218/2453 (90%)	2128 (96%)	90 (4%)	35	71
1	B	2218/2453 (90%)	2133 (96%)	85 (4%)	38	72
All	All	4436/4906 (90%)	4261 (96%)	175 (4%)	37	72

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	ATP	A	5400	-	27,33,33	1.01	1 (3%)	25,52,52	1.66	2 (8%)
3	ADP	A	5401	-	25,29,29	1.22	2 (8%)	24,45,45	1.57	4 (16%)
3	ADP	A	5402	-	25,29,29	1.03	1 (4%)	24,45,45	1.93	3 (12%)
4	SO4	A	5403	-	4,4,4	0.43	0	6,6,6	0.71	0
2	ATP	B	5400	-	27,33,33	1.01	1 (3%)	25,52,52	1.66	3 (12%)
3	ADP	B	5401	-	25,29,29	1.22	1 (4%)	24,45,45	1.90	4 (16%)
3	ADP	B	5402	-	25,29,29	1.00	1 (4%)	24,45,45	1.73	3 (12%)
4	SO4	B	5403	-	4,4,4	0.42	0	6,6,6	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5400	-	-	0/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	5401	-	-	0/12/32/32	0/3/3/3
3	ADP	A	5402	-	-	0/12/32/32	0/3/3/3
4	SO4	A	5403	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5400	-	-	0/18/38/38	0/3/3/3
3	ADP	B	5401	-	-	0/12/32/32	0/3/3/3
3	ADP	B	5402	-	-	0/12/32/32	0/3/3/3
4	SO4	B	5403	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5401	ADP	C2-N3	2.54	1.36	1.32
2	A	5400	ATP	C5-C4	2.99	1.47	1.40
3	A	5402	ADP	C5-C4	3.03	1.47	1.40
2	B	5400	ATP	C5-C4	3.07	1.47	1.40
3	B	5402	ADP	C5-C4	3.24	1.47	1.40
3	B	5401	ADP	C5-C4	3.27	1.47	1.40
3	A	5401	ADP	C5-C4	3.60	1.48	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5402	ADP	N3-C2-N1	-7.17	122.61	128.86
3	B	5401	ADP	N3-C2-N1	-6.89	122.86	128.86
3	B	5402	ADP	N3-C2-N1	-6.41	123.28	128.86
2	B	5400	ATP	N3-C2-N1	-5.84	123.77	128.86
2	A	5400	ATP	N3-C2-N1	-5.80	123.80	128.86
3	A	5401	ADP	N3-C2-N1	-4.95	124.55	128.86
3	A	5402	ADP	C4-C5-N7	-2.98	106.53	109.41
2	A	5400	ATP	C4-C5-N7	-2.93	106.58	109.41
2	B	5400	ATP	C4-C5-N7	-2.92	106.59	109.41
3	B	5402	ADP	C4-C5-N7	-2.53	106.97	109.41
3	B	5401	ADP	C4-C5-N7	-2.31	107.18	109.41
3	A	5401	ADP	C4-C5-N7	-2.25	107.23	109.41
3	B	5401	ADP	O2'-C2'-C3'	-2.02	105.35	111.83
2	B	5400	ATP	O3G-PG-O2G	2.14	116.24	107.61
3	B	5402	ADP	O3B-PB-O2B	2.16	116.31	107.61
3	B	5401	ADP	C4'-O4'-C1'	2.19	112.10	109.77
3	A	5401	ADP	N6-C6-N1	2.21	123.16	118.77
3	A	5401	ADP	C2'-C3'-C4'	2.47	107.43	102.62
3	A	5402	ADP	C4'-O4'-C1'	2.68	112.62	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 89 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.60	298 (11%) 6 6	88, 185, 310, 500	1 (0%)
1	B	2650/2695 (98%)	0.70	256 (9%) 8 9	96, 180, 317, 500	1 (0%)
All	All	5300/5390 (98%)	0.65	554 (10%) 7 7	88, 183, 311, 500	2 (0%)

All (554) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	35.5
1	B	33	GLU	29.8
1	B	83	GLY	27.1
1	B	69	ALA	26.7
1	A	131	MET	24.8
1	B	91	ILE	24.1
1	B	199	ALA	23.8
1	B	198	ILE	23.6
1	B	66	GLN	23.2
1	B	84	CYS	22.1
1	B	16	THR	21.6
1	B	92	SER	19.6
1	B	52	PRO	19.2
1	A	1460	GLY	18.9
1	B	15	PRO	18.5
1	B	35	ASP	17.9
1	B	4	LEU	15.6
1	B	155	TYR	15.3
1	A	132	PHE	15.1
1	B	34	ARG	15.1
1	B	200	TRP	15.1
1	B	189	ASP	14.8
1	B	50	GLU	14.2
1	B	152	PHE	14.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	95	GLU	13.6
1	B	14	GLN	13.1
1	B	68	MET	13.0
1	A	1459	LEU	12.9
1	B	32	TYR	12.4
1	B	17	ARG	12.3
1	B	186	PRO	12.1
1	B	88	ARG	11.7
1	B	87	GLU	11.5
1	B	89	ALA	11.5
1	B	18	LEU	10.9
1	A	27	TYR	10.5
1	B	48	GLY	10.5
1	A	143	ASN	10.3
1	B	149	HIS	10.0
1	B	65	THR	9.8
1	B	5	GLY	9.8
1	B	151	ASP	9.7
1	A	31	LEU	9.4
1	B	90	GLU	9.4
1	A	3580	ASN	9.2
1	A	1483	TYR	8.6
1	B	171	ALA	8.6
1	B	1483	TYR	8.4
1	A	42	ASN	8.3
1	B	194	SER	8.2
1	A	108	ILE	8.2
1	B	36	GLU	8.1
1	B	168	CYS	8.0
1	A	3575	GLY	8.0
1	B	45	PHE	7.8
1	A	3581	ASP	7.7
1	B	73	TYR	7.6
1	B	70	ILE	7.5
1	B	193	LYS	7.5
1	B	53	ASN	7.5
1	A	115	GLU	7.4
1	A	28	GLU	7.4
1	A	210	GLY	7.3
1	A	202	LEU	7.3
1	B	11	GLY	7.3
1	B	6	TYR	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	40	TRP	7.1
1	B	8	LYS	7.1
1	B	19	LEU	7.1
1	B	3580	ASN	7.1
1	B	96	GLY	7.1
1	A	35	ASP	7.0
1	A	3578	LEU	6.8
1	A	148	THR	6.7
1	A	3979	ASN	6.7
1	B	3	ILE	6.7
1	A	1549	ILE	6.7
1	A	2364	ASP	6.4
1	B	72	ARG	6.3
1	A	1500	ILE	6.3
1	B	143	ASN	6.3
1	A	2687	GLY	6.3
1	A	134	ASP	6.2
1	B	174	LYS	6.2
1	B	2941	THR	6.1
1	A	173	PRO	6.0
1	A	2942	ASP	6.0
1	A	2362	ALA	6.0
1	B	94	LEU	6.0
1	A	29	GLU	5.9
1	A	1458	ILE	5.9
1	A	1504	ASN	5.9
1	B	3567	LEU	5.9
1	A	1445	TRP	5.9
1	B	3300	THR	5.8
1	B	55	PRO	5.8
1	B	172	PHE	5.8
1	A	1390	SER	5.8
1	A	1490	ALA	5.8
1	B	190	LYS	5.7
1	A	150	PRO	5.7
1	A	130	LYS	5.7
1	A	1548	ILE	5.6
1	B	2938	MET	5.6
1	B	169	LEU	5.6
1	A	3306	TRP	5.6
1	B	1669	PHE	5.5
1	A	54	LEU	5.5

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1388	HIS	4.4
1	A	133	GLU	4.4
1	A	81	LEU	4.3
1	B	3024	LEU	4.3
1	A	144	GLY	4.3
1	B	74	ILE	4.3
1	A	216	PRO	4.3
1	B	67	SER	4.2
1	A	32	TYR	4.2
1	A	129	LEU	4.2
1	B	1394	LEU	4.1
1	B	3542	GLN	4.1
1	B	1458	ILE	4.1
1	B	3734	PRO	4.1
1	B	154	LEU	4.1
1	A	2854	ASN	4.1
1	B	3016	PHE	4.0
1	B	86	LYS	4.0
1	A	3301	PHE	4.0
1	A	75	ALA	4.0
1	A	1493	LEU	4.0
1	B	153	MET	4.0
1	B	192	LEU	4.0
1	A	3583	LEU	4.0
1	B	24	GLU	4.0
1	B	1485	MET	4.0
1	B	3304	GLU	4.0
1	B	1727	LEU	4.0
1	A	209	PHE	3.9
1	B	3573	SER	3.9
1	B	145	ASP	3.9
1	B	3763	PHE	3.9
1	A	1492	GLN	3.9
1	A	3739	ASP	3.9
1	B	3303	LYS	3.9
1	A	1452	TRP	3.9
1	A	3017	VAL	3.9
1	B	202	LEU	3.8
1	A	2941	THR	3.8
1	B	3585	VAL	3.8
1	A	1546	LEU	3.8
1	B	4035	GLN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3564	LYS	3.8
1	A	1479	LEU	3.8
1	B	31	LEU	3.8
1	B	1945	LEU	3.8
1	B	42	ASN	3.8
1	B	64	LEU	3.8
1	B	1	SER	3.7
1	A	1644	ILE	3.7
1	B	9	ILE	3.7
1	B	2172	ASP	3.7
1	A	1572	ILE	3.7
1	A	4034	LEU	3.7
1	A	1394	LEU	3.7
1	A	3591	LYS	3.7
1	B	1502	ILE	3.7
1	A	142	LEU	3.7
1	A	86	LYS	3.7
1	B	3703	PHE	3.7
1	A	2852	LEU	3.6
1	B	1383	TYR	3.6
1	A	1378	TRP	3.6
1	A	1602	ILE	3.6
1	A	19	LEU	3.6
1	A	147	VAL	3.6
1	B	1705	TYR	3.6
1	A	1530	GLN	3.5
1	A	2965	VAL	3.5
1	A	2676	THR	3.5
1	B	1762	TYR	3.5
1	A	2916	TRP	3.5
1	B	2364	ASP	3.5
1	B	3617	GLU	3.5
1	B	3020	GLY	3.5
1	A	3920	ILE	3.5
1	A	3024	LEU	3.5
1	A	211	GLY	3.5
1	B	63	LYS	3.5
1	A	3589	ASN	3.5
1	B	1456	TYR	3.5
1	A	2937	PRO	3.4
1	A	1550	GLY	3.4
1	A	138	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1738	ASN	3.4
1	B	135	ARG	3.4
1	A	1401	LEU	3.4
1	A	3570	LEU	3.4
1	A	2574	TYR	3.4
1	A	1391	GLY	3.4
1	A	72	ARG	3.4
1	B	3569	GLU	3.4
1	A	1489	ARG	3.3
1	A	151	ASP	3.3
1	B	44	LYS	3.3
1	A	2371	PHE	3.3
1	B	3919	LYS	3.3
1	A	1472	GLU	3.3
1	B	3571	ASN	3.3
1	A	171	ALA	3.3
1	B	3579	GLU	3.3
1	A	18	LEU	3.3
1	A	2611	LEU	3.2
1	B	148	THR	3.2
1	A	2870	GLU	3.2
1	A	1441	ILE	3.2
1	A	2029	LEU	3.2
1	B	1445	TRP	3.2
1	B	3543	ARG	3.2
1	B	3984	GLN	3.2
1	B	3566	LEU	3.2
1	A	16	THR	3.2
1	A	87	GLU	3.2
1	A	3561	ASN	3.2
1	B	131	MET	3.1
1	B	3572	ASN	3.1
1	A	3551	LEU	3.1
1	B	23	LEU	3.1
1	A	1565	MET	3.1
1	A	1607	TRP	3.1
1	A	1597	GLU	3.1
1	A	1636	ILE	3.1
1	A	109	ALA	3.1
1	A	57	TYR	3.1
1	B	4052	THR	3.1
1	A	1581	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2918	GLY	3.1
1	A	3584	MET	3.1
1	A	88	ARG	3.1
1	B	3028	VAL	3.0
1	B	1767	GLU	3.0
1	A	2368	PHE	3.0
1	B	1898	LEU	3.0
1	A	137	CYS	3.0
1	B	2942	ASP	3.0
1	A	3019	VAL	3.0
1	A	2303	GLN	3.0
1	B	3873	MET	3.0
1	B	3568	GLU	3.0
1	B	51	PHE	2.9
1	B	132	PHE	2.9
1	A	2179	PRO	2.9
1	B	2173	ASN	2.9
1	A	4029	ILE	2.9
1	B	1590	LEU	2.9
1	A	33	GLU	2.9
1	A	3425	LYS	2.9
1	B	1549	ILE	2.9
1	A	1486	ILE	2.9
1	A	1578	PHE	2.9
1	A	2359	ILE	2.9
1	B	185	ILE	2.9
1	B	3715	TYR	2.9
1	A	2582	VAL	2.9
1	B	1486	ILE	2.9
1	B	1513	ILE	2.9
1	B	3577	MET	2.9
1	A	2130	PHE	2.9
1	A	3436	PHE	2.9
1	B	3927	TYR	2.9
1	B	1460	GLY	2.9
1	B	1441	ILE	2.8
1	B	1449	GLN	2.8
1	B	82	GLY	2.8
1	A	2361	ILE	2.8
1	A	3484	HIS	2.8
1	B	3564	LYS	2.8
1	A	3554	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1452	TRP	2.8
1	A	2943	PHE	2.8
1	B	2022	PHE	2.8
1	A	3309	THR	2.8
1	A	3594	ALA	2.8
1	A	3868	HIS	2.8
1	A	1519	ILE	2.8
1	A	2091	MET	2.8
1	B	1937	MET	2.8
1	A	3020	GLY	2.8
1	A	2249	LEU	2.8
1	B	188	ILE	2.7
1	B	60	GLY	2.7
1	A	2689	ILE	2.7
1	A	4036	GLN	2.7
1	A	1526	PHE	2.7
1	A	1760	PHE	2.7
1	A	3026	GLU	2.7
1	A	1562	MET	2.7
1	A	4033	LEU	2.7
1	B	3744	LEU	2.7
1	A	92	SER	2.7
1	A	3313	PHE	2.7
1	A	2938	MET	2.7
1	A	1505	PHE	2.7
1	A	3446	PHE	2.7
1	B	3025	ASN	2.7
1	B	3934	TRP	2.7
1	B	1719	SER	2.7
1	B	3017	VAL	2.7
1	B	3581	ASP	2.7
1	B	3747	LEU	2.7
1	B	3853	THR	2.7
1	A	2190	PHE	2.6
1	B	1596	ILE	2.6
1	A	94	LEU	2.6
1	A	3025	ASN	2.6
1	B	75	ALA	2.6
1	B	1683	LEU	2.6
1	B	144	GLY	2.6
1	A	1456	TYR	2.6
1	B	1476	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1497	ILE	2.6
1	A	3567	LEU	2.6
1	A	76	ASP	2.6
1	B	1905	ARG	2.6
1	A	3865	ALA	2.6
1	B	1952	PHE	2.6
1	B	3867	GLU	2.6
1	A	2838	ALA	2.6
1	B	3582	GLU	2.6
1	A	2739	VAL	2.6
1	B	1480	THR	2.6
1	B	191	TYR	2.5
1	B	1505	PHE	2.5
1	B	3576	ASN	2.5
1	B	2024	SER	2.5
1	A	3873	MET	2.5
1	B	3618	TYR	2.5
1	A	1476	PHE	2.5
1	B	1415	MET	2.5
1	A	2682	PRO	2.5
1	A	2121	ALA	2.5
1	A	1469	LEU	2.5
1	A	2681	LEU	2.5
1	B	3726	LEU	2.5
1	B	3904	LEU	2.5
1	A	2581	LEU	2.5
1	A	2853	LEU	2.5
1	B	3686	PHE	2.5
1	B	3026	GLU	2.5
1	A	1590	LEU	2.5
1	A	146	HIS	2.5
1	A	3305	ARG	2.5
1	B	3557	LEU	2.5
1	A	1506	ASP	2.5
1	A	4035	GLN	2.5
1	A	36	GLU	2.5
1	B	1864	ASN	2.5
1	A	2607	TYR	2.5
1	A	1559	SER	2.5
1	A	3847	SER	2.5
1	B	3019	VAL	2.5
1	B	3587	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	2.4
1	A	3014	GLN	2.4
1	A	62	VAL	2.4
1	B	1760	PHE	2.4
1	B	156	ASP	2.4
1	A	11	GLY	2.4
1	A	200	TRP	2.4
1	A	1898	LEU	2.4
1	A	3028	VAL	2.4
1	A	1669	PHE	2.4
1	A	1705	TYR	2.4
1	B	1672	TYR	2.4
1	B	2943	PHE	2.4
1	A	1423	ILE	2.4
1	A	3415	ILE	2.4
1	B	3555	TYR	2.4
1	B	175	LEU	2.4
1	A	2656	PHE	2.4
1	A	2844	PHE	2.4
1	B	3565	ARG	2.4
1	A	2782	VAL	2.4
1	A	1494	ASP	2.4
1	A	3357	ALA	2.4
1	A	1640	VAL	2.4
1	A	2024	SER	2.4
1	A	2129	LEU	2.4
1	B	197	TYR	2.4
1	A	10	LYS	2.4
1	A	2876	TRP	2.4
1	B	1850	PHE	2.4
1	B	1572	ILE	2.4
1	A	2038	LEU	2.4
1	A	1426	GLN	2.4
1	A	3007	TYR	2.4
1	A	3326	ILE	2.4
1	B	2014	PHE	2.3
1	A	3875	MET	2.3
1	B	4092	MET	2.3
1	A	22	TYR	2.3
1	B	47	LEU	2.3
1	A	93	MET	2.3
1	B	1589	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2444	ASN	2.3
1	B	2302	PHE	2.3
1	B	1423	ILE	2.3
1	B	1953	LEU	2.3
1	A	3593	GLU	2.3
1	A	3559	LEU	2.3
1	A	2385	VAL	2.3
1	A	71	ILE	2.3
1	B	3768	PHE	2.3
1	A	73	TYR	2.3
1	A	3021	LEU	2.3
1	B	1664	LEU	2.3
1	B	3562	LEU	2.3
1	A	2912	CYS	2.3
1	A	2977	TYR	2.3
1	A	3542	GLN	2.3
1	B	2962	ARG	2.3
1	B	3839	ILE	2.3
1	A	1588	GLU	2.3
1	B	2122	THR	2.3
1	A	2856	LEU	2.3
1	A	2367	SER	2.3
1	A	2470	GLY	2.2
1	A	3563	GLU	2.2
1	A	2022	PHE	2.2
1	A	2784	PRO	2.2
1	B	1942	SER	2.2
1	A	3590	LEU	2.2
1	A	2314	ILE	2.2
1	A	2874	TYR	2.2
1	A	1540	LEU	2.2
1	A	2366	LEU	2.2
1	A	2150	ILE	2.2
1	A	61	ASP	2.2
1	A	1762	TYR	2.2
1	B	2990	GLY	2.2
1	B	3847	SER	2.2
1	B	3415	ILE	2.2
1	B	1666	THR	2.2
1	A	2686	LEU	2.2
1	A	2940	PHE	2.2
1	B	2021	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2310	LEU	2.2
1	A	3884	LEU	2.2
1	B	2795	PHE	2.2
1	B	3725	VAL	2.2
1	B	3948	HIS	2.2
1	B	3841	LEU	2.2
1	A	2962	ARG	2.2
1	A	1537	PHE	2.2
1	A	2603	CYS	2.2
1	B	3589	ASN	2.2
1	A	1509	LEU	2.1
1	B	1546	LEU	2.1
1	B	2006	LEU	2.1
1	B	2190	PHE	2.1
1	A	3899	ASP	2.1
1	A	1474	SER	2.1
1	B	1605	GLN	2.1
1	B	1668	GLN	2.1
1	A	149	HIS	2.1
1	A	3869	GLU	2.1
1	B	1603	GLN	2.1
1	B	4045	LEU	2.1
1	A	1428	CYS	2.1
1	A	1935	GLN	2.1
1	B	1500	ILE	2.1
1	B	3923	VAL	2.1
1	A	3557	LEU	2.1
1	A	4019	ASP	2.1
1	A	3426	THR	2.1
1	A	1603	GLN	2.1
1	B	2295	ILE	2.1
1	A	3994	TYR	2.1
1	B	3958	ASP	2.1
1	A	43	LYS	2.1
1	B	3390	PHE	2.1
1	A	2106	THR	2.1
1	A	2252	LEU	2.1
1	B	1420	TYR	2.1
1	B	3027	SER	2.1
1	A	2292	VAL	2.1
1	A	2673	LEU	2.1
1	A	3480	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2474	LEU	2.1
1	A	2999	LEU	2.1
1	B	3657	PHE	2.1
1	B	1828	TYR	2.1
1	A	1412	LEU	2.1
1	A	1571	SER	2.1
1	A	2170	LEU	2.1
1	A	1566	PHE	2.0
1	B	3895	PHE	2.0
1	A	1538	TYR	2.0
1	A	2237	LEU	2.0
1	B	1386	ILE	2.0
1	B	2989	PRO	2.0
1	A	2257	PHE	2.0
1	A	1612	ASP	2.0
1	B	1412	LEU	2.0
1	A	3448	SER	2.0
1	A	2599	LEU	2.0
1	B	3816	LEU	2.0
1	A	1645	PHE	2.0
1	B	3767	PHE	2.0
1	A	1582	VAL	2.0
1	A	2592	PHE	2.0
1	A	2304	ASN	2.0
1	A	1481	SER	2.0
1	A	2316	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	MG	B	5404	1/1	0.90	0.30	1.51	107,107,107,107	0
2	ATP	A	5400	31/31	0.94	0.31	1.08	122,147,224,246	0
4	SO4	A	5403	5/5	0.92	0.23	0.70	101,136,142,145	0
2	ATP	B	5400	31/31	0.91	0.27	0.62	124,160,195,221	0
3	ADP	B	5401	27/27	0.94	0.27	0.39	98,121,138,153	0
3	ADP	B	5402	27/27	0.87	0.33	0.34	108,145,183,194	0
3	ADP	A	5401	27/27	0.89	0.28	-0.18	126,146,191,198	0
3	ADP	A	5402	27/27	0.93	0.25	-0.69	134,176,208,218	0
4	SO4	B	5403	5/5	0.91	0.16	-0.78	139,143,171,171	0
5	MG	A	5404	1/1	0.77	0.17	-2.20	97,97,97,97	0

6.5 Other polymers

There are no such residues in this entry.